Hole-transporting Poly(dendrimer)s as Electron Donors for Low Donor Organic Solar Cells with Efficient Charge Transport

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di- and tri-demethylate byproducts

A: Aluminum chloride, sodium iodide, toluene, 60 °C, 27%; B: Dimethyl carbonate, tetra-*n*-butylammonium bromide, potassium carbonate, reflux, 57%.

Figure S1 Strategy for recovering dendrimer 1 from the di- and tri-demethylated side products.



Figure S2 DSC plots for the three poly(dendrimer)s (solid lines) in comparison with the corresponding monomers (dash-dot lines) and that of dendrimer 1. The plots shown are for the second heating process at scan rate of 50 $^{\circ}$ C/min.



Figure S3 TGA plots for 1 and the poly(dendrimer)s.



(b)



(c)



Figure S4 Current density-voltage (*J-V*) curves of BHJ devices with a) **P1**:PC₇₀BM, b) **P2**:PC₇₀BM, and c) **P3**:PC₇₀BM of different poly(dendrimer) blend concentrations.

Table S1 Averaged device performance parameters from at least 4 cells for P1:PC₇₀BM (a), P2:PC₇₀BM (b), and P3:PC₇₀BM (c) of different poly(dendrimer) blend concentrations. Among devices with different polymer content, the device with 6 wt% performed the best with a high J_{sc} and *FF*. By increasing the donor content up to 50 wt%, the reduction in photocurrent generation is responsible for the substantial decrease of the J_{sc} , which at least in part due to the fact that the poly(dendrimer) does not absorb strongly at visible wavelengths. In addition, for the low donor content films, the balanced electron-hole transport results in the high *FF* due to the suppressed bimolecular recombination.

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Blends [P1 (wt%):PC ₇₀ BM]	J _{sc} (mA/cm ²)	V _{oc} (V)	FF	РСЕ (%)
6	2.94±0.07	0.57±0.01	0.60±0.01	1.00±0.03
11	2.05±0.08	0.49±0.01	0.59±0.01	0.60±0.04
20	1.82±0.02	0.67±0.01	0.53±0.01	0.65±0.01

50 0.09±0.02 0.54±0.02 0.15±0.01 0.01±	=0.00
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(b)

	Blends [P2 (wt%):PC ₇₀ BM]	J _{sc} (mA/cm ²)	V _{oc} (V)	FF	РСЕ (%)
	1.2	2.92±0.08	0.78±0.01	0.51±0.01	1.16±0.06
	6	3.41±0.06	$0.79{\pm}0.01$	0.60±0.01	1.63±0.04
	11	2.67±0.07	0.77±0.01	0.63±0.01	1.29±0.05
	20	2.61±0.08	0.77±0.01	0.56±0.01	1.14 ± 0.07
	50	0.56±0.05	$0.84{\pm}0.02$	0.29±0.00	0.13±0.01
(c))				

Blends [P3 (wt%):PC ₇₀ BM]	J _{sc} (mA/cm ²)	V _{oc} (V)	FF	PCE (%)	
6	3.50±0.03	0.79±0.01	0.63±0.00	1.74±0.03	
11	2.64±0.14	0.77 ± 0.01	0.62±0.01	1.26±0.09	
20	2.53±0.07	0.78 ± 0.00	0.57±0.01	1.12±0.04	
50	0.91±0.06	0.85±0.01	0.29±0.01	0.22±0.02	



Figure S5 Resistance dependent PhotoVoltage (RPV) transient measurements on films of neat (a) dendrimer 1 and (b) and P2.



Figure S6 EQEs as a function of the photocurrent normalized to the space-charge-limited photocurrent (I_{SCLC}) for the dendrimer 1:PC₇₀BM blend at short-circuit conditions as well as for the **P2**:PC₇₀BM blend at short-circuit and maximum power point. The EQE was obtained from the intensity dependent photocurrent (IPC) measurements as described in the main text and the I_{SCLC} was calculated according to previously reported work from the slower carrier mobility (**Figure 4** in the main text) by assuming a Langevin recombination coefficient.¹ Ref. 1 demonstrated how the charge transport parameters determine the bimolecular recombination losses that manifest in the deviation from a constant EQE *vs*. photocurrent or laser power. The figure shows that the I_{SCLC} , as predicted from the slower carrier mobility obtained from RPV, coincides with the experimentally measured EQE deviation. This confirms that the hole mobilities as obtained by RPV are relevant for understanding the device performance. Note, we could not reach the I_{SCLC} with the available laser power for the **P2**:PC₇₀BM blend device at short-circuit conditions due to the relatively thin active layer and high hole mobility. We note that the intensity was increased until ~3 equivalent

suns, which implies that the linear photocurrent would be expected to continue until much higher intensities (>30 suns). Therefore, we applied a forward bias of 0.64 V (corresponding to the voltage at the maximum power point) to increase the carrier transit time and decrease the critical I_{SCLC} .



Figure S7 EQE as a function of the photocurrent normalized to the photocurrent at the maximum power point (I_{MP}) in **P2**:PC₇₀BM blend at maximum power point conditions (V_{MP}). The flat EQE demonstrates the absence of second-order bimolecular recombination losses even at V_{MP} due to the high hole mobilities and the relatively thin active layer, giving rise to the high *FF* of 0.65.

REFERENCE

1. Stolterfoht, M.; Armin, A.; Philippa, B.; White, R. D.; Burn, P. L.; Meredith, P.; Juška, G.; Pivrikas, A., Photocarrier drift distance in organic solar cells and photodetectors. *Scientific Reports* **2015**, *5*, 9949.