Supplementary Information

Actuation performance of a photo-bending crystal modeled by machine learning-based regression

Kazuki Ishizaki,^a Ryota Sugimoto,^b Yuki Hagiwara,^a Hideko Koshima,^c Takuya Taniguchi,^{*d} Toru Asahi^{a, b, c}

- a. Department of Advanced Science and Engineering, Graduate school of Advanced Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan.
- b. Department of Life Science and Medical Bioscience, School of Advanced Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan.
- c. Research Organization for Nano & Life Innovation, Waseda University, 513 Wasedatsurumaki-cho, Shinjuku-ku, Tokyo 162-0041, Japan.
- d. Center for Data Science, Waseda University, 1-6-1 Nishiwaseda, Shinjuku-ku, Tokyo 169-0042, Japan.
- * Correspondence to takuya.taniguchi@aoni.waseda.jp

1. Supplementary Figures



Supplementary Figure 1. Differential scanning calorimetry (DSC) measurement of the enol-(S)-1 crystal. DSC curve measured in the temperature range of 30–160 °C on heating and subsequent cooling.



Supplementary Figure 2. Young's moduli of the enol-(S)-1 crystal. (a,b) Calculation of Young's modulus by (a) beam bending and (b) compression test. (c–e) Typical *P-D* curves loaded on (c) (001) top face, (d) (010) side face, and (e) (100) cross-section face. The moduli when loaded on (001) and (010) faces were measured by bending test, and the modulus loaded on (100) face was measured by compression test. Such bending or compression test was repeated three times using different crystals of enol-(S)-1, and the average and the standard error are written in each panel.

2. Supplementary Tables

	enol-(<i>S</i>)-1	
Crystal system	Orthorhombic	
Space group	$P2_{1}2_{1}2_{1}$	
<i>a</i> (Å)	6.3282(8)	
<i>b</i> (Å)	9.8266(12)	
<i>c</i> (Å)	39.383(5)	
α (°)	90	
β (°)	90	
γ (°)	90	
$V(Å^3)$	2449.0(5)	
Ζ	4	
d (g/cm ³)	1.051	
$R_{I}\left[I > 2\sigma(I)\right]$	0.0589	
$wR_2 \left[I > 2\sigma(I)\right]$	0.1545	

Supplementary Table 1. Crystallographic data of an enol-(*S*)-1 crystal.

Supplementary Table 2. Change of unit cell before and under UV irradiation at 365 nm.

	Before UV irradiation	Under UV irradiation	Relative change (%)
<i>a</i> (Å)	6.345	6.328	-0.27
<i>b</i> (Å)	9.839	9.847	0.08
<i>c</i> (Å)	39.442	39.440	-0.01
α (°)	90.03	90.13	0.11
eta (°)	89.99	90.20	0.23
γ (°)	90.06	90.02	-0.04
$V(Å^3)$	2462	2457	0.20

3. Supplementary Movies

Supplementary Movie 1. Observation of bending motion of an enol-(*S*)-1 crystal ($2185 \times 571 \times 92$ μ m³) upon UV light irradiation (play speed at $10 \times$ speed).