

Electronic Supplementary Information for:

Small Molecules Based on 2,7-Carbazole for Efficient Solution-Processed Organic Solar Cells

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X-ray diffraction

The crystallinity of the active layer was analyzed using Grazing incidence wide-angle x-ray diffraction (GIWAXD) measurements. All the films were spin-coated from chlorobenzene solution on glass substrates. All measurements were performed with the diffractometer D8 Discover (Bruker, Germany) ($\lambda = 1.54 \text{ \AA}$). A fixed grazing incidence angle of 0.2° was used to reduce the scattering from substrates.

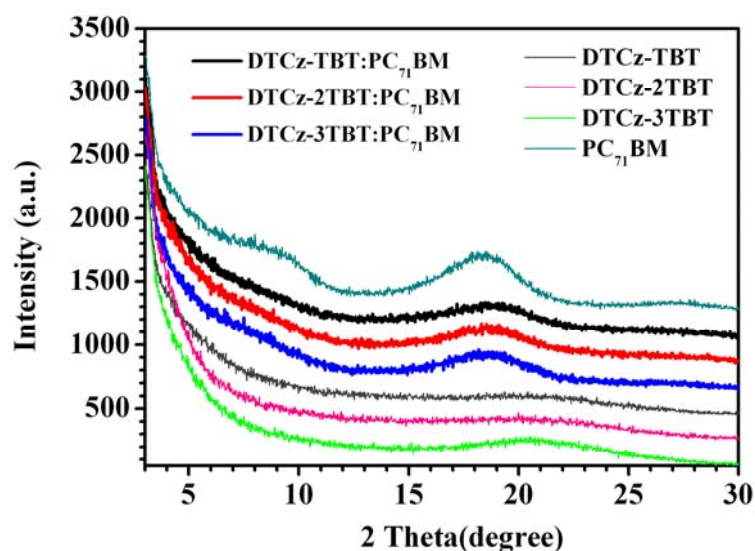


Figure S1. XRD diffraction patterns of films of DTCz-TBT, DTCz-2TBT, DTCz-3TBT, PC₇₁BM, DTCz-TBT:PC₇₁BM(1:2), DTCz-2TBT:PC₇₁BM(1:2), DTCz-3TBT:PC₇₁BM(1:2)

As shown in Figure S1, no clear reflection peak was observed for all the pristine films of the three molecules. The blended films only exhibited the weak diffraction pattern of PC₇₁BM.

Thermal Stability of the Devices

To examine the thermal stability of the devices, device performances obtained from DTCz-TBT/PC₇₁BM, DTCz-TBT/PC₇₁BM and DTCz-TBT/PC₇₁BM under the optimized conditions after post-production annealing at 80 °C for 0.5–12 h were compared. Related data were summarized in Figure S2 and Table S1.

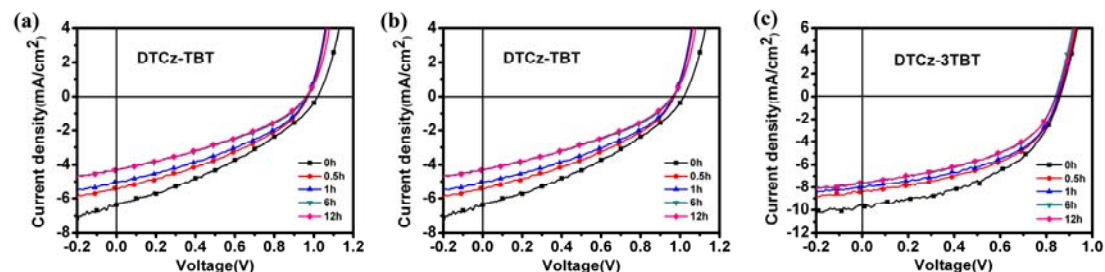


Figure S2. Current density-voltage (J - V) curves of devices processed from DTCz-TBT/PC₇₁BM(a), DTCz-TBT/PC₇₁BM(b) and DTCz-TBT/PC₇₁BM(c), during annealing at 80 °C for different time.

Table S1 photovoltaic performance with different thermal annealing time at 80 °C for devices based on compounds **DTCz-TBT**, **DTCz-2TBT** and **DTCz-3TBT**

Donor	Annealing time	V_{oc} (V)	J_{sc} (mA/cm ²)	FF	PCE	PCE decay ratio
DTCz-TBT	0h	1.02	6.36	0.35	2.26%	
	0.5h	0.97	5.41	0.37	1.96%	13%
	1h	0.97	5.05	0.37	1.83%	19%
	6h	0.97	4.28	0.37	1.52%	33%
	12h	0.96	4.24	0.36	1.48%	35%
DTCz-2TBT	0h	0.93	8.31	0.45	3.48%	
	0.5h	0.91	7.50	0.44	2.97%	15%
	1h	0.92	7.35	0.42	2.84%	18%
	6h	0.89	5.82	0.43	2.23%	36%
	12h	0.89	5.80	0.43	2.21%	36%
DTCz-3TBT	0h	0.86	9.59	0.48	3.94%	
	0.5h	0.85	8.36	0.49	3.45%	12%
	1h	0.85	7.90	0.50	3.33%	15%
	6h	0.84	7.64	0.47	3.00%	24%
	12h	0.85	7.59	0.46	2.96%	25%