Supplementary Information for:

The effect of different binding sites on the optical and electronic properties of tetraphenylethylene-substituted thiophene isomers

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1. General characterizations

1.1 ^{1}H NMR and ^{13}C NMR spectra

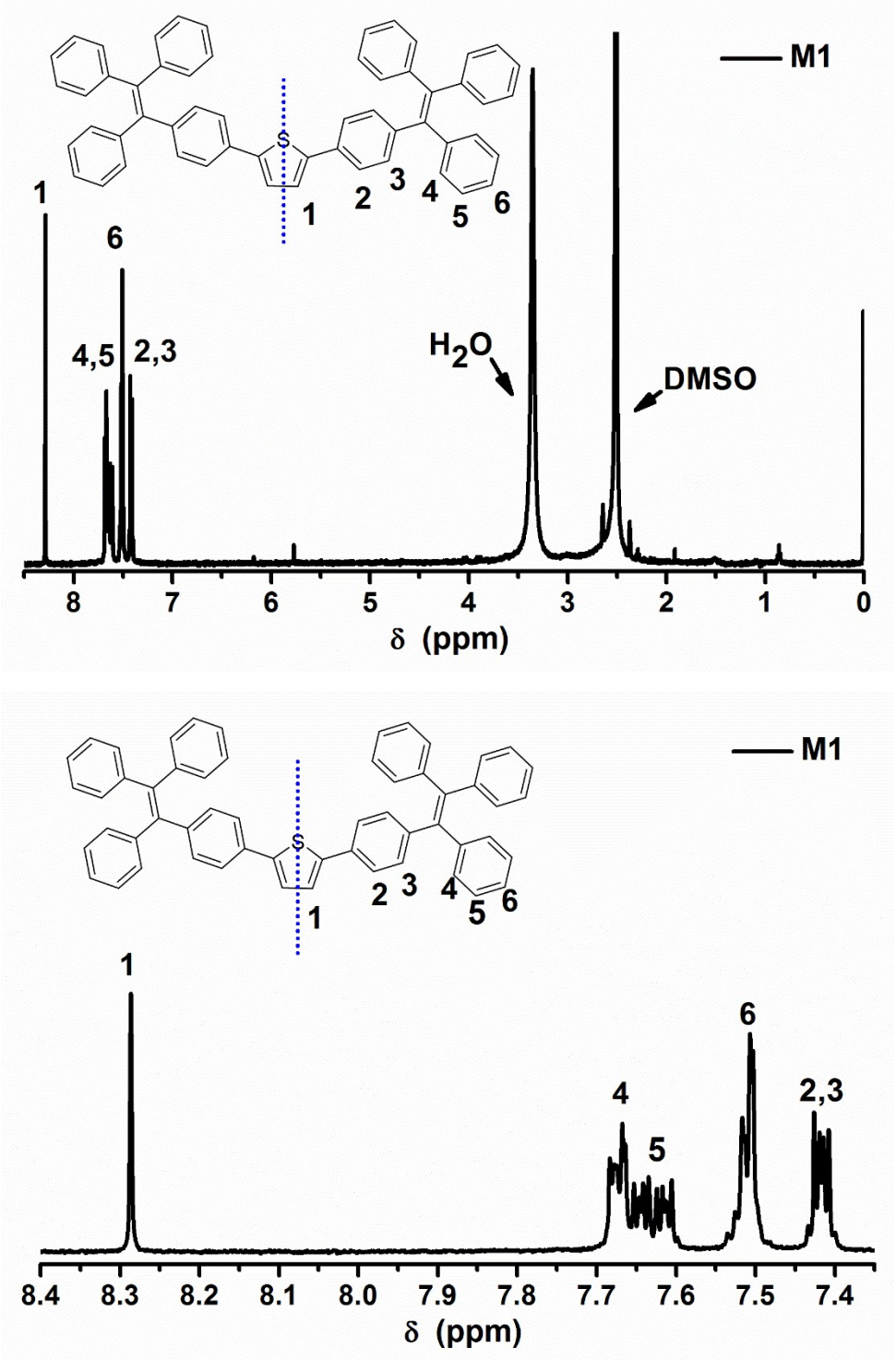


Fig. S1 ^{1}H NMR spectra of M1 in DMSO at room temperature.

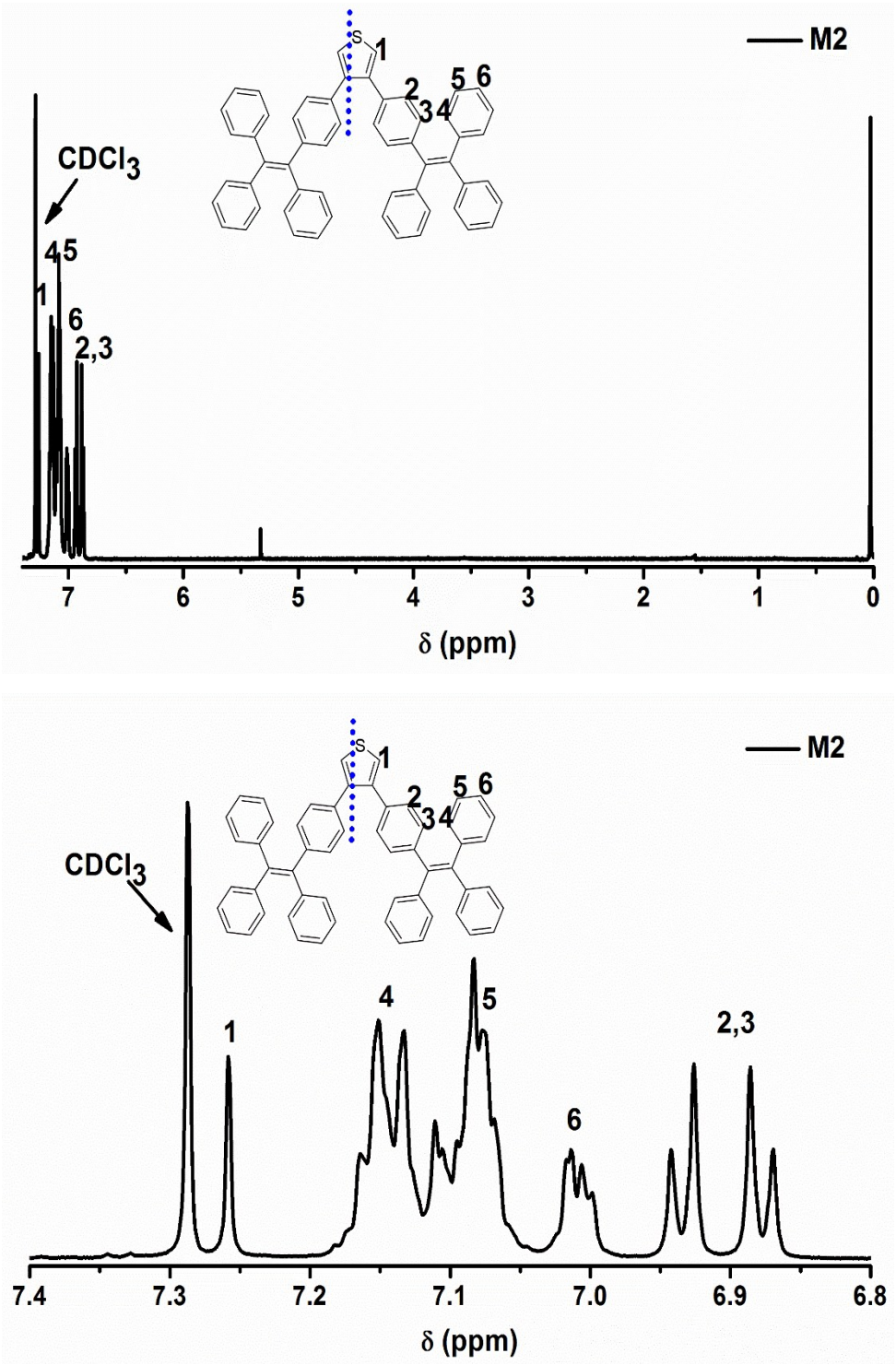


Fig. S2 ^{1}H NMR spectra of M2 in $CDCl_3$ at room temperature.

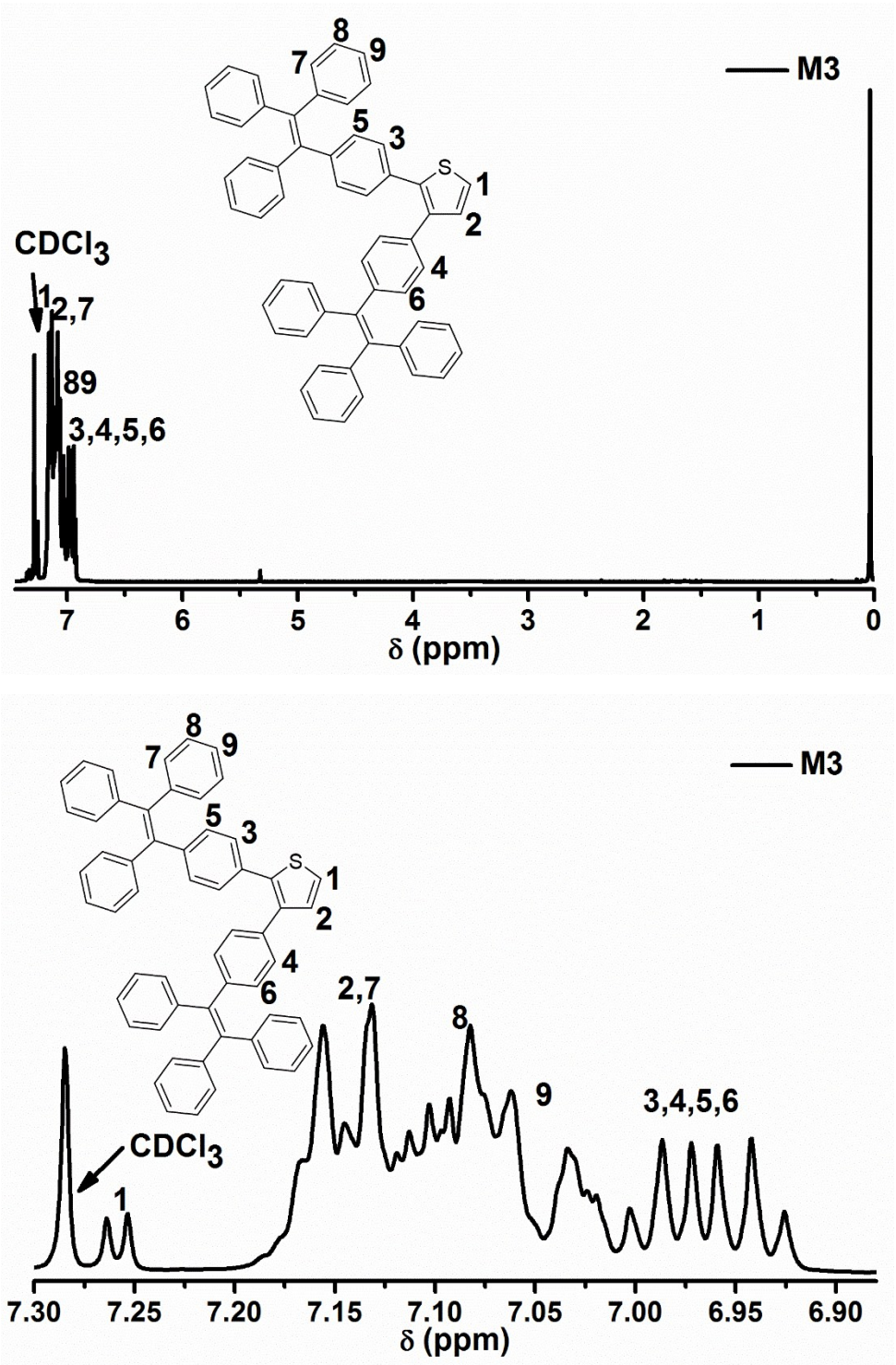


Fig. S3 ^{1}H NMR spectra of M3 in $CDCl_3$ at room temperature.

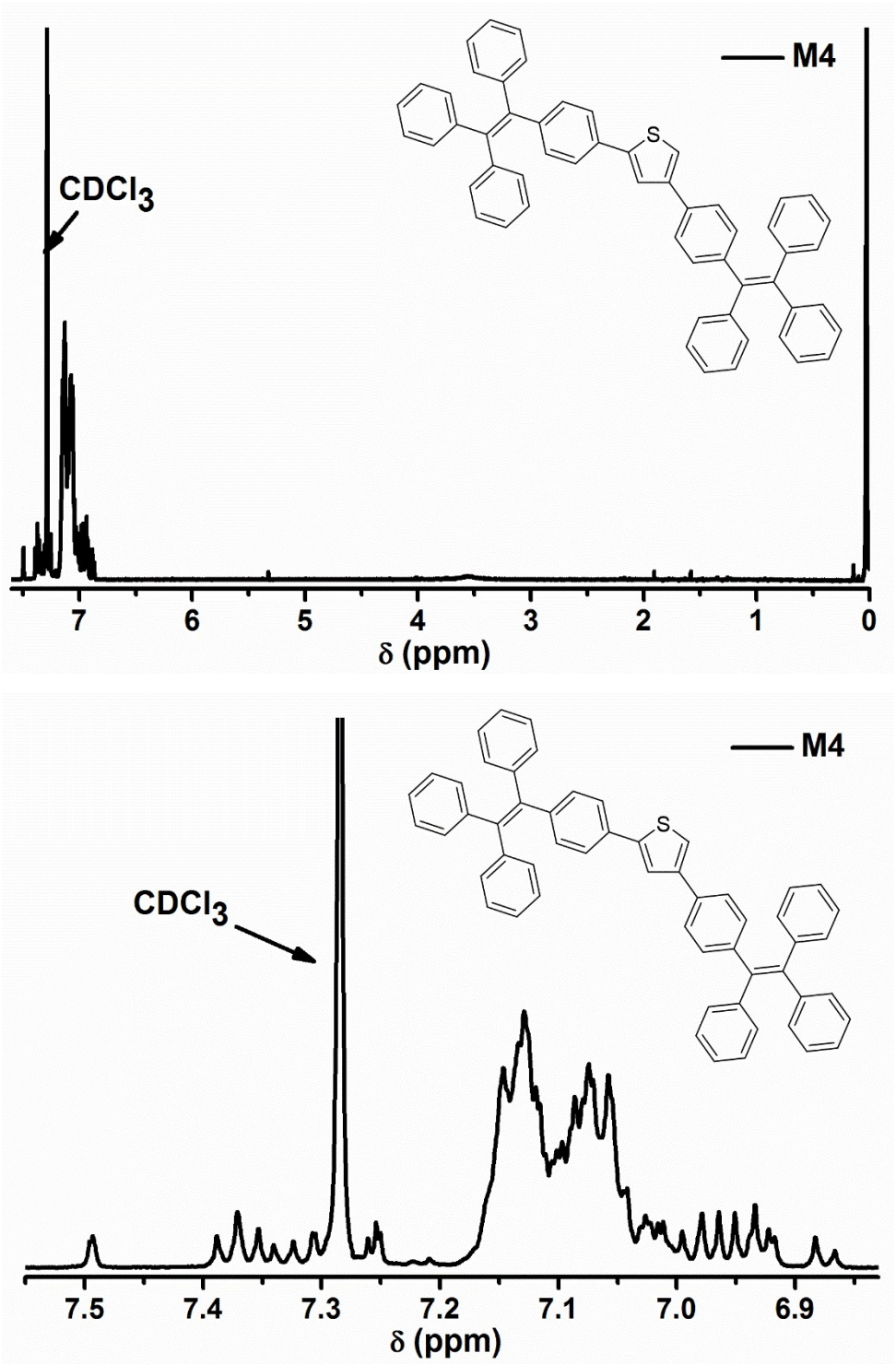


Fig. S4 ^{1}H NMR spectra of M4 in $CDCl_3$ at room temperature.

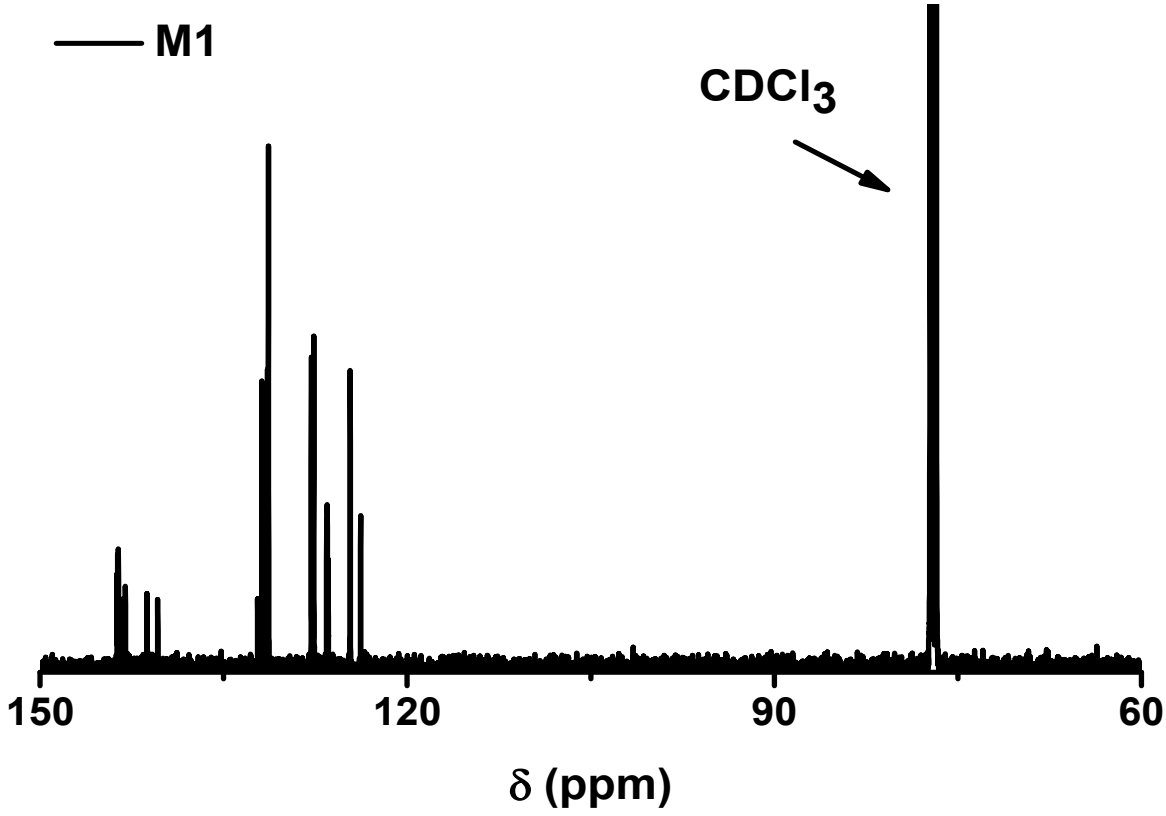


Fig. S5 ^{13}C NMR spectra of M1 in $CDCl_3$ at room temperature.

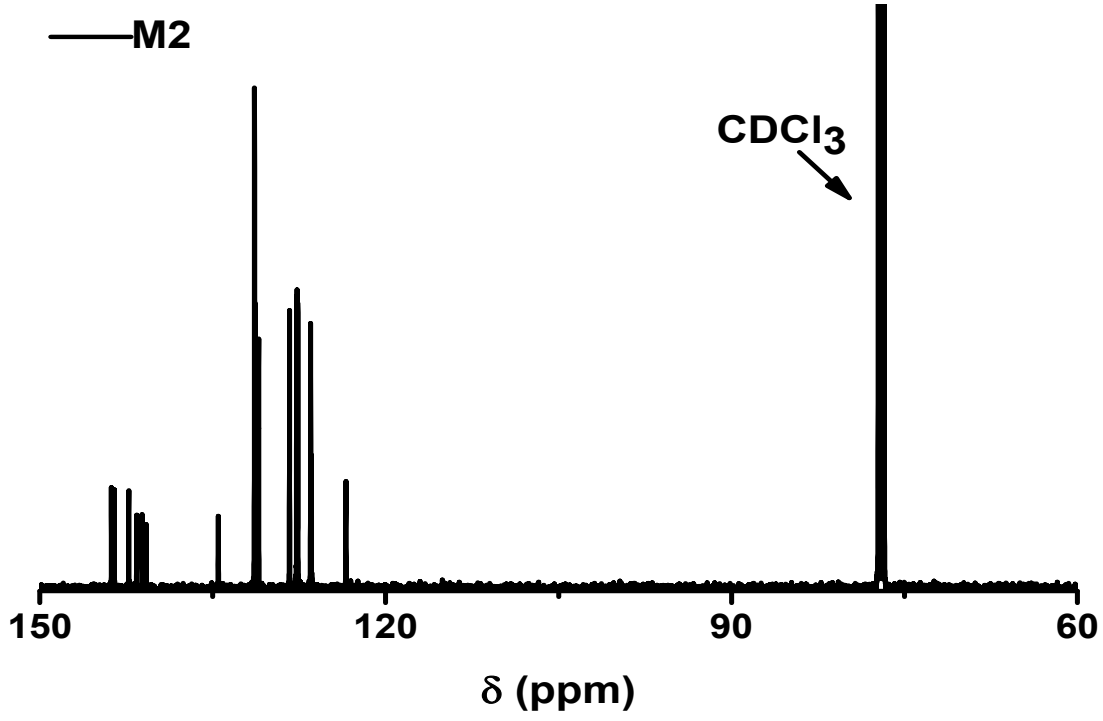


Fig. S6 ^{13}C NMR spectra of M2 in $CDCl_3$ at room temperature.

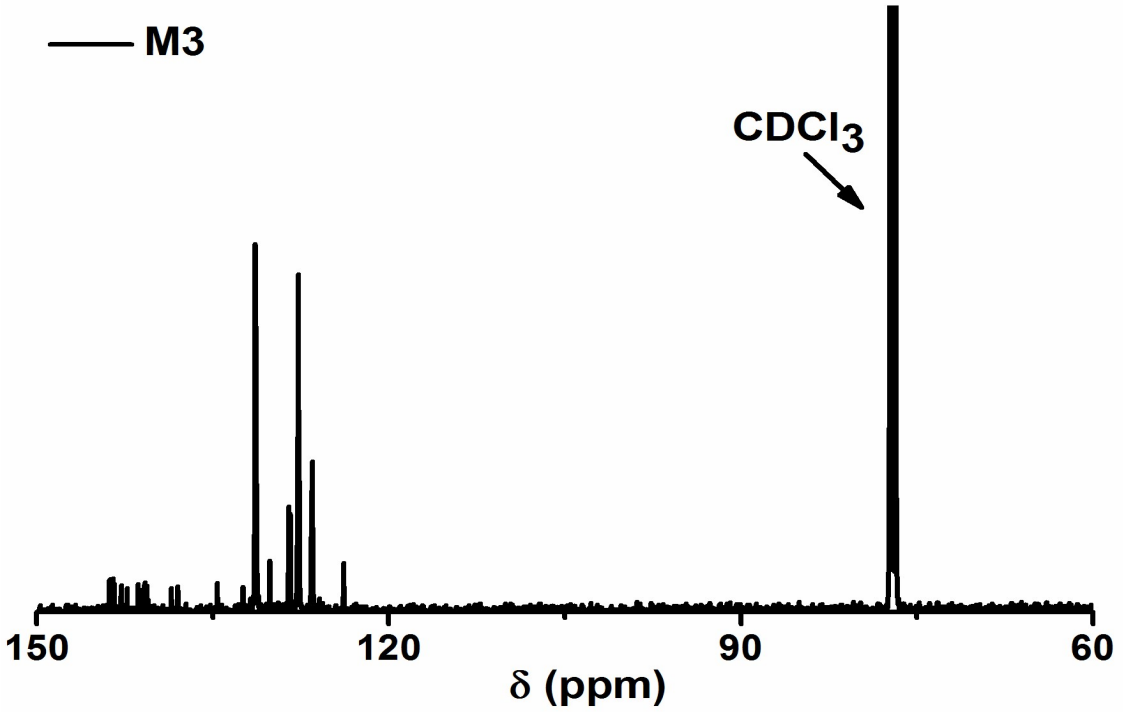


Fig. S7 ^{13}C NMR spectra of M3 in $CDCl_3$ at room temperature.

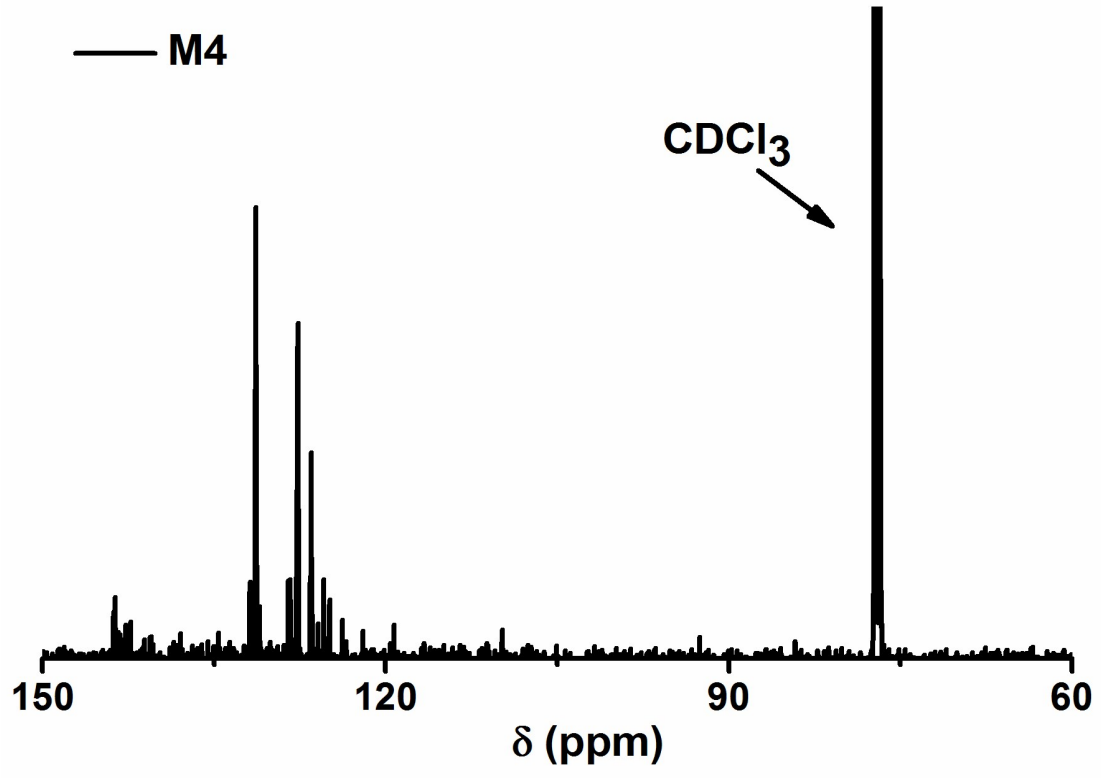


Fig. S8 ^{13}C NMR spectra of M4 in $CDCl_3$ at room temperature.

1.2 Mass spectra

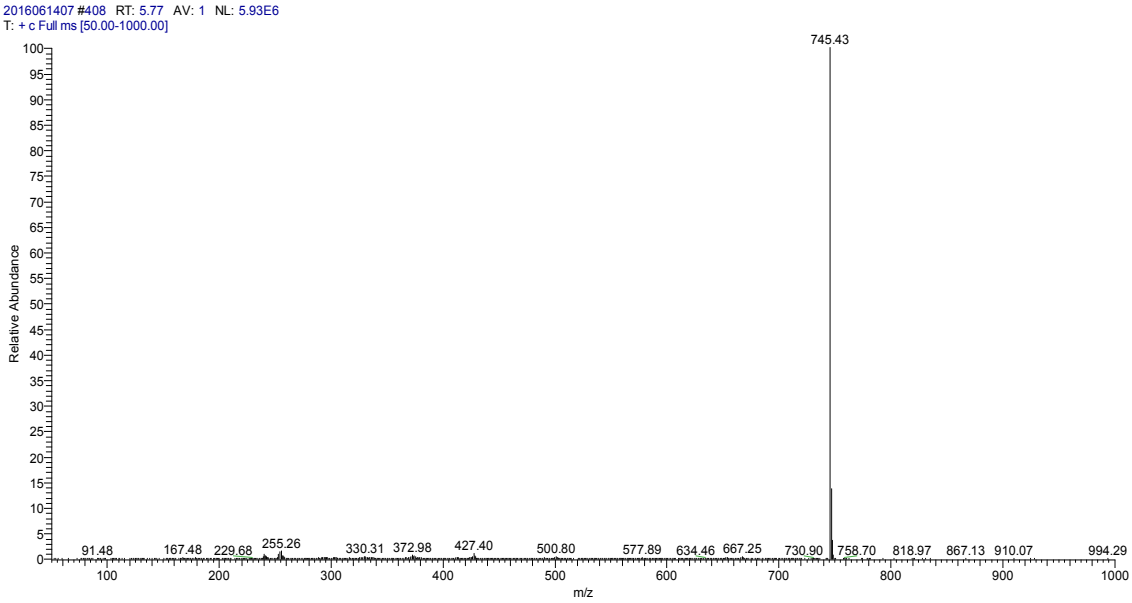


Fig. S9 Mass spectra of M1.

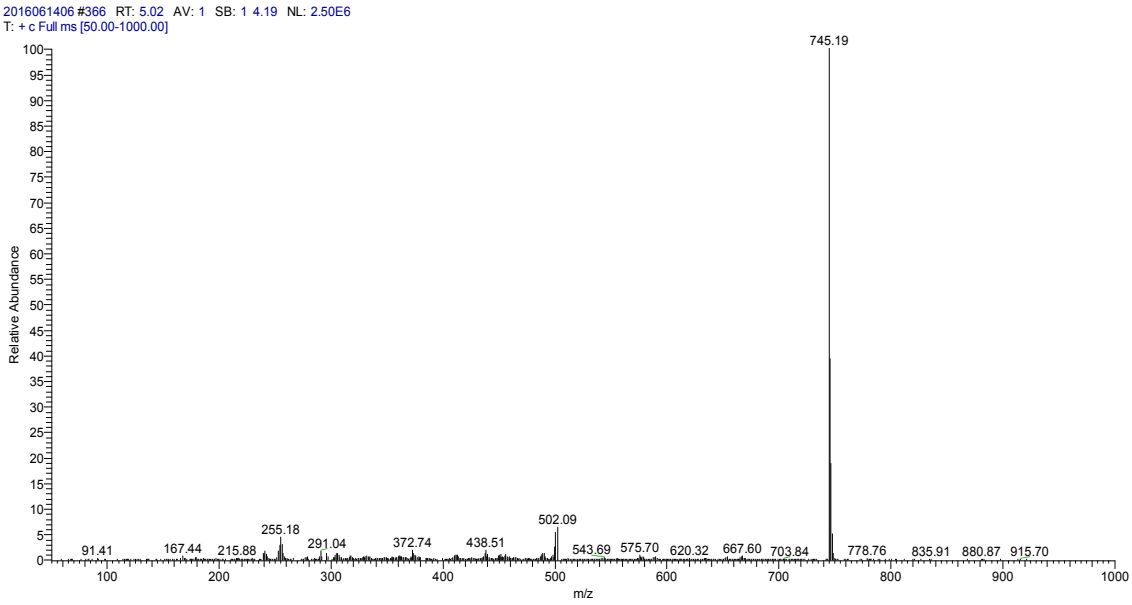


Fig. S10 Mass spectra of M2.

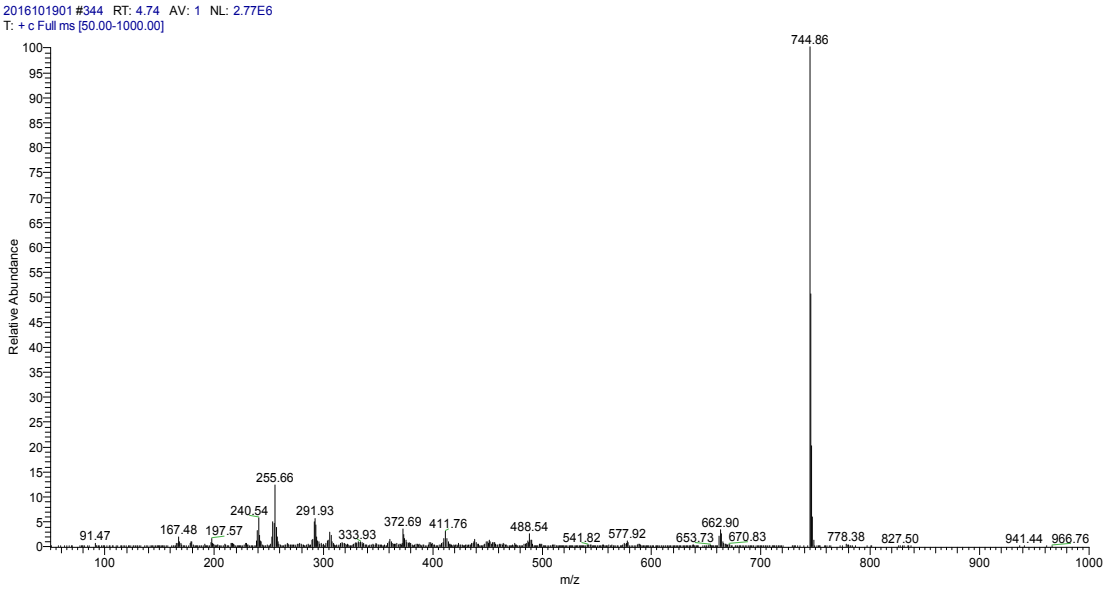


Fig. S11 Mass spectra of M3.

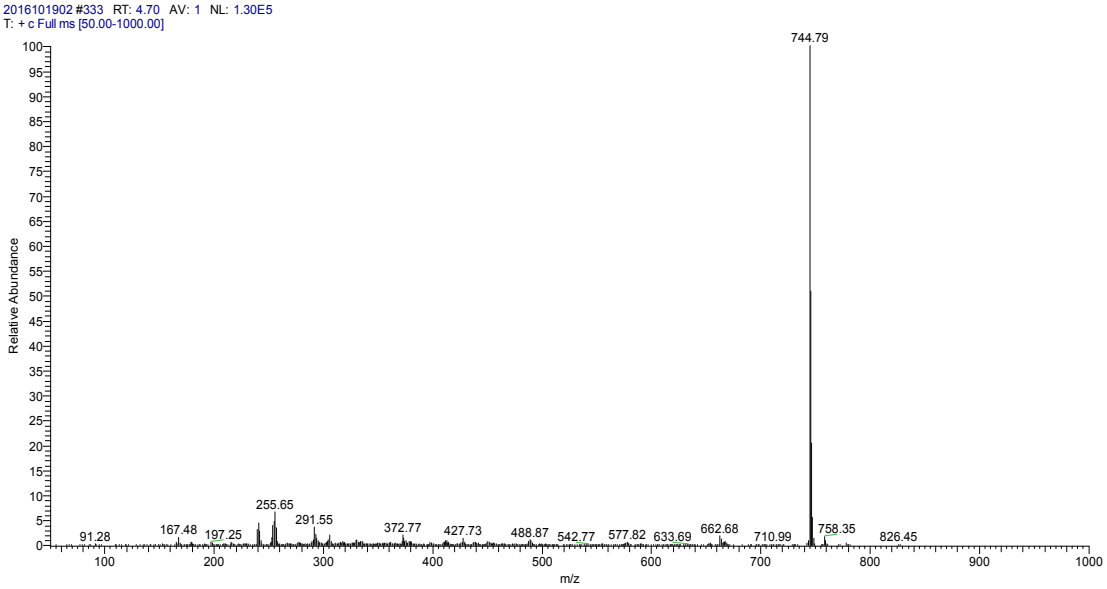


Fig. S12 Mass spectra of M4.

2. Photophysical property of M1-M4

2.1 Photophysical property

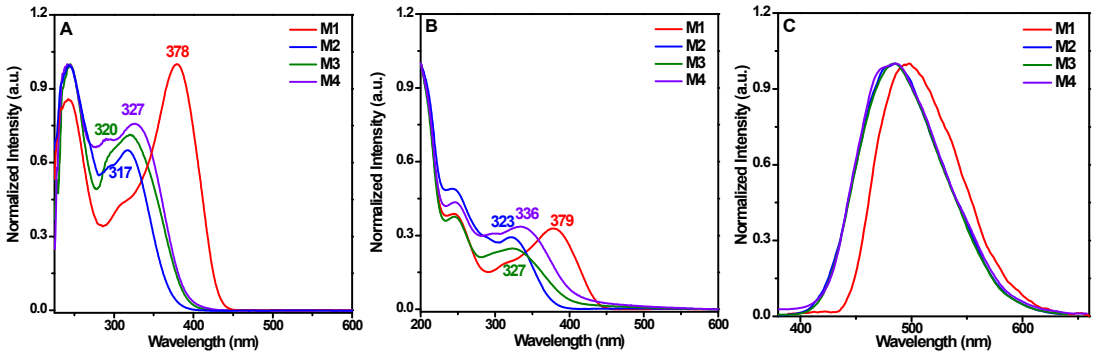
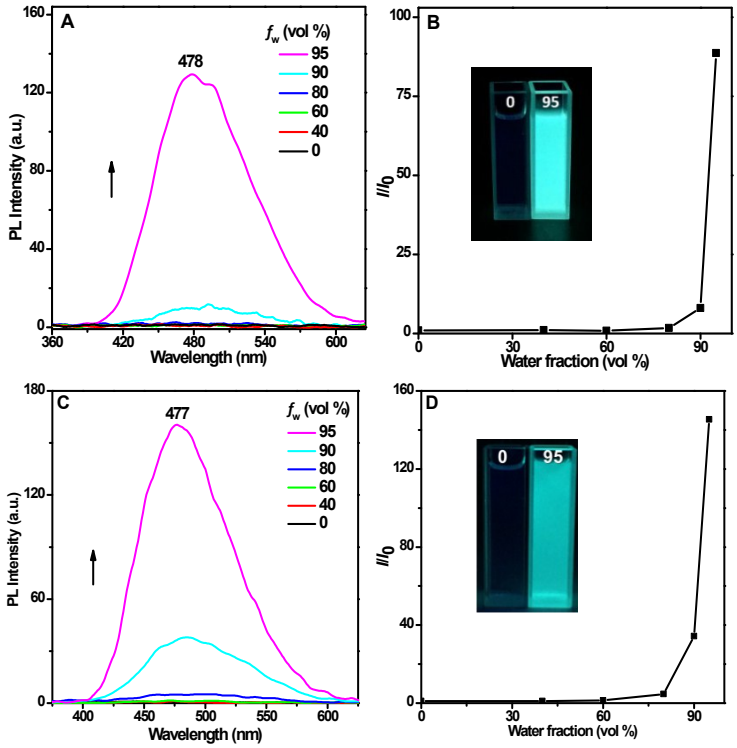


Fig. S13 (A) Normalized UV spectra of M1-M4 in dilute THF (10^{-5} M) solution. (B) and (C) Normalized UV and PL spectra of M1-M4 in thin films spin-coated from 10^{-3} M THF solution at 1500 rpm, respectively.

2.2 AIE property



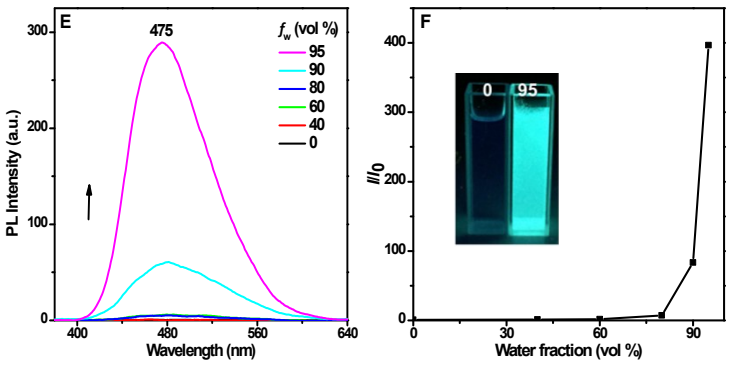


Fig. S14 (A), (C) and (E) are PL spectra of M2, M3 and M4, respectively, in THF-water mixtures with different water fractions (f_w). (B), (D) and (F) are plots of the relative PL intensity (I/I_0) versus the compositions of THF-water mixtures of M2, M3 and M4, respectively. M2, M3 and M4 concentration: 10 μM; excitation wavelength: 317 nm, 320 nm and 327 nm. Inset in (B), (D) and (F) are the fluorescent photographs at f_w = 0 and 95% taken under a 365 nm UV lamp.

3. EL property of M1-M4

3.1 EL performance of M1-M4

We have constructed the devices of different emissive isomers with the same device structure. One is ITO/PEDOT-PSS (30 nm)/NPB (50 nm)/EML (20 nm)/TPBi (30 nm)/LiF (1.2 nm)/Al (100 nm), another is ITO/HATCN (6 nm)/TAPC (50 nm)/EML (20 nm)/TPBi (30 nm)/LiF (1.2 nm)/Al (100 nm). The data are shown below.

Table S1 EL performance of M1-M4.

Isomers	HTL[a]	V_{on}[b] [V]	L_{max}[c] [cd·m^{-2}]	LE_{max}[d] [cd·A^{-1}]	$\lambda_{EL,\,max}$[e] [nm]	EQE[f] [%]
M1	NPB	3.5	65210	11.21	492	4.49
	TAPC	3.4	22010	8.28	480	3.68
M2	NPB	4.3	4070	2.22	440	1.65
	TAPC	3.9	9630	5.79	472	3.00
M3	NPB	3.5	16050	4.95	460	2.56
	TAPC	3.5	15340	6.07	492	2.53
M4	NPB	3.5	18100	6.86	464	3.03
	TAPC	3.4	17400	8.62	492	3.48

Abbreviation: [*a*] HTL = Hole-transporting layer; [*b*] V_{on} = turn on voltage; [*c*] L_{max} = the maximum luminance; [*d*] LE_{max} = the maximum luminance efficiency; [*e*] $\lambda_{EL,max}$ = the maximum electroluminescent wavelength; [*f*] EQE = the maximum external quantum efficiency.

3.2 Single-carrier devices of M1 and M2

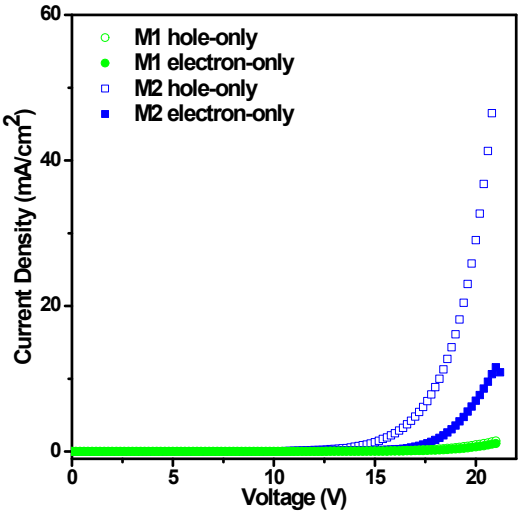


Fig. S15 Current density-voltage characteristics of hole-only and electron-only devices of M1 and M2, respectively.

3.3 Summary of EL performance

Table S2 Summary of key EL performance data of OLEDs using TPE and thiophene derivatives as the emitters in recent years.

Materials	V_{on}[a] [V]	L_{max}[b] [cd·m^{-2}]	LE_{max}[c] [cd·A^{-1}]	$\lambda_{EL,max}$[d] [nm]	EQE[e] [%]	CIE (x,y)	Ref.
M1	3.5	65210	11.21	492	4.49	(0.232,0.398)	this work
M2	3.9	9630	5.79	472	3.00	(0.192,0.279)	this work
M3	3.5	15340	6.07	492	2.53	(0.222,0.371)	this work
M4	3.4	17400	8.62	492	3.48	(0.223,0.365)	this work
TPE	~2.9	1800	0.45	445	~0.4	-	[1]
TPEBPh	5.0	10680	5.15	476	2.56	-	[1]
TPTPE	4.2	10800	5.8	488	2.7	-	[2]
BTPTPE	5.2	3530	2.8	448	1.6	-	[2]
BTPE	4.0	11180	7.26	488	3.17	-	[3]
3,4-BTPEMTPS	6.2	3980	4.96	520	1.66	-	[3]
2,5-BTPEMTPS	5.2	12560	6.40	552	1.98	-	[3]
2,5-BTPEMTPS (20 wt%):BTPE	4.6	10480	7.02	544	2.18	-	[3]
TPEPy	3.6	13400	7.3	484	3.0	-	[4]

TPEBPy	4.6	25500	6.0	516	2.1	-	[4]
TPE-2-Np	3.8	19800	7.3	492	2.7	-	[4]
TTPEPy	3.6	36300	12.3	488	4.95	-	[5]
BPBAPE	8.1	-	10.33	475	-	(0.195,0.303)	[6]
TPVAn	4.9	4165	5.3	456	5.3	(0.14,0.12)	[7]
DPDPyE	3.2	49830	10.2	516	3.3	-	[8]
2TPATPE	3.2	33770	13.0	512	4.4	-	[9]
3TPETPA	4.5	6935	4.0	499,513	1.5	-	[10]
4TPEDTPA	4.1	10723	8.0	488	3.7	-	[10]
DTDAE	3.6	40940	11.2	524	-	-	[11]
TPECaP	4.4	12930	5.5	496	2.2	-	[12]
TTPECaP	3.6	9048	6.3	490	2.3	-	[12]
(*Z*)-*o*-BCaPTPE	4.5	8010	7.9	492	3.1	-	[13]
BTPEBCF	5.5	13760	7.2	508	2.6	(0.24,0.42)	[14]
BAnBCF	4.4	8170	2.2	472	1.0	(0.19,0.24)	[14]
$TPESiPh_3$	5	5672	2.1	452	1.6	-	[15]
$VP_3{\cdot}(TPE)_3$	6	1908		474	-	(0.18,0.31)	[16]
BTPEAn	4.8	7900	3.2	464	2.1	-	[17]
BTPETD	3.9	13540	5.2	540	1.5	-	[18]
BTPETTD	5.4	8330	6.4	592	3.1	-	[18]
BTPEBTTD	4.4	1640	0.4	668	1.0	-	[18]
F1-TPE	5.8	1300	2.6	468	-	-	[19]
1TPE	3.5	2585	3.5	492	-	(0.18,0.34)	[20]
BTPEPBN	6.4	1375	4.43	516	1.52	-	[21]
$TPE(PF)_2$	4.6	14500	7.2	510	2.6	-	[22]
DBTO-*p*TPE	4.3	21984	8.66	-	3.62	-	[23]
TPE-TPDB	4.1	46030	5.1	485	2.6	(0.18,0.29)	[24]
TPE-2PN2PB	3.4	11665	8.3	543	2.6	(0.37,0.54)	[25]
TPE-TPAPBI	3.2	125300	16.8	520	5.8	(0.27,0.50)	[26]
TPE-DPBI	4.0	53070	6.6	518	2.3	(0.25,0.46)	[26]
CFT2P	2.2	48800	11.15	509	0.46	(0.27,0.61)	[27]
CFTP	4.1	7277	2.48	480	0.16	(0.16,0.36)	[27]
TPE-NPB	3.9	12607	13.1	516	4.2	-	[28]
CzPySiTPE	3.0	1063	1.51	468	1.12	(0.16,0.17)	[29]
IV	3.6	10954	6.82	484	3.3	-	[30]
6	4.0	1200	1.13	485	0.61	(0.170,0.331)	[31]
Si-*p*TPE	3.5	28718	7.40	512	2.92	(0.21,0.37)	[32]
Si-*m*TPE	3.7	4411	1.39	432	1.21	(0.16,0.12)	[32]
SFTPE	2.6	8196	3.33	466	-	(0.18,0.24)	[33]
TTPEBTTD	4.2	3750	2.4	650	3.7	(0.67,0.32)	[34]
PDA-TPE	2.4	53600	15.9	523	5.9	-	[35]
TPA-TPE	2.6	58300	14.3	515	4.5	-	[35]
N	4.2	65150	8.60	513	3.28	(0.23,0.46)	[36]

TPE-PNPB	3.2	49993	15.7	516	5.12	(0.27,0.51)	[37]
TPE-NB	3.3	42924	10.5	544	3.24	(0.35,0.55)	[37]
*o*TPE-*p*TPE	3.9	3166	2.2	454	1.7	(0.16,0.14)	[38]
*m*TPE-*p*TPE	4.1	3266	2.8	459	1.9	(0.16,0.16)	[38]
TPE-BFDB	3.2	92810	12.2	497	5.3	(0.20,0.37)	[39]
DPE-BFDB	5.0	33610	10.9	530	3.6	(0.29,0.53)	[39]

Abbreviations: [a]V_{on} = turn on voltage; [b]L_{max} = the maximum luminance; [c]LE_{max} = the maximum luminance efficiency; [d]$\lambda_{EL,max}$ = the maximum electroluminescent wavelength; [e]EQE = the maximum external quantum efficiency.

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4. Stacking modes and crystal data and structure refinements of M2, M3 and M4

4.1.1 Crystal data and structure refinements of M2.

Table S3 Crystal data and structure refinements of M2.

Compound	**M2**
Chemical formula	$C_{56}H_{40}S$
Formula weight	744.94
T/K	293
Crystal system	Triclinic
Space group	*P*-1
a [Å]	12.154(2)
b [Å]	13.157(3)
c [Å]	14.471(3)
α [°]	67.38(3)
β [°]	83.54(3)
γ [°]	79.95(3)
V [Å^3]	2100.7(7)
Z	2
λ [Å]	0.71073
F [000]	784
Density/mg·m^{-3}	1.178
Absorption coefficient [mm^{-1}]	0.114
θ [°]	3.05-27.47
Limiting indices	-15≤h≤15 -14≤k≤17 -18≤l≤18
Reflections collected / unique	20511/9430
GOF	0.985

R_1 [I>2σ(I)]	0.0602
wR_2 [I>2σ(I)]	0.1576
R_1 (all data)	0.1261
wR_2 (all data)	0.1962

4.1.2 The ORTEP of M2 and its crystal photograph

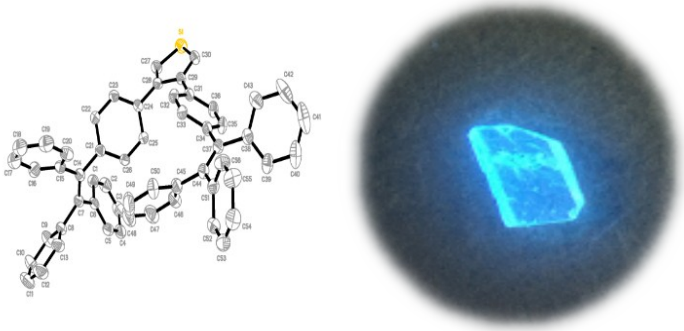

Fig. S16 ORTEP representation of M2 and its crystal photograph taken under the optical microscope under a 365 nm UV lamp.

4.2.1 Crystal data and structure refinements of M3.

Table S4 Crystal data and structure refinements of M3.

Compound	**M3**
Chemical formula	$C_{56}H_{40}S$
Formula weight	744.94
T/K	293
Crystal system	Triclinic
Space group	*P*-1
a [Å]	11.335(2)
b [Å]	11.899(2)
c [Å]	16.207(3)
α [°]	78.13(3)
β [°]	76.41(3)
γ [°]	86.87(3)
V [Å^3]	2079.3(7)
Z	2
λ [Å]	0.71073
F [000]	784
Density/mg·m^{-3}	1.190
Absorption coefficient [mm^{-1}]	0.116
θ [°]	3.05-25.00
	-13≤h≤13

Limiting indices	-14≤k≤14
	-19≤l≤19
Reflections collected / unique	15383/7084
GOF	1.044
R_1 [I>2σ(I)]	0.0583
wR_2 [I>2σ(I)]	0.1505
R_1 (all data)	0.1138
wR_2 (all data)	0.1778

4.2.2 The ORTEP of M3 and its crystal photograph

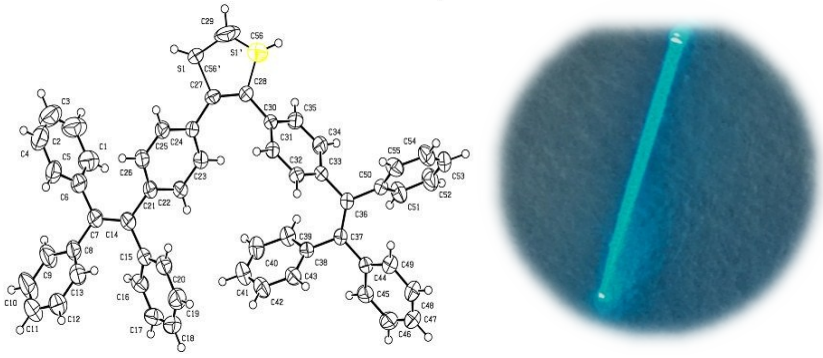

Fig. S17 ORTEP representation of M3 and its crystal photograph taken under the optical microscope under a 365 nm UV lamp.

4.3.1 Crystal data and structure refinements of M4.

Table S5 Crystal data and structure refinements of M4.

Compound	**M4**
Chemical formula	$C_{56}H_{40}S+C_{0.5}H_{0.5}Cl_{1.5}$
Formula weight	804.62
T/K	293
Crystal system	Triclinic
Space group	*P*-1
a [Å]	9.4004(19)
b [Å]	11.442(2)
c [Å]	21.172(4)
α [°]	82.07(3)
β [°]	84.57(3)
γ [°]	87.47(3)
V [Å^3]	2244.2(8)
Z	2
λ [Å]	0.71073
F [000]	842

Density/mg·m^{-3}	1.191
Absorption coefficient [mm^{-1}]	0.198
θ [°]	3.01-25.00
Limiting indices	-10≤h≤11 -13≤k≤13 -25≤l≤25
Reflections collected / unique	17582/7843
GOF	1.002
R_1 [I>2σ(I)]	0.0713
wR_2 [I>2σ(I)]	0.2139
R_1 (all data)	0.1313
wR_2 (all data)	0.2663

4.3.2 The ORTEP of M4 and its crystal photograph

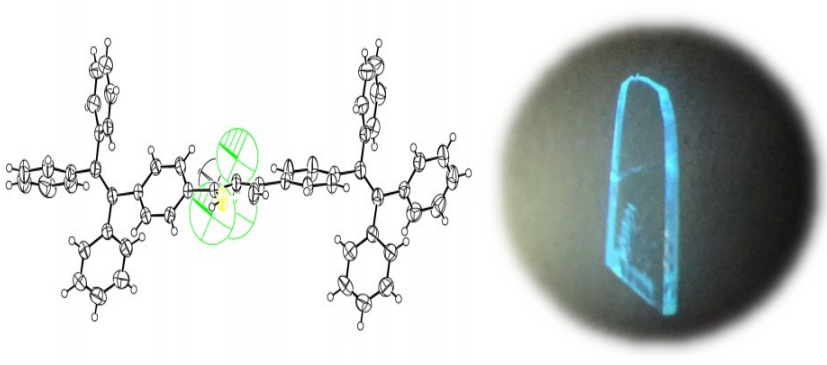

Fig. S18 ORTEP representation of M4 and its crystal photograph taken under the optical microscope under a 365 nm UV lamp.