

Electronic Supplementary Information

Photoinduced shape changes of diarylethene single crystals: correlation between shape changes and molecular packing†

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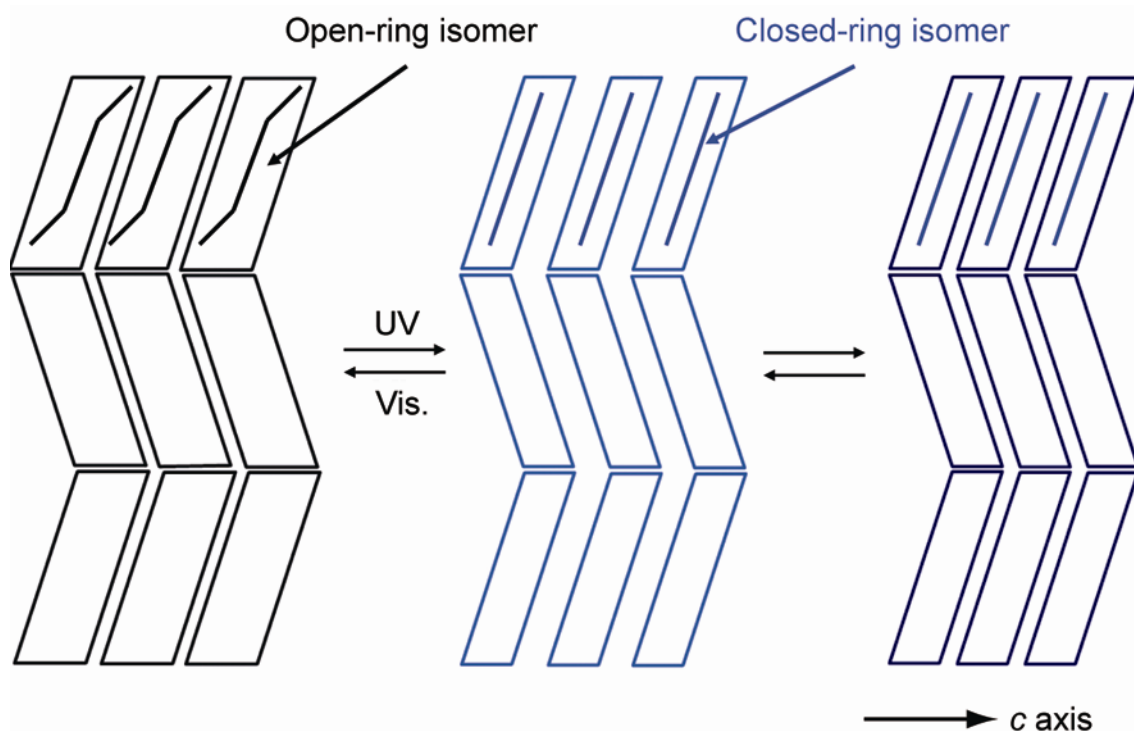


Fig. S1 Schematic illustration of photocontraction of a crystal viewed from (010) face. Upon irradiation with UV light the open-ring isomers (black line) converted to the closed-ring isomers (blue line). The thickness of the molecules is reduced as the molecules convert from the open- to the closed-ring isomers. The thin-shaped closed-ring isomers were stacked one by one. The molecular stacking resulted in the macroscopic contraction of the crystal along the *c* axis.

Table S1 Crystal data for **3a**, **3a'**, **3b** and **4a**.

	3a	3a' ^a	3b ^b	4a
CCDC No.	713392	713393	713394	713395
Empirical formula	C ₂₇ H ₂₀ F ₆ N ₂ S ₂	C ₂₇ H ₂₀ F ₆ N ₂ S ₂	C ₂₇ H ₂₀ F ₆ N ₂ S ₂	C ₃₁ H ₂₆ F ₆ S ₂
Formula weight	550.59	550.59	550.59	576.66
<i>T</i> / K	123	123	123	123
Crystal system	orthorhombic	orthorhombic	monoclinic	orthorhombic
Space group	<i>Pbcn</i>	<i>Pbcn</i>	<i>P2₁/c</i>	<i>Pbcn</i>
<i>a</i> / Å	21.5461(15)	21.586(2)	9.5508(8)	21.307(6)
<i>b</i> / Å	10.8096(8)	10.8692(11)	19.4249(15)	12.193(4)
<i>c</i> / Å	10.8098(8)	10.7268(11)	13.5268(11)	10.669(3)
α / °	90	90	90	90
β / °	90	90	95.7430(10)	90
γ / °	90	90	90	90
<i>V</i> / Å ³	2517.7(3)	2516.7(4)	2469.9(3)	2771.8(14)
<i>Z</i>	4	4	4	4
<i>D_c</i> / g cm ⁻³	1.453	1.453	1.465	1.382
Reflections collected	15259	9707	13830	14494
Independent reflections	2727	1514	5649	3196
<i>R</i> _{int}	0.0445	0.0445	0.0240	0.0310
Goodness-of-fit	1.042	1.013	0.970	1.031
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0385	0.0332	0.0393	0.0360
<i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0882	0.0731	0.1208	0.0889
<i>R</i> ₁ (all data)	0.0602	0.0463	0.0538	0.0531
<i>wR</i> ₂ (all data)	0.1002	0.0807	0.1355	0.0995

^a Irradiated with 365 nm light for 4 h. The reaction conversion is 6%.

^b Prepared by recrystallization of isolated closed-ring isomer **3b**.

Table S2 Crystal data for micrometer-size small crystals **1a** and **1a'**.

	1a	1a' ^a
CCDC No.	713390	713391
Empirical formula		C ₂₉ H ₂₂ F ₆ S ₂
Formula weight		548.61
Crystal size		20 × 15 × 8 μm ³
<i>T</i> / K		100
Crystal system		orthorhombic
Space group		<i>Pbcn</i>
<i>a</i> / Å	22.239(5)	22.30(3)
<i>b</i> / Å	10.971(3)	11.026(18)
<i>c</i> / Å	10.585(3)	10.542(18)
α / °	90	90
β / °	90	90
γ / °	90	90
<i>V</i> / Å ³	2594.1(12)	2593(7)
<i>Z</i>	4	4
<i>D_c</i> / g cm ⁻³	1.405	1.405
Reflections collected	2601	2224
Independent reflections	1481	1010
<i>R</i> _{int}	0.0977	0.1613
Goodness-of-fit	0.916	1.133
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0627	0.1009
<i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0766	0.2138
<i>R</i> ₁ (all data)	0.2024	0.2251
<i>wR</i> ₂ (all data)	0.1057	0.2612

^a Irradiated with 365 nm light for 1 min. The reaction conversion is 12%.