

Simple and low-cost thiophene and benzene-conjugated triarylamines as hole-transporting materials for perovskite solar cells

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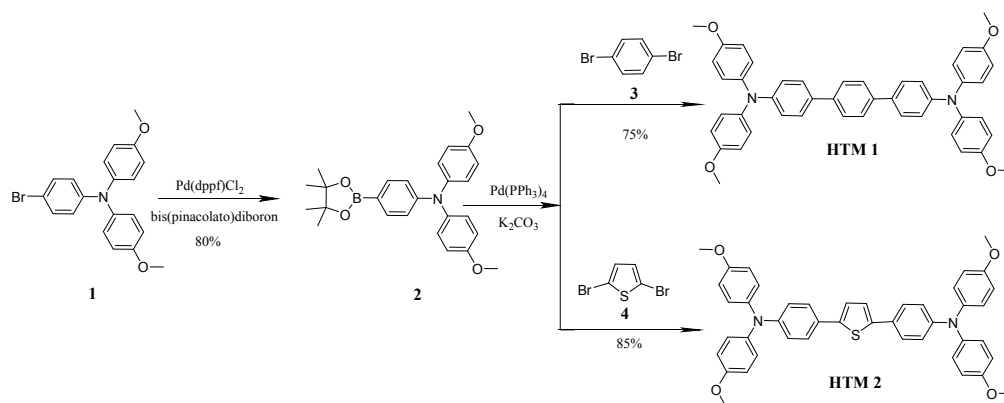
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FTO/PEDOT:PSS/HTM/Au.

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Scheme S1. Synthetic scheme for the preparation of HTM1 and HTM2.

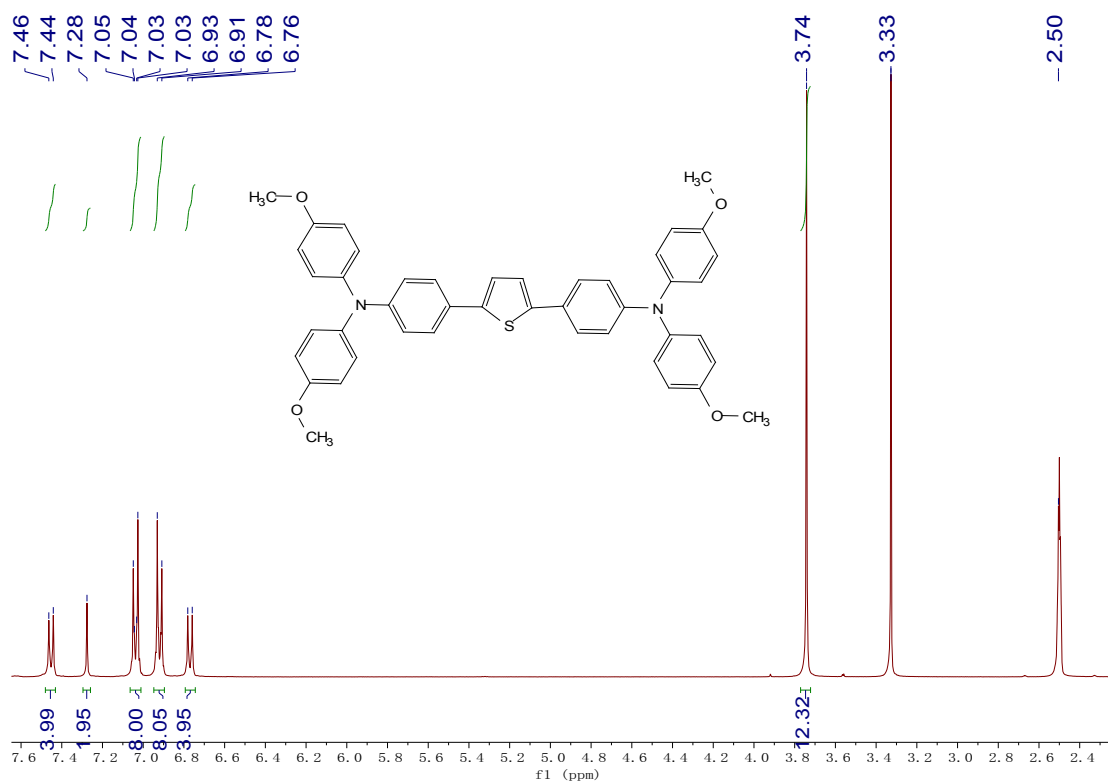


Figure S1. $^1\text{H NMR}$ of HTM1 in $\text{DMSO-}d_6$.

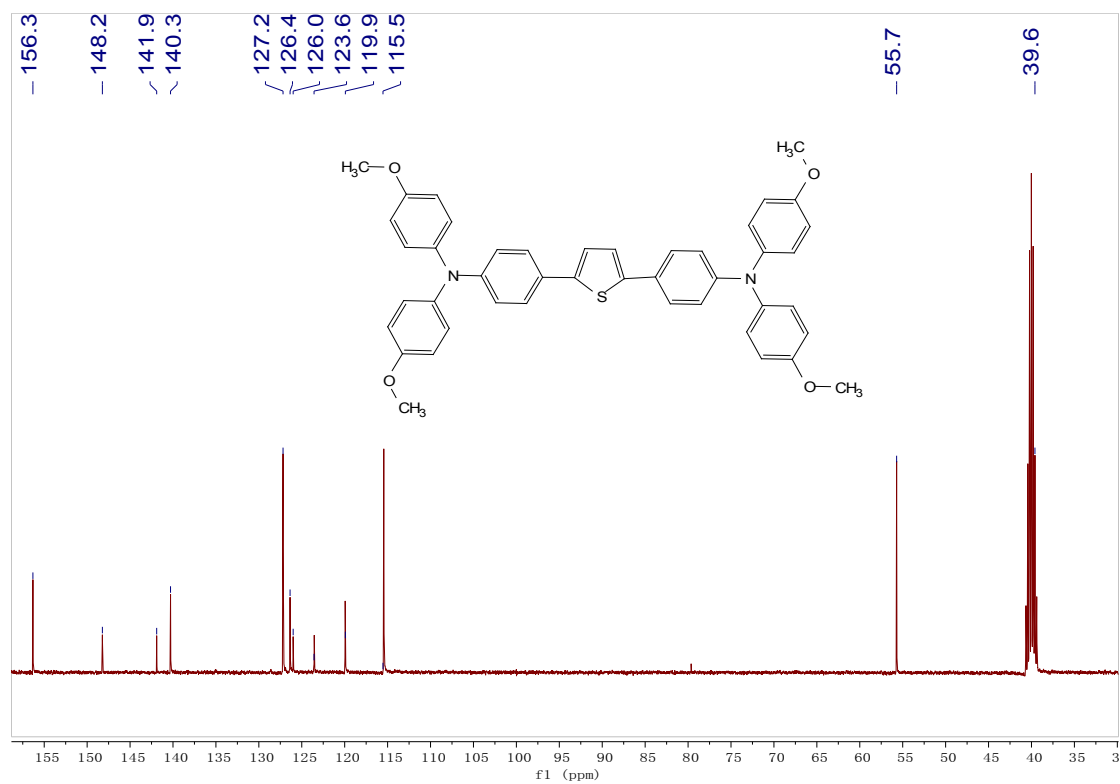


Figure S2. ^{13}C NMR of HTM1 in $\text{DMSO-}d_6$.

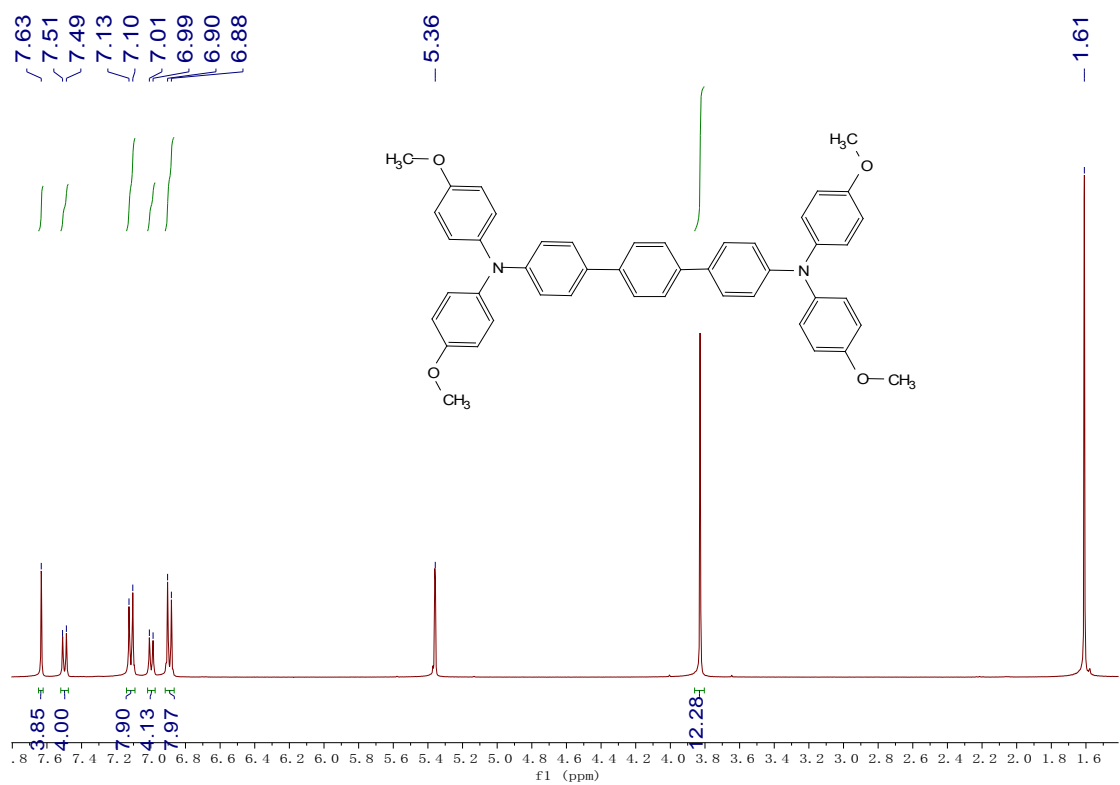


Figure S3. ^1H NMR of HTM2 in CD_2Cl_2 .

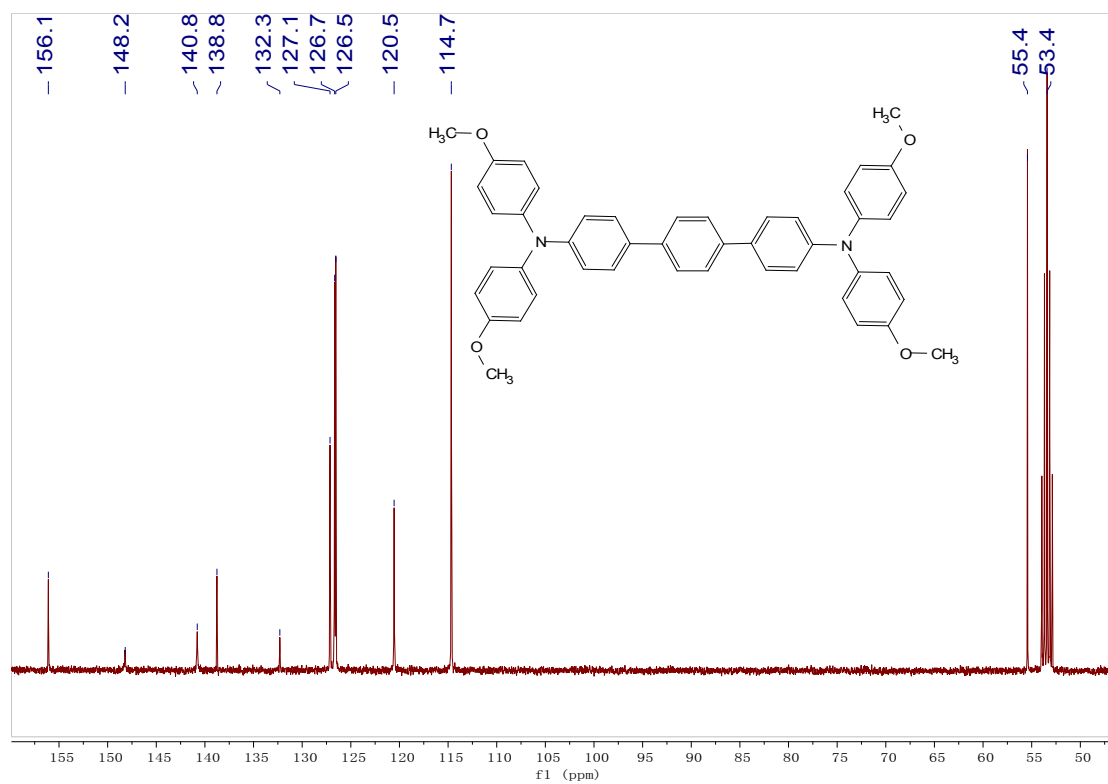


Figure S4. ^{13}C NMR of HTM2 in CD_2Cl_2 .

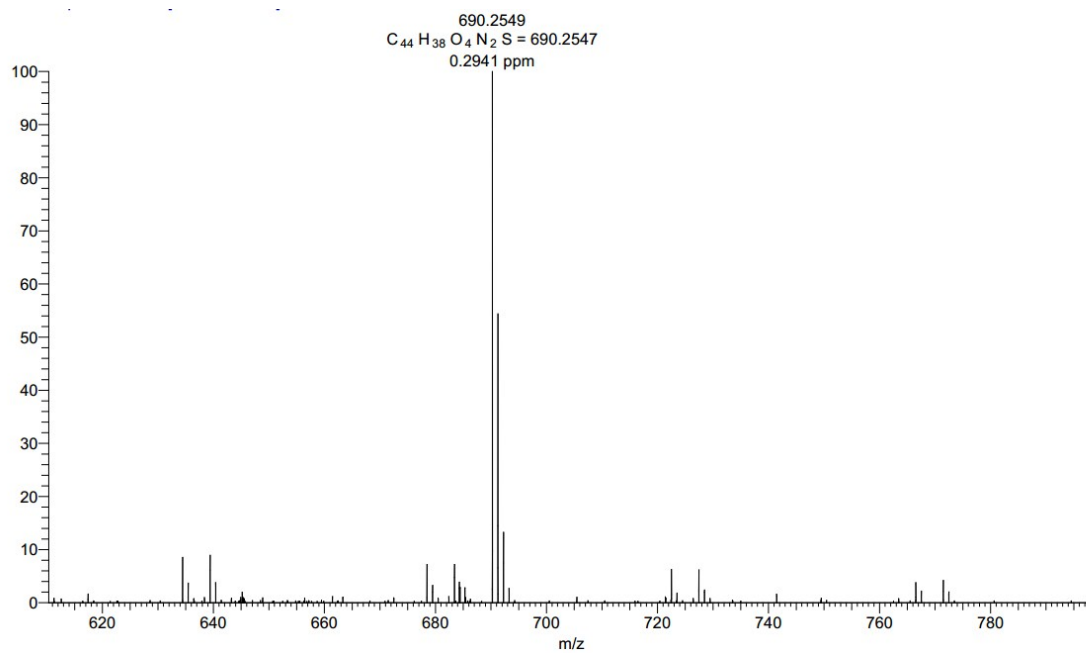


Figure S5. HRMS of HTM1.

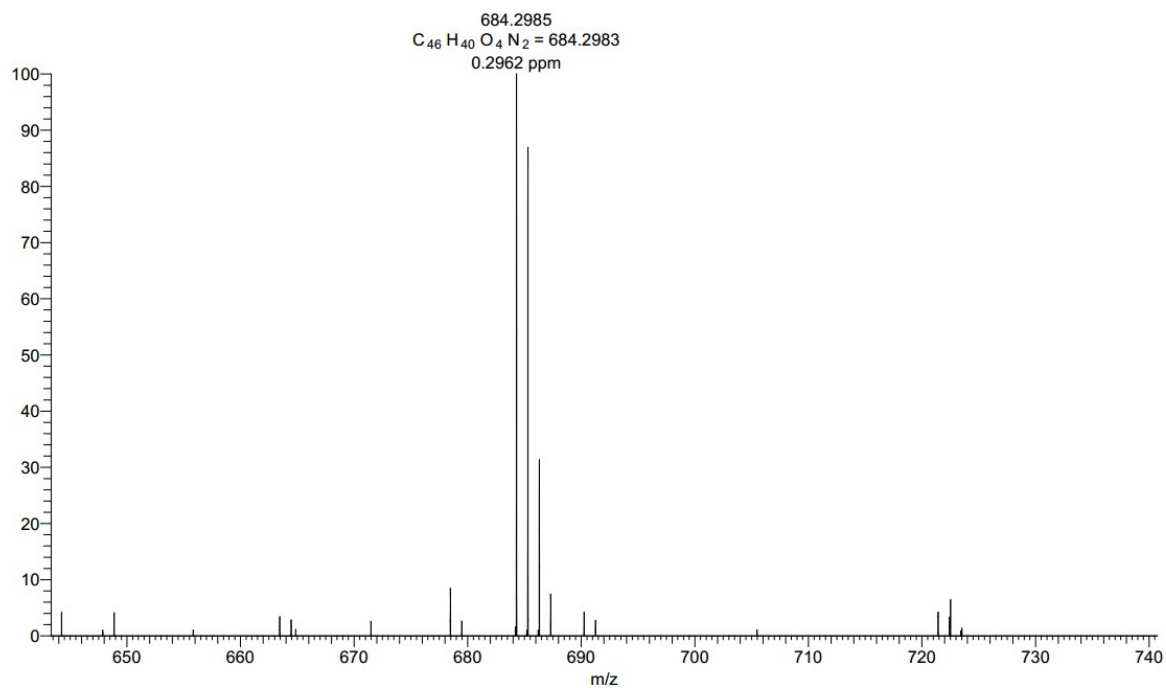


Figure S6. HRMS of HTM2.

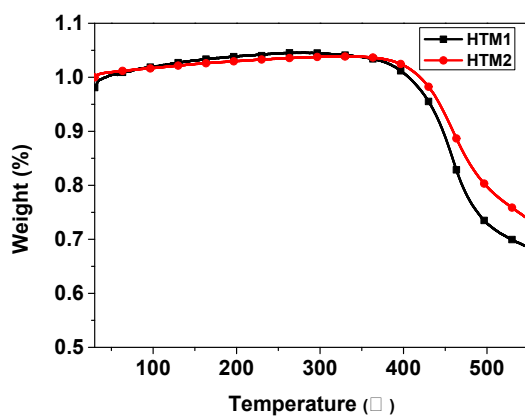


Figure S7. TGA of HTM1 and HTM2

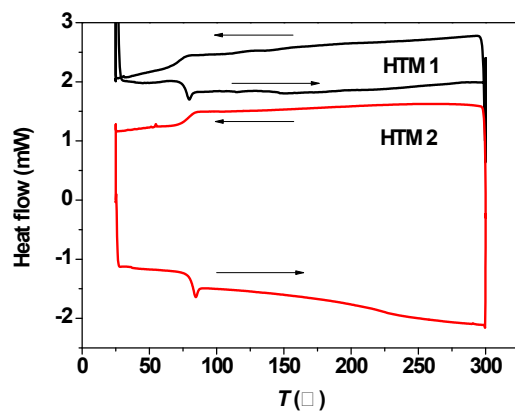


Figure S8. DSC of HTM1 and HTM2

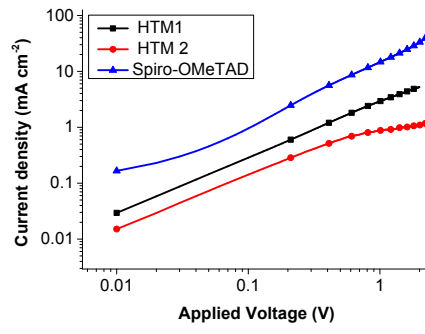


Figure S9. SCLC measurement of the HTMs films. Hole-only devices structure:

FTO/PEDOT:PSS/HTM/Au.

Table S1. Materials, quantities and cost for the synthesis of HTM1 and HTM2

Chemical	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical (\$/kg)	Cost of chemical (\$/g product)	Total Cost (\$/g)
4-bromo-N,N-bis(4-methoxyphenyl)aniline	1.11			1185.19	1.32	
bis(pinacolato)diboron	0.88			362.67	0.32	
Pd(dppf)Cl ₂	0.12			9822.22	1.18	
KOAc	0.84			32.00	0.03	
dioxane		15.00		8.00	0.12	
CH ₂ Cl ₂			20.00	4.44	0.09	
water			10.00		0.00	
methanol			15.00	4.00	0.06	
OMT BPIN						3.11
OMT BPIN	1.61			3109.63	5.01	
2,5-dibromothiophene	0.41			710.52	0.29	
Pd(PPh ₃) ₄	0.10			16000.00	1.60	
THF		17.80		11.85	0.21	
K ₂ CO ₃	1.17			7.41	0.01	
water		10.00			0.00	
CH ₂ Cl ₂			80.00	4.44	0.36	
Na ₂ SO ₄			5.00	3.26	0.02	
Petroleum ether			100.00	7.41	0.74	
silica gel			30.00	10.96	0.33	
2,5-bis(4,4'- bis(methoxyphenyl)aminophen-4''-yl)- thiophene (HTM 1)						8.56
OMT BPIN	1.84			3109.63	5.72	
2,5-dibromobenzene	0.46			120.44	0.06	
Pd(PPh ₃) ₄	0.11			16000.00	1.76	
THF		17.80		11.85	0.21	
K ₂ CO ₃	1.34			7.41	0.01	
water			10.00			
CH ₂ Cl ₂			80.00	4.44	0.36	
Na ₂ SO ₄			5.00	3.26	0.02	
Petroleum ether			100.00	7.41	0.74	
silica gel			40.00	10.96	0.44	
2,5-bis(4,4'- bis(methoxyphenyl)aminophen-4''-yl)-						9.31

thiophene (HTM 2)
