Electronic Supplementary Material (ESI) for Chemical Science.

Controllably Realizing Elastic/Plastic Bending based on a Room Temperature Phosphorescent Waveguiding Organic Crystal

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General Information

Emission spectrum was measured by a Fluoromax-4 spectrometer. Phosphorescent lifetime was measured by an Edinburgh FLS920 spectrometer. The crystal was irradiated by a Nd:YAG (355 nm) laser with a repetition rate of 10 Hz and the emission spectra of crystal ends were measured by a Maya2000 Pro CCD spectrometer. The crystal structure has been measured again. The lattice parameters (a = 6.005(9) Å, b = 25.999 (3) Å, c = 4.0357 (5) Å, α = 90°, β = 90°, γ = 90°) are consistent with the previous result (CCDC 707769: a = 5.9307(12) Å, b = 26.138(6) Å, c = 3.9251(8) Å, α = 90°, β = 90°, γ = 90°).[1]

Bending Strain Formula

The bending of organic crystals could be regarded as a pure bending process without any shear components. Thus, bending strain is calculated using the Euler-Bernoulli equation.[2]

$$\varepsilon\ (\%) = y/R \times 100 \qquad (1)$$

y is the distance of the considered plane from the neutral plane whose length remains invariant under bending process, and R is the radius of curvature of the neutral plane. Thus, the maximum bending strains reflect on the outlayer and baselayer of crystals.

The crystal with a thickness t, the formula (1) equals to:

$$\varepsilon\ (\%) = t/(2R+t) \times 100 \qquad (2)$$

To simplify this computational procedure, the value of R was fixed by a ballpoint pen refill with a radius of 2.25 mm. Thus, the bending strains are only dependent on the thickness of crystals.

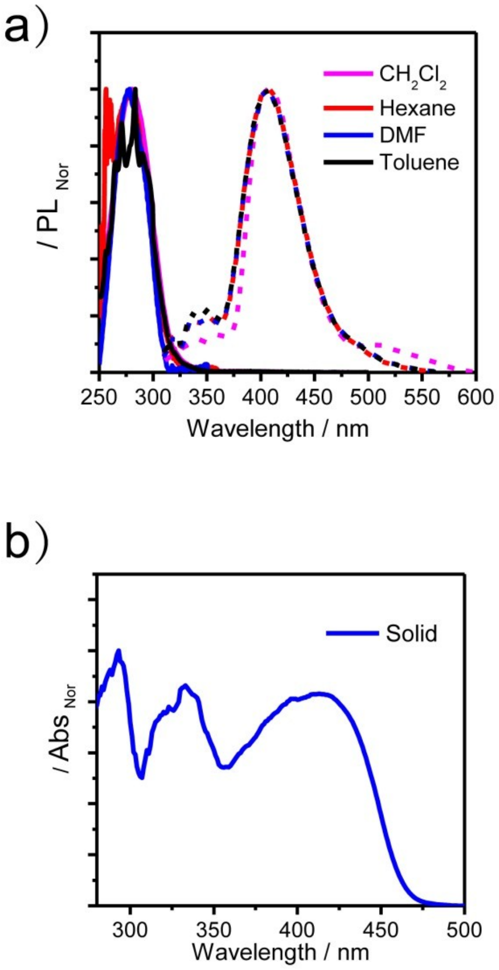

Figure S1. Absorption and emission spectra of **DBBZL** in different solvents (a), and absorption spectrum of crystals **DBBZL** (b).

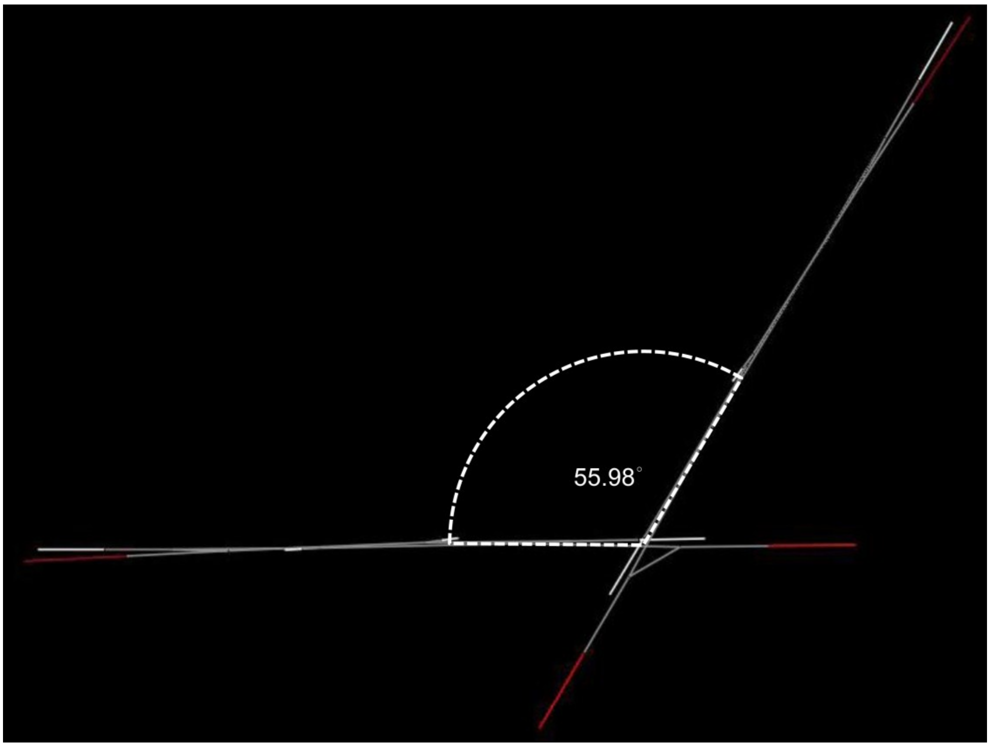

Figure S2. Twist conformation of molecule **DBBZL**. The angle between two benzene rings is given.

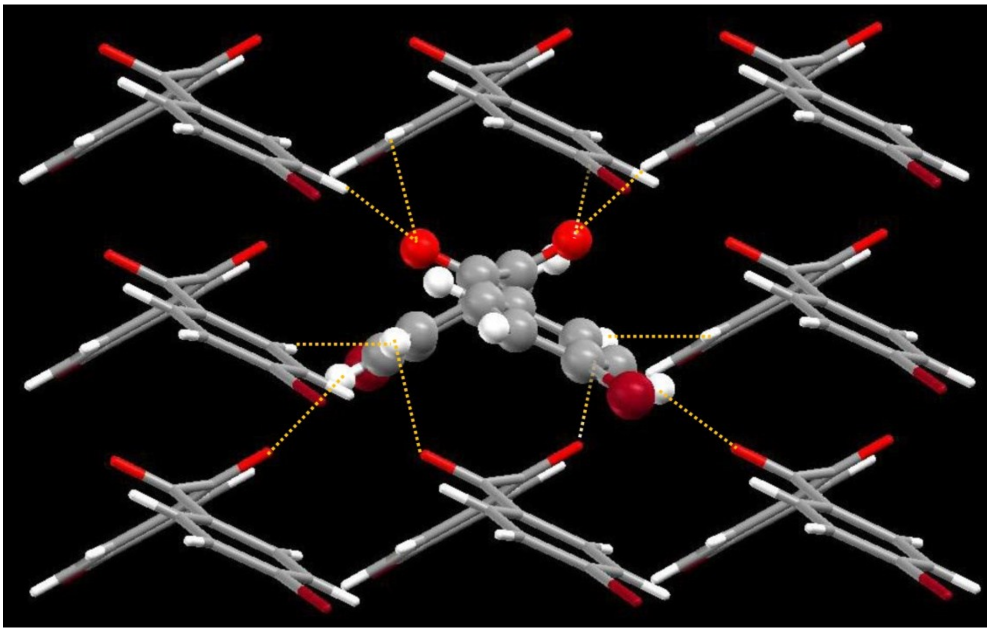

Figure S3. Interactions connected one molecule **DBBZL** with other molecules.

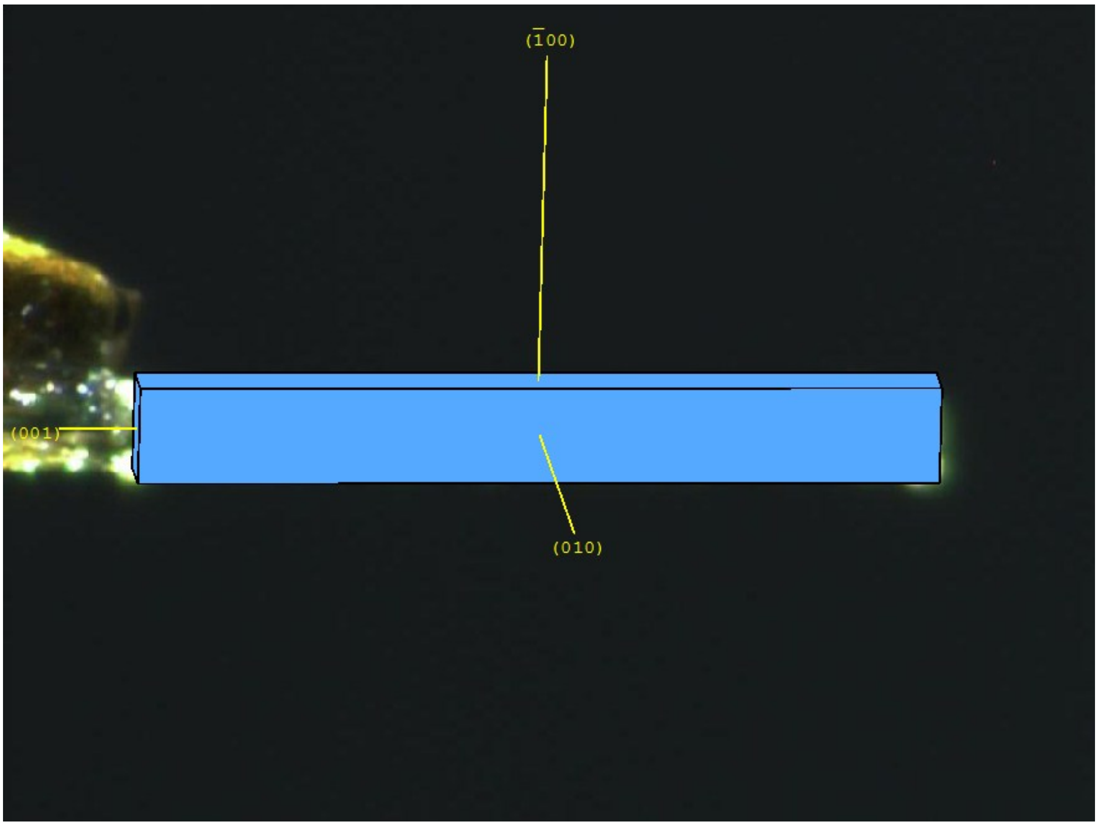

Figure S4. Determination of bending plane by X-ray diffraction.

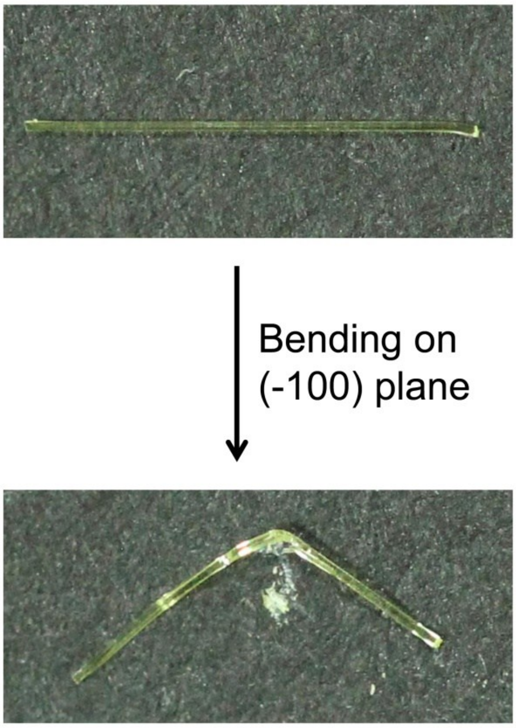

Figure S5. The bending process which occurred on (-100) plane.

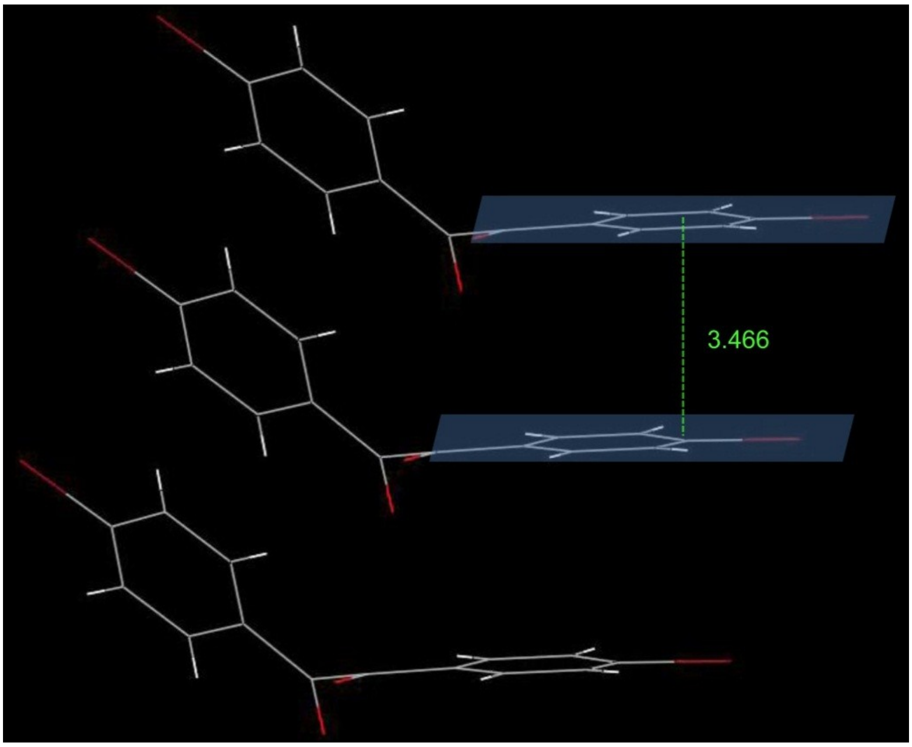

Figure S6. Distance between the parallel benzene rings.

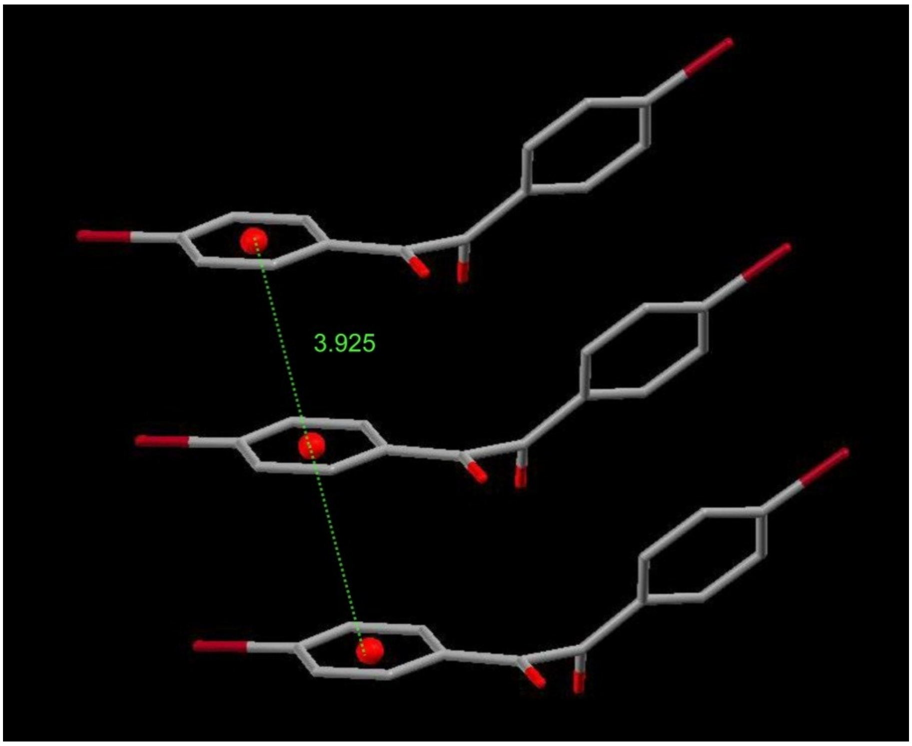

Figure S7. Distance between the centroids of benzene rings.

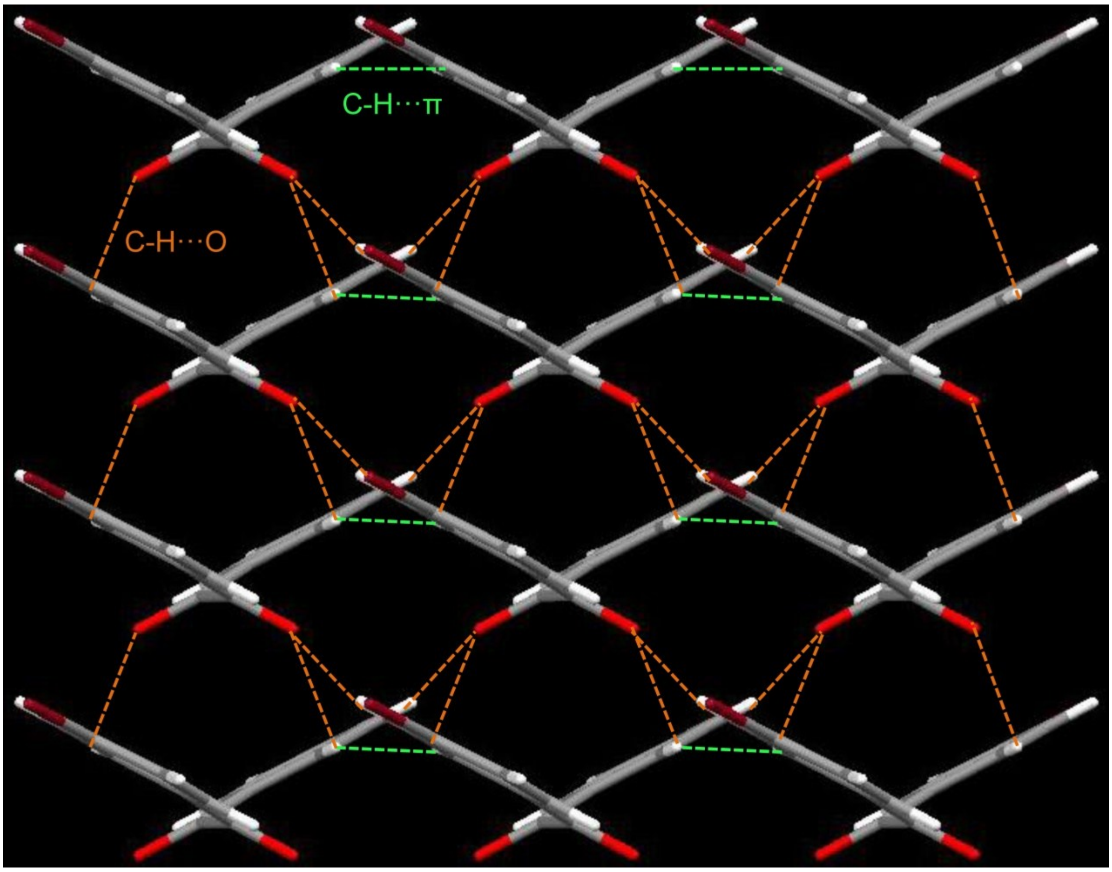

Figure S8. Crystal structure viewed down the major bending face (010), the orange lines represent C–H···O interactions and the green lines represent C–H···π interactions.

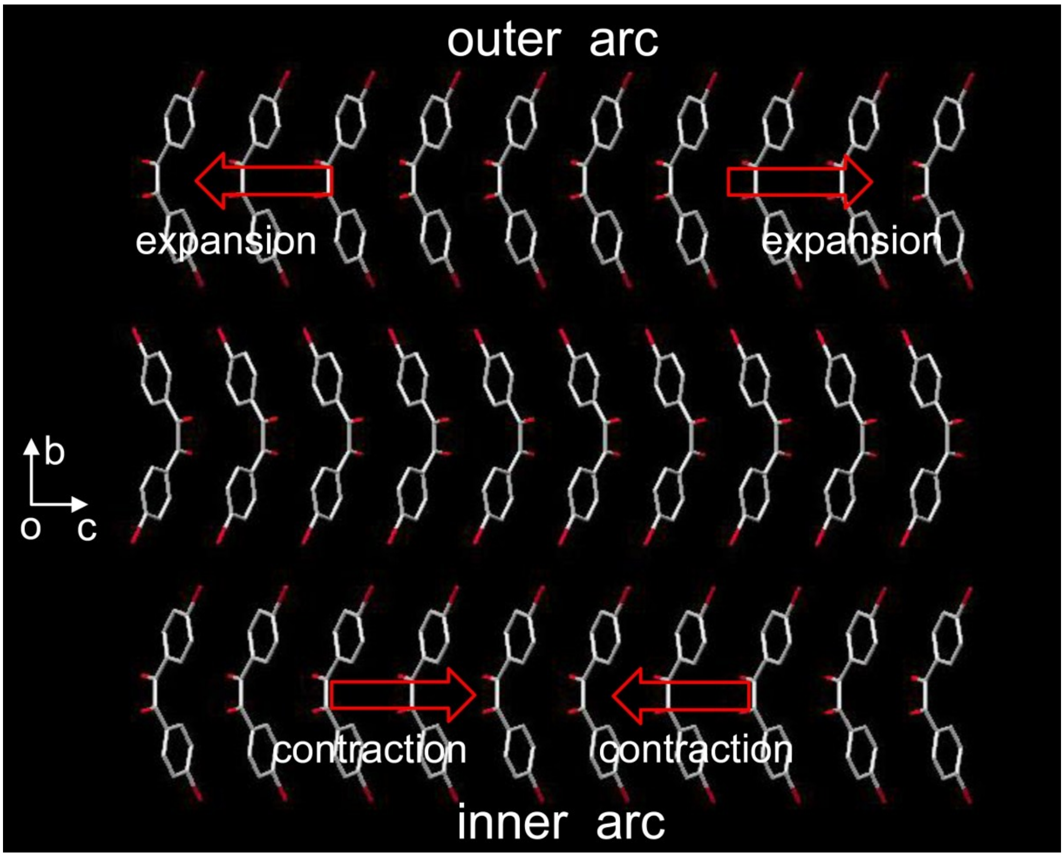

Figure S9. Molecular packing structure viewed down the (-100) plane along the b axis.

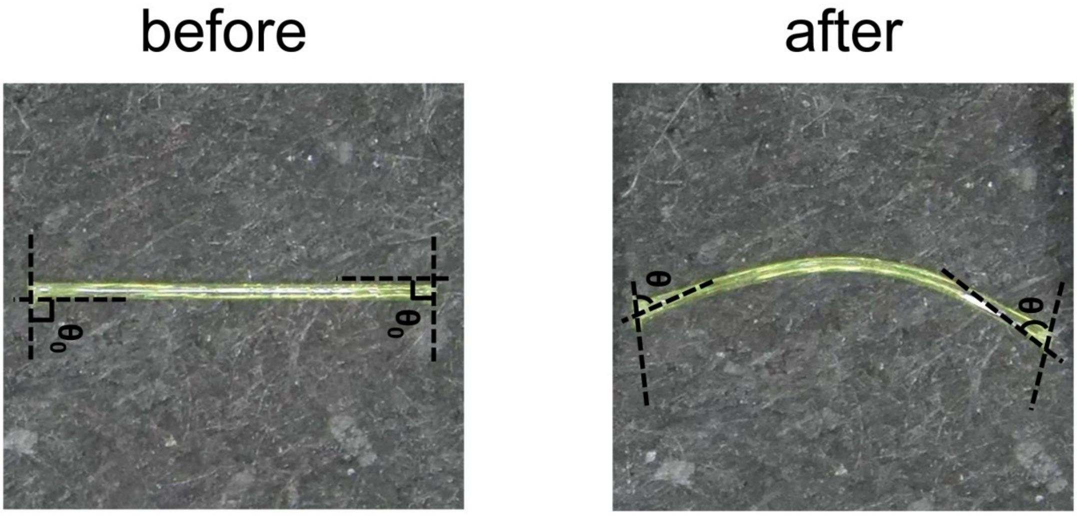

Figure S10. Photographs of the plastic bending process (the black dash lines represent the ends of crystal tops and bending faces; θ_0 and θ represent the angles before bending and after bending).

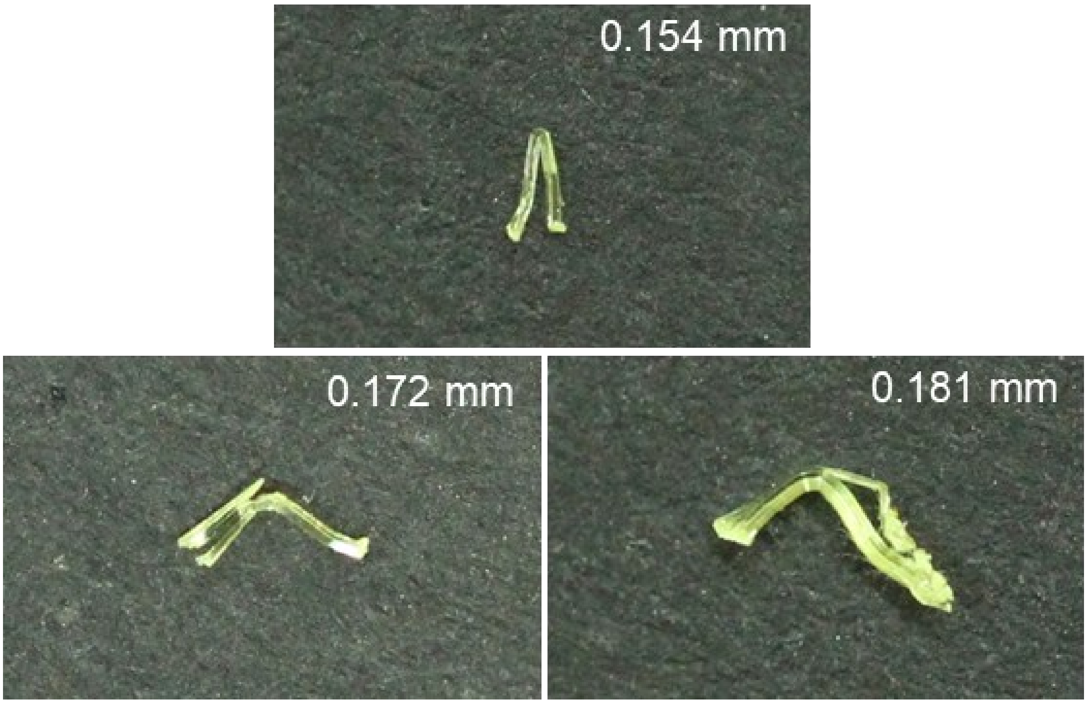

Figure S11. Photographs of the plastic bending of DBBZL crystals with various thicknesses (the thickness of each crystal is marked in the figure).

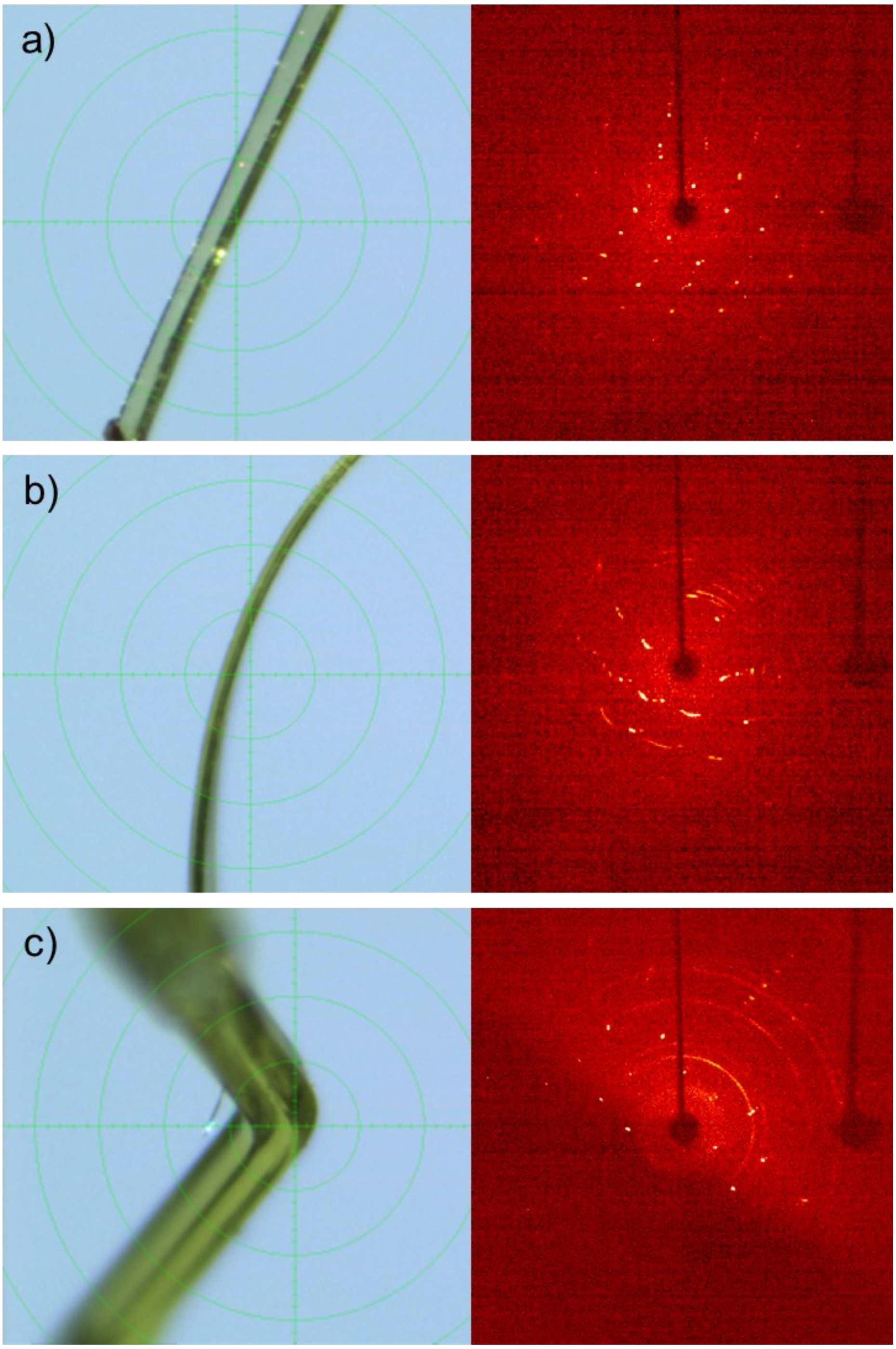

Figure S12. X-ray diffraction patterns of **DBBZL** crystals: a) straight crystal, b) elastically bended crystal, c) plastically bended crystal.

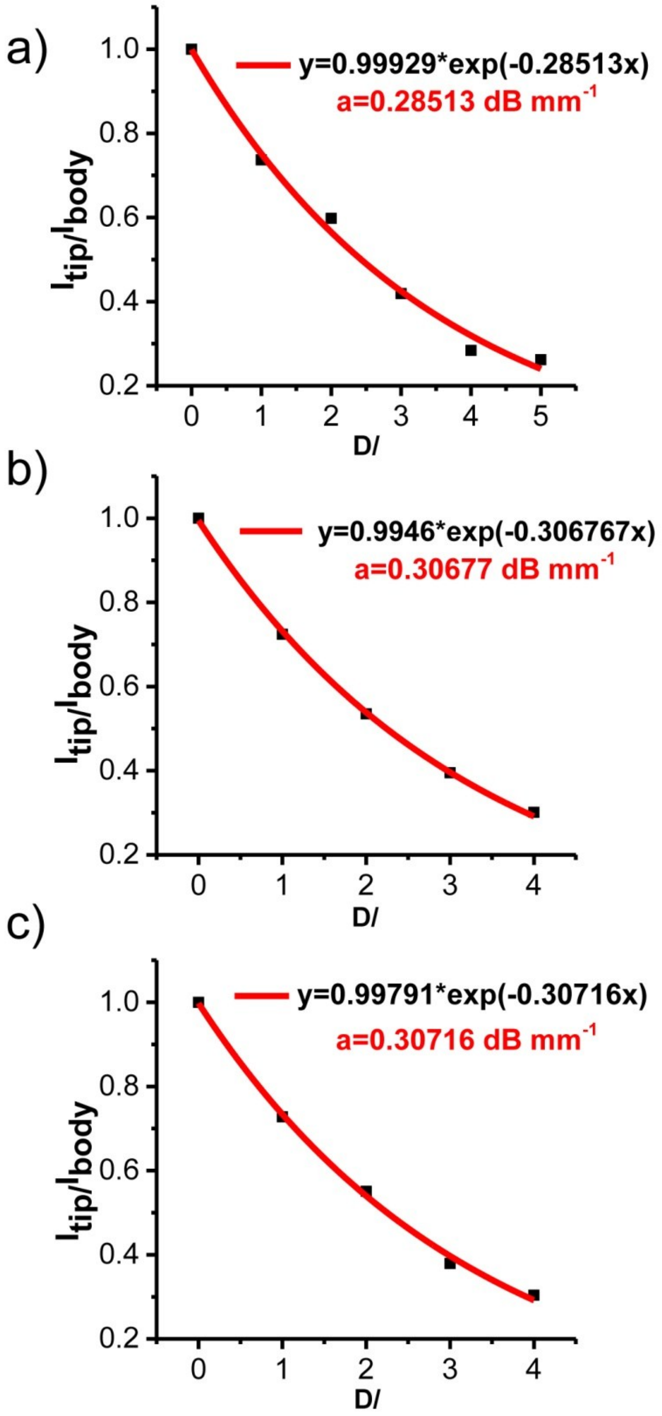

Figure S13. The I_{tip}/I_{body} decays of single **DBBZL** crystals in the straight state (a), elastic bent state (b) and plastic bent state (c).

References

1. T. Kawasaki, Y. Harada, K. Suzuki, T. Tobita, N. Florini, G. Pályi and K. Soai, *Org Lett,* **2008**, *10,* 4085.
2. S. Timoshenko, *Strength of materials*, D. Van Nostrand Company, New York, **1940**.