Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Isomeric Organic Semiconductors Containing Fused-Thiophene Cores: Molecular Packing and Charge Transport

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Fig. S1. The UV-Vis spectra of TF1 and TF2 in gas phase by TD-DFT.

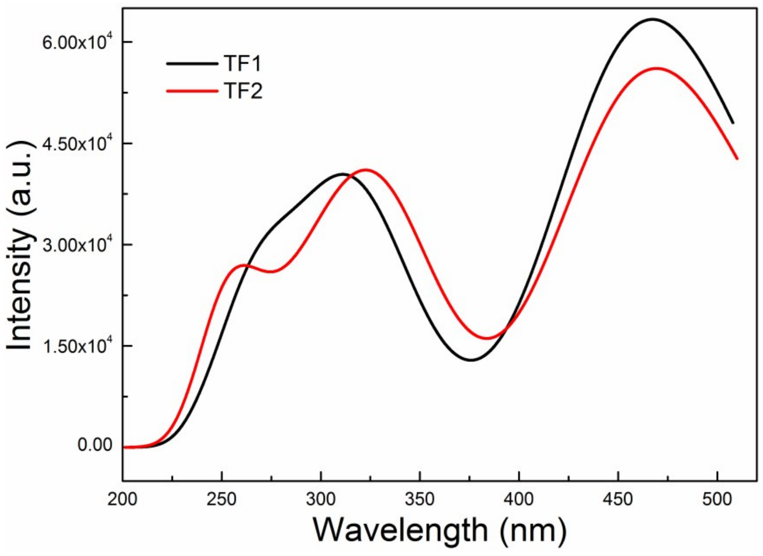


Fig. S2. The UV-Vis spectra of TF1 (a) and TF2 (b) in *o*-DCB solution at 25° and 50°.

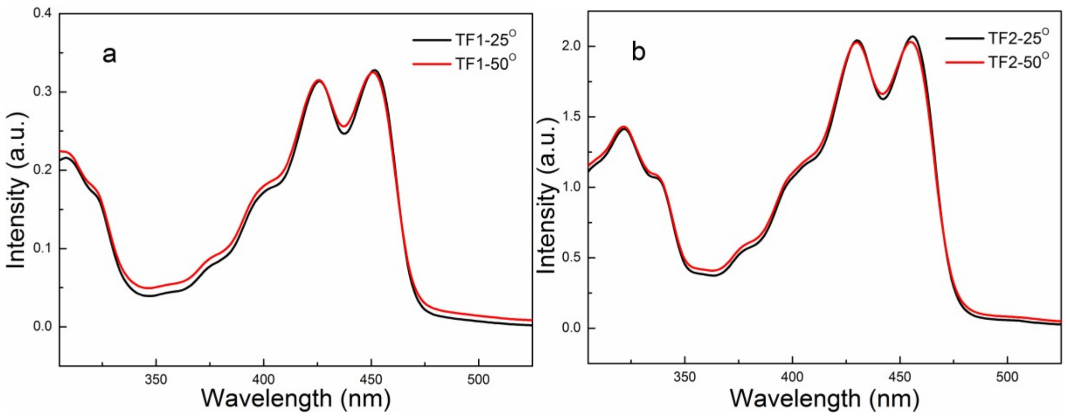


Fig. S3. The UV-Vis spectra of TF1 (a) and TF2 (b) in thin films with and without annealing (140° and 120° for TF1 and TF2, respectively).

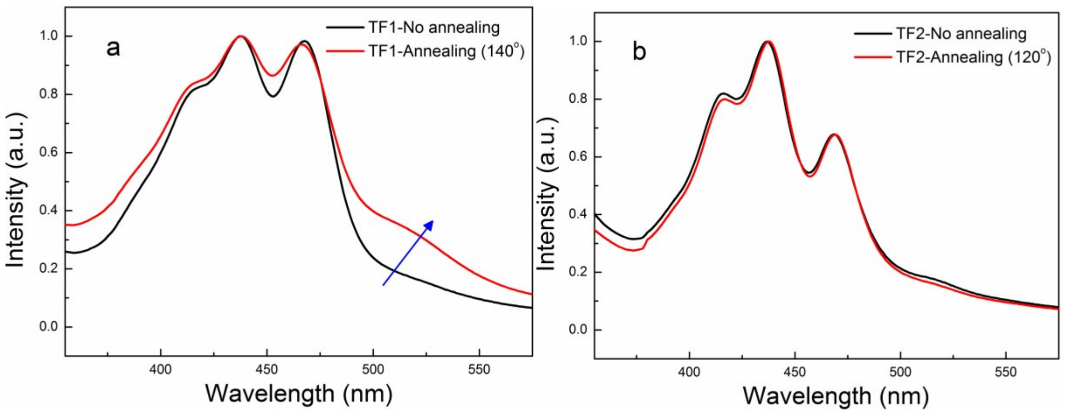


Fig. S4. The X-ray diffractions of TF1 and TF2 in thin films.

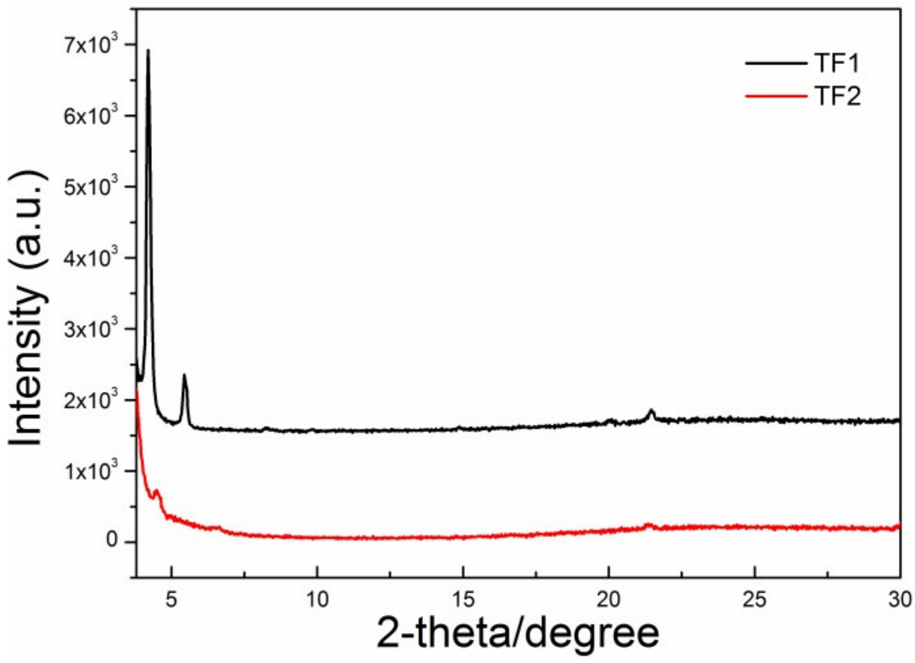


Fig. S5. Output (a, c) and transfer (b, d) characteristics of TF1 and TF2-based OFETs devices at room temperature.

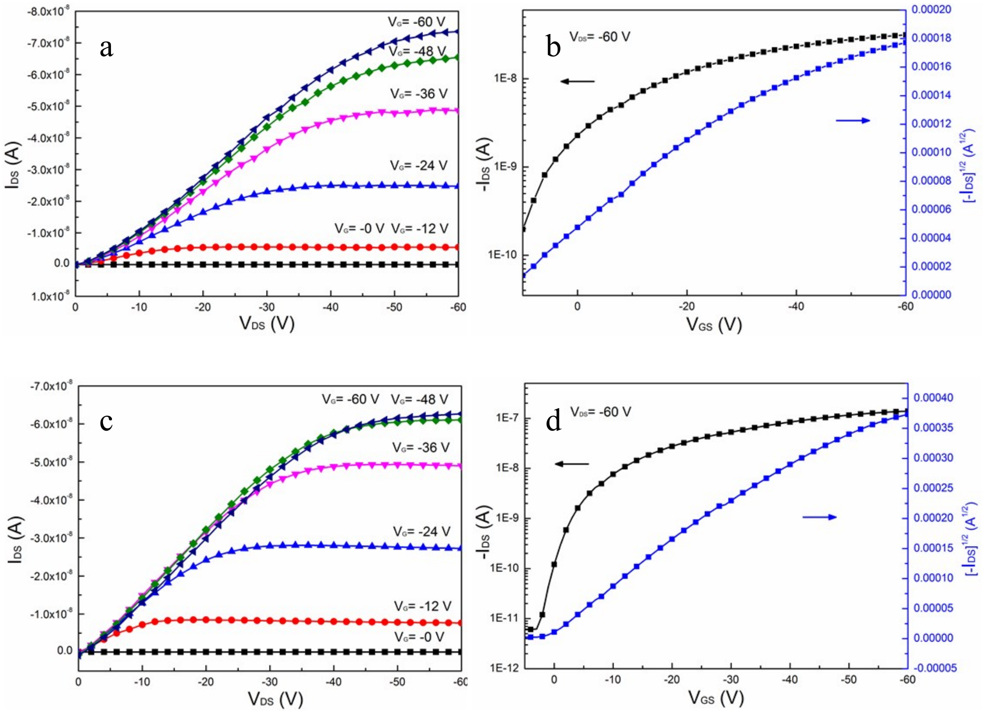
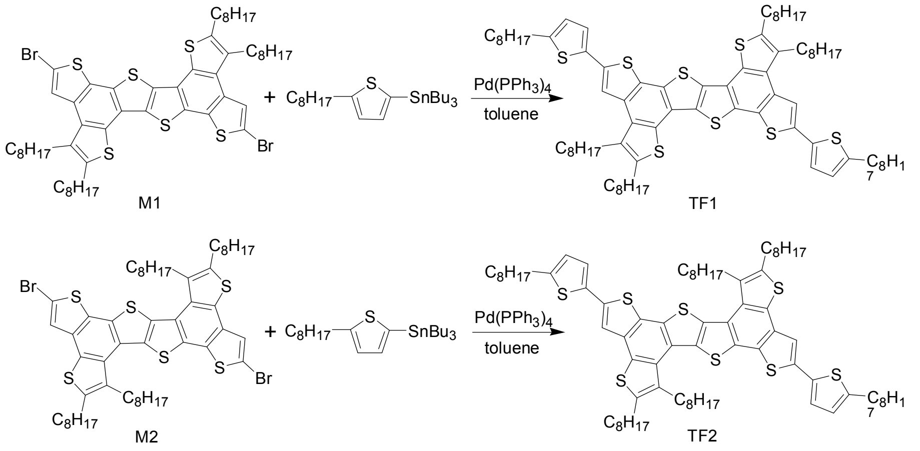


Table S1. Optical properties of TF1 and TF2.

Compounds	UV		PL	
	λ_{abs} [a] (nm)	λ_{abs} [b] (nm)	λ_{em} [a] (nm)	λ_{em} [b] (nm)
TF1	300, 428, 457	300, 424, 454, 483	465, 493, 530	565
TF2	308, 433, 455	312, 428, 448, 480	472, 499, 533	567

[a] In solution; [b] In films.

Scheme S1. Synthetic routes of TF1 and TF2.



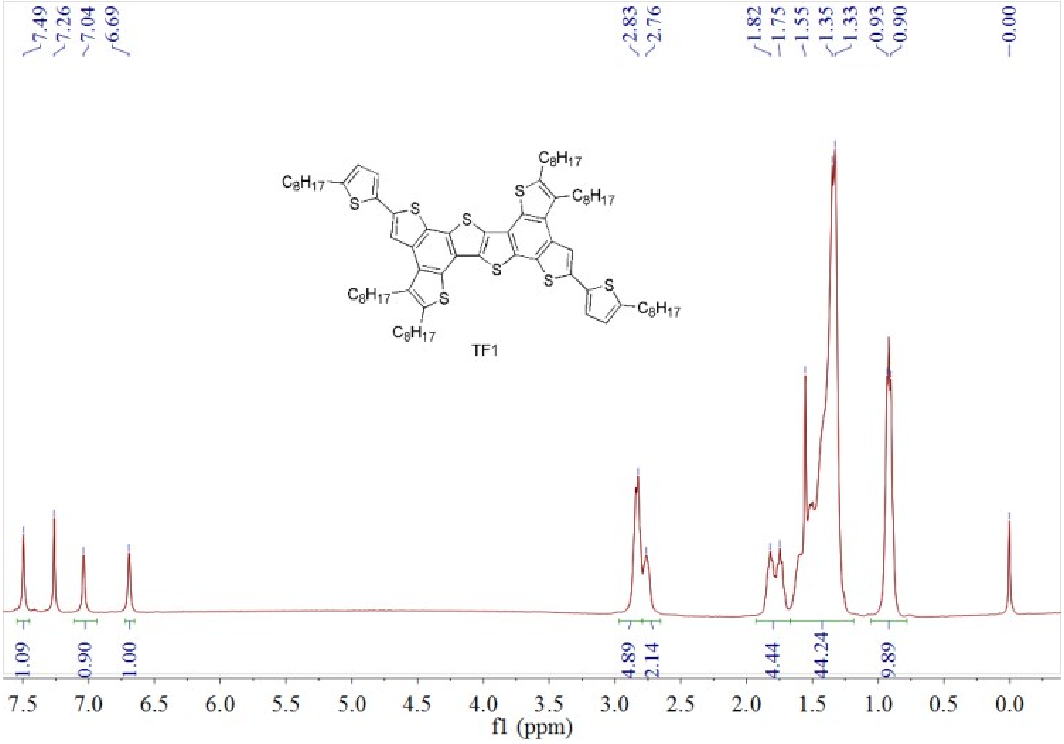
Synthesis of TF1 and TF2

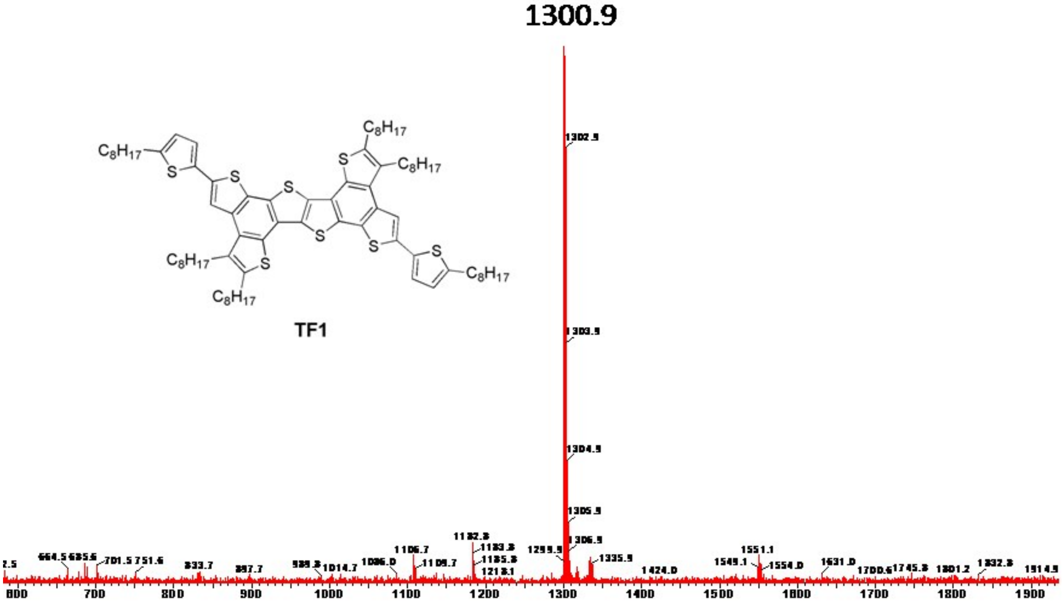
In a 50 mL two-neck flask, tetrakis-(triphenylphosphine)palladium(0) [$Pd(PPh_3)_4$] (10 mg) was added to the solution of tributyl-(5-octyl-thiophen-2-yl)-stannane (63.6 mg, 0.13 mmol) and M1 (50.1 mg, 0.05 mmol) in 30 mL toluene under nitrogen and then stirred at 110 ^oC overnight. After cooled downed to room temperature (RT), the solvent was removed under reduced pressure and then poured into methanol to get the precipitation. Finally, TF1 was purified through recrystallization by using THF and ethanol as dark-orange solid (44.6 mg, 68.6%). ^1H NMR (400 MHz, $CDCl_3$) δ (ppm), 7.49 (s, 2H), 7.04 (s, 2H), 6.99 (s, 2H), 2.90–2.80 (m, 8H), 2.80–2.70 (m, 4H), 1.85–1.70 (m, 8H), 1.58–1.29 (m, 64H), 0.95–0.80 (m, 18H). MS (MALDI-TOF) m/z: M^+ calculated for $C_{78}H_{108}S_8$, 1300.6, found 1300.9.

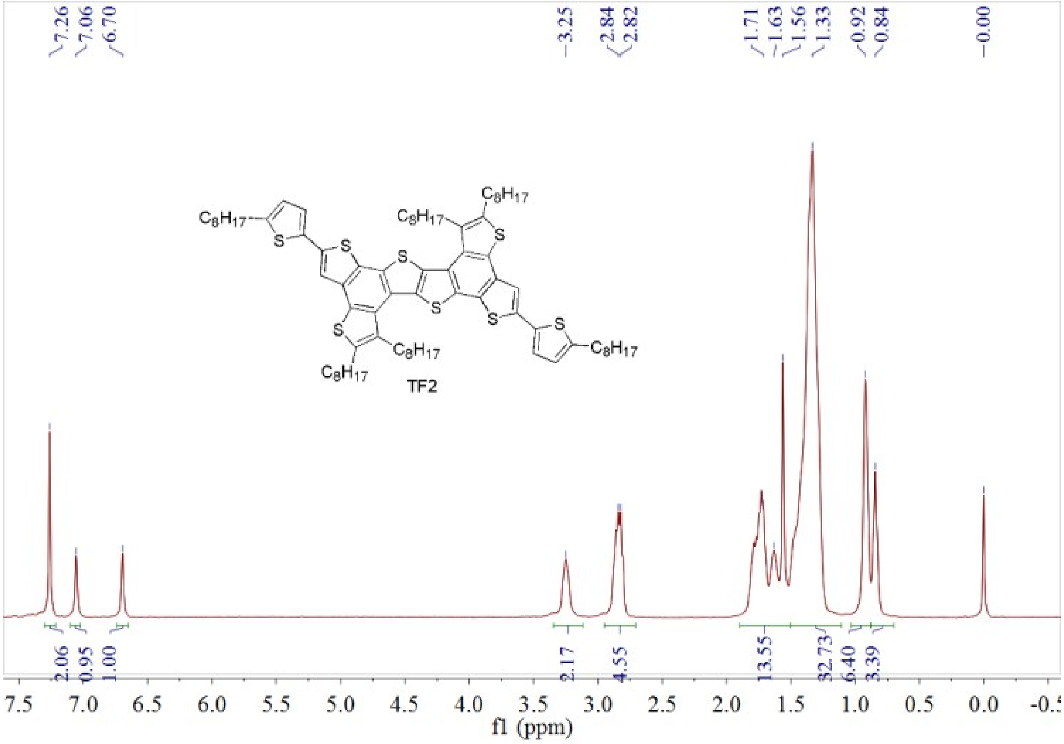
The synthetic procedure to TF2 is similar to that of TF1 with a yield of 78.5% as bright yellow solid. ^1H NMR (400 MHz, $CDCl_3$) δ (ppm), 7.27 (s, 2H), 7.06 (s, 2H), 6.70 (s, 2H), 3.41–3.30 (m, 4H), 2.89–2.78 (m, 8H), 1.76–1.60 (m, 12H), 1.58–1.25

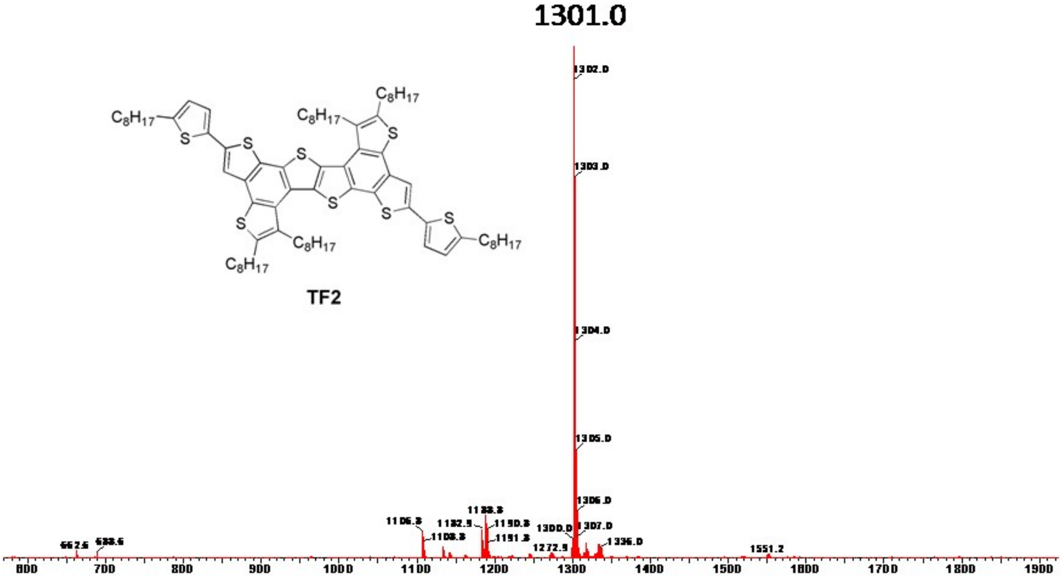
(m, 60H), 0.98–0.81 (m, 18H). MS (MALDI-TOF) m/z: M^+ calculated for $C_{78}H_{108}S_8$, 1300.6, found 1301.0.

NMR and MALDI-TOF spectra


7.49
7.26
7.04
6.69
2.83
2.76
1.82
1.75
1.55
1.35
1.33
0.93
0.90
-0.00
C_8H_{17}
TF1
1.09
0.90
1.00
4.89
2.14
4.44
44.24
9.89
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


1300.9
C_8H_{17}
TF1
1302.9
1303.9
1304.9
1305.9
1306.9
1299.9
1335.9
2.5
664.5
685.6
701.5
751.6
833.7
897.7
989.3
1014.7
1086.0
1106.7
1109.7
1182.8
1183.8
1185.8
1218.1
1424.0
1549.1
1551.1
1554.0
1631.0
1700.6
1745.8
1801.2
1832.8
1914.9
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900


7.26
7.06
6.70
3.25
2.84
2.82
1.71
1.63
1.56
1.33
0.92
0.84
-0.00
C8H17
S
TF2
2.06
0.95
1.00
2.17
4.55
13.55
32.73
6.40
3.39
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


1301.0
1302.0
1303.0
1304.0
1305.0
1306.0
1307.0
1300.0
1336.0
1272.9
1551.2
1106.3
1108.3
1182.5
1188.3
1190.3
1191.3
662.5
688.6
C8H17
S
TF2
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900