Supporting Information

Elastic Bending Flexibility of Fluorescent Organic Single Crystal: New Aspects of Commonly Used Building Block "4,7-Dibromo-2,1,3-benzothiadiazole"

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Materials and Methods

Chemicals

4,7-Dibromo-2,1,3-benzothiadiazole (Aldrich) were used as received. Solvents were used as received.

Measurements

UV-vis absorption spectra were obtained on an Ocean Optics USB4000-XR1 fiber spectrometer with DH2000-BAL tungsten halogen light source. Fluorescence spectra were obtained on an Ocean Optics USB4000 fiber spectrometer with PX-2 pulsed xenon light source. Absolute quantum yield were obtained by Hamamatsu C9920-02. The single crystal X-ray diffraction data for single crystals were collected at room temperature using SMART APEX II (Bruker AXS) with a CCD detector. The crystal structures were solved by the direct method and refined by full matrix least-squares using SHELXTL. XRD analysis was performed by JEOL JDX-3530 X-ray diffractometer system. Crystal images were obtained by optical microscope, KEYENCE VH-Z500R. DSC analysis was performed by a Shimadzu DS-60, which measured during heating from room temperature to 250 ^{o}C at heating rate of 10 ^{o}C/min in nitrogen.

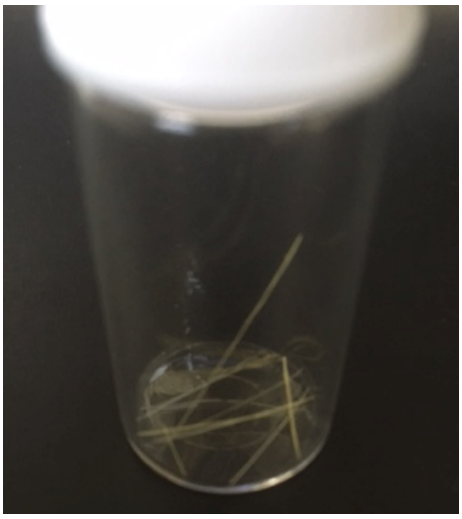

Figure S1. Single crystals of **DBBT**.

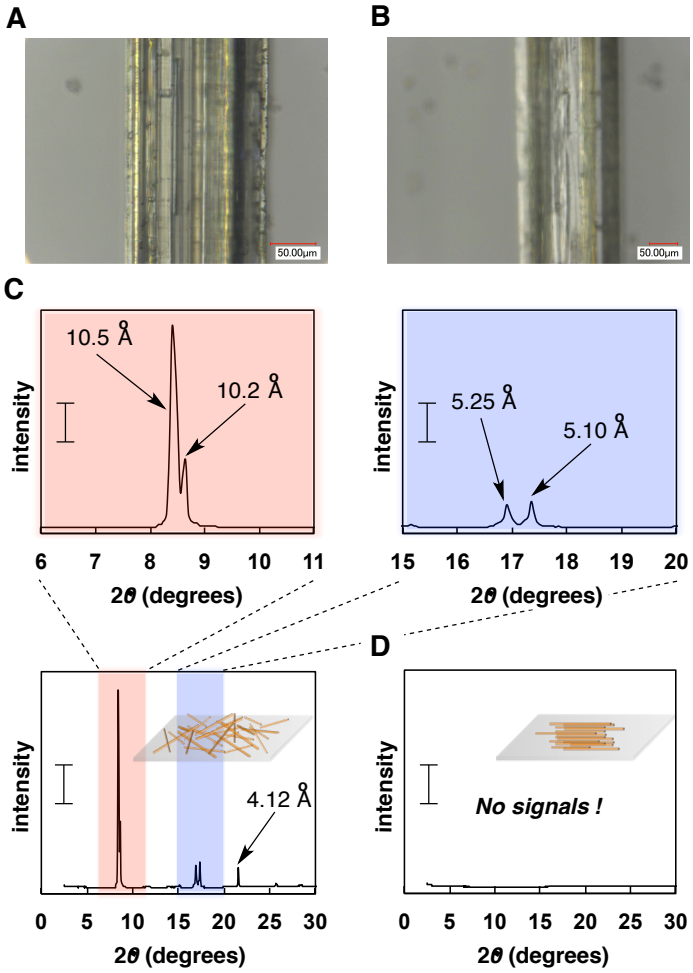

Figure S2. (A, B) Optical images of the crystal. (C) XRD patterns of the crystal when the crystals were randomly set on the substrate. (D) XRD profile of the crystals when the crystals were set on the parallel to the substrate. Scale: 10000 counts.

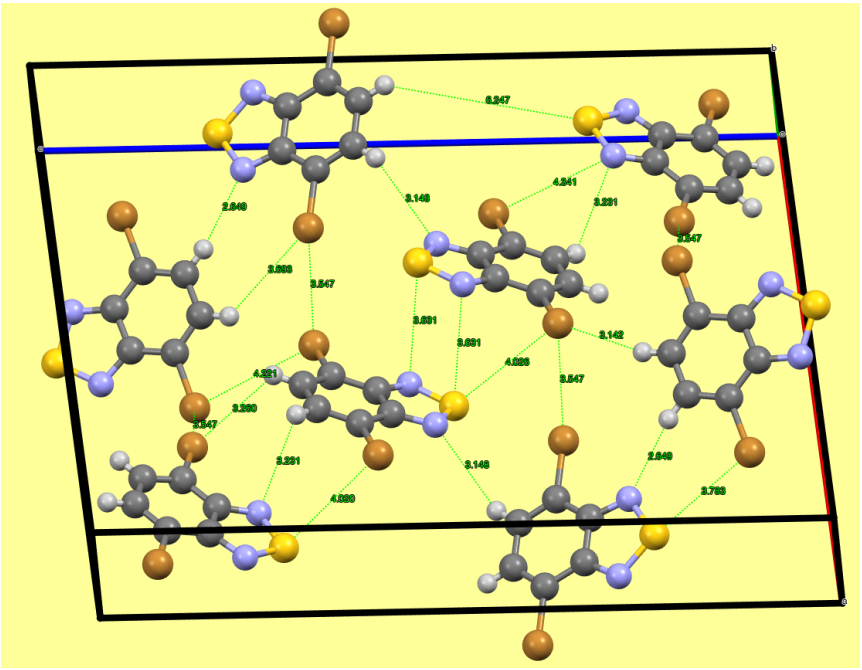

Figure S3. Crystal Structure of **DBBT**.

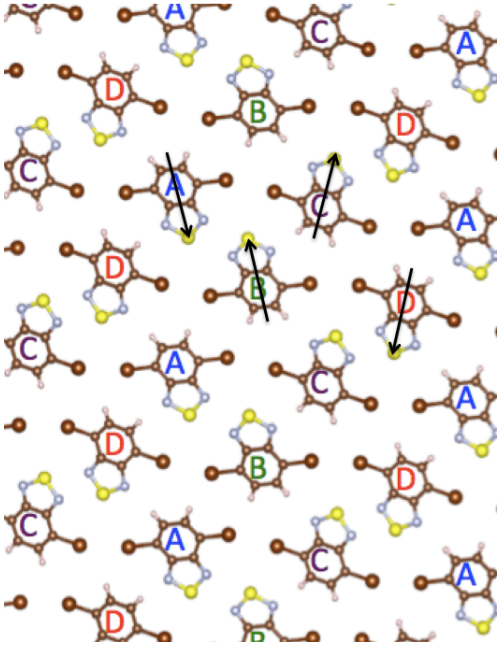

Figure S4. Crystal Structure of **DBBT** at (100) face.

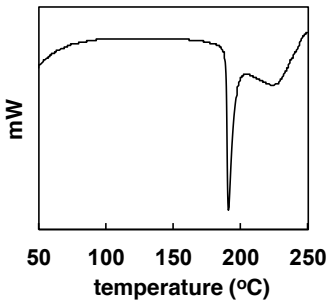

Figure S5. DSC trace of the crystal.

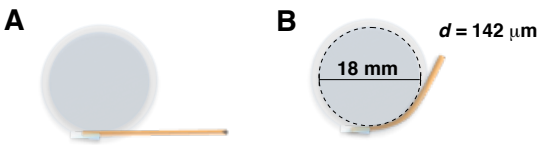

Figure S6. Illustration of straight (A) and bent (B) crystals.

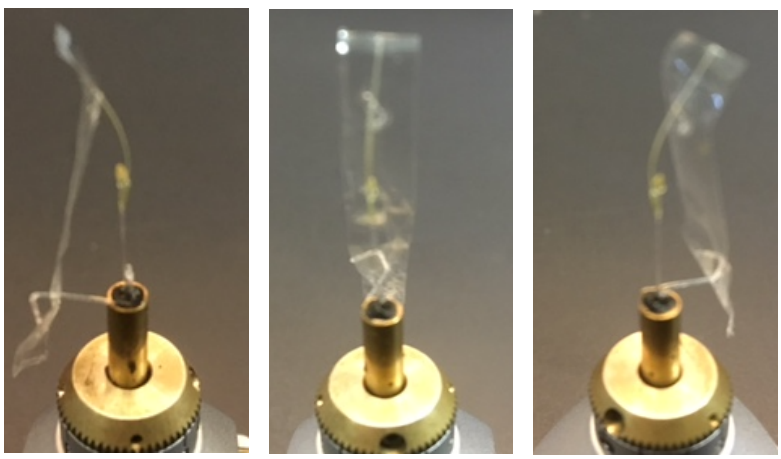

Figure S7. Photograph of bent crystal fixed by capillary and PE.

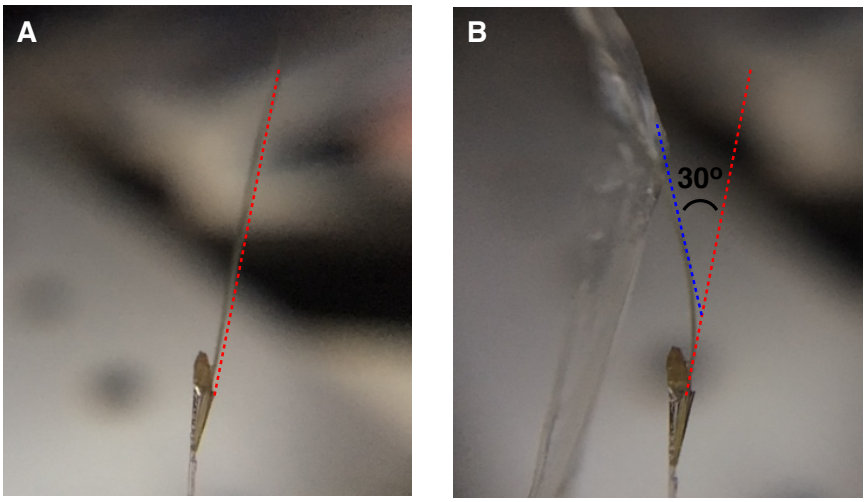

Figure S8. (A) Original crystal. (B) Bent crystal.

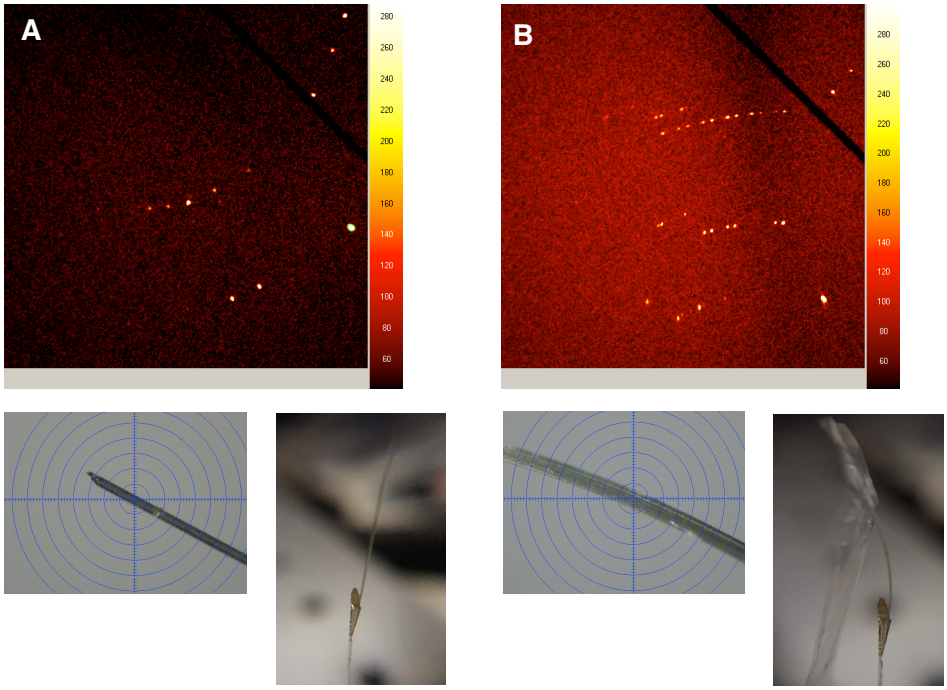

Figure S9. SCXRD patterns of (A) original crystal and (B) bent crystal.

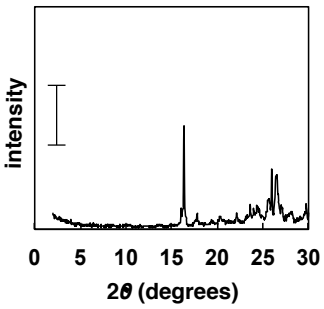

Figure S10. XRD patterns of **DBBT** in powder. Scale: 1000 counts.

Table S1. Crystal data and structure refinement for **DBBT**.

Identification code	global	
Empirical formula	C6 H2 Br2 N2 S	
Formula weight	293.98	
Temperature	300.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 18.3706(13) Å	α = 90°.
	b = 3.9543(2) Å	β = 97.441(3)°.
	c = 22.1361(17) Å	γ = 90°.
Volume	1594.49(19) $Å^3$	
Z	8	
Density (calculated)	2.449 mg/m^3	
Absorption coefficient	10.356 mm^{-1}	
F(000)	1104	
Crystal size	0.200 x 0.140 x 0.020 mm^3	
Theta range for data collection	2.24 to 26.04°.	
Index ranges	-22<=h<=22, -4<=k<=3, -27<=l<=25	
Reflections collected	17190	
Independent reflections	3105 [R(int) = 0.0531]	
Completeness to theta = 26.04°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.82 and 0.52	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3105 / 0 / 200	
Goodness-of-fit on F^2	1.169	
Final R indices [I>2sigma(I)]	R1 = 0.0526, wR2 = 0.1662	
R indices (all data)	R1 = 0.0739, wR2 = 0.1859	
Extinction coefficient	0.0060(7)	
Largest diff. peak and hole	1.620 and -1.691 $e.Å^{-3}$	