Electronic Supplementary Information

Cold Crystallization and Photo-induced Thermal Behavior of Alkyl-derivatized Diarylethene Molecules

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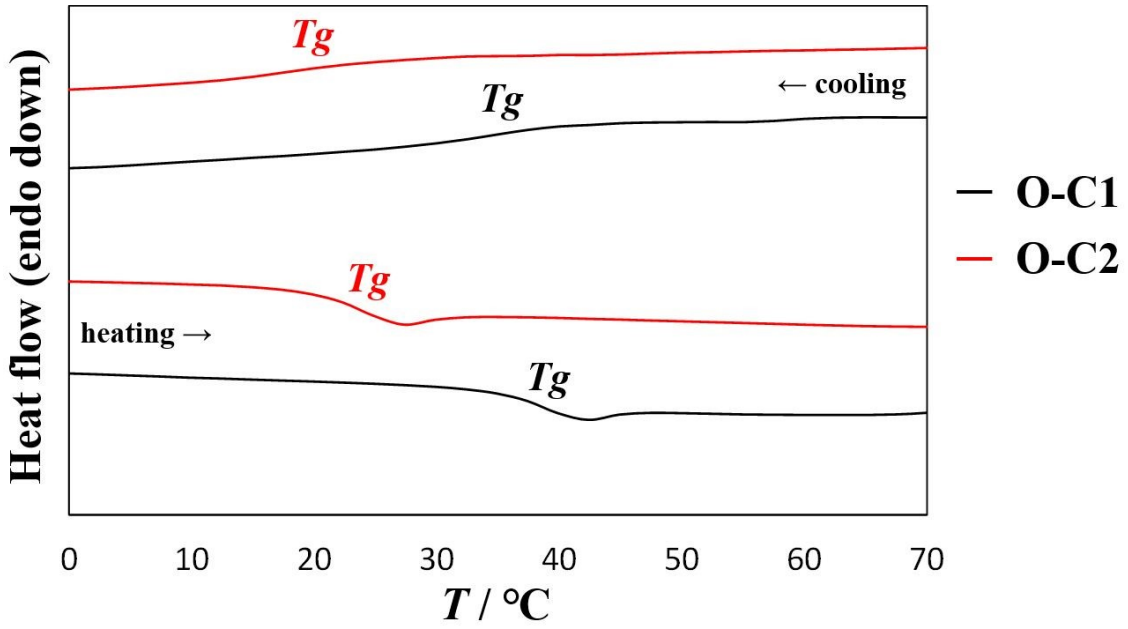


Fig. S1 Enlarged view of glass transitions of O-DAE-C1 and O-DAE-C2.

Single crystal X-ray structural analysis

The single crystal of DAE-C2 for X-ray crystallography was obtained by the slow evaporation of the hexane solution. A single crystal was mounted on a glass capillary, transferred to a Bruker AXS SMART diffractometer that was equipped with a CCD area detector and Mo Kα (λ = 0.71073 Å) radiation, and centered on the beam at 173 K. The structures were solved and refined by SHELX employing the direct method and expanded by Fourier techniques. All the non-hydrogen and hydrogen atoms were refined anisotropically and isotropically, respectively.

The crystallographic data are shown in Table S1, and the analyzed molecular structure is shown in Fig. S2.

Table S1. Crystallographic data of DAE-C2

		DAE-C2
Formula		$C_{20}H_{23}NO_2S_2$
Fw		373.51
T / K		173
Crystal system		Orthorhombic
Space group		Pna21
Unit cell	*a* / Å	16.8639(16)
	b / Å	9.6675(9)
	c / Å	12.0818(12)
	α / deg	90
	β / deg	90
	γ / deg	90
Volume / Å^3		1969.7(3)
Z		4
δ_{calc} / Mgm^{-3}		1.260
GOF		1.561
Final *R*	*R*1	0.1073
Indices [$I > 2\sigma(I)$]	*wR*2	0.3309
R indices	*R*1	0.1085
(all data)	*wR*2	0.3327

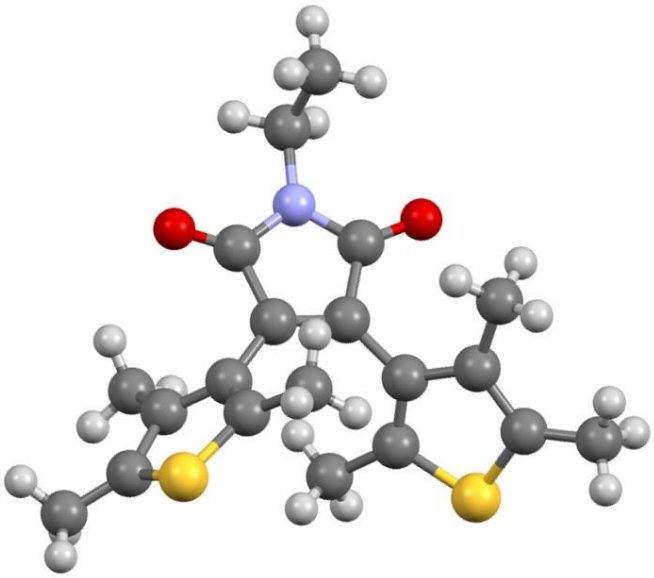
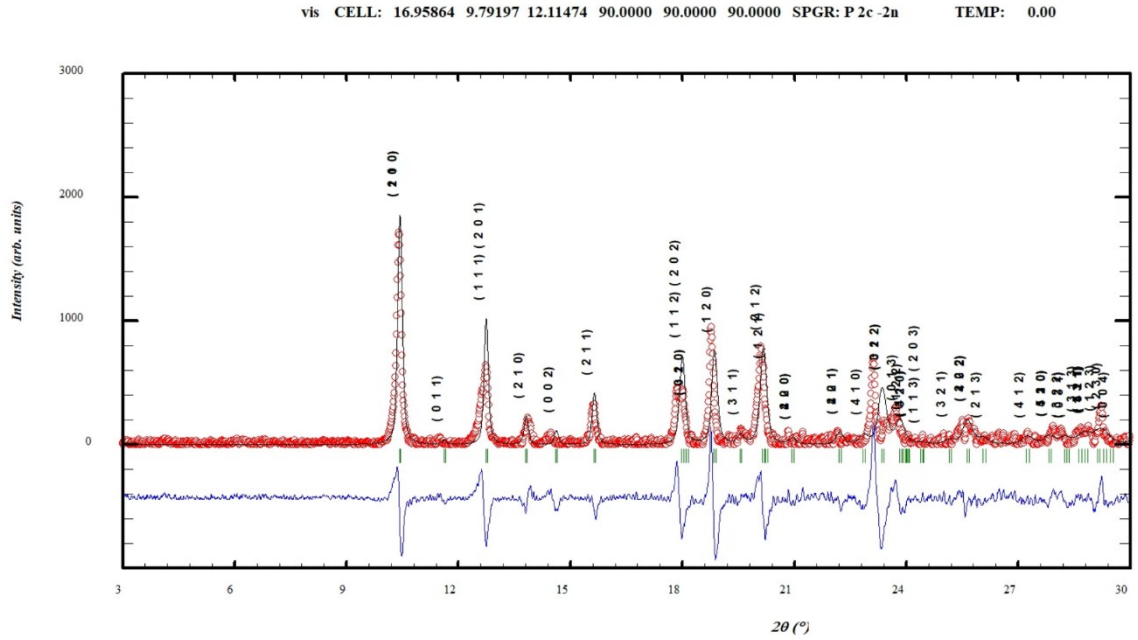


Fig. S2 Molecular structure in single crystal of DAE-C2.

(a)



(b)

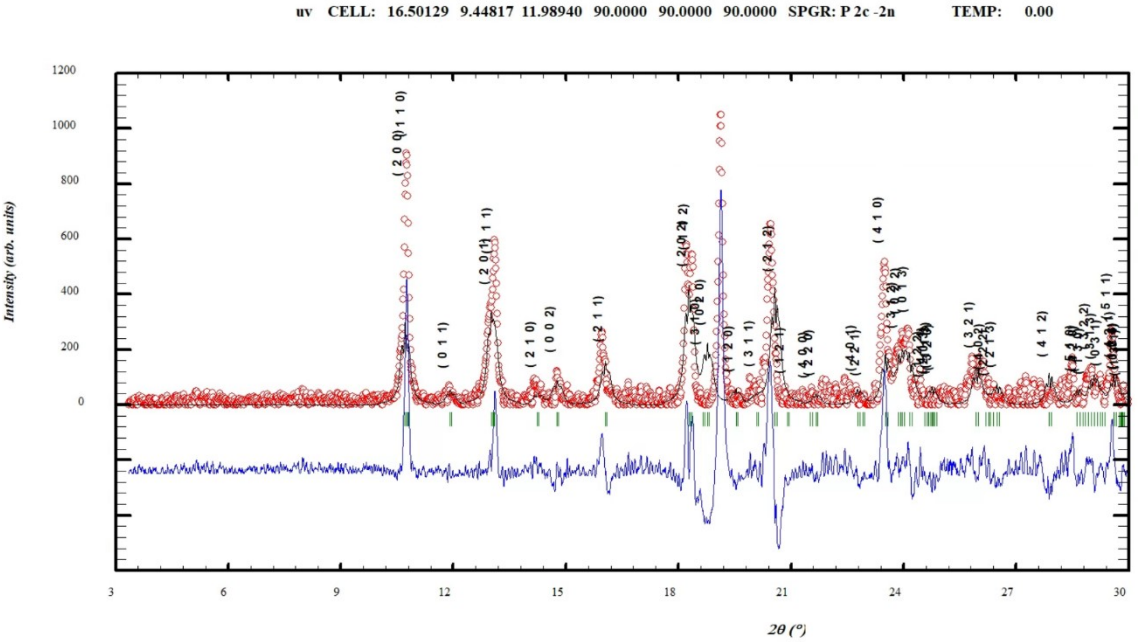


Fig. S3 Le Bail refinement of PXRD data of cold-crystallized samples under (a) visible-light irradiation and (b) UV irradiation. Red line shows the measured data. Black line shows the refined data. Blue line shows the residual.