Wide Band Gap Copolymers Based on Phthalimide: Synthesis, Characterizations, and Photovoltaic Properties with 3.70% Efficiency

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Electron mobility measurement.

The devices were fabricated with configuration of ITO/TIPD/polymer: $PC_{71}BM$/Al according to the method reported in literature.[1] Titanium (diisopropoxide) bis(2,4-pentanedionate) (TIPD) was purchased from Alfa Aesar in isopropanol solution. TIPD in isopropanol solution (3.5% v/v) was spin-coated on pre-cleaned ITO with 3000 rpm and then thermal annealing at 150 °C for 10 min. Polymer/PC71BM was the spin-coated on to the ITO/TIPD substrate. Finally, the Al was deposited on active layer with thickness of 100 nm. The *I-V* curves were tested under dark on a computer-controlled Keithley 2400 Source Measure Unit. The results were plotted as $Ln(JL^3V^2)$ vs. $(V/L)^{0.5}$, as shown in Figure S5.

Table S1. photovoltaic performances of P2 and P3 with PC71BM as acceptor material under different D/A ratios.

polymer	D/A ratio	J_{sc} (mA/cm^2)	V_{oc} (V)	*FF*(%)	*PCE* (avg %)
P2	2:1	2.87	0.71	41.3	0.84(0.82)
	1:1	0.80	3.43	54.7	1.50(1.46)
	1:2	2.87	0.79	61.5	1.39(1.36)
P3	2:1	5.54	0.80	40.0	1.79(1.74)
	1:1	6.76	0.81	51.6	2.83(2.79)
	1:2	0.89	7.01	58.6	3.70(3.65)
	1:3	5.73	0.91	59.5	3.10(3.05)

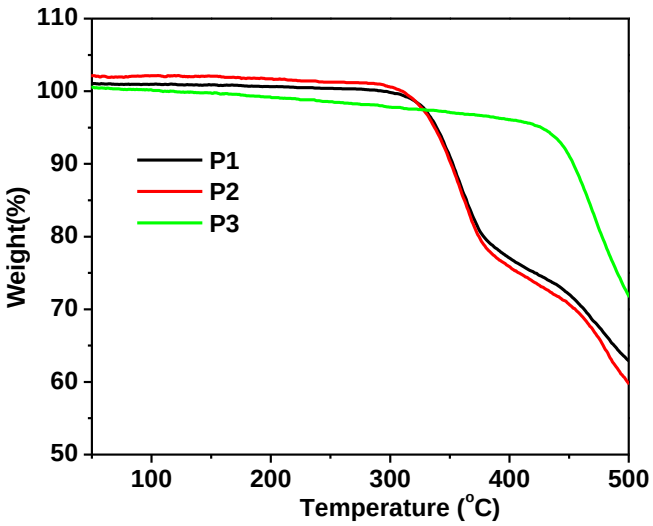

Figure S1. TGA curves of P1, P2, and P3.

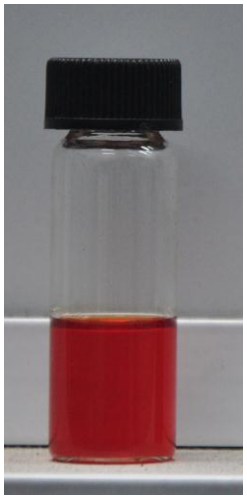

Figure S2. Solution appearance of PhI-based polymer P3 with a concentration of 5 mg/mL in $CHCl_3$.

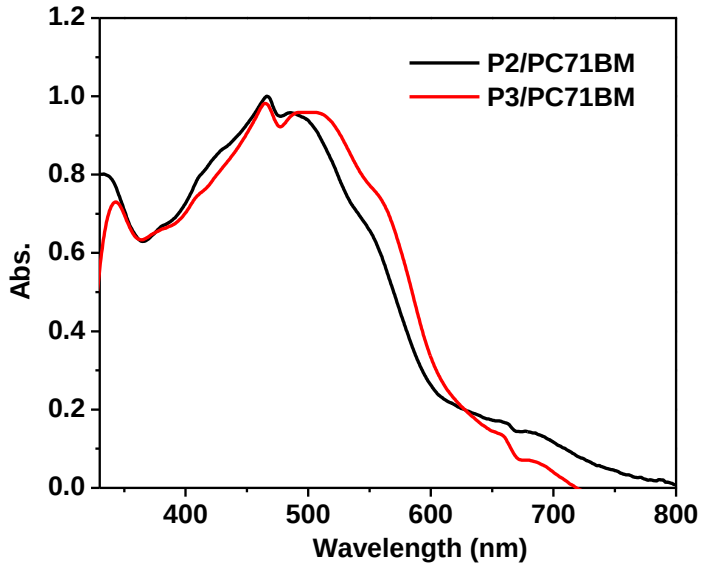

Figure S3. UV-vis absorption spectrum of P2/PC71BM and P3/PC71BM.

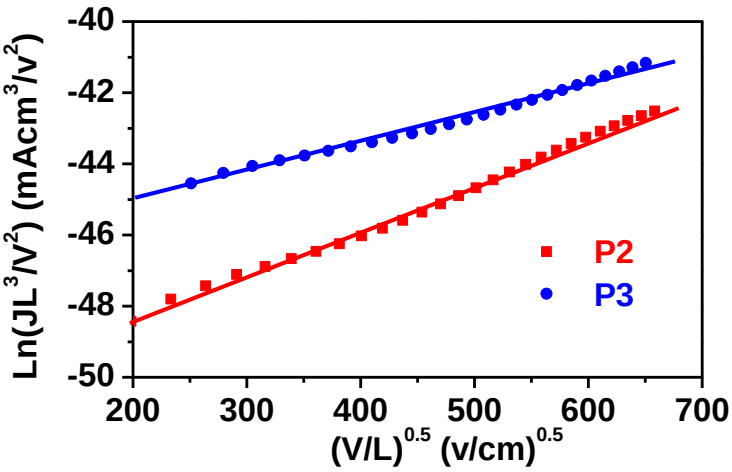

Figure S4. Plots of $\ln(JL^3/V^2)$ vs. $(V/L)^{0.5}$ of P2/PC71BM and P3/PC71BM.

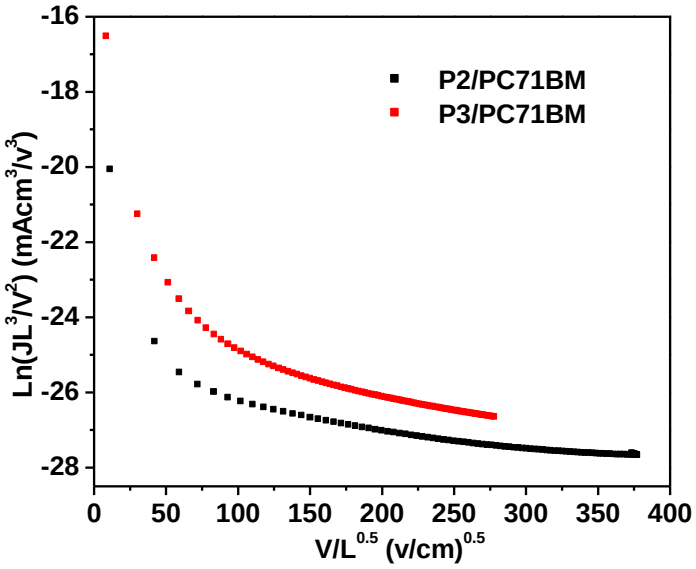

Figure S5. Plots of $\ln(JL^3/V^2)$ vs. $(V/L)^{0.5}$ of P2/PC71BM and P3/PC71BM with the device configuration of ITO/TIPD/active layer/Al.[1]

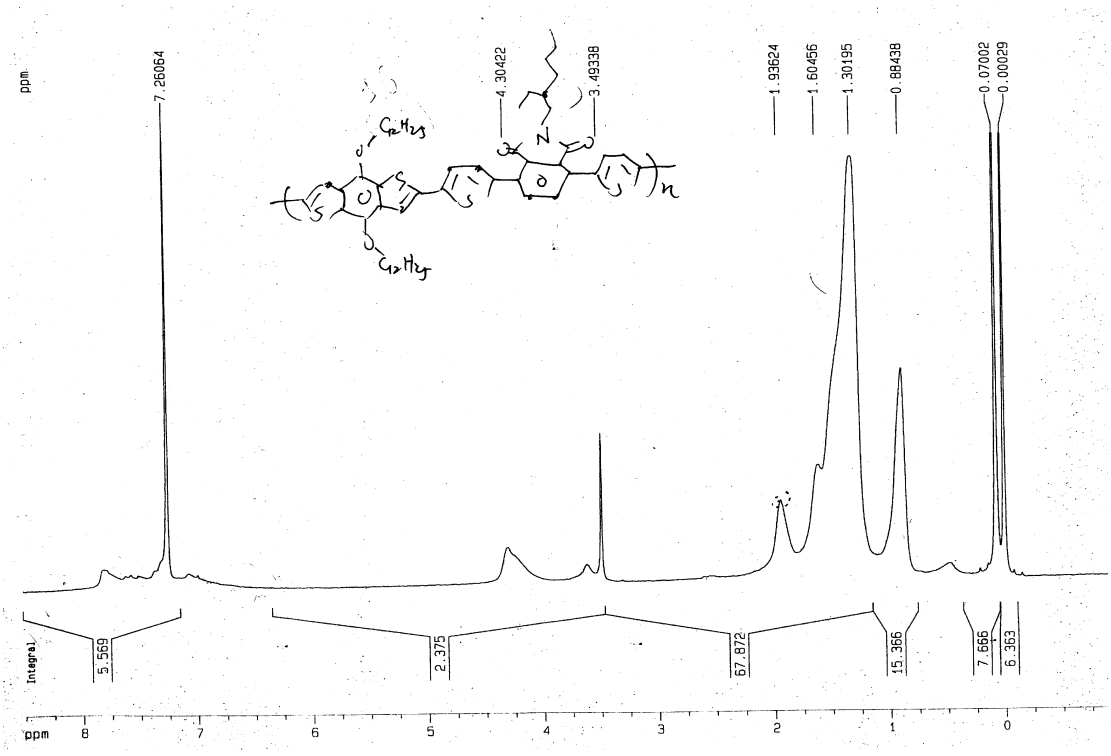

Figure S6 ^{1}HNMR spectra of P2.

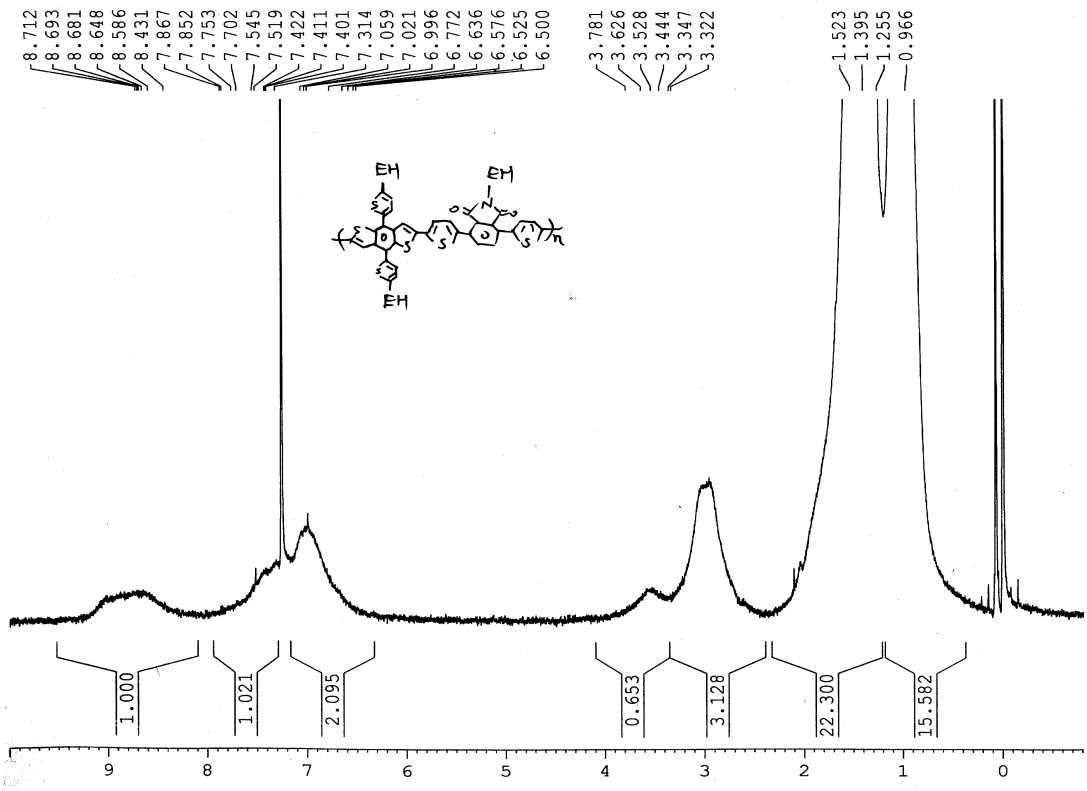

Figure S7 ^{1}HNMR spectra of P3.

Reference

1. Z. Tan, W. Zhang, Z. Zhang, D. Qian, Y. Huang, J. Hou, and Y. Li, *Adv. Mater*., 2012, **24**, 1476.