SUPPORTING INFORMATION

Synthesis, characterization of a dual-stimuli-responsive cobalt(III) complex: comparison of photo/thermo mechanical behaviour in crystal and polymer composite

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Table S1. Crystallographic data of complex **C-1**.

Identification code	**C-1**
CCDC	2320472
Empirical formula	$C_{18}H_{31}CoN_8O_{12}$
M_r [g mol^{-1}]	610.44
T [K]	293(2)
Crystal system	Monoclinic
Space group	P21/n
a [Å]	14.2165(3)
b [Å]	6.20030(11)
c [Å]	28.4449(5)
α [deg]	90
β [deg]	92.0239(18)
γ [deg]	90
V [Å^3]	2505.75(8)
Z	4
ρ_{calc} [g cm^{-3}]	1.618
μ [mm^{-1}]	0.764
F (000)	1272.0
Crystal size[mm^3]	0.020 × 0.015 × 0.008
Radiation	MoKα (λ = 0.71073)
$\theta_{min}/\theta_{max}$ [deg]	6.502 to 54.696
Index ranges	-18 ≤ h ≤ 17, -7 ≤ k ≤ 8, -36 ≤ l ≤ 36
Reflections collected	33972
Independent reflections	5424 [R_{int} = 0.0409, R_{sigma} =0.0311]
Data/restraints/ parameters	5424/6/381
GOF on F^2	1.163
final *R* indices [$I > 2\sigma(I)$]	$R1$ = 0.0548, wR_2 = 0.1295
R indices (all data)	R_1 = 0.0587, wR_2 = 0.1309
largest diff peak/hole [e Å^{-3}]	1.06/-0.56

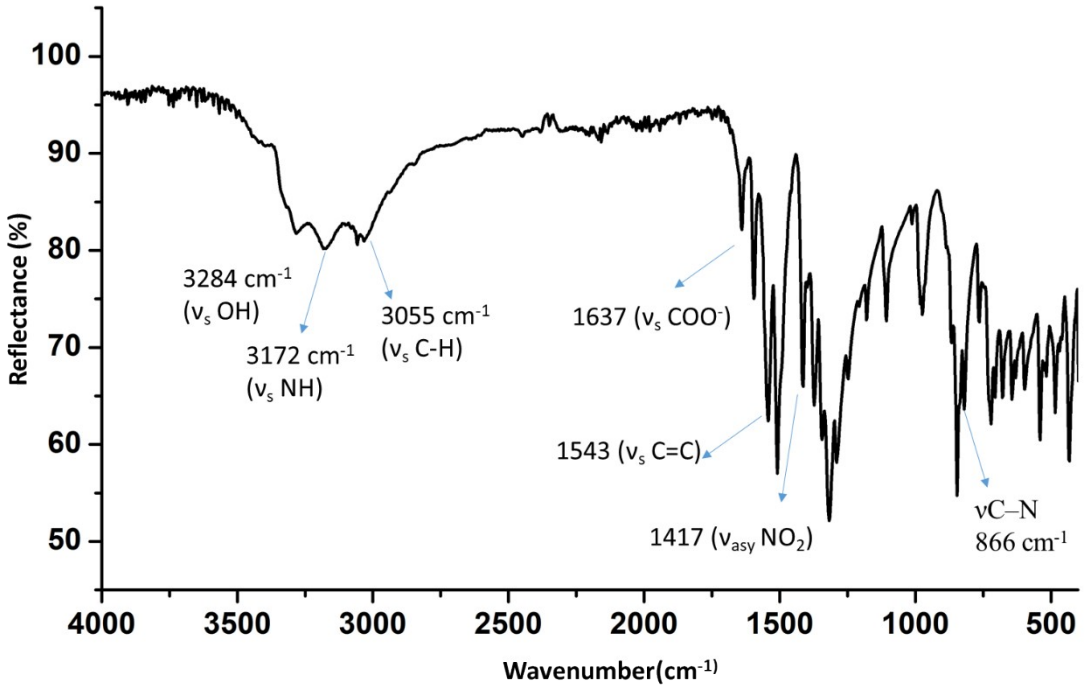

Fig. S1 FTIR spectrum of **C-1.**

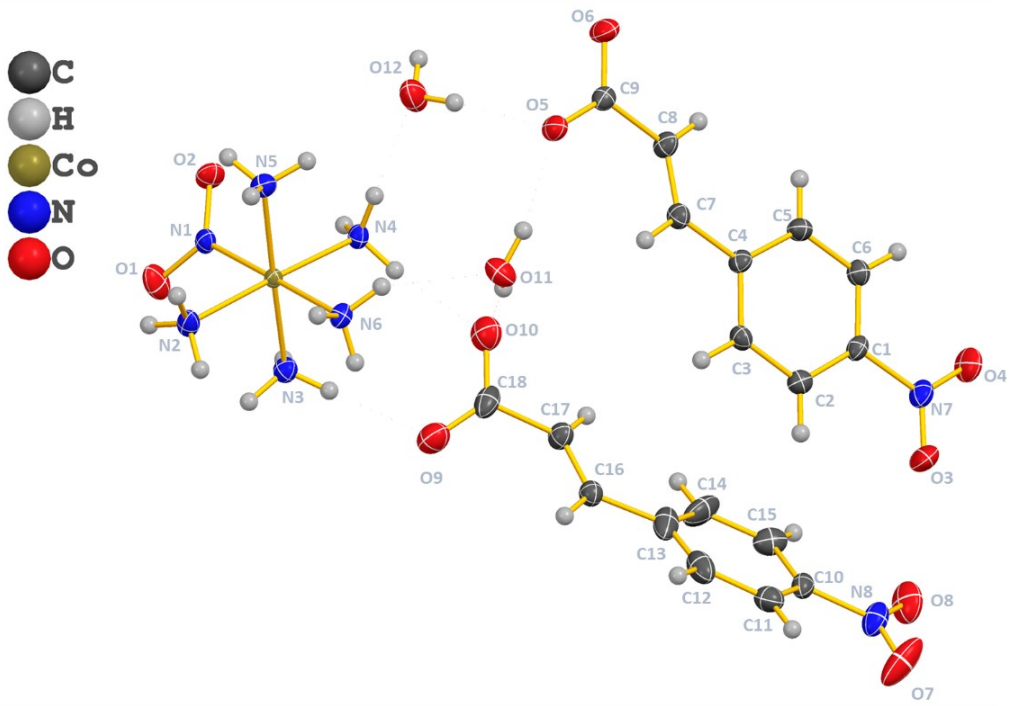

Fig. S2 ORTEP diagram of **C-1** with atoms numbering scheme. Thermal ellipsoid set at 40 % probability.

Table S2 Selected bond lengths **(Å)** and bond angles **(°)** observed for complex **C-1**.

C-1	
Atoms	**Bond Length (Å)**
Co1N4	1.957(3)
Co1N6	1.977(3)
Co1N1	1.917(3)
Co1N5	1.953(3)
Co1N2	1.962(3)
Co1N3	1.960(3)
C-1	
Atoms	**Bond Angle (°)**
N4 Co1 N6	90.55(13)
N4 Co1 N2	177.83(14)
N4 Co1 N3	88.32(13)
N1 Co1 N4	91.15(13)
N1 Co1 N6	177.98(13)
N1 Co1 N5	90.58(14)
N1 Co1 N2	88.77(13)
N1 Co1 N3	89.80(14)
N5 Co1 N4	90.56(13)
N5 Co1 N6	88.32(13)
N5 Co1 N2	91.61(13)
N5 Co1 N3	178.82(13)
N2 Co1 N6	89.56(13)
N3 Co1 N6	91.33(13)
N3 Co1 N2	89.51(14)

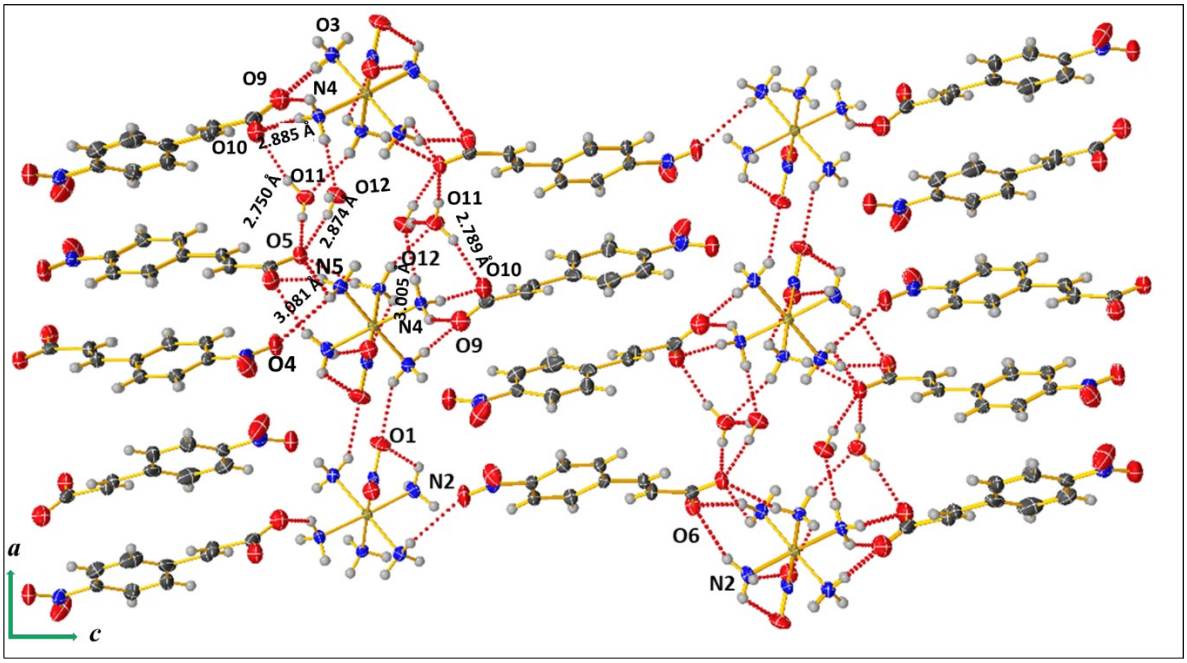

Fig. S3 Hydrogen bonding network of complex **C-1**.

Table S3 Hydrogen bonding distance **(Å)** and angles **(°)** of complex **C-1**.

D	H	A	d(D H)/Å	d(H···A)/Å	d(D···A)/Å	D H···A/°
O11	H11A	O10	0.85	1.96	2.789(4)	166.4
O11	H11B	O5	0.85	1.91	2.750(4)	168.1
O12	H12A	O5	0.85	2.03	2.874(4)	173.2
O12	H12B	O11[1]	0.85	2.02	2.861(4)	171.7
N4	H4A	O10	0.89	2.00	2.885(4)	172.2
N4	H4B	O12	0.89	2.12	3.005(4)	176.8
N4	H4C	O9[1]	0.89	2.20	2.963(4)	143.5
N6	H6A	O2[2]	0.89	2.33	2.915(4)	123.6
N6	H6B	O5[3]	0.89	2.20	3.076(4)	167.3
N6	H6C	O11	0.89	2.14	2.952(4)	150.9
N5	H5B	O6[3]	0.89	2.02	2.882(4)	161.4
N5	H5C	O5[4]	0.89	2.59	3.168(4)	123.0
N5	H5C	O4[5]	0.89	2.44	3.081(4)	128.9
N2	H2A	O2[2]	0.89	2.22	3.043(4)	154.5
N2	H2C	O6[3]	0.89	2.16	3.008(4)	159.3
N3	H3A	O9	0.89	2.12	3.008(4)	177.8
N3	H3C	O1[6]	0.89	2.19	2.983(4)	147.5

[1]+X,-1+Y,+Z; [2]+X,1+Y,+Z; [3]1/2-X,1/2+Y,3/2-Z; [4]1/2-X,-1/2+Y,3/2-Z; [5]1/2+X,1/2-Y,1/2+Z; [6]3/2-X,1/2+Y,3/2-Z

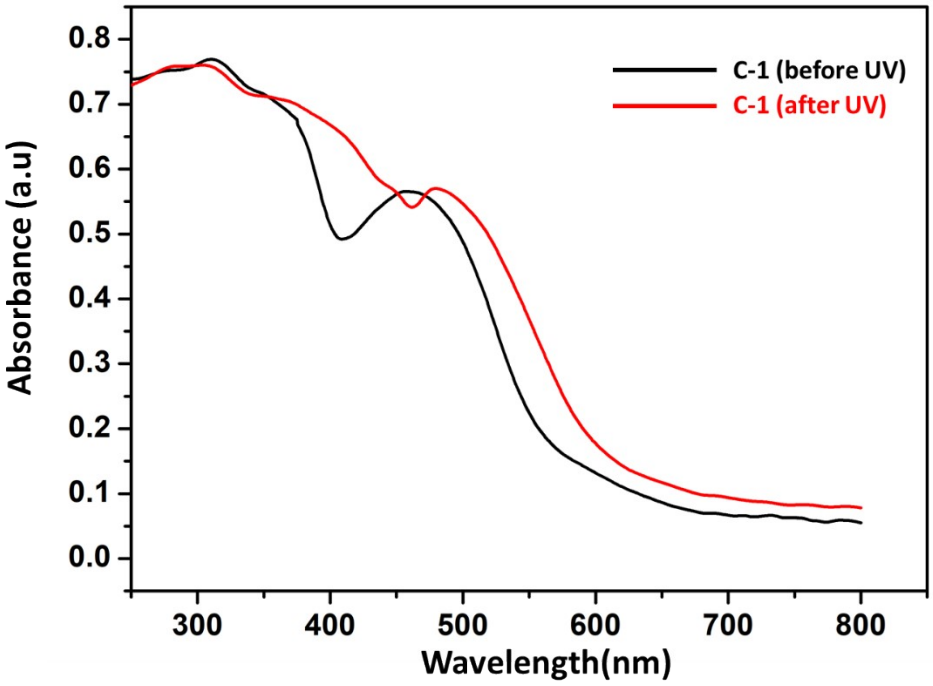

Fig. S4 Solid-state UV spectra of **C-1** (before and after UV irradiation).

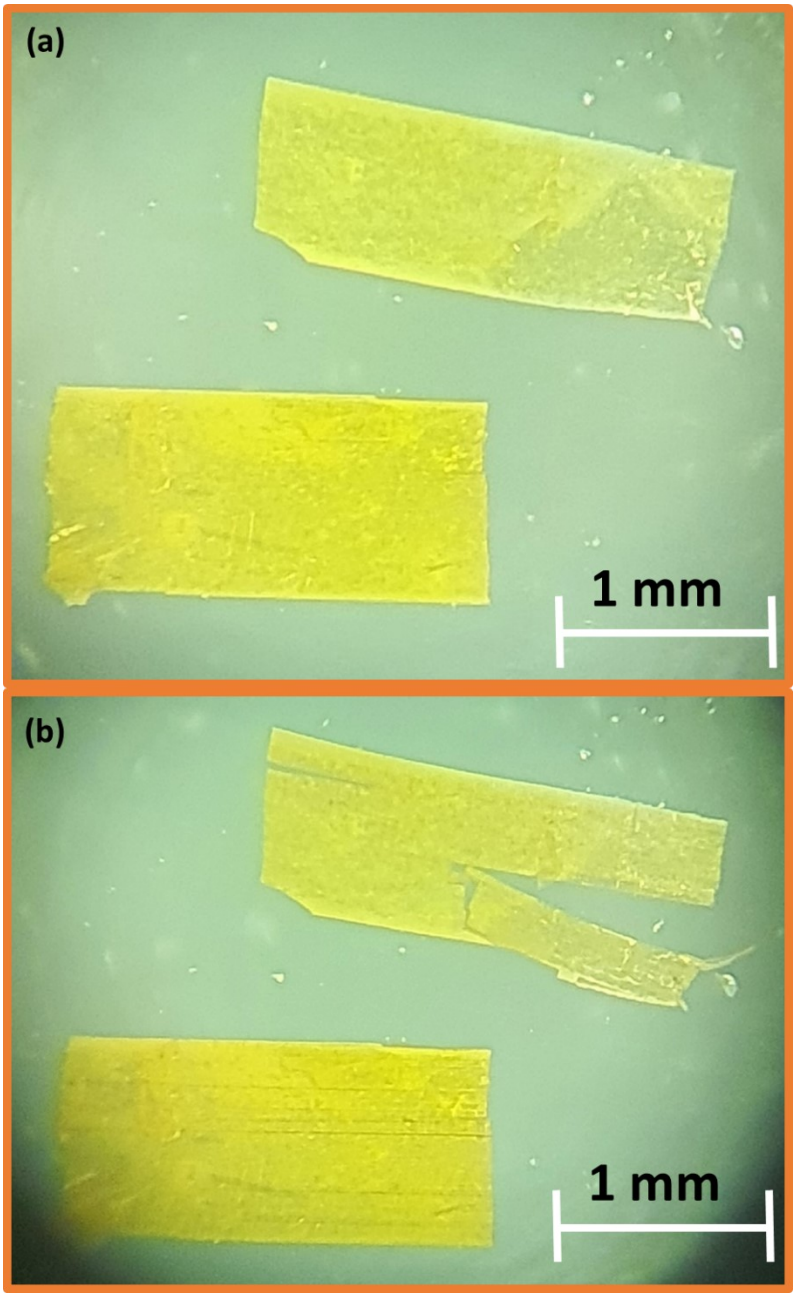

Fig. S5 Optical Microscope image of **C-1** crystals before (a) and after (b) UV irradiation.

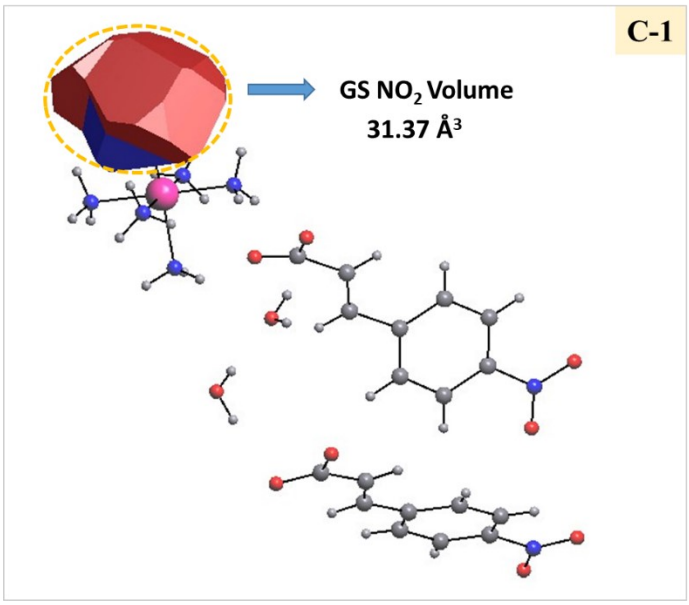

Fig. S6 VDP diagram of the ground state (GS) NO_2 using TOPOS software of complex **C-1**.

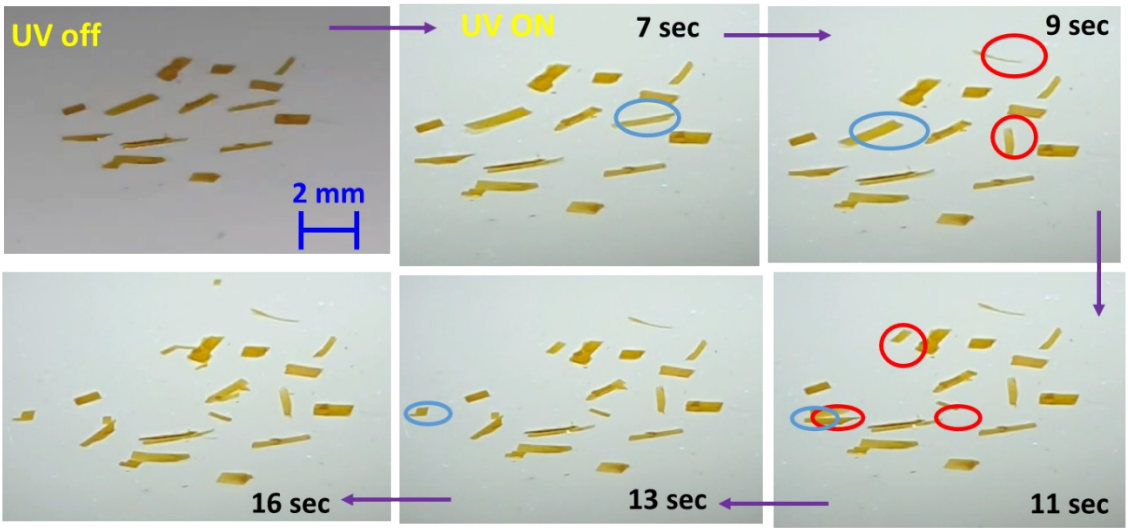

Fig. S7 Single crystals of **C-1** showing photomechanical motion under UV light. The initial and final positions are marked as blue and red circles respectively. The images were extracted from Video S2.

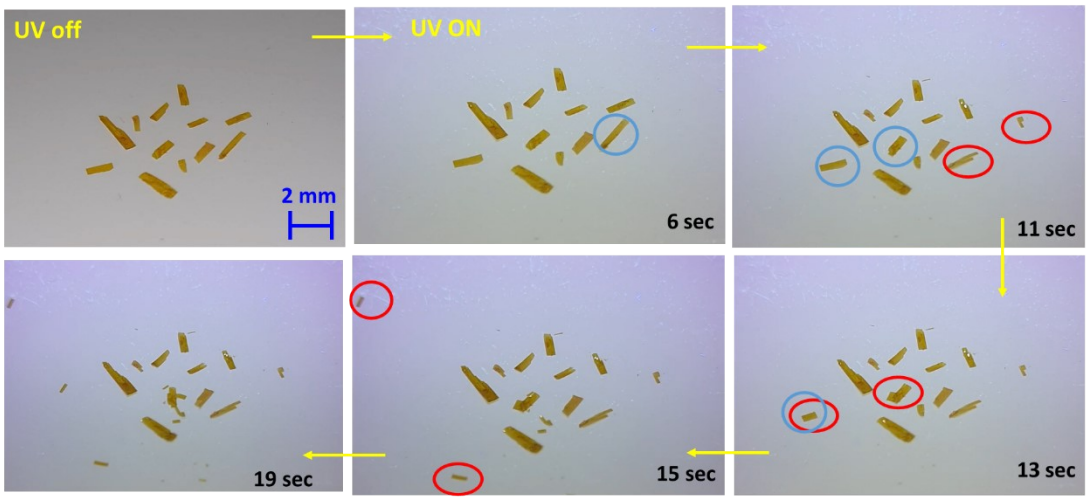

Fig. S8 Single crystals of **C-1** showing photomechanical motion under UV light. The initial and final positions are marked as blue and red circles respectively. The images were extracted from video S3.

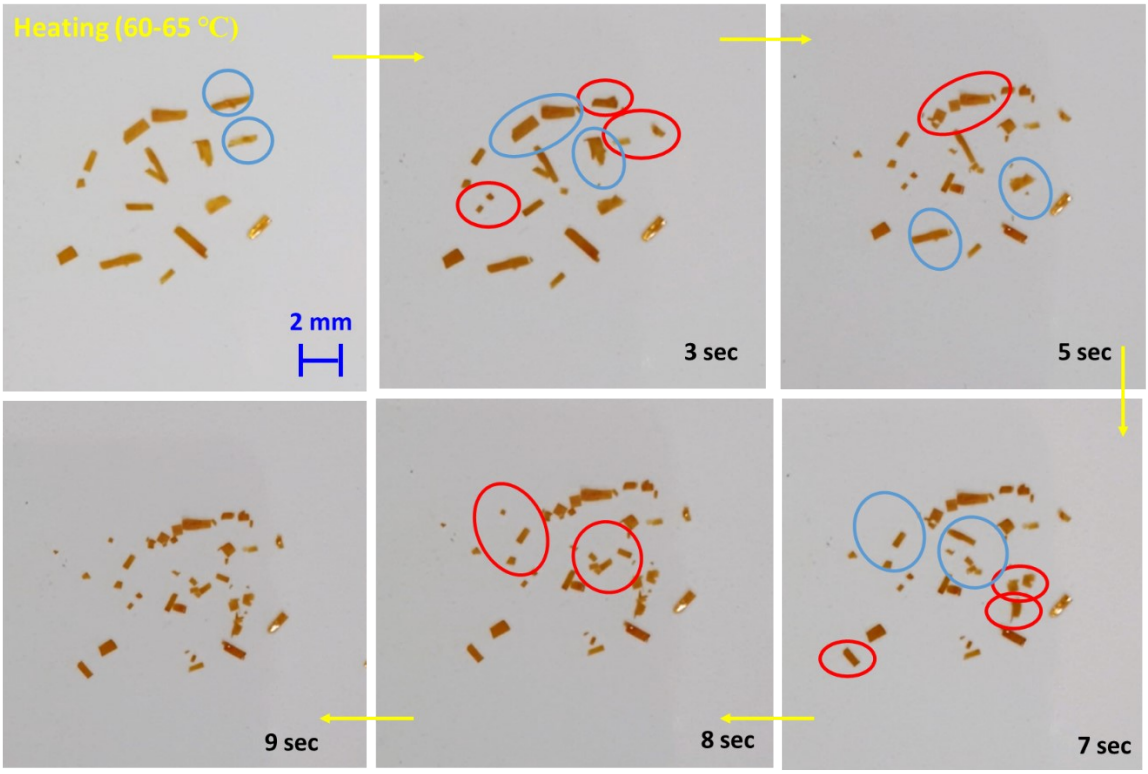

Fig. S9 Single crystals of **C-1** showing the thermomechanical motion at temperature 60-65 °C. The initial and final positions are marked as blue and red circles respectively. The images were extracted from Video S6.

Table S4. Distance transverse by the crystal of different sizes

Crystals (size)	**Distance transverse (mm) (photomechanical)**
2.0 mm×0.7mm×0.05	3.68
1.7 mm×0.5mm×0.04	2.77
1.7 mm×0.3mm×0.05	1.98 , 2.80, 2.07
1.0 mm×0.3mm×0.02	2.55
2.0 mm×0.8mm×0.05	1.1
1.5 mm×0.6mm×0.05	1.5
1.0 mm×0.5mm×0.06	3.1
Crystals	**Distance transverse (mm) (Thermomechanical)**
1.8 mm×0.5mm×0.05	1.8
1.7 mm×0.6mm×0.05	1.2
1.5 mm×0.5mm×0.04	1.1
2.0 mm×0.7mm×0.03	2.2
1.3 mm×0.5mm×0.04	1.9

Table S5. Lattice parameters of **C-1** extracted from the VT-PXRD data (30 and 60℃).

Parameters	**C-1 (30 ℃)**	**C-1 (60 ℃)**	**Change**	**% change**
a	15.7307	15.7337	0.003	0.019
b	4.7402	6.2307	1.49	31.43
c	28.6694	28.6808	0.005	0.017
V	1940.70	2551.38	610.68	31.46

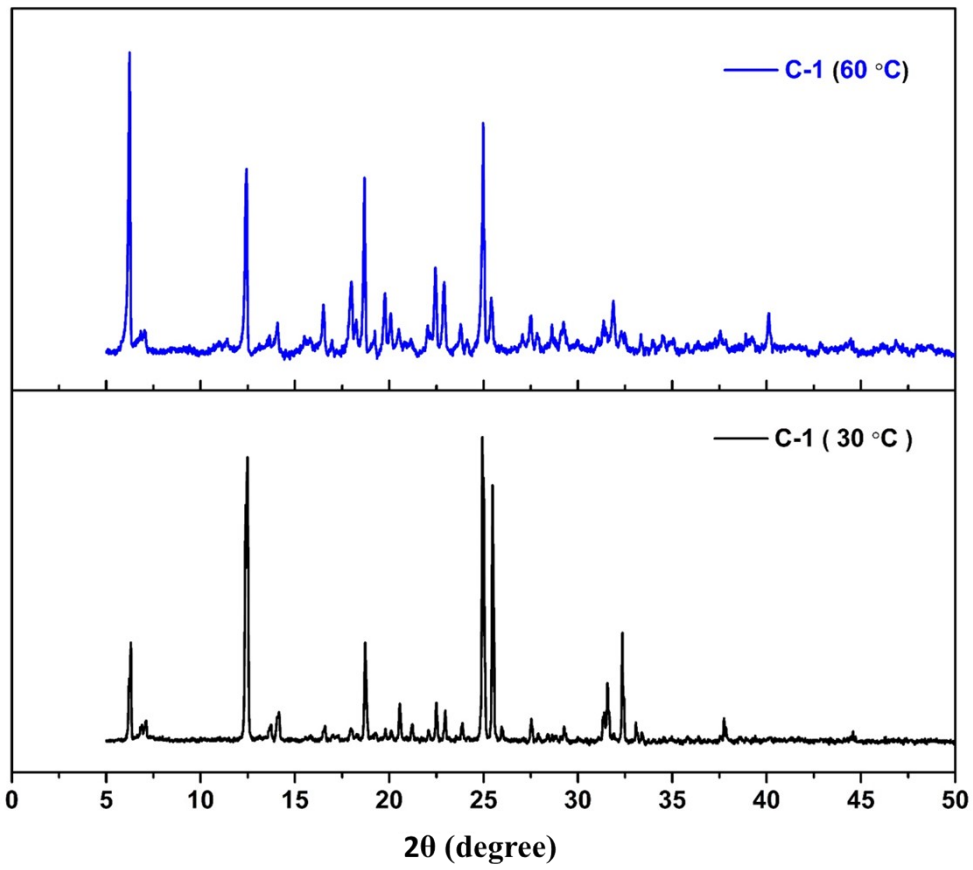

Fig. S10. PXRD pattern of **C-1** (30 and 60℃).

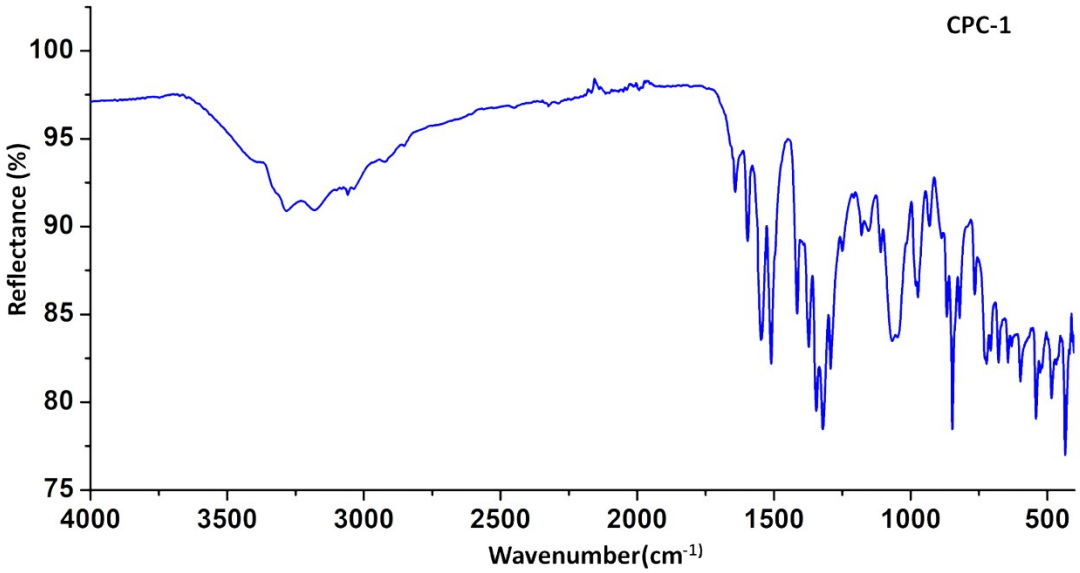

Fig. S11 FTIR Spectrum of **CPC-1**.

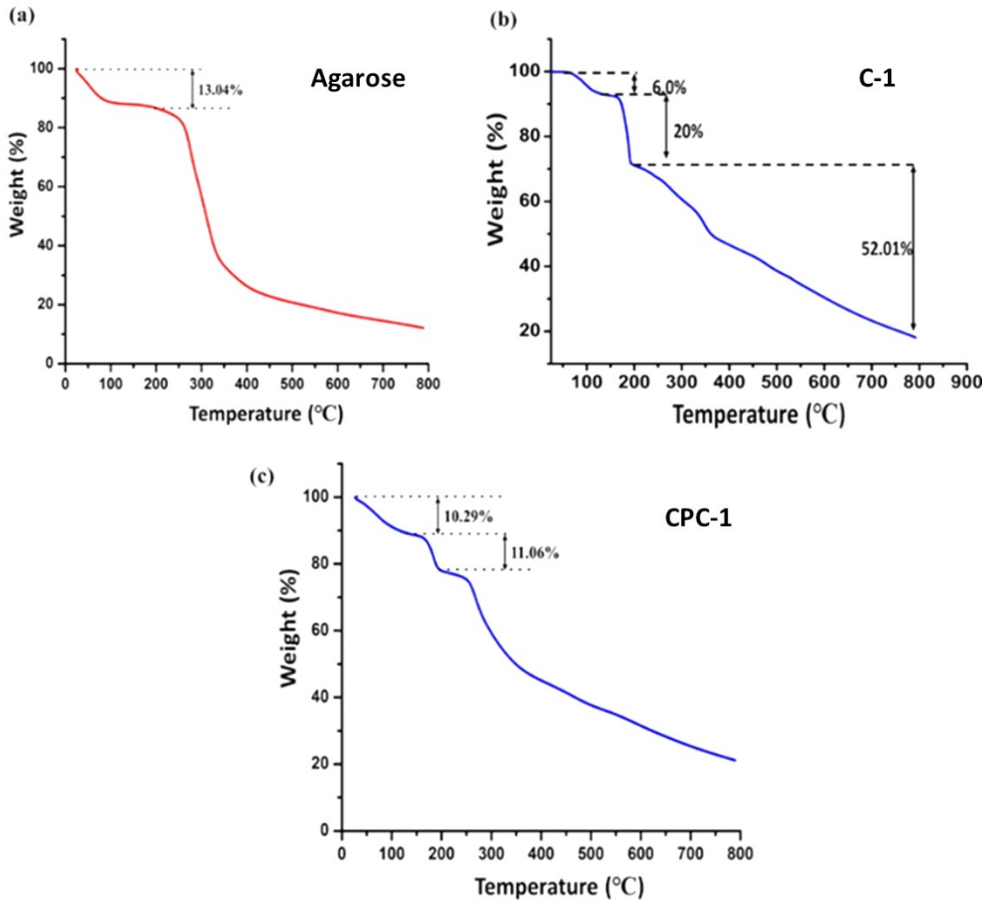

Fig. S12 TGA curves of (a) agarose film (b) **C-1** crystals (c) **CPC-1**.

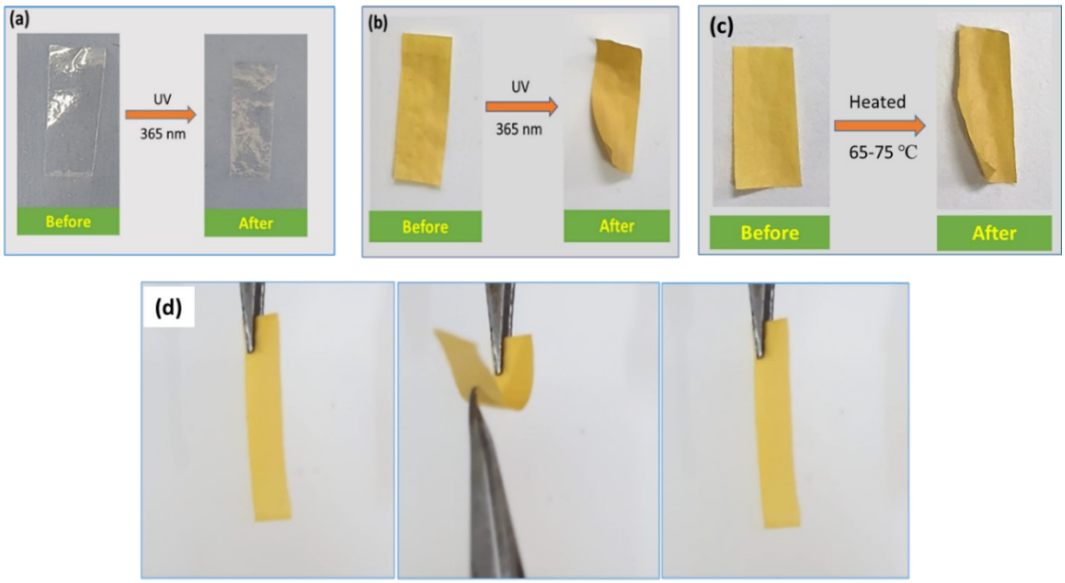

Fig. S13 (a) Pure Agarose Film (b) **CPC-1** under UV light (c) **CPC-1** film under heating (d) Flexibility test of **CPC-1** film.

Video Description

Video S1-3: Photomechanical behaviour of **C-1** crystals.

Video S4: Photomechanical behaviour (bending) of a single crystal of **C-1**.

Video S5-6: Thermomechanical behaviour of **C-1** crystals.

Video S7: Flexibility test of **CPC-1** Film.

Video S8: Photomechanical behaviour of **CPC-1** film.

Video S9: Thermomechanical behaviour of **CPC-1** film.