Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting information

Facile star shape tetraphenylethylene-based molecules with fused ring-terminated diarylamine as interfacial hole transporting materials for inverted perovskite solar cells

Yung-Chung Chen[a,b*], Ding-Zhi Lin[a], Jhong-Ci Wang[c], Jen-Shyang Ni[a], Yang-Yen Yu [c*]and Chih-Ping Chen[c*]

[a] Department of Chemical and Materials Engineering, National Kaohsiung University of Science and Technology, 415 jiangong Rd., Sanmin District, Kaohsiung City 80778, Taiwan

[b] Photo-SMART (Photo-sensitive material advanced research and technology center), National Kaohsiung University of Science and Technology, 415, Jiangong Rd., Sanmin District, Kaohsiung City 80778, Taiwan

[c] Department of Materials Engineering, Ming Chi University of Technology, 84 Gunjuan Road, Taishan, New Taipei City, 24301, Taiwan

Corresponding authors: Yung-Chung Chen (chenyc@nkust.edu.tw), Yang-Yen Yu (yyyu@mail.mcut.edu.tw), Chih-Ping Chen (cpchen@mail.mcut.edu.tw)

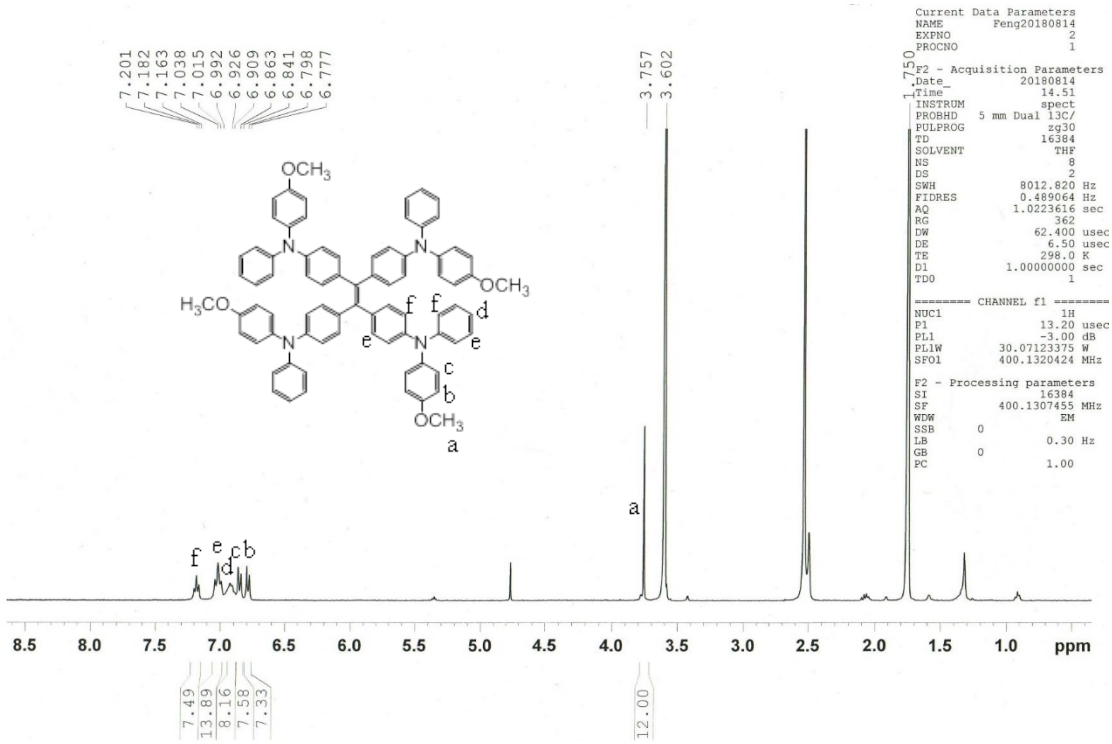


Fig. S1 ^{1}H NMR spectrum of the **CL-1**.

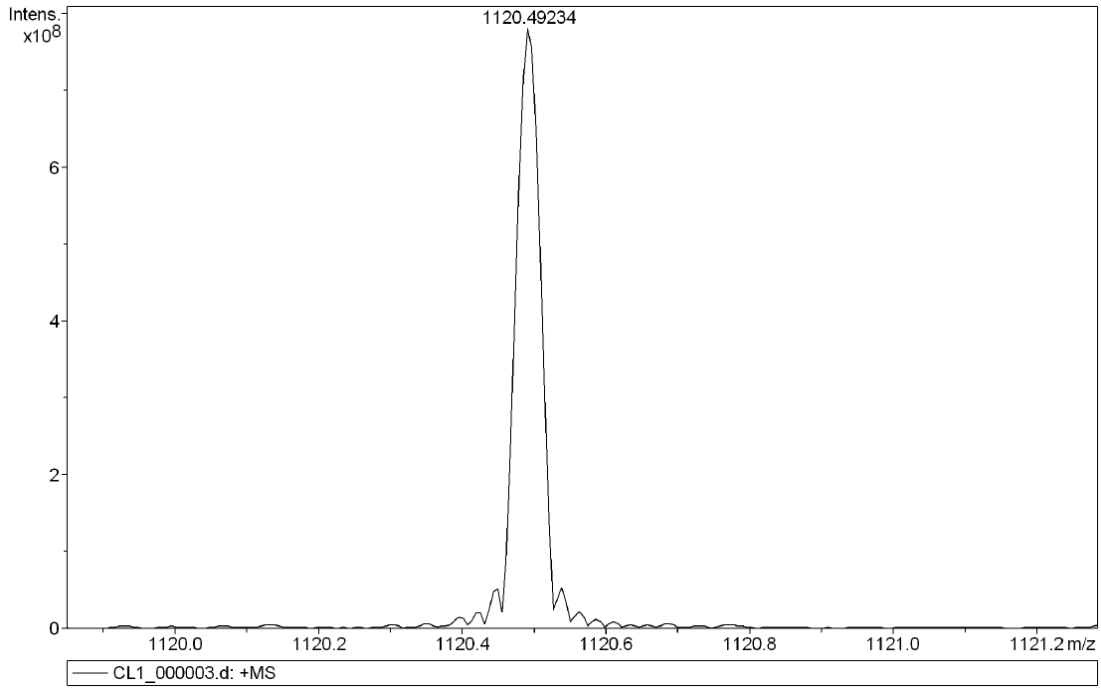


Fig. S2 HRMS spectrum of the **CL-1**.

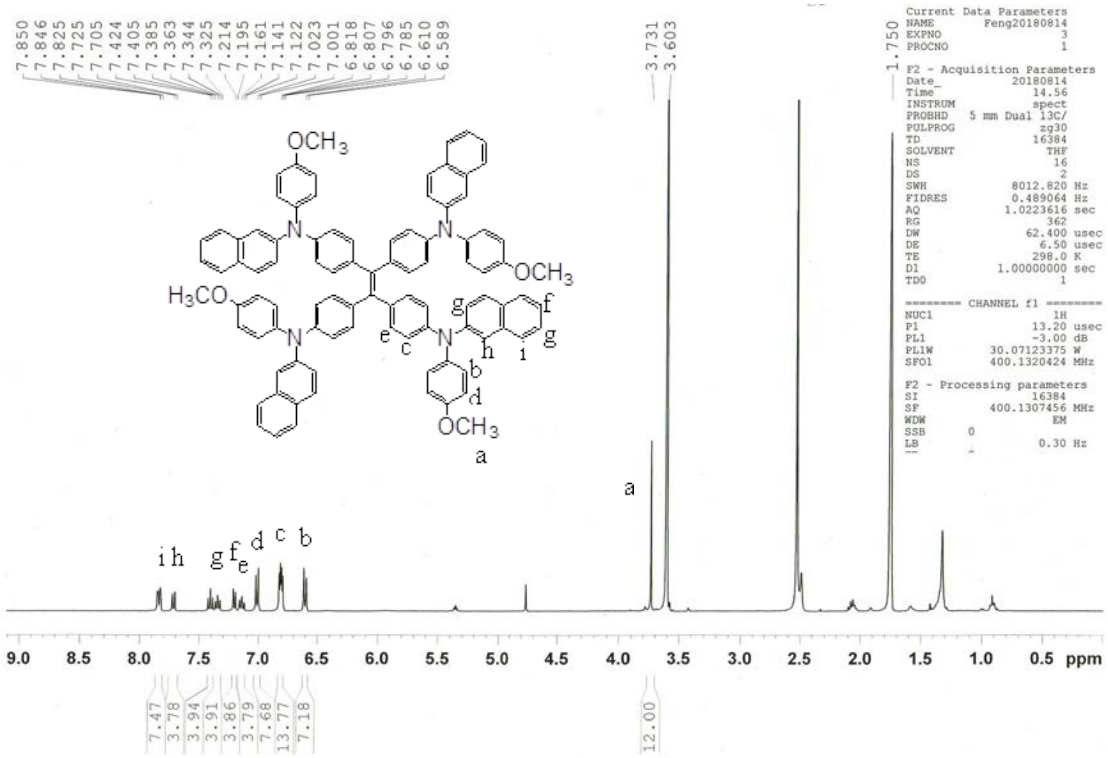


Fig. S3 ^{1}H NMR spectrum of the **CL-2**.

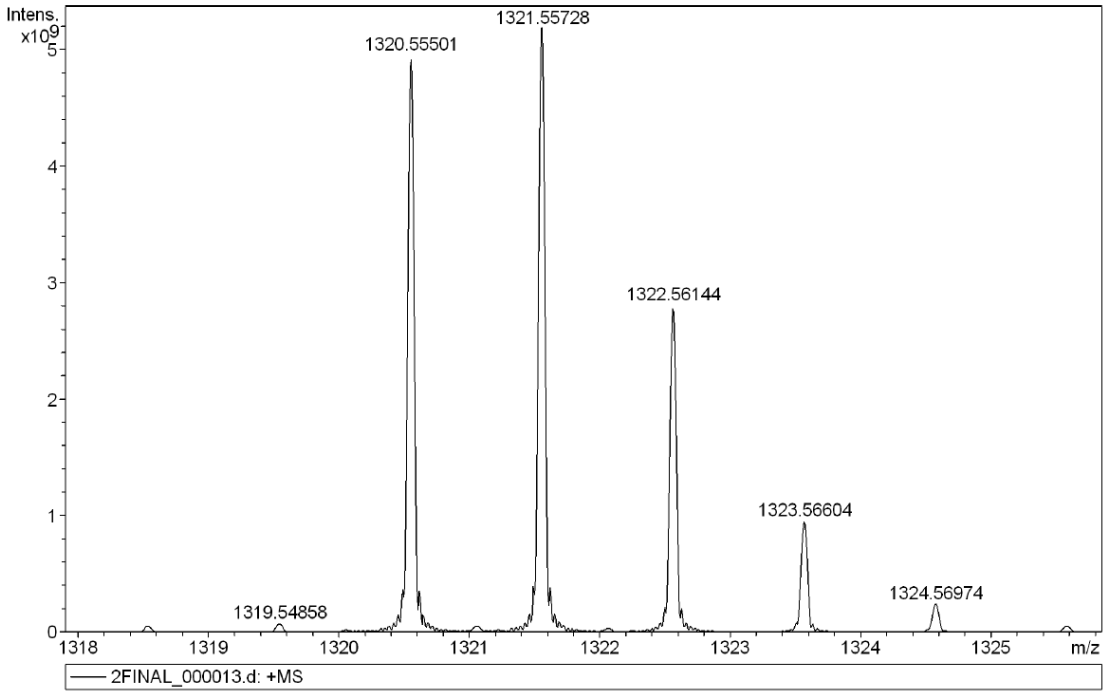


Fig. S4 HRMS spectrum of the **CL-2**.

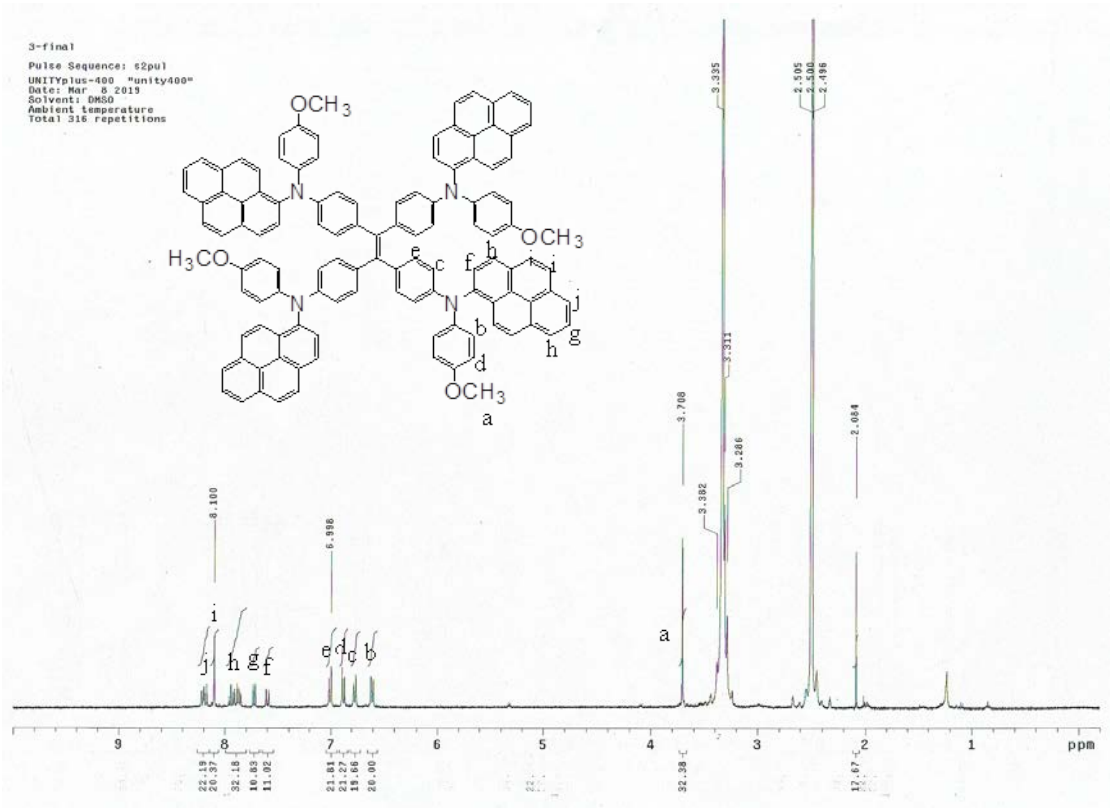


Fig. S5 ^{1}H NMR spectrum of the **CL-3**.

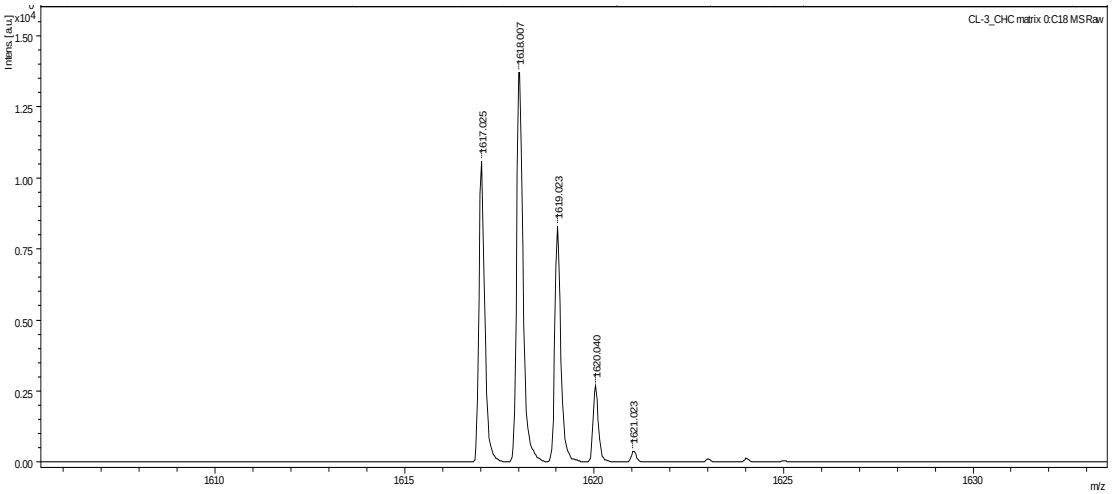


Fig. S6 MALDI/TOF spectrum of the **CL-3**.

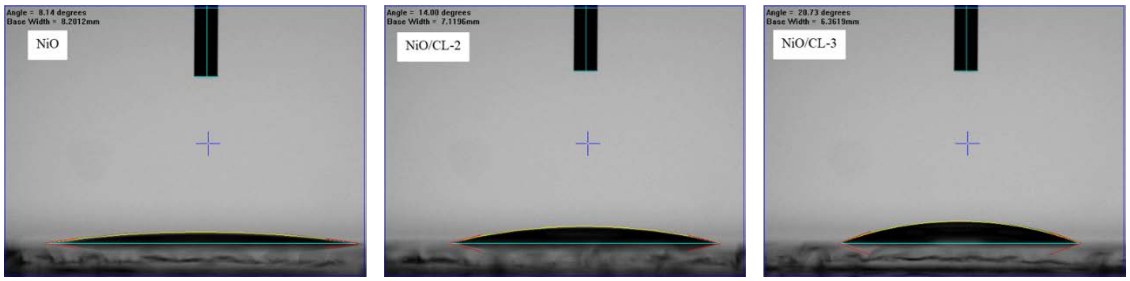


Fig. S7 Water contact angle of various HTLs spin-coated onto the ITO glass.

Table S1 Device performance based on ITO/HTMs/$CH_3NH_3PbI_3$/$PC_{61}BM$/BCP/Ag configuration

HTM	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	η_{avg} (%)	η_{max} (%)
CL-2	18.91±1.29	0.99±0.37	70.30±2.29	13.09±0.52	14.01
CL-3	17.93±0.69	0.99±0.05	66.98±2.44	11.84±0.49	12.46

[a] Calculated from 10 devices.

Table S2 Lifetimes of perovskite thin films of MAPbI3-based perovskite devices

Sample	τ_1 (ns)	A_1	τ_2 (ns)	A_2	$\tau_{Average}$ (ns)
NiOx/PVSK	7.4	32%	53.3	68%	38.7
NiOx/CL-2PVSK	8.1	34%	49.9	66%	35.6
NiOx/CL-3PVSK	6.8	35%	48.7	65%	34.1

The lifetime was obtained by fitting the PL data measured from the perovskite films with a biexponential decay function of the form: $\tau_{Average} = A_1 e^{-t/\tau_1} + A_2 e^{-t/\tau_2}$

Table S3 FWHM and crystallite size results of the perovskite films with different HTL layers

HTL	FWHM	Crystallite size[a] (nm)
NiOx	0.37239	21.74
NiOx/CL-2	0.37199	21.77
NiOx/CL-3	0.36944	21.92

[a] The crystallite size is determined by the peak of (110) at 2θ of around 14.1° and calculated from the Debye–Scherrer equation $\tau = k\lambda/B\cos\theta$ (τ = crystallite size).

Table S4 EIS results of the perovskite devices based on various HTLs[a]

Sample	Rs	Rp	CPE-T	CPE-P
NiOx	16	467	7.94E-9	0.98
NiOx/CL-3	12	265	5.44E-9	1.03

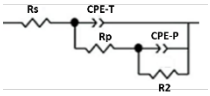
[a] Equivalent circuit model: 

Table S5 Contact angles and surface energies of various HTLs

HTL	θ_{Water}[°]	θ_{DIM}[°]	γ_{polar}[mN m^{-1}]	$\gamma_{dispersive}$[mN m^{-1}]	γ_{total}[mN m^{-1}]
CL-2	73.58	15.36	9.85	49.98	58.87
CL-3	72.90	14.24	10.11	49.02	59.37
NiOx	11.45	10.36	35.29	49.98	85.27
NiOx/**CL-2**	13.37	21.31	35.62	47.44	83.06
NiOx/**CL-3**	20.51	22.546	33.86	47.06	80.92