

Supplimentary infomation

A nuanced approach for assessing OPV materials for large scale applications

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Table S1: Cost calculation of the reaction components for SF(DPPB)₄.

Material	AUD/g or L	Unit	Usage for 100 g	Unit Price for 100 g acceptor	Price per g	
18-crown-6	AUD 5,080	kg	23.4 g	\$	119	
2-ethylhexyl bromide	AUD 640	kg	458.6 g	\$	294	
2-thiophenecarbonitrile	AUD 702	kg	300.2 g	\$	211	
Acetic acid	AUD 7.20	L	2.3 L	\$	17	
Phenylboronic acid	AUD 318	kg	64.9 g	\$	21	
Bis(pinacolato)diboron	AUD 509	kg	105.3 g	\$	54	
Chloroform	AUD 7.20	L	16.1 L	\$	116	
dimethyl succinate	AUD 109	kg	134.0 g	\$	15	
N,N-Dimethylformamide anhydrous	AUD 12	L	5.6 L	\$	70	
Ethanol	AUD 3.00	L	1.2 L	\$	4	
potassium carbonate, anhydrous	AUD 176	kg	922.8 g	\$	162	
Potassium acetate	AUD 189	kg	80.3 g	\$	15	
liquid nitrogen	AUD 3	kg	128.2 L	\$	385	
Methanol	AUD 2.75	L	4.6 L	\$	13	
N-bromosuccinimide	AUD 234	kg	175.8 g	\$	41	
tetrakis(triphenylphosphine)palladium(0)	AUD 5,408	kg	28.6 g	\$	155	
[1,1'-Bis(diphenylphosphino)ferrocene]dichloropalladium(II)	AUD 15,269	kg	11.1 g	\$	169	
potassium tert-butoxide	AUD 288	kg	367.2 g	\$	106	
2-methyl-2-butanol	AUD 70	L	3.0 L	\$	211	
2,2',7,7'-Tetrabromo-9,9'-spirobifluorene	AUD 1,400	kg	44.3 g	\$	62	
Tetrahydrofuran	AUD 17.00	L	4.2 L	\$	71	
Toluene	AUD 5.25	L	19.4 L	\$	102	
Sum of reactants				\$	2,408	\$ 24.08
Work-up						
CH ₂ Cl ₂	AUD 5.00	L	184.45 L	\$	922	
ethyl acetate	AUD 3.25	L	108.76 L	\$	353	
hexane	AUD 5.00	L	208.76 L	\$	1,044	
hexanes	AUD 7.37	L	11.52 L	\$	85	
methanol	AUD 2.75	L	13.86 L	\$	38	
MgSO ₄	AUD 27	kg	0.39 kg	\$	10	
Na ₂ SO ₄	AUD 64	kg	0.06 kg	\$	4	
petroleum ether	AUD 7.20	L	58.52 L	\$	421	
silica	AUD 10.2	kg	111.34 kg	\$	1,133	
Sum of Work-up				\$	4,011	\$ 40.11
Total sum for reactants and work-up				\$	6,419	\$ 64.19

Table S 2: Cost calculation of the reaction components for [60]PCBM.

Material	AUD/g or L	Unit	Usage for 100 g	Unit	Price for 100 g acceptor	Price per g
4-benzoylbutyric acid	\$ 1,755.97	kg	140.23 g	g	\$ 246.24	
methanol	\$ 2.75	L	1.87 g	g	\$ 5.15	
hydrochloric acid	\$ 3.80	L	0.03 g	g	\$ 0.11	
p-toluene-sulfonyl hydrazide	\$ 35.63	kg	149.92 L	L	\$ 5.34	
pyridine anhydrous	\$ 40.80	L	4.83 g	g	\$ 196.94	
sodium methoxide	\$ 152.00	kg	36.20 L	L	\$ 5.50	
C60	\$ 22,903.97	kg	231.69 g	g	\$ 5,306.67	
o-dichlorobenzene	\$ 17.20	L	16.09 L	L	\$ 276.74	
o-DCB	\$ 17.20	L	10.20 L	L	\$ 175.51	
Sum of reactants					\$ 6,218	\$ 62.18
Work-up						
methanol	\$ 2.75	L	10.439 L	L	\$ 28.71	
silica	\$ 10.18	L	23.324 L	L	\$ 237.42	
chlorobenzene	\$ 8.00	L	23.324 L	L	\$ 186.59	
toluene	\$ 5.25	L	93.295 L	L	\$ 489.80	
Sum of Work-up					\$ 943	\$ 9.43
Total sum for reactants and work-up					\$ 7,161	\$ 71.61