Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary information

A Photoluminescent Organosuperelastic Crystal of 7-Amino-4-Methylcoumarin

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Table of contents

Other supplementary material

Movie S1. Superelastic behavior of a single crystal of **1** sheared by tweezers under PW light.

Movie S2. Superelastic behavior of a single crystal of **1** sheared by tweezers under PW light (left) and PW+UV light (right).

Movie S3. Superelastic behavior of a single crystal of **1** sheared by a glass jig under PW light (left) and UV light (right).

Mechanical characterization

Table S1. Mechanical parameters of superelastic molecular crystals.

Entry	σ_f / MPa[a]	σ_r / MPa[a]	E_s / kJ m^{-3}[b]	η[c]	χ[d]	θ / °[e]
1-PW	0.63	0.04	4	0.07	0.01	3.8
1-UV	0.63	0.04	3	0.06	0.01	3.8
TPA[f]	0.50	0.46	62	0.93	0.13	6.5
FBA[g]	0.07	0.01–0.03	12	0.29	0.26	27.8
BPPB[h]	0.53	0.42	50	0.79	0.10	5.3
MNA[i]	0.03	0.01	4	0.39	0.20	20.5
PDA[j]	0.49	0.28	110	0.61	0.29	23.9
DCB[k]	0.03	0.02	8	0.77	0.28	18.6
FPC[l]	0.35	0.03	8	0.08	0.04	16.3
MPU[m]	0.25	0.16	8	0.64	0.04	2.9
7Cl[n]	1.53	0.66	560	0.43	0.51	42.1
TCNB[o]	0.11	0.04	15	0.35	0.19	21.4
MNBA[p]	0.69	0.38	31	0.55	0.06	3.3
PFPI[q]	0.28	0.19	72	0.69	0.31	22.2
TClB[r]	0.18	0.02	1.6	0.09	0.02	5.84~

[a]Effective shear stress for deformation: proceeding in the forward (σ_f) and reverse (σ_r) directions. [b]Energy storage density ($E_s=W_{out}/V$). The symbols W_{out} and V represent the output work and volume, respectively, in a deformed region of a specimen during superelastic deformation. [c]Energy storage efficiency ($\eta=W_{out}/W_{in}$) where W_{in} represents input work. [d]Superelastic index ($\chi=2E_s/(\sigma_f+\sigma_r)$). [e]Representative crystal bending angles: a crystal bending angle is variable depending on a crystal morphology. [f]Terephthalamide.[S1] [g]3,5-difluorobenzoic acid.[S2] [h]5-tetrabutyl-*n*-phosphonium tetraphenylborate.[S3] [i]*N*,*N*-dimethyl-4-nitroaniline.[S4] [J]Pentadecanoic acid.[S5] [k]1,4-dicyanobenzene[S6] [l]4,5,7,8,12,13,15,16-octafluoro[2.2]paracyclophane.[S7] [m]1,3-bis(4-methoxyphenyl)urea.[S8] [n]7-chloro-2-(2'-hydroxyphenyl)imidazo[1,2-*a*]pyridine.[S9] [o]1,3,5-tricyanobenzene.[S10] [p]3-methyl-4-nitrobenzoic acid.[S11] [q]*N*-(2,3,4,5,6-pentafluorophenyl)-1-phenylmethanimine.[S12] [r]1,3,5-trichlorobenzene.[S13]

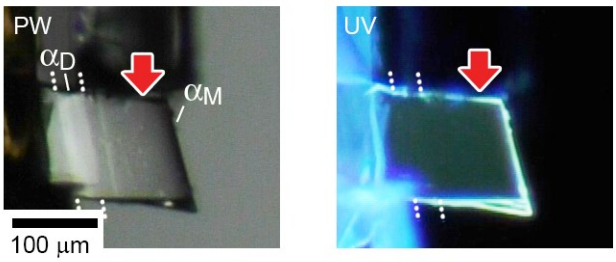

Figure S1. Photographic images of a deformed crystal of **1** under PW light (left) and UV light (right).

Crystallographic studies

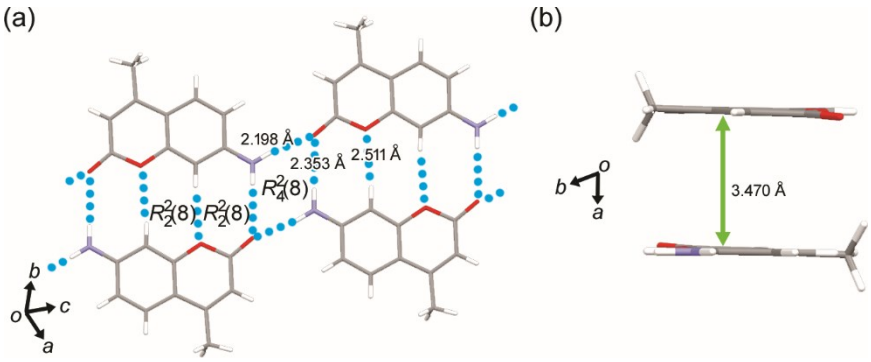

Figure S2. (a) Hydrogen bonding networks with graph set denotations[S14–S17] and (b) π-π interactions in the crystalline state.

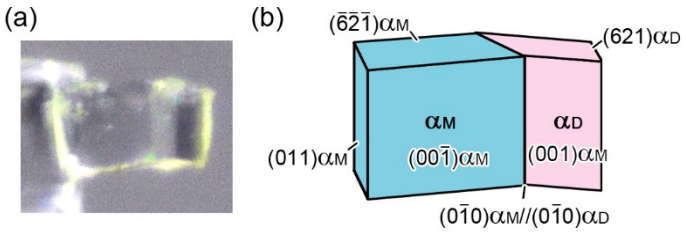

Figure S3. (a) A photographic image of a twinned crystal of **1** and (b) its face indices.

Table S2. Crystallographic parameters of a mechanically twinned crystal of **1**.

Sample	Mechanically twinned	
Domain	α_M	α_D
T / K	296	296
Molecular formula	$C_{10}H_9NO_2$	$C_{10}H_9NO_2$
Crystal size/mm^3	0.245x0.124x0.099	0.171x0.115x0.082
Molecular weight	175.18	175.18
Crystal system	triclinic	triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a / Å	6.9349(19)	6.9361(7)
b / Å	7.1467(15)	7.1569(6)
c / Å	9.558(2)	9.5654(9)
α / °	71.817(6)	71.825(3)
β / °	84.968(8)	84.915(3)
γ / °	70.026(8)	69.902(3)
V / Å^3	422.89(18)	423.58(7)
Z	2	2
D_{calcd} / Mg m^{-3}	1.376	1.374
μ (Mo Kα) / mm^{-1}	0.097	0.097
Reflections collected	5217	5247
Independent reflections (R_{int})	1468 (0.0610)	1473 (0.0449)
Goodness of fit	1.653	1.060
R_1 ($I > 2\sigma$ (all data))	0.1819 (0.2083)	0.0632 (0.0803)
$_wR_2$ ($I > 2\sigma$ (all data))	0.4492 (0.4751)	0.1731 (0.1973)
Largest diff. peak (hole)/eÅ^3	1.328 (-0.538)	0.281 (-0.225)
CCDC No.	2069188	2069189

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