Electronic Supplementary Material (ESI) for CrystEngComm.

Photomechanical Response of Sulfonylhydrazone Molecular Crystals

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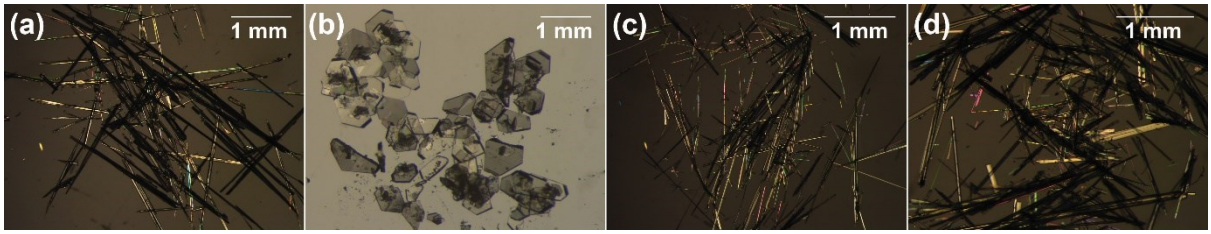


Figure S1. Optical microscopic images of the crystals of (a) **SH-1**, (b) **SH-2**, (c) **SH-3** and (d) **SH-4**.

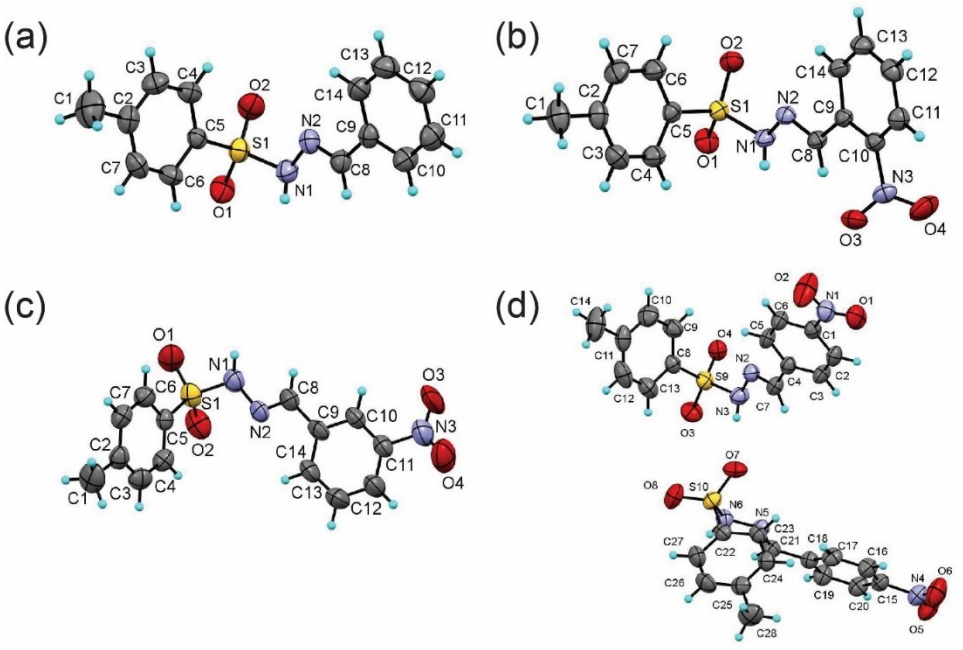


Figure S2. ORTEP diagrams of (a) **SH-1**, (b) **SH-2**, (c) **SH-3** and (d) **SH-4** with 50% probability ellipsoids.

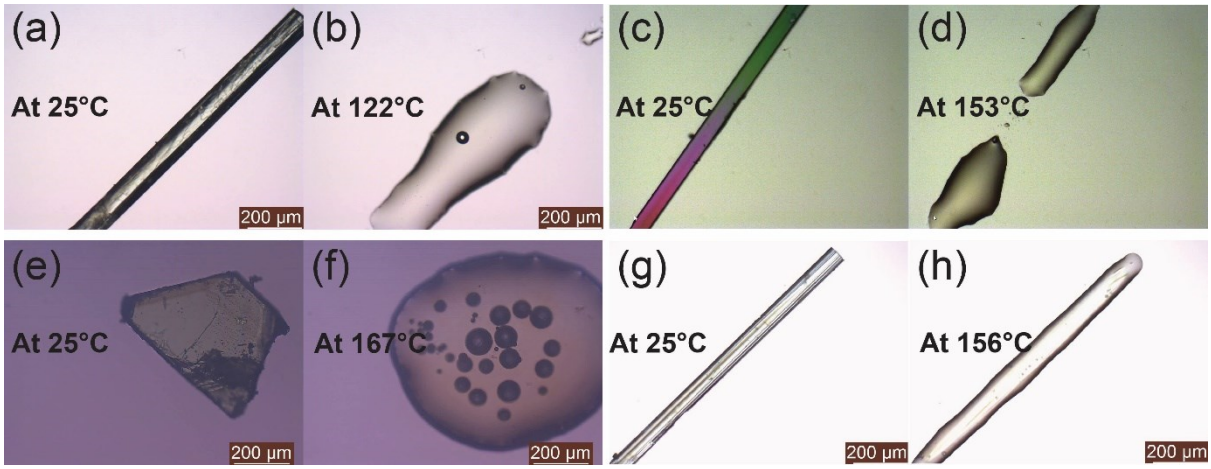


Figure S3. Thermal microscopy images show the melting of (a), (b) **SH-1**, (c), (d) **SH-2** (e), (f) **SH-3** and (g), (h) **SH-4** crystals.

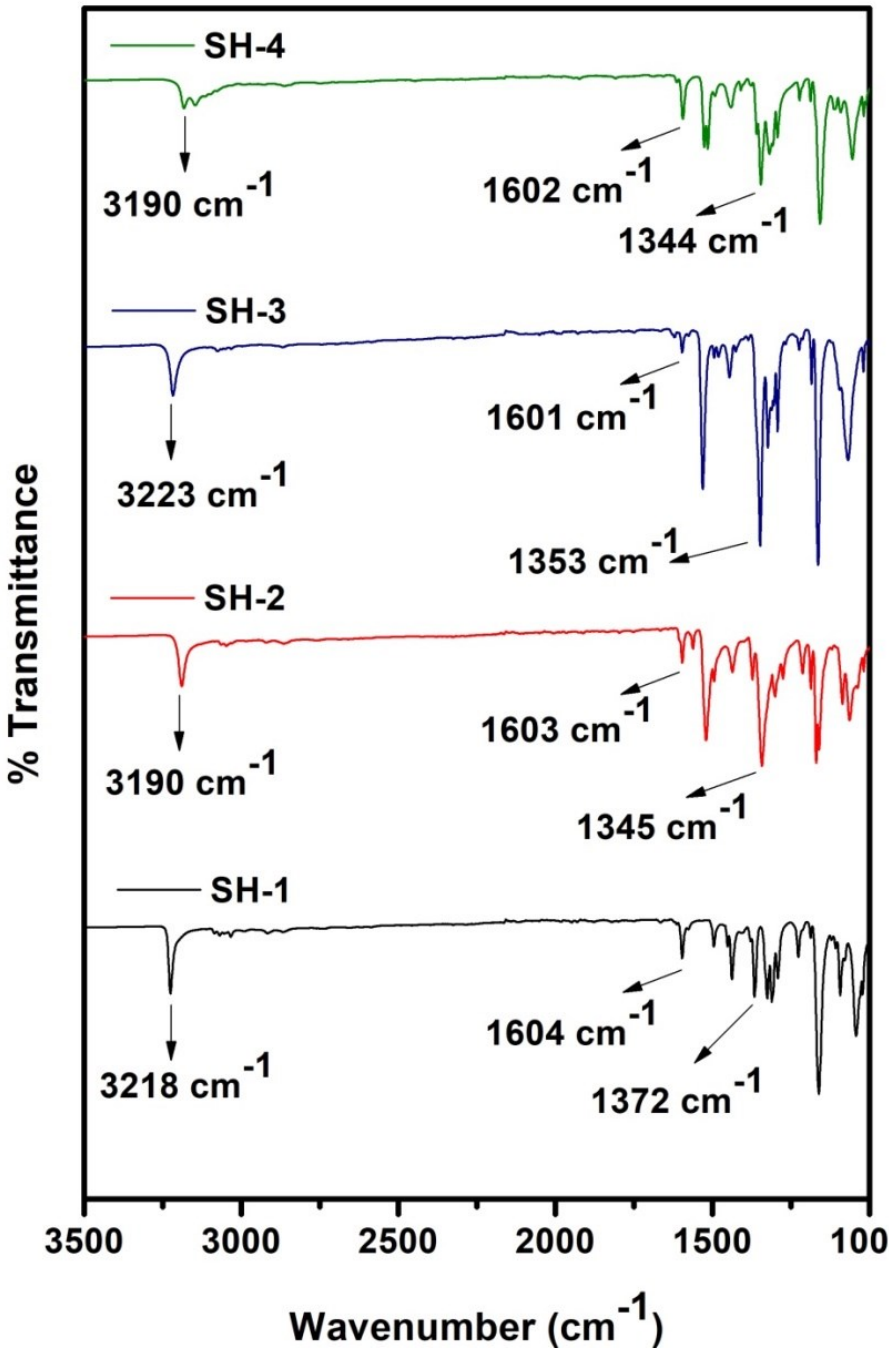
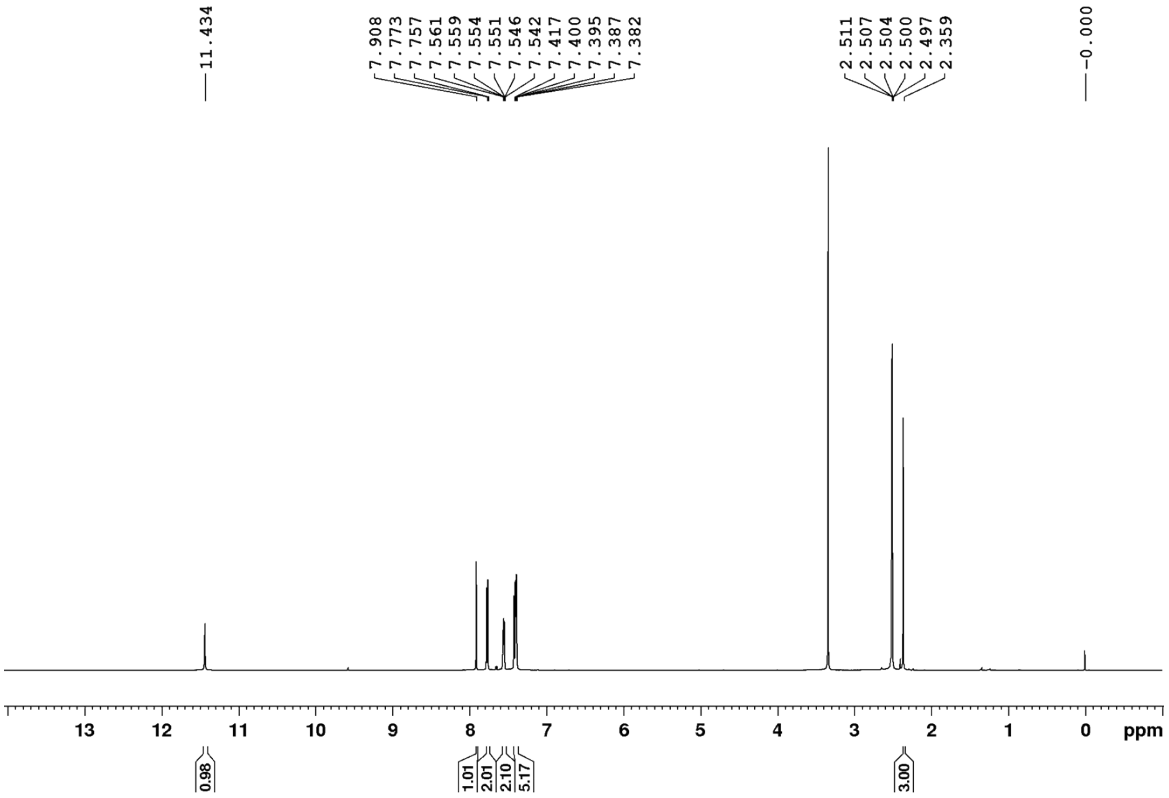
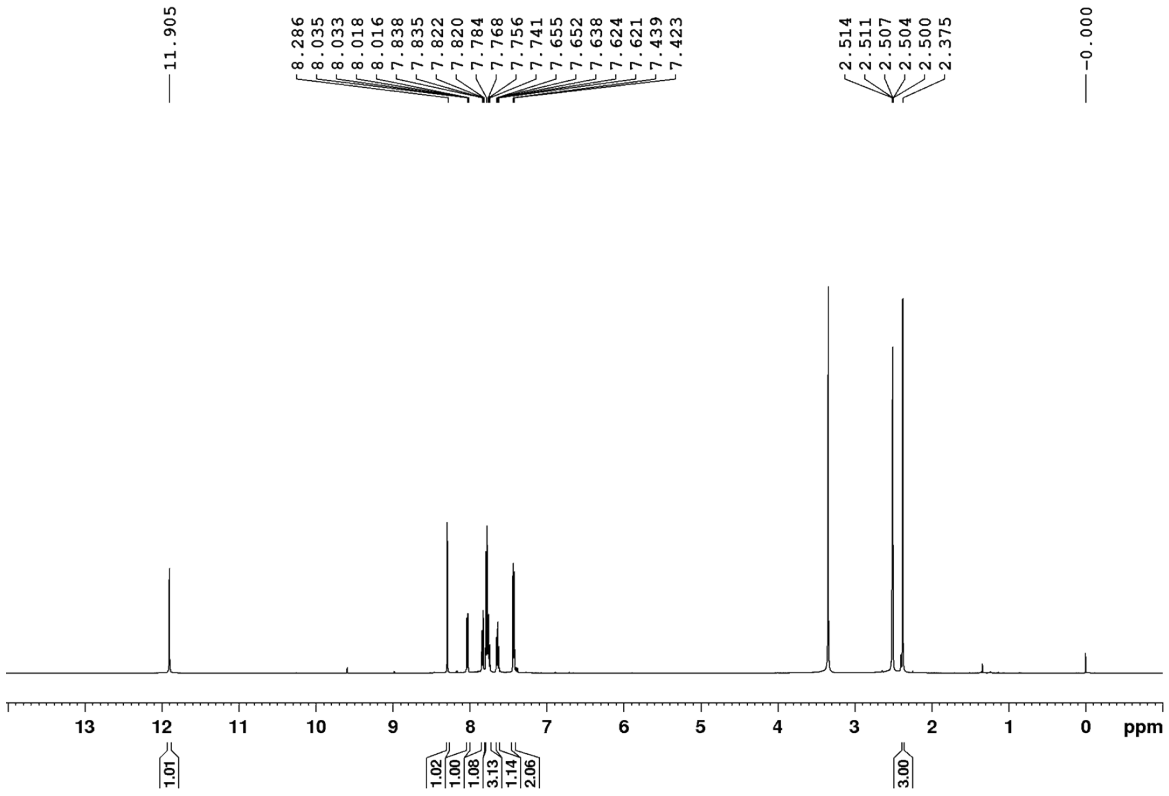


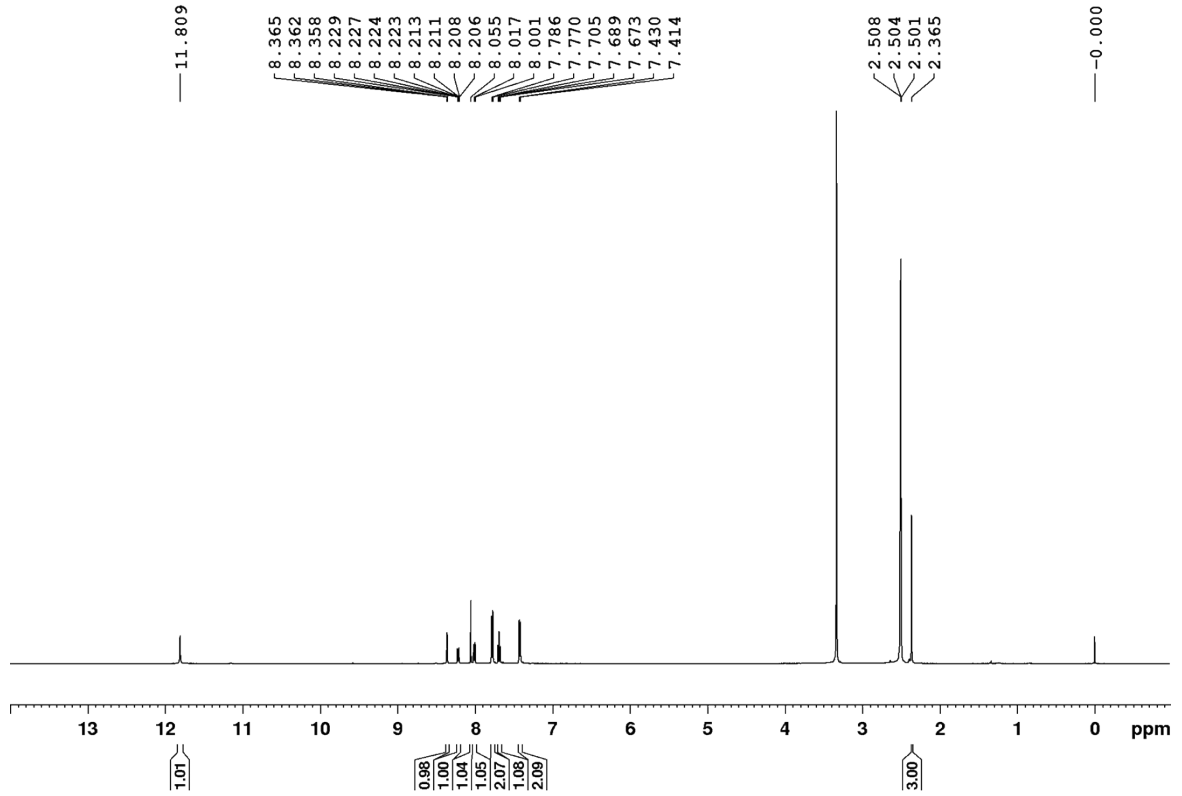
Figure S4. FT-IR spectra of **SH-1** (black), **SH-2** (red), **SH-3** (blue) and **SH-4** (green).


11.434
7.908
7.773
7.757
7.561
7.559
7.554
7.551
7.546
7.542
7.417
7.400
7.395
7.387
7.382
2.511
2.507
2.504
2.500
2.497
2.359
-0.000
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.01
2.01
2.10
5.17
3.00

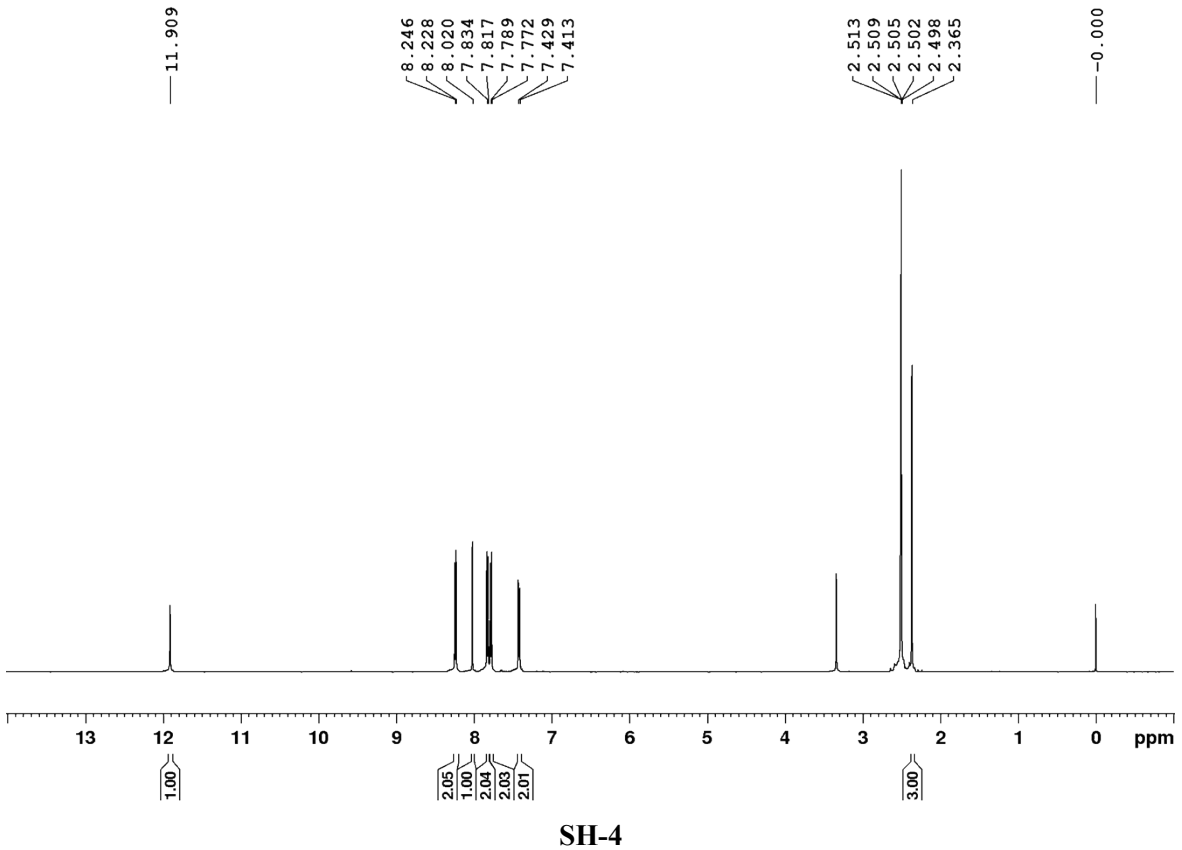
SH-1


11.905
8.286
8.035
8.033
8.018
8.016
7.838
7.835
7.822
7.820
7.784
7.768
7.756
7.741
7.655
7.652
7.638
7.624
7.621
7.439
7.423
2.514
2.511
2.507
2.504
2.500
2.375
-0.000
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.02
1.00
1.08
3.13
1.14
2.06
3.00

SH-2



SH-3



SH-4

Figure **S5**. 1H NMR spectra of **SH-1**, **SH-2**, **SH-3** and **SH-4** in DMSO-D6 solvent.

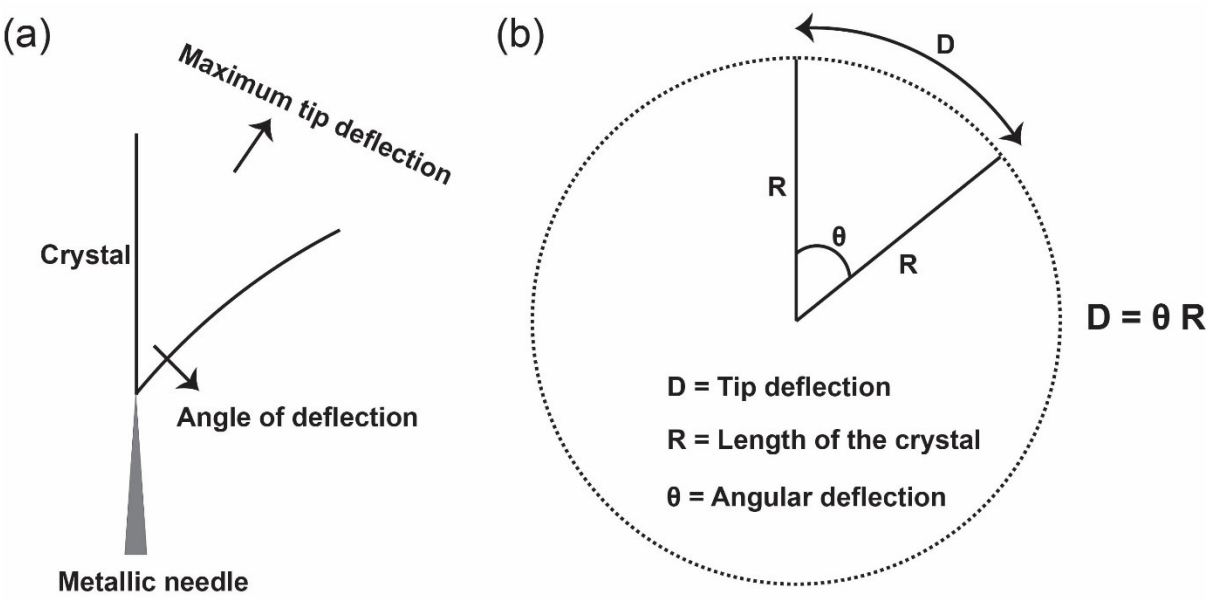


Figure S6. An illustrative representation of the photomechanical bending of the **SH** crystals attached to a metallic needle (a) and the designation of the metric parameters (b).

Table S1. Crystallization solvent and crystal dimensions of **SH-1**, **SH-2**, **SH-3**, and **SH-4**.

Comp.	Solvent of Crystallization	Length (mm) mini-max	Width (mm) min- maxi	Thickness (mm) min-max
SH-1	Methanol	1.70-6.39	0.02-0.11	0.02-0.07
SH-3	Methanol	1.68-5.51	0.03-0.11	0.01-0.11
SH-4	Methanol	1.26-4.65	0.05-0.17	0.02-0.07

Table S2. Basic crystallographic parameters of **SH-1**, **SH-2**, **SH-3**, and **SH-4**.

	SH-1	**SH-2**	**SH-3**	**SH-4**
Temperature / K	296.15	296.15	296.15	296.15
Radiation Source	Mo	Mo	Mo	Mo
Formula weight	274.35	319.34	319.34	319.34
Crystal system	Monoclinic	Triclinic	Orthorhombic	Monoclinic
Space group	$P2_1/c$	$P\bar{1}$	$Pna2_1$	$P\ 2_1/c$
a / Å	11.540(5)	5.6676(3)	11.443(3)	20.0412(9)
b / Å	5.320(2)	10.5227(5)	25.579(5)	10.2280(5)
c / Å	22.800(11)	12.1824(6)	5.1731(9)	15.0199(7)
α / °	90	93.860(2)	90	90
β / °	100.001(12)	94.947(2)	90	102.816(3)
γ / °	90	98.214(2)	90	90
Volume / Å^3	1378.4(11)	714.07(6)	1514.2(5)	3002.1(3)
Z	4	2	4	8
Density / (g cm^{-3})	1.3219	1.4851	1.4007	1.4130
μ / mm^{-1}	0.234	0.249	0.235	0.237
F_{000}	576.7401	332.4164	664.8327	1329.6654
h_{min}, h_{max}	-13, 13	-6, 6	-5, 13	-23, 23
k_{min}, k_{max}	-6, 6	-12, 12	-27, 30	-12, 12
l_{min}, l_{max}	-26, 26	-14, 14	-6, 6	-17, 17
No. of measured reflections	14369	15815	8208	63436
No. of unique reflections	2185	2511	2632	5362
No. of reflections used	1596	2322	1685	3816
R_{all}, R_{obs}	0.0774, 0.0481	0.0358, 0.0329	0.1160, 0.0693	0.0788, 0.0480
$wR_{2,all}$, $wR_{2,obs}$	0.1154, 0.1044	0.1106, 0.1056	0.1811, 0.1567	0.1133, 0.0999
$\Delta\rho_{min,max}$ / (e Å^{-3})	-0.3994, 0.3456	-0.3250, 0.2802	-0.4850, 0.3819	-0.4565, 0.3262
GooF	1.0617	0.9873	1.0407	1.0714
CCDC No.	2076195	2076196	2076194	2076197

Table S3. Mathematical equations used for the calculation of the various quantifiable parameters. For simplification, the radius (length of the crystal) is considered to be constant throughout the deflection. The equation $\boldsymbol{D = \theta R}$ is a rational approximation for small angles of photomechanical bending. The mathematical equations used for the calculation of various quantifiable parameters are given below.

Quantifiable parameter	**Mathematical formulae**
Tip displacement/ Tip deflection (D)	D (mm) = $[(x_2 - x_1)^2 + (y_2 - y_1)^2]^{1/2}$, where x_1, x_2 are the x coordinates and y_1, y_2 are the y coordinates of any two consecutive points on the trajectories of the crystal's tip.
Angle of deflection (θ)	θ (rad) = (Tip displacement, D in mm) / (Length of the crystal, R in mm rad^{-1}) Also, θ (°) = (180/π) × θ (rad)
Linear velocity (v)	v (mm s^{-1}) = (Tip displacement, D in mm) / (Change in time, t in s)
Angular velocity (ω)	1. ω (° s^{-1}) = (Angular displacement, θ in °)/ (Change in time, t in s) 2. Alternatively, ω (rad s^{-1}) = (Linear velocity, v in mm s^{-1})/ (Length of the crystal, R in mm rad^{-1}) Also, ω (° s^{-1}) = (180/π) × ω (rad s^{-1})
Linear acceleration (a)	a (mm s^{-2}) = (Change in linear velocity, v in mm s^{-1}) / (Change in time, t in s)
Angular acceleration (α)	1. α (° s^{-2}) = (Change in angular velocity, ω in ° s^{-1}) / (Change in time, t in s) 2. Alternatively, α (rad s^{-2}) = (Linear acceleration, a in mm s^{-2})/ (Length of the crystal, R in mm rad^{-1}) Also, α (° s^{-2}) = (180/π) × α (rad s^{-2})

Legends to the supporting movies:

Video S1: Photomechanical bending of **SH-1** crystals.

Video S2: Photomechanical bending of **SH-3** crystals.

Video S3: Photosalient effect of **SH-3** crystals.

Video S4: Wave like motion of **SH-3** crystals.

Video S5: Photomechanical bending of **SH-4** crystals.