

Heterologous Perylene Diimides Arrays: Potential Non-fullerene Acceptors in Organic Solar Cells

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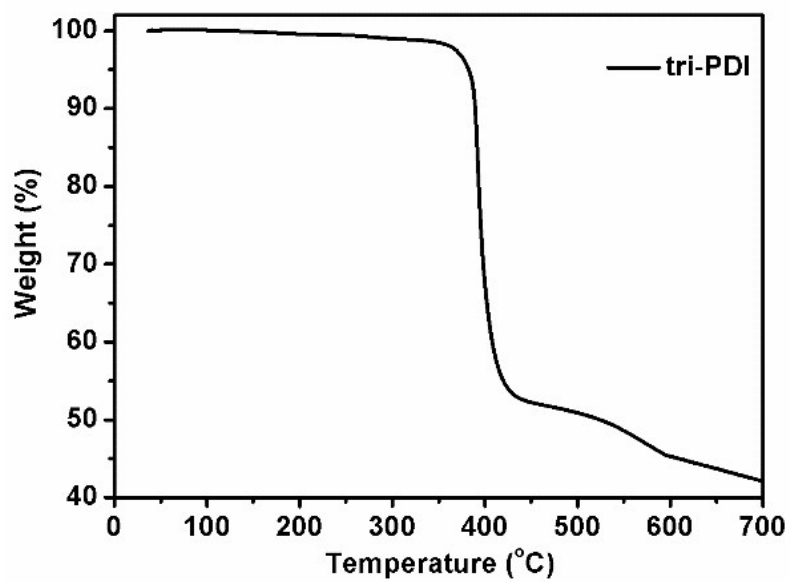
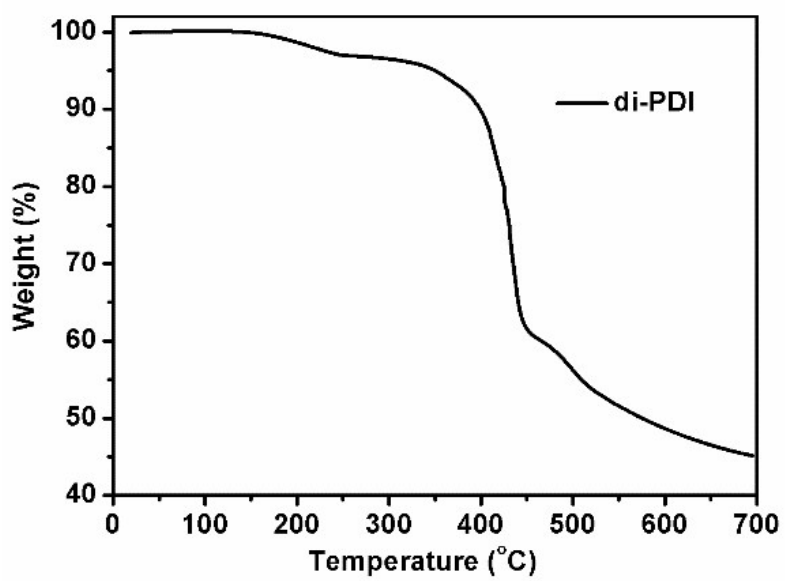


Fig. S1 TGA plots of **di-PDI** and **tri-PDI** (10 °C/min under N₂).

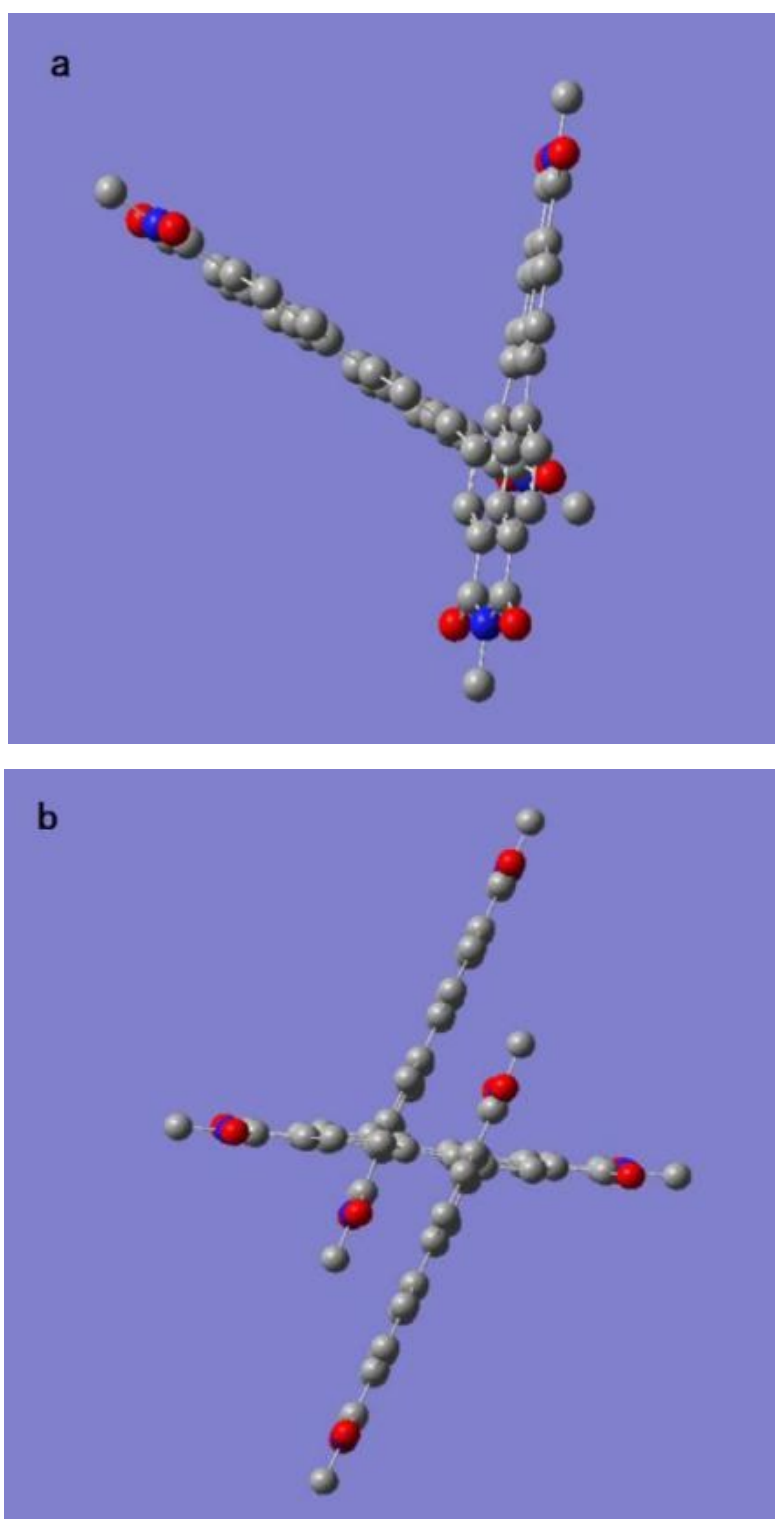


Fig. S2 Ground-state geometries of **di-PDI** and **tri-PDI** calculated from DFT.

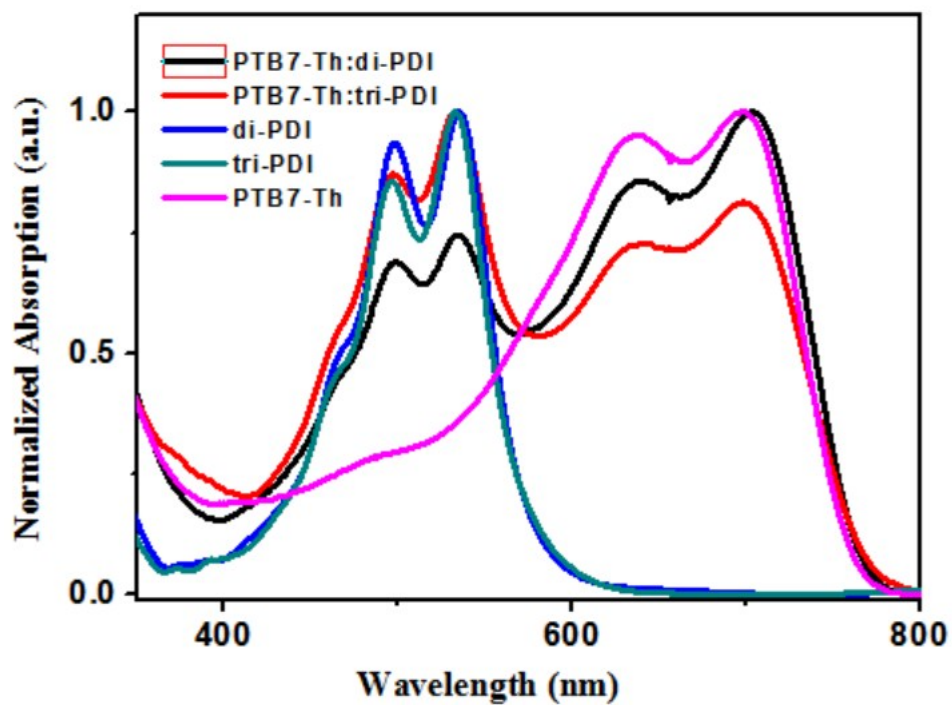


Fig. S3 Normalized UV-vis absorption spectra of **di-PDI**, **tri-PDI**, **PTB7-Th**, and their blend films in solid state.

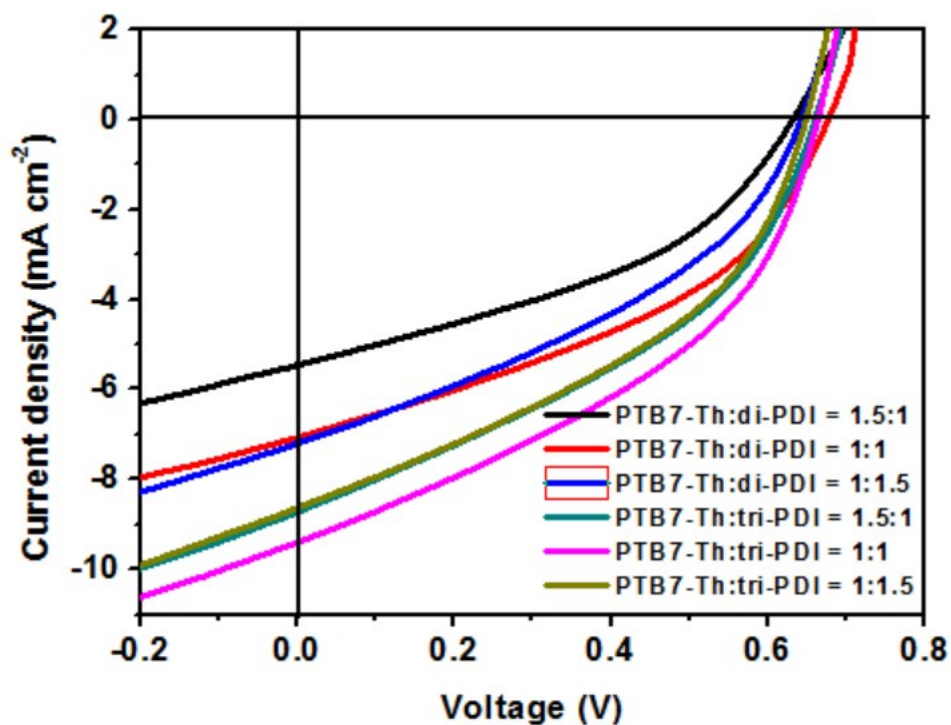


Fig. S4 J - V curves of PTB7-Th:tri-PDI (di-PDI) with different D/A ratios.

Table S1. Summary of device parameters of PTB7-Th:tri-PDI (di-PDI) with different D/A ratios.

Blend films	Ratio [wt/wt]	J_{sc} [mA/cm ²]	V_{oc} [V]	FF [%]	$PCE_{ave(max)}$ [%]
PTB7-Th: di-PDI	1.5:1	5.33±0.14 (5.46)	0.623±0.005 (0.628)	39.9±0.4 (40.2)	1.26 (1.38)
	1:1	6.96±0.12 (7.08)	0.669±0.003 (0.673)	40.5±0.3 (40.8)	1.81 (1.95)
	1:1.5	7.09±0.11 (7.20)	0.649±0.006 (0.655)	36.7±0.5 (37.2)	1.59 (1.74)
PTB7-Th: tri-PDI	1.5:1	8.53±0.14 (8.67)	0.662±0.005 (0.667)	38.9±0.2 (39.1)	2.12 (2.26)
	1:1	9.24±0.12 (9.36)	0.659±0.002 (0.661)	41.1±0.2 (41.2)	2.41 (2.54)
	1:1.5	8.49±0.14 (8.63)	0.657±0.004 (0.661)	38.7±0.5 (39.1)	2.08 (2.23)

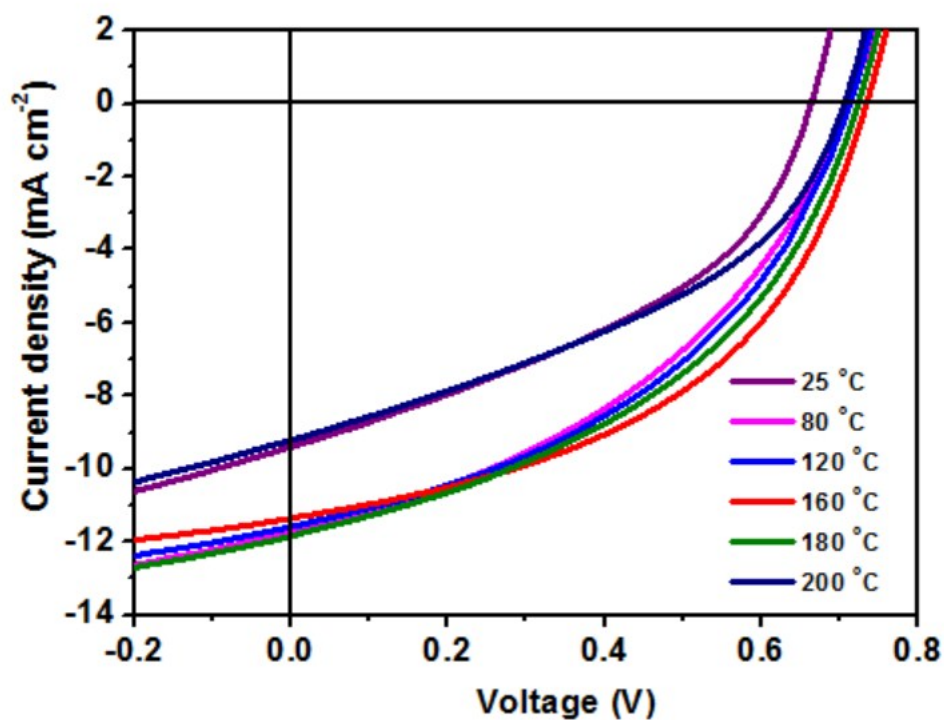


Fig. S5 J - V curves of PTB7-Th:tri-PDI (1:1) with different annealing temperature

Table S2. Summary of device parameters of PTB7-Th:tri-PDI (1:1) with different annealing temperature.

Temp. [°C]	J_{SC} [mA/cm ²]	V_{OC} [V]	FF [%]	$PCE_{ave(max)}$ [%]
25	9.24±0.12 (9.36)	0.659±0.002 (0.661)	41.1±0.2 (41.2)	2.41 (2.54)
80	11.59±0.14 (11.73)	0.706±0.005 (0.711)	40.8±0.4 (41.1)	3.27 (3.42)
120	11.48±0.12 (11.59)	0.713±0.003 (0.716)	42.4±0.4 (42.8)	3.39 (3.55)
160	11.22±0.13 (11.35)	0.731±0.005 (0.735)	46.9±0.3 (47.2)	3.82 (3.94)
180	11.73±0.12 (11.84)	0.735±0.002 (0.737)	42.1±0.4 (42.4)	3.59 (3.70)
200	9.07±0.14 (9.21)	0.716±0.005 (0.720)	39.1±0.5 (39.4)	2.48 (2.61)

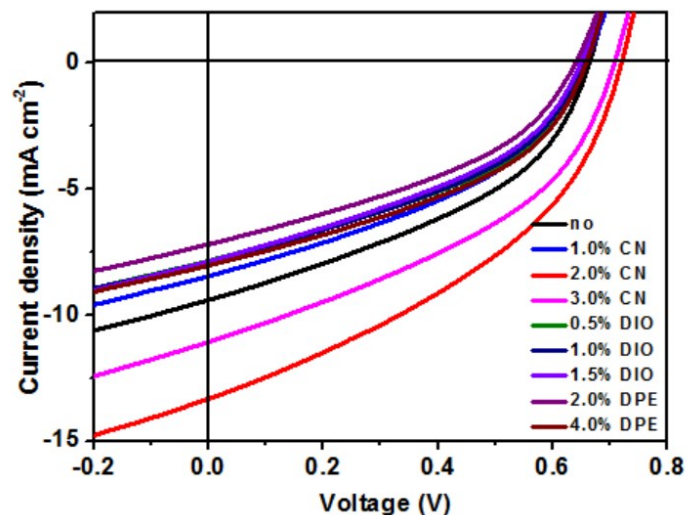


Fig. S6 J - V curves of PTB7-Th:tri-PDI (1:1) with different additives.

Table S3. Summary of device parameters of PTB7-Th:tri-PDI (1:1) with different additives.

Additives [volume]	J_{sc} [mA/cm ²]	V_{oc} [V]	FF [%]	$PCE_{ave(max)}$ [%]
No	9.24±0.12 (9.36)	0.659±0.002 (0.661)	41.1±0.2 (41.2)	2.41 (2.54)
1.0% CN	8.38±0.13 (8.51)	0.656±0.003 (0.659)	39.1±0.5 (39.6)	2.08 (2.22)
2.0% CN	13.28±0.13 (13.41)	0.709±0.004 (0.713)	39.6±0.4 (40.0)	3.70 (3.82)
3.0% CN	11.06±0.11 (11.16)	0.699±0.004 (0.703)	40.2±0.3 (40.4)	3.04 (3.17)
0.5% DIO	7.54±0.14 (7.68)	0.652±0.004 (0.656)	41.4±0.3 (41.7)	2.01 (2.10)
1.0% DIO	7.58±0.14 (7.71)	0.653±0.002 (0.655)	40.8±0.4 (41.1)	2.03 (2.07)
1.5% DIO	7.59±0.11 (7.70)	0.651±0.005 (0.655)	39.8±0.3 (40.1)	1.89 (2.02)
2.0% DPE	7.03±0.13 (7.15)	0.632±0.004 (0.633)	39.9±0.2 (40.1)	1.69 (1.81)
4.0% DPE	8.18±0.12 (8.30)	0.658±0.002 (0.660)	39.8±0.3 (40.0)	2.07 (2.19)

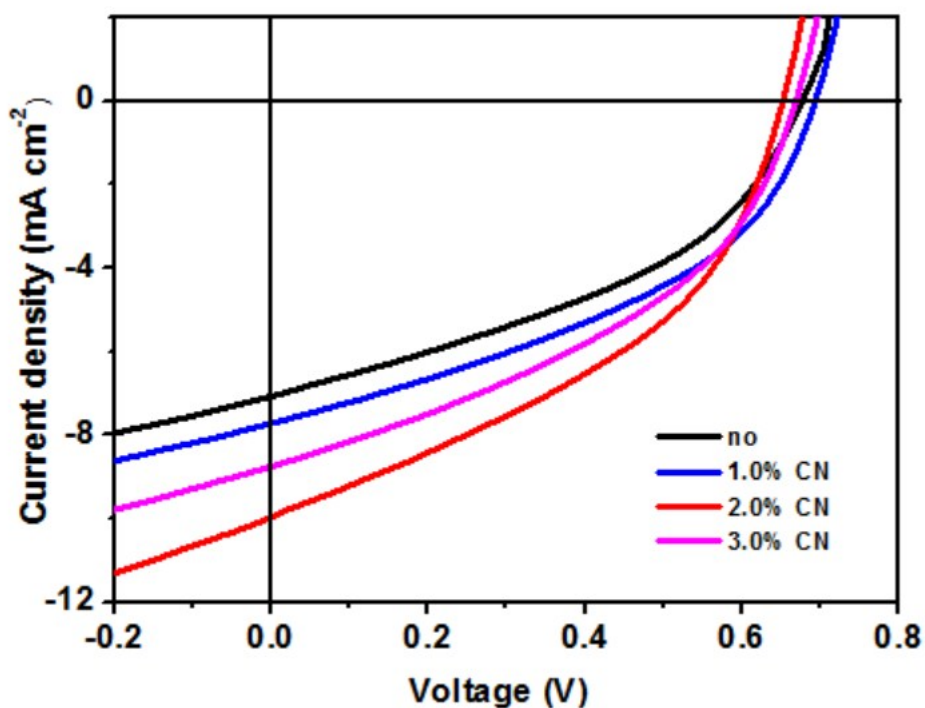


Fig. S7 J - V curves of PTB7-Th:di-PDI (1:1) with different CN concentrations.

TableS4. Summary of device parameters of PTB7-Th:di-PDI (1:1) with different CN concentrations.

Additives [volume]	J_{SC} [mA/cm ²]	V_{OC} [V]	FF [%]	$PCE_{ave(max)}$ [%]
No	6.96±0.12 (7.08)	0.669±0.003 (0.673)	40.5±0.3 (40.8)	1.81 (1.95)
1.0% CN	7.57±0.15 (7.72)	0.695±0.005 (0.700)	40.8±0.3 (41.1)	2.11 (2.22)
2.0% CN	9.85±0.13 (9.98)	0.655±0.006 (0.661)	40.4±0.2 (40.6)	2.56 (2.68)
3.0% CN	8.65±0.11 (8.76)	0.666±0.002 (0.668)	40.3±0.4 (40.7)	2.27 (2.38)

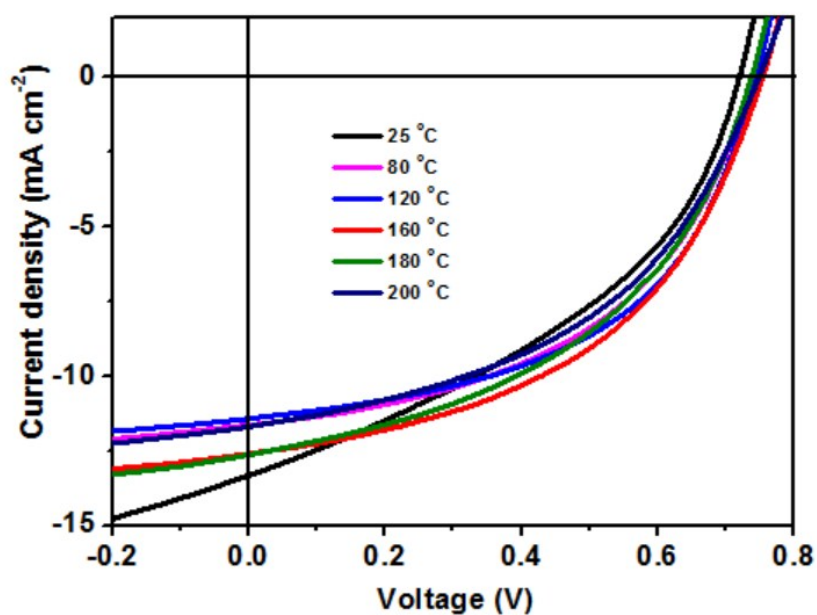


Fig. S8 J - V curves of PTB7-Th:tri-PDI (1:1) using 2.0% CN as additive with different annealing temperature.

Table S5. Summary of device parameters of PTB7-Th:tri-PDI (1:1) using 2.0% CN as additive with different annealing temperature.

Temp. [°C]	J_{sc} [mA/cm ²]	V_{oc} [V]	FF [%]	$PCE_{ave(max)}$ [%]
25	13.28±0.13 (13.41)	0.709±0.004 (0.713)	39.6±0.4 (40.0)	3.70 (3.82)
80	11.51±0.14 (11.64)	0.726±0.005 (0.731)	49.2±0.2 (49.4)	4.07 (4.20)
120	11.31±0.13 (11.43)	0.748±0.006 (0.754)	50.4±0.2 (50.6)	4.21 (4.36)
160	12.51±0.11 (12.61)	0.749±0.003 (0.751)	47.8±0.3 (48.1)	4.43 (4.55)
180	12.51±0.14 (12.64)	0.735±0.005 (0.740)	45.2±0.5 (45.5)	4.12 (4.26)
200	11.54±0.15 (11.69)	0.749±0.005 (0.754)	45.5±0.2 (45.6)	3.86 (4.02)

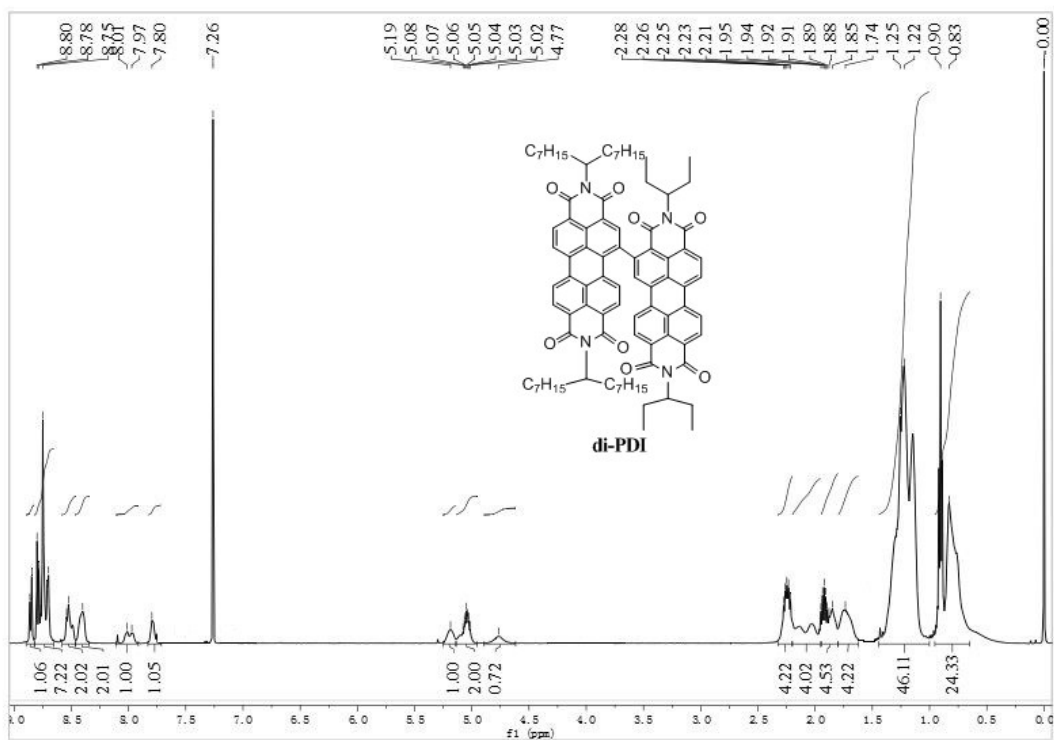


Fig. S9 ¹H NMR spectrum of di-PDI in CDCl₃.

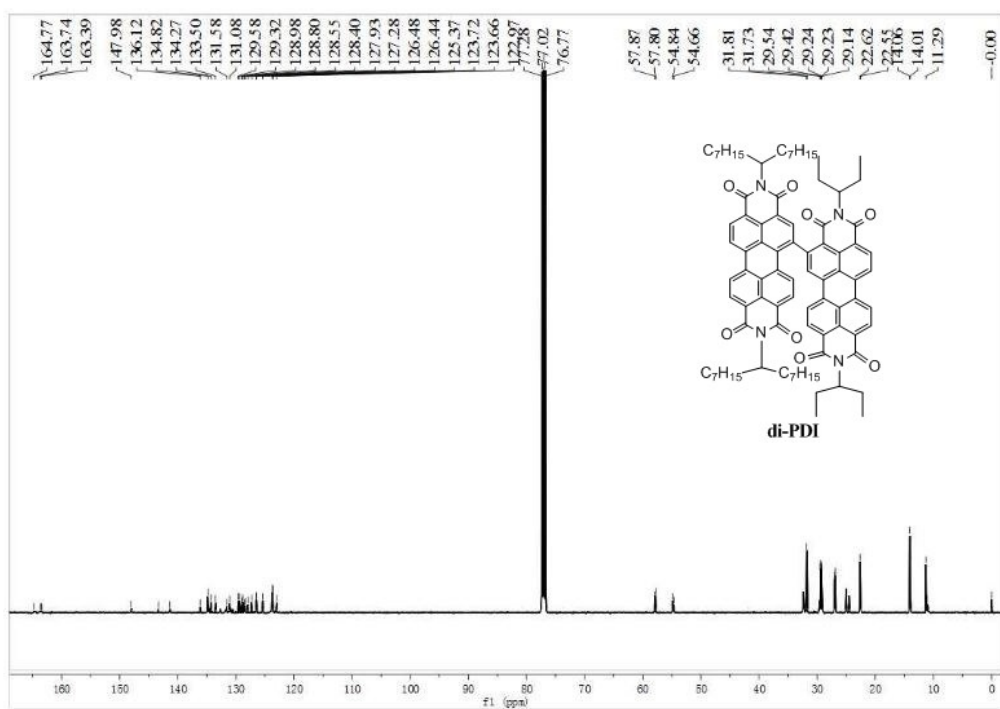


Fig. S10 ¹³C NMR spectrum of di-PDI in CDCl₃.

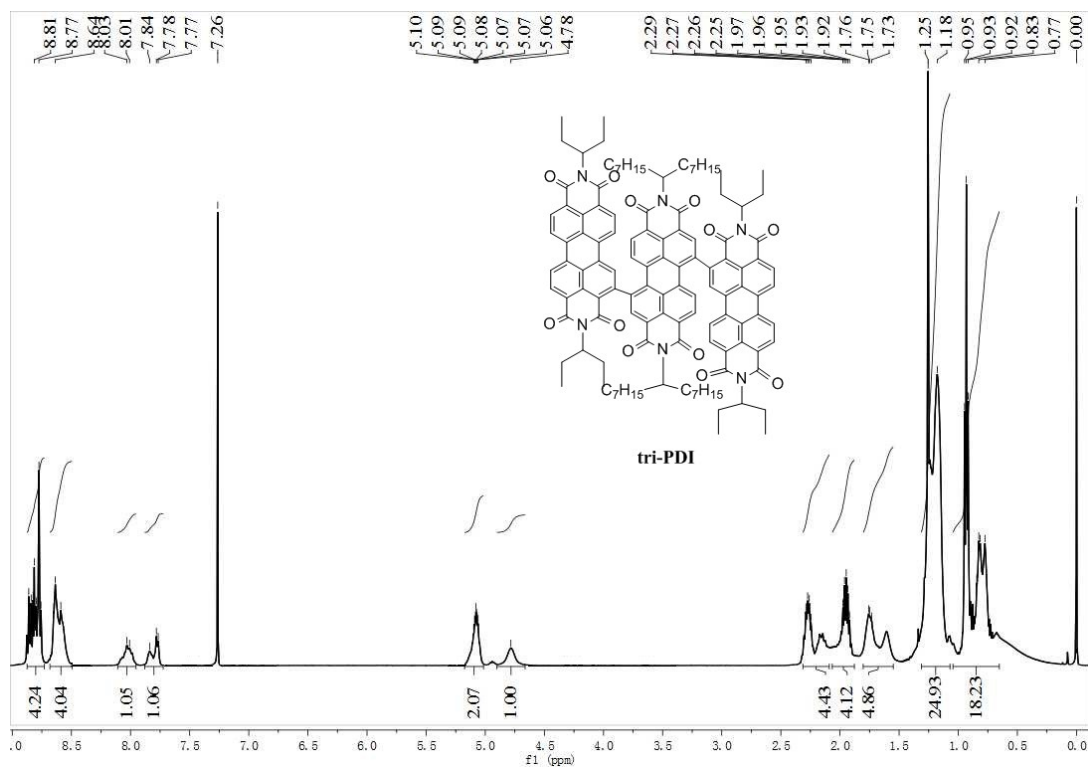


Fig. S11 ¹H NMR spectrum of tri-PDI in CDCl₃.

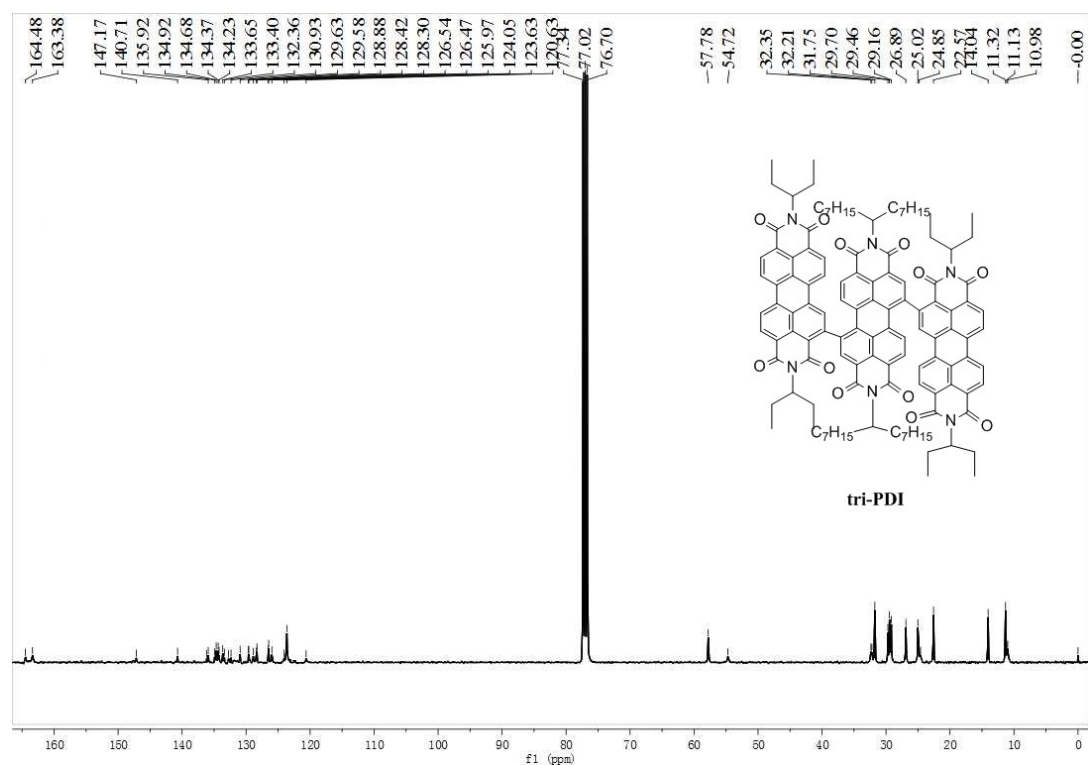


Fig. S12 ¹³C NMR spectrum of tri-PDI in CDCl₃.