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Supporting information for article:

**Crystal Packing Control of Trifluoromethyl-Substituted
Furan/Phenylene Co-oligomer**

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S1. Characterization

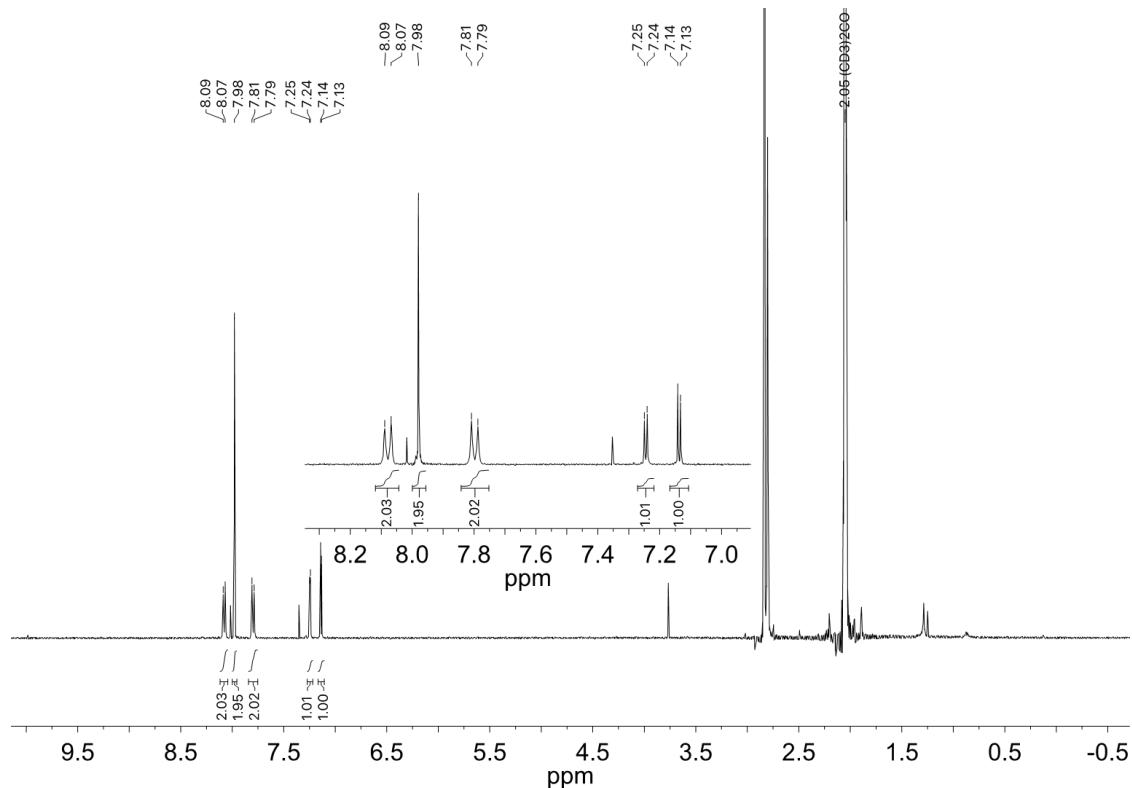


Figure S1 ^1H NMR spectrum of 1,4-bis(5-(4-(trifluoromethyl)phenyl)furan-2-yl)benzene in $(\text{CD}_3)_2\text{CO}$.

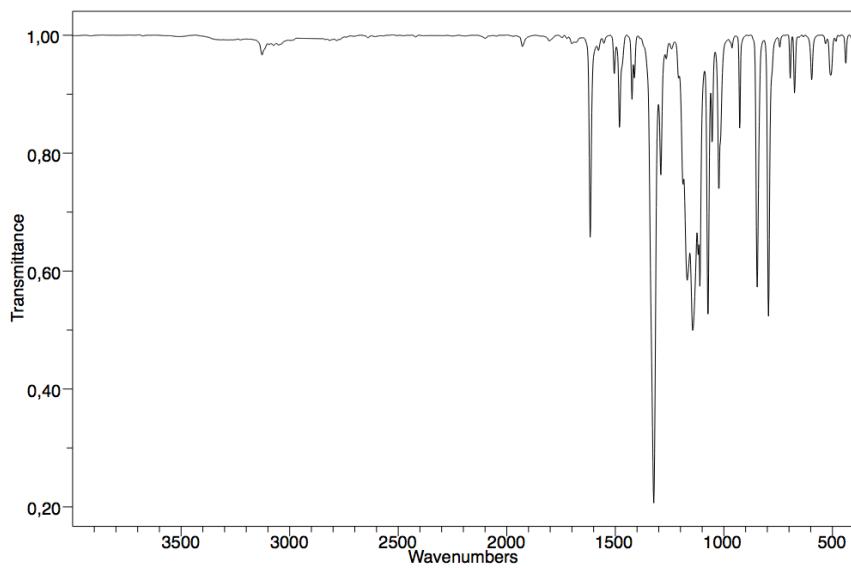


Figure S2 FT IR spectrum of 1,4-bis(5-(4-(trifluoromethyl)phenyl)furan-2-yl)benzene in KBr.

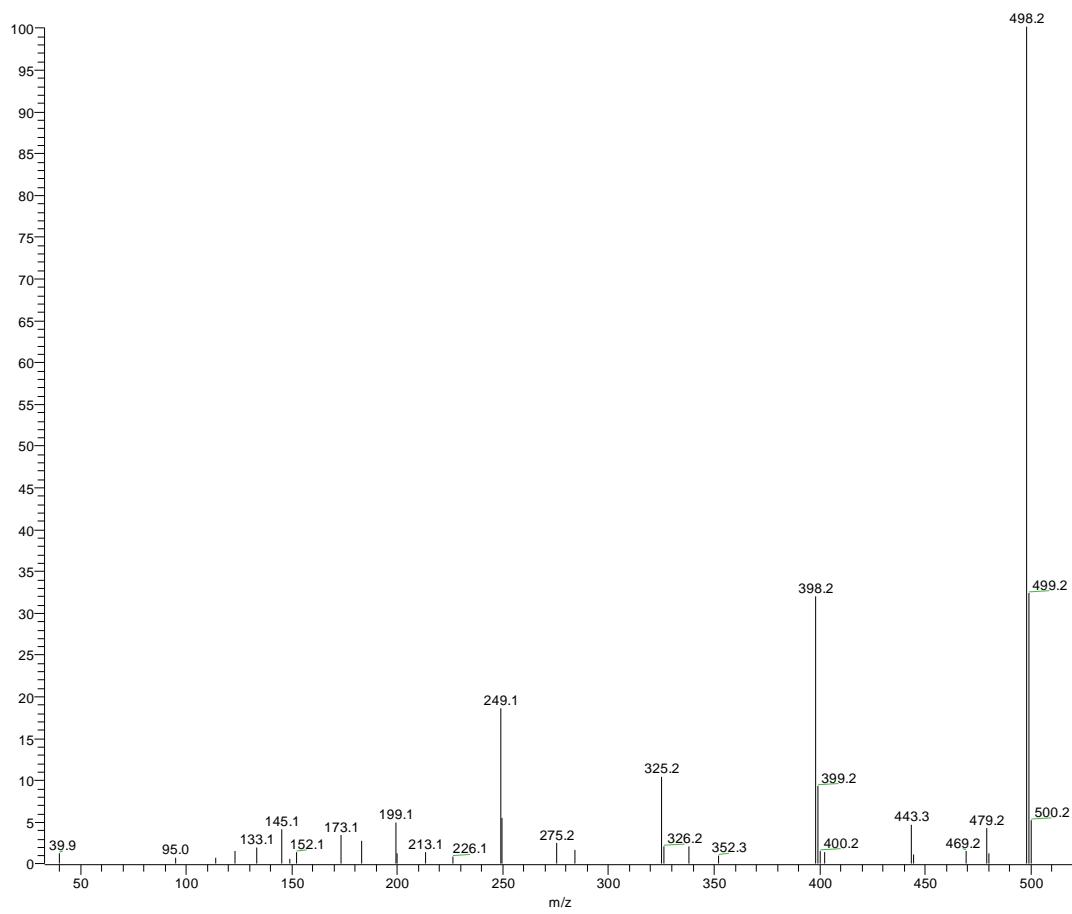


Figure S3 HRMS spectrum of 1,4-bis(5-(4-(trifluoromethyl)phenyl)furan-2-yl)benzene.

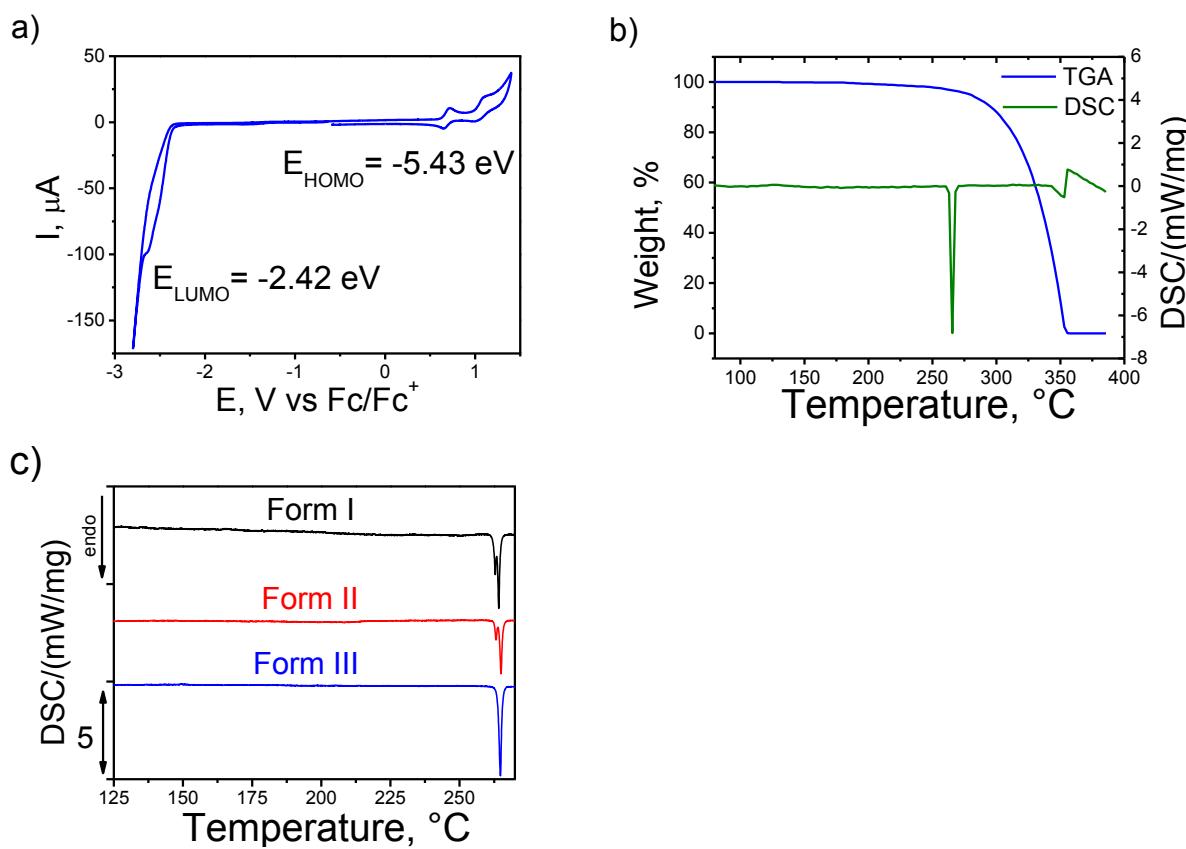


Figure S4 a) Cyclic voltammogramm of $\text{CF}_3\text{-BPFB}$ in CH_2Cl_2 solution; b) Thermal gravimetric and differential scanning calorimetric analyses of $\text{CF}_3\text{-BPFB}$ powder in He atmosphere; c) Differential scanning calorimetric analyses of $\text{CF}_3\text{-BPFB}$ polymorphs in He atmosphere.

S2. X-ray data

Table S1 Crystal data, data collection and structure refinement parameters for crystal structures of $\text{CF}_3\text{-BPFB}$.

	I	II	III
Chemical formula		$\text{C}_{28}\text{H}_{16}\text{F}_6\text{O}_2$	
$M_r/\text{g}\cdot\text{mol}^{-1}$	498.41		
Crystal system, space group		Monoclinic, $P2_1/c$	
Z	2	2	8
Crystal size (mm)	$0.25 \times 0.24 \times 0.008$	$0.60 \times 0.18 \times 0.05$	$1.00 \times 0.12 \times 0.02$
	23.238 (4),	11.505 (5),	20.544 (1),

a, b, c (Å)	7.529 (1), 6.2437 (9)	6.2350 (6), 16.012 (2)	6.2569 (3), 35.797 (2)
β (°)	92.830 (6)	109.293 (6)	106.649 (3)
V (Å ³)	1091.1 (3)	1084.1(2)	4408.4(4)
D_{calc} /g·cm ⁻³	1.517	1.527	1.502
μ (mm ⁻¹)	0.13	0.13	0.13
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8904, 1882, 1221	8382, 1919, 1436	50554, 7767, 3615
R_{int}	0.048	0.023	0.093
θ_{\min} (°)	3.225	3.535	1.035
θ_{\max} (°)	24.876	25.027	25.027
Range of			
h	-27 → 25	-13 → 13	-24 → 24
k	- 8 → 8	- 7 → 7	- 7 → 7
l	-7 → 7	-18 → 19	-42 → 42
$R1, wR(F^2), S$	0.042, 0.093, 1.05	0.032, 0.087, 1.03	0.060, 0.193, 1.06
No. of parameters	190	190	757
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.13, -0.17	0.14, -0.17	0.23, -0.21

Table S2 The distances and angles of noncovalent interactions C_{sp2}-H···π, C_{sp3}-F···π and C_{sp2}-H···F for polymorphic forms.

form	interaction	d(X···Cg)/d(H···F), Å	D _{pln} /d(C···F), Å	C-X...Cg/C-H...F, °
I	C2-H···Cg (2)	2.87	2.85	136
	C8-H···Cg (3)	2.95	2.92	137
II	C8-H···Cg (2)	3.00	2.93	127
	C11-H···Cg (3)	3.05	3.01	143
	F2(F5)···C5	3.36 (3.43)	3.05 (3.15)	145 (135)
	C3-H···F1(F4)	2.78 (2.75)	3.65 (3.62)	156 (157)

	C9-H···F4	2.69	3.51	147
III	C11'-H···Cg (3B)	3.04	3.01	139
	C2'-H···Cg (2A)	2.89	2.87	136
	C8'-H···Cg (2B)	3.04	2.99	130
	C8-H···Cg (3A)	2.90	2.89	134
	C8B-H···Cg (2')	3.01	2.97	128
	C2A-H···Cg (2')	2.92	2.88	137
	C8A-H···Cg (3)	2.87	2.86	136
	C2B-H···F6 (F3)	2.55 (2.60)	3.31 (3.40)	139 (145)
	C9'-H···F4B	2.65	3.41	140
	C3-H···F4B	2.71	3.53	148
	C2-H···F6B	2.62	3.41	142
	C10-H···F6A	2.66	3.22	119
	F2B···C4	3.64	3.15	141
	C3B-H···F1'	2.76	3.64	158
	F4···C3B	3.85	3.22	118
	C10'-H···F3'	2.74	3.26	117
	C10-H···F6A	2.66	3.22	119
	C10A-H···F3A	2.73	3.27	118
	C10A-H···F5	2.69	3.41	135

***Cg** is the aromatic ring center; **D_{pln}** is the nearest distance between X-atom (H/F-atom) and aromatic ring plane; Cg (1; 1'; 1A; 1B), is the furan ring; Cg (2; 2'; 2A; 2B) is the terminal phenyl ring; Cg (3; 3A; 3B) is the central phenyl ring (Fig. 1).

Table S3 The distances and the angles for F···F interactions and aggregates for polymorphic forms. (θ_1 and θ_2 are the angles $C_{sp^3}-F_1\cdots F_2$ and $F_1\cdots F_2-C_{sp^3}$ of $C_{sp^3}-F_1\cdots F_2-C_{sp^3}$ contact).

form	interaction	d(F···F), Å	θ_1 , °	θ_2 , °
I	F4···F5	2.70	154	166
	F1···F1	2.70	158	158

	F2···F5	2.87	127	104
	F1···F3(F6)	3.16 (3.17)	99 (106)	121 (120)
	F4···F6	3.21	104	108
	F3···F5	3.23	124	97
II	F1···F5	2.82	127	118
	F6···F1(F4)	3.07 (3.11)	129 (124)	96 (95)
	F1(F4)···F2(F5)	3.02 (3.05)	107 (122)	126 (113)
III (M-M')	F1···F3'(F6')	2.78 (2.88)	177 (165)	112 (108)
	F5···F2a	2.79	140	147
	F5a···F2'	2.68	148	118
III (MA)	F4a···F6a(F3a)	2.77 (2.79)	171 (167)	113 (110)
III (MB)	F3b···F5b	2.84	149	109
	F1b···F6b	2.88	141	116

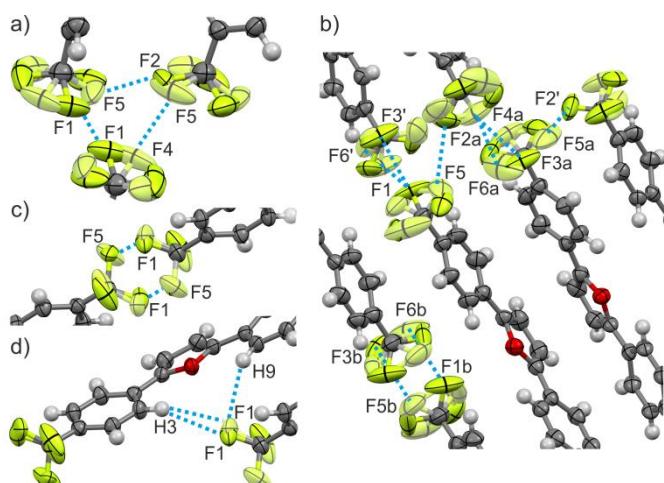


Figure S5 Noncovalent F···F interactions for disordered CF₃ groups of form I (a), form II (c, d) and form III (b).