

Supplementary Information

Trans-scale crystal dynamics for controlling kinetic responses in organic molecular systems

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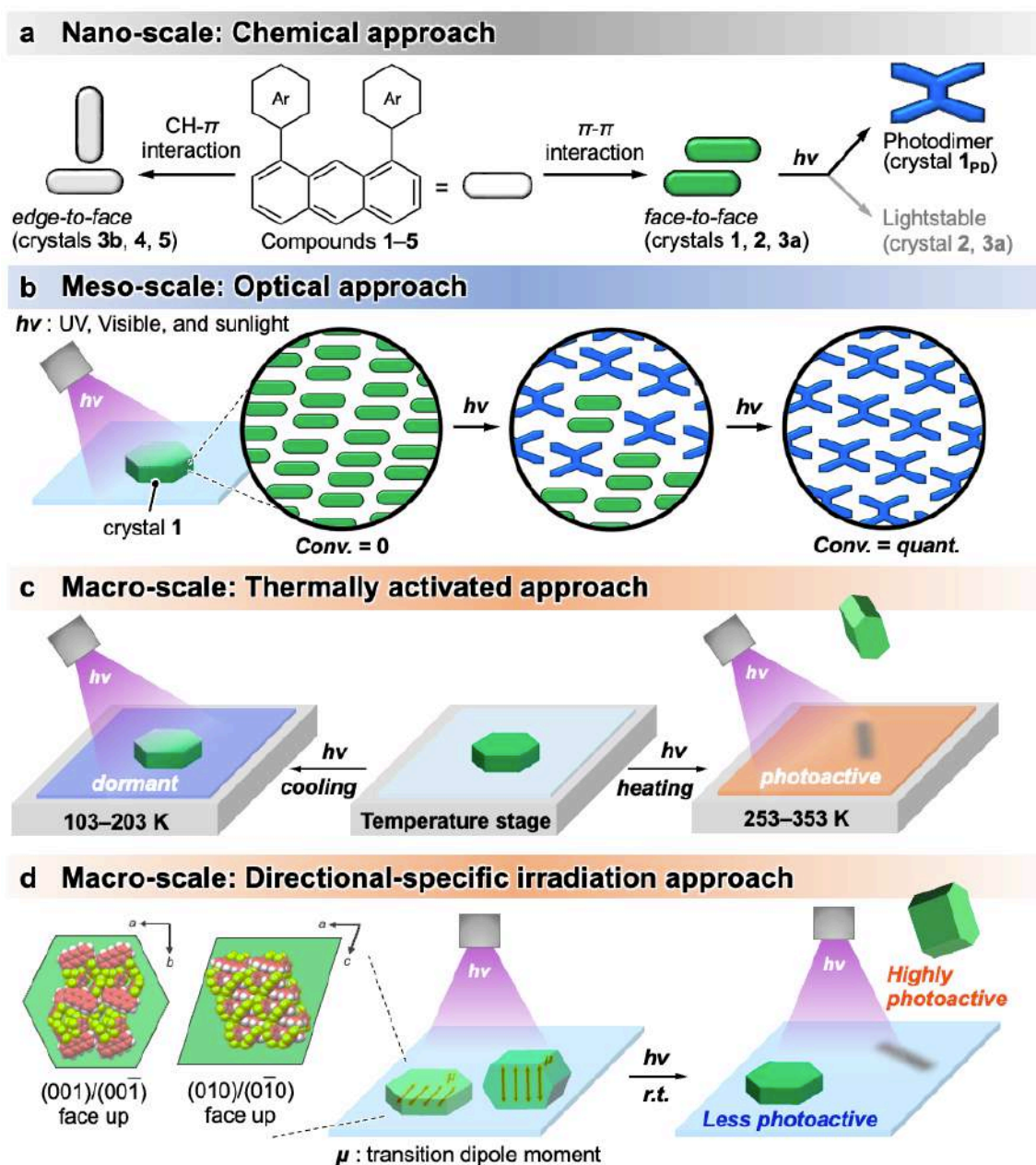
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1. Schematic framework of this work

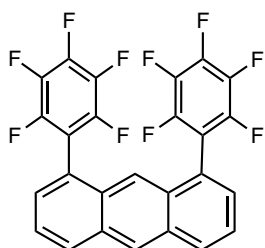


Supplementary Fig. 1. Schematic representation of trans-scale approach toward crystal dynamics.

Controlling crystal dynamics by **a**, chemical; **b**, optical; **c**, thermally activated; and **d**, directional-specific irradiation approaches. **1**, 1,8-bis(pentafluorophenyl)anthracene; **2**, 1,8-bis(4-fluorophenyl)anthracene; **3**, 1,8-diphenylanthracene; **4**, 1,8-bis(4-methylphenyl)anthracene; **5**, 1,8-bis(4-methoxyphenyl)anthracene; **1_{PD}**, 1,8-bis(pentafluorophenyl)anthracene photodimer; crystal **3a**, *face-to-face* structure of **3**; crystal **3b**, *edge-to-face* stacking structure of **3**.

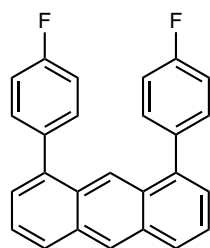
2. Synthesis

1,8-Bis(pentafluorophenyl)anthracene, **1**



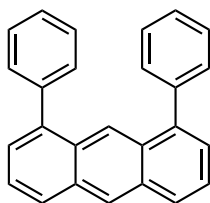
1,8-Dibromoanthracene (100 mg, 0.30 mmol), Pd(OAc)₂ (13 mg, 0.06 mmol), S-Phos (49 mg, 0.12 mmol), and K₂CO₃ (125 mg, 1.1 mL) were combined in a reaction vial with a magnetic stirrer bar. The vial was filled with argon. Pentafluorobenzene (75 mg, 0.60 mmol), and isopropyl acetate (0.6 mL) were then added. The resulting mixture was stirred at 80 °C for 77 h. The reaction mixture was quenched with brine, allowing the organic layer to separate. The aqueous layer was extracted with ethyl acetate. The combined organic solution was washed with brine, dried over MgSO₄, filtered, and concentrated by rotary evaporation. The crude product was purified by flash column chromatography on silica gel (*n*-hexane). The crude product was dissolved in chloroform recrystallized to obtain the **1** as pale-yellow powder (115 mg, 75%). ¹H NMR (CDCl₃, 400 MHz) δ: 8.63 (s, 1H), 8.18 (d, 2H, *J* = 8.4 Hz), 7.62–7.58 (m, 3H), 7.49 (d, 2H, *J* = 6.8 Hz). ¹³C NMR (CDCl₃, 100 MHz) δ: 146.0 (C), 143.6 (C), 139.9 (C), 132.0 (C), 130.5 (CH), 130.0 (C), 129.7 (CH), 128.3 (CH), 125.3 (CH), 124.4 (CH), 120.9 (C), 112.5 (C). The ¹H and ¹³C NMR spectra are in accordance with the literature.¹

1,8-Bis(4-fluorophenyl)anthracene, **2**



1,8-Dibromoanthracene (100 mg, 0.30 mmol), Pd(PPh₃)₄ (17 mg, 0.015 mmol), and 4-fluorophenylboronic acid (100 mg, 0.72 mmol) were combined in a two-necked flask with a magnetic stirrer bar. The flask was filled with argon. K₂CO₃ aq. (2 M, 1.5 mL) and toluene (1.5 mL) were then added. The resulting mixture was stirred at 110 °C for 24 h. The reaction mixture was quenched with brine, allowing the organic layer to separate. The aqueous layer was extracted with chloroform. The combined organic solution was washed with brine, dried over MgSO₄, filtered, and concentrated by rotary evaporation. The crude product was purified by flash column chromatography on silica gel (chloroform). The crude product was dissolved in chloroform recrystallized to obtain the **2** as pale-yellow powder (64 mg, 58%). ¹H NMR (CDCl₃, 400 MHz) δ: 8.55 (s, 1H), 8.47 (s, 1H), 8.04 (d, 2H, *J* = 8.0 Hz), 7.52 (dd, 2H, *J* = 8.0, 1.6 Hz), 7.44–7.41 (m, 4H), 7.36 (dd, 2H, *J* = 6.8, 0.8 Hz), 7.13–7.08 (m, 4H). ¹³C NMR (CDCl₃, 100 MHz) δ: 163.6 (C), 139.5 (C), 136.5 (C), 131.9 (C), 131.5 (CH, *J*_{CF} = 8.6 Hz), 130.3 (C), 127.9 (CH), 127.0 (CH), 126.4 (CH), 125.4 (CH), 123.5 (CH), 115.1 (CH, *J*_{CF} = 21.1 Hz). The ¹H and ¹³C NMR spectra are in accordance with the literature.²

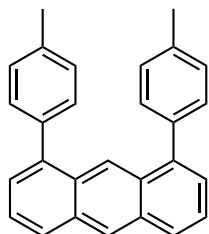
1,8-Diphenylanthracene, **3**



1,8-Dibromoanthracene (100 mg, 0.30 mmol), Pd(PPh₃)₄ (17 mg, 0.015 mmol), and phenylboronic acid (146 mg, 1.2 mmol) were combined in a two-necked flask with a magnetic stirrer bar. The flask was filled with argon. K₂CO₃ aq. (2 M, 2 mL) and toluene (2 mL) were then added. The resulting mixture was stirred at 110 °C for 24 h.

The reaction mixture was quenched with brine, allowing the organic layer to separate. The aqueous layer was extracted with chloroform. The combined organic solution was washed with brine, dried over MgSO₄, filtered, and concentrated by rotary evaporation. The crude product was purified by flash column chromatography on silica gel (chloroform). The crude product was dissolved in chloroform recrystallized to obtain the **3** as pale-yellow powder (84 mg, 85%). ¹H NMR (CDCl₃, 300 K, 400 MHz) δ: 8.63 (s, 1H), 8.53 (s, 1H), 8.03 (d, 2H, *J* = 8.4 Hz), 7.55–7.35 (m, 14H). ¹³C NMR (CDCl₃, 300 K, 100 MHz) δ: 140.7 (C), 140.6 (C), 132.0 (C), 130.2 (C), 130.1 (CH), 128.2 (CH), 127.7 (CH), 127.3 (CH), 126.8 (CH), 126.2 (CH), 125.4 (CH), 124.1 (CH). The ¹H and ¹³C NMR spectra are in accordance with the literature.³

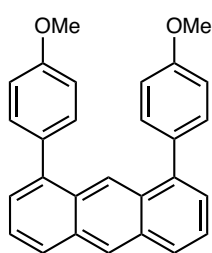
1,8-Bis(4-methylphenyl)anthracene, **4**



1,8-Dibromoanthracene (100 mg, 0.30 mmol), Pd(PPh₃)₄ (17 mg, 0.015 mmol), and 4-methylphenylboronic acid (98 mg, 0.72 mmol) were combined in a two-necked flask with a magnetic stirrer bar. The flask was filled with argon. K₂CO₃ aq. (2 M, 1 mL) and toluene (1 mL) were then added. The resulting mixture was stirred at 110 °C for 24 h.

The reaction mixture was quenched with brine, allowing the organic layer to separate. The aqueous layer was extracted with chloroform. The combined organic solution was washed with brine, dried over MgSO₄, filtered, and concentrated by rotary evaporation. The crude product was purified by flash column chromatography on silica gel (chloroform). The crude product was dissolved in chloroform recrystallized to obtain the **4** as pale-yellow powder (75 mg, 70%). ¹H NMR (CDCl₃, 300 K, 400 MHz) δ: 8.62 (s, 1H), 8.52 (s, 1H), 8.01 (d, 2H, *J* = 8.4 Hz), 7.51 (dd, 2H, *J* = 8.0, 1.6 Hz), 7.41–7.37 (m, 6H), 7.22 (d, 4H, *J* = 7.6 Hz), 2.42 (s, 6H). ¹³C NMR (CDCl₃, 300 K, 100 MHz) δ: 140.7 (C), 137.7 (C), 136.9 (C), 132.0 (C), 130.3 (C), 130.0 (CH), 128.9 (CH), 127.5 (CH), 126.6 (CH), 125.9 (CH), 125.4 (CH), 124.4 (CH), 21.30 (CH₃). The ¹H and ¹³C NMR spectra are in accordance with the literature.²

1,8-Bis(4-methoxyphenyl)anthracene, **5**

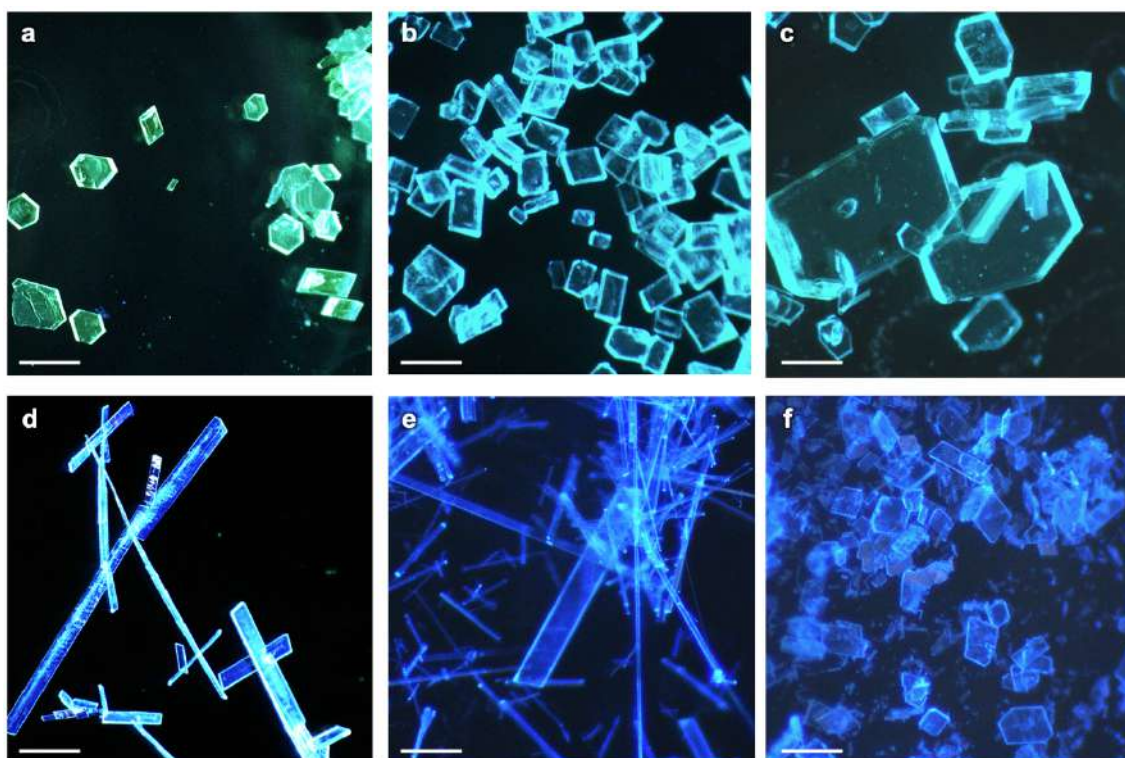


1,8-Dibromoanthracene (150 mg, 0.45 mmol), Pd(PPh₃)₄ (51 mg, 0.045 mmol), and 4-methoxyphenylboronic acid (203 mg, 1.34 mmol) were combined in a two-necked flask with a magnetic stirrer bar. The flask was filled with argon. K₂CO₃ aq. (2 M, 1.5 mL) and toluene (1.5 mL) were then added. The resulting mixture was stirred at 110 °C for 48 h. The reaction mixture was quenched with brine, allowing the organic layer to separate. The aqueous layer was extracted with chloroform. The combined organic solution was washed with brine, dried over MgSO₄, filtered, and concentrated by rotary evaporation. The crude product was purified by flash column chromatography on silica gel (chloroform). The crude product was dissolved in chloroform recrystallized to obtain the **5** as pale-yellow powder (172 mg, 98%). ¹H NMR (CDCl₃, 300 K, 400 MHz) δ: 8.65 (s, 1H), 8.52 (s, 1H), 8.00 (d, 2H, *J* = 8.8 Hz), 7.50 (dd, 2H, *J* = 8.0, 1.2 Hz), 7.45–7.41 (m, 4H), 7.38 (d, 2H, *J* = 6.4 Hz), 6.98–6.95 (m, 4H), 3.87 (s, 6H). ¹³C NMR (CDCl₃, 300 K, 100 MHz) δ: 159.0 (C), 140.3 (C), 133.1 (CH), 132.0 (C), 131.2 (CH), 130.4 (C), 127.4 (CH), 126.8 (CH), 126.0 (CH), 125.4 (CH), 124.2 (CH), 113.8 (CH), 55.46 (OCH₃). The ¹H and ¹³C NMR spectra are in accordance with the literature.²

3. X-ray crystallographic and theoretical analysis

3.1 Crystallization

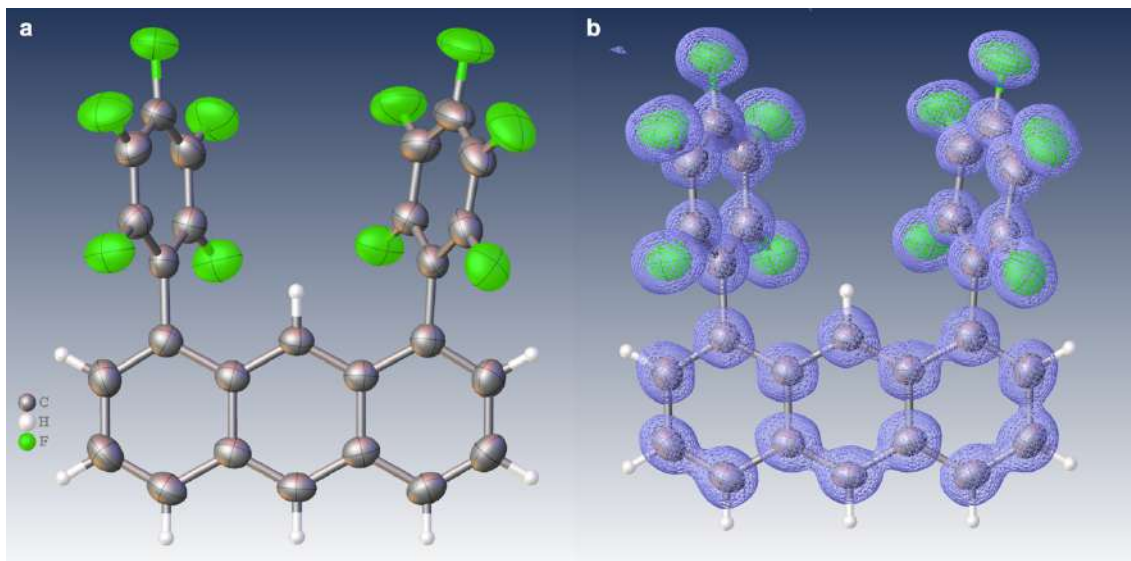
A 1,2-dichloroethane solution of **1** (10 mM, 1 mL) was vapor diffusion with methanol (ca. 2 mL) at 300 K for 24 h to obtain single crystalline **1** as green PL block-shaped crystals under UV irradiation. A 1,2-dimethoxyethane solution of **2** (10 mM, 1 mL) was slowly evaporated at 300 K for 24 h to obtain single crystalline **2** as blue PL plate-shaped crystals under UV irradiation. A chloroform solution of **3** (30 mM, 1 mL) was vapor diffusion with methanol (ca. 2 mL) at 300 K for 24 h to obtain single crystalline **3** as blue PL plate-shaped polymorphic crystals **3a** under UV irradiation. A chloroform solution of **3** (15 mM, 1 mL) was vapor diffusion with methanol (ca. 2 mL) at 300 K for 24 h to obtain single crystalline **3** as green PL plate-shaped polymorphic crystals **3b** under UV irradiation. A toluene solution of **4** (10 mM, 1 mL) was slowly evaporated at 300 K for 24 h to obtain single crystalline **4** as blue PL plate-shaped crystals under UV irradiation. A toluene solution of **5** (10 mM, 1 mL) was slowly evaporated at 300 K for 24 h to obtain single crystalline **5** as blue PL plate-shaped crystals under UV irradiation. One of the crystals was removed from the solution, mounted on a single crystal X-ray diffractometer using a nylon loop, and used for diffraction data collection.



Supplementary Fig. 2. Optical microscopy images.

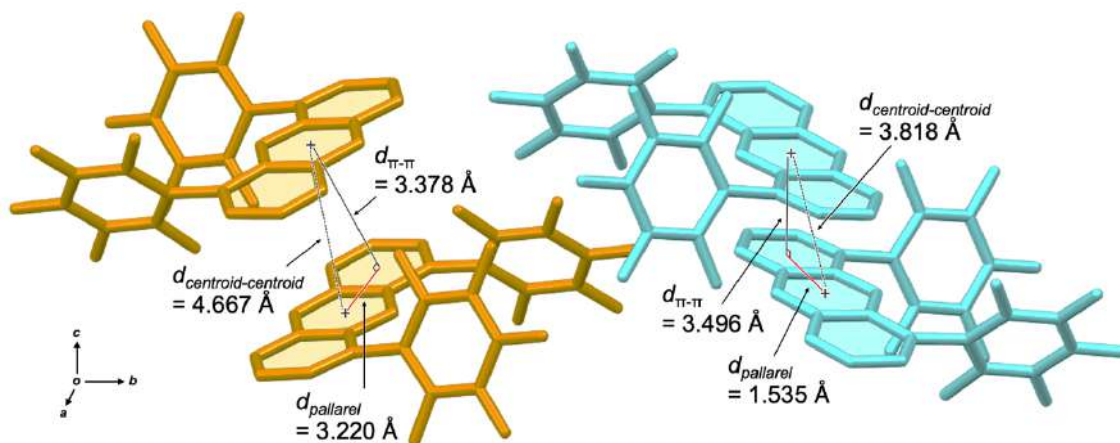
Optical microscopy images of crystals under UV irradiation. **a**, Crystal **1**. **b**, Crystal **2**. **c**, Crystal **3a**. **d**, Crystal **3b**. **e**, Crystal **4**. **f**, Crystal **5**. Scale bar, 100 μm .

3.2 X-Ray crystallographic analysis



Supplementary Fig. 3. Crystal structure of 1 at 303 K.

Crystal structures of **1** (CCDC reference number 2456683). **a**, ORTEP drawing (50% anisotropic displacement parameters) and **b**, electron density maps ($2F_o - F_c$; purple isomesh, $0.1/\text{\AA}^3$).

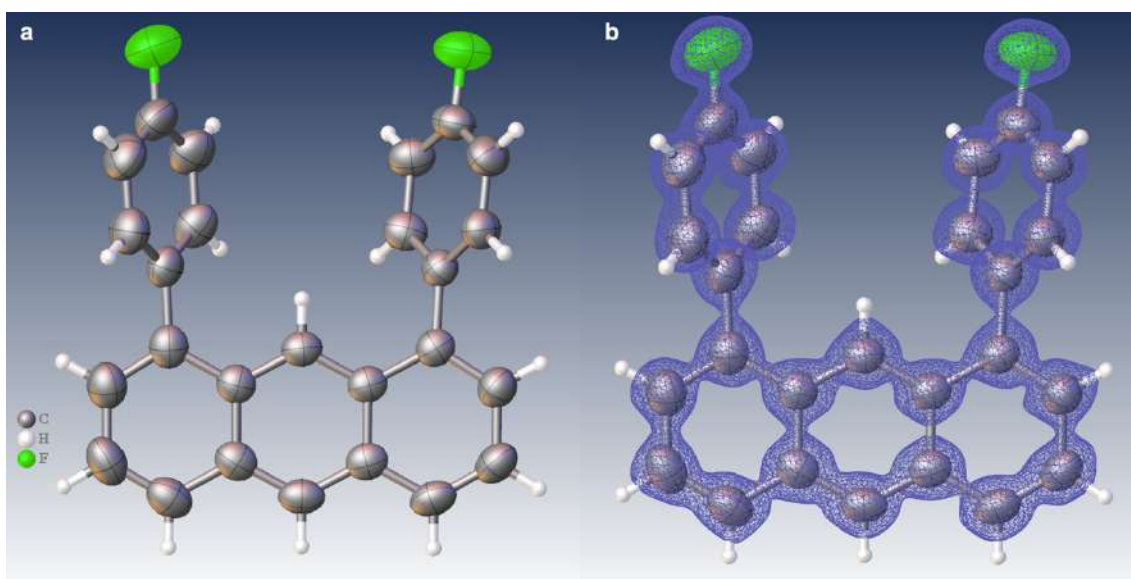


Supplementary Fig. 4. Face-to-face structures of 1 at 303 K.

Face-to-face structures of **1** are shown in capped-stick model. Hydrogen atom is omitted. Intermolecular distances ($d_{\text{centroid-centroid}}$, $d_{\pi-\pi}$, d_{parallel}) of Unit 1 and Unit 2 are shown for clarity. Unit 1, blue; Unit 2, orange.

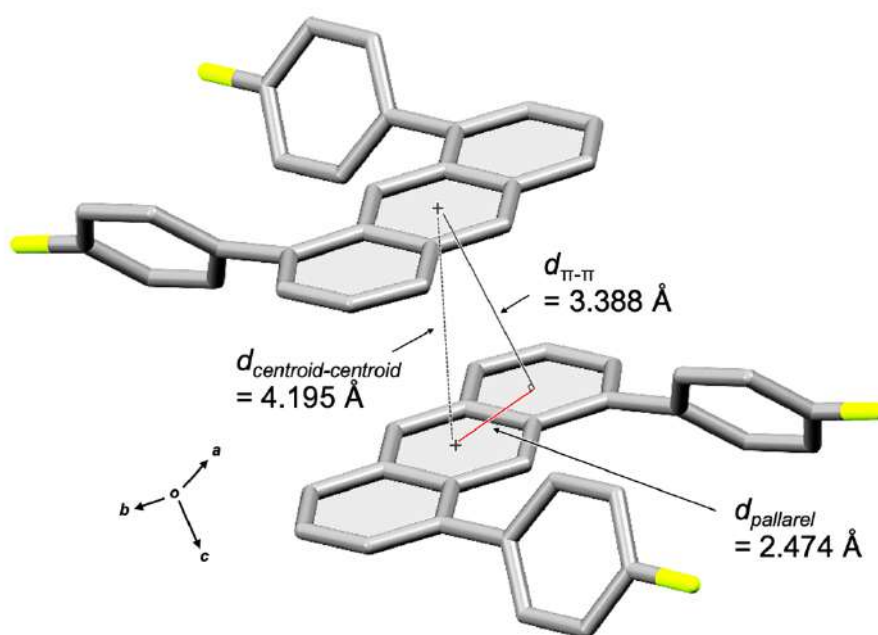
Supplementary Table 1. Crystal Data and Structural Refinement for the **1**

CCDC deposit number	2456683	
Empirical formula	C ₂₆ H ₈ F ₁₀	
Formula weight	510.32	
Temperature	303.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.5728(5) Å	<i>α</i> = 90°
	<i>b</i> = 24.6728(9) Å	<i>β</i> = 107.954(5)°
	<i>c</i> = 7.9791(3) Å	<i>γ</i> = 90°
Volume	1980.08(15) Å ³	
<i>Z</i>	4	
Density (calculated)	1.712 g/cm ³	
Absorption coefficient	0.165 mm ⁻¹	
<i>F</i> (000)	1016	
Crystal size	0.849 × 0.576 × 0.363 mm ³	
<i>θ</i> range for data collection	5.226 to 52.74°	
Index ranges	-13 ≤ <i>h</i> ≤ 13, -30 ≤ <i>k</i> ≤ 30, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	17204	
Independent reflections	4035 [<i>R</i> (int) = 0.0218]	
Data / restraints / parameters	4035 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.079	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0420, <i>wR</i> ₂ = 0.1085	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0559, <i>wR</i> ₂ = 0.1164	
Largest diff. peak and hole	0.15/-0.23 e.Å ⁻³	



Supplementary Fig. 5. Crystal structure of 2 at 303 K.

Crystal structures of **2** (CCDC reference number 2456863). **a**, ORTEP drawing (50% anisotropic displacement parameters) and **b**, electron density maps ($2F_o - F_c$; purple isomesh, $0.1 \text{ /e\AA}^{-3}$).

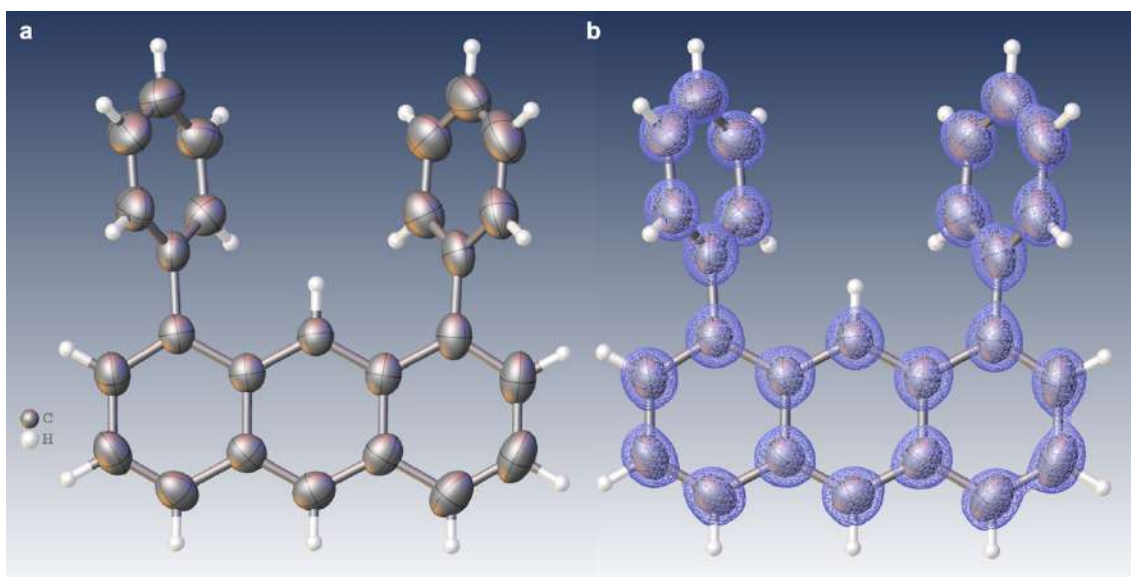


Supplementary Fig. 6. Face-to-face structure of 2 at 303 K.

Face-to-face structure of **2** is shown in capped-stick model. Hydrogen atom is omitted. Intermolecular distances ($d_{\text{centroid-centroid}}$, $d_{\pi-\pi}$, d_{parallel}) are shown. C, grey; F, yellow.

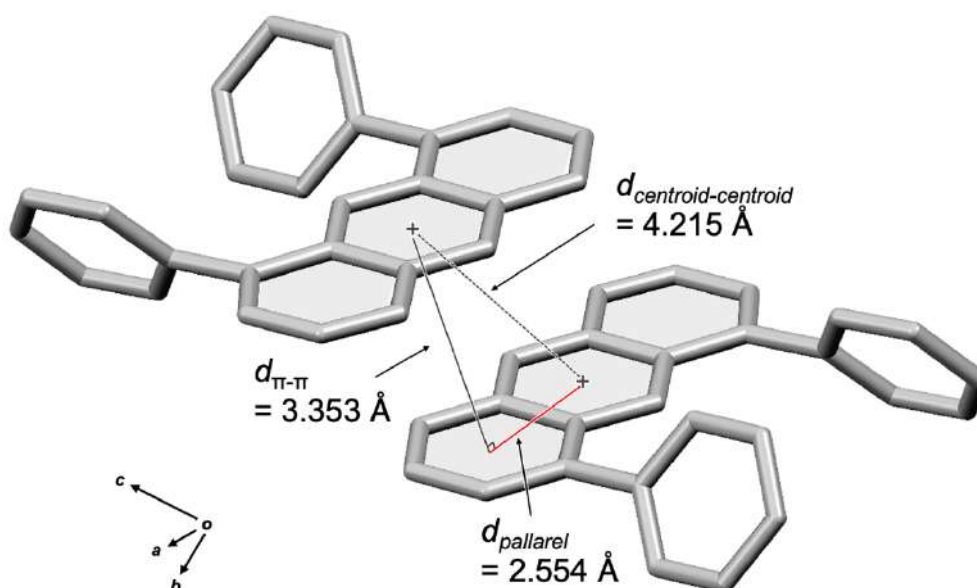
Supplementary Table 2. Crystal Data and Structural Refinement for the **2**

CCDC deposit number	2456863	
Empirical formula	C ₂₆ H ₁₆ F ₂	
Formula weight	366.39	
Temperature	303.15	
Wavelength	0.71073 nm	
Crystal system	triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	$a = 6.8546(7) \text{ \AA}$	$\alpha = 77.958(5)^\circ$
	$b = 9.7096(6) \text{ \AA}$	$\beta = 77.950(6)^\circ$
	$c = 14.2260(8) \text{ \AA}$	$\gamma = 81.435(7)^\circ$
Volume	900.07(12) Å ³	
<i>Z</i>	2	
Density (calculated)	1.352 g/cm ³	
Absorption coefficient	0.092 mm ⁻¹	
<i>F</i> (000)	380.0	
Crystal size	0.216 × 0.102 × 0.076 mm ³	
2 θ range for data collection	4.316 to 59.722°	
Index ranges	-8 ≤ <i>h</i> ≤ 9, -12 ≤ <i>k</i> ≤ 13, -18 ≤ <i>l</i> ≤ 19	
Reflections collected	10888	
Independent reflections	4328 [<i>R</i> (int) = 0.0581]	
Data / restraints / parameters	4328 / 0 / 253	
Goodness-of-fit on <i>F</i> ²	1.009	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0647, <i>wR</i> ₂ = 0.1693	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1100, <i>wR</i> ₂ = 0.1999	
Largest diff. peak and hole	0.24/-0.16 e.Å ⁻³	



Supplementary Fig. 7. Crystal structure of 3a at 303 K.

Crystal structures of **3a** (CCDC reference number 2456867). **a**, ORTEP drawing (50% anisotropic displacement parameters) and **b**, electron density maps ($2F_o - F_c$; purple isomesh, $0.1 \text{ /e\AA}^{-3}$).

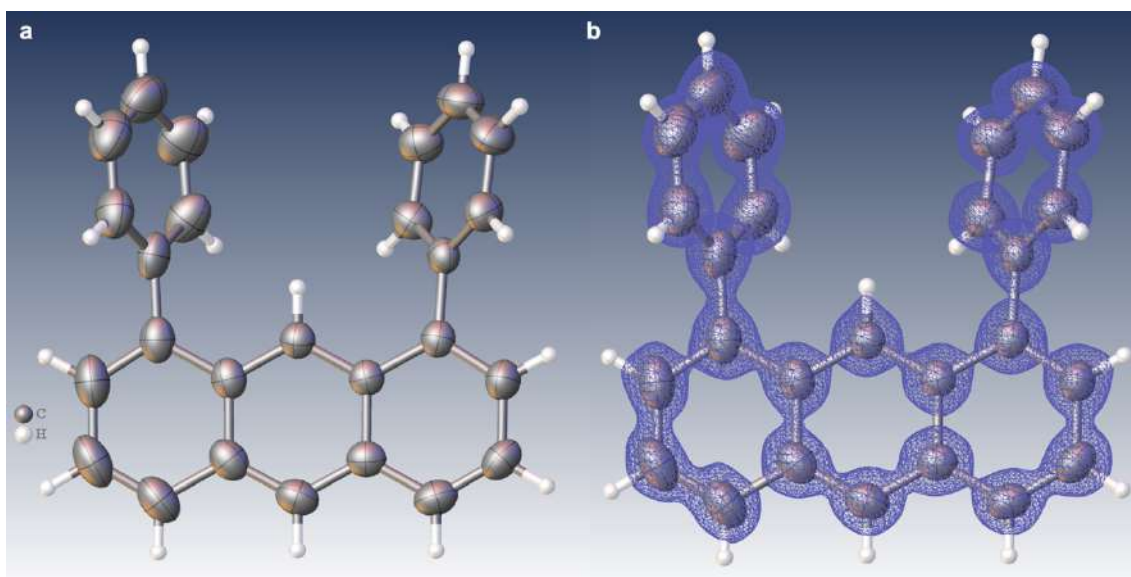


Supplementary Fig. 8. Face-to-face structure of 3a at 303 K.

Face-to-face structure of **3a** is shown in capped-stick model. Hydrogen atom is omitted. Intermolecular distances ($d_{\text{centroid-centroid}}$, $d_{\pi-\pi}$, d_{parallel}) are shown. C, gray.

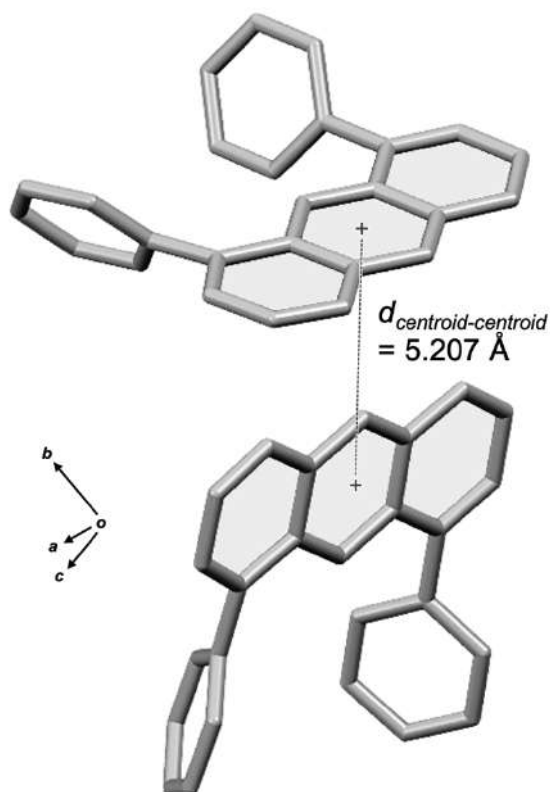
Supplementary Table 3. Crystal Data and Structural Refinement for the **3a**

CCDC deposit number	2456867	
Empirical formula	C ₂₆ H ₁₈	
Formula weight	330.40	
Temperature	303.15	
Wavelength	0.71073 nm	
Crystal system	triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	$a = 6.7141(3) \text{ \AA}$	$\alpha = 77.954(4)^\circ$
	$b = 9.6727(5) \text{ \AA}$	$\beta = 79.869(3)^\circ$
	$c = 14.2242(4) \text{ \AA}$	$\gamma = 80.885(4)^\circ$
Volume	882.21(7) Å ³	
<i>Z</i>	2	
Density (calculated)	1.244 g/cm ³	
Absorption coefficient	0.070 mm ⁻¹	
<i>F</i> (000)	348.0	
Crystal size	0.264 × 0.166 × 0.074 mm ³	
2 θ range for data collection	4.778 to 60.23°	
Index ranges	-9 ≤ <i>h</i> ≤ 8, -13 ≤ <i>k</i> ≤ 13, -19 ≤ <i>l</i> ≤ 17	
Reflections collected	10394	
Independent reflections	4221 [<i>R</i> (int) = 0.0258]	
Data / restraints / parameters	4221 / 0 / 235	
Goodness-of-fit on <i>F</i> ²	1.061	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0493, <i>wR</i> ₂ = 0.1308	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0730, <i>wR</i> ₂ = 0.1437	
Largest diff. peak and hole	0.13/-0.16 e.Å ⁻³	



Supplementary Fig. 9. Crystal structure of 3b at 303 K.

Crystal structures of **3b** (CCDC reference number 2456866). **a**, ORTEP drawing (50% anisotropic displacement parameters) and **b**, electron density maps ($2F_o - F_c$; purple isomesh, $0.1 / \text{e}\text{\AA}^{-3}$).

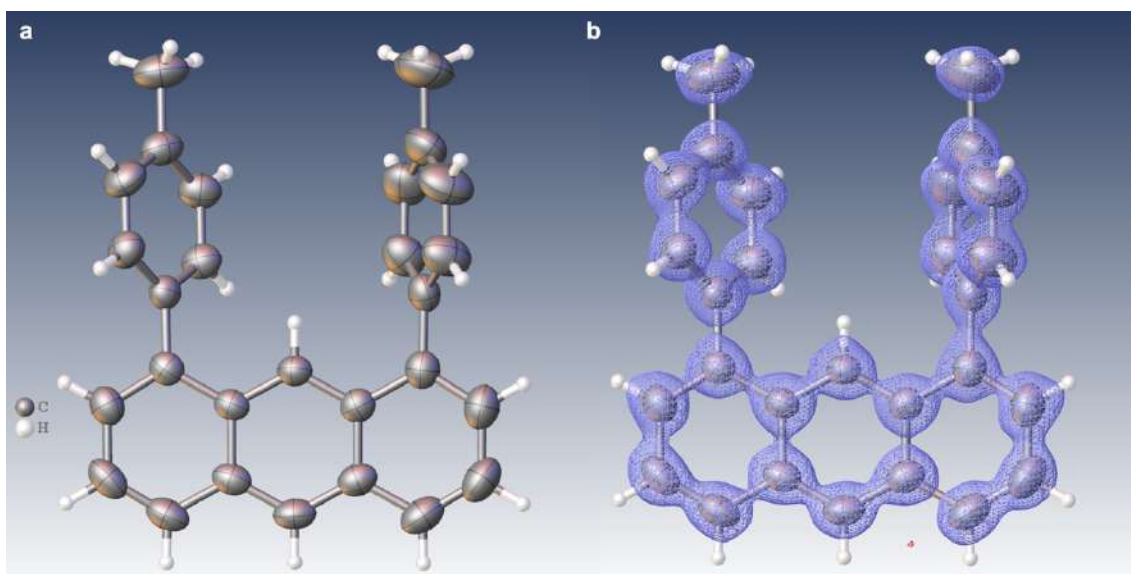


Supplementary Fig. 10. Edge-to-face structure of 3b at 303 K.

Edge-to-face structure of **3b** is shown in capped-stick model. Hydrogen atom is omitted. Intermolecular distance ($d_{\text{centroid-centroid}}$) is shown. C, gray.

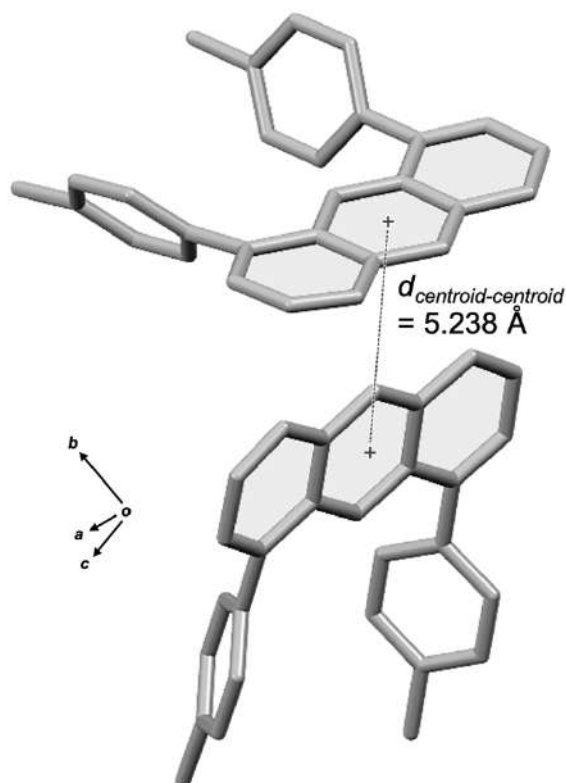
Supplementary Table 4. Crystal Data and Structural Refinement for the **3b**

CCDC deposit number	2456866	
Empirical formula	C ₂₆ H ₁₈	
Formula weight	330.40	
Temperature	303.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 9.9447(5) Å	<i>α</i> = 90°
	<i>b</i> = 27.1765(10) Å	<i>β</i> = 105.003(5)°
	<i>c</i> = 6.9805(3) Å	<i>γ</i> = 90°
Volume	1822.26(14) Å ³	
<i>Z</i>	4	
Density (calculated)	1.204 g/cm ³	
Absorption coefficient	0.068 mm ⁻¹	
<i>F</i> (000)	696.0	
Crystal size	0.335 × 0.236 × 0.106 mm ³	
2 θ range for data collection	4.24 to 60.322°	
Index ranges	-11 ≤ <i>h</i> ≤ 13, -37 ≤ <i>k</i> ≤ 35, -9 ≤ <i>l</i> ≤ 8	
Reflections collected	16371	
Independent reflections	4440 [<i>R</i> (int) = 0.0203]	
Data / restraints / parameters	4440 / 0 / 235	
Goodness-of-fit on <i>F</i> ²	1.042	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0446, <i>wR</i> ₂ = 0.1105	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0654, <i>wR</i> ₂ = 0.1219	
Largest diff. peak and hole	0.11/-0.17 e.Å ⁻³	



Supplementary Fig. 11. Crystal structure of 4 at 303 K.

Crystal structures of **4** (CCDC reference number 2456864). **a**, ORTEP drawing (50% anisotropic displacement parameters) and **b**, electron density maps ($2F_o - F_c$; purple isomesh, $0.1 \text{ /e\AA}^{-3}$).

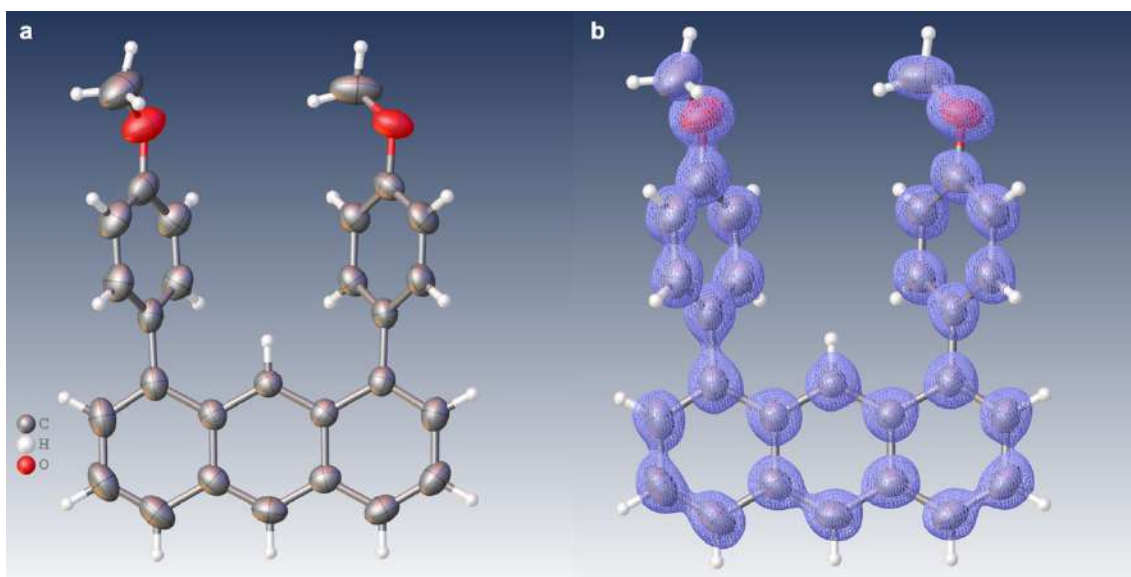


Supplementary Fig. 12. Edge-to-face structure of 4 at 303 K.

Edge-to-face structure of **4** is shown in capped-stick model. Hydrogen atom is omitted. Intermolecular distance ($d_{\text{centroid-centroid}}$) is shown. C, gray.

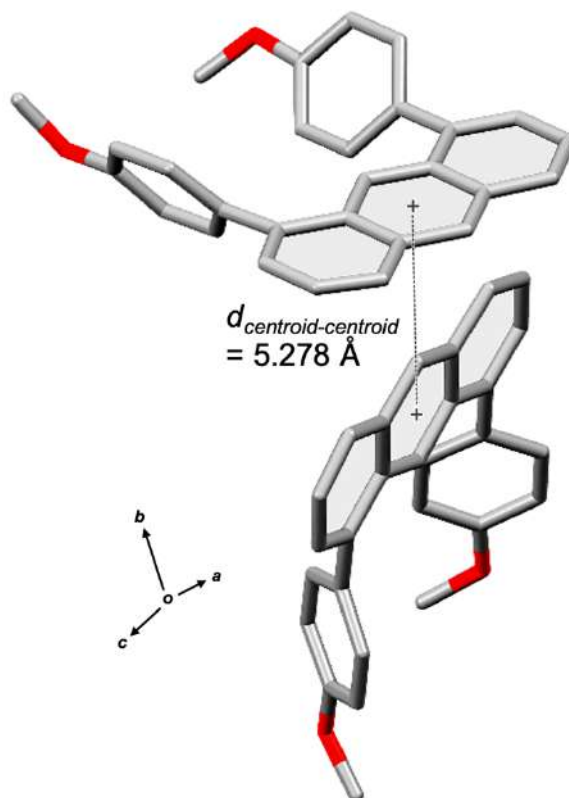
Supplementary Table 5. Crystal Data and Structural Refinement for the **4**

CCDC deposit number	2456864	
Empirical formula	C ₂₈ H ₂₂	
Formula weight	358.45	
Temperature	303.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 9.8376(5) Å	<i>α</i> = 90°
	<i>b</i> = 29.0057(11) Å	<i>β</i> = 106.438(5)°
	<i>c</i> = 7.3731(3) Å	<i>γ</i> = 90°
Volume	2017.89(16) Å ³	
<i>Z</i>	4	
Density (calculated)	1.180 g/cm ³	
Absorption coefficient	0.067 mm ⁻¹	
<i>F</i> (000)	760.0	
Crystal size	0.998 × 0.306 × 0.07 mm ³	
2 θ range for data collection	4.316 to 60.254°	
Index ranges	-12 ≤ <i>h</i> ≤ 13, -40 ≤ <i>k</i> ≤ 39, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	18564	
Independent reflections	4940 [<i>R</i> (int) = 0.0246]	
Data / restraints / parameters	4940 / 0 / 255	
Goodness-of-fit on <i>F</i> ²	1.045	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0491, <i>wR</i> ₂ = 0.1261	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0756, <i>wR</i> ₂ = 0.1405	
Largest diff. peak and hole	0.16/-0.16 e.Å ⁻³	



Supplementary Fig. 13. Crystal structure of 5 at 303 K.

Crystal structures of **5** (CCDC reference number 2456865). **a**, ORTEP drawing (50% anisotropic displacement parameters) and **b**, electron density maps ($2F_o - F_c$; purple isomesh, $0.1 \text{ /e\AA}^{-3}$).



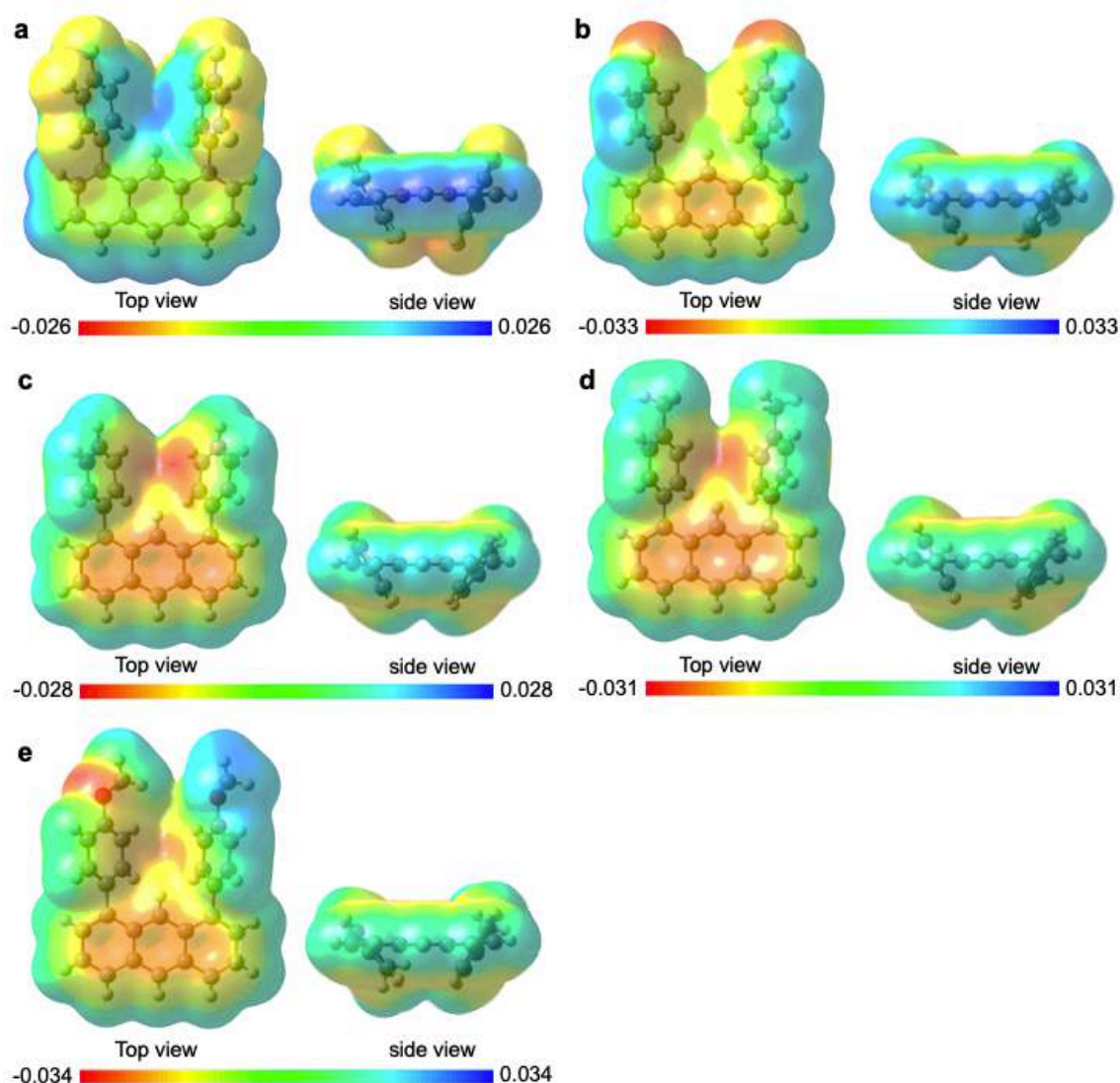
Supplementary Fig. 14. Edge-to-face structure of 5 at 303 K.

Edge-to-face structure of **5** is shown in capped-stick model. Hydrogen atom is omitted. Intermolecular distance ($d_{\text{centroid-centroid}}$) is shown. C, gray; O, red.

Supplementary Table 6. Crystal Data and Structural Refinement for the **5**

CCDC deposit number	2456865	
Empirical formula	C ₂₈ H ₂₂ O ₂	
Formula weight	390.45	
Temperature	303.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>a</i>	
Unit cell dimensions	<i>a</i> = 7.4965(13) Å	<i>α</i> = 90°
	<i>b</i> = 28.6848(13) Å	<i>β</i> = 137.43(3)°
	<i>c</i> = 13.969(2) Å	<i>γ</i> = 90°
Volume	2032.0(10) Å ³	
<i>Z</i>	4	
Density (calculated)	1.276 g/cm ³	
Absorption coefficient	0.079 mm ⁻¹	
<i>F</i> (000)	824.0	
Crystal size	0.325 × 0.213 × 0.072 mm ³	
2 θ range for data collection	4.31 to 60.276°	
Index ranges	-9 ≤ <i>h</i> ≤ 7, -38 ≤ <i>k</i> ≤ 38, -17 ≤ <i>l</i> ≤ 17	
Reflections collected	14248	
Independent reflections	4899 [<i>R</i> (int) = 0.0221]	
Data / restraints / parameters	4899 / 0 / 273	
Goodness-of-fit on <i>F</i> ²	1.045	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0501, <i>wR</i> ₂ = 0.1291	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0875, <i>wR</i> ₂ = 0.1477	
Largest diff. peak and hole	0.29/-0.27 e.Å ⁻³	

3.3 Molecular electrostatic potential analysis

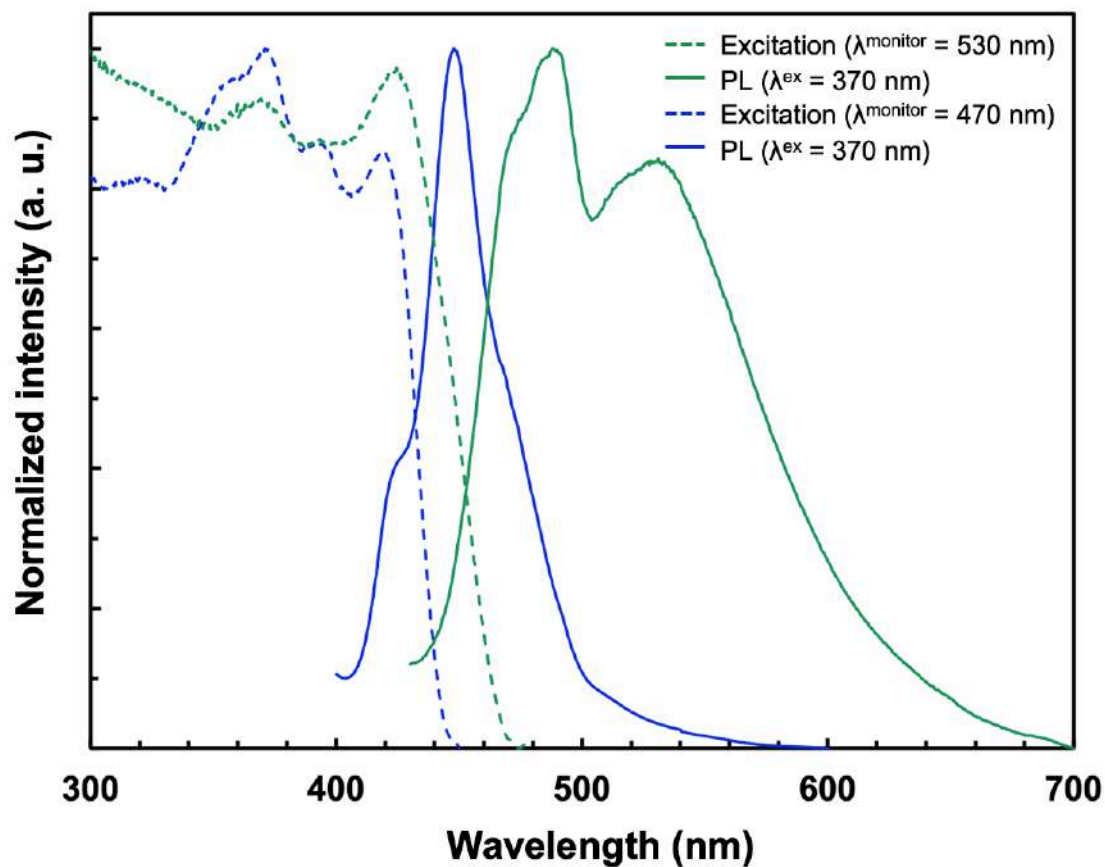


Supplementary Fig. 15. Molecular electrostatic potential maps.

Molecular electrostatic potential maps for the ground state of **a**, **1**, **b**, **2**, **c**, **3**, **d**, **4**, and **e**, **5** at the B3LYP/6-31+G(d,p) level (density isovalue: 0.004 au). The atomic coordinates were obtained from the crystal structures of single molecules. Isoelectronic density surface of electrostatic potential: red; negative charge, blue; positive charge.

4. Optical property

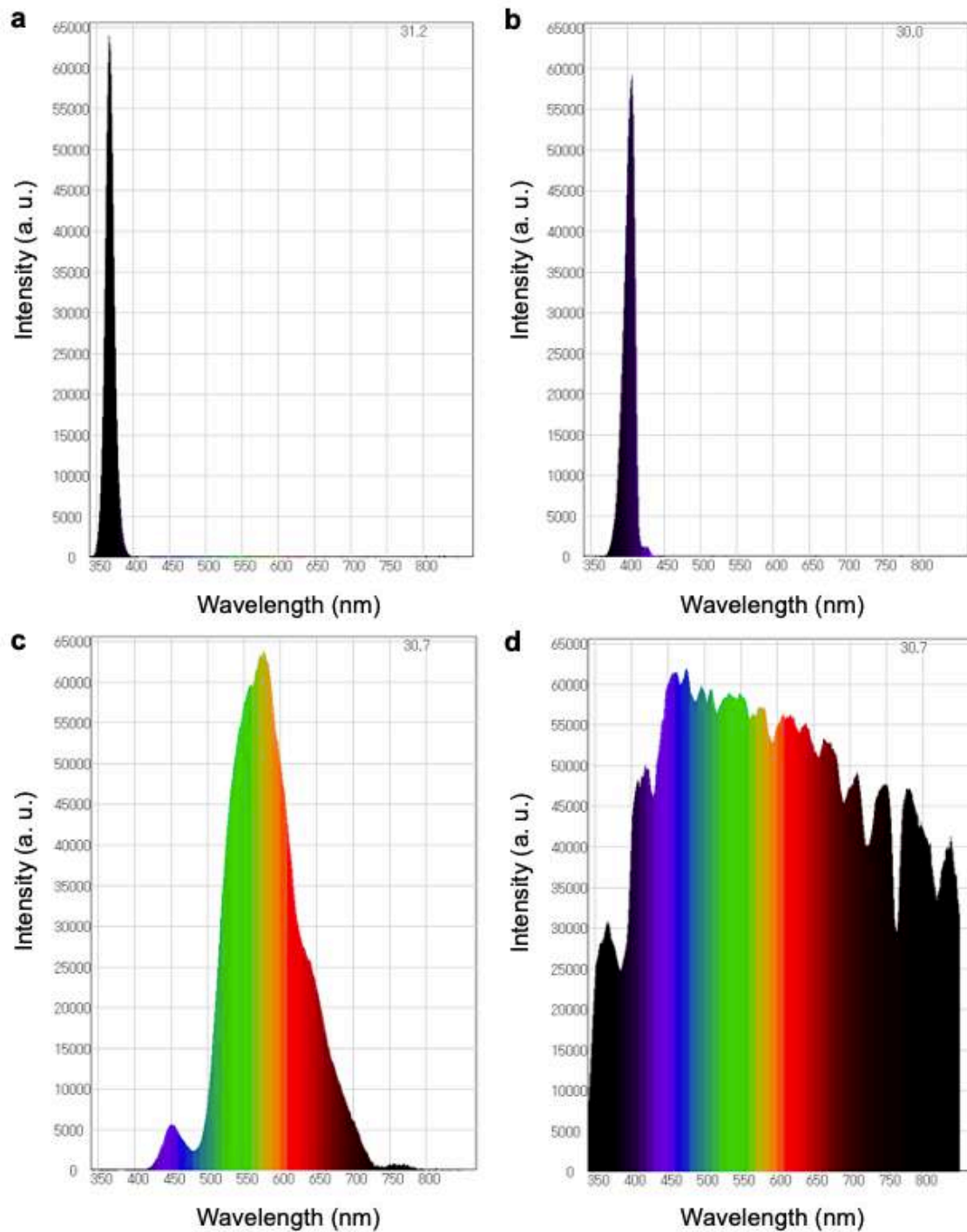
4.1 Optical absorption and photoluminescence bands



Supplementary Fig. 16. Solid-state optical property.

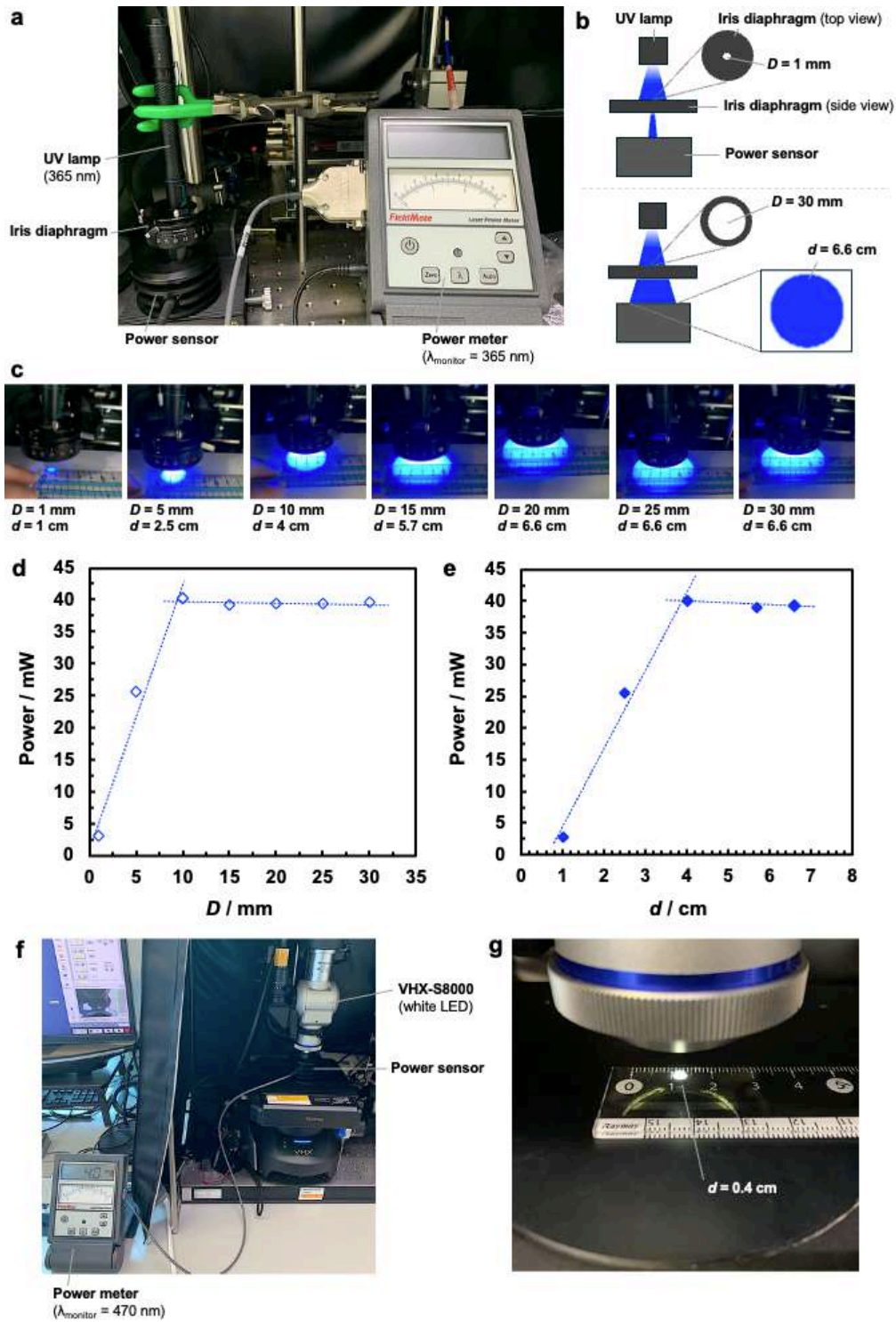
Fluorescence excitation (solid line) and PL (dashed line) spectra of crystal **1** (green) and **1_{PD}** (blue). The fluorescence excitation spectrum of crystal **1** shows an absorption edge at 470 nm, indicating that photochemical reactions are initiated within the optical absorption band below this wavelength.

4.2 Light source



Supplementary Fig. 17. Light source spectra.

Emission spectra of various light sources: **a**, UV lamp, **b**, blue laser, **c**, white LED, and **d**, sunlight.



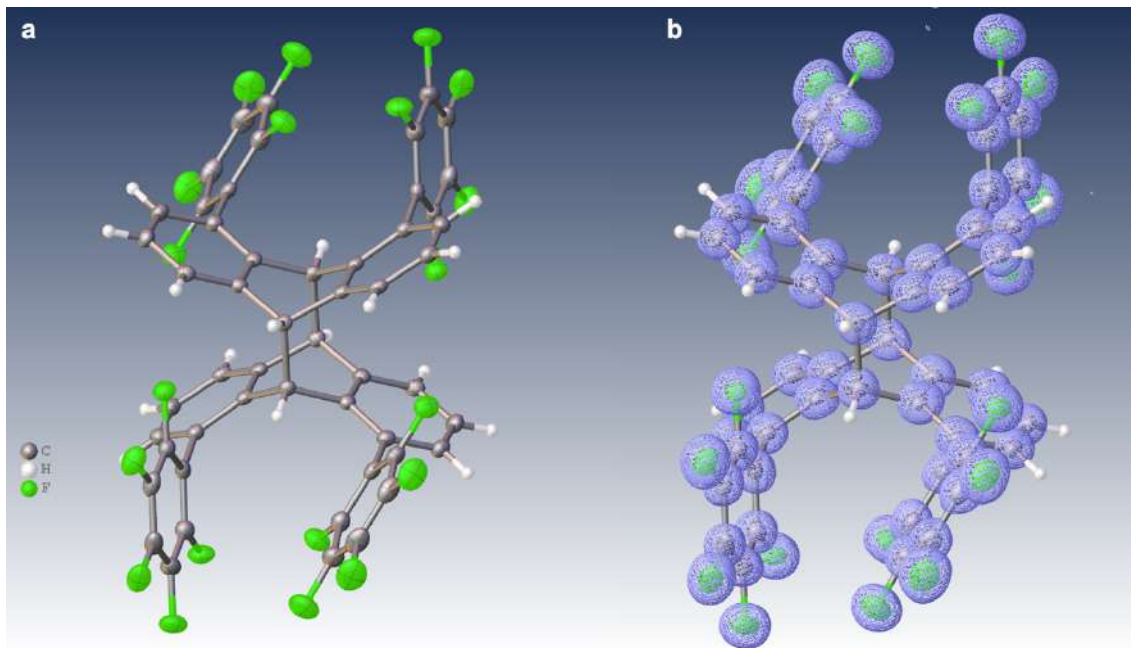
Supplementary Fig. 18. Power density calculation of light sources.

- a**, Experimental setup for UV irradiation. **b**, Schematic illustration of the measurement. **c**, Definition of the iris aperture diameter (D) and the actual illuminated spot diameter (d). **d**, Optical power of the UV source measured at aperture diameter D . **e**, Optical power corresponding to the effective radius d . **f**, Experimental setup for white LED irradiation. **g**, Definition of the illuminated spot diameter d for the white light source.

5. Solid-state [4+4] photoreaction

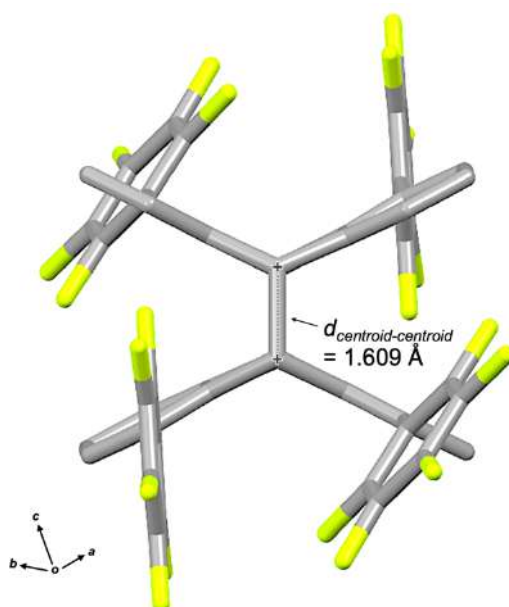
5.1 X-Ray crystallographic observation of **1_{PD}**

Crystal **1** was irradiated sunlight at 298 ± 5 K to obtain single crystalline **1_{PD}**.



Supplementary Fig. 19. Crystal structure of **1_{PD} at 103 K.**

Crystal structures of **1_{PD}** (CCDC reference number 2456868). **a**, ORTEP drawing (50% anisotropic displacement parameters) and **b**, electron density maps ($2F_o - F_c$; purple isomesh, $0.1 \text{ /e\AA}^{-3}$).



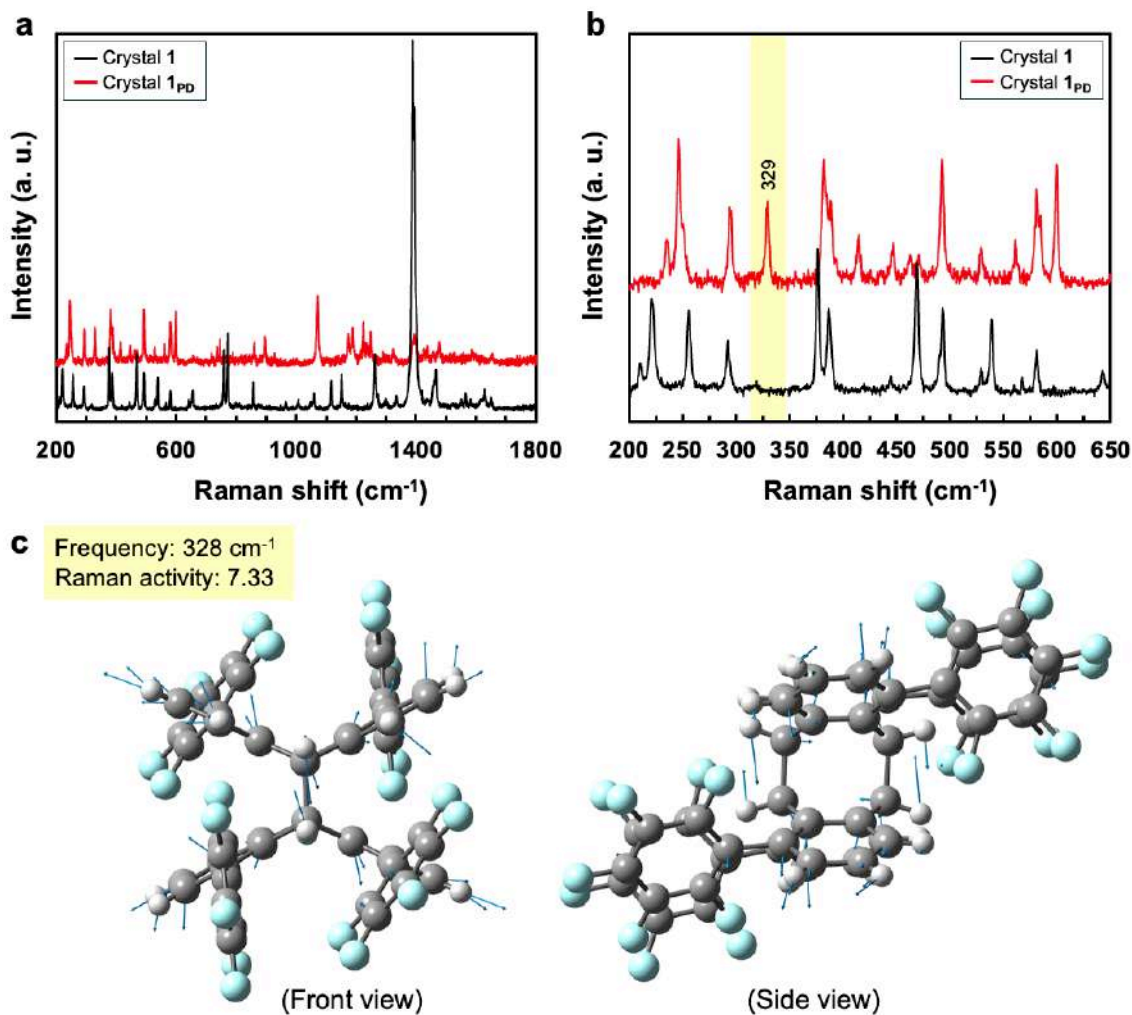
Supplementary Fig. 20. Photodimerized structure of **1_{PD} at 103 K.**

Photodimerized structure of **1_{PD}** is shown in capped-stick model. Hydrogen atom is omitted. Intermolecular distance ($d_{\text{centroid-centroid}}$) is shown. C, grey; F, yellow.

Supplementary Table 7. Crystal Data and Structural Refinement for the **1_{PD}**

CCDC deposit number	2456868	
Empirical formula	C ₅₂ H ₁₆ F ₂₀	
Formula weight	1020.65	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 9.9678(4) Å	<i>α</i> = 90°
	<i>b</i> = 24.3947(9) Å	<i>β</i> = 96.794(4)°
	<i>c</i> = 7.9092(4) Å	<i>γ</i> = 90°
Volume	1909.71(14) Å ³	
<i>Z</i>	2	
Density (calculated)	1.775 g/cm ³	
Absorption coefficient	0.172 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.307 × 0.246 × 0.078 mm ³	
2 θ range for data collection	3.34 to 52.742°	
Index ranges	-12 ≤ <i>h</i> ≤ 12, -27 ≤ <i>k</i> ≤ 27, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	12838	
Independent reflections	3895 [<i>R</i> (int) = 0.0344]	
Data / restraints / parameters	3895 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.052	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0384, <i>wR</i> ₂ = 0.0948	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0531, <i>wR</i> ₂ = 0.1020	
Largest diff. peak and hole	0.27/-0.23 e.Å ⁻³	

5.2 Raman spectroscopic observation of the structural transition.

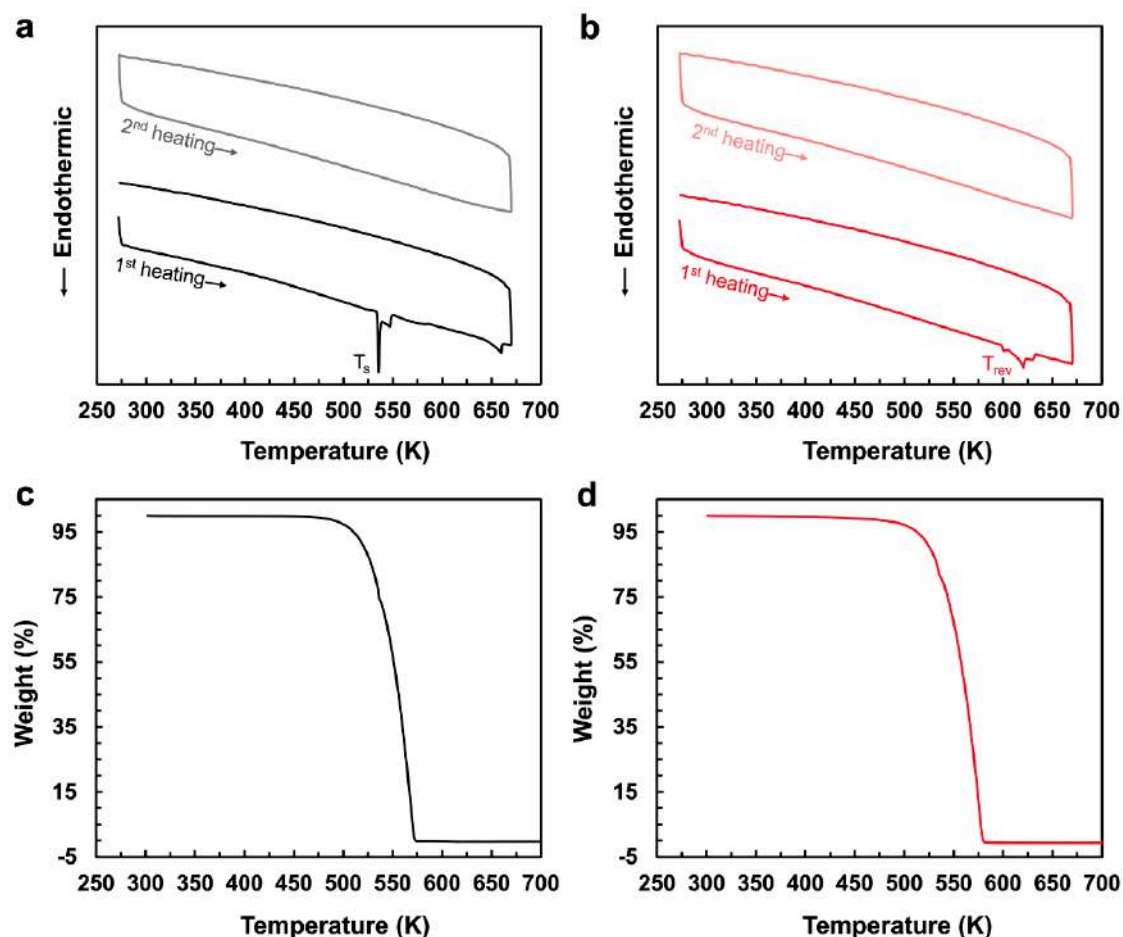


Supplementary Fig. 21. Direct evidence of photodimerization by Raman spectroscopy.

Spectral evolution of the photoreaction observed by Raman spectroscopy. **a**, full range from 200–1800 cm⁻¹, and **b**, the intramolecular vibration region. Spectra of crystal **1** (black) and its photodimer **1_{PD}** (red) are compared. **c**, Raman vibrational mode at 328 cm⁻¹ for **1_{PD}** calculated at the B3LYP/6-31G(d,p) level. Displacement vector, blue arrows.

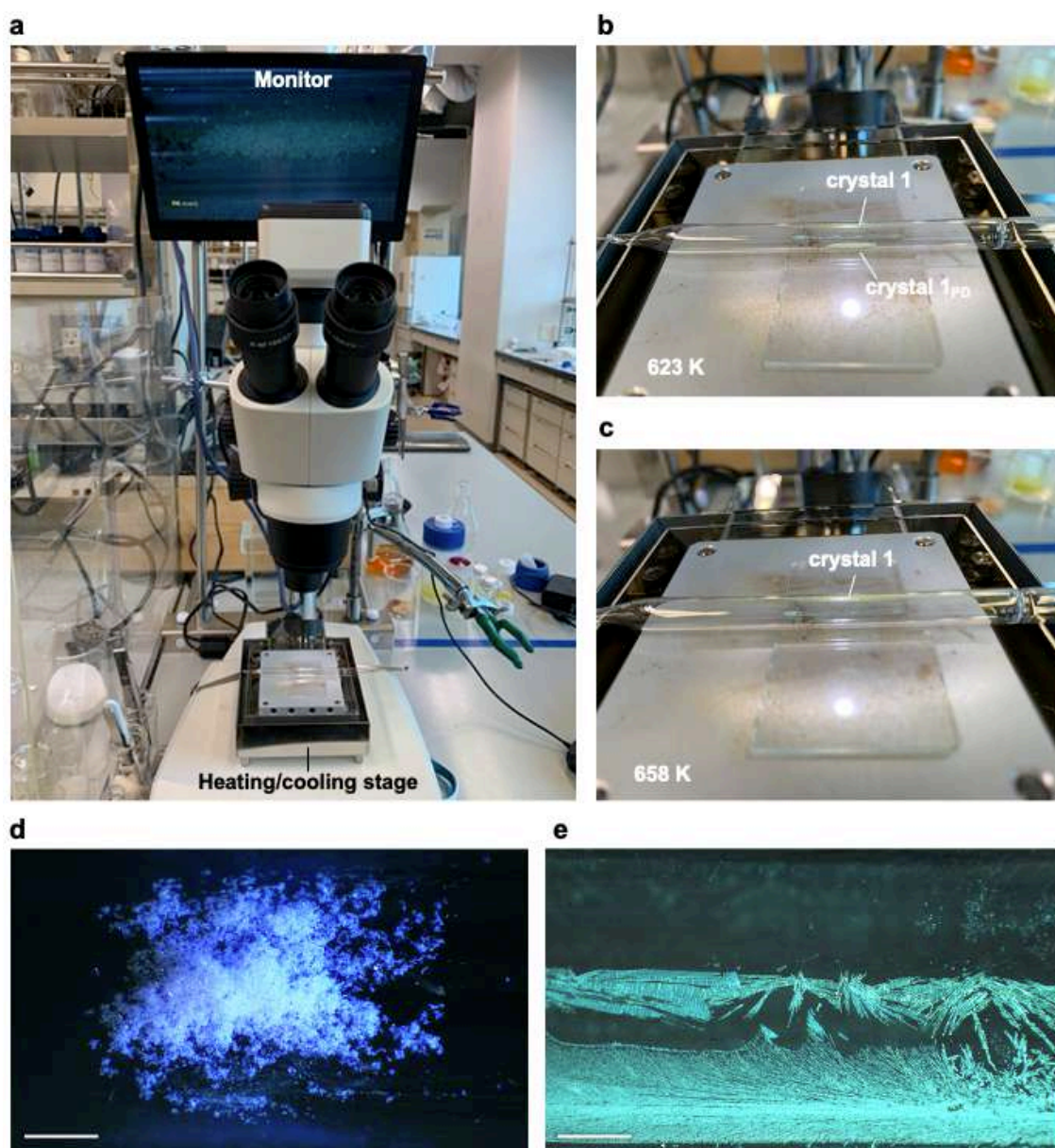
5.3 Solid-state retro reaction

Crystals **1_{PD}** was heated at 623–658 K in a glass tube to afford crystals **1**. ¹H NMR spectrum was recorded by adding CDCl₃ directly to the same glass tube to dissolve the sample. X-ray diffraction measurements of the thermally obtained crystals **1** was carried out at 103 K (CCDC reference number 2456715).



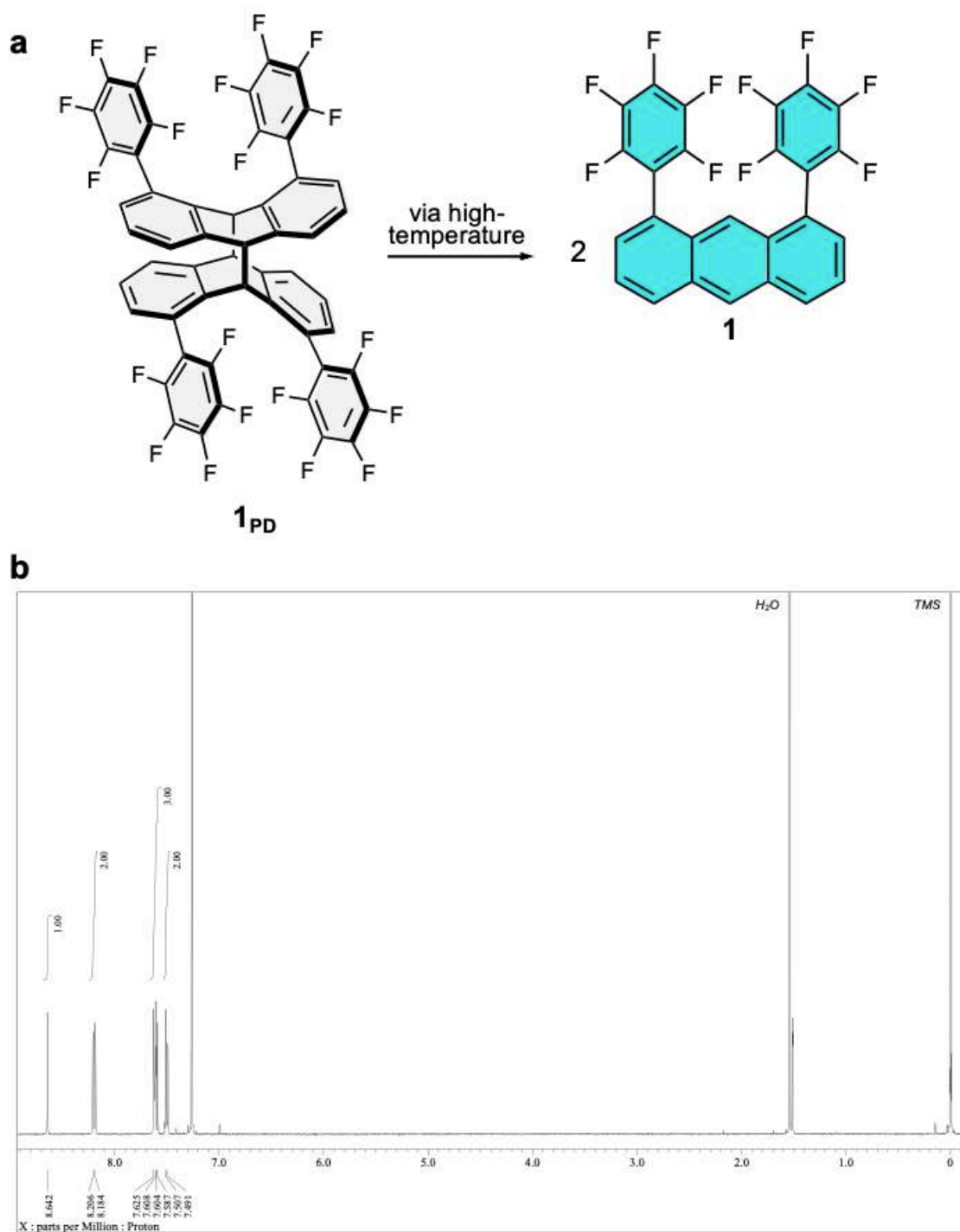
Supplementary Fig. 22. Thermal properties.

Thermal properties of crystal **1** and **1_{PD}**. DSC plots of **a**, crystal **1** and **b**, **1_{PD}** during the first two heating and cooling cycles, recorded at a heating/cooling rate of 10 K/min. T_s is sublimation temperature, T_{rev} is thermal reversion temperature. TGA plots of **c**, crystal **1** and **d**, **1_{PD}** with heating rate of 10 K/min.



Supplementary Fig. 23 Thermally induced retro reaction.

Experimental setup for the solid-state retro reaction of **1_{PD}** to **1**. **a**, Simultaneous reaction and observation system. Photographs of the reaction at **b**, 623 K and **c**, 658 K under ambient light. Optical microscopy images of **d**, before and **e**, after heating crystals under UV irradiation. Scale bar, 500 μm .



Supplementary Fig. 24. Experimental evidence obtained from ^1H NMR spectrum.

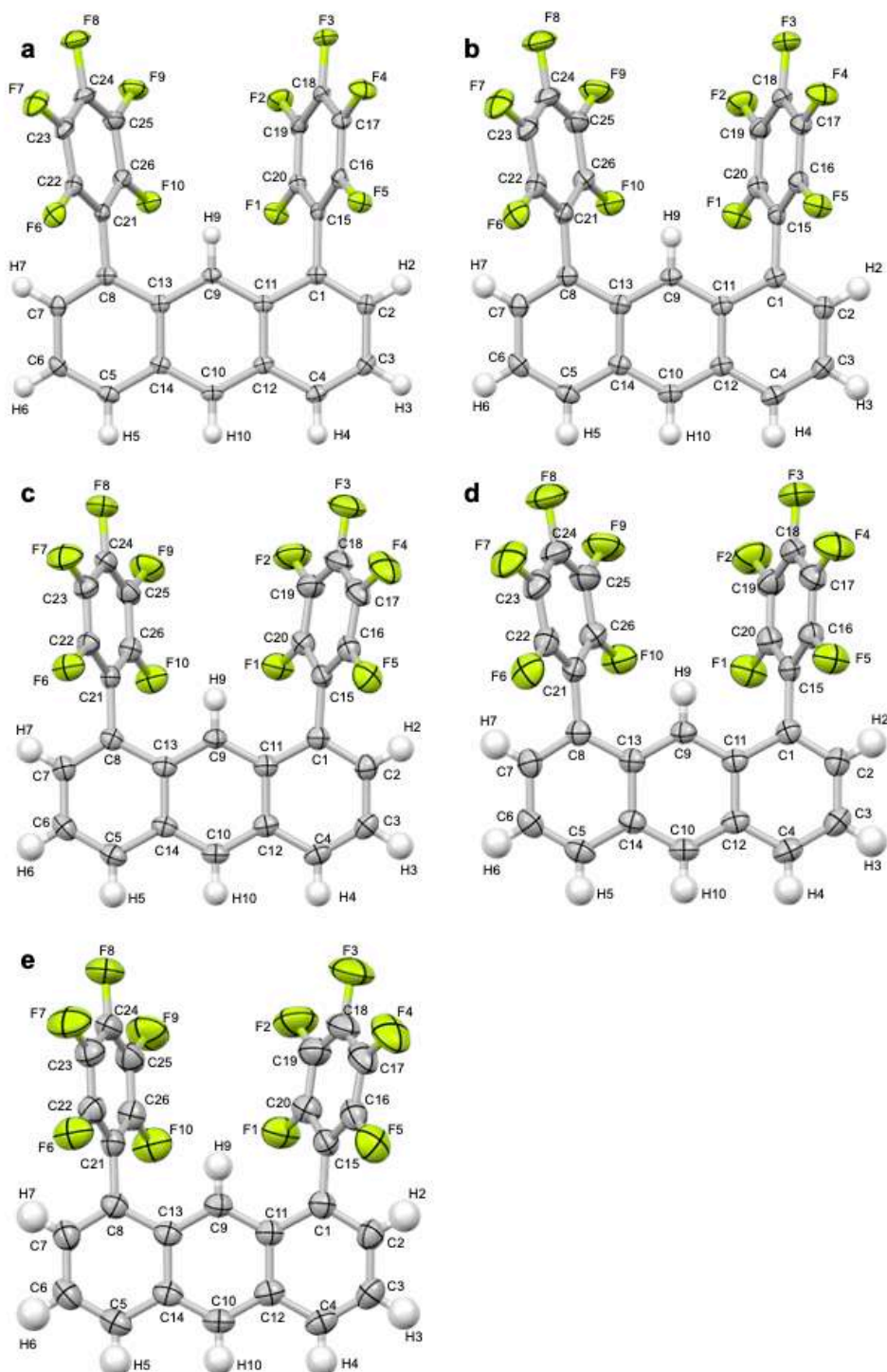
a, Solid-state retro reaction of **1_{PD}** to **1**. **b**, ^1H NMR (400 MHz, $CDCl_3$) spectrum of **1** obtained after thermal treatment.

Supplementary Table 8. Crystal Data for the Thermally Obtained **1**

CCDC deposit number	2456715	
Empirical formula	C ₂₆ H ₈ F ₁₀	
Formula weight	510.32	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.5116(5) Å	<i>α</i> = 90°
	<i>b</i> = 24.5436(10) Å	<i>β</i> = 108.471(5)°
	<i>c</i> = 7.8671(3) Å	<i>γ</i> = 90°
Volume	1925.09(15) Å ³	
<i>Z</i>	4	
Density (calculated)	1.761 g/cm ³	
Absorption coefficient	0.170 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.254 × 0.063 × 0.049 mm ³	
2 θ range for data collection	4.41 to 60.122°	
Index ranges	-14 ≤ <i>h</i> ≤ 13, -21 ≤ <i>k</i> ≤ 31, -9 ≤ <i>l</i> ≤ 5	
Reflections collected	12629	
Independent reflections	4550 [<i>R</i> (int) = 0.0576]	
Data / restraints / parameters	4550 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.032	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0586, <i>wR</i> ₂ = 0.1177	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1140, <i>wR</i> ₂ = 0.1359	
Largest diff. peak and hole	0.33/-0.34 e.Å ⁻³	

6. Thermal control of photoinduced crystal dynamics

6.1 Temperature-dependent X-ray crystallographic analysis



Supplementary Fig. 25. Crystal structure of 1 at 103–303 K.

Crystal structures of **1** at **a**, 103 K, **b**, 153 K, **c**, 203 K, **d**, 253 K, and **e**, 303 K. ORTEP drawing (50% anisotropic displacement parameters).

Supplementary Table 9. Crystal Data and Structural Refinement for the **1** at 103 K

Identification code	exp_373	
CCDC deposit number	2456716	
Empirical formula	C ₂₆ H ₈ F ₁₀	
Formula weight	510.32	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.5069(4) Å	<i>α</i> = 90°
	<i>b</i> = 24.5538(6) Å	<i>β</i> = 108.438(3)°
	<i>c</i> = 7.8617(2) Å	<i>γ</i> = 90°
Volume	1924.08(10) Å ³	
<i>Z</i>	4	
Density (calculated)	1.762 g/cm ³	
Absorption coefficient	0.170 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.692 × 0.45 × 0.426 mm ³	
2 θ range for data collection	4.41 to 52.742°	
Index ranges	-13 ≤ <i>h</i> ≤ 12, -30 ≤ <i>k</i> ≤ 23, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	15223	
Independent reflections	3926 [<i>R</i> (int) = 0.0321]	
Data / restraints / parameters	3926 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.073	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0364, <i>wR</i> ₂ = 0.0918	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0445, <i>wR</i> ₂ = 0.0973	
Largest diff. peak and hole	0.27/-0.27 e.Å ⁻³	

Supplementary Table 10. Crystal Data and Structural Refinement for the **1** at 153 K

Identification code	exp_374	
CCDC deposit number	2456717	
Empirical formula	C ₂₆ H ₈ F ₁₀	
Formula weight	510.32	
Temperature	153.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.5291(4) Å	$\alpha = 90^\circ$
	<i>b</i> = 24.5899(7) Å	$\beta = 108.263(4)^\circ$
	<i>c</i> = 7.8915(3) Å	$\gamma = 90^\circ$
Volume	1940.27(13) Å ³	
<i>Z</i>	4	
Density (calculated)	1.747 g/cm ³	
Absorption coefficient	0.169 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.8 × 0.503 × 0.379 mm ³	
2 θ range for data collection	4.398 to 52.74°	
Index ranges	-11 ≤ <i>h</i> ≤ 13, -30 ≤ <i>k</i> ≤ 29, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	16282	
Independent reflections	3956 [<i>R</i> (int) = 0.0423]	
Data / restraints / parameters	3956 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.070	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0377, <i>wR</i> ₂ = 0.0980	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0463, <i>wR</i> ₂ = 0.1037	
Largest diff. peak and hole	0.20/-0.26 e.Å ⁻³	

Supplementary Table 11. Crystal Data and Structural Refinement for the **1** at 203 K

Identification code	exp_375	
CCDC deposit number	2456718	
Empirical formula	C ₂₆ H ₈ F ₁₀	
Formula weight	510.32	
Temperature	203.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.5371(4) Å	$\alpha = 90^\circ$
	<i>b</i> = 24.6150(7) Å	$\beta = 108.167(4)^\circ$
	<i>c</i> = 7.9202(3) Å	$\gamma = 90^\circ$
Volume	1951.87(13) Å ³	
<i>Z</i>	4	
Density (calculated)	1.737 g/cm ³	
Absorption coefficient	0.168 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.547 × 0.444 × 0.428 mm ³	
2 θ range for data collection	5.246 to 52.744°	
Index ranges	-13 ≤ <i>h</i> ≤ 13, -30 ≤ <i>k</i> ≤ 30, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	16519	
Independent reflections	3983 [<i>R</i> (int) = 0.0357]	
Data / restraints / parameters	3983 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.069	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0390, <i>wR</i> ₂ = 0.0990	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0483, <i>wR</i> ₂ = 0.1043	
Largest diff. peak and hole	0.17/-0.26 e.Å ⁻³	

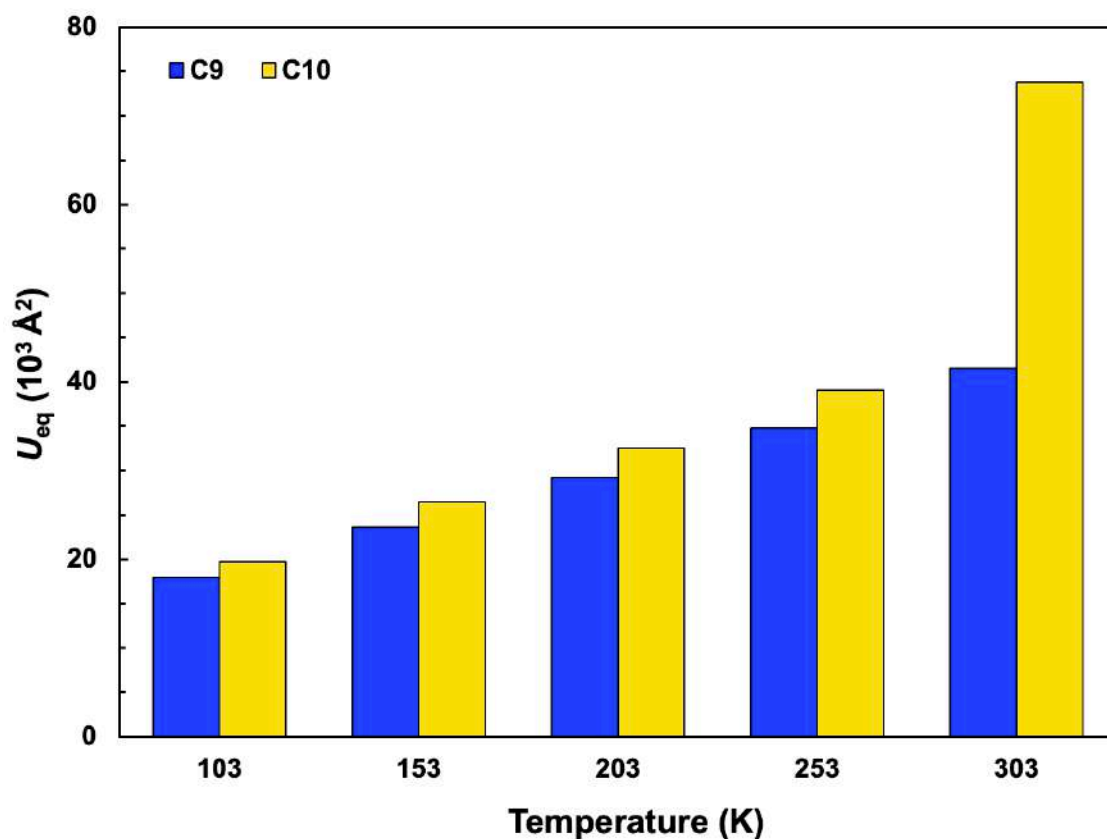
Supplementary Table 12. Crystal Data and Structural Refinement for the **1** at 253 K

Identification code	exp_376	
CCDC deposit number	2456719	
Empirical formula	C ₂₆ H ₈ F ₁₀	
Formula weight	510.32	
Temperature	253.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.5309(4) Å	$\alpha = 90^\circ$
	<i>b</i> = 24.6653(7) Å	$\beta = 108.061(4)^\circ$
	<i>c</i> = 7.9592(3) Å	$\gamma = 90^\circ$
Volume	1971.12(13) Å ³	
<i>Z</i>	4	
Density (calculated)	1.720 g/cm ³	
Absorption coefficient	0.166 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.772 × 0.532 × 0.35 mm ³	
2 θ range for data collection	4.38 to 52.744°	
Index ranges	-13 ≤ <i>h</i> ≤ 13, -30 ≤ <i>k</i> ≤ 30, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	17690	
Independent reflections	4024 [<i>R</i> (int) = 0.0264]	
Data / restraints / parameters	4024 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.078	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0408, <i>wR</i> ₂ = 0.1016	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0531, <i>wR</i> ₂ = 0.1090	
Largest diff. peak and hole	0.15/-0.24 e.Å ⁻³	

Supplementary Table 13. Equivalent Isotropic Displacement Parameters, U_{eq} ($\text{\AA}^2 \times 10^3$) for **1**.

Atom	103 K	153 K	203 K	253 K	303 K
F1	29.1(2)	40.5(3)	51.7(3)	62.0(3)	72.9(3)
C1	19.0(3)	25.0(3)	31.6(3)	36.5(3)	44.8(4)
C2	21.8(3)	49.3(3)	70.8(4)	77.2(4)	52.3(4)
F2	35.5(3)	29.6(3)	36.6(4)	44.3(4)	99.1(5)
F3	32.8(2)	32.2(4)	38.6(4)	48.4(4)	54.5(4)
C3	23.6(3)	45.5(3)	78.4(4)	71.8(4)	110.2(5)
C4	21.9(3)	47.4(3)	35.4(3)	76.0(4)	50.0(4)
F4	33.9(3)	29.7(3)	70.3(4)	44.1(4)	99.0(5)
F5	28.2(2)	28.3(3)	54.4(3)	42.5(4)	77.1(3)
C5	21.7(3)	39.3(2)	37.2(4)	62.2(3)	52.1(4)
C6	22.9(3)	43.4(3)	40.0(4)	65.9(3)	57.6(5)
F6	31.7(2)	30.9(3)	50.4(3)	46.1(4)	74.4(3)
C7	22.0(3)	29.3(3)	61.5(3)	84.5(4)	91.3(4)
F7	40.9(3)	56.0(3)	36.8(4)	44.4(4)	52.9(4)
C8	20.0(3)	25.8(3)	58.3(3)	37.6(3)	43.7(4)
F8	46.1(3)	62.7(4)	30.8(3)	94.5(5)	86.0(4)
C9	17.9(3)	23.6(3)	29.2(3)	34.8(3)	41.5(3)
F9	41.7(3)	56.7(3)	62.9(3)	84.7(4)	91.6(4)
C10	19.7(3)	26.5(3)	32.5(3)	39.1(4)	73.8(3)
F10	30.6(2)	41.6(3)	50.7(3)	62.0(3)	46.0(4)
C11	17.9(3)	23.7(3)	29.7(3)	34.8(3)	41.2(3)
C12	18.9(3)	25.1(3)	31.3(3)	36.9(3)	43.5(4)
C13	18.0(3)	23.9(3)	29.3(3)	34.8(3)	40.9(3)
C14	18.8(3)	25.1(3)	31.3(3)	36.7(3)	43.6(4)
C15	18.7(3)	24.3(3)	33.5(3)	36.5(3)	46.9(4)
C16	20.9(3)	28.3(3)	38.4(4)	42.9(4)	53.9(4)
C17	23.6(3)	31.9(3)	47.6(4)	49.2(4)	66.2(5)
C18	23.5(3)	31.6(4)	51.8(5)	49.2(4)	71.3(6)
C19	22.9(3)	31.0(3)	48.2(4)	48.1(4)	67.4(5)
C20	20.0(3)	27.2(3)	39.4(4)	41.5(4)	55.3(4)
C21	20.2(3)	27.1(3)	30.7(3)	39.7(4)	43.4(4)
C22	23.3(3)	32.0(3)	33.8(3)	47.1(4)	49.5(4)
C23	28.9(4)	38.7(4)	39.6(4)	57.8(5)	57.9(5)
C24	31.0(4)	41.8(4)	40.0(4)	61.8(5)	58.2(5)
C25	29.0(4)	38.5(4)	40.8(4)	56.1(5)	58.4(5)
C26	22.7(3)	31.2(3)	35.7(3)	46.0(4)	51.0(4)

U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.



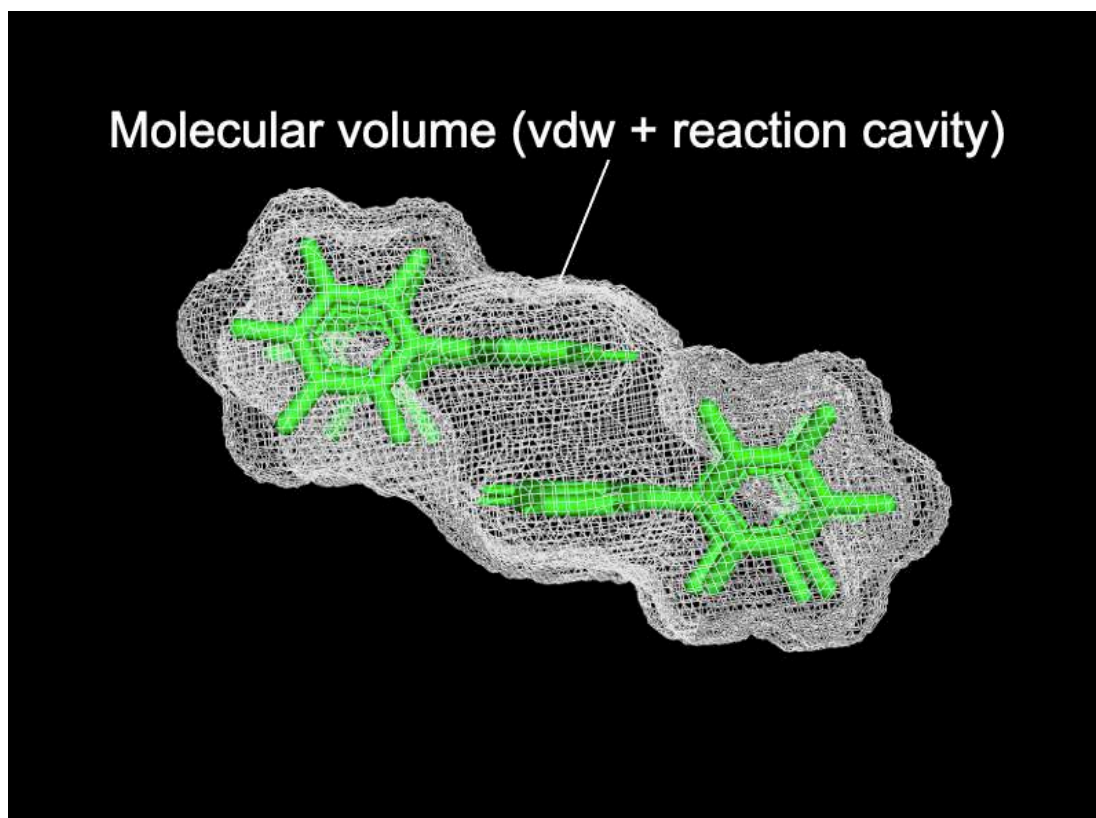
Supplementary Fig. 26. Thermal evolution of atomic coordinates in **1**.
Temperature dependence of U_{eq} values in crystal **1**.

Supplementary Table 14. Geometry Parameters of the Unit **1**

Temp. / K	$d_{\pi-\pi}$ / Å	$d_{centroid-centroid}$ / Å	$d_{parallel}$ / Å
103	3.440	3.745	1.480
153	3.456	3.764	1.491
203	3.469	3.782	1.507
253	3.487	3.804	1.520
303	3.496	3.818	1.535

Supplementary Table 15. Geometry Parameters of the Unit **2**

Temp. / K	$d_{\pi-\pi}$ / Å	$d_{centroid-centroid}$ / Å	$d_{parallel}$ / Å
103	3.315	4.611	3.205
153	3.334	4.625	3.205
203	3.348	4.637	3.208
253	3.367	4.658	3.219
303	3.378	4.667	3.220



Supplementary Fig. 27. Simulated molecular volumes.

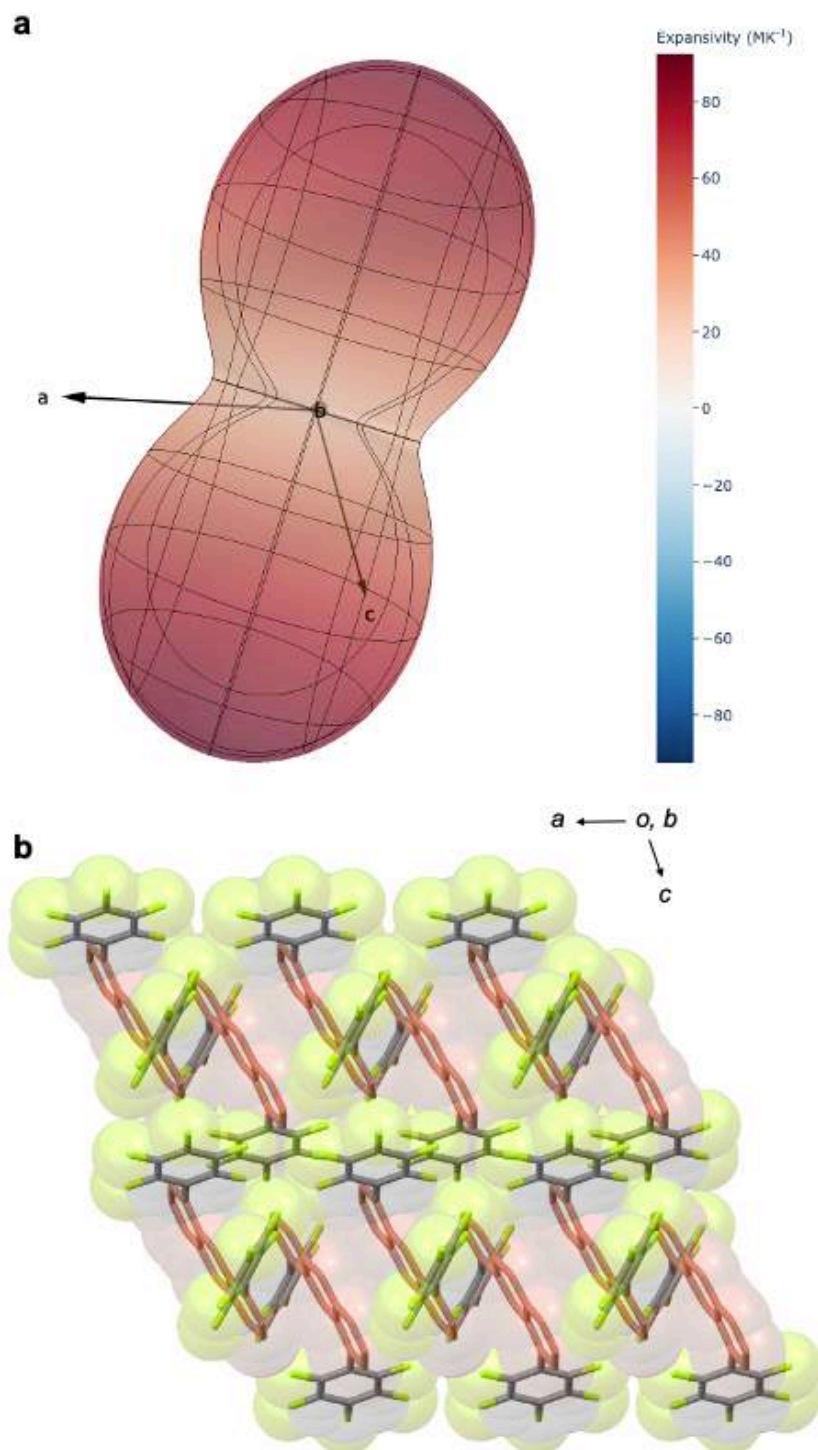
Molecular structure and surface maps of the. Crystal **1**. Molecular volume are MoloVol program⁴ was used for the calculation. Parameters were set as follows; one probe mode, probe radius: 1.2 Å, grid resolution: 0.2 Å, optimization depth: 4 and Elements radii (H: 1.2 Å, F: 1.46 Å, C: 1.77 Å).

Supplementary Table 16. Total Volumes of the Unit 1

Temp. / K	Molecular volume/Å ³	vdw volume/Å ³	Reaction cavity/Å ³
103	812.352	735.184	77.168
153	812.632	735.136	77.496
203	811.208	733.304	77.904
253	812.992	733.016	79.976
303	812.104	732.000	80.104

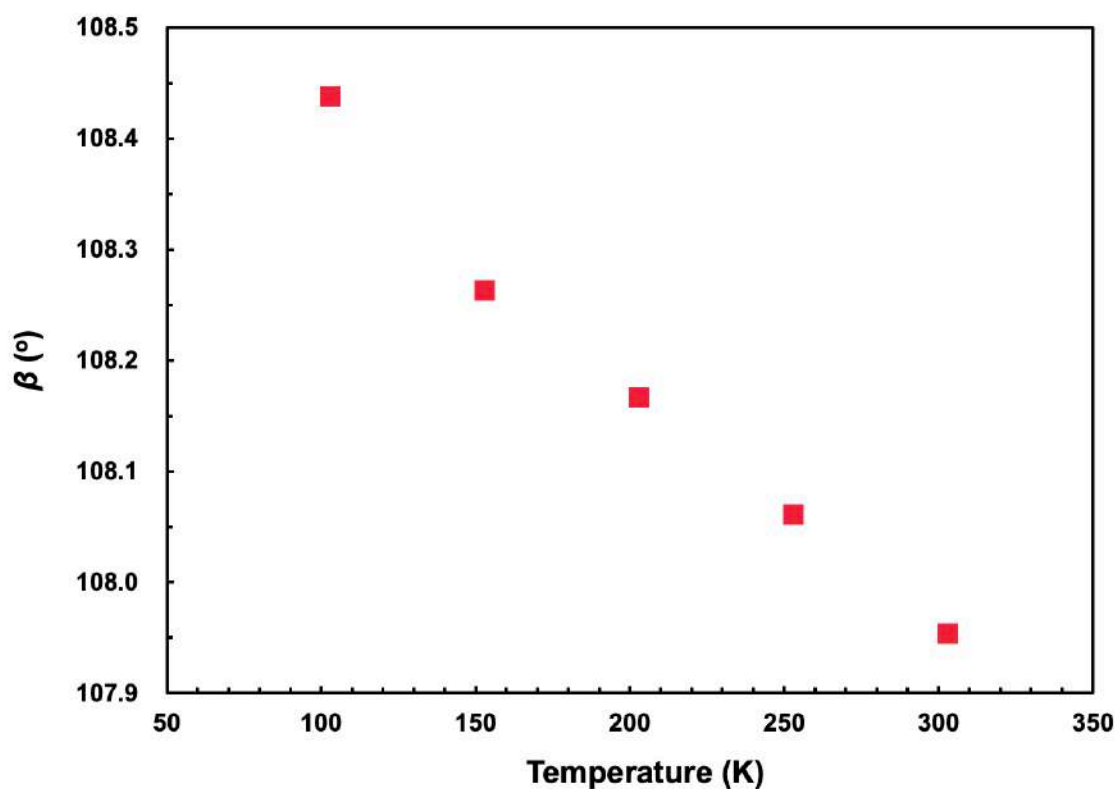
Supplementary Table 17. Total Volumes of the Unit 2

Temp. / K	Molecular volume/Å ³	vdw volume/Å ³	Reaction cavity/Å ³
103	806.472	734.912	71.560
153	807.608	734.696	72.912
203	807.248	733.504	73.744
253	807.512	733.264	74.248
303	806.464	731.672	74.792

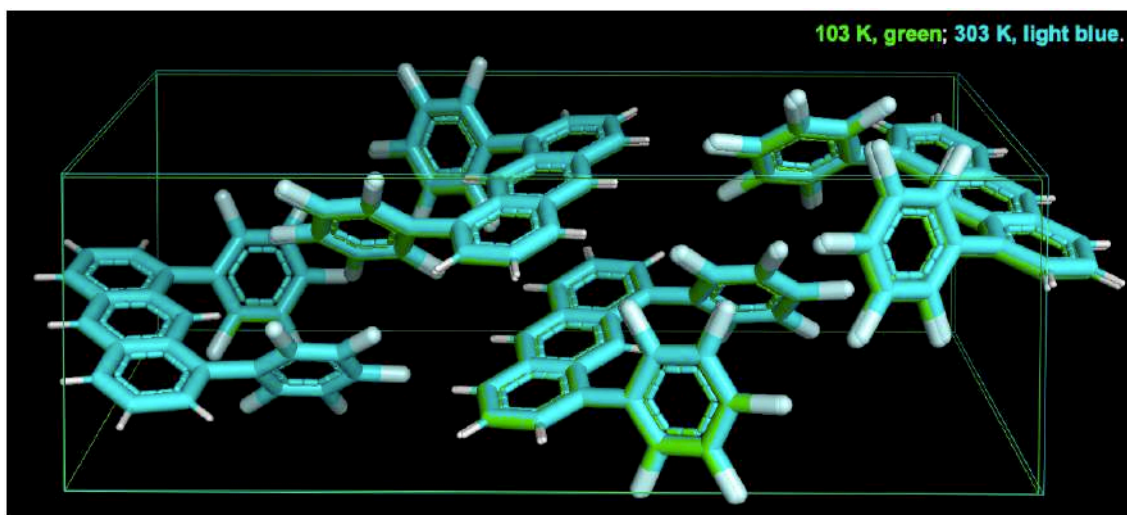


Supplementary Fig. 28. Anisotropic thermal expansion of crystal 1.

Thermal expansivity tensor and the corresponding crystal structure. **a**, Expansivity indicatrix of **1** determined using the PASCAL program^{5,6}, showing the spatial orientation of positive (red) and negative (blue) thermal expansion at 103–303 K. **b**, Packing structure viewed along the *b*-axis.



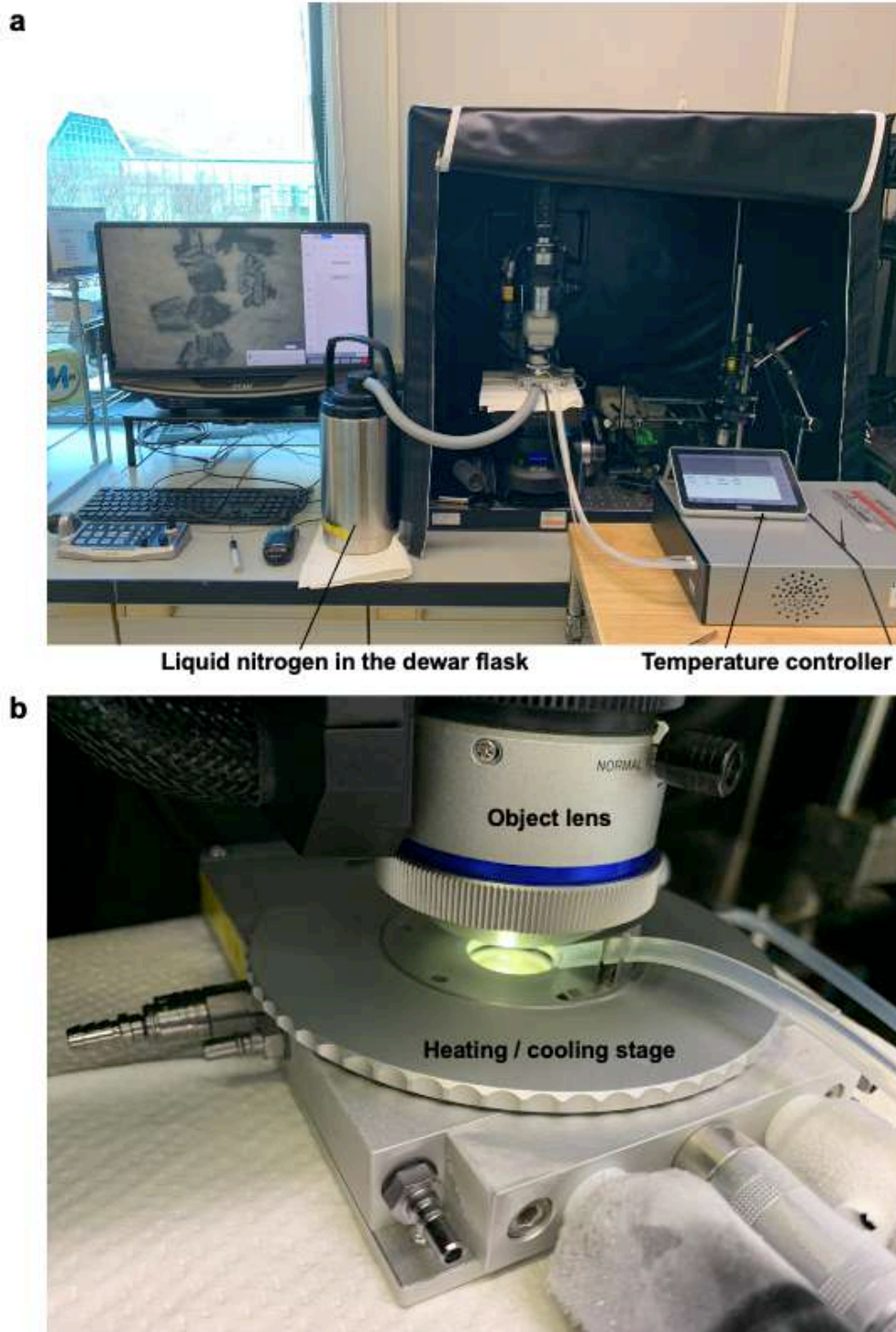
Supplementary Fig. 29. Temperature-induced lattice deformation in crystal 1
Temperature dependence of the angle β in crystal 1.



Supplementary Fig. 30. Superimposed crystal structures of 1 at 103 K (green) and 303 K (light blue).

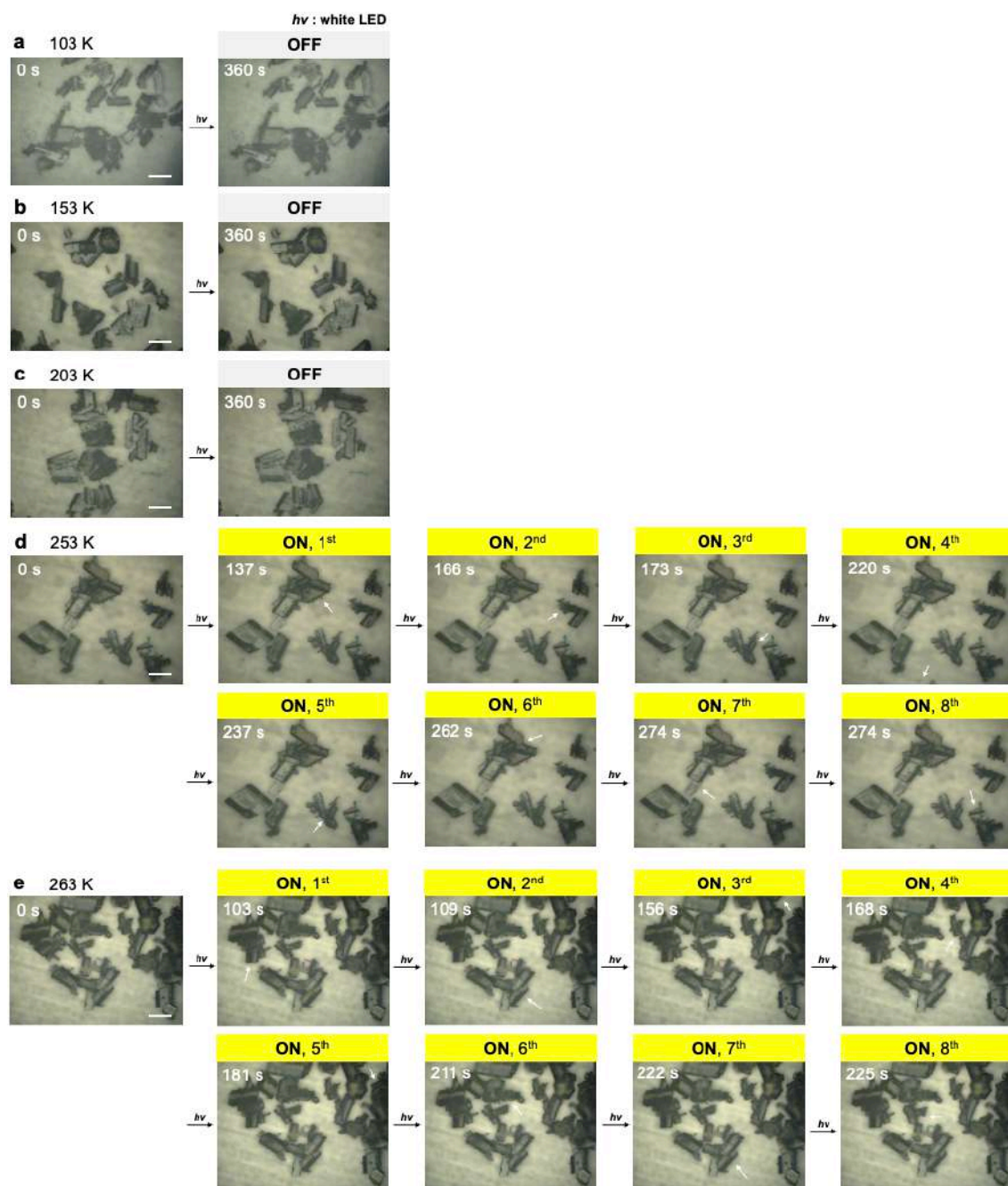
The structures are overlaid to highlight temperature-dependent changes in molecular packing and unit cells.

6.2 Temperature-dependent photoinduced crystal dynamics



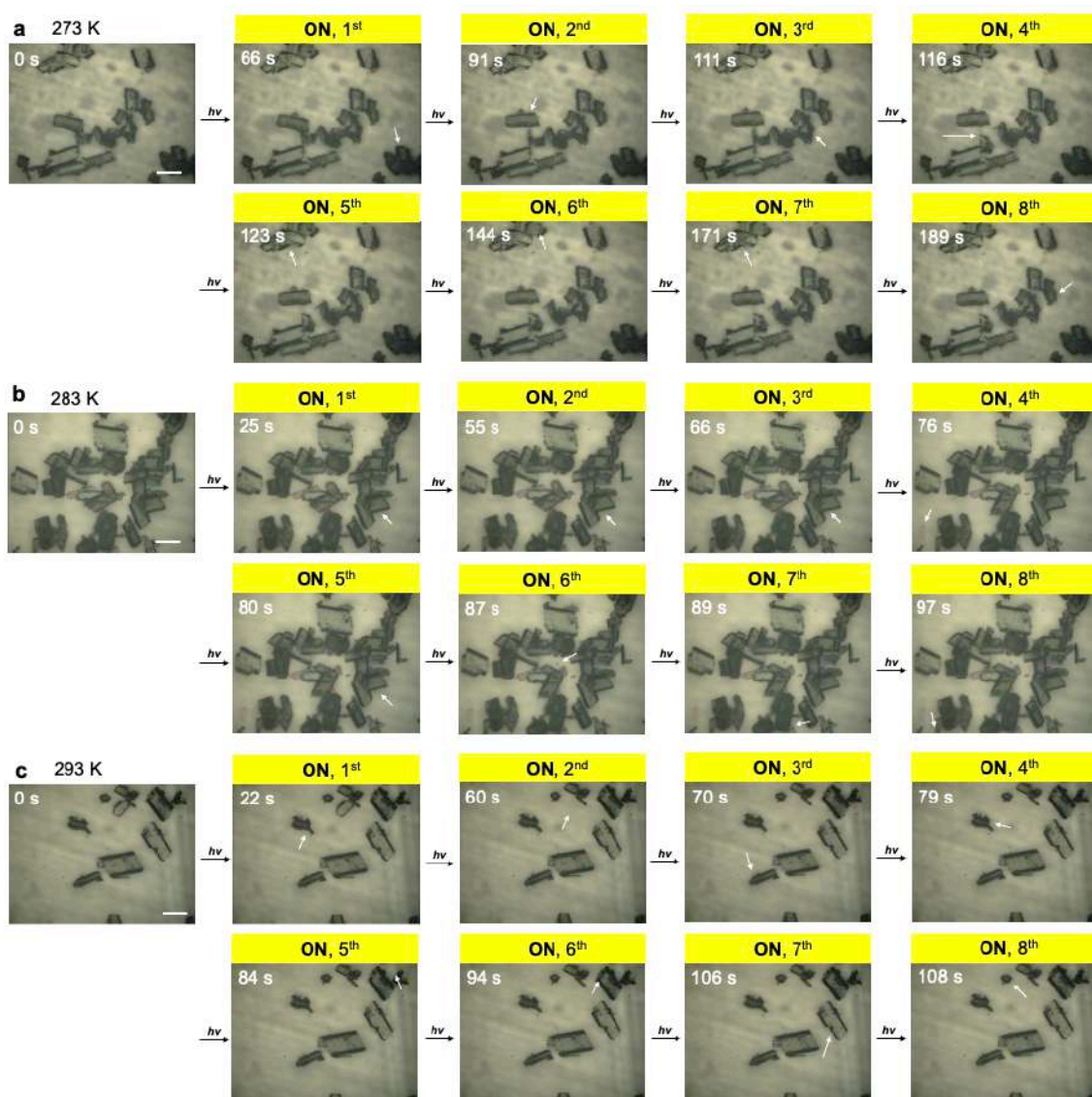
Supplementary Fig. 31. Thermal control system for observing crystal dynamics.

Experimental setup for observing photoinduced crystal dynamics at 103–353 K under white LED irradiation. **a**, Overall view of the observation system. **b**, Crystals placed on the heating/cooling stage.



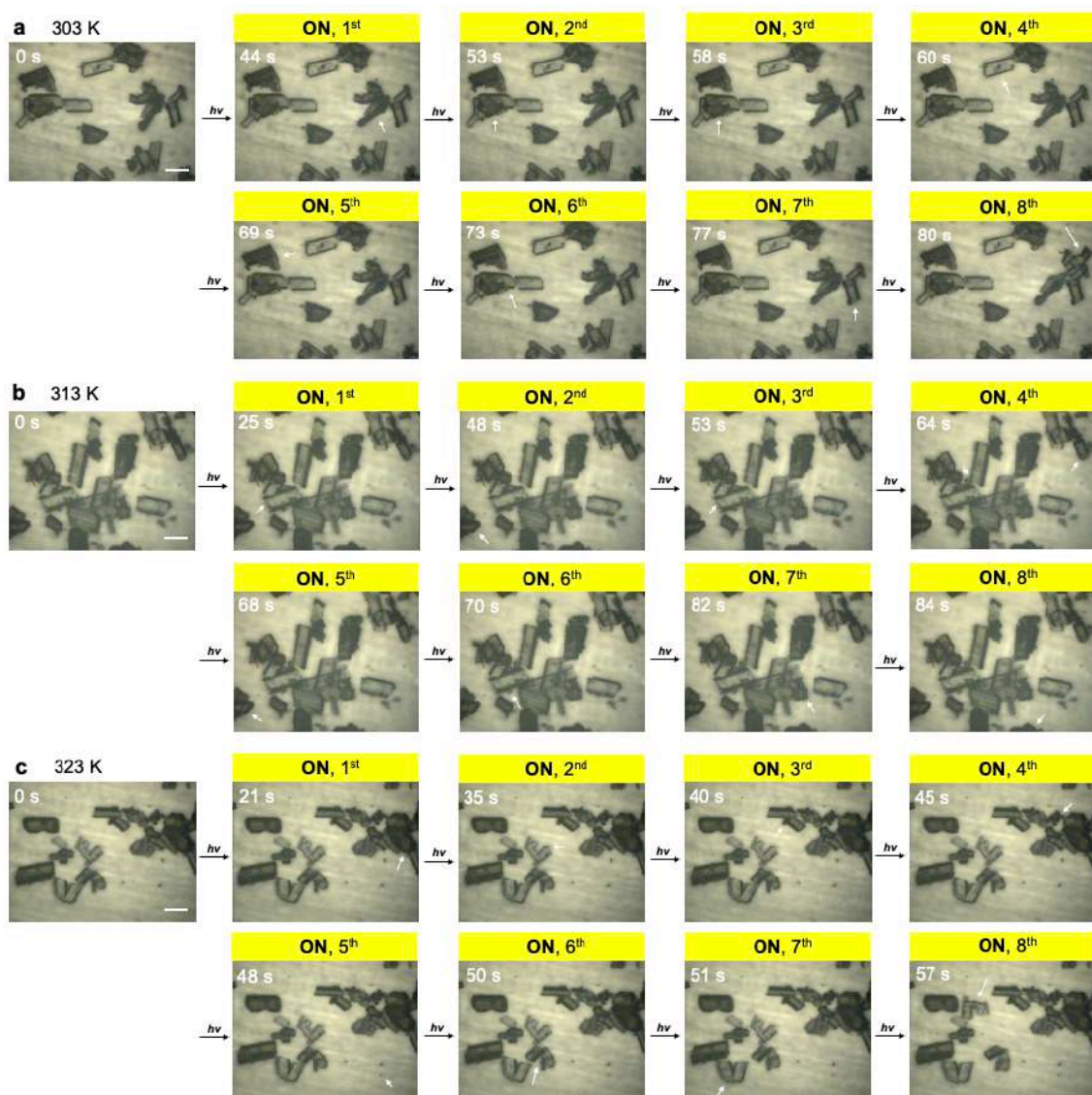
Supplementary Fig. 32. Thermal control of photoinduced crystal dynamics.

Photoinduced crystal dynamics at 103–263 K under white LED irradiation: **a**, 103 K, **b**, 153 K, **c**, 203 K, **d**, 253 K, and **e**, 263 K. White arrows indicate the locations where the mechanical response was observed. Scale bar, 200 μm .



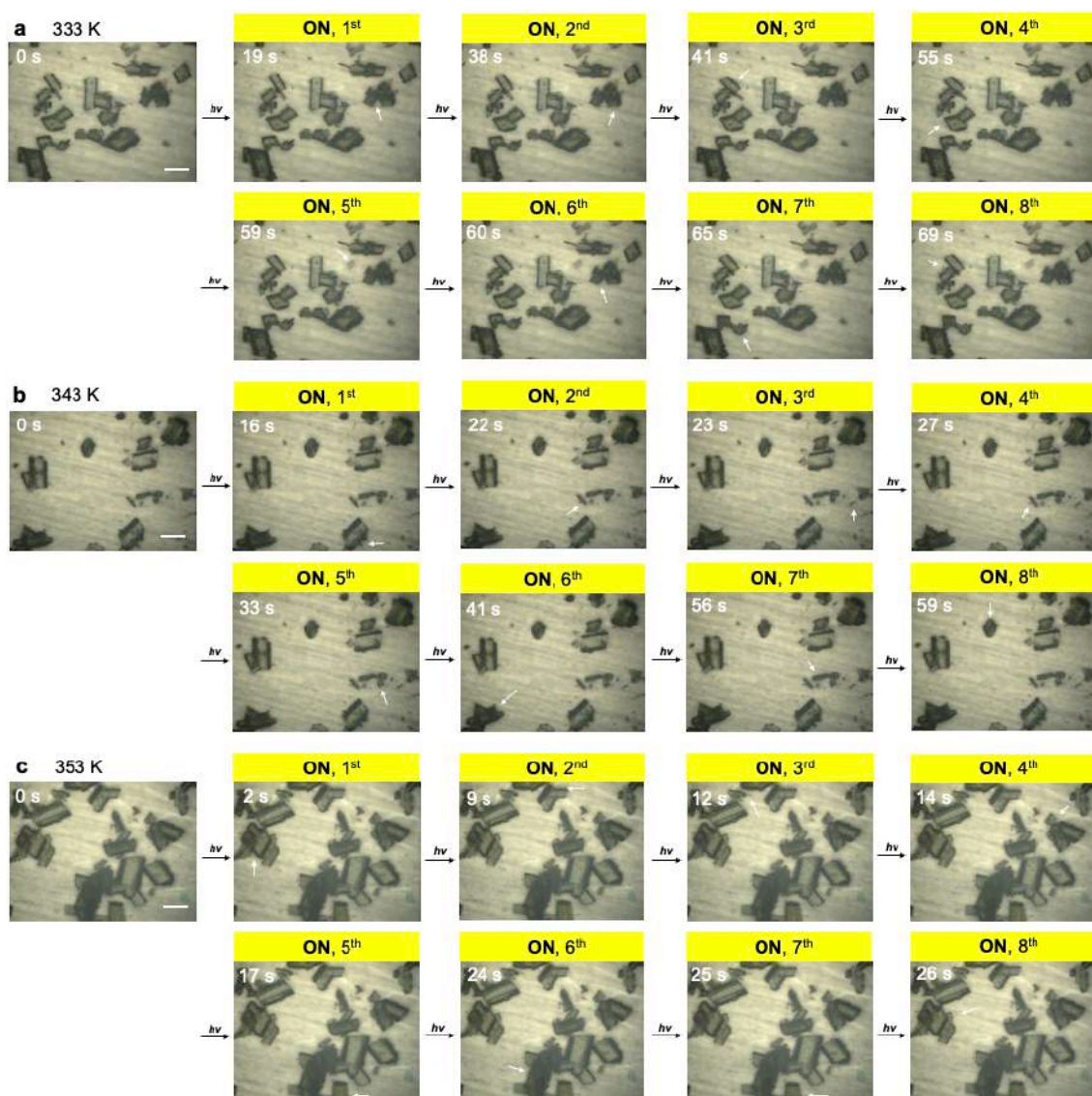
Supplementary Fig. 33. Thermal control of photoinduced crystal dynamics.

Photoinduced crystal dynamics at 273–293 K under white LED irradiation: **a**, 273 K, **b**, 283 K, and **c**, 293 K. White arrows indicate the locations where the mechanical response was observed. Scale bar, 200 μm .



Supplementary Fig. 34. Thermal control of photoinduced crystal dynamics.

Photoinduced crystal dynamics at 303–323 K under white LED irradiation: **a**, 303 K, **b**, 313 K, and **c**, 323 K. White arrows indicate the locations where the mechanical response was observed. Scale bar, 200 μm .

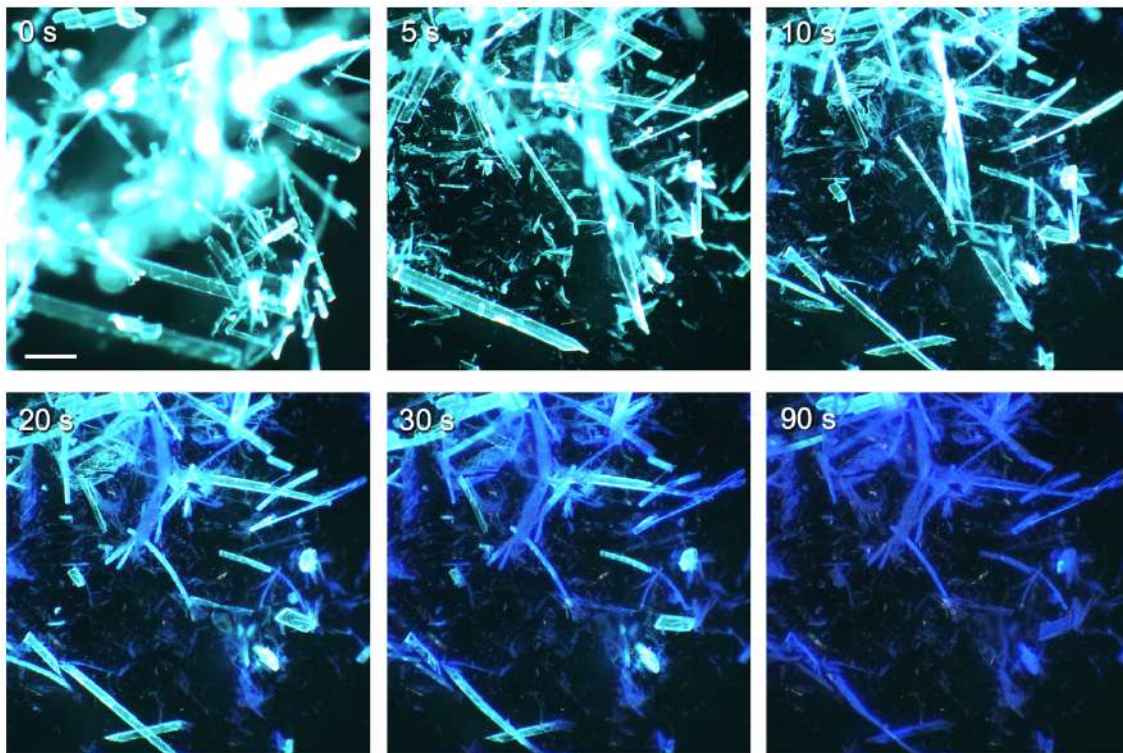


Supplementary Fig. 35. Thermal control of photoinduced crystal dynamics.

Photoinduced crystal dynamics at 333–353 K under white LED irradiation: **a**, 333 K, **b**, 343 K, and **c**, 353 K. White arrows indicate the locations where the mechanical response was observed. Scale bar, 200 μm .

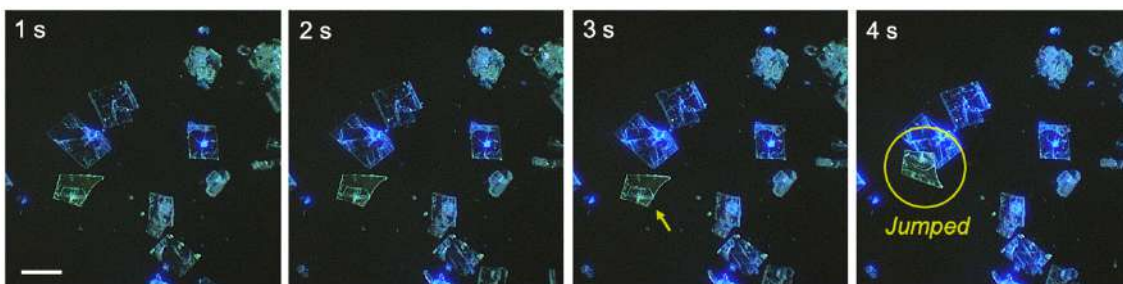
7. Photophysical control of crystal dynamics

7.1 Photophysical-parameter-dependent crystal dynamics



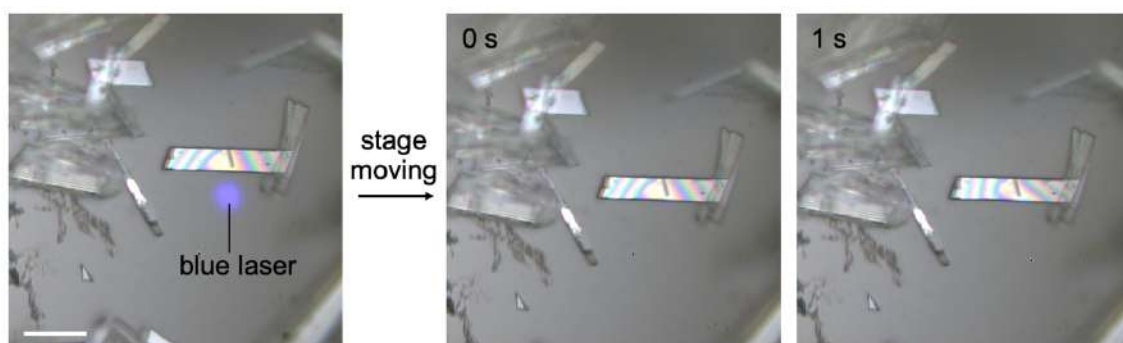
Supplementary Fig. 36. UV-light-induced crystal dynamics.

Optical microscopy images of crystals **1** under UV irradiation at 298 ± 5 K. Scale bar, 300 μm .



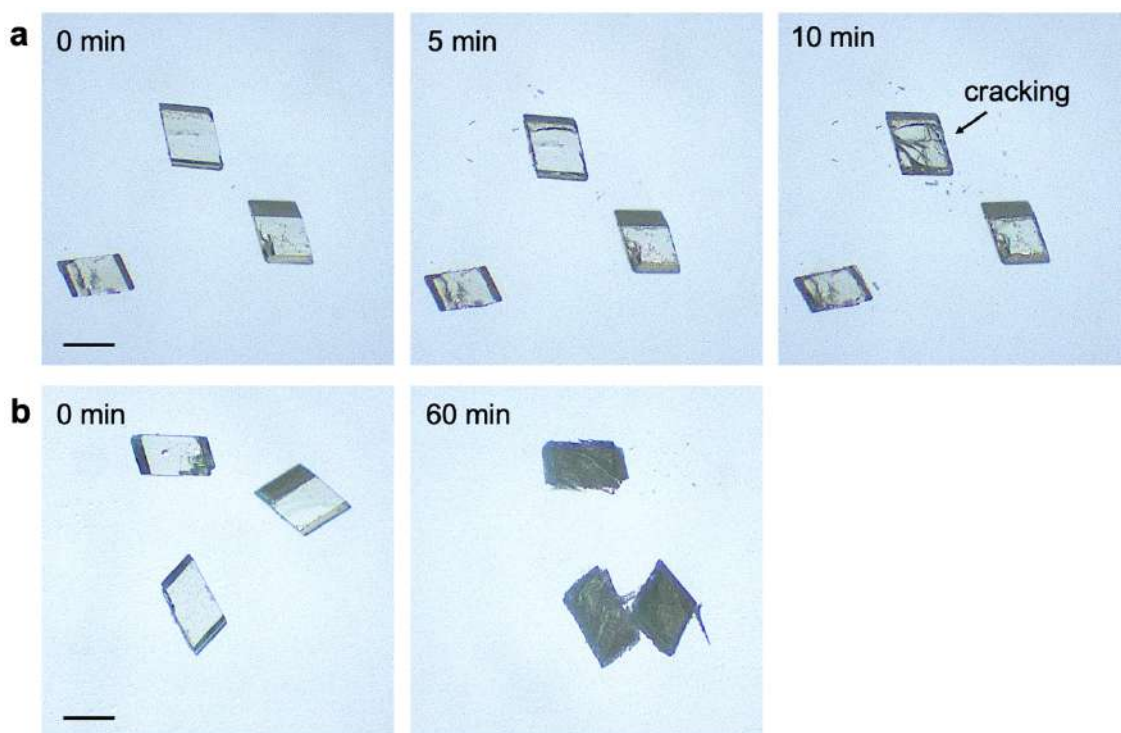
Supplementary Fig. 37. UV-light-induced crystal jumping.

Optical microscopy images of crystals **1** under UV irradiation at 298 ± 5 K. Scale bar, 300 μm .



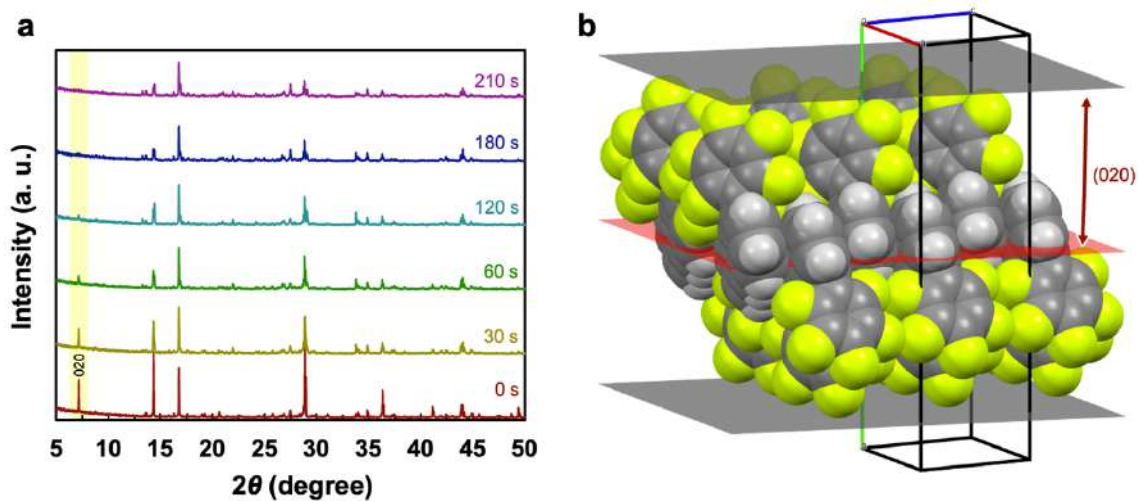
Supplementary Fig. 38. Remote control of crystal dynamics using a blue laser.

Optical microscopy images of crystals **1** under blue laser irradiation at 298 ± 5 K. Blue laser exposure of a chosen crystal resulted in modified interference fringes. Scale bar, 20 μm .



Supplementary Fig. 39. Sunlight-induced cracking of the crystal.

Optical microscopy images of crystals **1** under sunlight at 298 ± 5 K: **a**, 0 min–10 min and **b**, 0 min–60 min. Sunlight exposure led to cracking of the crystals. Scale bar, 20 μm .

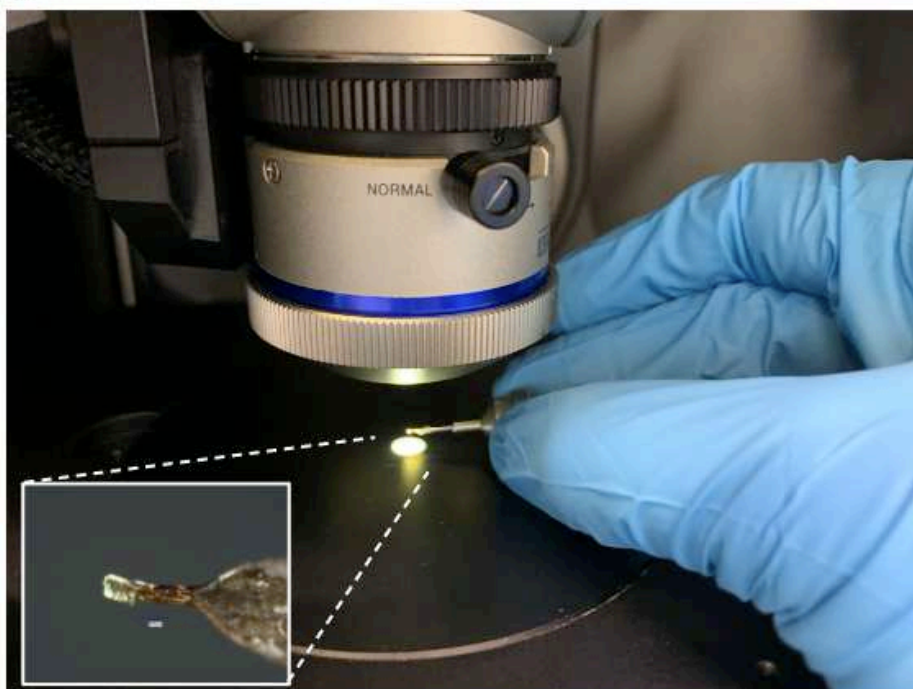


Supplementary Fig. 40. Time-resolved X-ray diffraction of photodimerization under UV irradiation.

a, The initial pattern at 0 s corresponds to crystal **1**, with the peak at $2\theta = 7.2^\circ$ indexed as {020}. **b**, Crystal structure of **1**. The molecular packing is illustrated, with the interplanar spacing of the (020) reflection ($2\theta = 7.2^\circ$) marked.

7.2 X-Ray crystallographic observation of intermediate states

a



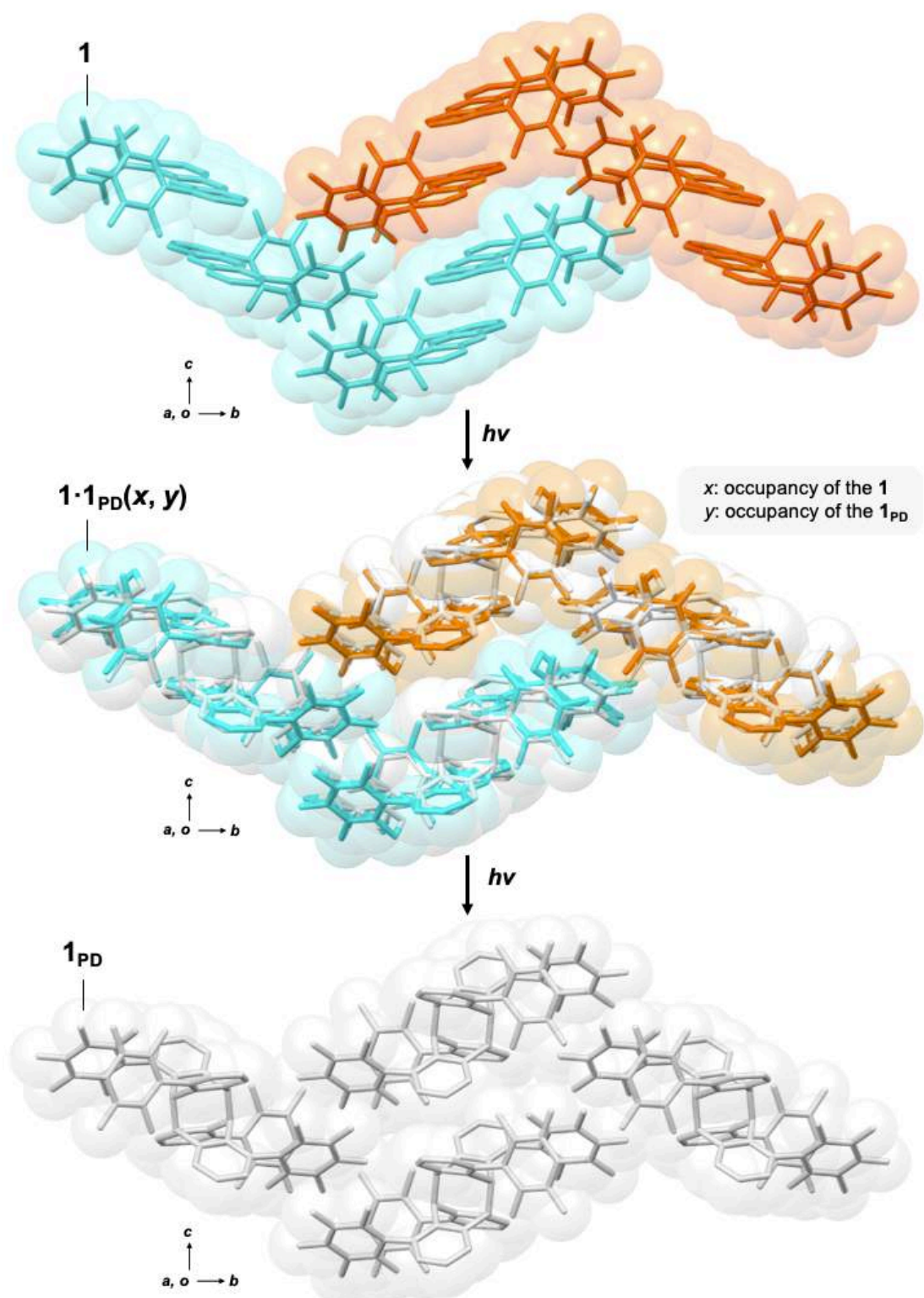
b

Blackout curtains for shading



Supplementary Fig. 41. Direct observation of intermediate states.

Experimental setup for capturing intermediate states during structural transitions under white LED irradiation. **a**, A white LED was used to irradiate the sample while crystal **1** was rotated 360 degrees. **b**, SCXRD measurements were conducted in a darkened room.



Supplementary Fig. 42. Nano-to-mesoscale observation of dynamics processes.

Crystal structures of **1**, **1·1_{PD}(x, y)**, and **1_{PD}**, shown as capped-sticks and space-filling models. Hydrogen atom is omitted. **1**, Blue and orange; **1_{PD}**, white.

Supplementary Table 18. Crystal Data and Structural Refinement for the **1**

Identification code	exp_346	
CCDC deposit number	2456869	
Empirical formula	C ₂₆ H ₈ F ₁₀	
Formula weight	510.32	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.5021(4) Å	<i>α</i> = 90°
	<i>b</i> = 24.5534(7) Å	<i>β</i> = 108.391(4)°
	<i>c</i> = 7.8616(3) Å	<i>γ</i> = 90°
Volume	1923.67(12) Å ³	
<i>Z</i>	4	
Density (calculated)	1.762 g/cm ³	
Absorption coefficient	0.170 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.309 × 0.262 × 0.153 mm ³	
2 θ range for data collection	4.412 to 52.734°	
Index ranges	-13 ≤ <i>h</i> ≤ 12, -30 ≤ <i>k</i> ≤ 30, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	12284	
Independent reflections	3929 [<i>R</i> (int) = 0.0497]	
Data / restraints / parameters	3929 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.070	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0391, <i>wR</i> ₂ = 0.0985	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0486, <i>wR</i> ₂ = 0.1050	
Largest diff. peak and hole	0.29/-0.22 e.Å ⁻³	

Supplementary Table 19. Crystal Data and Structural Refinement for the **1·1_{PD}(0.861, 0.139)**

Identification code	exp_347	
CCDC deposit number	2456870	
Empirical formula	C ₂₆ H ₈ F ₁₀	
Formula weight	510.32	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.4714(4) Å	<i>α</i> = 90°
	<i>b</i> = 24.5654(7) Å	<i>β</i> = 107.629(4)°
	<i>c</i> = 7.8582(3) Å	<i>γ</i> = 90°
Volume	1926.47(12) Å ³	
<i>Z</i>	4	
Density (calculated)	1.760 g/cm ³	
Absorption coefficient	0.170 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.284 × 0.162 × 0.131 mm ³	
2 θ range for data collection	4.406 to 60.364°	
Index ranges	-12 ≤ <i>h</i> ≤ 13, -29 ≤ <i>k</i> ≤ 32, -8 ≤ <i>l</i> ≤ 9	
Reflections collected	13247	
Independent reflections	4591 [<i>R</i> (int) = 0.0297]	
Data / restraints / parameters	4591 / 102 / 650	
Goodness-of-fit on <i>F</i> ²	1.051	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0409, <i>wR</i> ₂ = 0.0948	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0598, <i>wR</i> ₂ = 0.1040	
Largest diff. peak and hole	0.44/-0.34 e.Å ⁻³	

A- and B-level alerts in the Checkcif file:

A-Level alerts

“The absolute value of parameter shift to su ratio > 0.20”

This alert is derived from the low quality of data due to the mixed crystal.

“Maximum Shift/Error 5.01 Why ?”

This alert is derived from photoproduct, which is slightly disordered.

“Atom C109 (Anion/Solvent) ADP max/min Ratio 7.3 prolat”

This alert is derived from photoproduct, which is slightly disordered.

B-Level alerts

“Poor Data / Parameter Ratio 7.06 Note”

This alert is derived from the low quality of data due to the mixed crystal.

“ADP of Atom F101, Atom F102, Atom C101, Atom C102, Atom C106, Atom C112, Atom C113, Atom C115, Atom C116, Atom C117, Atom C118, Atom C119, and Atom C120 are N.P.D. or (nearly) 2D .”

These alerts are derived from photoproduct, which is slightly disordered.

“Atom C114 and Atom C123 (Anion/Solvent) ADP max/min Ratio”

These alerts are derived from photoproduct, which is slightly disordered.

“Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range 10.0 Ratio 5.4 prolat”

These alerts are derived from photoproduct, which is slightly disordered.

Nota on the structure refinement:

1,8-bis(pentafluorophenyl)anthracene photodimer may be present, but it could not be definitively assigned due to either low occupancy.

Supplementary Table 20. Crystal Data and Structural Refinement for the **1·1_{PD}(0.736, 0.264)**

Identification code	exp_348	
CCDC deposit number	2456871	
Empirical formula	C ₂₆ H ₈ F ₁₀	
Formula weight	510.32	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.4329(7) Å	<i>α</i> = 90°
	<i>b</i> = 24.6081(11) Å	<i>β</i> = 106.521(7)°
	<i>c</i> = 7.8634(5) Å	<i>γ</i> = 90°
Volume	1935.5(2) Å ³	
<i>Z</i>	4	
Density (calculated)	1.751 g/cm ³	
Absorption coefficient	0.169 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.278 × 0.202 × 0.147 mm ³	
2 θ range for data collection	4.072 to 60.244°	
Index ranges	-13 ≤ <i>h</i> ≤ 12, -27 ≤ <i>k</i> ≤ 32, -11 ≤ <i>l</i> ≤ 9	
Reflections collected	16246	
Independent reflections	4900 [<i>R</i> (int) = 0.0338]	
Data / restraints / parameters	4690 / 102 / 650	
Goodness-of-fit on <i>F</i> ²	1.041	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0496, <i>wR</i> ₂ = 0.1278	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0811, <i>wR</i> ₂ = 0.1460	
Largest diff. peak and hole	0.20/-0.21 e.Å ⁻³	

A- and B-level alerts in the Checkcif file:

(There is no A-level alerts)

B-Level alerts

“Poor Data / Parameter Ratio 7.22 Note”

This alert is derived from the low quality of data due to the mixed crystal.

“Atom C117 (Anion/Solvent) ADP max/min Ratio 5.9 prolat”

This alert is derived from photoproduct, which is slightly disordered.

Supplementary Table 21. Crystal Data and Structural Refinement for the **1·1_{PD}(0.633, 0.367)**

Identification code	exp_349	
CCDC deposit number	2456872	
Empirical formula	C ₂₆ H ₈ F ₁₀	
Formula weight	510.32	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.3382(18) Å	<i>α</i> = 90°
	<i>b</i> = 24.587(2) Å	<i>β</i> = 104.463(19)°
	<i>c</i> = 7.8557(16) Å	<i>γ</i> = 90°
Volume	1933.5(6) Å ³	
<i>Z</i>	4	
Density (calculated)	1.753 g/cm ³	
Absorption coefficient	0.169 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.28 × 0.197 × 0.158 mm ³	
2 θ range for data collection	4.394 to 60.252°	
Index ranges	-12 ≤ <i>h</i> ≤ 12, -33 ≤ <i>k</i> ≤ 32, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	15766	
Independent reflections	4623 [<i>R</i> (int) = 0.0748]	
Data / restraints / parameters	4623 / 102 / 650	
Goodness-of-fit on <i>F</i> ²	1.047	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0735, <i>wR</i> ₂ = 0.1975	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1426, <i>wR</i> ₂ = 0.2393	
Largest diff. peak and hole	0.22/-0.22 e.Å ⁻³	

A- and B-level alerts in the Checkcif file:

(There is no A-level alerts)

B-Level alerts

“Poor Data / Parameter Ratio 7.11 Note”

This alert is derived from the low quality of data due to the mixed crystal.

Supplementary Table 22. Crystal Data and Structural Refinement for the **1·1_{PD}(0.493, 0.507)**

Identification code	exp_350	
CCDC deposit number	2456873	
Empirical formula	C ₅₂ H ₁₆ F ₂₀	
Formula weight	1020.65	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.2366(12) Å	<i>α</i> = 90°
	<i>b</i> = 24.5406(17) Å	<i>β</i> = 101.428(13)°
	<i>c</i> = 7.8620(12) Å	<i>γ</i> = 90°
Volume	1935.9(4) Å ³	
<i>Z</i>	2	
Density (calculated)	1.751 g/cm ³	
Absorption coefficient	0.169 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.323 × 0.195 × 0.144 mm ³	
2 θ range for data collection	4.386 to 52.744°	
Index ranges	-12 ≤ <i>h</i> ≤ 10, -30 ≤ <i>k</i> ≤ 30, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	12502	
Independent reflections	3949 [<i>R</i> (int) = 0.0391]	
Data / restraints / parameters	3949 / 102 / 650	
Goodness-of-fit on <i>F</i> ²	1.070	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0641, <i>wR</i> ₂ = 0.1281	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1076, <i>wR</i> ₂ = 0.1515	
Largest diff. peak and hole	0.18/-0.19 e.Å ⁻³	

A- and B-level alerts in the Checkcif file:

(There is no A-level alerts)

B-Level alerts

“Poor Data / Parameter Ratio 6.08 Note”

This alert is derived from the low quality of data due to the mixed crystal.

“Atom C20 has ADP max/min Ratio 4.8 oblate”

This alert is derived from photoreactant, which is highly disordered.

Supplementary Table 23. Crystal Data and Structural Refinement for the **1·1_{PD}(0.359, 0.641)**

Identification code	exp_351	
CCDC deposit number	2456874	
Empirical formula	C ₅₂ H ₁₆ F ₂₀	
Formula weight	1020.65	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.1635(9) Å	<i>α</i> = 90°
	<i>b</i> = 24.5361(13) Å	<i>β</i> = 99.624(8)°
	<i>c</i> = 7.8585(7) Å	<i>γ</i> = 90°
Volume	1932.1(3) Å ³	
<i>Z</i>	2	
Density (calculated)	1.754 g/cm ³	
Absorption coefficient	0.170 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.282 × 0.188 × 0.14 mm ³	
2 θ range for data collection	4.064 to 52.74°	
Index ranges	-12 ≤ <i>h</i> ≤ 10, -30 ≤ <i>k</i> ≤ 28, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	12307	
Independent reflections	3940 [<i>R</i> (int) = 0.0406]	
Data / restraints / parameters	3940 / 102 / 650	
Goodness-of-fit on <i>F</i> ²	1.067	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0567, <i>wR</i> ₂ = 0.1366	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0903, <i>wR</i> ₂ = 0.1570	
Largest diff. peak and hole	0.21/-0.23 e.Å ⁻³	

A- and B-level alerts in the Checkcif file:

(There is no A-level alerts)

B-Level alerts

“Poor Data / Parameter Ratio 6.06 Note”

This alert is derived from the low quality of data due to the mixed crystal.

“Atom C121 and Atom C123 has ADP max/min Ratio ”

These alerts are derived from photoreactant, which is highly disordered.

Supplementary Table 24. Crystal Data and Structural Refinement for the **1·1_{PD}(0.230, 0.770)**

Identification code	exp_353	
CCDC deposit number	2456875	
Empirical formula	C ₅₂ H ₁₆ F ₂₀	
Formula weight	1020.65	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.1108(5) Å	<i>α</i> = 90°
	<i>b</i> = 24.5235(9) Å	<i>β</i> = 98.557(5)°
	<i>c</i> = 7.8720(4) Å	<i>γ</i> = 90°
Volume	1930.15(16) Å ³	
<i>Z</i>	2	
Density (calculated)	1.756 g/cm ³	
Absorption coefficient	0.170 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.304 × 0.192 × 0.152 mm ³	
2 θ range for data collection	3.322 to 60.294°	
Index ranges	-12 ≤ <i>h</i> ≤ 10, -34 ≤ <i>k</i> ≤ 32, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	13540	
Independent reflections	4599 [<i>R</i> (int) = 0.0301]	
Data / restraints / parameters	4599 / 102 / 650	
Goodness-of-fit on <i>F</i> ²	1.040	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0455, <i>wR</i> ₂ = 0.1109	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0659, <i>wR</i> ₂ = 0.1243	
Largest diff. peak and hole	0.22/-0.35 e.Å ⁻³	

A- and B-level alerts in the Checkcif file:

A-Level alerts

“The absolute value of parameter shift to su ratio > 0.20 ”

This alert is derived from the low quality of data due to the mixed crystal.

“Maximum Shift/Error 2.42 Why ?”

This alert is derived from photoreactant, which is highly disordered.

B-Level alerts

“Poor Data / Parameter Ratio 7.08 Note”

This alert is derived from the low quality of data due to the mixed crystal.

“ADP of Atom C121, Atom C123, and Atom C126 are N.P.D. or (nearly) 2D.”

These alerts are derived from photoreactant, which is highly disordered.

“Atom C108 (Anion/Solvent) ADP max/min Ratio 5.2 prolat”

This alert is derived from photoreactant, which is highly disordered.

Supplementary Table 25. Crystal Data and Structural Refinement for the **1·1_{PD}(0.155, 0.845)**

Identification code	exp_354	
CCDC deposit number	2456876	
Empirical formula	C ₅₂ H ₁₆ F ₂₀	
Formula weight	1020.65	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.0742(4) Å	<i>α</i> = 90°
	<i>b</i> = 24.5203(7) Å	<i>β</i> = 97.881(3)°
	<i>c</i> = 7.8996(3) Å	<i>γ</i> = 90°
Volume	1932.95(12) Å ³	
<i>Z</i>	2	
Density (calculated)	1.754 g/cm ³	
Absorption coefficient	0.169 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.342 × 0.209 × 0.135 mm ³	
2 θ range for data collection	3.322 to 52.742°	
Index ranges	-12 ≤ <i>h</i> ≤ 9, -30 ≤ <i>k</i> ≤ 25, -9 ≤ <i>l</i> ≤ 8	
Reflections collected	13491	
Independent reflections	3939 [<i>R</i> (int) = 0.0283]	
Data / restraints / parameters	3939 / 102 / 650	
Goodness-of-fit on <i>F</i> ²	1.041	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0378, <i>wR</i> ₂ = 0.0920	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0504, <i>wR</i> ₂ = 0.0999	
Largest diff. peak and hole	0.29/-0.31 e.Å ⁻³	

A- and B-level alerts in the Checkcif file:

A-Level alerts

“The absolute value of parameter shift to su ratio > 0.20”

This alert is derived from the low quality of data due to the mixed crystal.

“Maximum Shift/Error 3.11 Why ?”

This alert is derived from photoreactant, which is highly disordered.

“Atom C105 and Atom C118 (Anion/Solvent) ADP max/min Ratio 5.2 prolat”

These alerts are derived from photoreactant, which is highly disordered.

B-Level alerts

“Poor Data / Parameter Ratio 6.06 Note”

This alert is derived from the low quality of data due to the mixed crystal.

“ADP of Atom F107, Atom C101, Atom C115, Atom C116, Atom C117, Atom C119, Atom C123 and Atom C124 are N.P.D. or (nearly) 2D.”

These alerts are derived from photoreactant, which is highly disordered.

“Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range 10.0 Ratio”

This alert is derived from photoreactant, which is highly disordered.

Nota on the structure refinement:

1,8-bis(pentafluorophenyl)anthracene may be present, but it could not be definitively assigned due to either low occupancy.

Supplementary Table 26. Crystal Data and Structural Refinement for the **1·1_{PD}(0.128, 0.872)**

Identification code	exp_355	
CCDC deposit number	2456877	
Empirical formula	C ₅₂ H ₁₆ F ₂₀	
Formula weight	1020.65	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.0528(4) Å	<i>α</i> = 90°
	<i>b</i> = 24.5186(7) Å	<i>β</i> = 97.513(4)°
	<i>c</i> = 7.9026(3) Å	<i>γ</i> = 90°
Volume	1931.12(12) Å ³	
<i>Z</i>	2	
Density (calculated)	1.755 g/cm ³	
Absorption coefficient	0.170 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.318 × 0.189 × 0.149 mm ³	
2 θ range for data collection	4.412 to 52.742°	
Index ranges	-12 ≤ <i>h</i> ≤ 10, -30 ≤ <i>k</i> ≤ 30, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	12697	
Independent reflections	3929 [<i>R</i> (int) = 0.0287]	
Data / restraints / parameters	3929 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.097	
Final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0625, <i>wR</i> ₂ = 0.1617	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0768, <i>wR</i> ₂ = 0.1730	
Largest diff. peak and hole	1.13/-0.46 e.Å ⁻³	

A- and B-level alerts in the Checkcif file:

(There is no A-level alerts)

B-Level alerts

“Large Reported Max. (Positive) Residual Density 1.13 eA-3”

This alert is derived from photoreactant, which is slightly disordered.

Nota on the structure refinement:

1,8-bis(pentafluorophenyl)anthracene may be present, but it could not be definitively assigned due to either low occupancy.

Supplementary Table 27. Crystal Data and Structural Refinement for the **1·1_{PD}(0.081, 0.919)**

Identification code	exp_356	
CCDC deposit number	2456878	
Empirical formula	C ₅₂ H ₁₆ F ₂₀	
Formula weight	1020.65	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 10.0271(4) Å	<i>α</i> = 90°
	<i>b</i> = 24.4615(7) Å	<i>β</i> = 97.376(3)°
	<i>c</i> = 7.9076(3) Å	<i>γ</i> = 90°
Volume	1923.51(12) Å ³	
<i>Z</i>	2	
Density (calculated)	1.762 g/cm ³	
Absorption coefficient	0.170 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.275 × 0.253 × 0.146 mm ³	
2 θ range for data collection	3.33 to 52.734°	
Index ranges	-9 ≤ <i>h</i> ≤ 12, -30 ≤ <i>k</i> ≤ 29, -6 ≤ <i>l</i> ≤ 9	
Reflections collected	12991	
Independent reflections	3924 [<i>R</i> (int) = 0.0282]	
Data / restraints / parameters	3924 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.069	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0534, <i>wR</i> ₂ = 0.1386	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0641, <i>wR</i> ₂ = 0.1465	
Largest diff. peak and hole	0.86/-0.46 e.Å ⁻³	

Supplementary Table 28. Crystal Data and Structural Refinement for the **1_{PD}**

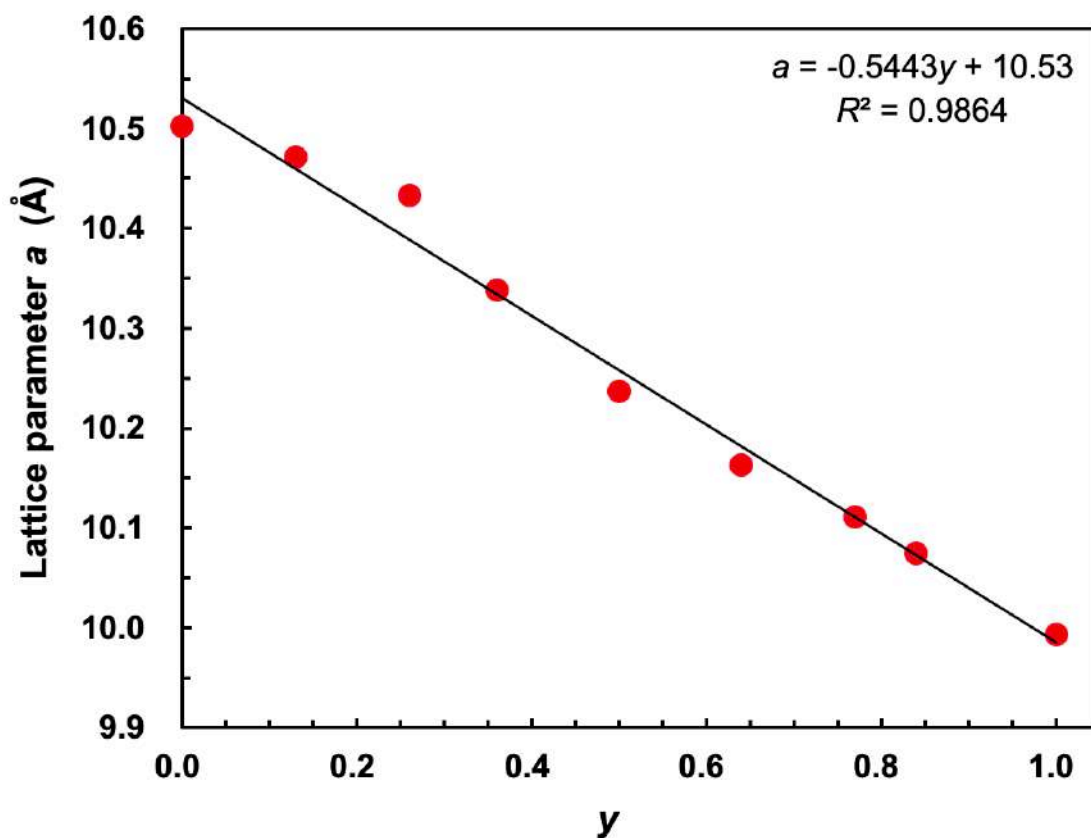
Identification code	exp_357	
CCDC deposit number	2456879	
Formula weight	C ₅₂ H ₁₆ F ₂₀	
Formula weight	1020.65	
Temperature	103.15	
Wavelength	0.71073 nm	
Crystal system	monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 9.9934(3) Å	$\alpha = 90^\circ$
	<i>b</i> = 24.4447(5) Å	$\beta = 97.139(3)^\circ$
	<i>c</i> = 7.9097(2) Å	$\gamma = 90^\circ$
Volume	1917.25(9) Å ³	
<i>Z</i>	2	
Density (calculated)	1.768 g/cm ³	
Absorption coefficient	0.171 mm ⁻¹	
<i>F</i> (000)	1016.0	
Crystal size	0.381 × 0.219 × 0.144 mm ³	
2 θ range for data collection	3.332 to 52.734°	
Index ranges	-12 ≤ <i>h</i> ≤ 11, -30 ≤ <i>k</i> ≤ 30, -9 ≤ <i>l</i> ≤ 8	
Reflections collected	13268	
Independent reflections	3914 [<i>R</i> (int) = 0.0289]	
Data / restraints / parameters	3914 / 0 / 325	
Goodness-of-fit on <i>F</i> ²	1.070	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0393, <i>wR</i> ₂ = 0.1000	
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0482, <i>wR</i> ₂ = 0.1061	
Largest diff. peak and hole	0.42/-0.27 e.Å ⁻³	

7.3 Estimation of the conversion ratio based on Vegard's law

Conversion ratios were estimated using Vegard's law.^{7,8} In this section, the non-stoichiometric $1 \cdot 1_{PD}(x, y)$ mixed crystal of the 1,8-bis(pentafluorophenyl)anthracene (**1**) and 1,8-bis(pentafluorophenyl)anthracene photodimer (**1_{PD}**) is modeled. The compositions of **1** and **1_{PD}** are denoted by x and y , respectively. The following relationship (Equation 1) holds between y and the lattice parameter a of $1 \cdot 1_{PD}(x, y)$.

$$a = ya_{1_{PD}} + (1 - y)a_1 \quad (1)$$

where $a_{1_{PD}}$ and a_1 are the equilibrium lattice parameters of the **1** and **1_{PD}**, respectively, and a is the lattice parameter of the $1 \cdot 1_{PD}(x, y)$.



Supplementary Fig. 43. Vegard's plot of the $1 \cdot 1_{PD}(x, y)$.

Linear fitting and R^2 for outputs versus lattice parameters are indicated.

Supplementary Table 29. Composition Date for the $1 \cdot 1_{PD}(x, y)$

Irradiation time / s	Lattice parameter a / Å	y	x
480	10.0528	0.872	0.128
540	10.0271	0.919	0.081

7.4 Photochemical reaction kinetics

Photochemical reaction in a single crystal was modeled using the Johnson–Mehl–Avrami–Kolmogorov (JMAK) equation (Equation (2a)).^{9,10}

$$y = 1 - e^{-(k't^n)} \quad (2a)$$

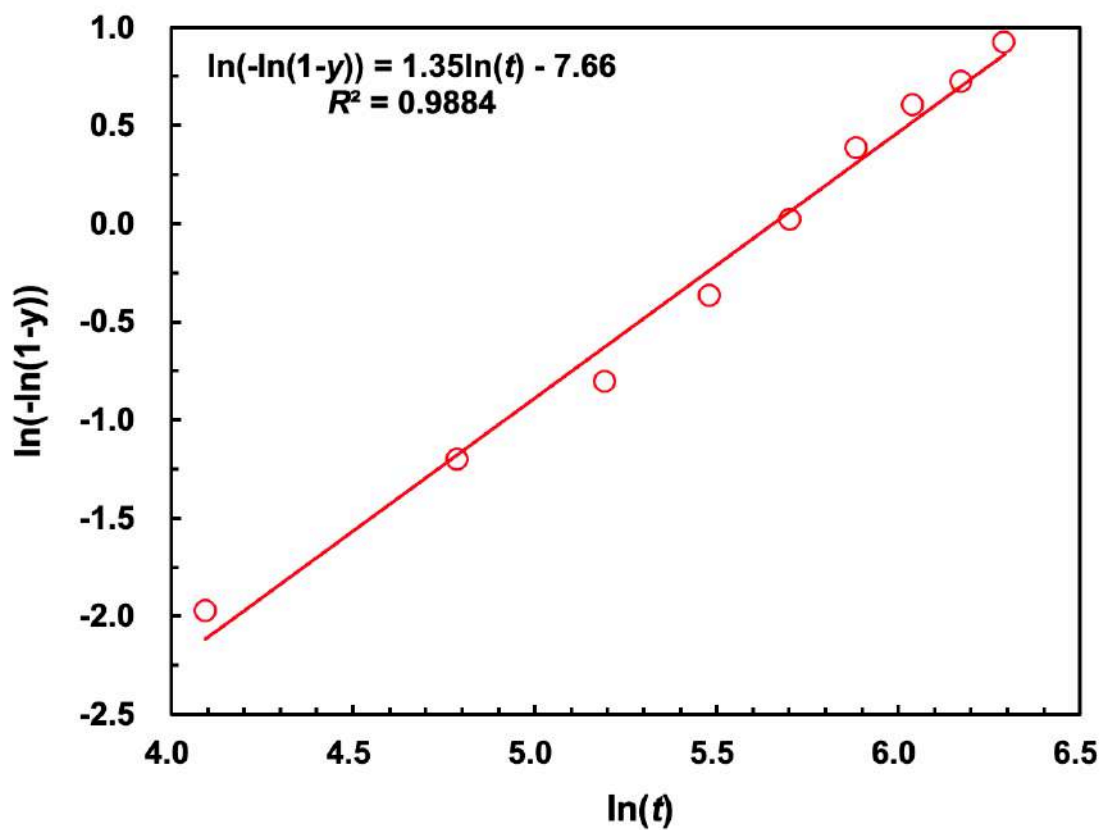
By substituting $k' = k^n$, Equation (2a) can be rewritten as Equation (2b).

$$y = 1 - e^{-(kt)^n} \quad (2b)$$

where y is the conversion ratio of **1_{PD}**, k and k' are the reaction rate constant, t is the irradiation time, and n is the Avrami exponent (reaction order). Furthermore, Equations (2a) and (2b) are derived from equations (2c) and (2d).

$$\ln(-\ln(1-y)) = n\ln(t) + \ln(k') \quad (2c)$$

$$\ln(-\ln(1-y)) = n\ln(t) + n\ln(k) \quad (2d)$$



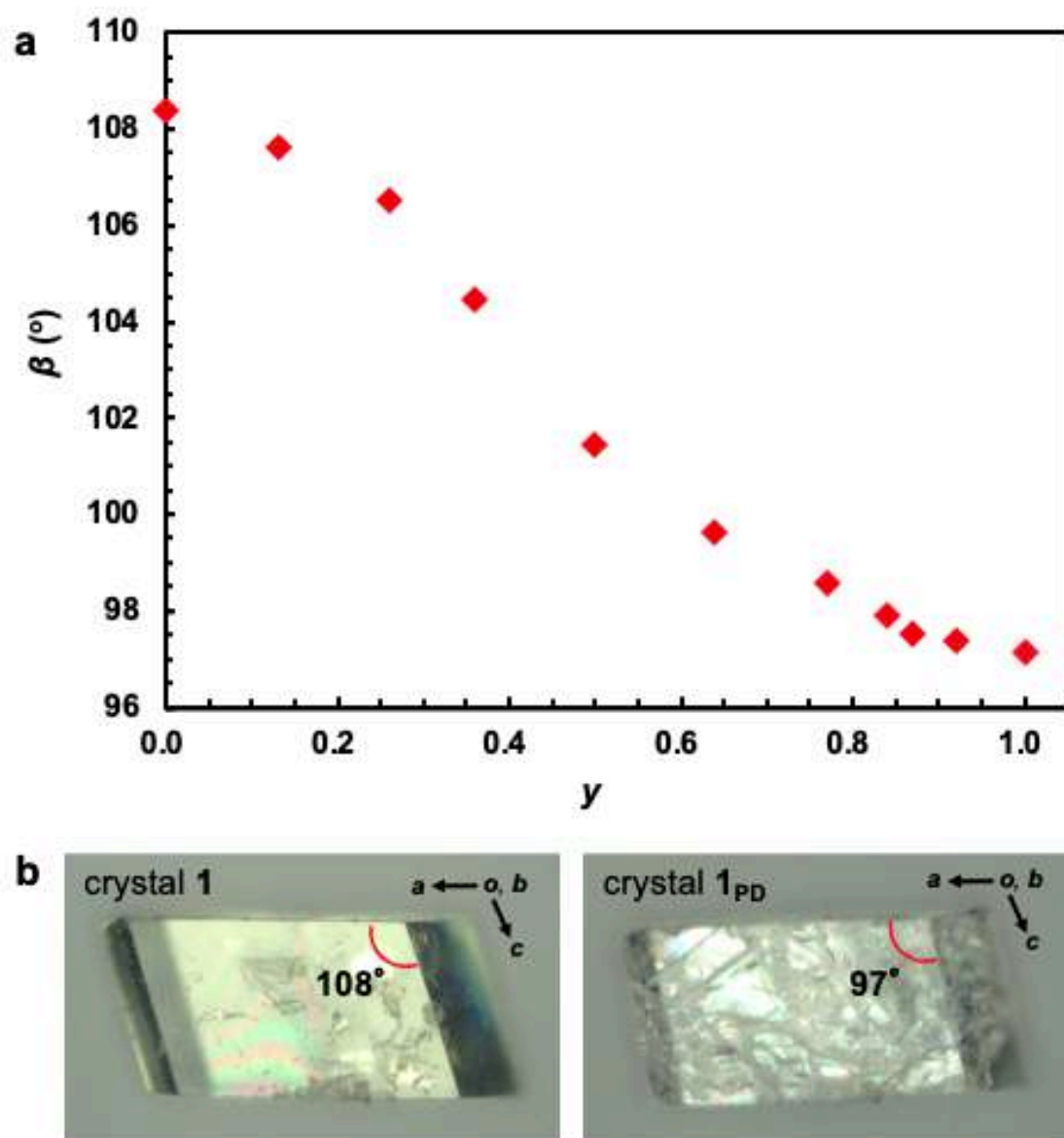
Supplementary Fig. 44. Avrami plot for photochemical reaction kinetics.

Linear fitting and R^2 are indicated.

Supplementary Table 30. Reaction Rate Constants and Avrami Exponent

k' / s^{-n}	k / s^{-1}	n
4.7×10^{-4}	3.5×10^{-3}	1.35

7.5 Relationship between conversion ratio and lattice strain

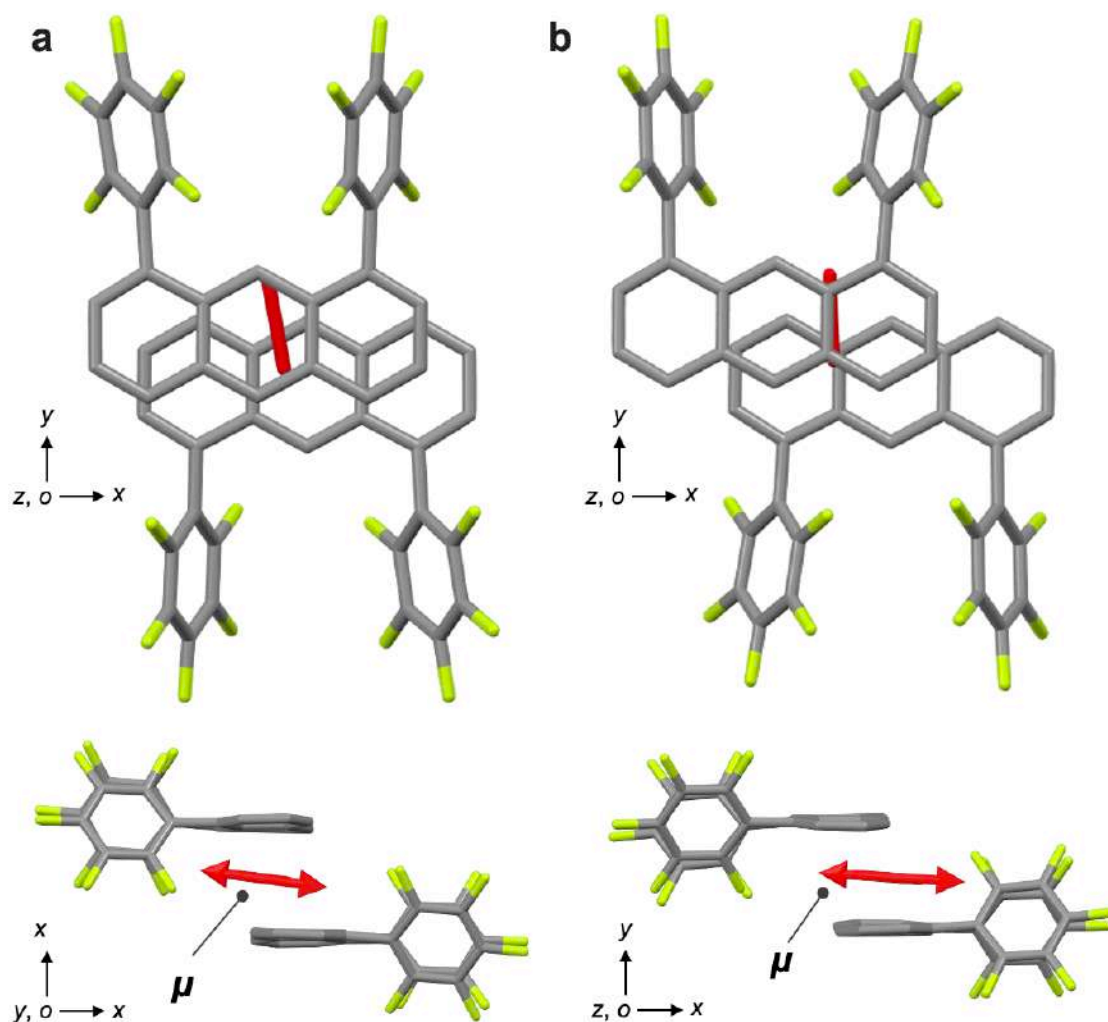


Supplementary Fig. 45. Change in lattice and crystal morphology.

a, Relationship between y and β . **b**, Crystal morphology of the crystals **1** and **1_{PD}**.

8. Anisotropic crystal dynamics

8.1 Excited-state characterization of 1 using TD-DFT



Supplementary Fig. 46. Transition dipole moment analysis of 1.

TD-DFT calculation of the ground-to-excited-state transition ($S_0 \rightarrow S_2$) of **a**, Unit 1 and **b**, Unit 2. Transition dipole moments (μ) of Orientation of the μ along the short axis of anthracene in both Unit 1 and Unit 2. μ , red.

Supplementary Table 31. Ground-to-Excited-State μ of Unit 1

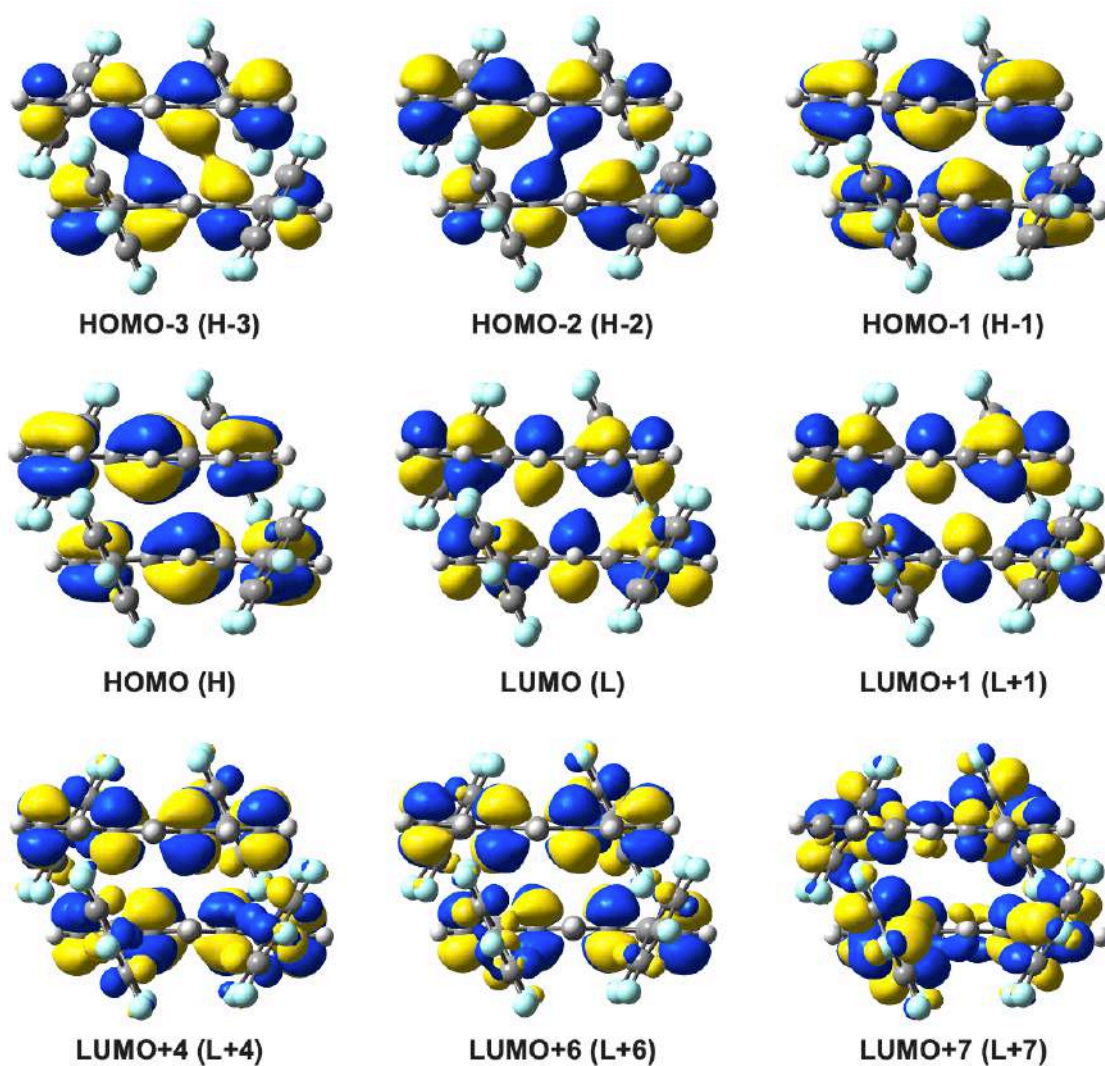
states	X	Y	Z	Dip. S.	Oci.
1	0.1071	0.0006	0.0283	0.0123	0.0011
2	-1.7375	-0.0018	-0.4460	3.2180	0.2800
3	0.0039	-0.0072	0.0027	0.0001	0.0000
4	-0.3608	-0.5152	-0.2220	0.4449	0.0419
5	-0.1046	0.0097	-0.0510	0.0136	0.0014
6	-0.0583	-0.0043	-0.0287	0.0042	0.0004

Supplementary Table 32. Ground-to-Excited-State μ of Unit 2

states	X	Y	Z	Dip. S.	Oci.
1	-0.0460	0.0134	-0.0101	0.0024	0.0002
2	-1.7048	-0.5065	-0.3625	3.2941	0.2878
3	0.3309	-0.0951	0.0025	0.1185	0.0115
4	-0.148	0.0087	-0.0009	0.0003	0.0000
5	-0.0063	-0.0158	-0.0004	0.0003	0.0000
6	-0.0876	-0.4191	0.00057	0.1834	0.0184

Supplementary Table 33. TD-DFT Vertical Excitation Energy and Oscillator Strength of Unit 1

Transition	Energy / eV	Wavelength / nm	Oci.	Contribution of Orbitals
$S_0 \rightarrow S_1$	3.5013	354.11	0.0011	H-1 $\rightarrow$ L (46.0%)
				H $\rightarrow$ L+1 (52.4%)
$S_0 \rightarrow S_2$	3.5520	349.05	0.2800	H-1 $\rightarrow$ L+1 (29.5%)
				H $\rightarrow$ L (67.8%)
$S_0 \rightarrow S_3$	3.8203	324.54	0.0000	H-3 $\rightarrow$ L (14.8%)
				H-2 $\rightarrow$ L+1 (14.7%)
				H-1 $\rightarrow$ L (48.5%)
				H $\rightarrow$ L+1 (42.9%)
$S_0 \rightarrow S_4$	3.8481	322.20	0.0419	H-3 $\rightarrow$ L+1 (13.3%)
				H-2 $\rightarrow$ L (15.3%)
				H-1 $\rightarrow$ L+1 (57.8%)
				H-1 $\rightarrow$ L+4 (14.6%)
				H $\rightarrow$ L (25.1%)
				H $\rightarrow$ L+6 (15.7%)
				H-3 $\rightarrow$ L (16.9%)
				H-3 $\rightarrow$ L+1 (25.3%)
$S_0 \rightarrow S_5$	4.1510	298.68	0.0014	H-2 $\rightarrow$ L (31.8%)
				H-2 $\rightarrow$ L+1 (15.9%)
				H-1 $\rightarrow$ L (10.7%)
				H-1 $\rightarrow$ L+1 (22.2%)
				H-1 $\rightarrow$ L+4 (21.1%)
				H-1 $\rightarrow$ L+6 (11.9%)
				H-1 $\rightarrow$ L+7 (10.5%)
				H $\rightarrow$ L (14.5%)
				H $\rightarrow$ L+4 (14.9%)
				H $\rightarrow$ L+6 (23.6%)
$S_0 \rightarrow S_6$	4.1529	298.55	0.0419	H-3 $\rightarrow$ L (28.3%)
				H-3 $\rightarrow$ L+1 (14.9%)
				H-2 $\rightarrow$ L (17.5%)
				H-2 $\rightarrow$ L+1 (29.9%)
				H-1 $\rightarrow$ L (17.4%)
				H-1 $\rightarrow$ L+1 (12.7%)
				H-1 $\rightarrow$ L+4 (12.7%)
				H-1 $\rightarrow$ L+6 (22.7%)
				H $\rightarrow$ L+1 (15.3%)
				H $\rightarrow$ L+4 (26.1%)
				H $\rightarrow$ L+6 (13.5%)

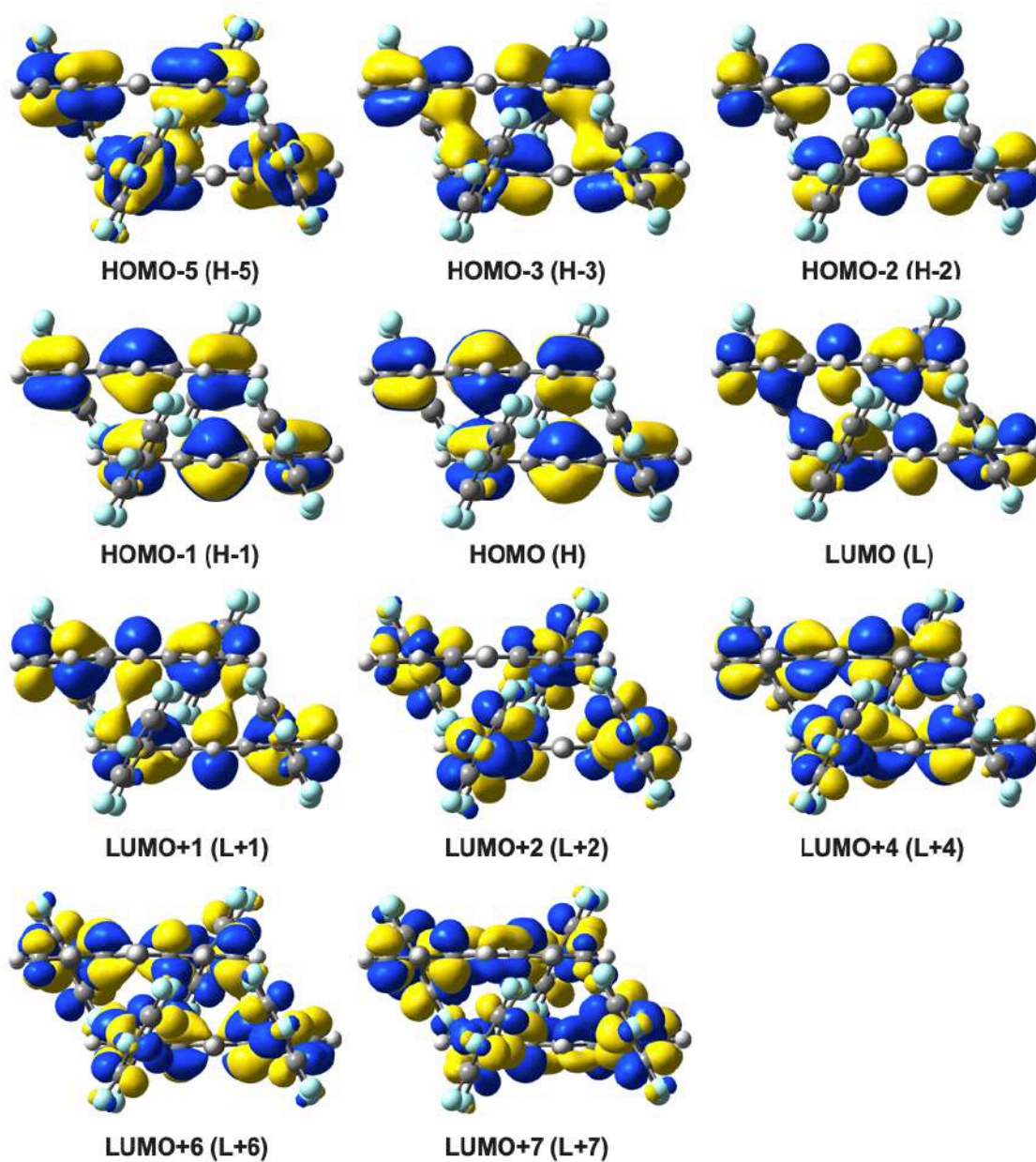


Supplementary Fig. 47. Kohn-Sham orbitals (isovalue = 0.02) of Unit 1 obtained from TD-DFT calculations.

The atomic coordinates were obtained from the crystal structure. Blue, positive lobes; yellow, negative lobes.

Supplementary Table 34. TD-DFT Vertical Excitation Energy and Oscillator Strength of Unit 2

Transition	Energy / eV	Wavelength / nm	Oci.	Contribution of Orbitals
$S_0 \rightarrow S_1$	3.5013	354.11	0.0011	H-1 $\rightarrow$ L+1 (27.1%) H $\rightarrow$ L (64.5%)
$S_0 \rightarrow S_2$	3.5520	349.05	0.2800	H-1 $\rightarrow$ L (56.3%) H $\rightarrow$ L (41.1%)
$S_0 \rightarrow S_3$	3.8203	324.54	0.0000	H-3 $\rightarrow$ L (14.8%) H-2 $\rightarrow$ L+1 (15.4%) H-1 $\rightarrow$ L (37.9%) H $\rightarrow$ L+1 (52.1%) H $\rightarrow$ L+6 (10.8%)
$S_0 \rightarrow S_4$	3.8481	322.20	0.0419	H-5 $\rightarrow$ L+1 (10.0%) H-3 $\rightarrow$ L+1 (17.8%) H-2 $\rightarrow$ L (41.7%) H-1 $\rightarrow$ L+1 (35.9%) H-1 $\rightarrow$ L+6 (18.0%) H-1 $\rightarrow$ L+7 (11.5%) H $\rightarrow$ L (12.8%) H $\rightarrow$ L+4 (22.3%)
$S_0 \rightarrow S_5$	4.1510	298.68	0.0014	H-3 $\rightarrow$ L+1 (14.8%) H-2 $\rightarrow$ L (28.0%) H-1 $\rightarrow$ L+1 (52.8%) H-1 $\rightarrow$ L+7 (10.5%) H $\rightarrow$ L (23.7%) H $\rightarrow$ L+4 (13.4%)
$S_0 \rightarrow S_6$	4.1529	298.55	0.0419	H-5 $\rightarrow$ L (13.4%) H-3 $\rightarrow$ L (25.0%) H-2 $\rightarrow$ L+1 (38.4%) H-1 $\rightarrow$ L (15.8%) H-1 $\rightarrow$ L+2 (10.7%) H-1 $\rightarrow$ L+4 (24.9%) H $\rightarrow$ L+1 (20.7%) H $\rightarrow$ L+6 (22.5%) H $\rightarrow$ L+7 (19.2%)



Supplementary Fig. 48. Kohn-Sham orbitals (isovalue = 0.02) of Unit 2 obtained from TD-DFT calculations.

The atomic coordinates were obtained from the crystal structure. Blue, positive lobes; yellow, negative lobes.

Supplementary Table 35. Atomic Coordinates of Unit 1

F	2.740849	-3.503867	1.593117
F	4.386158	-1.773138	-2.485254
F	5.129267	1.147793	-2.172047
F	5.236315	-4.060674	2.363027
F	7.332575	-3.558315	0.697958
F	3.803149	3.660928	1.595582
F	6.894758	-2.359549	-1.70575
F	6.324032	3.616253	2.49963
F	7.628032	1.03221	-1.206259
F	8.254738	2.289756	1.120523
C	2.50573	0.133956	-0.821968
H	3.358248	-0.029236	-0.436146
C	1.66852	-0.95052	-1.095858
C	-0.039817	0.619962	-1.848651
H	-0.917781	0.787116	-2.171562
C	0.34698	-0.695767	-1.601966
C	2.130586	1.445832	-1.097538
C	3.745595	-3.206632	0.751547
C	2.995914	2.575919	-0.889634
C	0.817022	1.700917	-1.63627
C	2.078053	-2.316619	-0.920144
C	3.471833	-2.615209	-0.47425
C	0.442892	3.035167	-1.964579
H	-0.421058	3.203316	-2.32237
C	1.297831	4.071063	-1.775863
H	1.035438	4.952176	-2.011684
C	4.368483	2.406812	-0.328557
C	-0.095409	-3.083145	-1.665518
H	-0.685534	-3.807155	-1.842126
C	6.090542	-3.224941	0.332915
C	-0.513192	-1.807496	-1.865561

H	-1.392688	-1.650123	-2.187474
C	4.571115	-2.333246	-1.278274
C	5.867122	-2.62566	-0.891898
C	2.584199	3.836331	-1.223711
H	3.171118	4.570022	-1.083407
C	5.031431	-3.503072	1.164025
C	4.726094	3.019776	0.86508
C	5.381917	1.731468	-0.996701
C	1.216702	-3.343477	-1.192485
H	1.50117	-4.240673	-1.065399
C	6.677852	1.675302	-0.516604
C	6.021442	2.992493	1.350783
C	6.994475	2.320515	0.656612
F	-2.740672	3.504321	-1.592322
F	-4.386539	1.7724	2.485533
F	-5.129918	-1.147568	2.172331
F	-5.236474	4.061041	-2.363603
F	-7.332734	3.558682	-0.698533
F	-3.802702	-3.661437	-1.594792
F	-6.894648	2.358954	1.705169
F	-6.323585	-3.616762	-2.49884
F	-7.628683	-1.031985	1.206543
F	-8.25407	-2.28916	-1.120587
C	-2.506381	-0.133731	0.822252
H	-3.358899	0.029461	0.43643
C	-1.668901	0.949782	1.096137
C	0.039657	-0.619595	1.848075
H	0.917621	-0.786748	2.170986
C	-0.346533	0.695258	1.602756
C	-2.129648	-1.446199	1.097469
C	-3.745417	3.207086	-0.750752
C	-2.995467	-2.576427	0.890424

C	-0.816845	-1.700462	1.637065
C	-2.077944	2.316023	0.919563
C	-3.471993	2.615576	0.473674
C	-0.442782	-3.035763	1.963998
H	0.420677	-3.204054	2.322648
C	-1.297991	-4.070695	1.775288
H	-1.034991	-4.952684	2.012474
C	-4.368373	-2.407408	0.327977
C	0.096078	3.083742	1.665454
H	0.685981	3.806646	1.842916
C	-6.090702	3.225308	-0.333491
C	0.512542	1.807721	1.865844
H	1.392529	1.65049	2.186898
C	-4.571274	2.333613	1.277699
C	-5.867281	2.626027	0.891322
C	-2.584359	-3.835964	1.223135
H	-3.171769	-4.569797	1.08369
C	-5.031591	3.503439	-1.164601
C	-4.726253	-3.019409	-0.865655
C	-5.381807	-1.732064	0.996121
C	-1.217083	3.342739	1.192764
H	-1.500232	4.240306	1.065329
C	-6.677183	-1.674706	0.516539
C	-6.022093	-2.992267	-1.350499
C	-6.994028	-2.321024	-0.655822

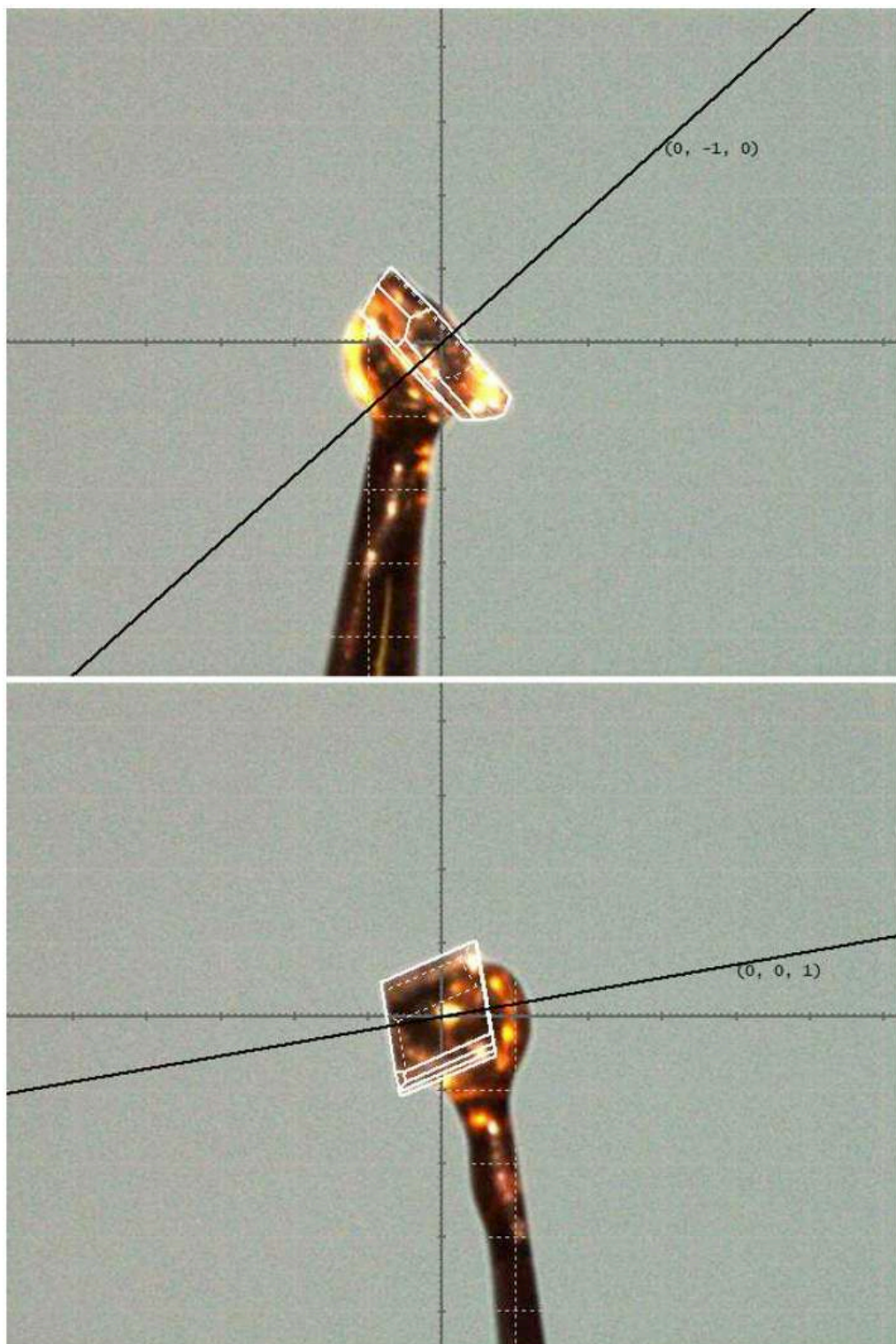
Supplementary Table 36. Atomic Coordinates of Unit 2

F	6.096864	3.217903	-2.10494
F	3.948871	1.576321	1.771432
F	3.271898	-1.358756	1.442565
F	8.452717	2.408107	-1.14277
F	8.606271	1.244611	1.31565
F	3.480265	-3.504818	-2.753932
F	6.332143	0.783849	2.738708
F	5.695055	-4.792993	-1.973831
F	5.542102	-2.584084	2.174848
F	6.756385	-4.333502	0.486902
C	2.822571	0.546236	-0.987077
H	3.687449	0.226415	-0.758808
C	2.610172	1.924705	-1.072285
C	0.31396	1.481371	-1.764755
H	-0.532259	1.799687	-2.057363
C	1.323018	2.404239	-1.497484
C	1.803646	-0.373637	-1.224453
C	6.118958	2.619245	-0.90299
C	1.972752	-1.794693	-1.079154
C	0.501898	0.106728	-1.618359
C	3.616699	2.890357	-0.726642
C	4.935607	2.425678	-0.203336
C	-0.555758	-0.825231	-1.818068
H	-1.414003	-0.50893	-2.075105
C	-0.361432	-2.155224	-1.646742
H	-1.082551	-2.760908	-1.772415
C	3.286513	-2.381198	-0.682422
C	2.100093	4.696417	-1.283568
H	1.941814	5.62972	-1.363839
C	7.4182	1.597114	0.812115
C	1.117005	3.815659	-1.598738

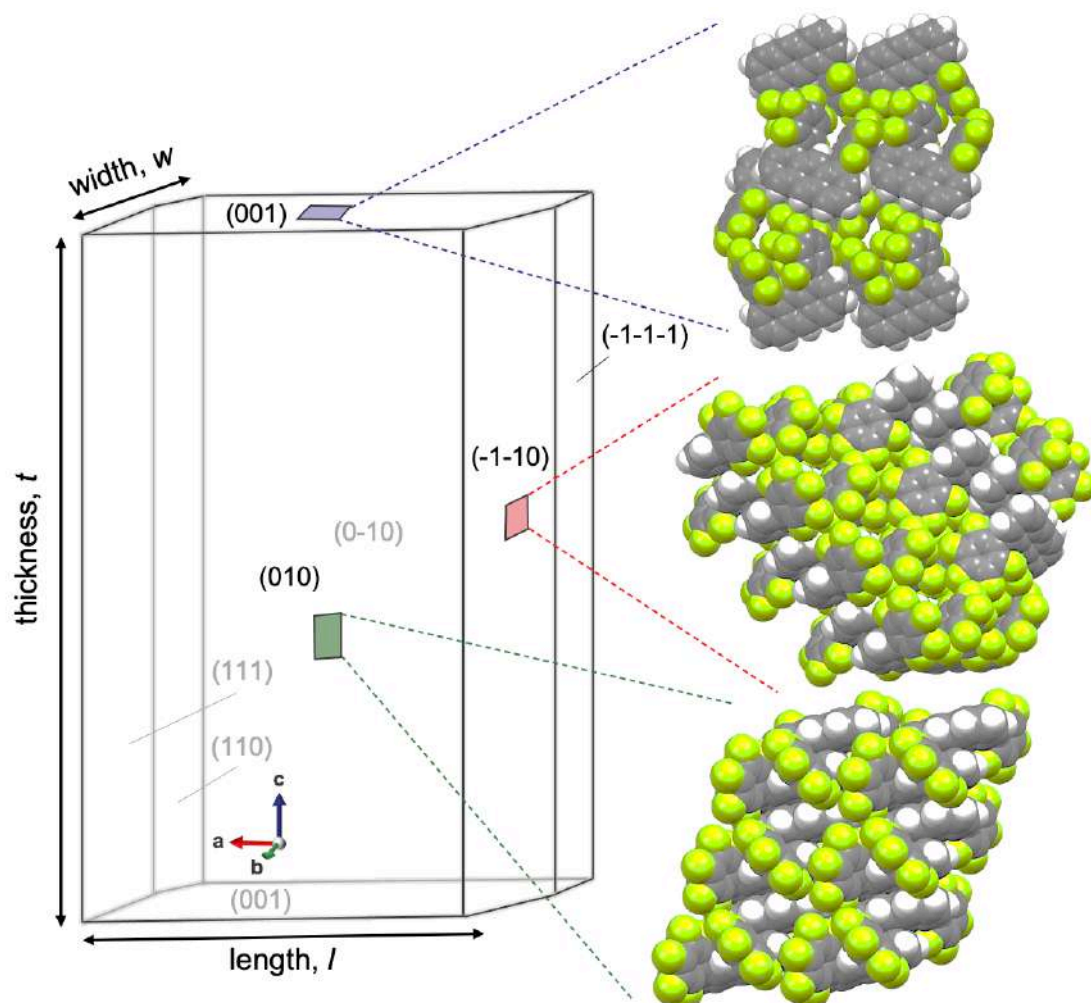
H	0.274899	4.143034	-1.891298
C	5.049079	1.788344	1.028101
C	6.26486	1.372881	1.539265
C	0.920152	-2.643492	-1.28245
H	1.04961	-3.578741	-1.177511
C	7.346207	2.207323	-0.417633
C	3.949778	-3.268013	-1.520941
C	3.867533	-2.167936	0.561433
C	3.363322	4.230614	-0.837201
H	4.04102	4.856135	-0.610299
C	5.030358	-2.802455	0.957046
C	5.101693	-3.930305	-1.135847
C	5.637641	-3.695558	0.104025
F	-6.097642	-3.218337	2.105385
F	-3.948287	-1.576714	-1.770608
F	-3.271679	1.357874	-1.443018
F	-8.452621	-2.40761	1.142607
F	-8.606175	-1.244115	-1.315813
F	-3.480423	3.505095	2.754711
F	-6.332179	-0.784952	-2.738219
F	-5.694958	4.793489	1.973669
F	-5.541264	2.583912	-2.174966
F	-6.756543	4.333778	-0.486124
C	-2.821732	-0.546407	0.986958
H	-3.686865	-0.226807	0.759631
C	-2.610075	-1.924208	1.072122
C	-0.313741	-1.482253	1.764302
H	0.531481	-1.800121	2.057808
C	-1.322922	-2.403742	1.497321
C	-1.804424	0.373203	1.224898
C	-6.118862	-2.618748	0.902827
C	-1.973275	1.79448	1.078657

C	-0.502676	-0.107162	1.618804
C	-3.616735	-2.89146	0.727131
C	-4.935511	-2.425181	0.203173
C	0.555855	0.825728	1.817905
H	1.41348	0.508717	2.074608
C	0.361274	2.1555	1.647521
H	1.082647	2.761405	1.772252
C	-3.287036	2.380985	0.681925
C	-2.099997	-4.69592	1.283405
H	-1.941718	-5.629224	1.363676
C	-7.418104	-1.596617	-0.812277
C	-1.116166	-3.815831	1.59862
H	-0.274315	-4.143427	1.892121
C	-5.04824	-1.788516	-1.02822
C	-6.264763	-1.372385	-1.539427
C	-0.920676	2.643279	1.281953
H	-1.050133	3.578527	1.177014
C	-7.346111	-2.206827	0.41747
C	-3.949682	3.26851	1.520778
C	-3.867436	2.168433	-0.561596
C	-3.363845	-4.230827	0.836704
H	-4.041798	-4.856569	0.610744
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C	-5.102217	3.930091	1.13535
C	-5.638164	3.695345	-0.104521

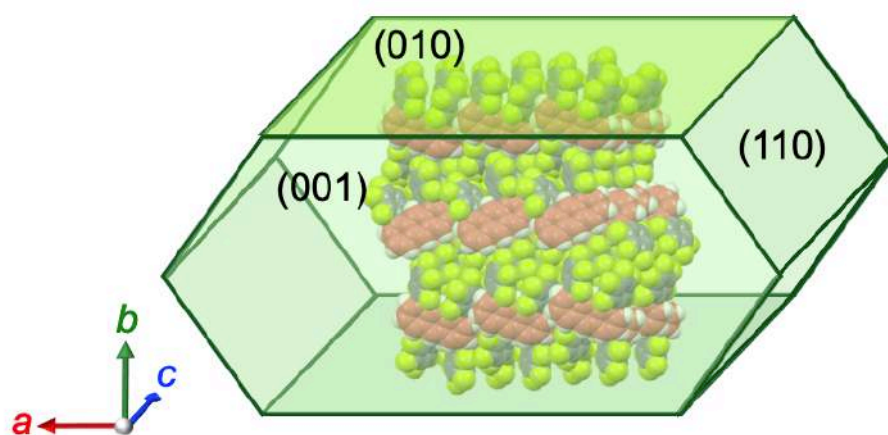
8.2 Transition dipole moment arrangement in crystal 1



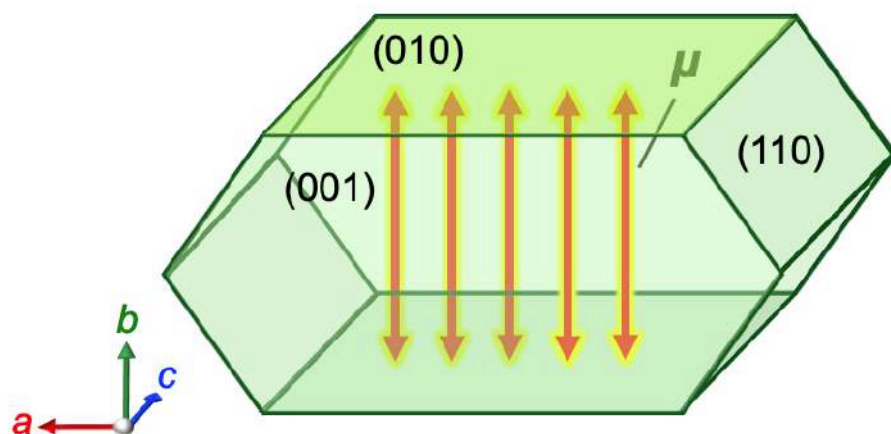
Supplementary Fig. 49. Indexing of single crystal X-ray diffraction images.
Relationship between crystal morphology and lattice plane of crystal 1.



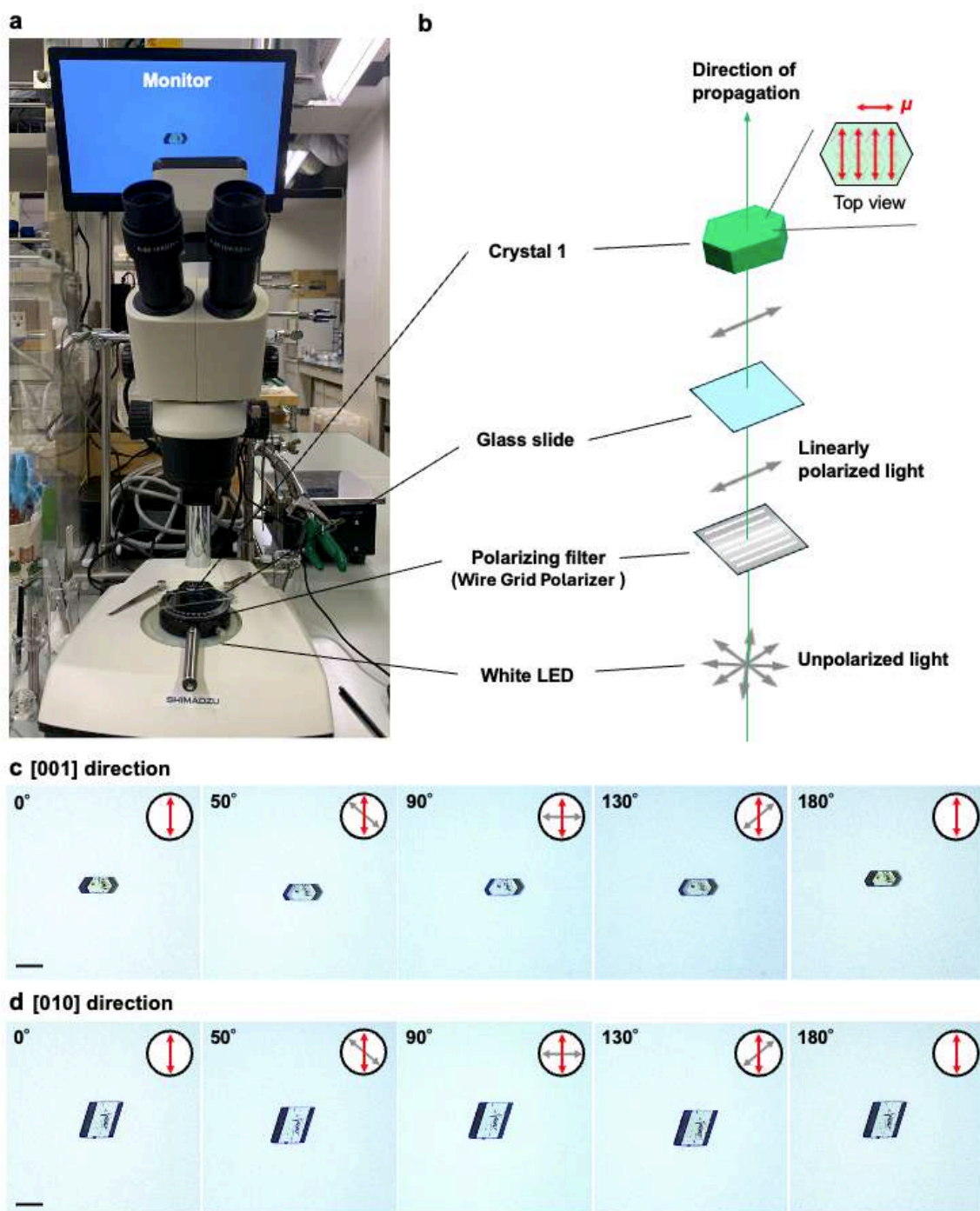
Supplementary Fig. 50. Crystal morphology and packing structure of 1.
 The short axis of the anthracene unit is oriented along the crystallographic *b*-axis.



II



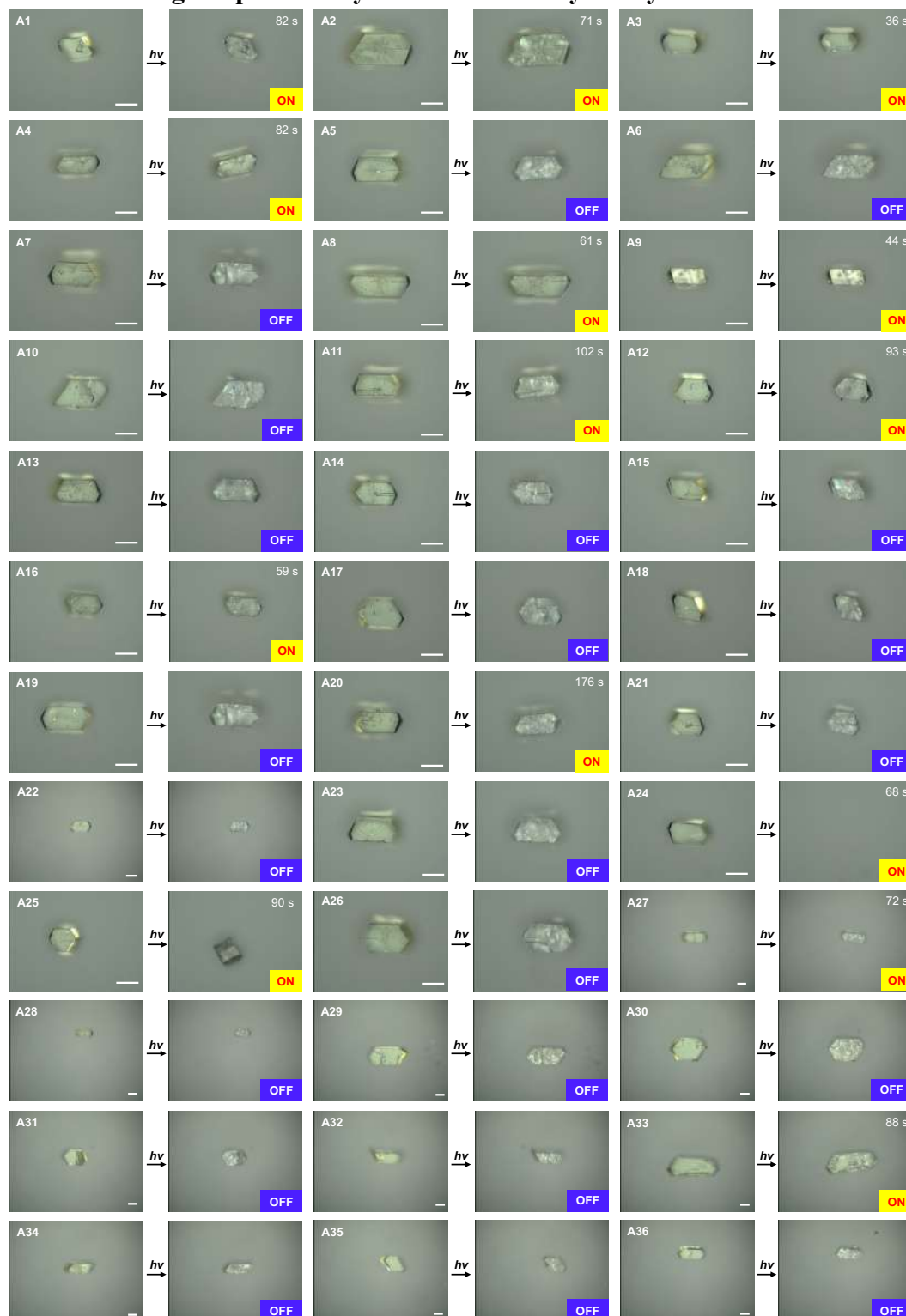
Supplementary Fig. 51. Crystal morphology and μ ($S_0 \rightarrow S_2$) of 1.
The μ is oriented along the crystallographic b -axis.



Supplementary Fig. 52. Anisotropic light absorption of the single crystal.

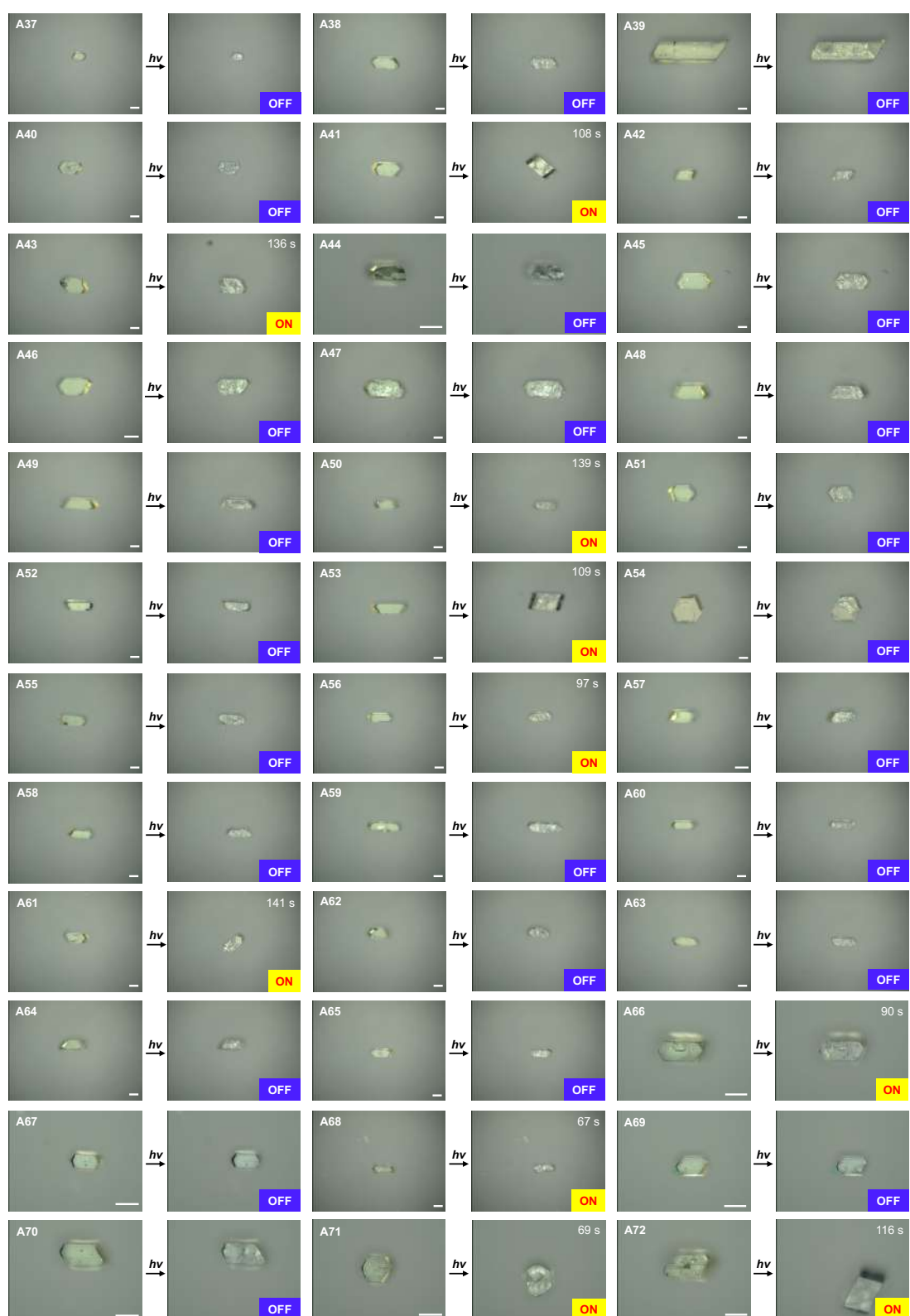
a, Photograph and **b**, schematic illustration of the experimental setup. Optical microscopy images of crystal 1 observed along the **c**, [001] and **d**, [010] directions under linearly polarized light. Differences in absorption along distinct crystallographic axes reveal optical anisotropy arising from the orientation of μ . Scale bar, 300 μm .

8.3 Controlling the probability of the onset of crystal dynamics



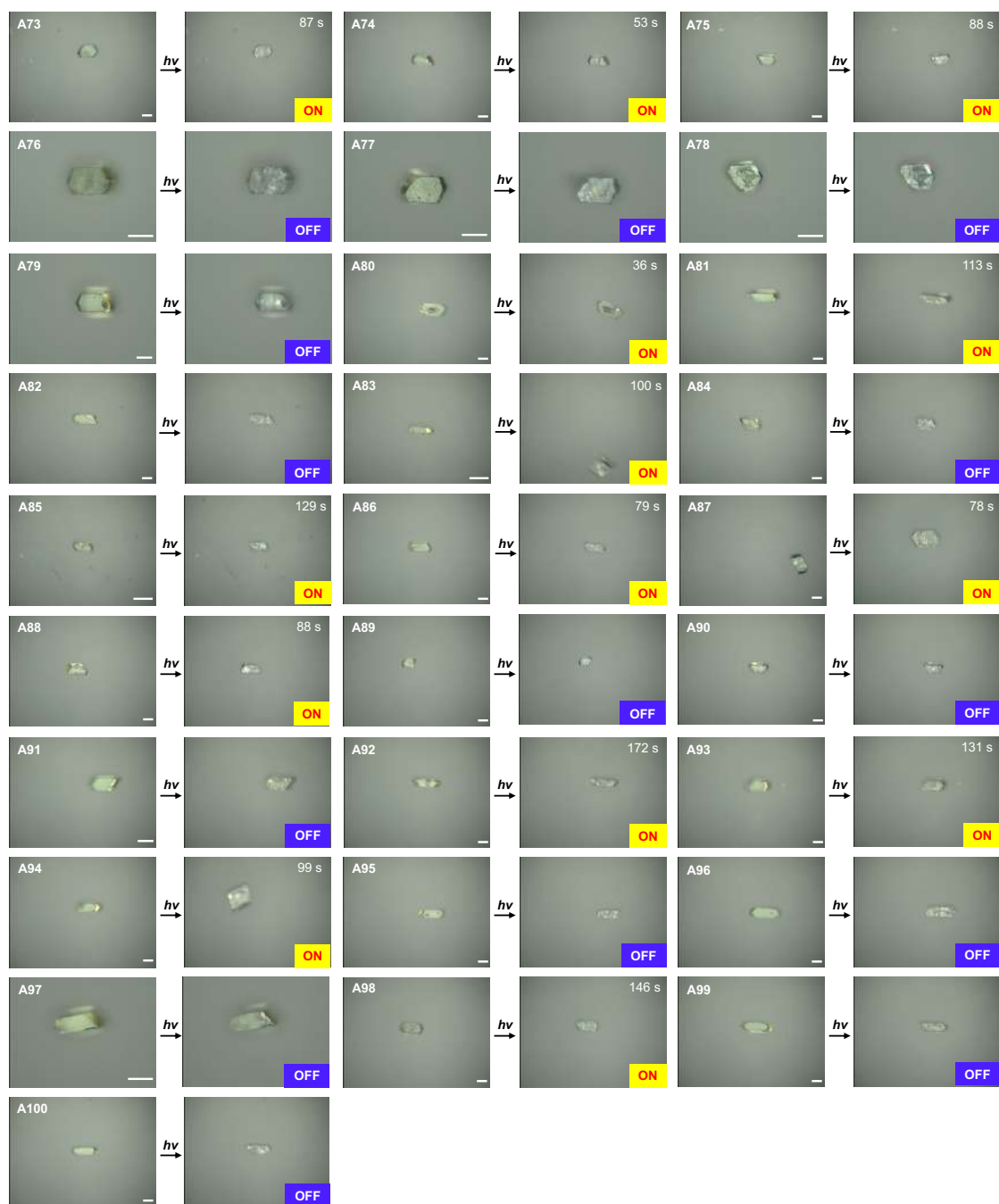
Supplementary Fig. 53. Observation of the crystal dynamics of crystals 1 under white LED irradiation along the [001] direction.

A1–A36. Scale bar, 300 μm .



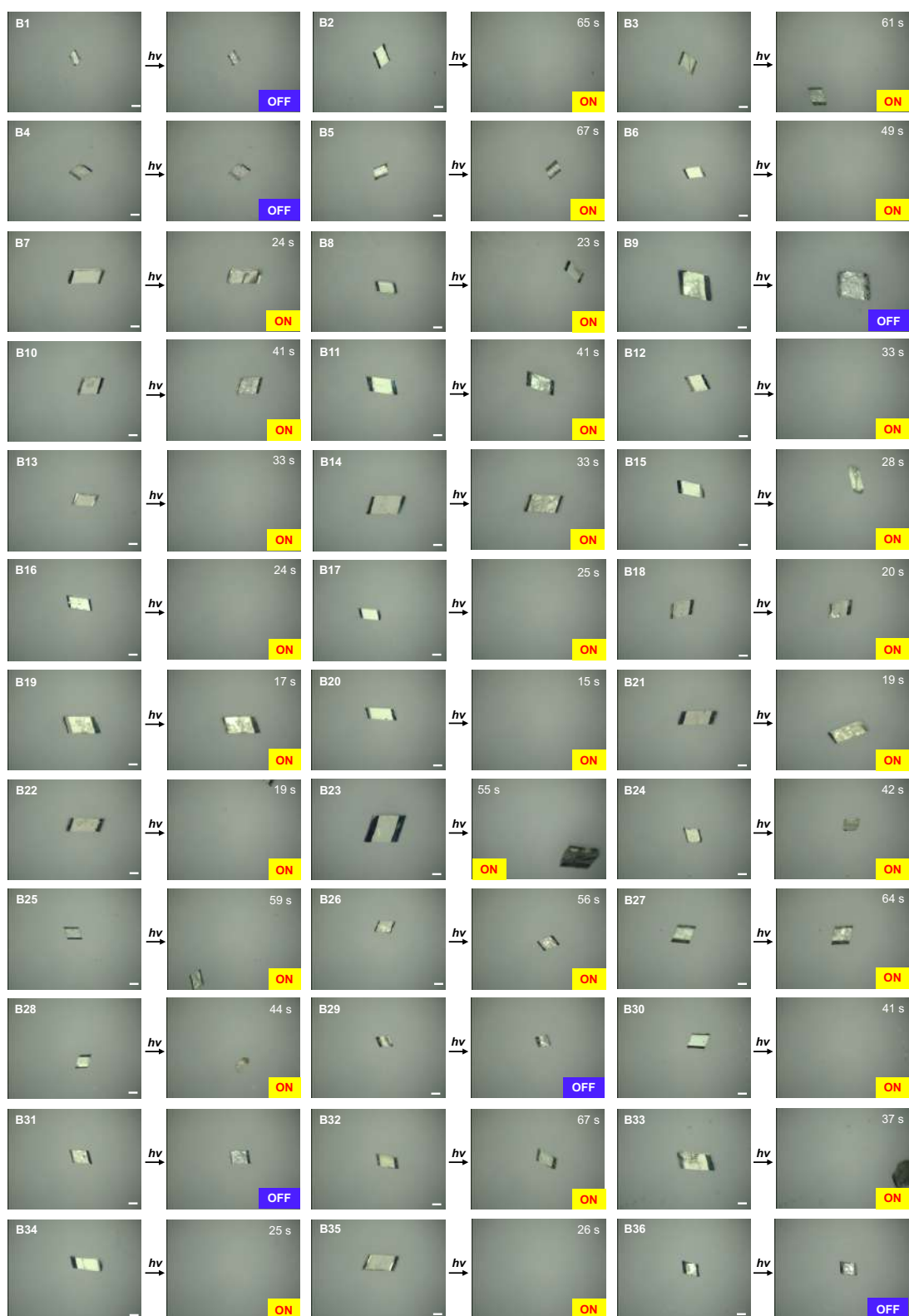
Supplementary Fig. 54. Observation of the crystal dynamics of crystals 1 under white LED irradiation along the [001] direction.

A37–A72. Scale bar, 300 μm .



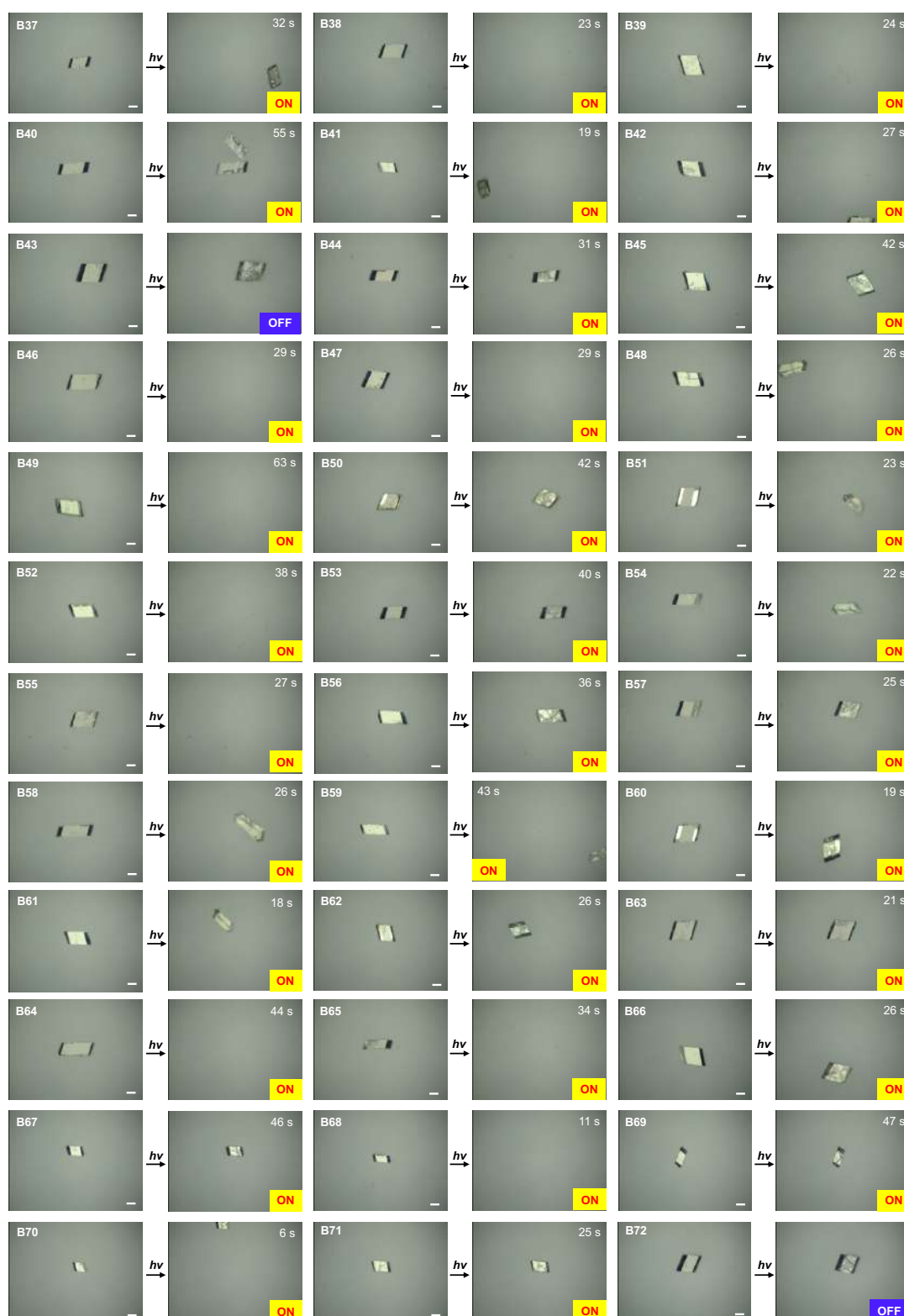
Supplementary Fig. 55. Observation of the crystal dynamics of crystals 1 under white LED irradiation along the [001] direction.

A73–A100. Scale bar, 300 μm .



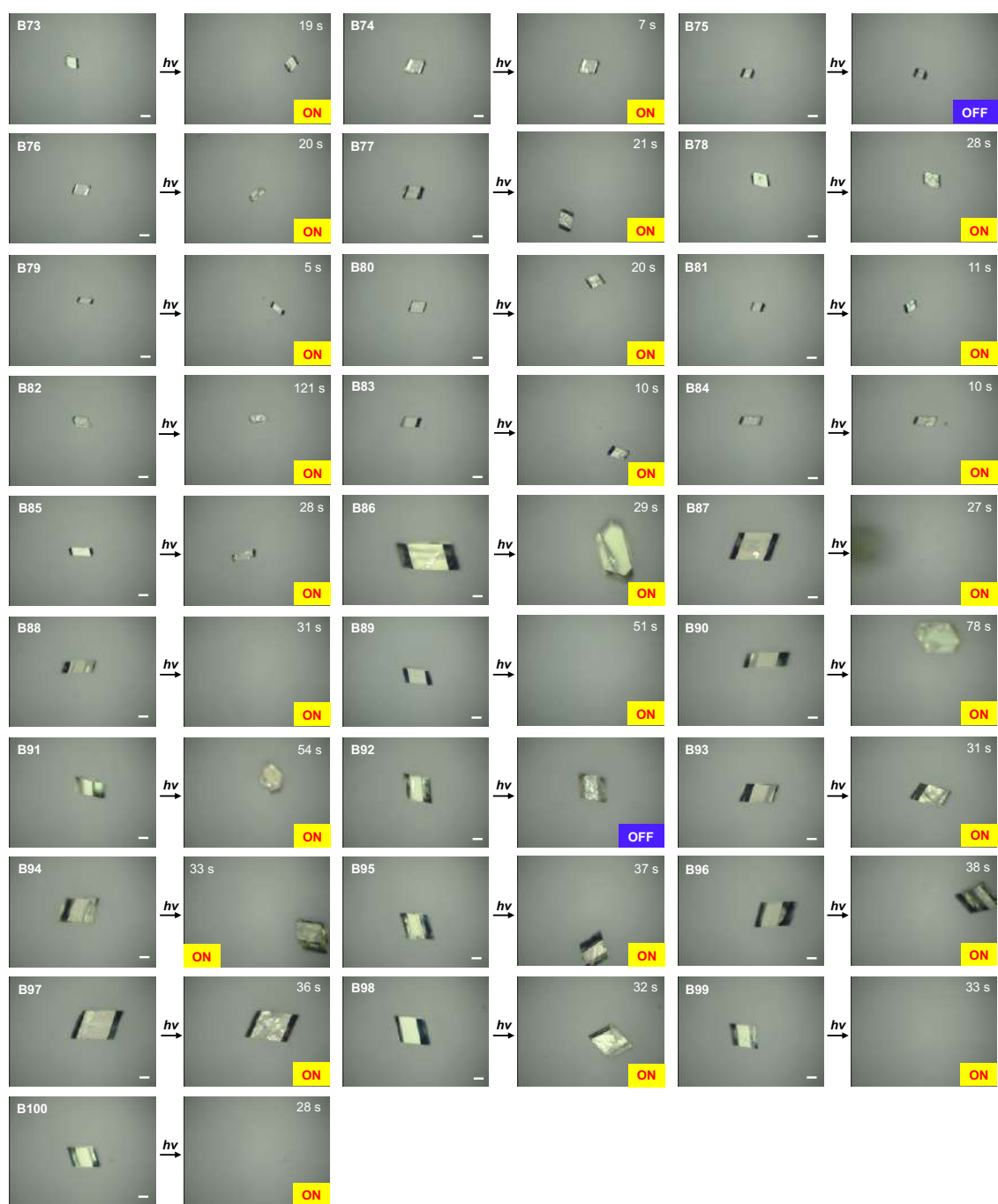
Supplementary Fig. 56. Observation of the crystal dynamics of crystals 1 under white LED irradiation along the [010] direction.

B1–B36. Scale bar, 300 μm.



Supplementary Fig. 57. Observation of the crystal dynamics of crystals 1 under white LED irradiation along the [010] direction.

B37–B72. Scale bar, 300 μm.



Supplementary Fig. 58. Observation of the crystal dynamics of crystals 1 under white LED irradiation along the [010] direction.

B73–B100. Scale bar, 300 μm.

Supplementary Table 37. Anisotropic Crystal Dynamics of **1**: [001] Direction

Entry	$l / \mu\text{m}$	$w / \mu\text{m}$	$t / \mu\text{m}$	Crystal dynamics	Response time/s
A1	136	88	93	ON	82
A2	293	136	107	ON	71
A3	180	73	99	ON	36
A4	213	80	107	ON	34
A5	240	108	103	OFF	—
A6	237	111	160	OFF	—
A7	233	97	187	OFF	—
A8	271	95	143	ON	61
A9	176	92	68	ON	44
A10	240	120	80	OFF	—
A11	213	93	147	ON	102
A12	173	99	88	ON	93
A13	221	101	89	OFF	—
A14	184	107	99	OFF	—
A15	175	87	135	OFF	—
A16	160	81	87	ON	59
A17	193	113	65	OFF	—
A18	167	101	97	OFF	—
A19	215	87	80	OFF	—
A20	207	99	145	ON	176
A21	148	95	93	OFF	—
A22	227	112	85	OFF	—
A23	223	112	129	OFF	—
A24	187	93	80	ON	68
A25	132	101	87	ON	90
A26	212	127	125	OFF	—
A27	260	108	165	ON	72
A28	175	80	133	OFF	—
A29	416	189	160	OFF	—
A30	400	253	128	OFF	—
A31	261	165	133	OFF	—
A32	328	107	259	OFF	—
A33	564	193	175	ON	88
A34	300	107	195	OFF	—

A35	355	152	111	OFF	—
A36	247	119	141	OFF	—
A37	149	84	75	OFF	—
A38	300	120	113	OFF	—
A39	827	193	299	OFF	—
A40	257	127	107	OFF	—
A41	320	132	161	ON	108
A42	243	105	164	OFF	—
A43	236	167	103	ON	136
A44	165	67	115	OFF	—
A45	393	167	127	ON	136
A46	247	128	111	OFF	—
A47	461	201	136	OFF	—
A48	388	149	281	OFF	—
A49	372	99	215	OFF	—
A50	259	87	167	ON	139
A51	287	173	140	OFF	—
A52	307	87	175	OFF	—
A53	371	107	189	ON	109
A54	367	296	155	OFF	—
A55	260	84	120	OFF	—
A56	273	113	253	ON	97
A57	268	80	140	OFF	—
A58	367	97	140	OFF	—
A59	284	88	147	OFF	—
A60	255	112	137	OFF	—
A61	219	100	177	ON	141
A62	287	85	113	OFF	—
A63	273	100	208	OFF	—
A64	236	83	101	OFF	—
A65	227	80	167	OFF	—
A66	137	89	55	ON	90
A67	232	65	125	OFF	—
A68	55	75	140	ON	67
A69	201	68	100	OFF	—
A70	200	107	93	OFF	—

A71	148	109	84	ON	69
A72	227	105	116	ON	116
A73	205	120	99	ON	87
A74	200	97	127	ON	53
A75	187	95	104	ON	88
A76	193	113	100	OFF	—
A77	147	91	73	OFF	—
A78	140	109	59	OFF	—
A79	295	101	148	OFF	—
A80	267	113	101	ON	36
A81	293	85	201	ON	113
A82	201	81	165	OFF	—
A83	255	61	68	ON	100
A84	213	101	120	OFF	—
A85	223	83	140	ON	129
A86	233	91	89	ON	79
A87	211	107	107	ON	78
A88	209	85	117	ON	88
A89	133	67	87	OFF	—
A90	307	80	212	OFF	—
A91	265	72	153	OFF	—
A92	227	87	193	ON	171
A93	224	107	213	ON	131
A94	188	76	167	ON	99
A95	303	73	101	OFF	—
A96	251	93	200	OFF	—
A97	120	60	171	OFF	—
A98	232	105	128	ON	146
A99	280	73	127	OFF	—
A100	247	75	120	OFF	—

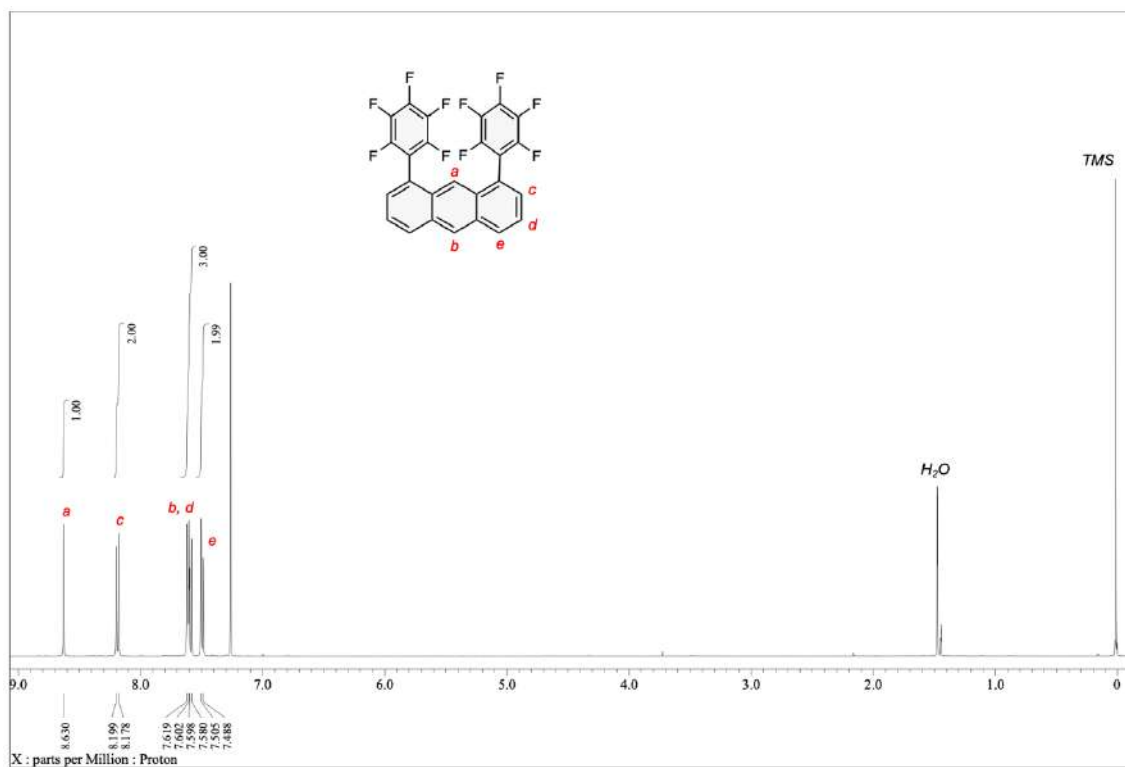
Supplementary Table 38. Anisotropic Crystal Dynamics of **1**: [010] Direction

Entry	$l / \mu\text{m}$	$w / \mu\text{m}$	$t / \mu\text{m}$	Crystal dynamics	Response time/s
B1	136	67	100	OFF	—
B2	173	80	193	ON	65
B3	200	87	160	ON	61
B4	187	53	147	OFF	—
B5	133	80	157	ON	67
B6	223	80	113	ON	49
B7	393	127	157	ON	24
B8	192	103	125	ON	23
B9	387	147	288	OFF	—
B10	255	107	187	ON	41
B11	336	125	161	ON	41
B12	240	93	189	ON	33
B13	271	80	132	ON	33
B14	400	147	201	ON	33
B15	307	111	140	ON	28
B16	280	80	127	ON	24
B17	243	107	107	ON	25
B18	269	143	165	ON	20
B19	315	129	197	ON	17
B20	333	119	127	ON	15
B21	413	157	155	ON	19
B22	407	173	153	ON	19
B23	387	127	308	ON	55
B24	187	67	153	ON	42
B25	137	67	185	ON	59
B26	196	61	131	ON	56
B27	220	120	205	ON	64
B28	144	85	140	ON	44
B29	148	93	120	OFF	—
B30	179	69	193	ON	41
B31	221	65	148	OFF	—
B32	253	113	124	ON	67
B33	411	147	176	ON	37
B34	375	123	125	ON	25

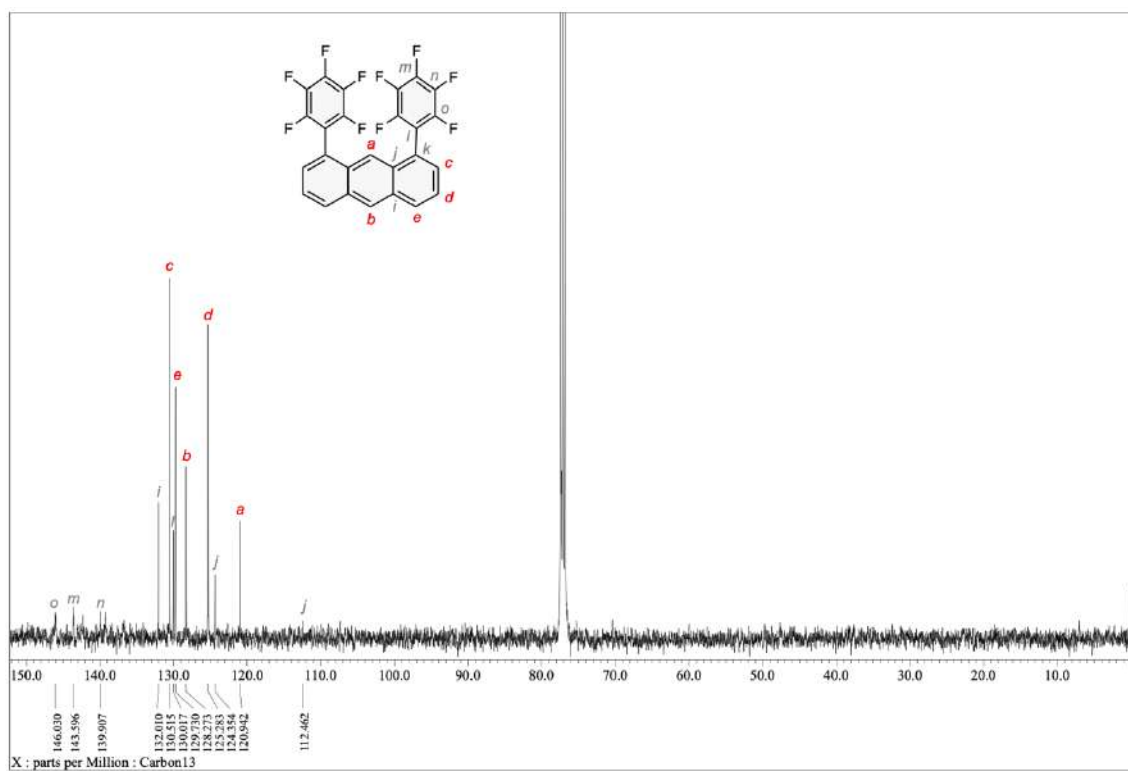
B35	352	149	165	ON	26
B36	188	73	135	OFF	—
B37	243	93	112	ON	32
B38	287	97	155	ON	23
B39	249	96	228	ON	24
B40	347	96	120	ON	55
B41	204	80	107	ON	19
B42	293	136	168	ON	27
B43	304	133	213	OFF	—
B44	269	103	192	ON	31
B45	276	116	193	ON	42
B46	367	121	167	ON	29
B47	269	111	187	ON	29
B48	309	109	136	ON	26
B49	316	132	160	ON	63
B50	232	116	195	ON	42
B51	253	133	203	ON	23
B52	291	103	136	ON	38
B53	277	120	135	ON	40
B54	313	104	136	ON	22
B55	276	103	172	ON	27
B56	309	119	140	ON	36
B57	240	105	176	ON	25
B58	401	137	125	ON	26
B59	308	89	101	ON	43
B60	271	123	188	ON	19
B61	255	103	137	ON	18
B62	184	112	179	ON	26
B63	264	113	103	ON	21
B64	167	67	99	ON	32
B65	385	108	144	ON	34
B66	295	85	187	ON	26
B67	187	76	117	ON	46
B68	188	107	79	ON	11
B69	207	92	81	ON	47
B70	145	52	76	ON	6

B71	208	67	113	ON	25
B72	235	97	187	OFF	—
B73	156	73	103	ON	19
B74	187	89	143	ON	7
B75	137	67	91	OFF	—
B76	180	73	112	ON	20
B77	203	87	125	ON	21
B78	193	69	128	ON	28
B79	169	87	52	ON	5
B80	165	65	111	ON	20
B81	148	61	91	ON	11
B82	173	91	95	ON	121
B83	183	73	108	ON	10
B84	196	95	105	ON	10
B85	236	93	79	ON	28
B86	611	281	268	ON	29
B87	437	173	299	ON	27
B88	333	187	123	ON	31
B89	305	116	149	ON	51
B90	257	289	139	ON	78
B91	360	223	125	ON	54
B92	281	153	247	OFF	—
B93	367	195	187	ON	31
B94	340	183	249	ON	33
B95	353	151	263	ON	37
B96	307	177	253	ON	38
B97	453	241	288	ON	36
B98	333	165	267	ON	32
B99	260	141	227	ON	33
B100	293	192	152	ON	28

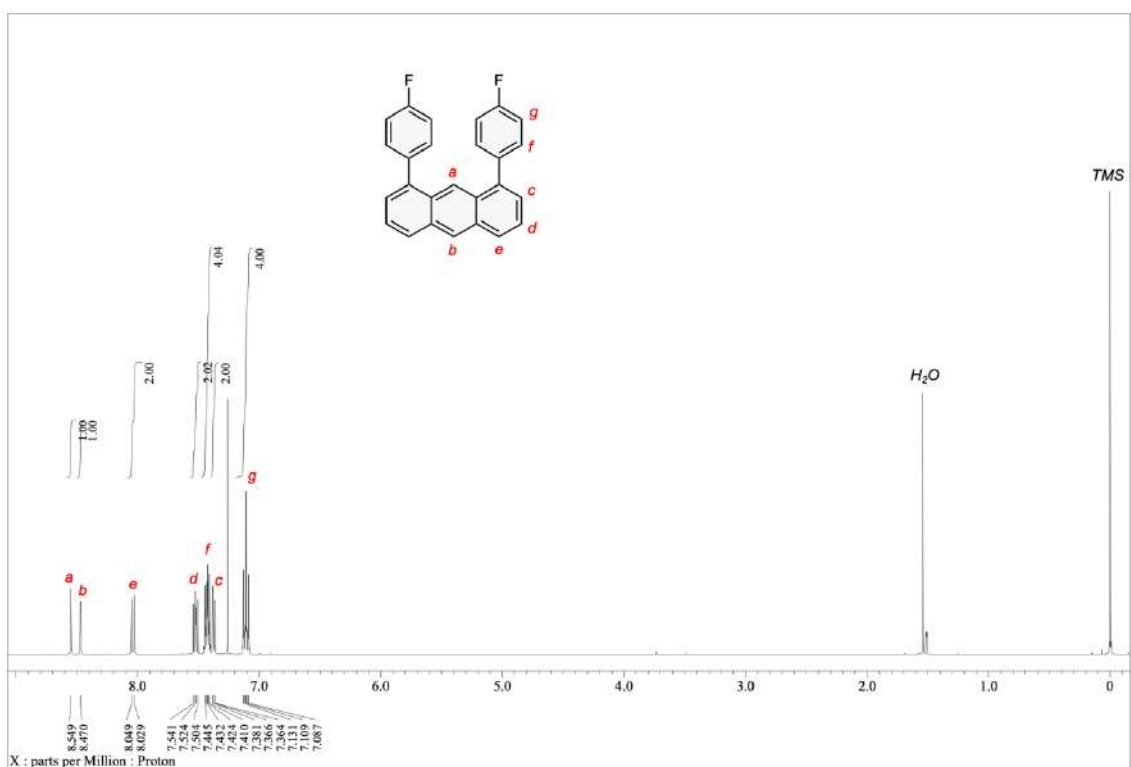
NMR spectra



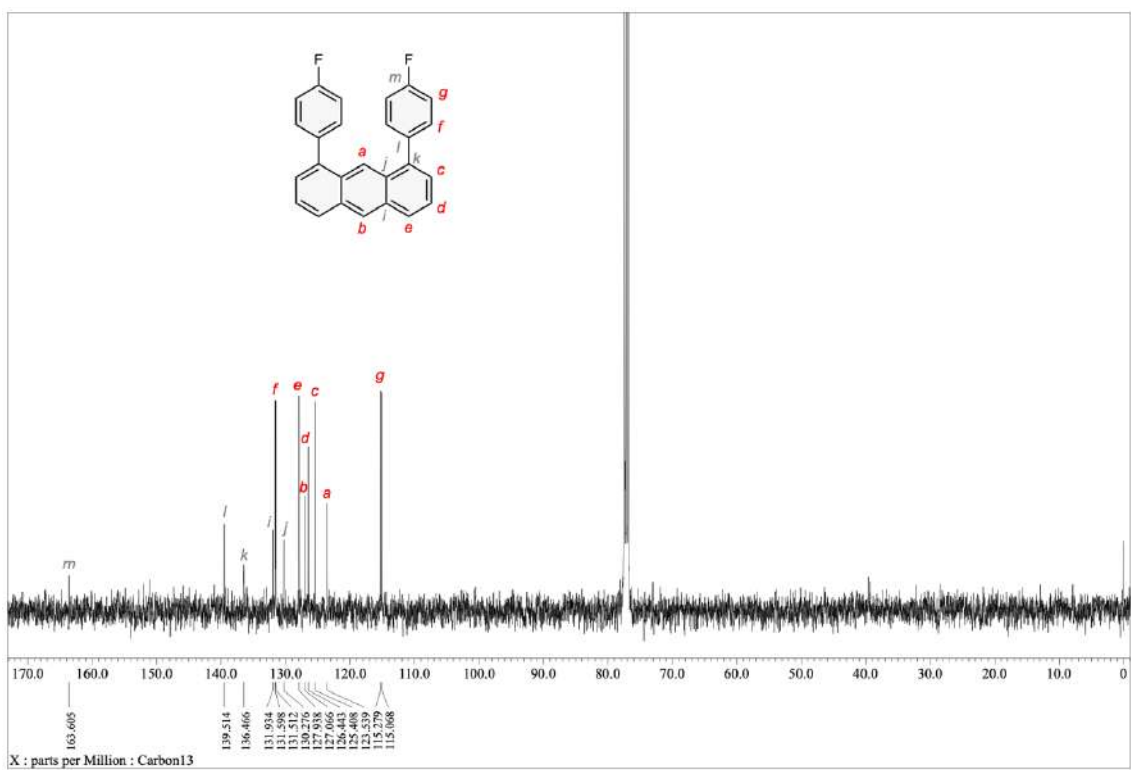
Supplementary Fig. 59. ¹H NMR (400 MHz, CDCl₃) spectrum of 1.



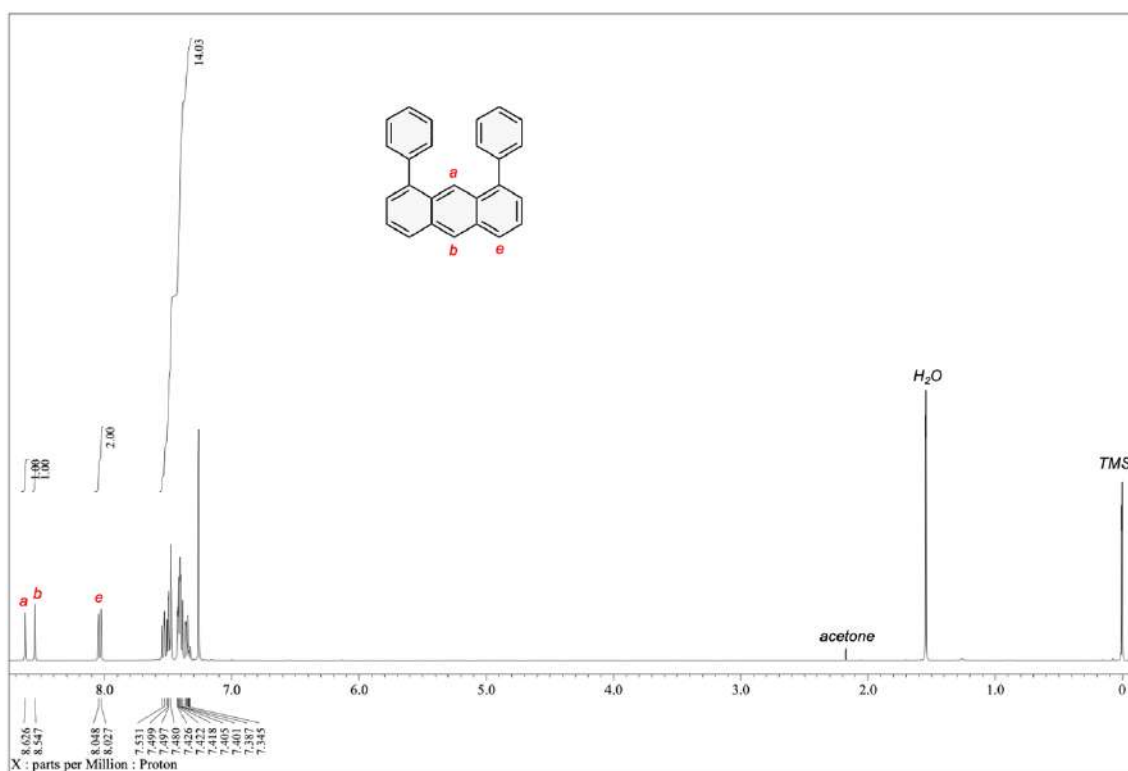
Supplementary Fig. 60. ¹³C NMR (100 MHz, CDCl₃) spectrum of 1.



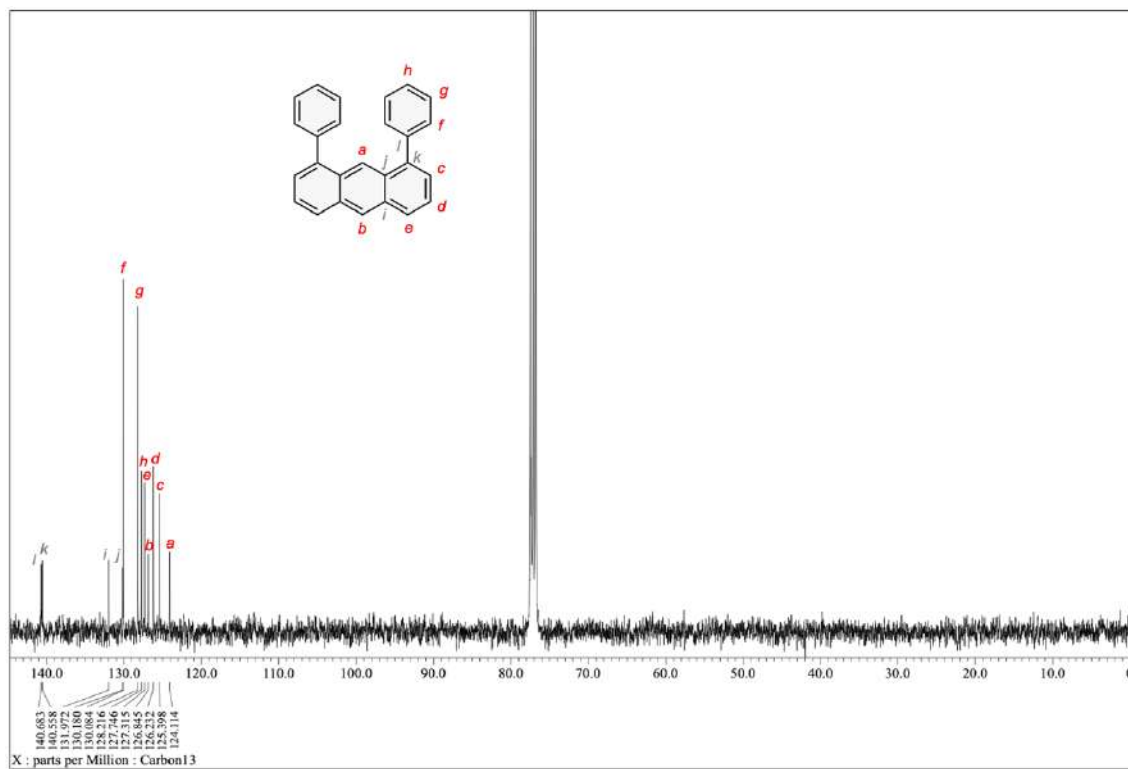
Supplementary Fig. 61. ^1H NMR (400 MHz, CDCl_3) spectrum of 2.



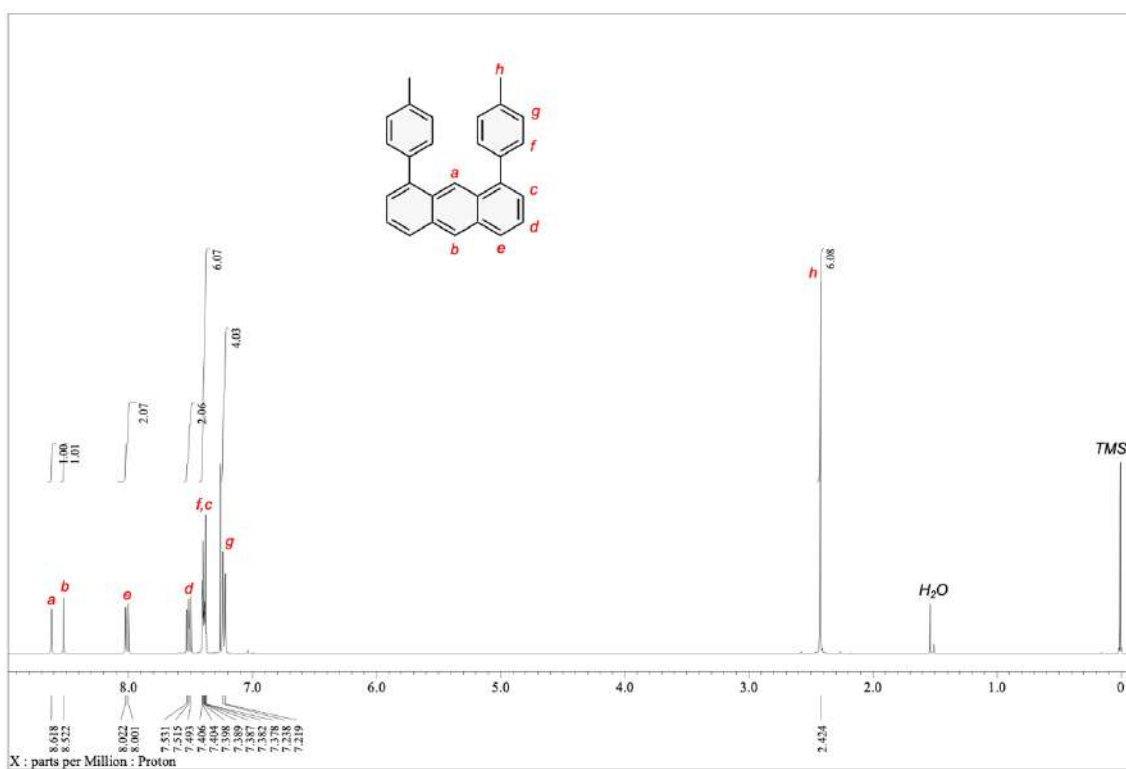
Supplementary Fig. 62. ^{13}C NMR (100 MHz, CDCl_3) spectrum of 2.



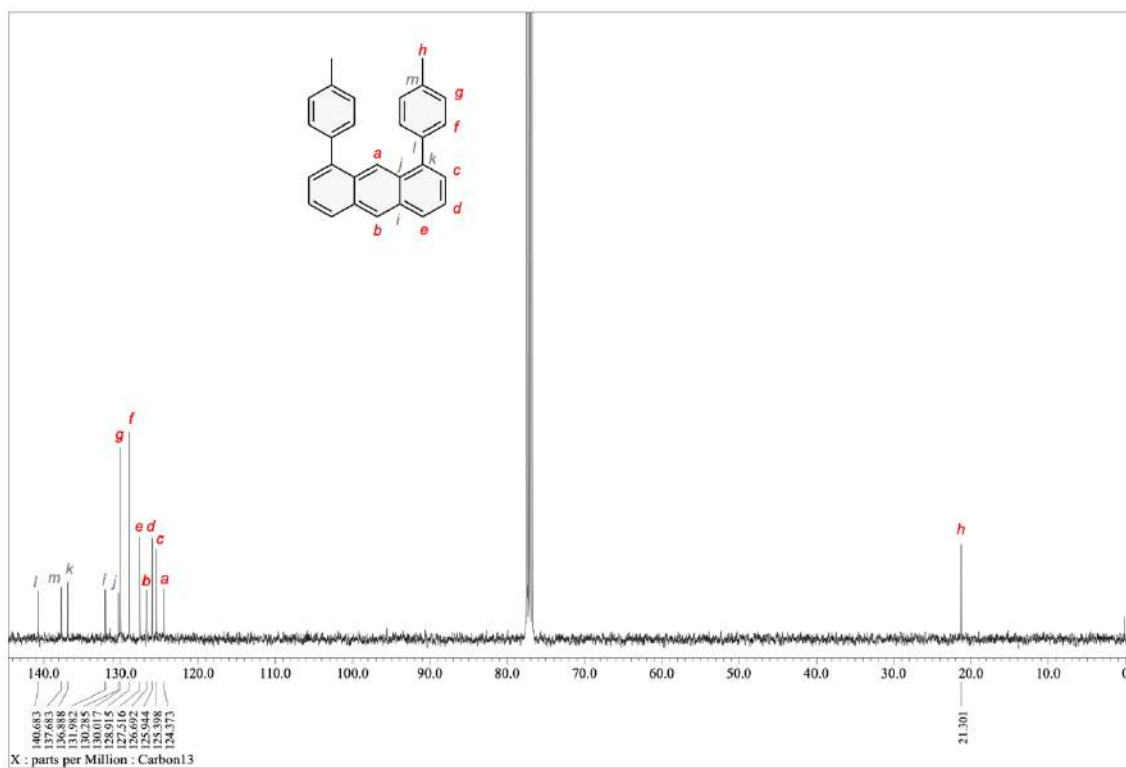
Supplementary Fig. 63. ¹H NMR (400 MHz, CDCl₃) spectrum of 3.



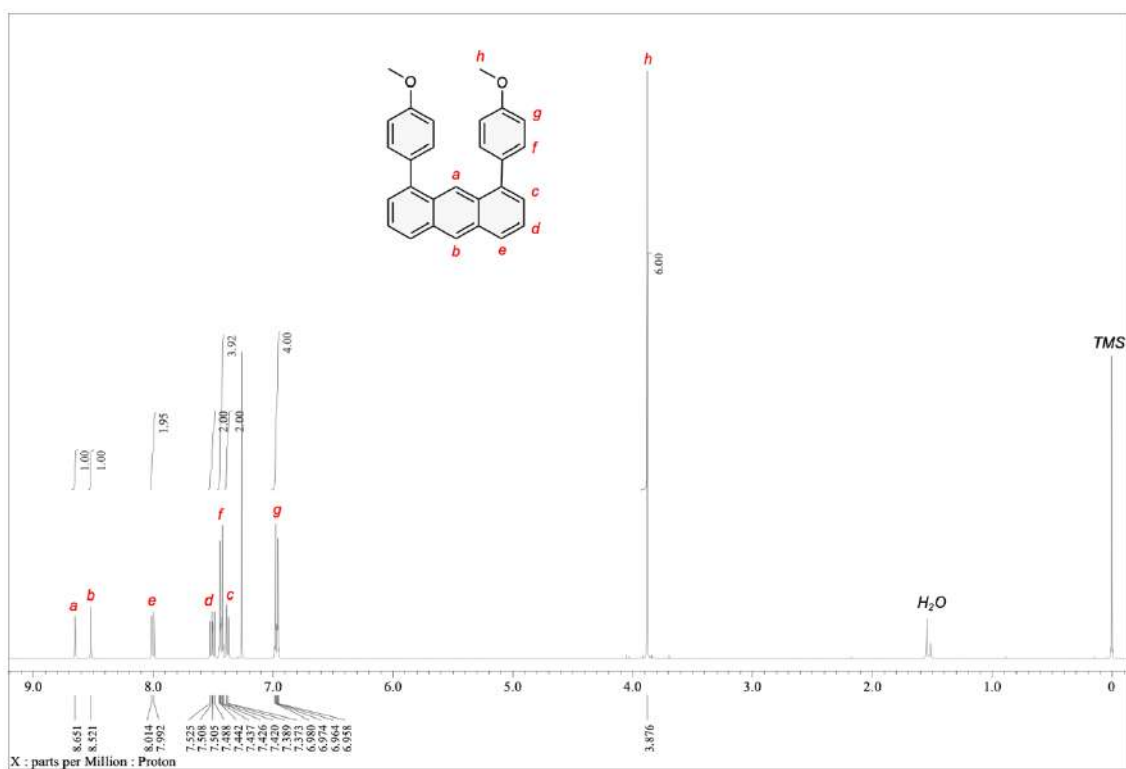
Supplementary Fig. 64. ¹³C NMR (100 MHz, CDCl₃) spectrum of 3.



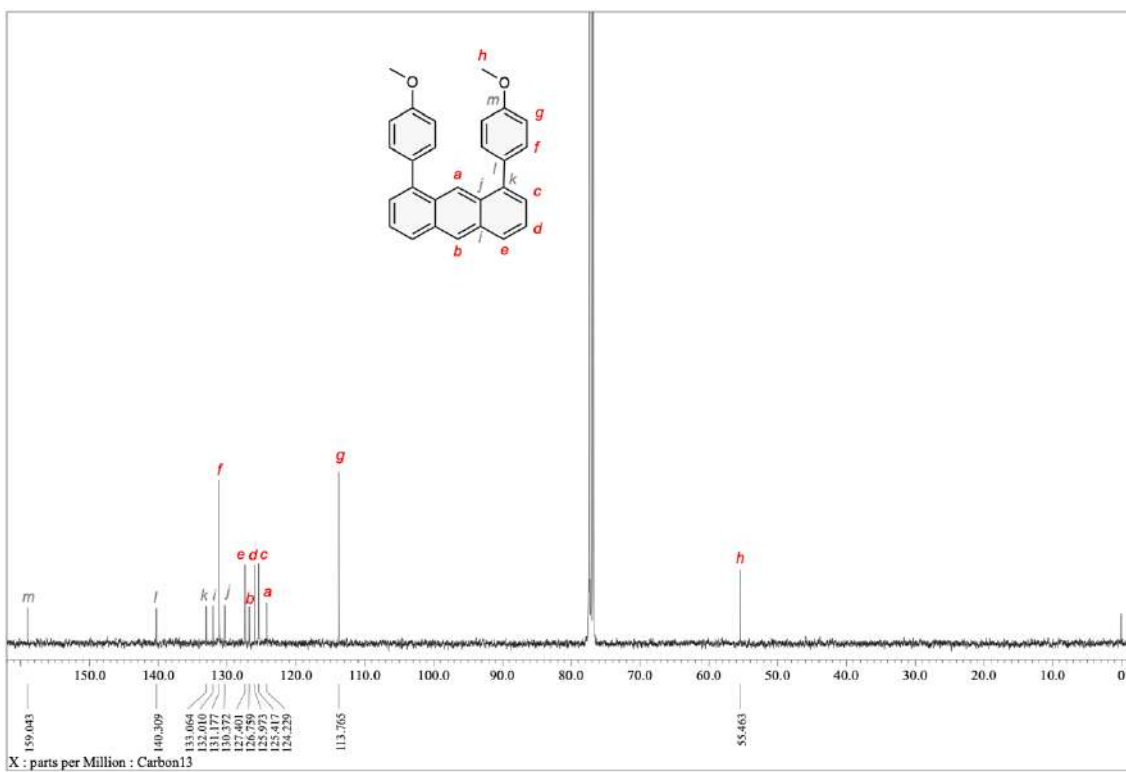
Supplementary Fig. 65. ^1H NMR (400 MHz, CDCl_3) spectrum of 4.



Supplementary Fig. 66. ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4.



Supplementary Fig. 67. ^1H NMR (400 MHz, CDCl_3) spectrum of 5.



Supplementary Fig. 68. ^{13}C NMR (100 MHz, CDCl_3) spectrum of 5.

Supplementary Movies

Hino, Y., Matsuo, T., & Hayashi, S. Trans-scale crystal dynamics for controlling kinetic responses in organic molecular systems. *Zenodo* <https://doi.org/10.5281/zenodo.15694836>, (2025)

checkCIF/PLATON reports



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

Bond precision:	C-C = 0.0025 Å	Wavelength=0.71073	
Cell:	a=10.5728 (5)	b=24.6728 (9)	c=7.9791 (3)
	alpha=90	beta=107.954 (5)	gamma=90
Temperature:	303 K		
	Calculated	Reported	
Volume	1980.08 (15)	1980.08 (15)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H8 F10	?	
Sum formula	C26 H8 F10	C26 H8 F10	
Mr	510.32	510.32	
Dx, g cm ⁻³	1.712	1.712	
Z	4	4	
Mu (mm ⁻¹)	0.165	0.165	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	13, 30, 9	13, 30, 9	
Nref	4038	4035	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.999

Theta(max)= 26.370

R(reflections)= 0.0420(3028)

wR2(reflections)=
0.1164(4035)

S = 1.079

Npar= 325

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check

Alert level G

PLAT434_ALERT_2_G	Short Inter HL..HL Contact F7	..F8	2.78 Ang.
	x,3/2-y,-1/2+z =	4_575	Check
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=	2.61	Note
	1 0 0, 1 1 0, 0 2 0,		
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2	Note
	1 0 0, 1 1 0,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.3	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	4.703	Note
	Predicted wR2: Based on SigI**2	2.47	or SHELX Weight 10.79
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

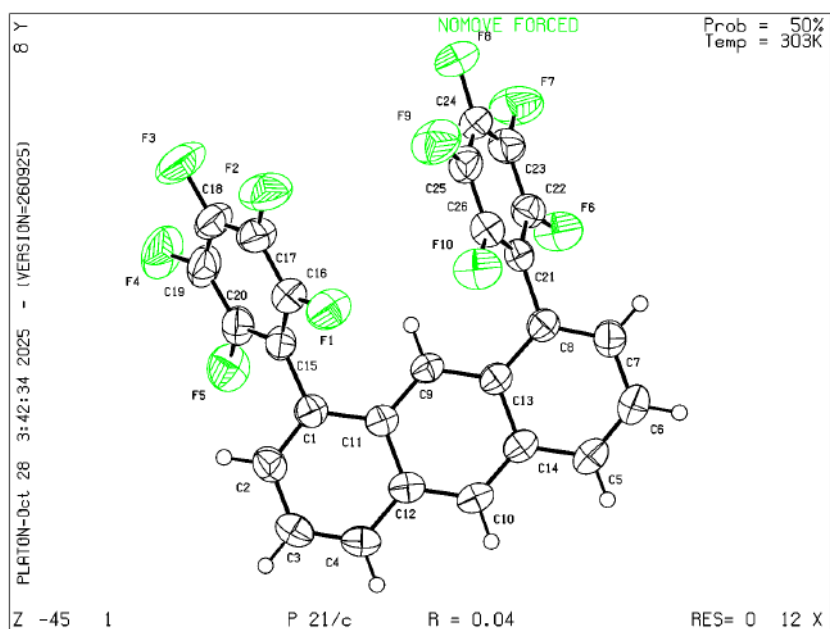
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

Datablock 1 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2

Bond precision:	C-C = 0.0031 Å	Wavelength=0.71073
Cell:	a=6.8546(7)	b=9.7096(6) c=14.2260(8)
	alpha=77.958(5)	beta=77.950(6) gamma=81.435(7)
Temperature:	303 K	
Volume	Calculated 900.07(12)	Reported 900.07(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H16 F2	?
Sum formula	C26 H16 F2	C26 H16 F2
Mr	366.39	366.39
Dx, g cm ⁻³	1.352	1.352
Z	2	2
Mu (mm ⁻¹)	0.092	0.092
F000	380.0	380.0
F000'	380.19	
h, k, lmax	9, 13, 19	9, 13, 19
Nref	5196	4328
Tmin, Tmax		
Tmin'		
Correction method=	Not given	

Data completeness= 0.833

Theta(max)= 29.861

R(reflections)= 0.0647(2337)

wR2(reflections)=
0.1999(4328)

S = 1.009

Npar= 253

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

● Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-0.915	Report
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	9 Report
	1 0 1, 0 2 2, 5 7 3, 5 8 3, -5 1 4,		1 4 4,
	-2 8 4, 4 0 6, -2 0 15,		

● Alert level G

PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=	2.16 Note
	0 0 1,	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600 857 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2 Note
	1 4 4, 0 2 2,	
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.5 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	1.821 Note
	Predicted wR2: Based on SigI**2 10.98 or SHELX Weight 19.80	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

A reduced cell check using CCDC's cellCheckCSD service has found that one or more structures in this CIF are similar to those previously published in the CSD or the ICSD.

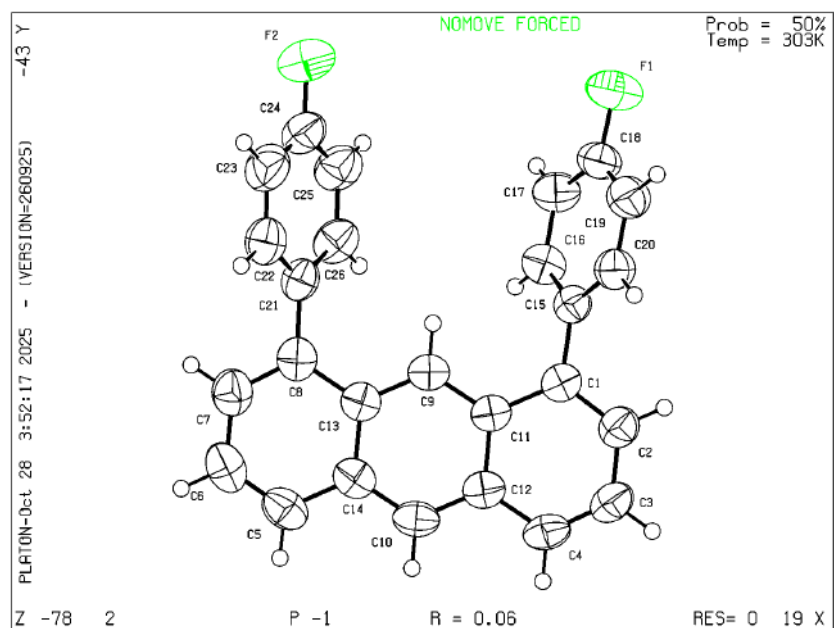
DATABLOCK: 2

- CSD Refcode: MACKAG



[Cell Parameters for MACKAG: 9.67,14.13,6.81(102.39,98.29,77.99)]

Datablock 2 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3a

Bond precision:	C-C = 0.0019 Å	Wavelength=0.71073
Cell:	a=6.7141(3)	b=9.6727(5) c=14.2242(4)
	alpha=77.954(4)	beta=79.869(3) gamma=80.885(4)
Temperature:	303 K	
Volume	Calculated 882.21(7)	Reported 882.21(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H18	?
Sum formula	C26 H18	C26 H18
Mr	330.40	330.40
Dx, g cm ⁻³	1.244	1.244
Z	2	2
Mu (mm ⁻¹)	0.070	0.070
F000	348.0	348.0
F000'	348.13	
h, k, lmax	9, 13, 20	9, 13, 19
Nref	5208	4221
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.810 Theta(max)= 30.115

R(reflections)= 0.0493(2752) wR2(reflections)=
0.1437(4221)

S = 1.061 Npar= 235

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

 **Alert level C**

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error)	...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error)	...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error)	...	Please Check
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C19 --C20 .	5.6 s.u.

 **Alert level G**

PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated	and Succeeded by SHELXL	2019/3 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min)[Deg]=		2.39 Note
	0 1 0, 0 0 1,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	978 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1 Note
	0 1 0,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.5 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		2.555 Note
	Predicted wR2: Based on SigI**2	5.62 or SHELX Weight 13.54	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2 Info

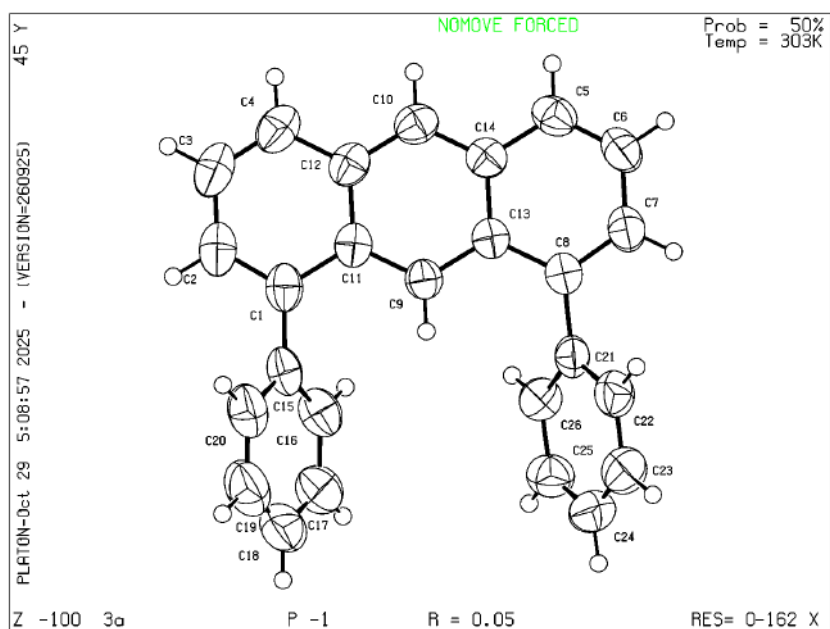
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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duplicate check

Datablock 3a - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3b

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3b

Bond precision:	C-C = 0.0018 Å		Wavelength=0.71073
Cell:	a=9.9447 (5)	b=27.1765 (10)	c=6.9805 (3)
	alpha=90	beta=105.003 (5)	gamma=90
Temperature:	303 K		
	Calculated	Reported	
Volume	1822.26 (14)	1822.26 (14)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H18	?	
Sum formula	C26 H18	C26 H18	
Mr	330.40	330.40	
Dx, g cm ⁻³	1.204	1.204	
Z	4	4	
Mu (mm ⁻¹)	0.068	0.068	
F000	696.0	696.0	
F000'	696.26		
h, k, lmax	14, 38, 9	13, 37, 9	
Nref	5367	4440	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.827 Theta(max)= 30.161

R(reflections)= 0.0446(3162) wR2(reflections)=
0.1219(4440)

S = 1.042 Npar= 235

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

 **Alert level C**

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error)	...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error)	...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error)	...	Please Check

 **Alert level G**

PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL		2019/3 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=	2.12	Note
	0 2 0,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	913 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.7	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	4.715	Note
	Predicted wR2: Based on SigI**2	2.59	or SHELX Weight 11.71
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by		2 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

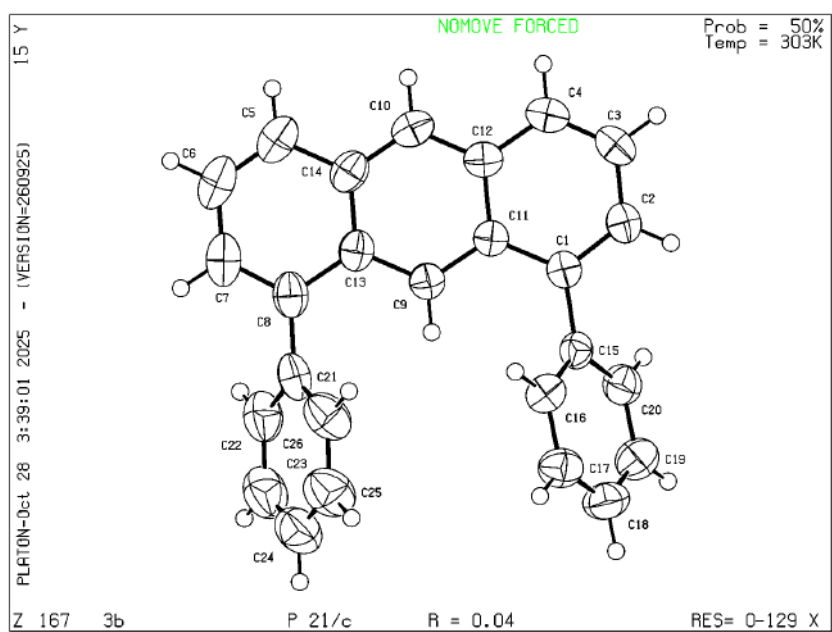
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PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

Datablock 3b - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 4

Bond precision:	C-C = 0.0022 Å		Wavelength=0.71073
Cell:	a=9.8376(5)	b=29.0057(11)	c=7.3731(3)
	alpha=90	beta=106.438(5)	gamma=90
Temperature:	303 K		
	Calculated	Reported	
Volume	2017.90(16)	2017.89(16)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C28 H22	?	
Sum formula	C28 H22	C28 H22	
Mr	358.46	358.45	
Dx, g cm-3	1.180	1.180	
Z	4	4	
Mu (mm-1)	0.067	0.067	
F000	760.0	760.0	
F000'	760.28		
h, k, lmax	13, 40, 10	13, 40, 9	
Nref	5968	4940	
Tmin, Tmax	0.976, 0.995		
Tmin'	0.935		
Correction method= Not given			

Data completeness= 0.828

Theta(max)= 30.127

R(reflections)= 0.0491(3356)

wR2(reflections)=
0.1405(4940)

S = 1.045

Npar= 255

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.1 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C19 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C18 Check
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist.	C15 -C20 .	1.37 Ang.

Alert level G

PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..	1.00 mm	
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !	
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3 Note	
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=	2.16 Note	
	0 2 0,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	957 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.8	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	4.762	Note
	Predicted wR2: Based on SigI**2	2.95 or SHELX Weight	13.45
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		5 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by		2 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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duplicate check

A reduced cell check using CCDC's cellCheckCSD service has found that one or more structures in this CIF are similar to those previously published in the CSD or the ICSD.

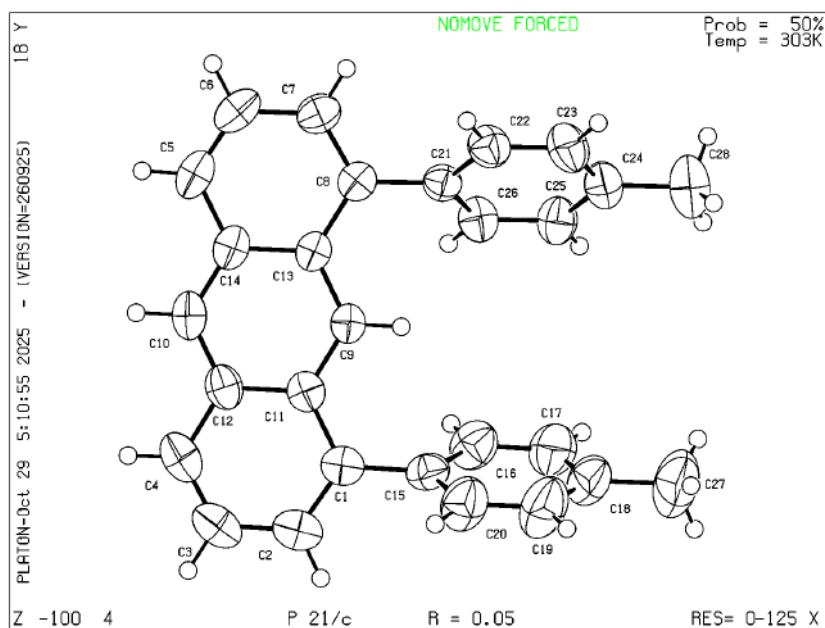
DATABLOCK: 4

- CSD Refcode: MACJOT



[Cell Parameters for MACJOT: 9.7784,28.975,7.3131(90,106.1,90)]

Datablock 4 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 5

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 5

Bond precision:	C-C = 0.0030 Å	Wavelength=0.71073
Cell:	a=7.4965 (13) alpha=90	b=28.6848 (13) beta=137.43 (3)
Temperature:	303 K	c=13.969 (2) gamma=90
	Calculated	Reported
Volume	2032.1 (12)	2032.0 (10)
Space group	P 21/a	P 21/a
Hall group	-P 2yab	-P 2yba
Moiety formula	C28 H22 O2	?
Sum formula	C28 H22 O2	C28 H22 O2
Mr	390.46	390.45
Dx, g cm ⁻³	1.276	1.276
Z	4	4
Mu (mm ⁻¹)	0.079	0.079
F000	824.0	824.0
F000'	824.36	
h, k, lmax	10, 40, 19	9, 38, 17
Nref	5996	4899
Tmin, Tmax		
Tmin'		
Correction method=	Not given	

Data completeness= 0.817 Theta(max)= 30.138

R(reflections)= 0.0501(3062) wR2(reflections)=
0.1477(4899)

S = 1.045 Npar= 273

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

 Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error)	...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error)	...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error)	...	Please Check
PLAT127_ALERT_1_C	Implicit Hall Symbol	Inconsistent with Explicit	-P 2yba Check

 Alert level G

PLAT128_ALERT_4_G	Alternate Setting for Input Space-group	P21/a	P21/c Note
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by	...	2 Units
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary	..	Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated	and Succeeded by SHELXL	2019/3 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min)[Deg]=	0 2 0,	2.16 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	870 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.9 Low
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ		2 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.		2 Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ		2 Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.		2 Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		4.173 Note
	Predicted wR2: Based on SigI**2	3.54 or SHELX Weight	14.13
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		3 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected
- 9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check
-

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PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

A reduced cell check using CCDC's cellCheckCSD service has found that one or more structures in this CIF are similar to those previously published in the CSD or the ICSD.

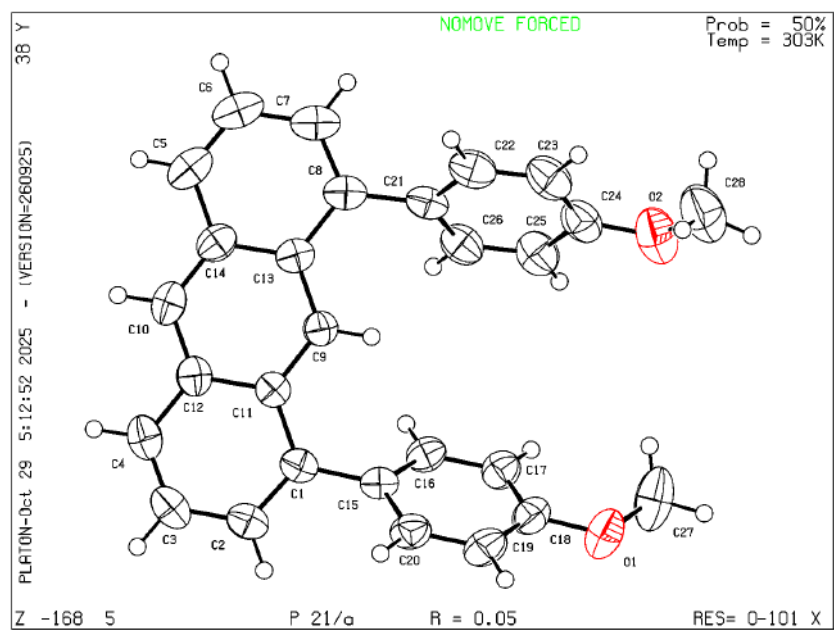
DATABLOCK: 5

- CSD Refcode: MACJUZ



[Cell Parameters for MACJUZ: 9.859,28.758,7.5196(90,106.373,90)]

Datablock 5 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Thermally_obtained_1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: Thermally_obtained_1

Bond precision:	C-C = 0.0042 Å	Wavelength=0.71073
Cell:	a=10.5116(5) alpha=90	b=24.5436(10) beta=108.471(5) c=7.8671(3) gamma=90
Temperature:	103 K	
Volume	Calculated 1925.09(15)	Reported 1925.09(15)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H8 F10	?
Sum formula	C26 H8 F10	C26 H8 F10
Mr	510.32	510.32
Dx, g cm ⁻³	1.761	1.761
Z	4	4
Mu (mm ⁻¹)	0.170	0.170
F000	1016.0	1016.0
F000'	1016.91	
h, k, lmax	14, 34, 11	14, 31, 9
Nref	5646	4550
Tmin, Tmax		
Tmin'		

Correction method= Not given

$$\text{Theta (max)} = 30.061$$

```
wR2 (reflections)=  
0.1359 ( 4550)
```

Npar= 325

- Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00417 Ang.	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	5.910 Check	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.147 Check	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & Sth/L=	0.600	13 Report
	2 29 0, -3 26 1, -3 28 1, -7 24 2, -4 24 2,	-5 25 2,	
	-4 25 2, -5 26 2, -4 26 2, -5 22 5, -6 23 5,	-5 23 5,	
	-4 24 5,		

- Alert level G

```

PLAT434_ALERT_2_G Short Inter HL..HL Contact F8      ..F9      .      2.72 Ang.
                                     x,1/2-y,1/2+z =      4_566 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....      34 Note
      C00B      C00C      H00C      C00D      H00D      C00E      C00F      C00G
      C00H      C00I      C00J      H00J      C00K      H00K      C00L      C00M
      H00M      C00N      C00O      H00O      C00P      H00P      C00Q      C00R
      C00S      C00T      C00U      H00U      C00V      C00W      C00X      C00Y
      C00Z      C010

PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..      Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated      and Succeeded by SHELXL      2019/3 Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]=      2.20 Note
      1      0      0,      0      2      0,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above Sth/L=      0.600      857 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      17 Note
      0      2      0,      -9      22      5,      3      14      8,      0      20      7,      -5      23      5,      -5      24      6,
      -7      23      5,      -8      23      5,      -5      22      5,      -6      24      6,      -4      24      5,      3      24      5,
      1      0      0,      -6      23      5,      -5      26      5,      -7      24      5,      -10      21      5,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....      2.8 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ      3 Unit
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.      2 Unit
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ      3 Unit
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.      2 Unit
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      2.368 Note
      Predicted wr2: based on SigI**2      5.74 or SHELX Weight 13.17

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      7 Info

```

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
14 **ALERT level G** = General information/check it is not something unexpected

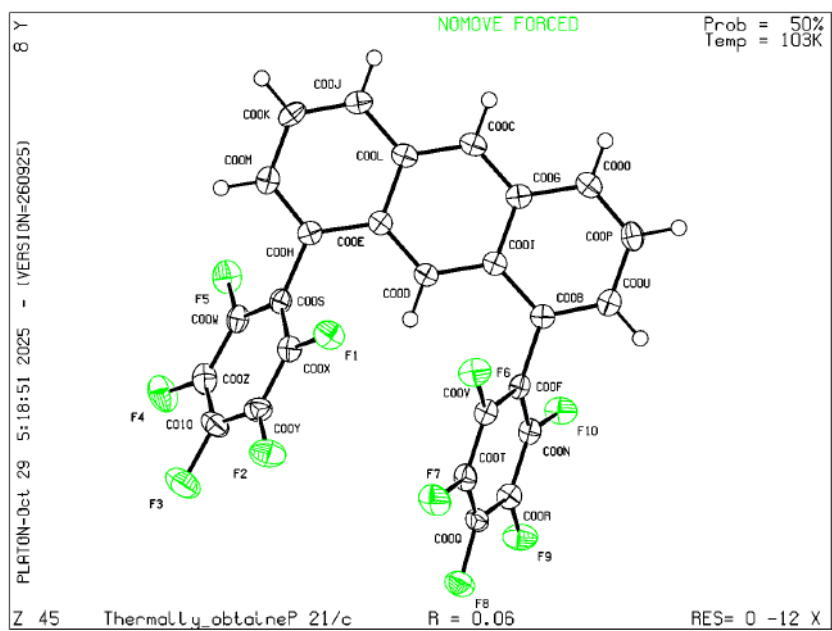
7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_373

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_373

Bond precision:	C-C = 0.0021 Å	Wavelength=0.71073	
Cell:	a=10.5069 (4)	b=24.5538 (6)	c=7.8617 (2)
	alpha=90	beta=108.438 (3)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1924.08 (11)	1924.08 (10)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H8 F10	?	
Sum formula	C26 H8 F10	C26 H8 F10	
Mr	510.32	510.32	
Dx, g cm ⁻³	1.762	1.762	
Z	4	4	
Mu (mm ⁻¹)	0.170	0.170	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	13, 30, 9	13, 30, 9	
Nref	3933	3926	
Tmin, Tmax			
Tmin'			
Correction method= Not given			

Data completeness= 0.998 Theta(max)= 26.371

R(reflections)= 0.0364(3279) wR2(reflections)=
0.0973(3926)

S = 1.073 Npar= 325

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

 **Alert level C**

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error)	...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error)	...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error)	...	Please Check

 **Alert level G**

PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3	..F4	2.72 Ang.
	x,1/2-y,-1/2+z =		4_565 Check
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL		2019/3 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min)[Deg]=		2.21 Note
	1 0 0, 0 2 0,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	6 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1 Note
	1 0 0,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.9 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		3.074 Note
	Predicted wR2: Based on SigI**2	3.16 or SHELX Weight	9.06
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		16 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

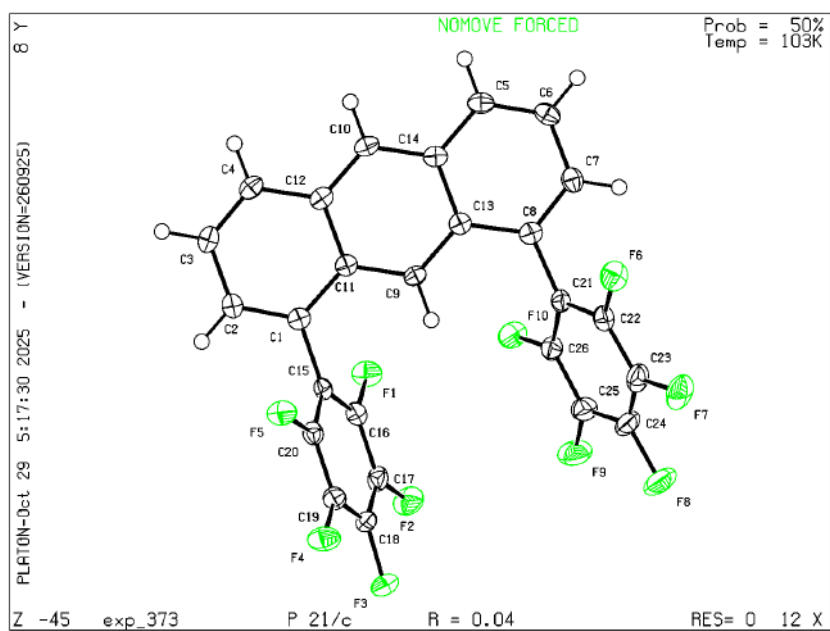
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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Datablock exp_373 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_374

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_374

Bond precision:	C-C = 0.0021 Å		Wavelength=0.71073
Cell:	a=10.5291 (4)	b=24.5899 (7)	c=7.8915 (3)
	alpha=90	beta=108.263 (4)	gamma=90
Temperature:	153 K		
	Calculated	Reported	
Volume	1940.27 (13)	1940.27 (13)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H8 F10	?	
Sum formula	C26 H8 F10	C26 H8 F10	
Mr	510.32	510.32	
Dx, g cm ⁻³	1.747	1.747	
Z	4	4	
Mu (mm ⁻¹)	0.169	0.169	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	13, 30, 9	13, 30, 9	
Nref	3958	3956	
Tmin, Tmax	0.903, 0.938		
Tmin'	0.874		

Correction method= Not given

$$\text{Theta (max)} = 26.370$$

```
wR2 (reflections)=  
0.1037 ( 3956)
```

Npar= 325

🟡 **Alert level C**

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
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PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..		0.80 mm
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3 ..F4 .	2.73 Ang.
	x,1/2-y,-1/2+z =	4.565 Check
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta (Min) [Deg]=	2.20 Note
	1 0 0, 0 2 0,	
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1 Note
	1 0 0,	
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.1 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.720 Note
	Predicted wR2: Based on SigI*2 3.81 or SHELX Weight	9.69
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	10 Info

- | | | |
|---|----------------------|--|
| 0 | ALERT level A | = Most likely a serious problem - resolve or explain |
| 0 | ALERT level B | = A potentially serious problem, consider carefully |
| 1 | ALERT level C | = Check. Ensure it is not caused by an omission or oversight |
| 9 | ALERT level G | = General information/check it is not something unexpected |
| 2 | ALERT type 1 | CIF construction/syntax error, inconsistent or missing data |
| 3 | ALERT type 2 | Indicator that the structure model may be wrong or deficient |
| 2 | ALERT type 3 | Indicator that the structure quality may be low |
| 2 | ALERT type 4 | Improvement, methodology, query or suggestion |
| 1 | ALERT type 5 | Informative message, check |

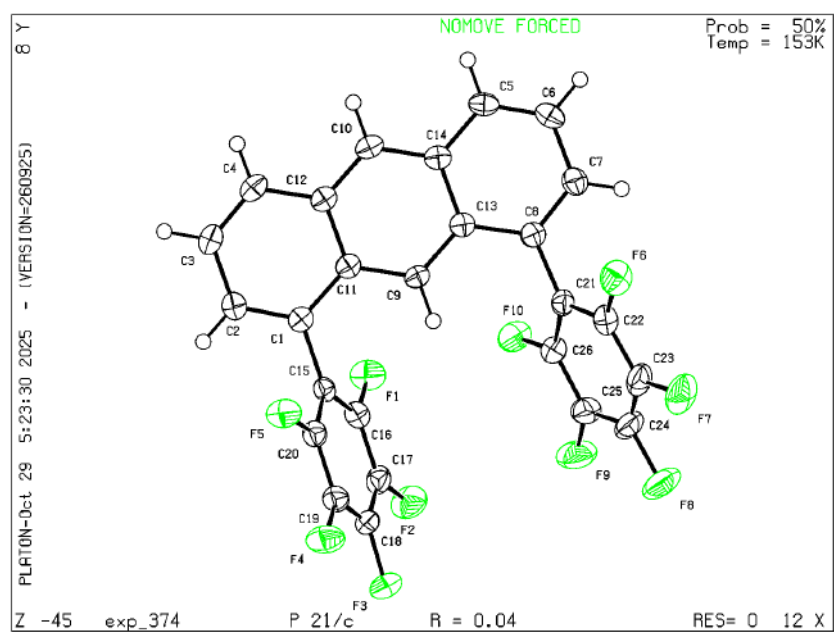
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Datablock exp_374 - ellipsoid plot





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Structure factors have been supplied for datablock(s) exp_375

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_375

Bond precision:	C-C = 0.0021 Å		Wavelength=0.71073
Cell:	a=10.5371 (4)	b=24.6150 (7)	c=7.9202 (3)
	alpha=90	beta=108.167 (4)	gamma=90
Temperature:	203 K		
	Calculated	Reported	
Volume	1951.87 (13)	1951.87 (13)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H8 F10	?	
Sum formula	C26 H8 F10	C26 H8 F10	
Mr	510.32	510.32	
Dx, g cm ⁻³	1.737	1.737	
Z	4	4	
Mu (mm ⁻¹)	0.168	0.168	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	13, 30, 9	13, 30, 9	
Nref	3986	3983	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.999

Theta(max)= 26.372

R(reflections)= 0.0390 (3249)

wR2(reflections)=
0.1043 (3983)

S = 1.069

Npar= 325

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check

Alert level G

PLAT434_ALERT_2_G	Short Inter HL..HL Contact F7	..F8	2.75 Ang.
	x, 3/2-y, 1/2+z	=	4_576 Check
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL		2019/3 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=		2.62 Note
	1 0 0, 1 1 0, 0 2 0,		
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		2 Note
	1 0 0, 1 1 0,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.1 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		2.905 Note
	Predicted wR2: Based on SigI**2	3.59 or SHELX Weight	9.76
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		8 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

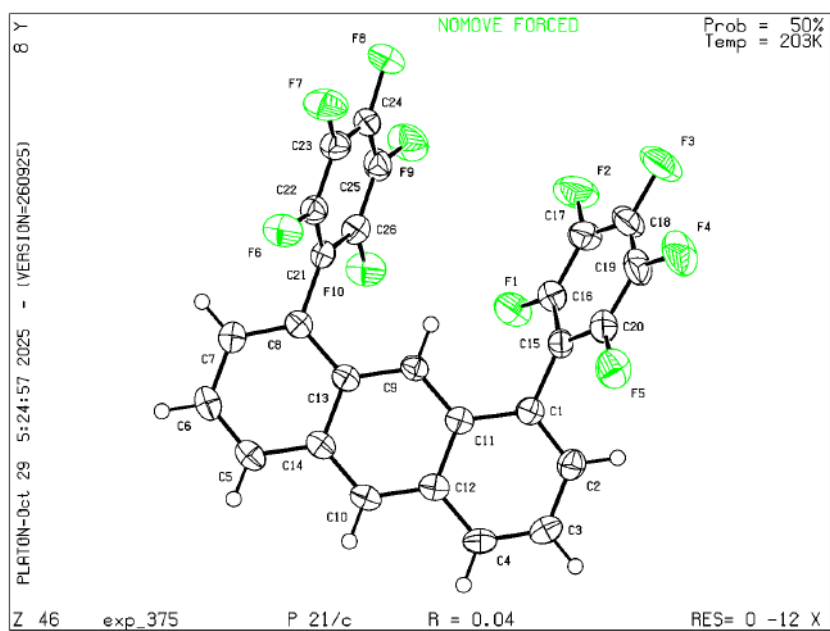
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

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No duplication found

Datablock exp_375 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_376

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_376

Bond precision:	C-C = 0.0023 Å	Wavelength=0.71073	
Cell:	a=10.5609 (4)	b=24.6653 (7)	c=7.9592 (3)
	alpha=90	beta=108.061 (4)	gamma=90
Temperature:	253 K		
	Calculated	Reported	
Volume	1971.12 (13)	1971.12 (13)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H8 F10	?	
Sum formula	C26 H8 F10	C26 H8 F10	
Mr	510.32	510.32	
Dx, g cm ⁻³	1.720	1.720	
Z	4	4	
Mu (mm ⁻¹)	0.166	0.166	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	13, 30, 9	13, 30, 9	
Nref	4026	4024	
Tmin, Tmax	0.899, 0.944		
Tmin'	0.880		

Correction method= Not given

$$\text{Theta (max)} = 26.372$$

```
wR2(reflections)=  
0.1090( 4024)
```

Npar= 325

🟡 **Alert level C**

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
-------------------	--------------------------------------	-----------	-------------

```

Alert level G
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..      0.77 mm
PLAT434_ALERT_2_G Short Inter HL..HL Contact F3 ..F4 ..      2.77 Ang.
                                     x,1/2-y,-1/2+z =      4_565 Check
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..      Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated and Succeeded by SHELXL      2019/3 Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta (Min) [Deg]=      2.19 Note
      1 0 0, 0 2 0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      1 Note
      1 0 0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....      4.4 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      3.942 Note
      Predicted wr2: Based on SigI**2 2.77 or SHELX Weight 10.12
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      2 Info

```

0	ALERT level A	= Most likely a serious problem - resolve or explain
0	ALERT level B	= A potentially serious problem, consider carefully
1	ALERT level C	= Check. Ensure it is not caused by an omission or oversight
9	ALERT level G	= General information/check it is not something unexpected

```
2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
```

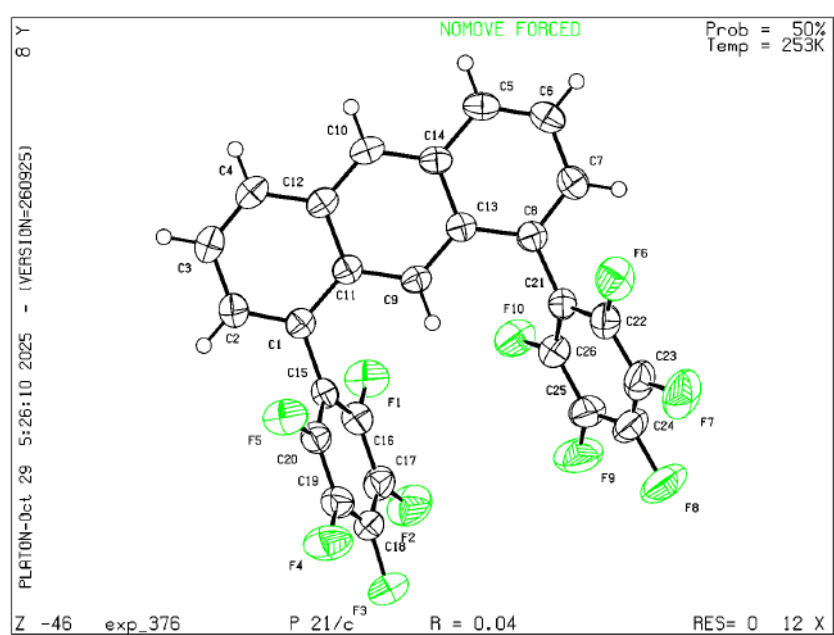
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

Datablock exp_376 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_346

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_346

Bond precision:	C-C = 0.0022 Å		Wavelength=0.71073
Cell:	a=10.5021 (4)	b=24.5534 (7)	c=7.8616 (3)
	alpha=90	beta=108.391 (4)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1923.67 (13)	1923.67 (12)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H8 F10	?	
Sum formula	C26 H8 F10	C26 H8 F10	
Mr	510.32	510.32	
Dx, g cm ⁻³	1.762	1.762	
Z	4	4	
Mu (mm ⁻¹)	0.170	0.170	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	13, 30, 9	13, 30, 9	
Nref	3933	3929	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.999 Theta(max)= 26.367

R(reflections)= 0.0391(3198) wR2(reflections)=
0.1050(3929)

S = 1.070 Npar= 325

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

 **Alert level C**

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error)	...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error)	...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error)	...	Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	2 Report
	10 0 0, 10 1 0,		

 **Alert level G**

PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3	..F4	.	2.72 Ang.
		x,1/2-y,-1/2+z =	4_565	Check
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..			Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL			2019/3 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=			2.21 Note
	1 0 0, 0 2 0,			
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			2 Note
	0 2 0, 1 0 0,			
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			3.1 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value			1.994 Note
	Predicted wR2: Based on SigI**2	5.26	or SHELX Weight	9.81
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			13 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

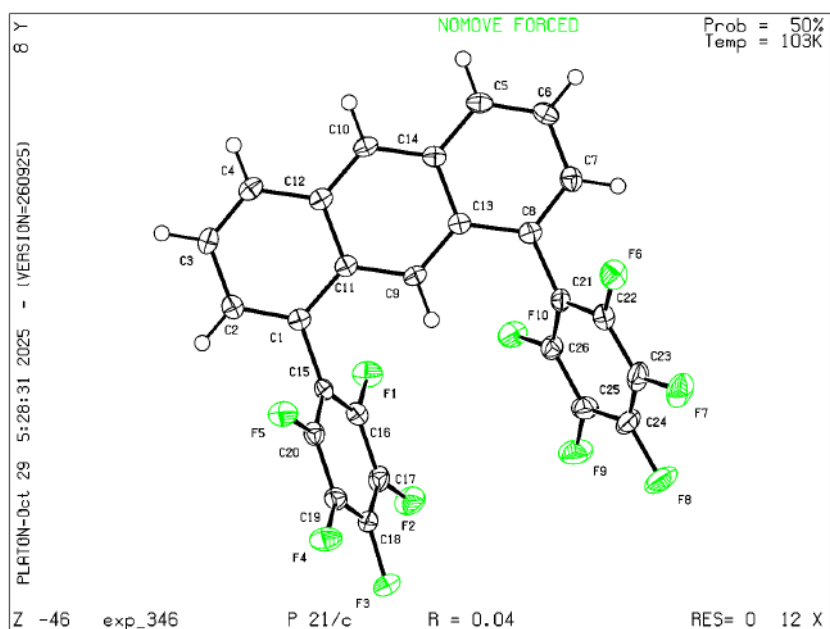
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

Datablock exp_346 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_347

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_347

Bond precision:	= 0.0000 Å	Wavelength=0.71073	
Cell:	a=10.4714 (4)	b=24.5654 (7)	c=7.8582 (3)
	alpha=90	beta=107.629 (4)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1926.47 (13)	1926.47 (12)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H8 F10	?	
Sum formula	C26 H8 F10	C26 H8 F10	
Mr	510.32	510.32	
Dx, g cm ⁻³	1.760	1.760	
Z	4	4	
Mu (mm ⁻¹)	0.170	0.170	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	14, 34, 11	13, 32, 9	
Nref	5718	4591	
Tmin, Tmax			
Tmin'			
Correction method= Not given			

Data completeness= 0.803 Theta(max)= 30.182

R(reflections)= 0.0409(3407) wR2(reflections)=
0.1040(4591)

S = 1.051 Npar= 650

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 5.014
Additional refinement cycles may be required.

Author Response: This alert is derived from the low quality of data due to the mixed cr

PLAT080_ALERT_2_A Maximum Shift/Error 5.01 Why ?

Author Response: This alert is derived from photoproduct, which is slightly disordered.

PLAT214_ALERT_2_A Atom C109 (Anion/Solvent) ADP max/min Ratio 7.3 prolat

Author Response: This alert is derived from photoproduct, which is slightly disordered.

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 7.06 Note

Author Response: This alert is derived from the low quality of data due to the mixed cr

PLAT212_ALERT_2_B ADP of Atom F101 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom F102 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C101 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C102 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C106 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C112 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C113 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C115 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C116 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C117 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C118 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C119 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT212_ALERT_2_B ADP of Atom C120 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoproduct, which is slightly disorder

Author Response: This alert is derived from photoproduct, which is slightly disordered.

Author Response: This alert is derived from photoproduct, which is slightly disordered.

Author Response: These alerts are derived from photoproduct, which is slightly disorder

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT214_ALERT_2_C	Atom C111 (Anion/Solvent) ADP max/min Ratio	4.1 oblate	

Author Response: This alert is derived from photoproduct, which is slightly disordered.

- Alert level G

[illegible]

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PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.          2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ          2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.          2 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.665 Note
                   Predicted wR2: Based on SigI**2  3.91 or SHELX Weight  9.88
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by        2 Check

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 3 ALERT level A = Most likely a serious problem - resolve or explain
17 ALERT level B = A potentially serious problem, consider carefully
 6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
84 ALERT level G = General information/check it is not something unexpected

 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 ALERT type 2 Indicator that the structure model may be wrong or deficient
67 ALERT type 3 Indicator that the structure quality may be low
 8 ALERT type 4 Improvement, methodology, query or suggestion
 4 ALERT type 5 Informative message, check

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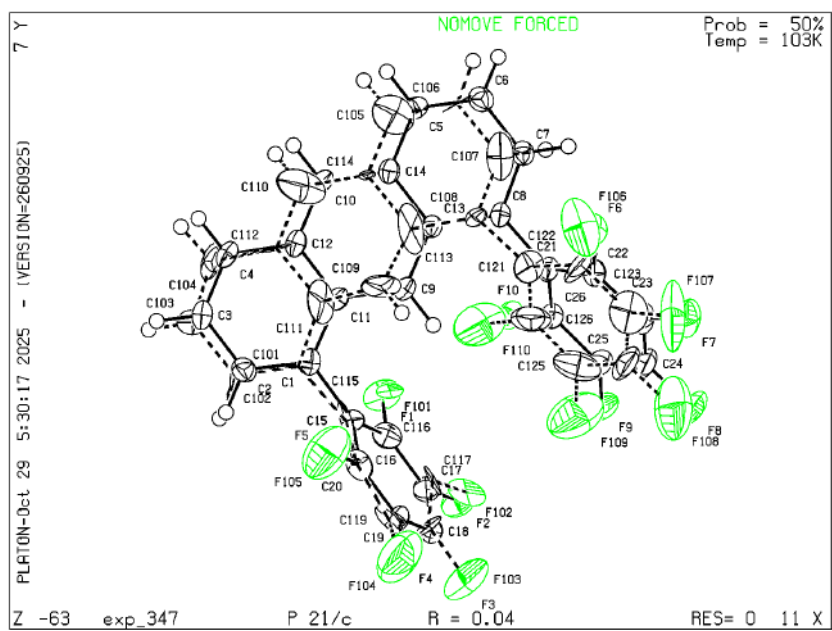
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

Datablock exp_347 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_348

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_348

Bond precision:	= 0.0000 Å	Wavelength=0.71073	
Cell:	a=10.4329 (7)	b=24.6081 (11)	c=7.8634 (5)
	alpha=90	beta=106.521 (7)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1935.5 (2)	1935.5 (2)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H8 F10	?	
Sum formula	C26 H8 F10	C26 H8 F10	
Mr	510.32	510.32	
Dx, g cm ⁻³	1.751	1.751	
Z	4	4	
Mu (mm ⁻¹)	0.169	0.169	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	14, 34, 11	13, 32, 11	
Nref	5704	4690	
Tmin, Tmax			
Tmin'			
Correction method= Not given			

Data completeness= 0.822 Theta(max)= 30.122

R(reflections)= 0.0496(3109) wR2(reflections)=
0.1460(4690)

S = 1.041 Npar= 650

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 7.22 Note

Author Response: This alert is derived from the low quality of data due to the mixed cr

PLAT214_ALERT_2_B Atom C117 (Anion/Solvent) ADP max/min Ratio 5.9 prolat

Author Response: This alert is derived from photoproduct, which is slightly disordered.

Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT214_ALERT_2_C Atom C112 (Anion/Solvent) ADP max/min Ratio 4.7 prolat

Author Response: This alert is derived from photoproduct, which is slightly disordered.

PLAT214_ALERT_2_C Atom C120 (Anion/Solvent) ADP max/min Ratio 4.9 prolat

Author Response: This alert is derived from photoproduct, which is slightly disordered.

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 2.2 Note
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for C109 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for C110 Check
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
 1 0 0,

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 72 Note
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 102 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report

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PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 1)	32.38	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	11.62	Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C109 --C110	1.88	Ang.
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	102	Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]= 0 2 0,	2.04	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	919	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.5	Low
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2	Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ	2	Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	3.422	Note
Predicted wR2: Based on SigI**2 4.27 or SHELX Weight 14.02			

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 2 **ALERT level B** = A potentially serious problem, consider carefully
 10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 79 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 6 ALERT type 2 Indicator that the structure model may be wrong or deficient
 68 ALERT type 3 Indicator that the structure quality may be low
 9 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check

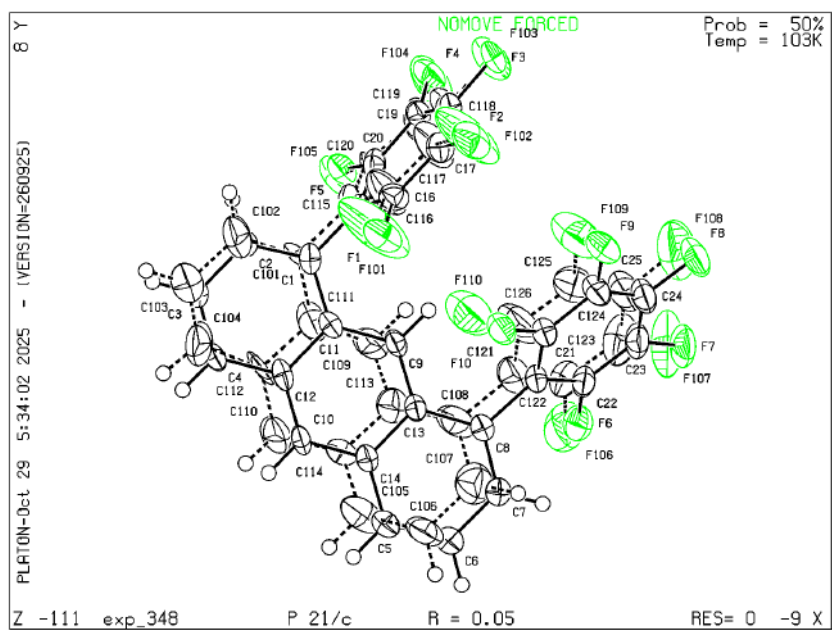
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

Datablock exp_348 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_349

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_349

Bond precision:	= 0.0000 Å		Wavelength=0.71073
Cell:	a=10.3382 (18)	b=24.587 (2)	c=7.8557 (16)
	alpha=90	beta=104.463 (19)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1933.5 (6)	1933.5 (6)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	0.245 (C52 H16 F20), 0.844 (C26 H8 F10)	?	
Sum formula	C34.67 H10.67 F13.33	C26 H8 F10	
Mr	680.43	510.32	
Dx, g cm-3	1.753	1.753	
Z	3	4	
Mu (mm-1)	0.169	0.169	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	14, 34, 11	12, 33, 9	
Nref	5702	4623	
Tmin, Tmax			
Tmin'			
Correction method= Not given			

Data completeness= 0.811 Theta(max)= 30.126

R(reflections)= 0.0735(2310) wR2(reflections)=
0.2393(4623)

S = 1.047 Npar= 650

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 7.11 Note

Author Response: This alert is derived from the low quality of data due to the mixed cr

Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings	Differ	Please Check
	Calc: C34.67 H10.67 F13.33			
	Rep.: C26 H8 F10			
PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given		Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...			Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...			Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...			Please Check
PLAT213_ALERT_2_C	Atom C122	has ADP max/min Ratio		3.4 oblate
PLAT213_ALERT_2_C	Atom C124	has ADP max/min Ratio		3.4 prolat
PLAT214_ALERT_2_C	Atom C23	(Anion/Solvent) ADP max/min Ratio		4.1 prolat
PLAT214_ALERT_2_C	Atom C24	(Anion/Solvent) ADP max/min Ratio		4.5 prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range			3.4 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C18	--C19	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C21	--C22	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C23	--C24	.	0.18 Ang.
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)			2.4 Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2)			2.9 Note
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist. C115	-C120	.	1.37 Ang.
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist. C21	-C26	.	1.37 Ang.
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...			-5.314 Report
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		7 Report
	1 2 1, 1 17 1, 2 8 2, 5 0 6, 5 1 6,			5 2 6,
	5 3 6,			

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	72	Note
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.750	Check
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	102	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report

[illegible]

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PLAT230_ALERT_2_G Hirshfeld Test Diff for F6 --C22 . 6.3 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 1) 32.30 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2) 27.85 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C109 --C110 1.71 Ang.
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 102 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated and Succeeded by SHELXL 2019/3 Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]= 2.20 Note
1 0 0, 0 2 0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 728 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
1 0 0, 1 17 1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.4 Low
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 2 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 2 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.101 Note
Predicted wR2: Based on SigI**2 7.72 or SHELX Weight 22.86

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0 ALERT level A = Most likely a serious problem - resolve or explain
1 ALERT level B = A potentially serious problem, consider carefully
19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
84 ALERT level G = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 ALERT type 2 Indicator that the structure model may be wrong or deficient
69 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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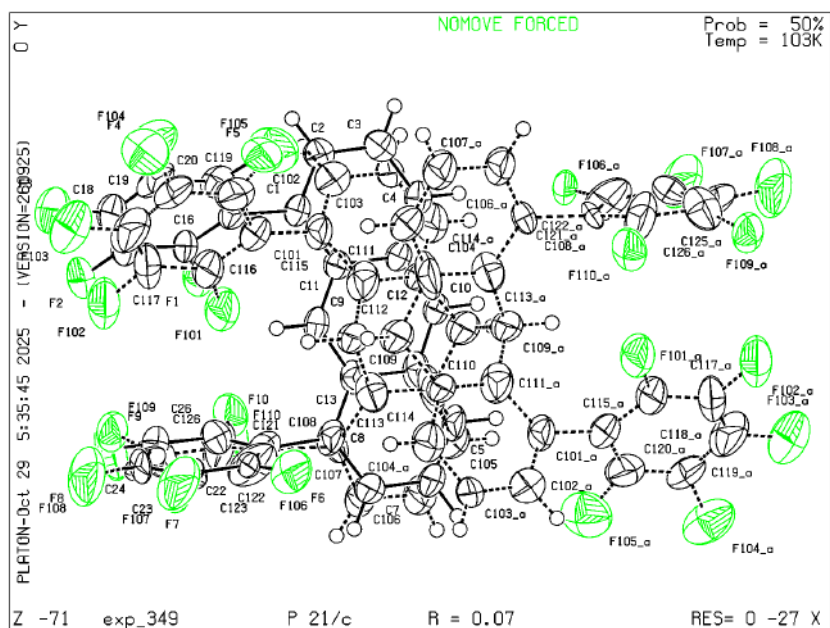
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PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

Datablock exp_349 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_350

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_350

Bond precision:	= 0.0000 Å		Wavelength=0.71073
Cell:	a=10.2366 (12)	b=24.5406 (17)	c=7.8620 (12)
	alpha=90	beta=101.428 (13)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1935.9(4)	1935.9(4)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	0.507(C52 H16 F20), 0.986(C26 H8 F10)	?	
Sum formula	C52 H16 F20	C52 H16 F20	
Mr	1020.65	1020.65	
Dx, g cm-3	1.751	1.751	
Z	2	2	
Mu (mm-1)	0.169	0.169	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	12, 30, 9	12, 30, 9	
Nref	3962	3949	
Tmin, Tmax			
Tmin'			
Correction method= Not given			

Data completeness= 0.997 Theta(max)= 26.372

R(reflections)= 0.0641(2452) wR2(reflections)=
0.1515(3949)

S = 1.070 Npar= 650

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.08 Note

Author Response: This alert is derived from the low quality of data due to the mixed cr

PLAT213_ALERT_2_B Atom C20 has ADP max/min Ratio 4.8 oblate

Author Response: This alert is derived from photoreactant, which is highly disordered.

Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT213_ALERT_2_C Atom C18 has ADP max/min Ratio 3.1 prolat

Author Response: This alert is derived from photoreactant, which is highly disordered.

PLAT234_ALERT_4_C Large Hirshfeld Difference C1 --C15 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C16 --C17 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C23 --C24 . 0.17 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.7 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 2.6 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 8 Report
7 5 3, 0 18 3, -3 0 4, 7 7 4, 2 16 4, 2 15 5,
-3 24 5, -3 2 9,

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 72 Note
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 102 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report

[illegible]

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PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 1) 44.62 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2) 21.69 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 102 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated and Succeeded by SHELXL 2019/3 Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]= 2.19 Note
1 0 0, 0 2 0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 4 Note
1 0 0, 0 18 3, -3 0 4, 2 16 4,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.2 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.278 Note
Predicted wR2: Based on SigI**2 4.62 or SHELX Weight 14.15

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0 ALERT level A = Most likely a serious problem - resolve or explain
2 ALERT level B = A potentially serious problem, consider carefully
11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
77 ALERT level G = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
68 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

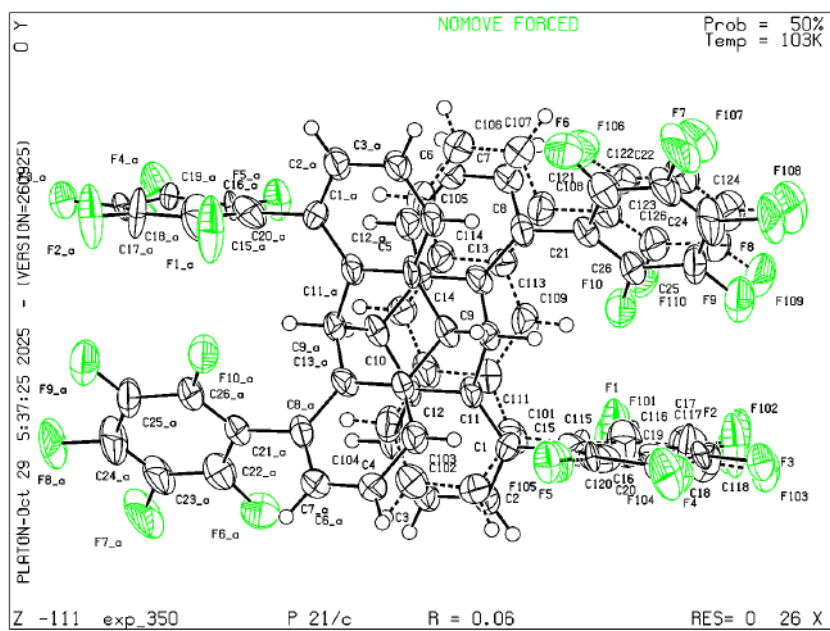
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_351

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_351

Bond precision:	= 0.0000 Å		Wavelength=0.71073
Cell:	a=10.1635 (9)	b=24.5361 (13)	c=7.8585 (7)
	alpha=90	beta=99.624 (8)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1932.1 (3)	1932.1 (3)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	1.282 (C52 H16 F20), 1.436 (C26 H8 F10)	?	
Sum formula	C104 H32 F40	C52 H16 F20	
Mr	2041.30	1020.65	
Dx, g cm-3	1.754	1.754	
Z	1	2	
Mu (mm-1)	0.170	0.170	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	12, 30, 9	12, 30, 9	
Nref	3945	3940	
Tmin, Tmax	0.962, 0.976		
Tmin'	0.953		
Correction method= Not given			

Data completeness= 0.999 Theta(max)= 26.370

R(reflections)= 0.0567 (2649) wR2(reflections)=
0.1570 (3940)

S = 1.067 Npar= 650

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.06 Note

Author Response: This alert is derived from the low quality of data due to the mixed cr

PLAT214_ALERT_2_B Atom C121 (Anion/Solvent) ADP max/min Ratio 5.2 oblate

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT214_ALERT_2_B Atom C123 (Anion/Solvent) ADP max/min Ratio 5.8 oblate

Author Response: These alerts are derived from photoreactant, which is highly disordere

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: C104 H32 F40
Rep.: C52 H16 F20
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT214_ALERT_2_C Atom F109 (Anion/Solvent) ADP max/min Ratio 4.3 prolat

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT234_ALERT_4_C Large Hirshfeld Difference F9 --C25 . 0.17 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 2.4 Note
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C115 -C120 . 1.37 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
-6 24 3, 7 0 6, 7 1 6,

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 72 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 102 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report

[illegible]

PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 1)	56.41	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	15.80	Check
PLAT793_ALERT_4_G	Model has Chirality at C9 (Centro SpGr)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C10 (Centro SpGr)		R Verify
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	2	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	102	Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta (Min) [Deg]= 0 2 0,	2.03	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.1	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	3.214	Note
Predicted wR2: Based on SigI**2 4.88 or SHELX Weight 14.71			

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 3 **ALERT level B** = A potentially serious problem, consider carefully
 8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 79 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 7 ALERT type 2 Indicator that the structure model may be wrong or deficient
 68 ALERT type 3 Indicator that the structure quality may be low
 10 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

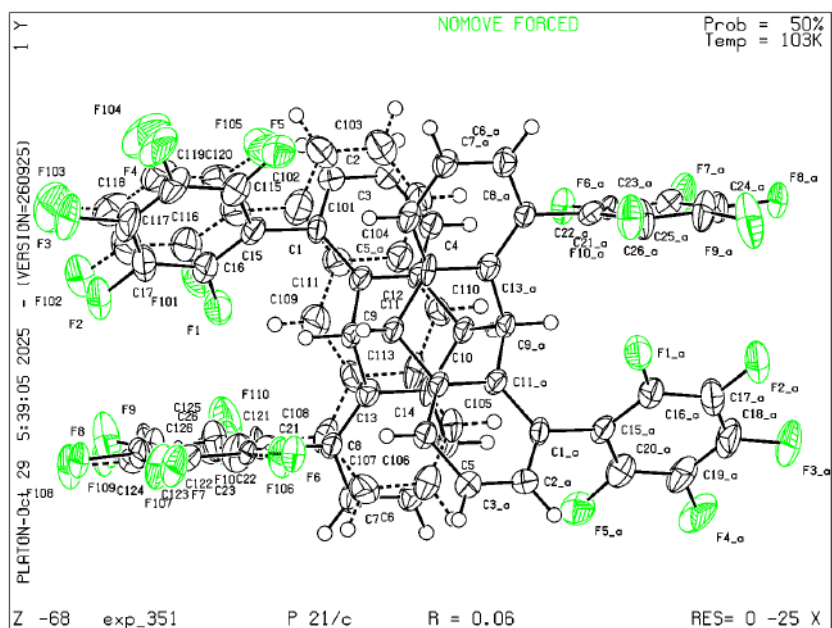
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

Datablock exp_351 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_353

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_353

Bond precision:	= 0.0000 Å		Wavelength=0.71073
Cell:	a=10.1108 (5)	b=24.5235 (9)	c=7.8720 (4)
	alpha=90	beta=98.557 (5)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1930.15 (16)	1930.15 (16)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	0.77 (C52 H16 F20), 0.46 (C26 H8 F10)		?
Sum formula	C52 H16 F20	C52 H16 F20	
Mr	1020.65	1020.65	
Dx, g cm-3	1.756	1.756	
Z	2	2	
Mu (mm-1)	0.170	0.170	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	14, 34, 11	12, 34, 9	
Nref	5710	4599	
Tmin, Tmax			
Tmin'			
Correction method= Not given			

Data completeness= 0.805 Theta(max)= 30.147

R(reflections)= 0.0455(3401) wR2(reflections)=
0.1243(4599)

S = 1.040 Npar= 650

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

 Alert level A

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 2.423
Additional refinement cycles may be required.

Author Response: This alert is derived from the low quality of data due to the mixed cr

PLAT080_ALERT_2_A Maximum Shift/Error 2.42 Why ?

Author Response: This alert is derived from photoreactant, which is highly disordered.

 Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 7.08 Note

Author Response: This alert is derived from the low quality of data due to the mixed cr

PLAT212_ALERT_2_B ADP of Atom C121 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordered

PLAT212_ALERT_2_B ADP of Atom C123 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordered

PLAT212_ALERT_2_B ADP of Atom C126 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordered

PLAT214_ALERT_2_B Atom C108 (Anion/Solvent) ADP max/min Ratio 5.2 prolat

Author Response: This alert is derived from photoreactant, which is highly disordered.

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2)		2.2 Note
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist. C115 -C120		1.36 Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & Sth/L=	0.600	3 Report
	1 0 0, 7 13 2, 9 1 3,		
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc)		1 Check
	0 2 0.		

●

[illegible]

PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C22 --C23 .	5.7	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C24 --C25 .	6.8	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C25 --C26 .	5.5	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 1)	67.76	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	10.12	Check
PLAT793_ALERT_4_G	Model has Chirality at C9 (Centro SpGr)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C10 (Centro SpGr)	R	Verify
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	3	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	102	Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please	Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	811	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
	1 0 0,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.9	Low
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	2	Units
PLAT956_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Hmax Differ	2	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	2	Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.992	Note
	Predicted wR2: Based on SigI**2 4.15 or SHELX Weight 11.94		

-
- 2 **ALERT level A** = Most likely a serious problem - resolve or explain
5 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
85 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

13 ALERT type 2 Indicator that the structure model may be wrong or deficient
68 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

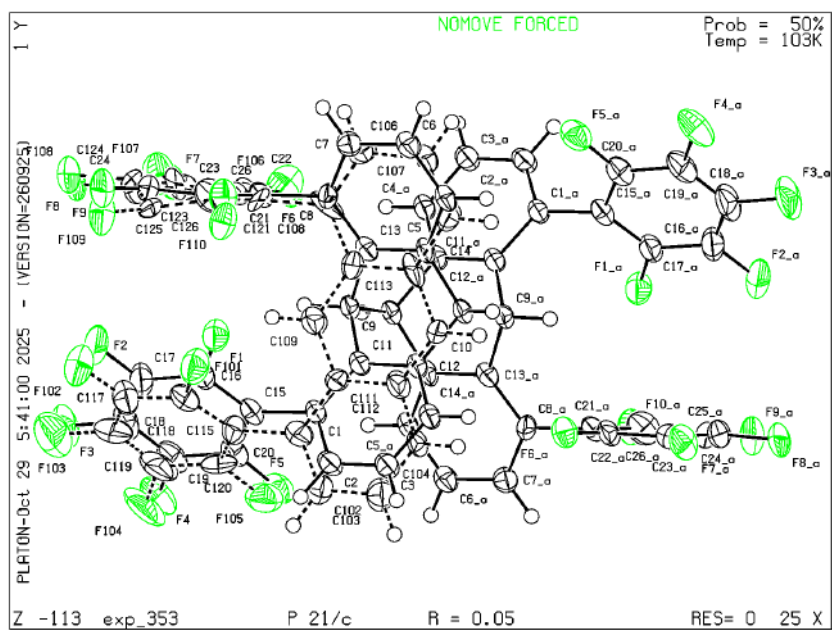
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

Datablock exp_353 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_354

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_354

Bond precision:	= 0.0000 Å	Wavelength=0.71073	
Cell:	a=10.0742 (4)	b=24.5203 (7)	c=7.8996 (3)
	alpha=90	beta=97.881 (4)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1932.95 (12)	1932.95 (12)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	0.845 (C52 H16 F20), 0.31 (C26 H8 F10)	?	
Sum formula	C52 H16 F20	C52 H16 F20	
Mr	1020.65	1020.65	
Dx, g cm-3	1.754	1.754	
Z	2	2	
Mu (mm-1)	0.169	0.169	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	12, 30, 9	12, 30, 9	
Nref	3942	3939	
Tmin, Tmax			
Tmin'			
Correction method= Not given			

Data completeness= 0.999 Theta(max)= 26.371

R(reflections)= 0.0378(3129) wR2(reflections)=
0.0999(3939)

S = 1.041 Npar= 650

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 3.110
Additional refinement cycles may be required.

Author Response: This alert is derived from the low quality of data due to the mixed cr

PLAT080_ALERT_2_A Maximum Shift/Error 3.11 Why ?

Author Response: This alert is derived from photoreactant, which is highly disordered.

PLAT214_ALERT_2_A Atom C105 (Anion/Solvent) ADP max/min Ratio 6.1 prolat

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT214_ALERT_2_A Atom C118 (Anion/Solvent) ADP max/min Ratio 10.7 prolat

Author Response: These alerts are derived from photoreactant, which is highly disordere

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.06 Note

Author Response: This alert is derived from the low quality of data due to the mixed cry

PLAT212_ALERT_2_B ADP of Atom F107 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT212_ALERT_2_B ADP of Atom C101 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT212_ALERT_2_B ADP of Atom C115 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT212_ALERT_2_B ADP of Atom C116 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT212_ALERT_2_B ADP of Atom C117 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT212_ALERT_2_B ADP of Atom C119 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT212_ALERT_2_B ADP of Atom C123 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT212_ALERT_2_B ADP of Atom C124 is N.P.D. or (nearly) 2D . Please Check

Author Response: These alerts are derived from photoreactant, which is highly disordere

PLAT221_ALERT_2_B Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range 10.0 Ratio

Author Response: This alert is derived from photoreactant, which is highly disordered.

 Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT221_ALERT_2_C Solv./Anion Resd 2 F Ueq(max)/Ueq(min) Range		7.4 Ratio

Author Response: This alert is derived from photoreactant, which is highly disordered.

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
1 0 0, -4 4 6,

 Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	72 Note
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records	102 Report

181

PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C19 --C20	6.7	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C24 --C25	6.0	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 1)	74.36	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	6.82	Check
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	5	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	102	Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
	1 0 0,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	3.172	Note
	Predicted wR2: Based on SigI**2 3.15 or SHELX Weight	9.58	

4 **ALERT level A** = Most likely a serious problem - resolve or explain
 10 **ALERT level B** = A potentially serious problem, consider carefully
 6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 78 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 18 ALERT type 2 Indicator that the structure model may be wrong or deficient
 67 ALERT type 3 Indicator that the structure quality may be low
 7 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

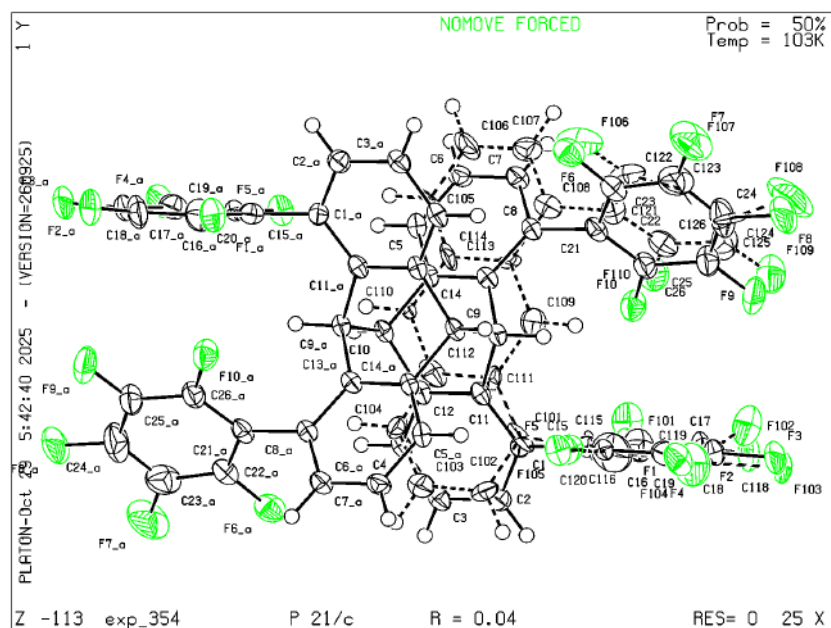
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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Datablock exp_354 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_355

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_355

Bond precision:	C-C = 0.0041 Å		Wavelength=0.71073
Cell:	a=10.0528 (4)	b=24.5186 (7)	c=7.9026 (3)
	alpha=90	beta=97.513 (4)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1931.12 (12)	1931.12 (12)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C52 H16 F20	?	
Sum formula	C52 H16 F20	C52 H16 F20	
Mr	1020.65	1020.65	
Dx, g cm ⁻³	1.755	1.755	
Z	2	2	
Mu (mm ⁻¹)	0.170	0.170	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	12, 30, 9	12, 30, 9	
Nref	3946	3929	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.996

Theta(max)= 26.371

R(reflections)= 0.0625(3139)

wR2(reflections)=
0.1730(3929)

S = 1.097

Npar= 325

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.13 eA-3

Author Response: This alert is derived from photoreactant, which is slightly disordered

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error)	...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error)	...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error)	...	Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		2.43 Report
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0041 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.073 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	14 Report
	5 1 1, 4 8 1, -1 10 1, -2 12 1, 1 0 2, 2 0 2,		
	-3 1 2, -2 1 2, 1 3 2, -4 2 3, 2 0 4, 2 2 4,		
	7 0 6, -5 2 9,		

Alert level G

PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3	..F4	.	2.73 Ang.
		x,1/2-y,1/2+z =		4_566 Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3	..F6	.	2.83 Ang.
		1+x,y,z =		1_655 Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F4	..F9	.	2.80 Ang.
		x,1/2-y,-1/2+z =		4_565 Check
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters			1 Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..			Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL			2019/3 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min)[Deg]=			2.21 Note
	1 0 0, 0 2 0,			
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		1 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			14 Note
	1 0 0, 0 2 0, 1 0 2, 2 0 2, -2 1 2, -2 12 1,			
	-3 1 2, -4 2 3, 2 2 4, -1 10 1, 5 1 1, 2 0 4,			
	1 3 2, 4 8 1,			
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			3.2 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value			5.119 Note

Predicted wR2: Based on SigI**2 3.38 or SHELX Weight 15.77
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
12 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

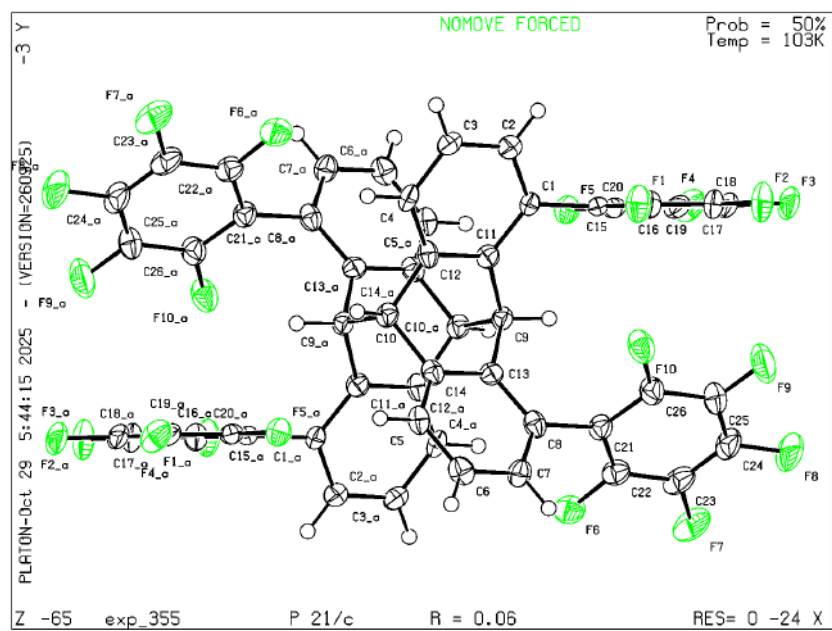
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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Datablock exp_355 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_356

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_356

Bond precision:	C-C = 0.0034 Å		Wavelength=0.71073
Cell:	a=10.0271 (4)	b=24.4615 (7)	c=7.9076 (3)
	alpha=90	beta=97.376 (3)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1923.51 (12)	1923.51 (12)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C52 H16 F20	?	
Sum formula	C52 H16 F20	C52 H16 F20	
Mr	1020.65	1020.65	
Dx, g cm ⁻³	1.762	1.762	
Z	2	2	
Mu (mm ⁻¹)	0.170	0.170	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	12, 30, 9	12, 30, 9	
Nref	3924	3924	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 1.000 Theta(max)= 26.367

R(reflections)= 0.0534(3251) wR2(reflections)=
 0.1465(3924)

S = 1.069 Npar= 325

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
 Click on the hyperlinks for more details of the test.

 Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
 The relevant atom site should be identified.

PLAT052_ALERT_1_C Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density	0.86 eA-3	

 Alert level G

PLAT434_ALERT_2_G Short Inter HL..HL Contact F2	..F7	.	2.78 Ang.
	x,3/2-y,1/2+z =		4_576 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F5	..F8	.	2.83 Ang.
	-1+x,y,z =		1_455 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F7	..F8	.	2.73 Ang.
	x,3/2-y,-1/2+z =		4_575 Check
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..			Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated and Succeeded by SHELXL			2019/3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity			3.3 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value			4.565 Note
	Predicted wR2: Based on SigI**2	3.21 or SHELX Weight	13.70
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.			5 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 8 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
 1 ALERT type 3 Indicator that the structure quality may be low
 1 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

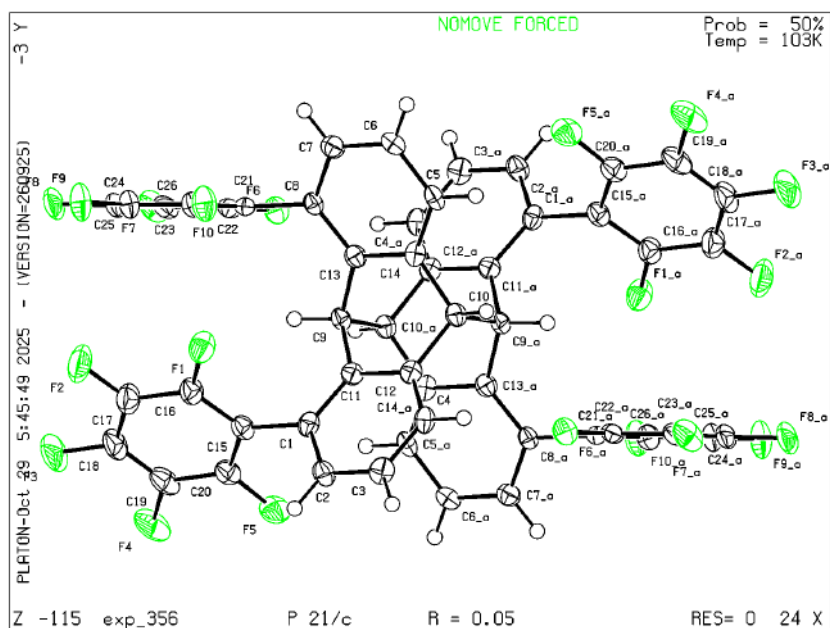
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Datablock exp_356 - ellipsoid plot





checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_357

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_357

Bond precision:	C-C = 0.0022 Å		Wavelength=0.71073
Cell:	a=9.9934 (3)	b=24.4447 (5)	c=7.9097 (2)
	alpha=90	beta=97.139 (3)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	1917.25 (9)	1917.25 (9)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C52 H16 F20	?	
Sum formula	C52 H16 F20	C52 H16 F20	
Mr	1020.65	1020.65	
Dx, g cm ⁻³	1.768	1.768	
Z	2	2	
Mu (mm ⁻¹)	0.171	0.171	
F000	1016.0	1016.0	
F000'	1016.91		
h, k, lmax	12, 30, 9	12, 30, 9	
Nref	3915	3914	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 1.000 Theta(max)= 26.367

R(reflections)= 0.0393(3257) wR2(reflections)=
0.1061(3914)

S = 1.070 Npar= 325

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

● Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error)	...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error)	...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error)	...	Please Check

● Alert level G

PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3	..F4	.	2.73 Ang.
		x,1/2-y,1/2+z =		4_566 Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3	..F6	.	2.82 Ang.
		1+x,y,z =		1_655 Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F4	..F9	.	2.77 Ang.
		x,1/2-y,-1/2+z =		4_565 Check
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary	..		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated	and Succeeded by SHELXL		2019/3 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			1 Note
	1 0 0,			
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			3.4 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value			3.310 Note
	Predicted wR2: Based on SigI**2	3.20 or SHELX Weight	9.92	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			16 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
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5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

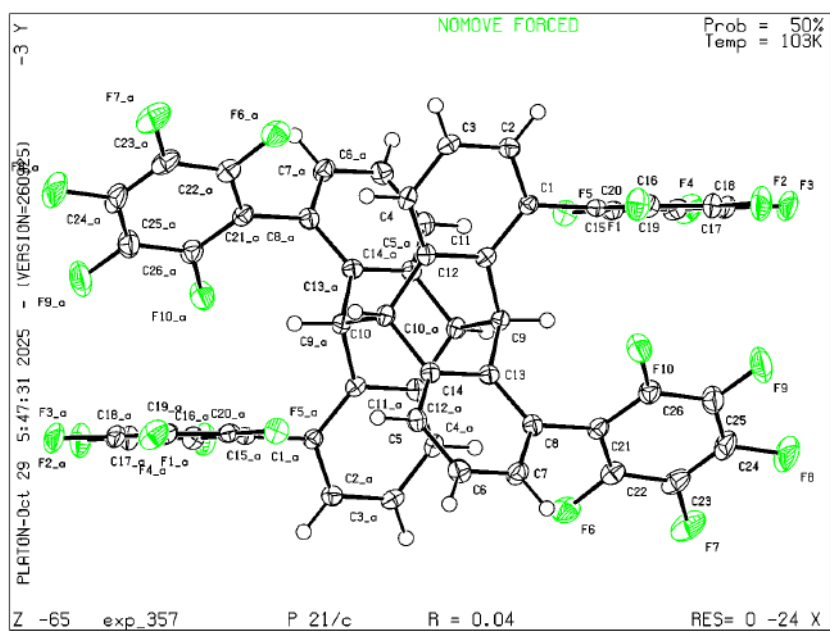
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PLATON version of 26/09/2025; check.def file version of 20/09/2025

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No duplication found

Datablock exp_357 - ellipsoid plot



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