Electronic Supplementary Material (ESI) for ChemComm.

Supporting information

Structural origins of two-dimensional elastic bending in a nonaromatic organic molecular crystal

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Experiment Section

Materials. Isosorbide 5-mononitrate (IMN) was purchased from Lunan Pharmaceutical Group with the mass fraction > 99% and used without further purification.

Preparation of single crystals

A propyl acetate solution of IMN (0.2915 g/g) was prepared at 40 ℃. Then the solution was extracted by syringes and injected into the glass bottle through a 0.22 μm organic membrane filter. The sealed glass bottle was kept in 20 ℃ for 12-24 h and then the long needle-like single crystals could be obtained.

SEM. Scanning electron microscopy (SEM, TM300, Hitachi, Japan) was used to observe the mechanical bending and splitting behaviors.

Single-Crystal X-ray Diffraction Experiment. A suitable single crystal was set on a ROD, Synergy Custom system, HyPix diffractometer. The data was collected in 160 K and 113.15 K controlled by an Oxford Cryostream 800 Cooler. Olex2 was used to solve the structure by intrinsic phasing methods (SHELXT) and complete and refine the structure models using the full-matrix least-squares methods on F2 (SHELXL).

Nanoindentation.

The nanomechanical test uses KLA-G200 to access the mechanical property of IMN. The (0 1 0) face of IMN were indented to a peak load of 5 mN with a loading/unloading rate of 0.25 mN s^{-1} in all tests. We chose the 20 single crystals (length:2-3cm; width of (0 1 0) plane: 50-120 μm; thickness of (1 0 0): 20-35 μm) to perform the mechanical property measurement. These single crystals were glued

down to a glass slide using a spread drop of cyanoacrylate adhesive. P-h curves were analyzed using the standard Oliver−Pharr method to extract the H and E values of the crystals where the Poisson's ratio (ν) is 0.18.

Computation. The energy of the targeted hydrogen bond was calculated based on its electron density at the bond critical point (ρ_{BCP}). M062x method with def2TZVPP basis set was applied to calculate the intermolecular interaction energies of the two IMN molecules in Gaussian 09. All of the calculated values were corrected by BSSEs according to the counterpoise method of Boys and Bernardi. The bond energy was calculated based on the equation of $\Delta E=-223.08\times\rho_{BCP}+0.7423$.

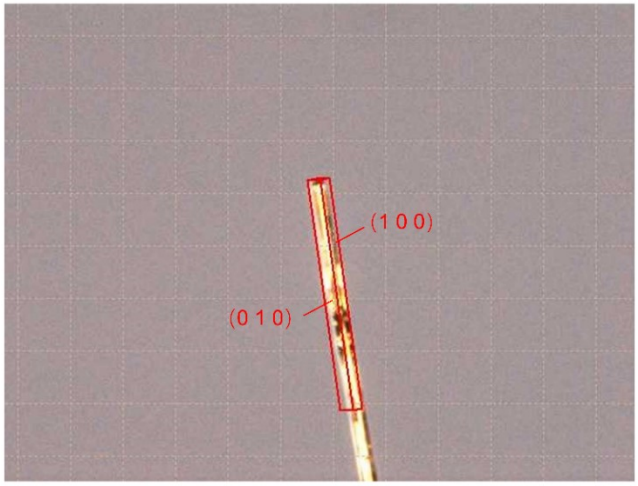

Fig.S1 Face indexing of IMN

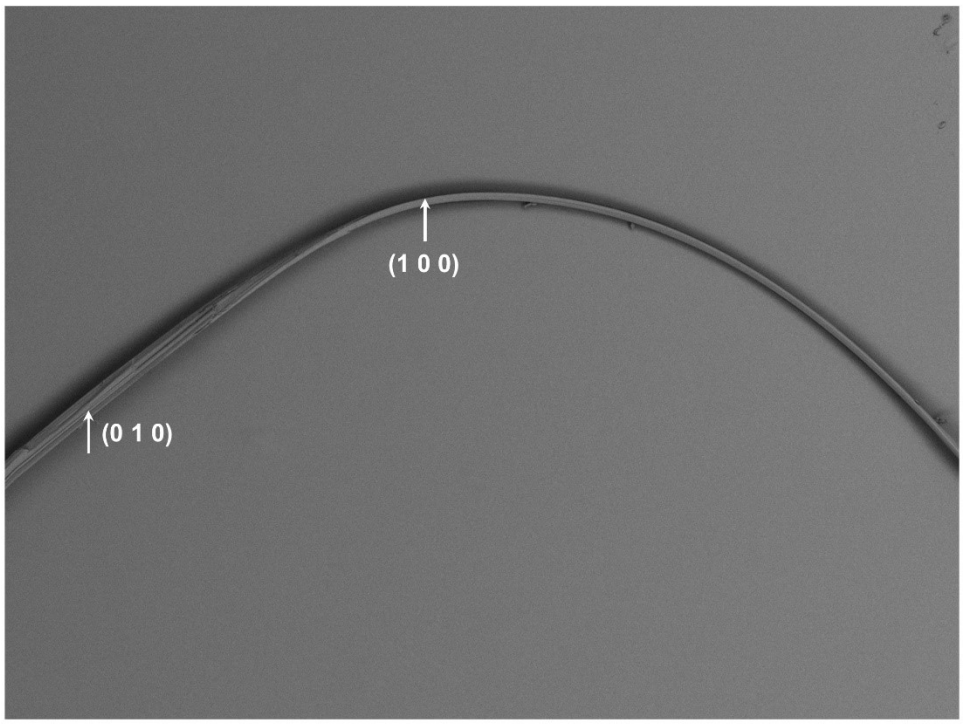

Fig.S2 SEM figures of the twist crystal of IMN.

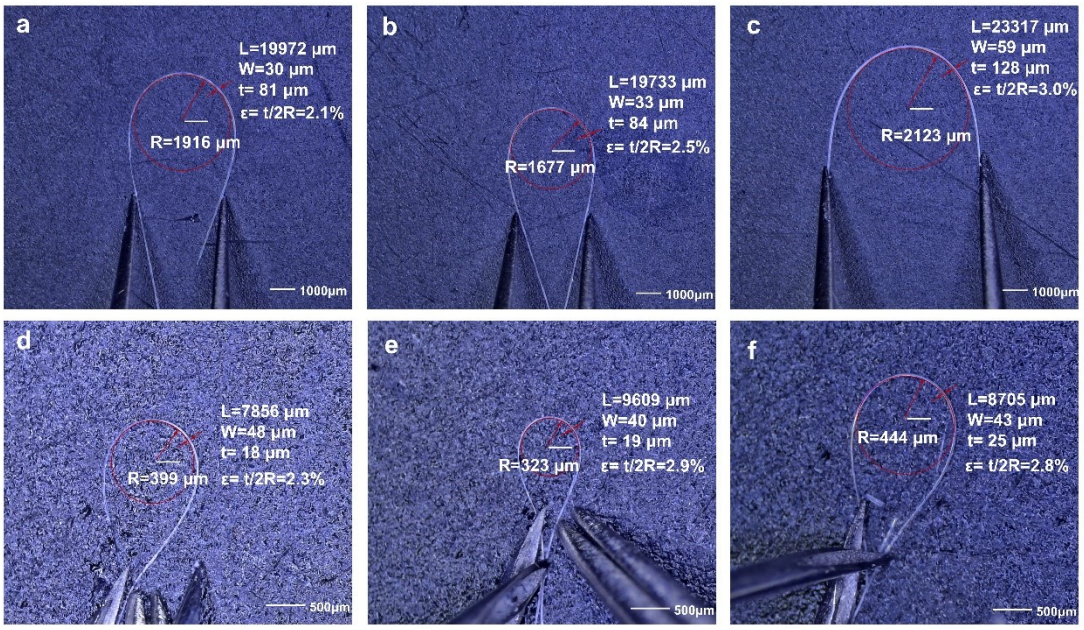

Fig.S3 Calculation of elastic strain by using the Euler-Bernoulli's beam bending theory. a-c) elastic strain when the bent plane is (1 0 0) plane, L represents the length of the single crystals, W is the width of the (1 0 0), t is the thickness of (0 1 0) plane; d-f) elastic strain when the bent plane is (0 1 0) plane. L represents the length of the single crystals, W is the width of the (0 1 0), t is the thickness of (1 0 0) plane.

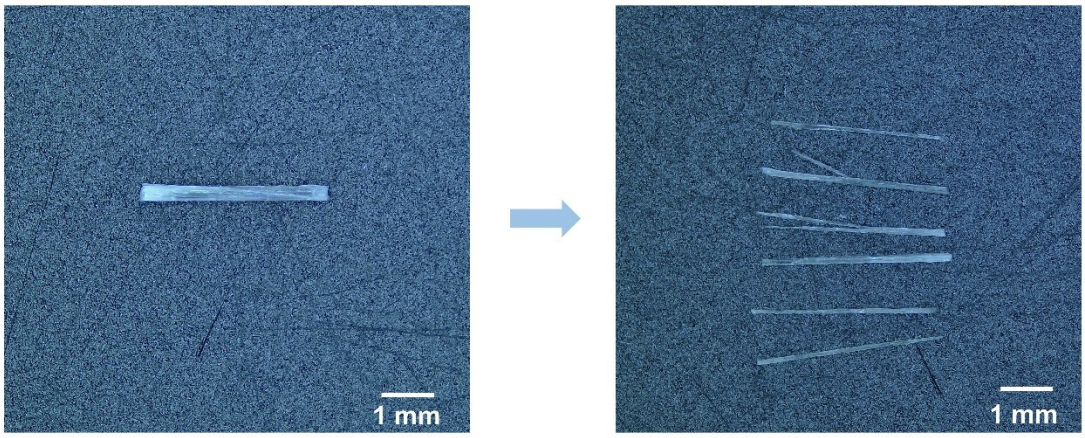

Fig.S4 Representative images of the mechanically induced splitting.

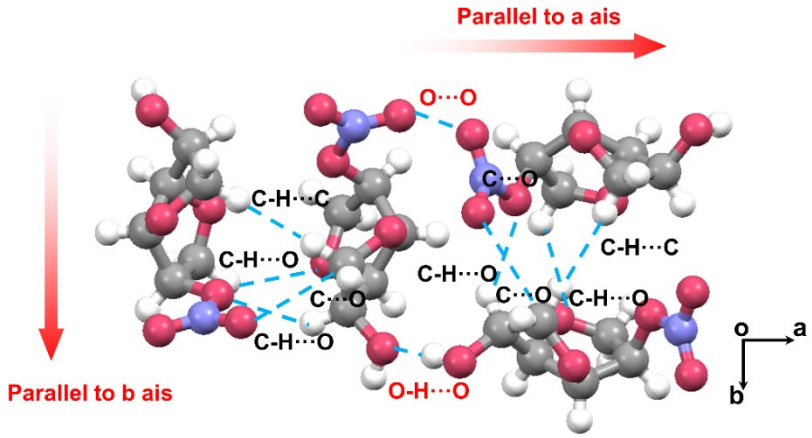

Fig.S5 The intermolecular interactions of the building units and their orientation.

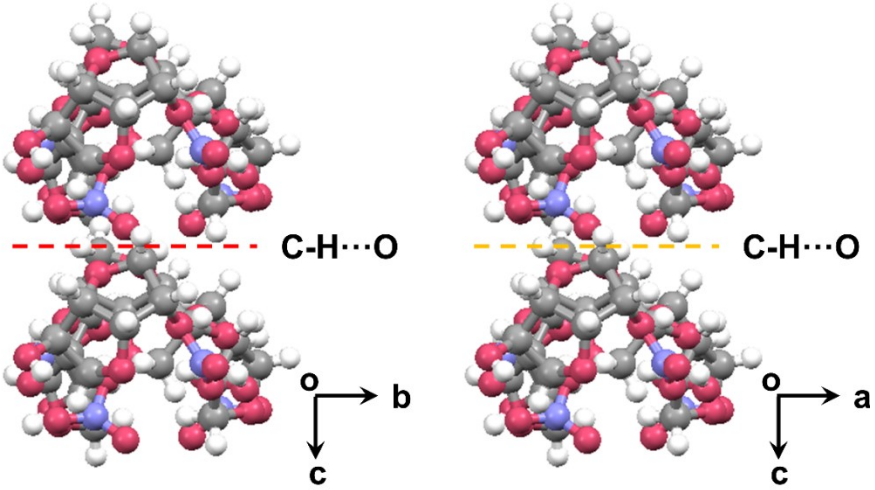

Fig.S6 The intermolecular interactions of the columns viewed from a axis and b axis along [0 0 1] direction.

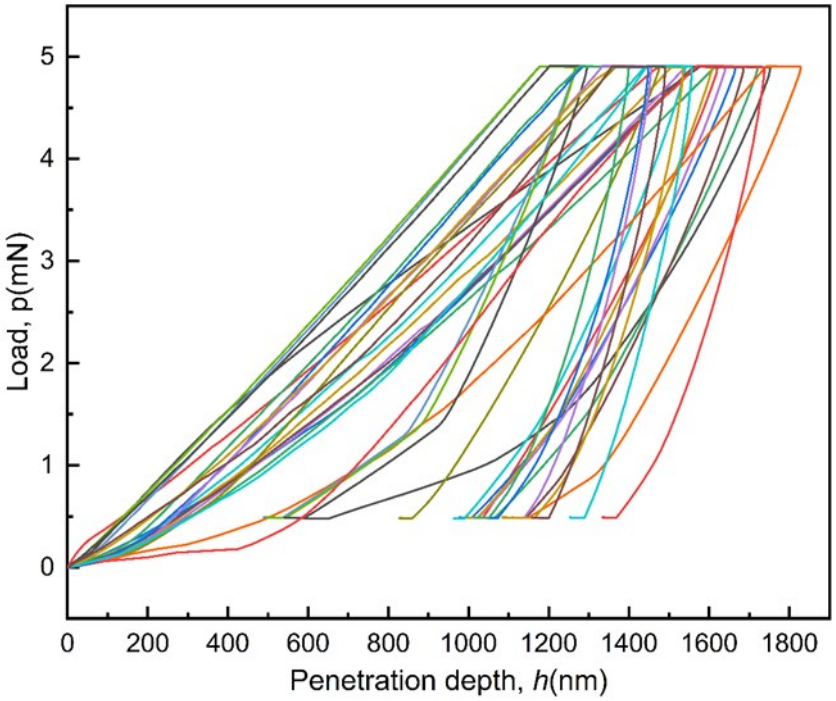

Fig.S7 (P−h) curves obtained from nanoindentation on 20 straight IMN crystals.

Table S1 Crystal data of the reported structure compared our resolved structure.

		Straight	Bent
Compounds	Isosorbide 5-mononitrate	Isosorbide 5-mononitrate	Isosorbide 5-mononitrate
Crystal system	tetragonal system	tetragonal system	tetragonal system
Temperature	223 K	160 K	113.15 K
Space group	$P4_3$	$P4_3$	$P4_3$
Z	8	8	8
Formula weight	191.14	191.14	191.14
Color	colourless	colourless	colourless
a (Å)	15.92600 (10)	15.86558 (18)	15.8980(6)
b (Å)	15.92600 (10)	15.86558 (18)	15.8980(6)
C (Å)	6.50900(10)	6.49316 (13)	6.4937(4)
α	90	90	90
β	90	90	90
γ	90	90	90
V	1650.93(3)	1634.43(5)	1641.26(16)
Density/ (g/cm3)	1.538	1.554	1.547
λ (Mo Kα) (Å)	1.54178	1.54184	0.71073
F_{000}	800	800	800
h_{min}, h_{max}	-18,18	-17,19	-19,19
k_{min}, k_{max}	-13,13	-19,19	-19,19
l_{min}, l_{max}	-7,7	-7, 7	-8,8
No. of measured reflections	8305	15280	14602
No. of unique reflections	2543	3159	3359
No. of reflections used	2747	3034	2673
No. of refinement	243	240	238

parameters			
CCDC number	1400345	2207949	2207955

Table S2 the obtained modulus, hardness and measured maximum displacement from the 20 single crystals.

Test	Modulus/GPa	Hardness/GPa	maximum displacement h_{max}/ (nm)
1	1.319	0.115	1824.977
2	1.354	0.13	1748.786
3	1.424	0.134	1717.545
4	1.444	0.148	1662.557
5	1.553	0.154	1617.399
6	1.605	0.145	1639.009
7	1.694	0.128	1683.656
8	1.722	0.201	1473.995
9	1.729	0.148	1606.403
10	1.927	0.158	1539.549
11	2.227	0.283	1262.967
12	2.336	0.268	1263.696
13	2.422	0.241	1294.054
14	2.765	0.1	1737.652
15	2.813	0.107	1534.667
16	3.267	0.112	1490.124
17	3.354	0.099	1556.582
18	3.454	0.147	1448.28
19	3.753	0.157	1398.758
20	3.782	0.143	1455.26