

Electronic Supplementary Information (ESI) for *Chemical Society Reviews*

Ternary organic solar cells: Optimizing the third components

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Table S1. Characteristics of the devices used in PDI derivatives based TOSCs and optoelectronic properties of NFAs (HOMO, LUMO, and E_g for A2).

D1	A1	A2	HOMO (eV)	LUMO (eV)	E_g (eV)	Additive (%)	Coating Solvent	Coating method	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)	Ref
PTB7-Th	SF-4PDI	TPE-4PDI	-6.29	-4.20	2.09	2.5% CN	CB	SC	15.09	0.85	48.6	6.19	s1
FBT	PC ₆₁ BM	PDI	-5.9	-3.7	2.2	1% anisaldehyde	o-xylene	SC	13.4	0.86	68.0	7.9	s2
PTB7-Th	ITIC	PDI	-6.10	-3.90	2.2	0.4% DIO	CF	SC	18.37	0.84	56.0	8.64	s3
PTB7-Th	PBI-Por	PDI-V	-5.99	-3.87	2.12		CB	SC	17.54	0.75	69.1	9.43	s4
PBDB-T	ITIC	PMIA-0	-5.93	-3.83	2.1	1% 1-CN	o-DCB	SC	17.38	0.89	61.0	9.77	s5
PTB7-th	IDT-2BR	PDI-2DTT	-5.60	-3.90	1.7	3% DPE	DCB	SC	14.8	1.04	65.4	10.1	s6
PDBT-T1	ITIC-Th	SdiPBI-Se	-6.09	-3.87	2.22	0.7% DIO	DCM	SC	15.50	0.93	70.8	10.27	s7
PTB7-Th	PC ₇₁ BM	TPE-4PDI	-5.95	-3.88	2.07	3% DIO	CB	SC	17.89	0.79	74.7	10.4	s8
PM6	Y6	TPA-4PDI	-6.04	-3.69	2.35	0.25% DIO	CF	SC	27.55	0.84	78.2	18.29	s9

Table S2. Characteristics of the devices used in IDT derivatives (IDIC, IEIC, IT-4F, ITIC-, ITM)-based TOSCs and optoelectronic properties of SMAs (HOMO, LUMO, and E_g for A2).

D1	A1	A2	HOMO (eV)	LUMO (eV)	E_g (eV)	Additive (%)	Coating Solvent	Coating method	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)	Ref
IDT													
PBTA-BO	PC ₆₁ BM	IFBR	-5.69	-3.64	2.05		DCB	SC	13.45	0.92	65.07	8.11	s10
PBTA-BO	PC ₇₁ BM	IffBR	-5.71	-3.77	1.94		CB	SC	14.66	0.91	68.12	9.06	s11
PTB7-Th:	EH-	EH-	-5.58	-3.90	1.68		oDCB	SC	15.39	0.97	60.5	9.19	s12
	5T-TTC	IDTBR											
PTB7-th	PC ₇₁ BM	IDT2BR	-5.52	-3.84	1.68	DIO	CB	SC	17.22	0.83	0.65	9.37	s13
PBDB-T	PC ₇₁ BM	IDT-OT	-5.11	-3.46	1.65	0.5%	CB	SC	15.35	0.86	68.1	9.09	s14
						DIO							
PBDB-T	PC ₇₁ BM	IDTC-4CI	-5.50	-3.79	1.71	0.5% CN	CF	SC	19.14	0.82	65.6	10.41	s15
PBDB-T	PC ₇₁ BM	IDT-2O	-5.72	-3.85	1.87	-	DCB	SC	17.20	0.88	73.49	10.67	s16
PCE10	IDTBR:	IDFBR	-5.75	-3.70	2.05		CB	SC	17.3	1.04	0.7	11.4	s17
T2-ORH	T2-ORH	EH-	-5.42	-3.60	1.82		CF	CB	17.51	1.0	63.0	11.55	s18
		IDTBR											
P1	ITCPTC	IDT6CN				0.3%	CB	SC	17.81	0.87	76.5	11.92	s19
						DIO							
PTB7-Th	F8IC	IDT-2BR.	-5.52	-3.69	1.83	0.5%	CF	SC	25.1	0.68	69.9	12.1	s20
						DIO							
PTB7-Th	T2-ORH	T2-OEHRH	-5.65	-3.58	2.07	1% DPE	ToI	SC	18.05	1.04	65.0	12.1	s21
BDB-T	ITIC	IDT-T	-5.73	3.59	2.14	0.5%	CB	SC	17.9	0.93	73.1	12.2	s22
						DIO							
PCE10	F8IC	Eh-IDTBR	-5.45	-3.90	1.55	0.5%	CB	SC	12.26	0.81	73.02	12.27	s23
						DPE							
PBDB-T	ITC6-2F	IDT-PDOT-C6	-5.47	-3.80	1.67		DCB	SC	21.73	0.85	72.06	13.36	s24
PM6	C8-SF	Y-MODF	-5.81	-3.90	1.91		CF	SC	20.88	0.84	75.87	13.39	s25
BDB-T	IDTT-OB	IDT-PDOT-C6	-5.59	-4.17	1.42	0.2%	o-DCB	SC	20.06	0.92	70.41	13.4	s26
						DIO							
PBDB-T	INPIC-Si	IDTO-T-4F	-5.58	-4.04	1.54	0.5%	CB	SC	22.55	0.87	74.18	14.55	s27
						DIO							
PBDB-T	IE4F-S	IBC-F	-5.62	-3.53	2.09		CB	SC	22.83	0.88	74.4	15.06	s28
PM6	Y6	O-IDTBR	-5.68	-4.13	1.55	1% 1-CN	CB	SC	25.75	0.85	0.76	16.60	s29
PM6	Y6	IDT-TNIC	-5.53	-3.92	1.61	1-CN	CF	SC	25.90	0.86	75.9	17.00	s30
PM6	Y6	IDT-T-PCN	-5.48	3.74	1.74	1% 1-CN	CF	SC	26.56	0.85	76.1	17.36	s31
PM6	BTP-eC9	IDTR	-5.29	-3.31	1.98	0.5% 1-CN	CF	SC	28.14	0.86	80.55	19.54	s32
PDCBT	PCBM	ITIC					DCM:DIM	SC	10.12	0.87	71.0	6.20	s33
PBTOTT	PC ₇₁ BM	ITIC	-5.64	-4.04	1.6	0.3%	CB	SC	15.0	0.88	64.2	8.18	s34
						DIO							
PBDB-T	PCBM	ITIC					CB	SC	15.0	0.87	65.0	8.6	s35
TP	IEICO-4F	ITIC	-5.48	-3.83	1.65	0.5%	CB	SC	18.00	0.87	58.0	9.10	s36
						DIO							

PBTTFB	PC ₇₀ BM	ITIC	-5.71	-4.12	1.59	3% DPE	CB	SC	13.73	1.01	71.0	9.73	s37
PBDB-T	ITIC	ITIC-Th	-5.66	-3.93	1.73	0.5 % DIO	CB	SC	16.5	0.91	67.0	9.76	s38
PTB7-Th	FBR-CN	ITIC-Th	-5.68	-4.11	1.57	3%-1- CN	CB	SC	17.76	0.80	69.9	9.82	s39
PBDB-T	PC ₇₁ BM	ITIC	-	-3.78		0.1% F4TCNQ	CB	SC	16.12	0.89	70.0	9.94	s40
P1	PC ₇₁ BM	ITIC	-5.49	-3.89	1.6	2% DPE	ToI	SC	17.80	0.92	63.7	10.21	s41
PDBT-T1	SdiPBI-Se	ITIC-Th	-5.66	-3.93	1.73	0.7% DIO	DCM	SC	15.50	0.93	70.8	10.27	s7
PTzBT	PC ₇₁ BM	ITIC	-5.68	-3.75	1.93		CB	SC	16.5	0.89	70.0	10.3	s42
PBDTBDD	PC ₆₀ BM	ITIC				0.5% DIO	DCM	SC	17.76	0.91	63.4	10.36	s43
PPBDTBT	PC ₇₁ BM	ITIC	-5.51	-3.78	1.73	0.2% DIO	DCM	SC	16.85	0.89	66.2	10.41	s44
PDBTT1	PC ₇₀ BM	ITIC-Th	-5.66	-3.93	1.73	1% DIO	CF	SC	15.72	0.93	71.1	10.48	s45
PBDB-T	ITIF	ITIC	-5.54	-3.84	1.7	0.5% DIO	CB	SC	17.31	0.86	70.0	10.53	s46
PBDB-T	SR197	ITIC	-5.48	-3.83	1.65		CB	SC	18.59	0.87	67.7	11.03	s47
PBDB-T	FBR	ITIC	-5.54	-3.84	1.7		CB	SC	18.73	0.91	65.0	11.17	s48
PDOT	PC ₇₁ BM	ITIC	-5.61	-3.89	1.72	1% DIO	CB	SC	17.49	0.96	66.8	11.21	s49
PTBTz-2	PC ₇₁ BM	ITIC	-5.63	-3.97	1.66	DIO			20.75	0.89	60.9	11.26	s50
PBDB-T	SR197	ITIC	-5.48	-3.83	1.65		CB	SC	18.23	0.87	67.7	11.03	s47
P3TCO-1	PC ₇₁ BM	ITIC	-5.51	-3.78	1.73		CB	SC	18.16	0.94	66.7	11.41	s51
J71	IT-M	ITIC	-5.58	-4.02	1.56	0.2% DIO	CF	SC	18.08	0.97	65.6	11.60	s52
FTAZ	IDIC	ITIC-Th- O	-5.36	-3.91	1.45	0.4% DIO	CF	SC	18.9	0.86	72.3	11.6	s53
J71	MeIC2	ITIC	-5.51	3.92	1.59		CF	SC	18.1	0.91	70.5	11.6	s54
PBDT-2TC	4TBA	6TBA	-				DCB	SC	16.6	0.96	73.0	11.73	s55
PBDB-T	IEICO-4F	4TIC				DIO	CB	SC	21.64	0.82	67.5	11.82	s56
PBDB-T	IDT6CN-M	ITCPTC.				0.3% DIO	CB	SC	17.81	0.87	76.2	11.92	s19
PBDTPD-HT	PC ₇₀ BM.	ITIC	-5.58	-4.02	1.56	0.8% DIO	CF	SC	17.38	0.95	74.0	12.09	s57
PTB7-Th	COi8DFIC	ITIC-4F	-5.90	-4.32	1.58	1% DIO	CB	SC	26.75	0.69	71.5	13.23	s58
PBT1-C	ICBA	ITIC-2Cl	-5.70	-4.14	1.56	DIO	CF	SC	19.69	0.91	77.1	13.41	s59
PTB7-Th	PC ₇₁ BM	3TT-FIC	-5.42	-4.17	1.25	DIO	CB	SC	27.73	0.66	73.0	13.54	s60
PT3	meta- TrBRCN	TCPTC	-5.50	-3.92	1.58	0.5% DIO	CB	SC	20.16	0.88	76.3	13.63	s61
PM6	PC ₆₁ BM	ITIC	-6.10	4.0	2.10	0.5% DIO	CB	SC	12.37	0.93	64.3	13.88	s62
PM-6	MeIC	ITCPTC	-5.62	-3.96	1.66	0.25% DIO	CF	SC	18.42	0.98	78.2	14.13	s63
PBTA-PS	LA1	6TIC	-5.45	-3.94	1.51		CB	SC	22.33	0.84	75.9	14.24	s64
PBDB-T:IPIC-4Cl	PC ₇₁ BM	IPIC-4Cl	-5.51	-3.95	1.56	0.5% DIO	CB	SC	23.3	0.82	74.6	14.3	s65
ZnP-TBO	6TIC	4TIC	-5.46	-4.06	1.4	0.3% DIO	CB	SC	24.58	0.80	74.9	14.73	s66
PM7	ITC-2Cl	IXIC-4Cl	-5.52	-4.13	1.39	0.25% DIO	CF	SC	23.99	0.85	74.7	15.37	s67
PM6	M36	ITCC-M	-5.53	-3.69	1.84	0.5% 1- CN	CF	SC	23.6	0.88	72.1	15.8	s68
PM6	Y7	ITIC-M	-5.58	-3.98	1.6	0.5% 1- CN	CB	SC	30.16	0.87	67.5	17.73	s69
PM6	BTP-eC9	ITIC-Th	-5.66	-3.93		DIO	CB	SC	28.0	0.87	77.0	18.7	s70
ITM													
PBDB-T	PC ₇₁ BM	IT-M	-5.58	-3.98	1.6	0.5%	CB	SC	16.59	0.92	67.58	10.16	s7

Table S3. Characteristics of the devices used in Y6 derivatives-based TOSCs and optoelectronic properties of small molecule acceptors (HOMO, LUMO, and E_g for A2).

D1	A1	A2	HOMO (eV)	LUMO (eV)	E_g (eV)	Additive (%)	Coating Solvent	Coating method	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)	Ref
P3HT	NC70BA	ZY-4Cl	-5.61	-3.67	1.94		CF	SC	17.98	0.87	66.07	10.53	s78
PCE10	YF-CN	Y6	-5.74	-4.02	1.72		CF	SC	27.92	0.68	63.11	12.03	s79
PBDB-T	ITCC	Y1	-5.47	-3.95	1.52	0.9% CN	CB	SC	21.5	0.93	67.8	13.1	s80
C2	DBTBT-IC	AQx-3	-5.68	-3.93	1.75		CF	SC	23.95	0.84	72.0	14.49	s81
PBDTNS- BDD	PC ₇₁ BM	Y6	-5.65	-4.10	1.55		CF	SC	24.7	0.81	74.4	14.88	s82
PBDB-T- 2Cl	MF1	BP-4F	-5.68	-3.88	1.8		CF	SC	22.02	0.89	78.05	15.31	s83
PM6	DTY6	Y-Me	-5.52	-3.70	1.82	0.5% CN	CF-O-Xy	SC	24.2	0.87	74.0	15.7	s84
PM6	PC ₇₁ BM	BTCT- 2Cl	-5.56	-3.95	1.61	0.5% DIO	CF	SC	25.1	0.88	72.6	16.1	s85
PBDB-T- SF	ITCT	Y6	-5.62	-4.11	1.51	0.5% CN	CF	SC	24.75	0.88	73.67	16.14	s86
PM6	BTO	Y6	-5.61	-3.98	1.63		paraxylene	SC	25.91	0.86	73.41	16.39	s87
PM6	Y6	L8BO- 2O	-5.58	-3.91	1.67	0.6% CN	CB	SC	25.21	0.85	76.66	16.4	s88
PFBDT- 8ttTPD	PC ₇₁ BM	Y6	-5.65	-4.29	1.36		CF	SC	25.96	0.85	74.0	16.43	s89
P106	DBTBTIC	Y18- DMO	-5.63	-3.93	1.7		CF	SC	24.82	0.91	73.0	16.49	s90
PM6	IDIC	Y6	-5.62	-4.11	1.51		CB	SC	25.39	0.86	74.92	16.51	s91
PBDB-TF	PC ₆₁ BM	Y6	-5.65	-4.10	1.55	0.8% CN	CF	SC	25.4	0.84	77.0	16.5	s92
PM6	Y-TNF	Y-TN	-5.46	-3.86	1.6	0.25% DIO	CF	SC	25.84	0.85	75.10	16.63	s93
PM6	PC ₇₁ BM	Y6	-5.70	-4.10	1.6	0.5% CN	CF	SC	25.70	0.85	76.35	16.67	s94
PTQ10	PC ₇₁ BM	Y6	-5.65	-4.10	1.55		CF	SC	25.32	0.85	74.69	16.07	s95
PM6	Y-TNF	Y-TN	-5.54	-3.97	1.57	0.25% DIO	CF	SC	25.84	0.85	75.10	16.63	s93
PM6	PC ₇₁ BM	Y6	-5.62	-4.11	1.51	0.75% CN	CF	SC	25.5	0.85	76.9	16.7	s96
PM6	FBTIC	Y6	-5.65	-4.10	1.55	0.5% CN	CF	SC	24.6	0.86	77.9	16.7	s97
PBDB-TF	DTNIF	Y6	-5.65	-4.10	1.55	0.5% CN	CF	SC	26.40	0.85	73.80	16.73	s98
PM6	PC ₇₁ BM	Y6	-5.62	-4.11	1.51	0.5% CN	CF	SC	25.1	0.86	77.2	16.7	s99
PM6	DIBC	Y6	-5.65	-4.10	1.55		CF	SC	27.02	0.83	76.32	16.81	s100
PM6	DRCN5T	BTP-4Cl	-5.67	-4.13	1.54	1.75% CN	CB	SC	25.85	0.87	74.41	16.83	s101
PM6	SR197	Y6	-5.65	-4.10	1.55	0.5% CN	CF	SC	26.87	0.83	75.08	16.83	s102
PM6	Y6	TF1	-5.38	-3.92	1.46	0.5	CF	SC	26.12	0.87	76.21	16.91	s103
PBDB-TF	Y6	APDC- TPDA	-5.65	-4.10	1.55	4% CN	CB	SC	25.98	0.84	77.50	16.96	s104
PM6	BTP-M	Y6	-5.65	-4.00	1.65	0.5% CN	CF	SC	26.56	0.87	73.46	17.03	s105
PM6	PC ₇₁ BM	CH1007	-5.59	-3.97	1.62	0.5% CN	CF	SC	27.48	0.82	75.61	17.08	s106
PM6	ABP6T-4F	CH1007	-5.63	-3.96	1.64	0.5% CN	CF	SC	26.52	0.85	75.87	17.10	s107
PM6	BTP-PIO	Y6	-5.65	-4.10			CF	SC	27.31	0.84	73.9	17.10	s108
PM6	DRTB-T- C4	Y6	-5.71	-4.34	1.37	0.5% CN	CF	SC	24.79	0.85	81.3	17.13	s109
PM6:	L8-BO-F	BTP-eC9				0.5% CN	CN	LBL	28.36	0.83	73.0	17.31	s110

PM6	IDT-T-PCN	Y6	-5.60	-4.10	1.5	CN	CF	SC	26.56	0.85	76.1	17.36	s31
PM6	ITCPTC	Y6	-5.60	-4.10	1.5	0.5% CN	CF	SC	25.67	0.86	78.8	17.42	s111
PM6	Y6	F6D	-5.61	-4.16	1.45	1%- CN	CF	SC	26.95	0.86	75.44	17.52	s112
PM6	Y6	BTP-CC	-5.50	-3.68	1.82	0.5%CN	CF	SC	26.98	0.84	76.98	17.55	s113
PTQ10	BTP-Ph	BTP-Th	-5.60	-3.78	1.82	0.75% CN	CF	SC	25.2	0.88	78.6	17.6	s114
PM6	PY-IT	L8-BO					CF	SC	24.45	0.95	76.38	17.74	s115
D18	BTP-Ec9-4f	SM16	-5.67	-3.93	1.74		CF	SC	27.26	0.88	75.16	18.20	s116
PM6	S9	S1					CF	SC	26.77	0.89	76.66	18.29	s117
D18	N3	Qx-p-C ₇ H ₈ O	-5.66	-3.91	1.75		CF	SC	27.85	0.87	75.88	18.49	s118
PM6	BTP-eC9	BTP-F	-5.59	-3.86	1.73				26.99	0.85	79.0	18.45	s119
PM6	BTP-eC9	QX-Ac	-5.54	-3.78	1.76		CF:CB	SC	26.69	0.87	79.35	18.51	s120
PM6	BO-5Cl	BO-4Cl	-5.68	-3.94	1.74	0.3% DIO	CF	SC	26.93	0.87	78.0	18.56	s121
PM6	N3	Norb-Y	-5.63	-3.63	2.0	DBCl	CF	SC	27.64	0.86	77.96	18.59	s122
PM6	L8-BO-F	BTP-eC9	-5.59	-3.98	1.61	0.5% DIO	CF	SC	27.35	0.85	80.0	18.66	s123
PM6	BTP-eC9	Y6-10	-5.75	-3.71	2.04	0.5% DIO	CF	SC	28.06	0.85	26.97	18.81	s124
PM6	ThMeCl-2	C5-16	-5.69	-4.03	1.66	0.25% DIO	CF	SC	27.8	0.86	79.3	18.9	s125
PBQx-TF	F-BTA3	ec9-2Cl	-5.57	-3.74	1.83	0.5% DIO	Tol	SC	26.8	0.87	79.0	18.7	s126
PM6	L8-BO	Cl-QTP-4F	-5.66	-3.72	1.94	0.4% DIM	CF	SC	26.86	0.88	79.5	19.0	s127
PM6	Z2	L8-BO	-5.73	-3.94	1.79	0.25% DIO	CF	SC	26.79	0.90	78.87	19.02	s128
PM6	BTP-ec9	Y-LC	-5.76	-3.77		DBCb	CF	SC	28.51	0.85	78.2	19.10	s129
PM6	Z3	L8-BO	-5.73	-3.94	1.79	0.25% DIO	CF	SC	26.79	0.90	78.87	19.02	s128
PM6	L8-BO	BTP-ThMeCl	-5.64	-3.81	1.83	0.25 % DIO	CF	SC	26.7	0.87	82.0	19.10	s130
LWPM6	Y6	TYT-S	-5.71	-4.01	1.70		CF	SC	28.63	0.85	79.12	19.23	s131
PM6	L8-BO	QEIP-4Cl	-5.73	-3.94	1.79	0.25 % DIO	CF	SC	27.24	0.89	79.07	19.27	s132
PY5	PNDIT-F3N	L8-BO	-5.67	-3.92	1.75	0.3% DIO	CF	SC	27.08	0.91	78.72	19.40	s133
D18	L8-BO	2T-BO-2	-5.61	-3.70	1.91	DIO	CF	SC	26.15	0.92	80.49	19.37	s134
PM6	N3	YIS-6F	-5.70	-3.96	1.40	DBCL	CF	SC	28.4	0.86	79.1	19.43	s135
PM6	oPhFO	BTP-ec9	-5.71	-3.92	1.79		CB	SC	27.6	0.878	80.6	19.5	s136
PM6	L8-BO	BTP-OS	-5.68	-3.91	1.77	0.25% DIO	CF	SC	27.77	0.901	78.82	19.72	s137
PM6	L8-BO	ZY-4Cl	-5.64	-3.67	1.97		CF	SC	27.51	0.908	79.67	19.90	s138
PM6	BTP-eC9	YQX-10	-5.8	-4.37	1.43	0.5% DIO	CF	SC	29.25	0.864	79.05	20.0	s139
PM6	PY-IT	AQI4				DIB	CB:OXY	SC	26.6	0.94	80.1	20.1	s140
PM6	L8-BO	C9-1F	-5.62	-3.89	1.73	DIB	CF	SC	26.96	0.92	81.18	20.16	s141
D18	L8-BO	BQx-O	-5.72	-3.66	2.06		CF	SC	26.77	0.932	80.59	20.11	s142
PM6	BTP-eC9	QD-1	-5.73	-3.80	1.93	0.3% DIO	CF	SC	28.98	0.873	79.82	20.19	s143
PM6	L8-BO	Z-Tri	-5.69	-3.88	1.81	DBCl	CF	SC	27.30	0.927	80.3	20.32	s144
PM6	PBTI-FR	L8-BO	-5.67	-3.97	1.7	0.25% DIO	SF	SC	28.07	0.89	82.55	20.52	s145

1,3-dibromo-5-chlorobenzene (DBCb)

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