Electronic Supplementary Material (ESI) for Energy Advances.

Supplementary Information for

Design and Development of Low-Cost Imidazole-Based Hole Transporting Material for Perovskite Solar Cell

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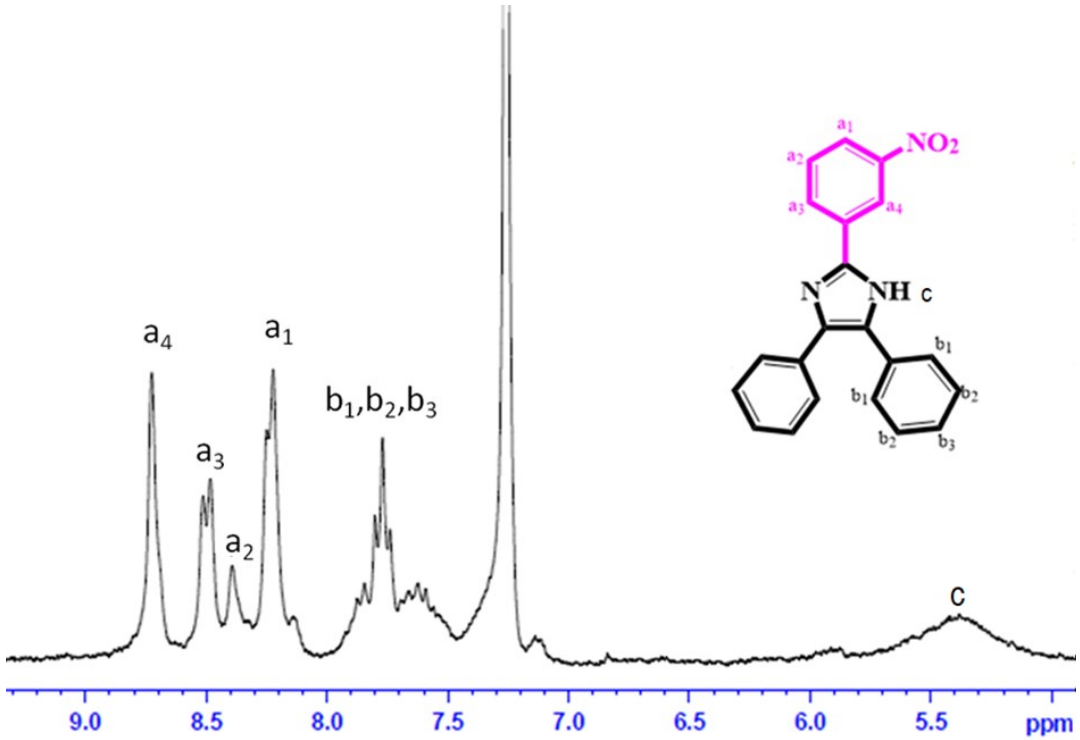


Fig. S1. [1]HNMR spectrum of HTM **1**.

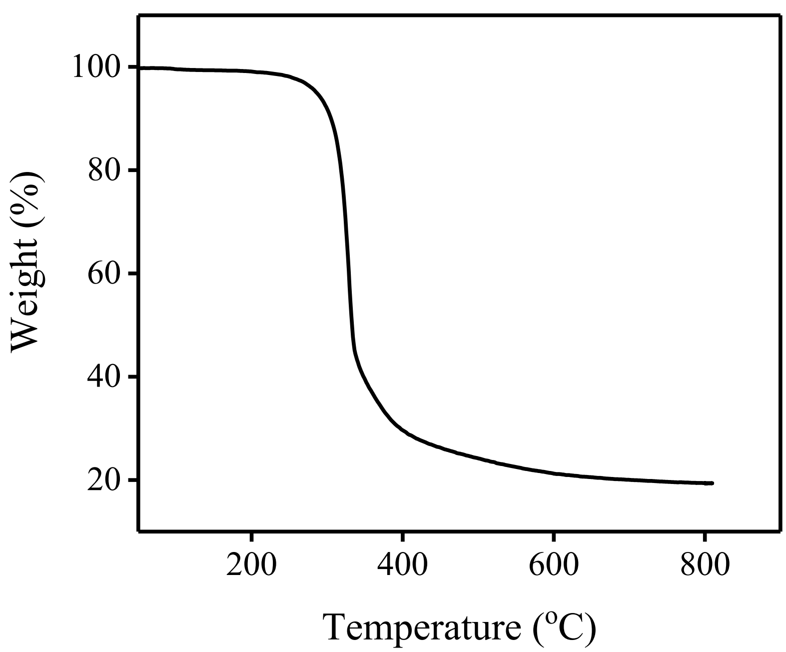


Fig. S2. TGA curve of the HTM **1** with scan rate of 10 °C min^{-1} under N_2 atmosphere.

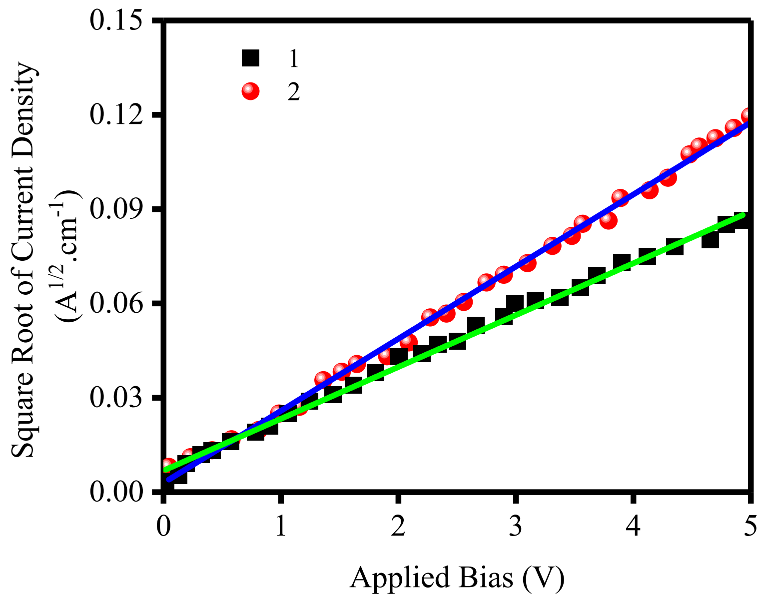


Fig. S3. Hole mobility measurements using space-charge limited currents for the devices fabricated with HTMs **1** and **2**.

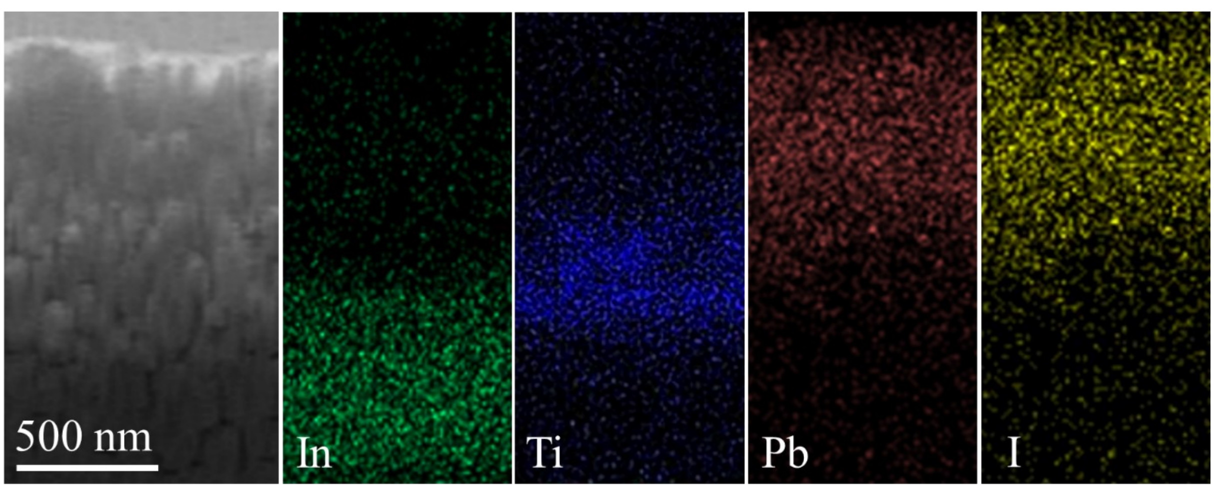


Fig. S4. Cross-sectional SEM images and corresponding EDX mapping images of the solar cell, indicating the distribution of elements In, Ti, Pb, and I.

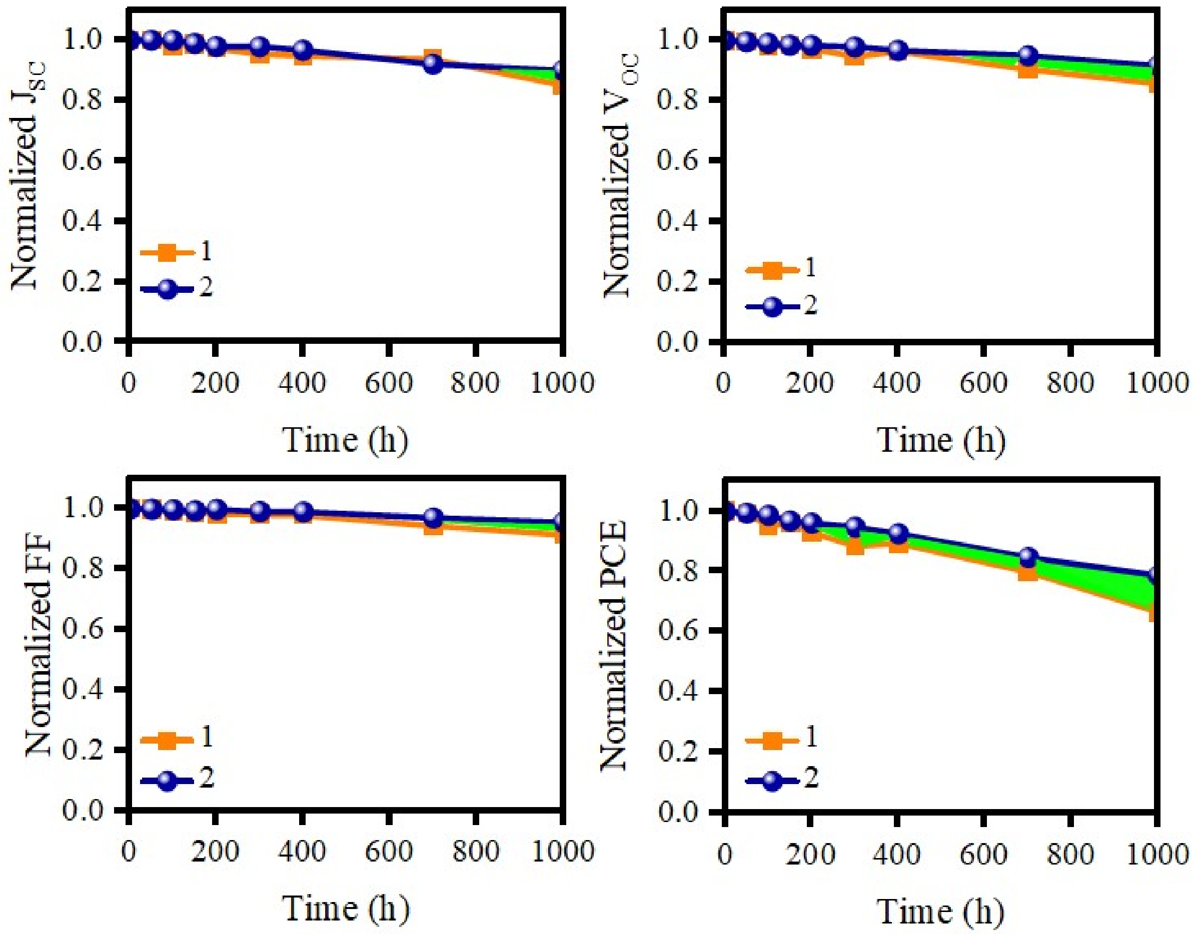


Fig. S5. Stability of the photovoltaic parameters of PSCs based on HTMs **1** and **2** under during exposure to full AM 1.5 simulated sunlight for 1000 hours (humidity ≈ 40%). Highlighted parts show the difference between photovoltaic performance of HTRMs **1**, and **2** over times.

Table S1. Quantities and cost of the materials used for the synthesis of 1 g of HTM **2**. Reproduced from ref. [1] with permission from the Royal Society of Chemistry, copyright 2016.

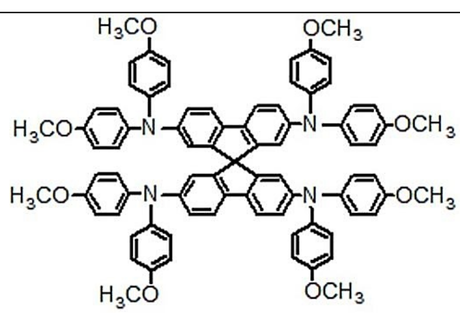
Chemical name	**Weight reagent (g/g)**	**Weight solvent (g/g)**	**Weight workup (g/g)**	**Price of chemical (\$/kg)**	**Material cost (\$/g product)**	**Cost per step (\$/step)**
2,2',7,7'-tetrabromo-9,9'-spirobi[9H-fluorene]	1.15			95900.00	110.29	
4,4'-dimethoxydiphenylamine	1.87			54900.00	102.66	273.62
t-BuONa	1.04			307.00	0.32	

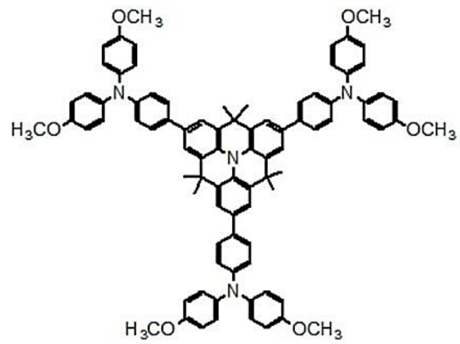
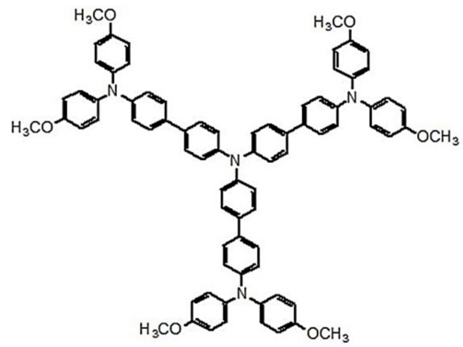
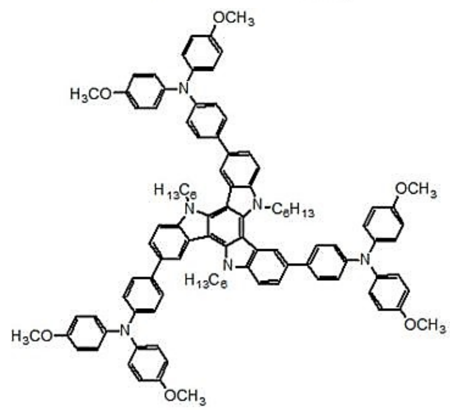
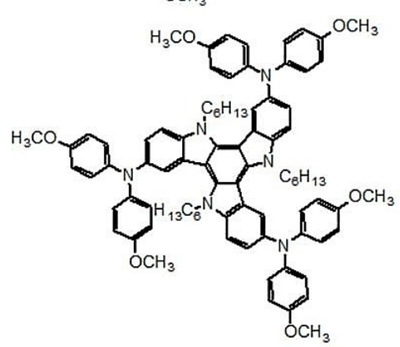
$Pd_2(dba)_3$	0.067			14900.00	1.00	
Toluene		12		69.48	0.83	
Ethyl acetate			135	80.16	10.82	
NaCl (brine)	2		1	50.70	0.05	
$MgSO_4$	0.05		1	144.20	0.14	
Ethyl acetate	1		120	80.16	9.62	
n-Hexane			176	117.91	20.75	
Silica gel 60	20		263	62.20	16.36	
Total						273.62

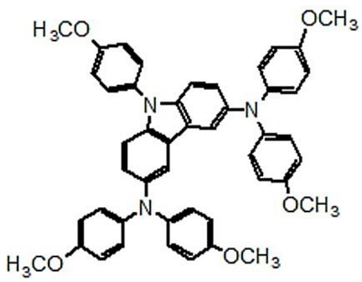
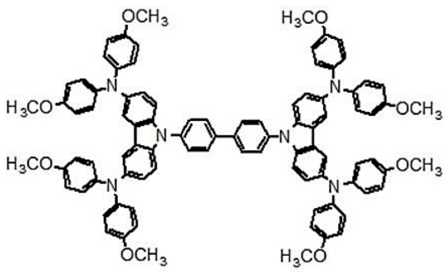
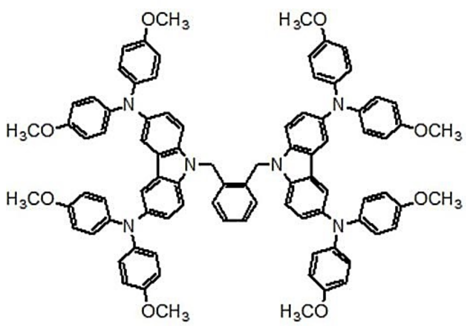
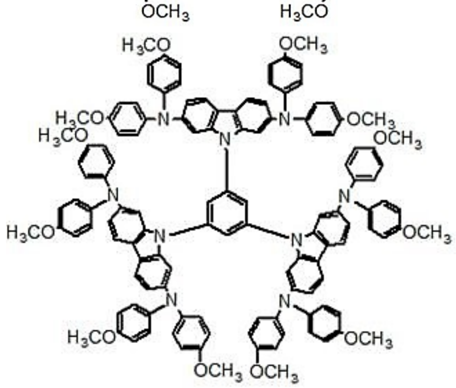
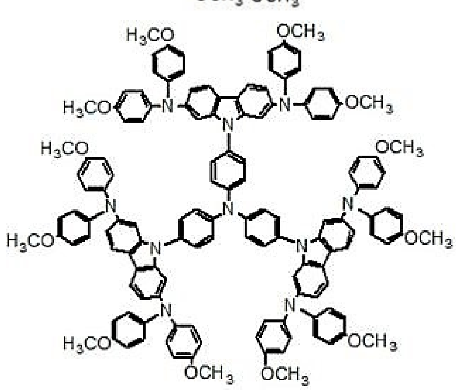
Table S2. Quantities and costs of the materials used for the synthesis of 1 g of HTM **1** together with sum of costs HTM [2, 3].

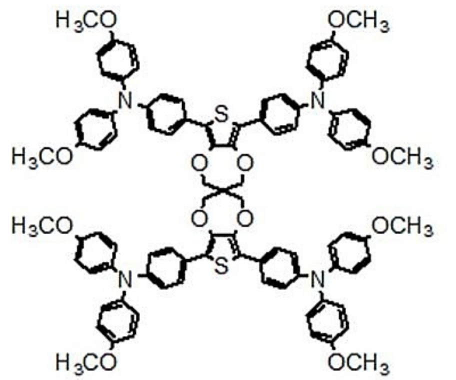
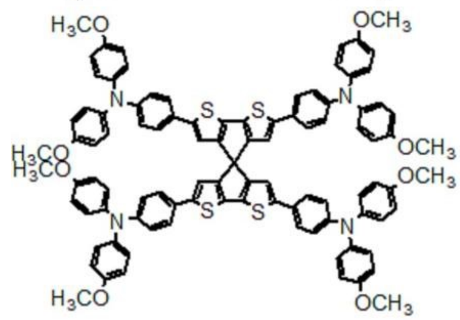
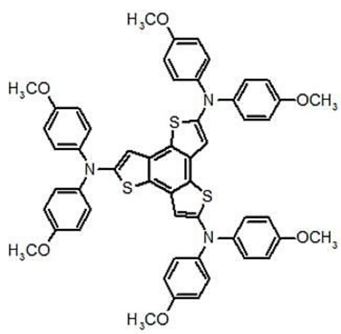
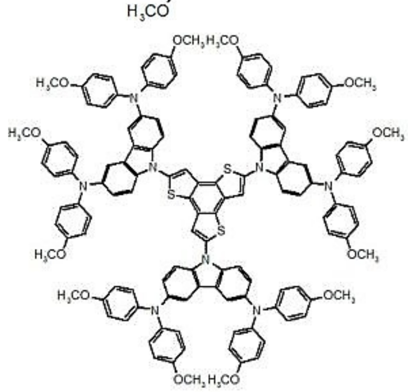
Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Benzil	0.62			120	0.072	
3-nitrobenzaldehyde	0.44			150	0.066	
Ammonium Acetate	3.66			90	0.33	1.66
Acetic Acid		10.5	5.50	50	0.80	
Ethanol			15.78	25	0.40	
Total						1.66

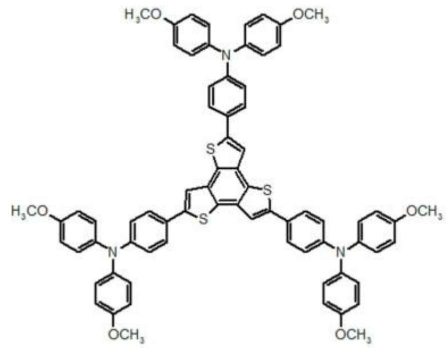
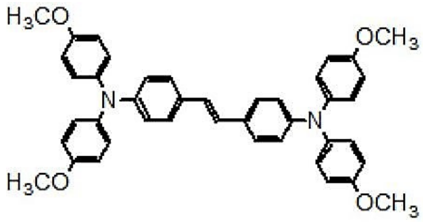
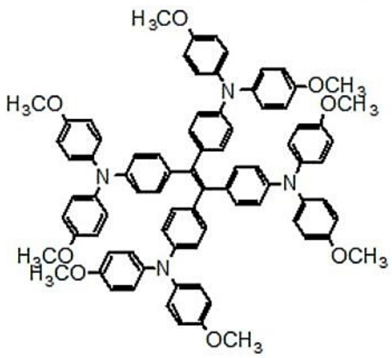
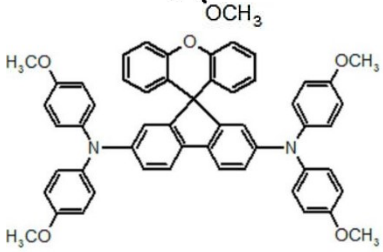
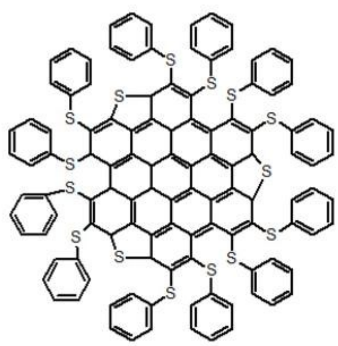
Table S3. The catalysts and cost for the synthesis of 1 g of organic HTMs and their photovoltaic characteristics.

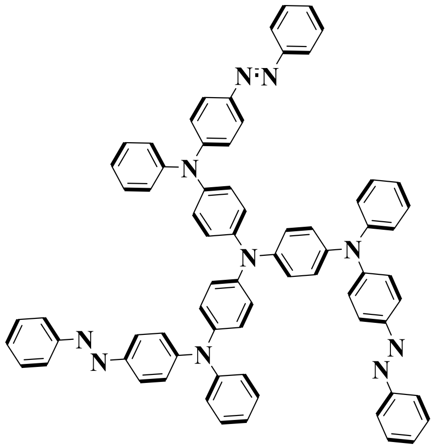
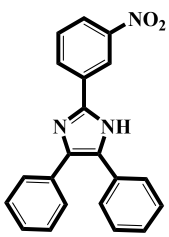
No.	HTM	Catalyst used for synthesis	Cost per 1 g	Jsc (mA cm^{-2})	Voc (V)	FF	η (%)	Ref.
1		t-BuONa Pd2(dba)3 P(t-Bu)3	273.62	20.7	1.00	0.71	14.9	4

2		$Pd(PPh_3)_4$ K_2CO_3	842.08	20.98	0.97	0.67	13.63	[5]
3		$Pd(PPh_3)_4$ K_2CO_3	420.22	20.88	0.95	0.62	12.31	[5]
4		$Pd(PPh_3)_4$ K_2CO_3	695.87	21.21	1.09	0.78	18.36	[6]
5		t-BuONa $Pd(OAc)_2$ $P(t\text{-}Bu)_3$	245.84	20.6	0.88	0.63	11.54	[6]

6		t-BuONa $P(t\text{-}Bu)_3$ $Pd_2(dba)_3$	148.57	20.4	1.13	0.68	15.8	[7]
7		CuI 1,10-phenanthroline K_2CO_3	216.46	23.2	1.02	0.79	18.6	[7]
8		t-BuONa $Pd(OAc)_2$ $[(t\text{-}Bu)_3PH]BF_4$	168.42	21.0	0.92	0.67	12.92	[8]
9		$Pd(OAc)_2$ Tri-t-butylphosphine t-BuONa	434.12	20.28	1.02	0.71	14.79	[9]
10		$Pd(OAc)_2$ Tri-t-butylphosphine t-BuONa	450.13	20.35	0.99	0.69	13.86	[9]

11		K_2CO_3 $Pd(PPh_3)_4$	579.16	17.63	1.02	0.73	13.44	10
12		K_2CO_3 $Pd(PPh_3)_4$	633.88	13.8	0.98	0.76	10.3	11
13		$Pd_2(dba)_3$ X-Phos t-BuONa	376.30	20.4	1.04	0.72	16.0	12
14		$Pd_2(dba)_3$ X-Phos t-BuONa	591.57	20.6	1.09	0.77	17.0	12

15		$Pd(PPh_3)_4$ K_3PO_4 NH_4Cl	800.49	21.9	1.07	0.77	18.2	[12]
16		Zn $TiCl_4$	101.34	18.2	1.03	0.61	11.4	[13]
17		Zn $TiCl_4$	52.59	21.2	0.92	0.67	13.1	[13]
18		t-BuONa P(t-Bu)$_3$ Pd(OAc)$_2$	112.23	23.4	1.13	0.73	19.8	[14]
19		AlC$_3$ $FeCl_3$	367.55	20.6	0.95	0.66	12.8	[15]

20		CuI Cs_2CO_3 1,10-phenanthroline	22.76	17.01	0.94	0.63	17.86	[16]
21		-	1.66	15.31	0.90	0.65	15.20	This work

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