

Supporting Information

One-Pot Synthesized Electron-Acceptor Composite Enables Efficient Fullerene-Free Ternary Organic Solar Cells

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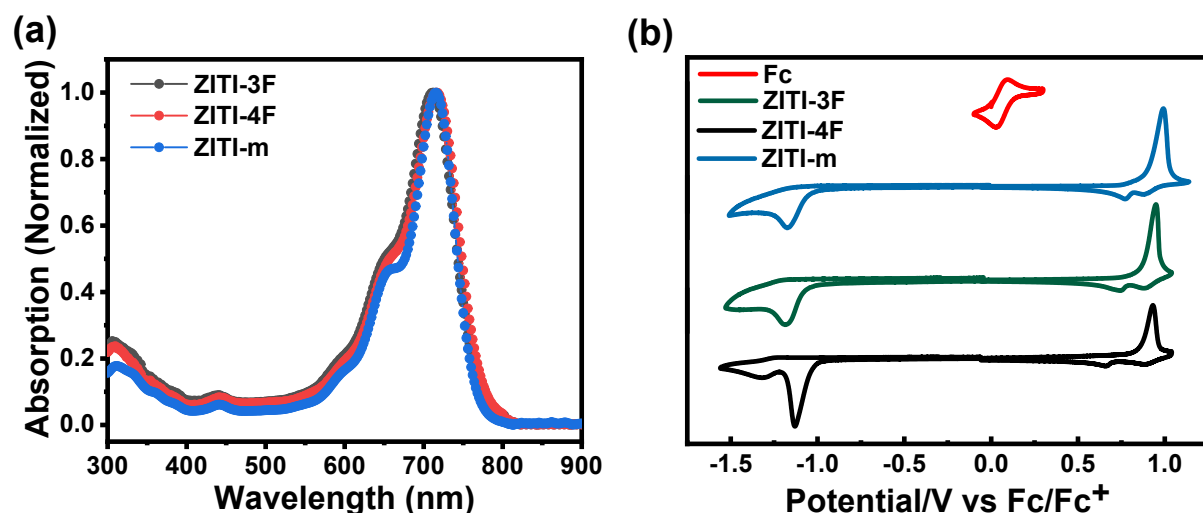


Fig. S1 (a) UV-vis-NIR absorption spectra of ZITI-3F, ZITI-4F and ZITI-m in chloroform. (b) Cyclic voltammogram of ZITI-3F, ZITI-4F and ZITI-m film in diluted CH₃CN solution with a scan rate of 100 mV s⁻¹.

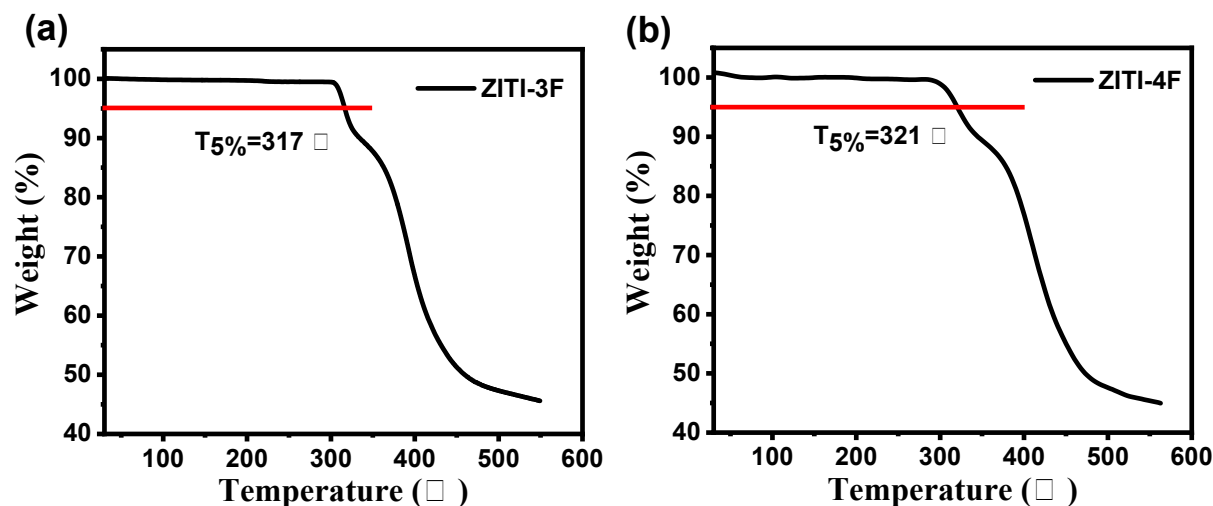


Fig. S2 Thermal gravimetric analysis curves of ZITI-3F (a) and ZITI-4F (b).

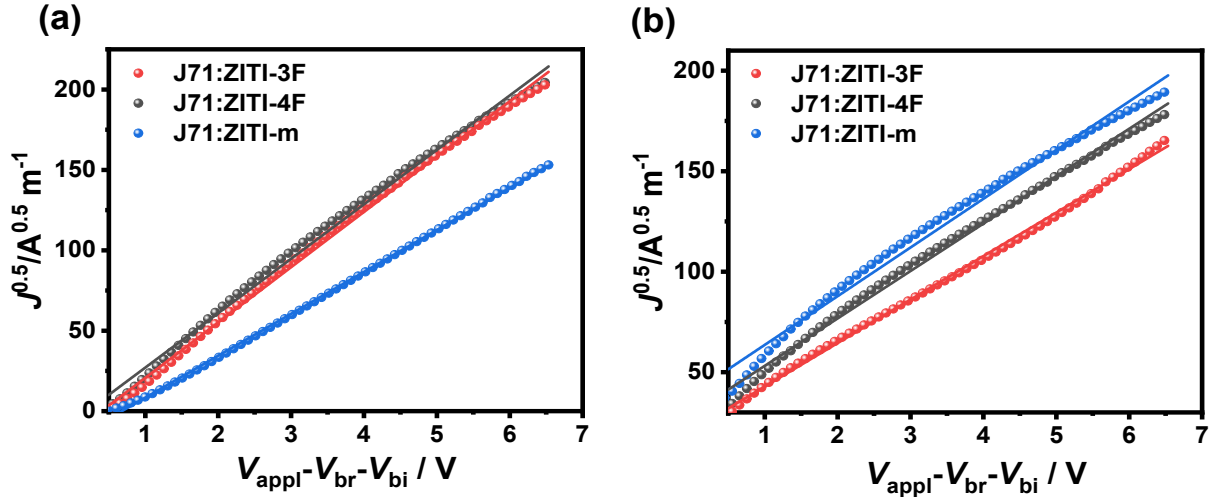


Fig. S3 $J^{0.5}$ vs V plots: J71:ZITI-3F, J71:ZITI-4F and J71:ZITI-m hole-only diode (a) and electron-only diode (b).

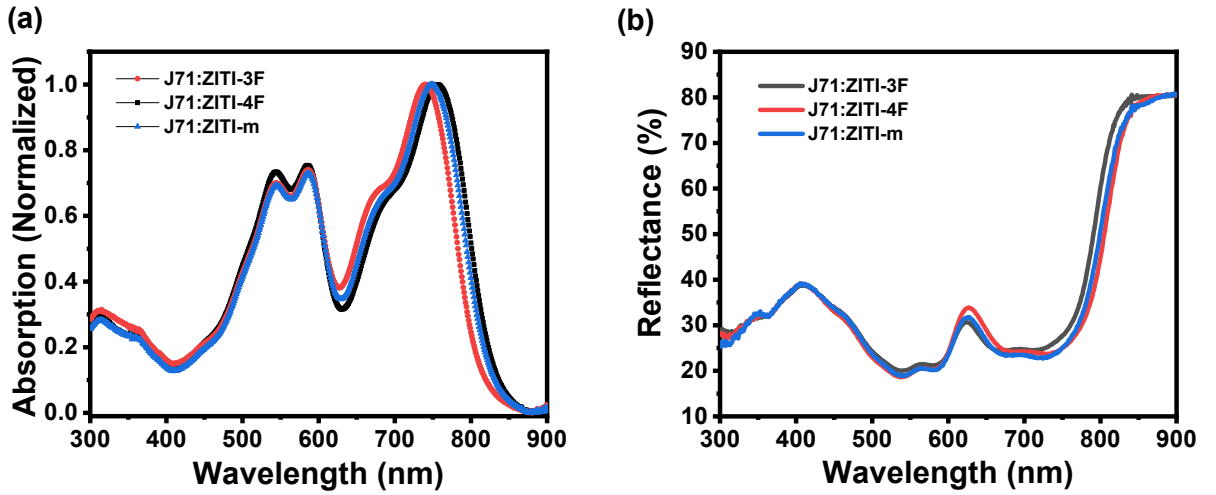


Fig. S4 (a) Normalized UV-vis-NIR absorption spectra and (b) reflectance spectra of J71:ZITI-3F, J71:ZITI-4F and J71:ZITI-m blend films at the best device performance conditions.

Table S1. Photovoltaic parameters of J71:ZITI-3F (A_1)-, J71:ZITI-4F (A_2)- and J71:ZITI-3F:ZITI-4F (with different ratios)-based devices.

D: A_1 : A_2	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF (%)	PCE _{avg} (PCE _{max}) (%)	μ_h ($\times 10^{-4} cm^2$ $V^{-1} s^{-1}$)	μ_e ($\times 10^{-4} cm^2$ $V^{-1} s^{-1}$)	μ_h/μ_e
1:1:0	0.897	20.67	71.53	12.97 $\pm$ 0.15 (13.15)	3.96	1.57	2.52
1:0.2:0.8	0.869	21.02	73.43	13.34 $\pm$ 0.10 (13.49)	3.17	1.78	1.78
1:0.4:0.6	0.878	21.64	72.91	13.51 $\pm$ 0.13 (13.64)	2.59	1.80	1.44
ZITI-m	0.882	21.57	73.10	13.65 $\pm$ 0.13 (13.85)	2.27	1.97	1.15
1:0.6:0.4	0.883	21.55	72.89	13.52 $\pm$ 0.12 (13.67)	2.54	1.93	1.32
1:0.8:0.2	0.885	20.99	72.39	13.33 $\pm$ 0.11 (13.46)	3.11	2.02	1.53
1:0:1	0.850	21.30	72.76	13.02 $\pm$ 0.13 (13.18)	3.83	1.86	2.06

^{a)} Average values with standard deviation were obtained from 15 devices.

Table S2. Photovoltaic parameters of J71:ZITI-3F-based solar cells with different D/A ratios.

J71:ZITI-3F D/A ratio	Thickness (nm)	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE (PCE _{max}) (%)
1:0.7	95	0.91	19.21	70.22	12.14±0.16(12.33)
1:1	110	0.90	20.67	71.53	12.97±0.15(13.15)
1:1.3	120	0.89	20.51	72.53	12.94±0.14(13.12)

Table S3. Photovoltaic parameters of J71:ZITI-4F-based solar cells with different D/A ratios.

J71:ZITI-4F D/A ratio	Thickness (nm)	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE _{avg} (PCE _{max}) (%)
1:0.7	95	0.86	20.65	71.12	12.56±0.12(12.70)
1:1	110	0.85	21.30	72.76	13.02±0.13(13.18)
1:1.3	120	0.85	21.74	70.87	12.89±0.14(13.13)

Table S4. Photovoltaic performance of J71:ZITI-3F-based solar cells at different thermal annealing temperatures.

J71:ZITI-3F TA	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE _{avg} (PCE _{max}) (%)
as-cast	0.93	18.95	65.98	11.58±0.09 (11.70)
100 °C/10 min	0.91	19.70	72.77	12.84±0.08 (12.97)
120 °C/10 min	0.90	20.67	71.53	12.97±0.15 (13.15)
140 °C/10 min	0.89	20.55	70.08	12.78±0.10 (12.90)
160 °C/10 min	0.88	19.05	68.30	11.43±0.13 (11.53)

Table S5. Photovoltaic parameters of J71:ZITI-4F-based solar cells at different thermal-annealing temperatures.

J71:ZITI-4F TA	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE _{avg} (PCE _{max}) (%)
as-cast	0.90	19.80	66.87	11.64±0.12 (11.89)
100 °C/10 min	0.86	21.22	68.60	12.71±0.10 (12.87)
120 °C/10 min	0.85	21.30	72.76	13.02±0.13 (13.18)
140 °C/10 min	0.84	21.39	72.84	12.95±0.15 (13.09)
160 °C/10 min	0.82	21.07	69.23	11.90±0.13 (12.05)

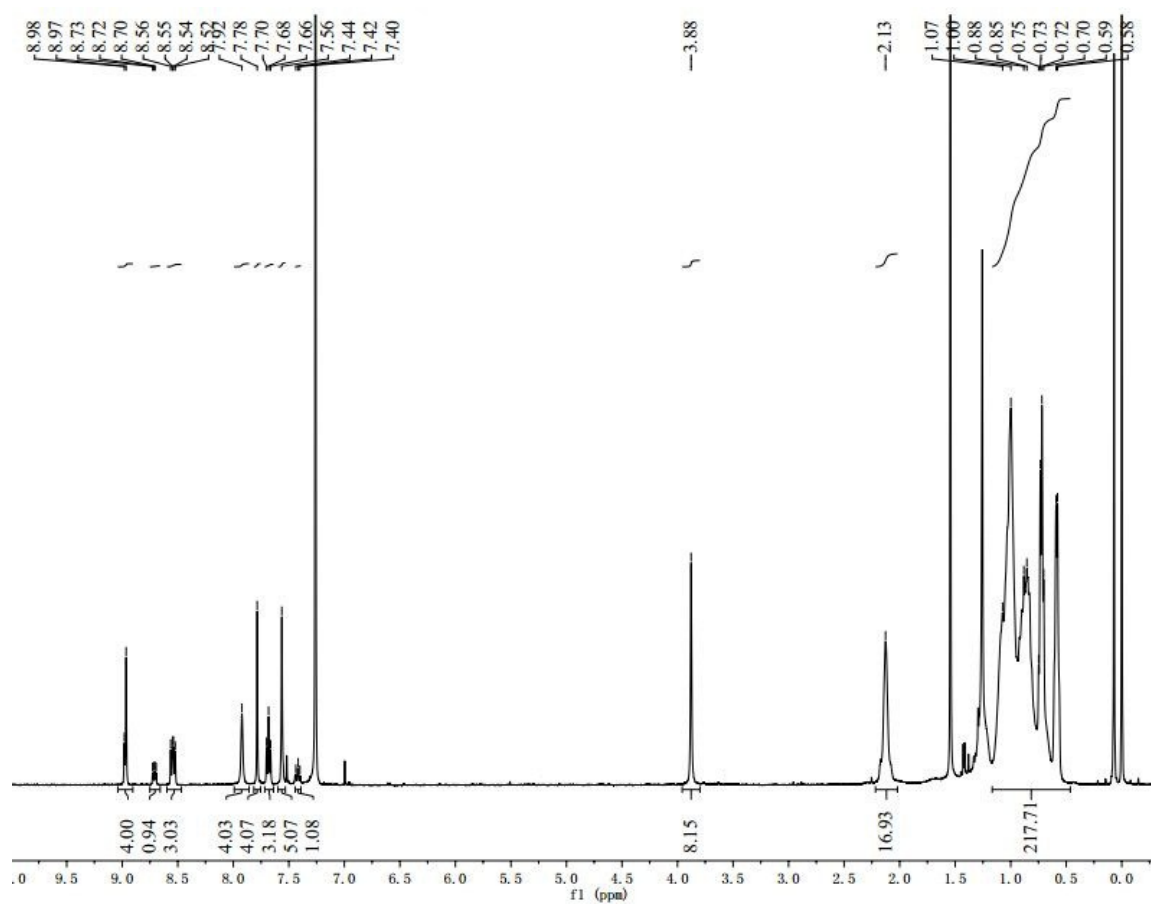
Table S6. Photovoltaic parameters of J71:ZITI-3F-based solar cells with different thicknesses.

J71:ZITI-3F rpm	Thickness (nm)	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE _{avg} (PCE _{max}) (%)
3500	95	0.89	20.02	73.07	12.88±0.15 (13.07)
3000	110	0.90	20.67	71.53	12.97±0.15 (13.15)
2500	120	0.89	20.73	71.42	13.00±0.15 (13.11)
2000	135	0.89	20.93	69.19	12.81±0.09 (12.92)

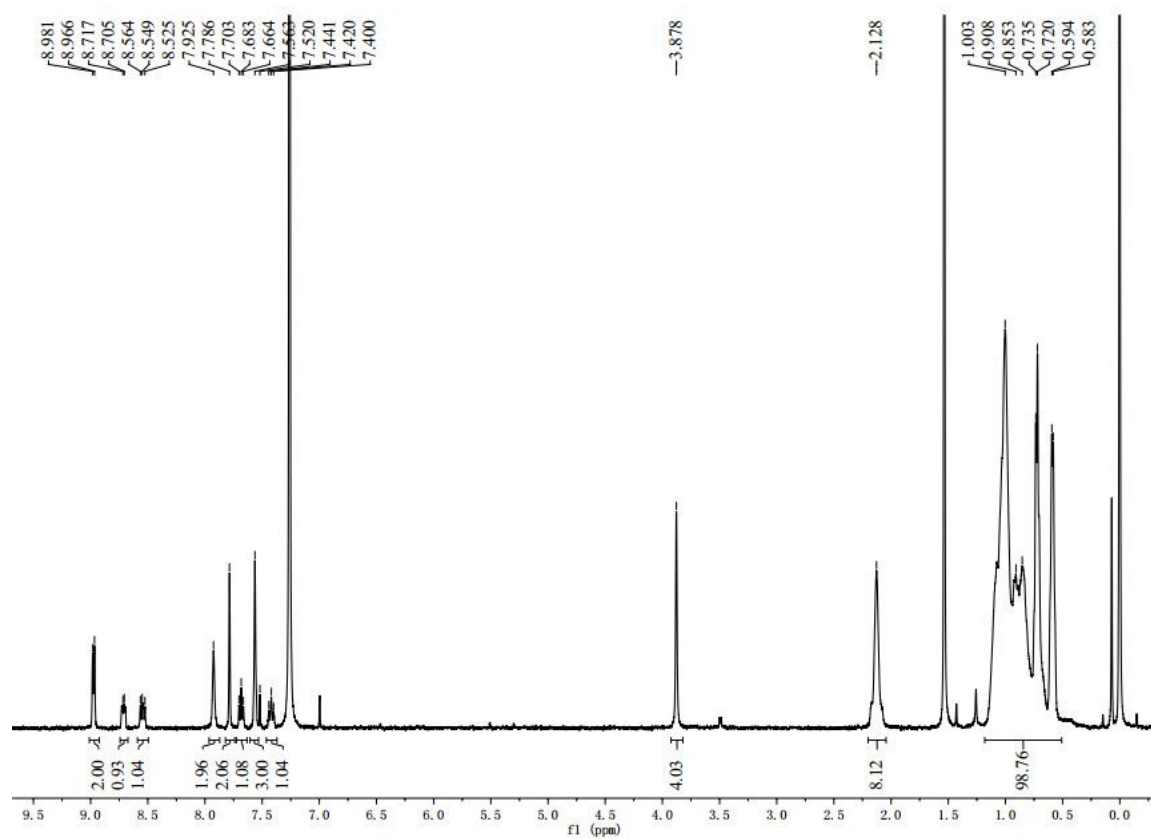
Table S7. Photovoltaic parameters of J71:ZITI-4F-based solar cells with different thicknesses.

J71:ZITI-4F rpm	Thickness (nm)	V_{oc} (V)	J_{sc} (mA cm⁻²)	FF (%)	PCE_{avg} (PCE_{max}) (%)
3500	95	0.85	20.63	73.38	12.71±0.15 (12.99)
3000	110	0.85	21.30	72.76	13.02±0.13 (13.18)
2500	120	0.85	21.46	71.17	12.99±0.16 (13.10)
2000	135	0.85	21.71	70.04	12.94±0.12 (13.02)

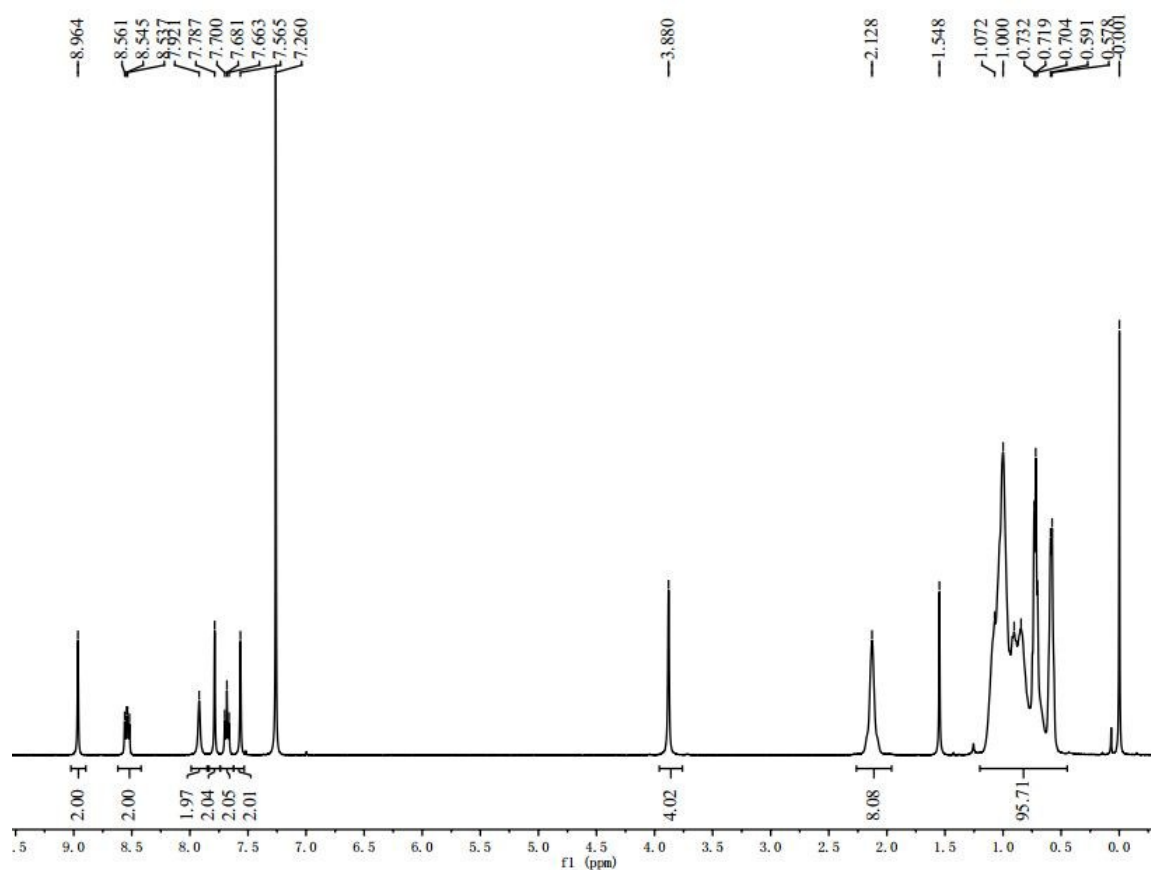
¹H NMR spectrum of ZITI-m.



¹H NMR spectrum of ZITI-3F.



^1H NMR spectrum of ZITI-4F.



^{13}C NMR spectrum of ZITI-4F.

