Supporting Information

Polymorphisms and morphological studies of a difluorobenzothiadiazole conjugated copolymer with 7.8% Polymer Solar Cells Efficiency

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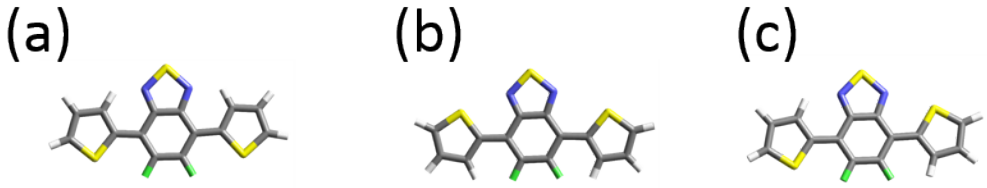

Scheme S1. Three possible conformations of Th_2FBT: (a) *syn1*, (b) *syn2* and (c) *anti*-conformation.

Table S1. Crystal data and structure refinement for $FBTTh_4$.

Identification code	ic16335	
Empirical formula	C14 H6 F2 N2 S3	
Formula weight	336.39	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 15.7727(9) Å	α= 90°.
	b = 4.8184(3) Å	β= 104.765(5)°.
	c = 17.7825(8) Å	γ = 90°.
Volume	1306.83(13) $Å^3$	
Z	4	
Density (calculated)	1.710 Mg/m^3	
Absorption coefficient	5.361 mm^{-1}	
F(000)	680	
Crystal size	0.25 x 0.15 x 0.10 mm^3	
Theta range for data collection	5.14 to 67.97°.	
Index ranges	-16<=h<=18, -5<=k<=5, -21<=l<=21	
Reflections collected	4717	
Independent reflections	2375 [R(int) = 0.0451]	
Completeness to theta = 67.97°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.73034	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2375 / 60 / 228	
Goodness-of-fit on F^2	1.140	
Final R indices [I>2sigma(I)]	R1 = 0.0641, wR2 = 0.1775	
R indices (all data)	R1 = 0.0915, wR2 = 0.1914	
Largest diff. peak and hole	0.723 and -0.250 $e.Å^{-3}$	

Table S2. Crystallographic Parameters of PTh_4FBT

(*hkl*) plane	Experimental *d*-spacing (nm)	Theoretical *d*-spacing (nm)
(100)	2.022	2.022
(200)	1.011	1.008
(300)	0.674	0.671
(400)	0.505	0.504
(020)	0.37	0.369
(005)	0.40	0.399

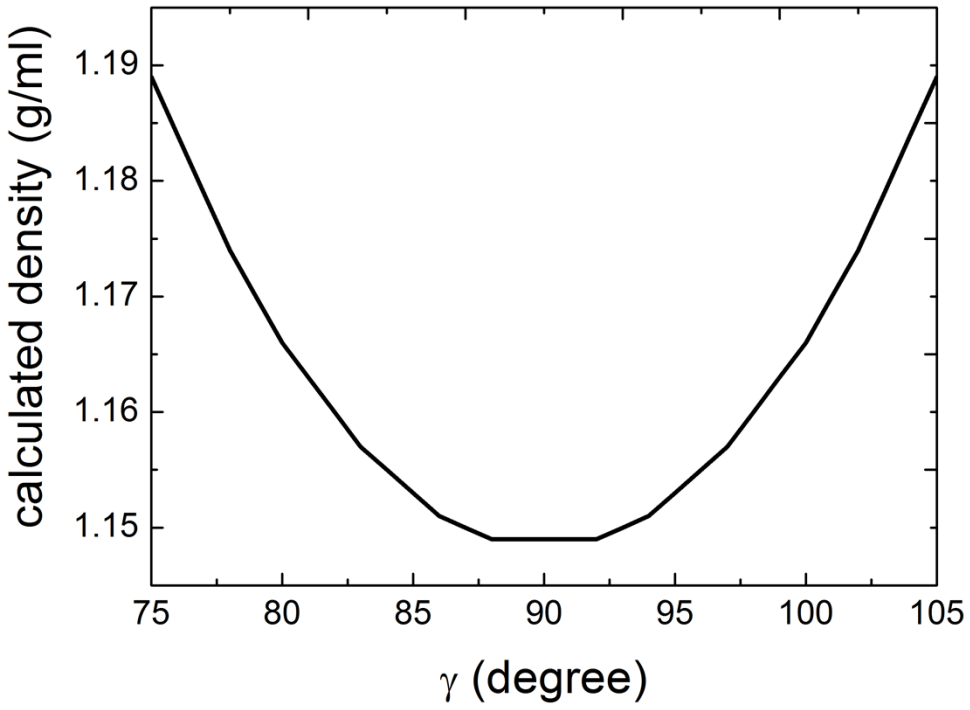

Figure S1. Calculated density at different γ.

Table S3. Unit cell parameters of PTh_4FBT (Mw=1033.88) and their calculated density.

a(Å)	*b*(Å)	*c*(Å)	*α*	*β*	*γ*	*V*(Å^3)	*Z*	*d(g/ml)*
20.2	7.4	20	90	90	105	2887.73	2	1.18
20.2	7.4	20	90	90	104	2900.80	2	1.18
20.2	7.4	20	90	90	103	2912.98	2	1.17
20.2	7.4	20	90	90	102	2924.27	2	1.17
20.2	7.4	20	90	90	101	2934.67	2	1.17
20.2	7.4	20	90	90	100	2944.18	2	1.16
20.2	7.4	20	90	90	99	2952.79	2	1.16
20.2	7.4	20	90	90	98	2960.51	2	1.16
20.2	7.4	20	90	90	97	2967.32	2	1.15
20.2	7.4	20	90	90	96	2973.22	2	1.15
20.2	7.4	20	90	90	95	2978.22	2	1.15
20.2	7.4	20	90	90	94	2982.32	2	1.15
20.2	7.4	20	90	90	93	2985.50	2	1.15
20.2	7.4	20	90	90	92	2987.78	2	1.14
20.2	7.4	20	90	90	91	2989.14	2	1.14
20.2	7.4	20	90	90	90	2989.60	2	1.14
20.2	7.4	20	90	90	89	2989.14	2	1.14
20.2	7.4	20	90	90	88	2987.78	2	1.14
20.2	7.4	20	90	90	87	2985.50	2	1.15
20.2	7.4	20	90	90	86	2982.32	2	1.15
20.2	7.4	20	90	90	85	2978.22	2	1.15
20.2	7.4	20	90	90	84	2973.22	2	1.15
20.2	7.4	20	90	90	83	2967.32	2	1.15
20.2	7.4	20	90	90	82	2960.51	2	1.16
20.2	7.4	20	90	90	81	2952.79	2	1.16
20.2	7.4	20	90	90	80	2944.18	2	1.16
20.2	7.4	20	90	90	79	2934.67	2	1.17
20.2	7.4	20	90	90	78	2924.27	2	1.17
20.2	7.4	20	90	90	77	2912.98	2	1.17
20.2	7.4	20	90	90	76	2900.80	2	1.18
20.2	7.4	20	90	90	75	2887.73	2	1.18