Supporting Information

Backbone Rigidity and Its Influences on the Morphology and Charge Mobility of FBT Based Conjugated Polymers

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Synthesis and characterization

Compound 1. To a round bottom flask was added 5,6-difluoro-4,7-diiodobenzo-2,1,3-thiadiazole (0.62 g, 1.46 mmol), 4-（2-octyldodecyl）-2-tributylstannyl thiophene (3 g, 5.68 mmol), degassed dry tetrahydrofuran (THF) (50 mL) and Bis(triphenylphosphine)palladium(II) dichloride ($PdCl_2(PPh_3)_2$) (0.05g, 0.073 mmol). The solution was stirred at 70 °C for 24 h, cooled down to room temperature, and passed through Celite. The product was reprecipitated from ethanol to give a yellow powder. Yield: 0.8 g (61%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.08 (s, 2H), 7.17 (s, 2H), 2.65 (d, J = 6.4 Hz, 4H), 1.68(m, 2H), 1.25 (br, 64H), 0.86（t, J = 5.2 Hz,12H).[1]

Compound 2. To a round bottom flask was added 5,6-difluoro-4,7-diiodobenzo-2,1,3-thiadiazole (0.5 g, 1.18 mmol), 4-dodecyl-2-tributylstannyl thiophene (1.96 g, 4.71 mmol), degassed dry tetrahydrofuran (THF) (50 mL) and $PdCl_2(PPh_3)_2$ (0.04g, 0.06 mmol). The solution was stirred at 70 °C for 18 hours, cooled down to room temperature, and passed through Celite. The product was reprecipitated from ethanol to give a yellow

powder. Yield: 0.55 g (69%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.12 (s, 2H), 7.20 (s, 2H), 2.71(t, *J* = 7.6Hz, 4H), 1.70 (m, 2H), 1.26 (br, 36H), 0.87 (t, *J* = 7.2 Hz, 6H).[1]

FBT-2. To a round bottom flask was added **1** (0.8 g, 0.9 mmol), N-bromosuccinimide (0.45 g, 2.2 mmol), chloroform (30 mL) and acetic acid (30 mL). After the mixture was stirred at room temperature for 12 hours, 100 mL water was added. The mixture was extracted with ether (100mL). The organic phase was washed with brine, and dried over anhydrous $MgSO_4$. After removal of the volatiles, the residue solid was recrystallied from ethanol to afford product as orange solid. Yield: 0.82 g (87%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.92 (s, 2H), 2.59 (d, *J* = 7.2 Hz, 4H), 1.74 (m, 2H), 1.25 (br, 64H), 0.86 (t, *J* = 6.4 Hz,12H).[1]

FBT-3. To a round bottom flask was added **2** (0.3 g, 0.45 mmol), N-bromosuccinimide (0.18 g, 1.0 mmol), chloroform (30 mL) and acetic acid (30 mL). After the mixture was stirred at room temperature for 12 hours, 100 mL water was added. The mixture was extracted with ether (100mL). The organic phase was washed with brine, and dried over anhydrous $MgSO_4$. After removal of the volatiles, the residue solid was recrystallized from ethanol to afford product as orange solid. Yield: 0.33 g (89%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.96 (s, 2H), 2.66 (t, *J* = 7.2Hz, 4H), 1.66 (m, 4H), 1.25 (br, *J* = 36 Hz), 0.87 (t, *J* = 5.2 Hz, 6H).[1]

Compound 3. To a round bottom flask was added 2-bromo-3-octyldodecylthiophene (2 g, 4.5 mmol) and THF (30 mL). *n*-butyl lithium (2.5 M in hexane, 2 mL) was added slowly into the flask at -78 ^{o}C. The solution was stirred at -78 ^{o}C for 30 mins before dimethylformamide (0.38 mL, 4.96 mmol) was added. After the mixture was stirred at

room temperature for 12 hours, 100 mL water was added. The mixture was extracted with hexane (100mL). The organic phase was washed with brine, and dried over anhydrous $MgSO_4$. The solvent was then evaporated by rotary evaporator under reduced pressure. The residue was subjected to column chromatography (SiO_2, hexane/ethyl acetate = 50/1 (v/v)). The product is yellow liquid. Yield: 1.3 g (73%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 10.02 (s, 1H), 7.63 (d, 1H), 6.98 (d, *J* = 3.2 Hz, 1H), 2.88 (d, *J* = 6.4 Hz, 2H), 1.65 (m, 1H), 1.24(br, 32H), 0.88 (t, *J* = 6.4 Hz, 6H).

Compound 5. To a round bottom flask was added 2-bromo-3-dodecylthiophene (5.6g, 16.9 mmol) and THF (40 mL). *n*-butyl lithium (2.5 M in hexane, 7.43 mL) was added slowly into the flask at -78 ^{o}C. The solution was stirred at -78 ^{o}C for 30 mins before dimethylformamide (1.43 mL, 18.6 mmol) was added. After the mixture was stirred at room temperature for 12 hours, 100 mL water was added. The mixture was extracted with hexane (100mL). The organic phase was washed with brine, and dried over anhydrous $MgSO_4$. The solvent was then evaporated by rotary evaporator under reduced pressure. The residue was subjected to column chromatography (SiO_2, hexane/ethyl acetate = 50/1 (v/v)). The product is yellow liquid. Yield: 2.3 g (48%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm)10.04 (s, 1H), 7.63 (d, 1H), 7.01 (d, *J* = 4.8Hz, 1H), 2.97 (t, *J* = 8.0 Hz, 2H), 1.66 (t, *J*=6.8Hz, 2H), 1.25 (br, 18H), 0.86 (t, *J* = 6.8 Hz, 3H).[2]

Compound 6. To a round bottom flask was added dried THF (30 mL). $TiCl_4$ (0.34 mL) and Zn powder (0.4 g) were added at 0 ^{o}C. The mixture was stir at 0 ^{o}C for 15 mins, and then refluxed for 1 hr. Mixture of **3** (0.56 g, 1.4 mmol) and pyridine (0.24 mL, 2.8 mmol) was then added into the flask and reflux for 3 hrs. After the solution was cooled to room temperature, water (100mL) was added. The mixture was extracted with hexane (100mL).

The organic phase was washed with brine, and dried over anhydrous $MgSO_4$. The solvent was then evaporated by rotary evaporator under reduced pressure. The residue was subjected to column chromatography (SiO_2, hexane). The product is yellow liquid. Yield: 0.375 g (69%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.04 (d, *J* = 5.2 Hz, 2H), 6.99 (s, 2H), 6.79 (d, *J* = 3.6 Hz, 2H), 2.58 (d, *J* = 7.2 Hz, 4H), 1.60 (m, 2H), 1.24 (br, 64H), 0.86 (t, *J* = 8.2 Hz,12H).

Compound 7.To a round bottom flask was added dried THF (50 mL). $TiCl_4$ (2.8 mL) and Zn powder (3.3 g) were added at 0 ^{o}C. The mixture was stir at 0 ^{o}C for 15 mins, and then refluxed for 1 hr. Mixture of **4** (1.2 g, 10.6 mmol) and pyridine (1.9 mL, 23.5 mmol) was then added into the flask and reflux for 3 hrs. After the solution was cooled to room temperature, water (100mL) was added. The mixture was extracted with ether (100mL). The organic phase was washed with brine, and dried over anhydrous $MgSO_4$. The solvent was then evaporated by rotary evaporator under reduced pressure. The residue was subjected to column chromatography (SiO_2, hexane). The product is yellow solid. Yield:), 7.04 (m, 4H) 7.00 (t, *J* = 2.8Hz, 2H)0.98 g (48%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.18 (d, *J* = 3.2Hz, 2H).[3]

Compound 8. To a round bottom flask was added dried THF (50 mL). $TiCl_4$ (1.5 mL) and Zn powder (1.7 g) were added at 0 ^{o}C. The mixture was stir at 0 ^{o}C for 15 mins, and then refluxed for 1 hr. Mixture of **5** (1.51 g, 5.38 mmol) and pyridine (0.84 mL, 10.76 mmol) was then added into the flask and reflux for 3 hrs. After the solution was cooled to room temperature, water (100mL) was added. The mixture was extracted with ether (100mL). The organic phase was washed with brine, and dried over anhydrous $MgSO_4$. The solvent was then evaporated by rotary evaporator under reduced pressure. The

residue was subjected to column chromatography (SiO_2, hexane). The product is yellow solid. Yield: 1.47 g (52%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.06 (d, J = 4.4 Hz, 2H), 6.99 (s, 2H), 6.84 (d, *J* = 4.0Hz, 2H), 2.65 (t, *J* = 7.6 Hz, 4H), 1.59 (m, 4H), 1.33 (br, 36H), 0.88 (t, *J* = 6.0Hz, 6H).[2]

DTV-1. To a round bottom flask was added **6** (0.26 g, 0.34 mmol), chloroform (10 mL) and acetic acid (5 mL). N-bromosuccinimide (0.12 g, 0.68 mmol) was dissolved in DMF (5mL), and then added slowly into the flask at 0 °C. After the mixture was stirred at room temperature for 2 hours, 100 mL water was added. The mixture was extracted with hexane (100mL). The organic phase was washed with brine, and dried over anhydrous $MgSO_4$. After removal of the solvent, the residue was subjected to column chromatography (SiO_2, hexane). The product is yellow liquid. Yield: 0.25 g (82%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 6.75 (s, 4H), 2.48 (d, *J* = 3.2 Hz, 4H), 1.59(m, 2H), 1.25 (br, 64H), 0.87 (t, *J* = 4.8 Hz, 12H).

DTV-2. To a round bottom flask was added **7** (0.5 g, 2.6 mmol) and THF (30 mL). *n*-butyl lithium (2.5 M in hexane, 2.1 mL) and TMEDA (0.78Ml, 5.2mmol) were added slowly into the flask at -78 °C. The solution was stirred at -78 °C for 30 mins and then heated to 80 °C for 10 minutes and cooled to -78 °C again. trimethyltin chloride was slowly added to the solution. After the mixture was stirred at room temperature for 12 hours, 100 mL water was added. The mixture was extracted with ether (100mL). The organic phase was washed with brine, and dried over anhydrous $MgSO_4$. The solvent was then evaporated by rotary evaporator under reduced pressure. the residue solid was recrystallized from ethanol to afford product as yellow solid. Yield: 0.83 g (62%). ^{1}H

NMR($CDCl_3$, 400MHz): δ (ppm) 7.12 (d, *J* = 2.4Hz, 2H), 7.09 (s, 2H) 7.08 (d, *J* =2.4Hz, 2H), 0.38(s, 18H).[3]

DTV-3. To a round bottom flask was added **8** (0.576 g, 1.09 mmol) and THF (30 mL). *n*-butyl lithium (2.5 M in hexane, 1.31 mL) and TMEDA (0.0.49mL, 3.27mmol) were added slowly into the flask at -78 °C. The solution was stirred at -78 °C for 30 mins and then heated to 80 °C for 10 minutes and cooled to -78 °C again. trimethyltin chloride was slowly added to the solution. After the mixture was stirred at room temperature for 12 hours, 100 mL water was added. The mixture was extracted with ether (100mL). The organic phase was washed with brine, and dried over anhydrous $MgSO_4$. The solvent was then evaporated by rotary evaporator under reduced pressure. the residue solid was recrystallized from ethanol to afford product as yellow solid. Yield: 0.72 g (78%). ^{1}H NMR($CDCl_3$, 400MHz): δ (ppm) 6.99 (s, 2H), 6.92(s, 2H), 2.65 (t, *J* = 7.61 Hz, 4H), 1.59 (m, 4H), 1.33(br, 36H), 0.88 (t, *J* = 6.8Hz, 6H), 0.36 (s, 18Hz).[2]

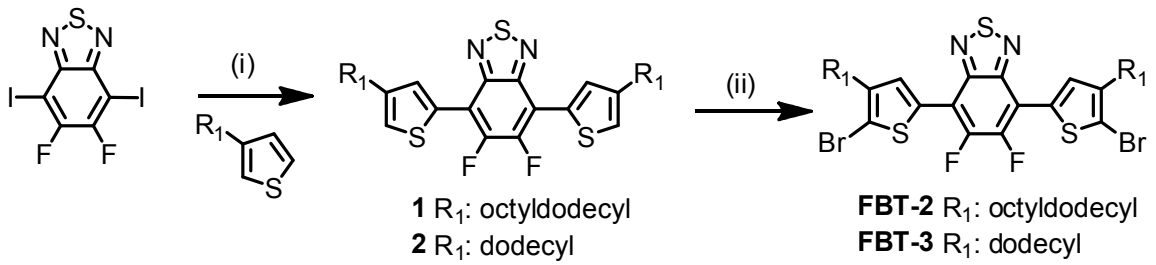
Synthesis of PVTh$_4$FBT-OD1. To a round bottom flask was added **FBT-1** (100.5 mg, 0.11 mmol), **DTV-1** (73.02 mg, 0.11 mmol), tris(dibenzylideneacetone)dipalladium(0) (4.1mg, 0.0045mmol) and tri(o-tolyl)phosphine (10.75 mg, 0.0352 mmol) was dissolved in dry chlorobenzene (5 mL). After the mixture was purged with nitrogen at room temperature for 10 minutes, the mixture was stirred at 120°C for 48 hours. Tributyl(thiophen-2-yl) stannane (41.94 mg, 0.11 mmol) was introduced to the mixture solution before the mixture solution was stirred at 120 °C for additional 12 hours. After stirred at 120 °C for 12 hours, 2-bromothiophene (36.05 mg, 0.22 mmol) was added to the solution and stirred at 120°C for 12 hours. After cooling to room temperature the solution was added dropwise to methanol. The precipitate was collected by filtration and

washed by Soxhlet extraction with acetone (24 hours), hexane (24 hours) and tetrahydrofuran (24 hours) sequentially. The residue solid was re-dissolved in hot toluene (100 mL). The Pd-thiol gel (Silicycle Inc.) was added to above toluene solution to remove the residual Pd catalyst at 100 ^{o}C for 12 hours. After filtration of solution and removal of the solvent under reduced pressure, the polymer solution was added into methanol to re-precipitate. The purified polymer was collected by filtration and dried under vacuum for 1 day to give a green solid. Yield: 88.0 mg (73.6%).

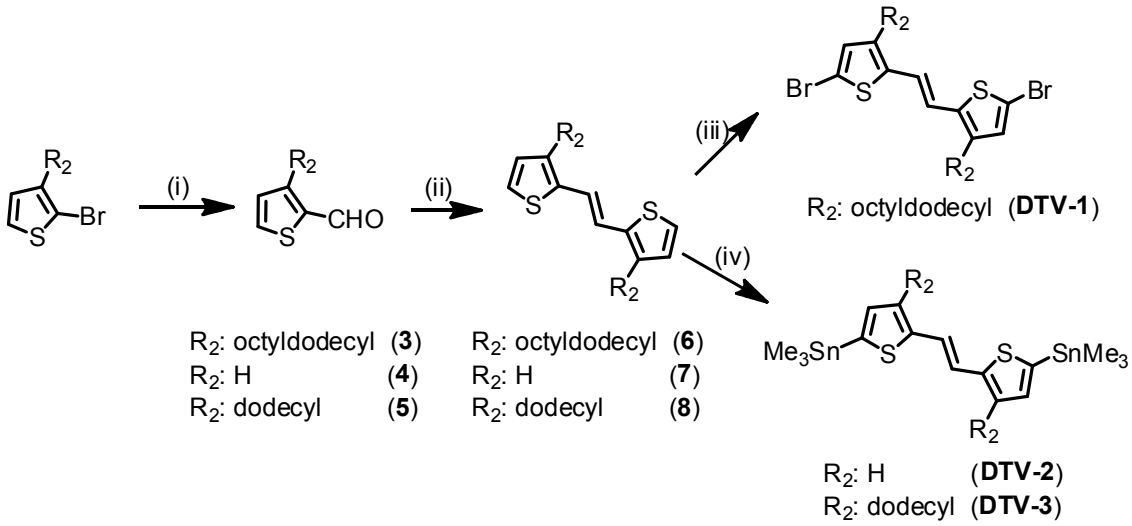
Synthesis of PVTh$_4$FBT-OD2. To a round bottom flask was added **FBT-2** (76.32 mg, 0.14 mmol), **DTV-2** (150 mg, 0.14 mmol), tris(dibenzylideneacetone)dipalladium(0) (5.2mg, 0.0056mmol) and tri(o-tolyl)phosphine (13.8 mg, 0.0448 mmol) was dissolved in dry chlorobenzene (5 mL). After the mixture was purged with nitrogen at room temperature for 10 minutes, the mixture was stirred at 120^{o}C for 48 hours. Tributyl(thiophen-2-yl) stannane (53.38 mg, 0.14 mmol) was introduced to the mixture solution before the mixture solution was stirred at 120^{o}C for additional 12 hours. After stirred at 120^{o}C for 12 hours, 2-bromothiophene (45.88 mg, 0.28 mmol) was added to the solution and stirred at 120^{o}C for 12 hours. After cooling to room temperature the solution was added dropwise to methanol. The precipitate was collected by filtration and washed by Soxhlet extraction with acetone (24 hours), hexane (24 hours) and tetrahydrofuran (24 hours) sequentially. The residue solid was re-dissolved in hot toluene (100 mL). The Pd-thiol gel (Silicycle Inc.) was added to above toluene solution to remove the residual Pd catalyst at 100 ^{o}C for 12 hours. After filtration of solution and removal of the solvent under reduced pressure, the polymer solution was added into methanol to re-precipitate.

The purified polymer was collected by filtration and dried under vacuum for 1 day to give a green solid. Yield: 95.0 mg (62.5%).

Synthesis of PVTh$_4$FBT-DD. To a round bottom flask was added **FBT-3** (300 mg, 0.70 mmol), **DTV-3** (74.5 mg, 0.12 mmol), tris(dibenzylideneacetone)dipalladium(0) (4.39mg, 0.0048mmol) and tri(o-tolyl)phosphine (11.62 mg, 0.0384 mmol) was dissolved in dry chlorobenzene (5 mL). After the mixture was purged with nitrogen at room temperature for 10 minutes, the mixture was stirred at 120^{o}C for 48 hours. Tributyl(thiophen-2-yl) stannane (45.75 mg, 0.12 mmol) was introduced to the mixture solution before the mixture solution was stirred at 120^{o}C for additional 12 hours. After stirred at 120^{o}C for 12 hours, 2-bromothiophene (39.33 mg, 0.24 mmol) was added to the solution and stirred at 120^{o}C for 12 hours. After cooling to room temperature the solution was added dropwise to methanol. The precipitate was collected by filtration and washed by Soxhlet extraction with acetone (24 hours), hexane (24 hours) and tetrahydrofuran (24 hours) sequentially. The residue solid was re-dissolved in hot toluene (100 mL). The Pd-thiol gel (Silicycle Inc.) was added to above toluene solution to remove the residual Pd catalyst at 100 ^{o}C for 12 hours. After filtration of solution and removal of the solvent under reduced pressure, the polymer solution was added into methanol to re-precipitate. The purified polymer was collected by filtration and dried under vacuum for 1 day to give a green solid. Yield: 56.0 mg (38.8%).



Scheme S1. Synthetic procedures of the FBT monomers. Reagents and conditions: (i) Bis(triphenylphosphine)palladium(II) dichloride, tetrahydrofuran, 70 °C, 18 hrs; (ii) N-bromosuccinimide, $CHCl_3$, acetic acid, room temperature, 12 hrs.



Scheme S2. Synthetic procedures of the DTV monomers. Reagents and conditions: (i) *n*-butyl lithium (2.5 M in hexane), dimethylformamide, THF, -78 °C to room temperature, 12 hrs; (ii) $TiCl_4$, Zn, pyridine, THF, reflux, 3 hrs; (iii) N-bromosuccinimide, $CHCl_3$, acetic acid, 0 °C, 2 hrs; (iv) *n*-butyl lithium (2.5 M in hexane), trimethyltin chloride, THF, tetramethylethylenediamine, -78 °C to room temperature, 12 hrs.

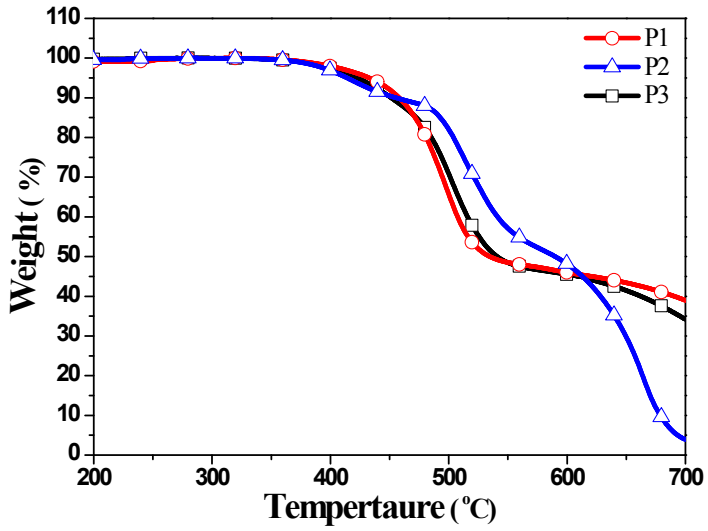


Figure S1. The TGA measurement of **PVTh$_4$FBT** polymers.

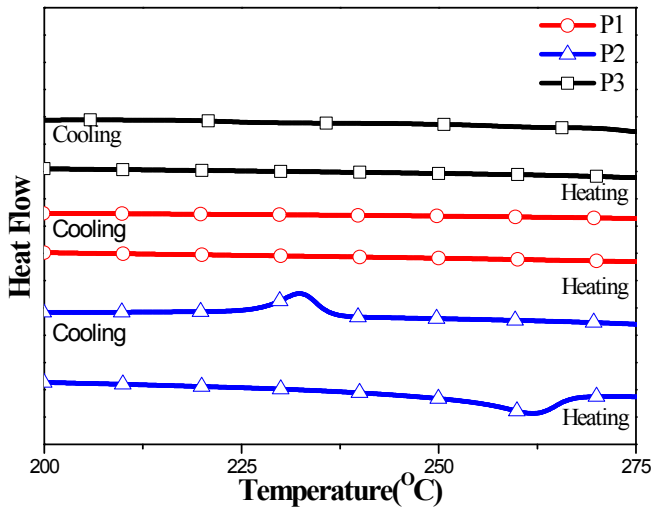


Figure S2. DSC thermograms of the **PVTh$_4$FBT** polymers.

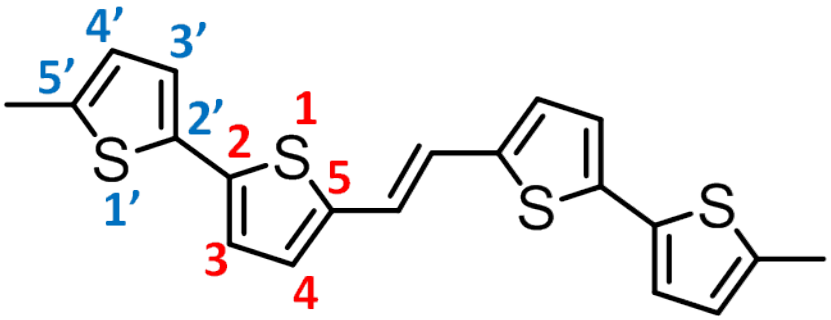
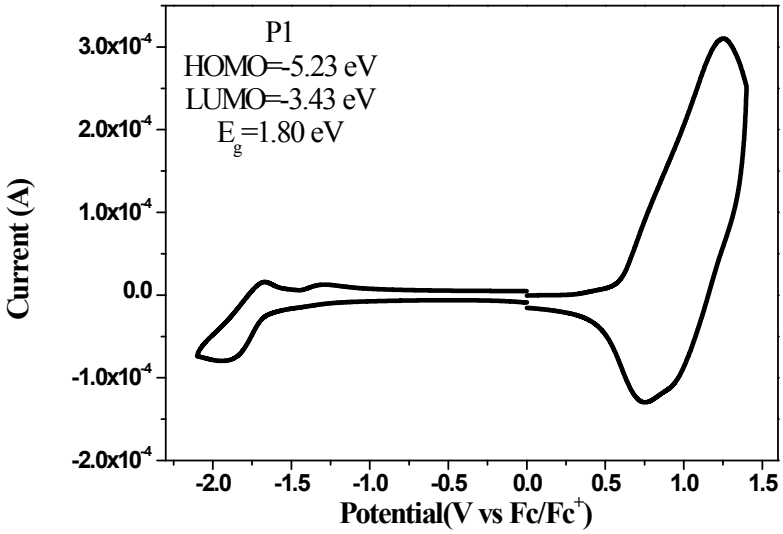
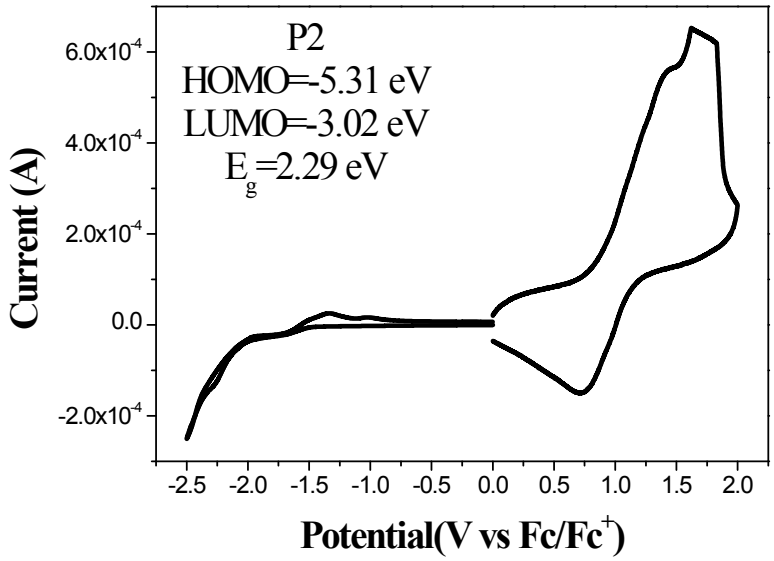


Figure S3. Number code on the (*E*)-1,2-bis(2,2'-bithiophen-5-yl)ethene structural unit





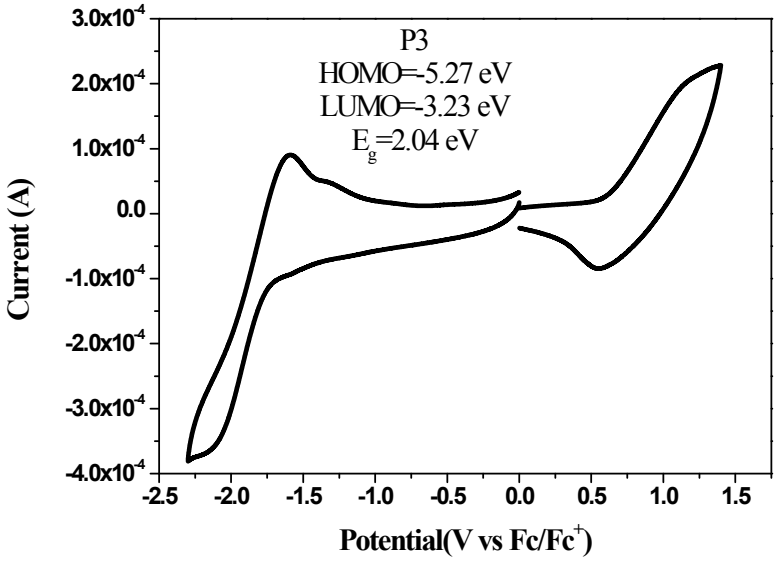
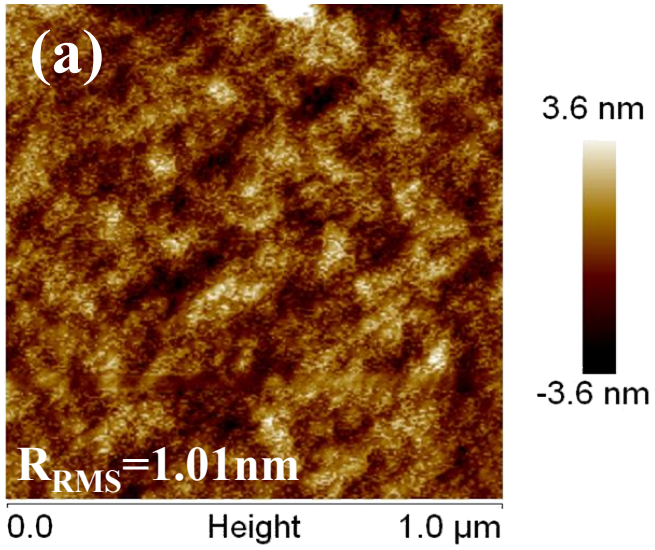
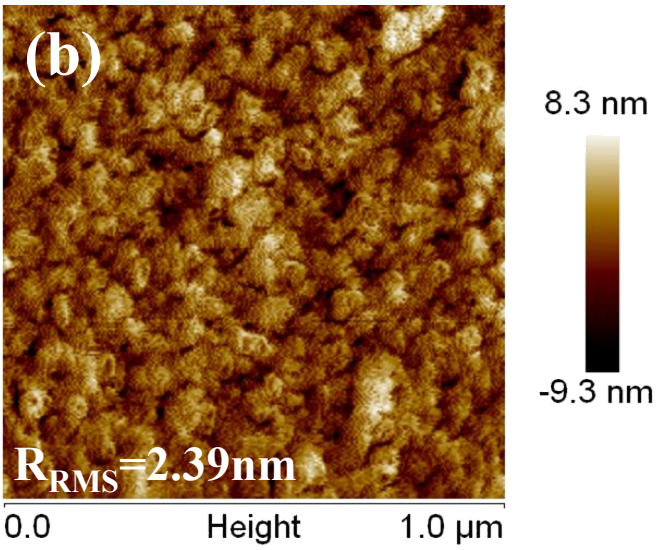


Figure S4. Cyclic voltammograms of the **PVTh$_4$FBT** polymers


(a)
3.6 nm
-3.6 nm
R_{RMS}=1.01nm
0.0
Height
1.0 μm


(b)
8.3 nm
-9.3 nm
R_{RMS}=2.39nm
0.0
Height
1.0 μm

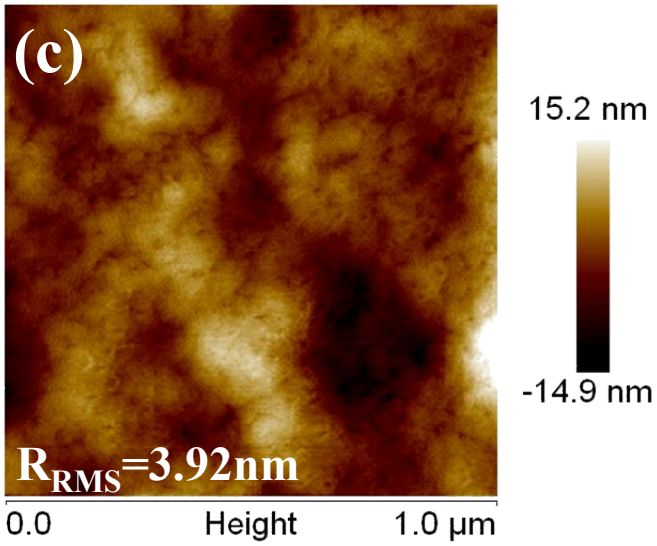
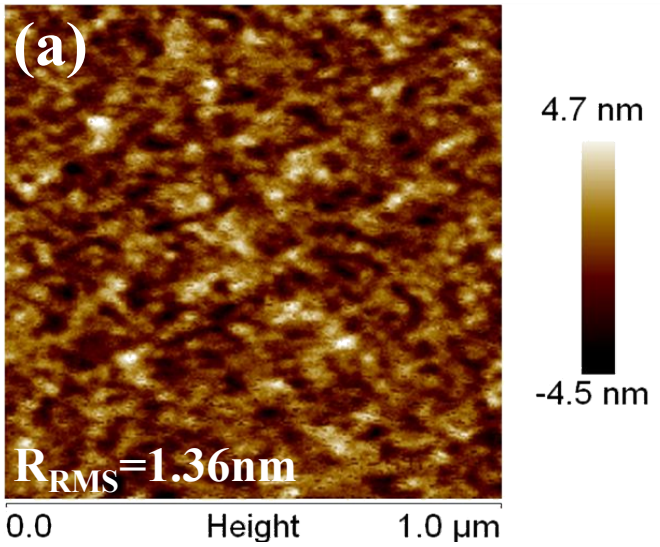


Figure S5. Tapping-mode AFM height images of (d) **P1**, (e) **P2** and (f) **P3**



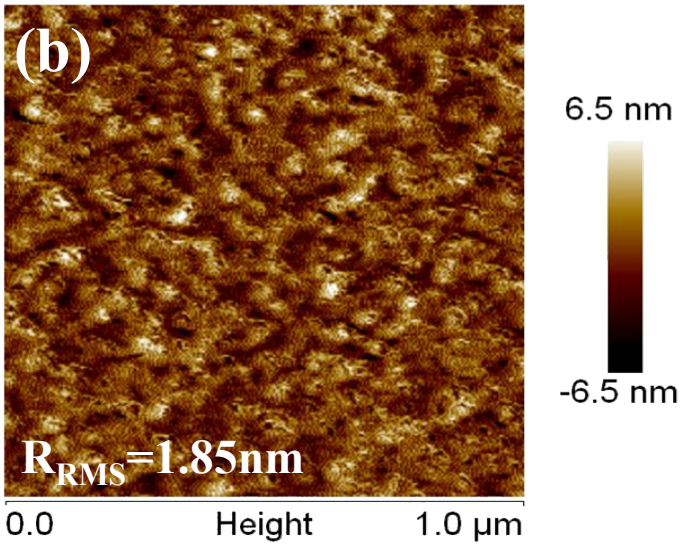


Figure S6. Tapping mode AFM height images of the **P2** thin films, which were prepared from (a) ODCB solution (2.5mg/mL), and (b) TCB solution (2.5mg/mL).

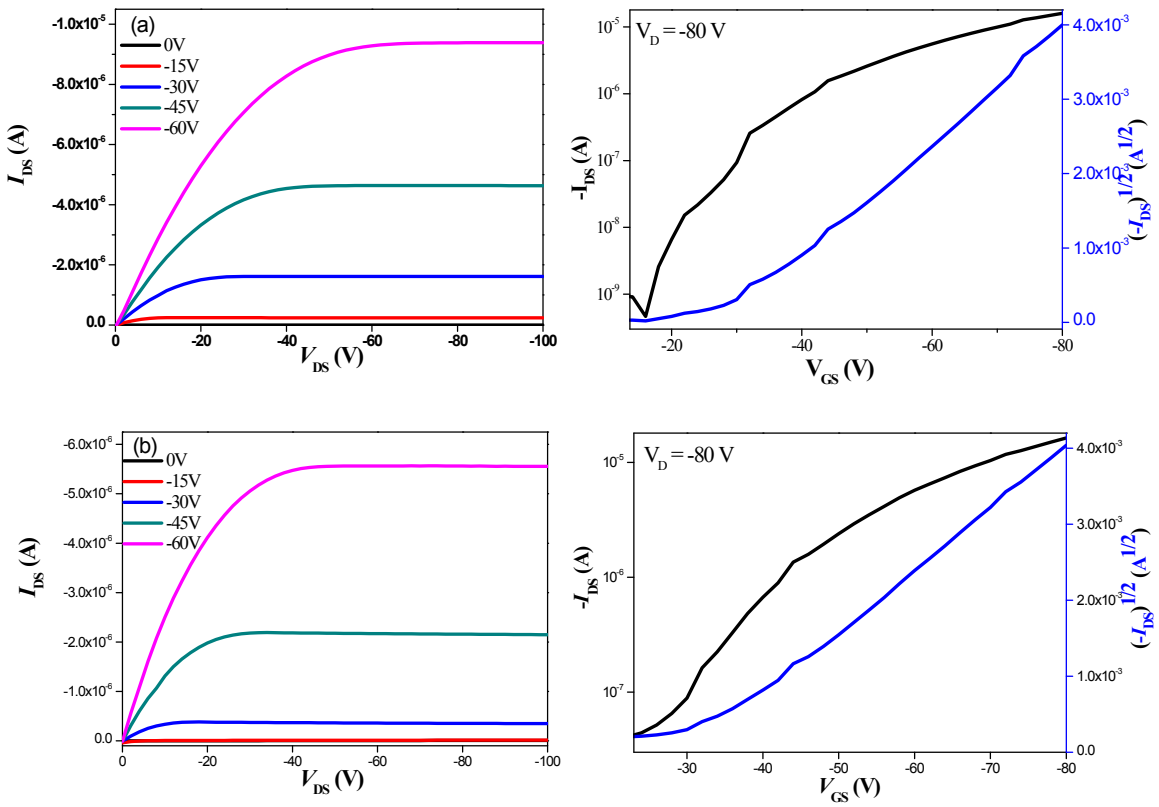


Figure S7. Transfer (right) and output (left) characteristics of the OFET devices of P2. Films were prepared by spin-coating from (a) the ODCB solutions (2.5 mg/mL) and (b)TCB solutions (2.5 mg/mL) before annealed at 250 °C for 30 min.

Cartesian coordination of optimized geometry of **$PVTh_4FBT$-backbone**, **PTh_4FBT–backbone**, **$PVTh_4FBT$-OD1**, **$PVTh_4FBT$-OD2** and **$PVTh_4FBT$-DD** from B3LYP/6-311G(d,p) level

$PVTh_4FBT$ -backbone

C	10.55443700	0.83593700	-0.05348500
C	11.97860400	0.56773100	0.08468200
C	12.46047300	-0.73702100	0.36959300
C	11.52004600	-1.70753400	0.50392600
C	10.12413100	-1.45692200	0.37088100
C	9.57225100	-0.22191100	0.09540200
H	13.51549600	-0.94497100	0.47379600
N	12.74400200	1.64575900	-0.08110900
N	10.29748800	2.11432200	-0.31993400
S	11.73646800	2.90040500	-0.38788800
F	11.86982700	-2.97263000	0.77341500
F	9.33470600	-2.53406900	0.53629600
C	8.14236800	0.00851600	-0.03613600
C	7.49991900	1.20216500	-0.31396000
S	6.94683500	-1.27535800	0.15837400
C	6.09882700	1.09729400	-0.38201700
H	8.04192400	2.12081400	-0.47002300
C	5.62446400	-0.17969000	-0.15704100
H	5.45181300	1.93460000	-0.60807800
C	4.26183900	-0.64886700	-0.15757900
C	3.78982000	-1.94546000	-0.18020700
S	2.92049300	0.48514500	-0.12447200
C	2.38343400	-2.03628000	-0.17926700
H	4.44513800	-2.80597800	-0.21299600
C	1.73958400	-0.81343000	-0.15885900
H	1.84137700	-2.97298800	-0.20202400
C	0.32018000	-0.59661700	-0.16066000
C	-0.32017900	0.59661600	-0.16066700
H	-0.26736800	-1.51173700	-0.16347900
H	0.26736900	1.51173600	-0.16348800
C	-1.73958300	0.81342900	-0.15887700
C	-2.38343300	2.03627900	-0.17930000
S	-2.92049200	-0.48514600	-0.12448900
C	-3.78981900	1.94545900	-0.18025000
H	-1.84137600	2.97298700	-0.20206000
C	-4.26183800	0.64886600	-0.15761600
H	-4.44513600	2.80597700	-0.21305000
C	-5.62446300	0.17968900	-0.15708300
C	-6.09882400	-1.09729700	-0.38205400
S	-6.94683600	1.27535900	0.15831300
C	-7.49991600	-1.20216800	-0.31400600

H	-5.45180900	-1.93460500	-0.60810300
C	-8.14236800	-0.00851700	-0.03619600
H	-8.04192000	-2.12081700	-0.47006700
C	-9.57225100	0.22191200	0.09533000
C	-10.55443700	-0.83593800	-0.05355600
C	-10.12413400	1.45692500	0.37079600
C	-11.97860500	-0.56773000	0.08459800
C	-11.52005000	1.70753700	0.50382900
C	-12.46047600	0.73702300	0.36949600
H	-13.51549900	0.94497400	0.47369000
N	-10.29748600	-2.11432500	-0.31999400
N	-12.74400200	-1.64576000	-0.08119000
S	-11.73646500	-2.90040800	-0.38795300
F	-9.33471100	2.53407300	0.53620800
F	-11.86983300	2.97263600	0.77330600

PTh$_4$FBT -backbone

C	10.98228600	-0.33310400	-0.29600300
C	9.59211700	-0.72509000	-0.11471300
C	8.52425600	0.25688000	-0.14410000
C	8.96334100	1.54838000	-0.35451900
C	10.32719400	1.92047300	-0.53065500
C	11.34599400	1.02290800	-0.50768000
H	12.37507900	1.32261400	-0.64316500
C	7.12462500	-0.09764700	0.03355400
C	6.59235100	-1.35501200	0.25602800
S	5.82371600	1.09411800	-0.02145200
C	5.19179700	-1.36908700	0.39385900
H	7.21173600	-2.23453200	0.32570800
C	4.60995000	-0.12314400	0.27911200
H	4.62400500	-2.26799800	0.59494100
C	3.21540800	0.23491500	0.37297300
C	2.64861800	1.47190600	0.59597300
S	1.96305200	-0.97987700	0.18888200
C	1.23825200	1.45185800	0.64503700
C	0.69328700	0.19854800	0.46056300
H	0.63551600	2.32823900	0.84386500
C	-0.69328800	-0.19855000	0.46056300
C	-1.23825300	-1.45186000	0.64503600
S	-1.96305200	0.97987500	0.18888200
C	-2.64861800	-1.47190700	0.59597300
H	-0.63551700	-2.32824100	0.84386400
C	-3.21540800	-0.23491700	0.37297300
C	-4.60995000	0.12314300	0.27911200
C	-5.19179700	1.36908600	0.39386000
S	-5.82371600	-1.09411900	-0.02145200

C	-6.59235100	1.35501100	0.25602900
H	-4.62400500	2.26799600	0.59494200
C	-7.12462500	0.09764700	0.03355400
H	-7.21173600	2.23453200	0.32570900
C	-8.52425600	-0.25688000	-0.14410000
C	-9.59211700	0.72509100	-0.11471300
C	-8.96334200	-1.54837900	-0.35451900
C	-10.98228500	0.33310600	-0.29600300
C	-10.32719500	-1.92047200	-0.53065500
C	-11.34599500	-1.02290500	-0.50768000
H	-12.37508000	-1.32261000	-0.64316500
N	11.83685500	-1.35400500	-0.24178000
N	9.44933300	-2.03533300	0.07056100
N	-9.44933100	2.03533400	0.07056100
N	-11.83685300	1.35400800	-0.24178000
S	10.94690000	-2.70437500	0.01842900
S	-10.94689800	2.70437700	0.01842900
F	10.56302800	3.22520100	-0.72394700
F	8.08477900	2.56622800	-0.40776300
F	-8.08478100	-2.56622900	-0.40776300
F	-10.56303100	-3.22519900	-0.72394700
H	-3.23825000	-2.36567000	0.75224000
H	3.23825000	2.36566800	0.75224100

PVTh$_4$FBT -OD1

C	-10.51781100	0.97186600	0.18845800
C	-11.94911200	0.74138300	0.05440300
C	-12.45920500	-0.51767900	-0.35814100
C	-11.53836200	-1.48183500	-0.61715500
C	-10.13605000	-1.26810700	-0.48945200
C	-9.55700900	-0.07831500	-0.09517400
H	-13.51955400	-0.69756300	-0.46033000
N	-12.69217400	1.80658900	0.35219600
N	-10.23339700	2.21010000	0.58473600
S	-11.65686200	3.00579800	0.76916300
F	-11.91567300	-2.70524600	-1.01313300
F	-9.36898600	-2.33310900	-0.78736700
C	-8.12143500	0.11516100	0.02865500
C	-7.45253800	1.26182800	0.41977300
S	-6.95198500	-1.15816500	-0.32912600
C	-6.05264000	1.12957000	0.44450900
H	-7.97527400	2.16621200	0.68604000
C	-5.60423500	-0.12239700	0.07173000
H	-5.38672500	1.92820300	0.74377800
C	-4.25030600	-0.60742900	-0.00945000
C	-3.80012700	-1.90053800	-0.16812000

S	-2.89026400	0.49387900	0.08686300
C	-2.39172400	-2.04001000	-0.20692600
H	-4.47352800	-2.74504000	-0.24572400
C	-1.73490100	-0.82002500	-0.07565500
C	-0.31756700	-0.59354800	-0.08483900
C	0.31756900	0.59356700	0.08476800
H	0.28115600	-1.48434500	-0.25163200
H	-0.28115400	1.48436400	0.25155900
C	1.73490400	0.82004400	0.07558600
C	2.39172600	2.04003000	0.20684900
S	2.89026700	-0.49386200	-0.08691500
C	3.80013000	1.90055700	0.16804900
C	4.25030800	0.60744700	0.00939000
H	4.47353200	2.74505900	0.24564100
C	5.60423700	0.12241300	-0.07178300
C	6.05264700	-1.12952800	-0.44464200
S	6.95197900	1.15814400	0.32919300
C	7.45254400	-1.26179400	-0.41987400
H	5.38673800	-1.92813300	-0.74399600
C	8.12143400	-0.11515800	-0.02865000
H	7.97528500	-2.16616000	-0.68619400
C	9.55700600	0.07830200	0.09523500
C	10.51781200	-0.97186300	-0.18844300
C	10.13604000	1.26806300	0.48961700
C	11.94911000	-0.74139500	-0.05432700
C	11.53834900	1.48177600	0.61737800
C	12.45919600	0.51763400	0.35832300
H	13.51954200	0.69750600	0.46055700
N	10.23340500	-2.21006700	-0.58481900
N	12.69217600	-1.80658400	-0.35217400
S	11.65687100	-3.00575800	-0.76926000
F	9.36897200	2.33304700	0.78758600
F	11.91565400	2.70515700	1.01345500
C	-1.69786800	-3.37244300	-0.34706500
H	-0.85338200	-3.27667300	-1.03741000
H	-2.39027400	-4.08082900	-0.81582800
C	-1.18355200	-3.98993800	0.97881800
H	-0.51464700	-3.25703400	1.44632300
C	-0.37160200	-5.25869900	0.68784700
H	0.02947400	-5.68827200	1.60995200
H	-0.99597700	-6.02205900	0.21087200
H	0.47078100	-5.05269200	0.02076100
C	-2.32369100	-4.27987100	1.96220400
H	-2.88735400	-3.37672400	2.20658900
H	-3.02372100	-5.01164400	1.54327700
H	-1.93363100	-4.69330300	2.89640400

C	1.69787100	3.37246500	0.34697300
H	0.85338200	3.27670100	1.03731700
H	2.39027500	4.08085500	0.81573000
C	1.18355700	3.98994600	-0.97891800
H	0.51465300	3.25703600	-1.44641600
C	2.32369800	4.27986800	-1.96230400
H	2.88736100	3.37671900	-2.20667800
H	1.93364000	4.69329000	-2.89650900
H	3.02372800	5.01164600	-1.54338400
C	0.37160600	5.25870900	-0.68796100
H	-0.02946700	5.68827300	-1.61007200
H	-0.47077800	5.05271000	-0.02087500
H	0.99598000	6.02207500	-0.21099300

PVTh$_4$FBT -OD2

C	10.65217800	0.26941100	0.07224700
C	12.03205700	-0.16594700	-0.08915200
C	12.35477700	-1.53049300	-0.31189100
C	11.30745300	-2.39322300	-0.36599900
C	9.95347400	-1.97861200	-0.20900700
C	9.55338800	-0.67613200	0.01122100
H	13.37574200	-1.86242600	-0.43289300
N	12.91864100	0.82538800	-0.00736200
N	10.54911700	1.58165000	0.27019300
S	12.06862300	2.20146300	0.25270700
F	11.50405300	-3.70250500	-0.57279200
F	9.04349600	-2.96589300	-0.29355300
C	8.16189400	-0.27988700	0.16975700
C	7.66832900	0.98304400	0.43022900
S	6.82296000	-1.41068000	0.03263500
C	6.25838600	1.07501300	0.53351500
H	8.32036900	1.83161800	0.56329700
C	5.64513700	-0.15917400	0.36016100
C	4.25693300	-0.56279200	0.45229900
C	3.77044800	-1.79267100	0.85084900
S	2.92291400	0.48001000	-0.02045900
C	2.36628300	-1.89903600	0.79265000
H	4.41775500	-2.58632100	1.19933300
C	1.73306700	-0.75444300	0.34875600
H	1.81847800	-2.78633700	1.08350700
C	0.31557500	-0.56189500	0.20632200
C	-0.31557600	0.56189800	-0.20631800
H	-0.27724800	-1.43611700	0.46545600
H	0.27724700	1.43612100	-0.46545200
C	-1.73306700	0.75444600	-0.34875200
C	-2.36628300	1.89903900	-0.79264700

S	-2.92291400	-0.48000800	0.02046300
C	-3.77044900	1.79267300	-0.85084600
H	-1.81847900	2.78634000	-1.08350300
C	-4.25693300	0.56279400	-0.45229600
H	-4.41775600	2.58632300	-1.19933100
C	-5.64513700	0.15917500	-0.36015900
C	-6.25838500	-1.07501200	-0.53351200
S	-6.82296100	1.41068000	-0.03263500
C	-7.66832800	-0.98304500	-0.43022800
C	-8.16189400	0.27988600	-0.16975700
H	-8.32036700	-1.83161900	-0.56329600
C	-9.55338800	0.67613100	-0.01122300
C	-10.65217800	-0.26941300	-0.07225000
C	-9.95347500	1.97861000	0.20900400
C	-12.03205800	0.16594400	0.08914700
C	-11.30745500	2.39322100	0.36599400
C	-12.35477800	1.53049000	0.31188500
H	-13.37574400	1.86242300	0.43288600
N	-10.54911600	-1.58165200	-0.27019600
N	-12.91864100	-0.82539200	0.00735700
S	-12.06862200	-2.20146600	-0.25271100
F	-9.04349800	2.96589200	0.29355100
F	-11.50405600	3.70250300	0.57278600
C	5.56183000	2.37576100	0.84923000
H	4.65167900	2.17254500	1.42011300
H	6.21165100	2.96482100	1.50694700
C	-5.56182800	-2.37576000	-0.84922600
H	-4.65167600	-2.17254400	-1.42010900
H	-6.21164700	-2.96482100	-1.50694400
C	-5.18988900	-3.25240800	0.37537600
H	-4.58993100	-2.63716200	1.05629800
C	-6.42294900	-3.73791300	1.14705500
H	-6.12484700	-4.34192000	2.00872500
H	-7.02624800	-2.90618000	1.51700100
H	-7.06199100	-4.36083000	0.51110100
C	-4.32602400	-4.43671600	-0.07778400
H	-3.41694000	-4.09873700	-0.58353600
H	-4.02728800	-5.05410900	0.77403800
H	-4.87700700	-5.07783500	-0.77461200
C	5.18989000	3.25240900	-0.37537100
H	4.58993100	2.63716400	-1.05629300
C	4.32602700	4.43671800	0.07779000
H	4.87701100	5.07783600	0.77461800
H	4.02729000	5.05411100	-0.77403200
H	3.41694300	4.09873900	0.58354300
C	6.42295000	3.73791400	-1.14705200

H	7.02624700	2.90618100	-1.51699900
H	6.12484600	4.34192100	-2.00872100
H	7.06199300	4.36083000	-0.51109800

$PVTh_4FBT$ -DD

C	10.61599000	-0.31179100	-0.10671700
C	11.99535500	0.02122500	0.21982300
C	12.32224500	1.21367600	0.91749100
C	11.27927200	2.01425300	1.25732700
C	9.92610000	1.69917600	0.94216700
C	9.52185500	0.56437300	0.26829300
H	13.34275500	1.46834100	1.16423300
N	12.87754700	-0.88681000	-0.19568300
N	10.50919300	-1.46642900	-0.76026400
S	12.02453700	-2.07009900	-0.94141200
F	11.47974400	3.16245200	1.91870800
F	9.02120900	2.60481800	1.35571400
C	8.13094200	0.26801200	-0.04157800
C	7.63018300	-0.83285100	-0.70743300
S	6.80154000	1.32465800	0.41795400
C	6.22387300	-0.85082900	-0.87514900
H	8.27448300	-1.61019300	-1.08794100
C	5.61987000	0.27007800	-0.32491500
C	4.23423000	0.69311000	-0.29729200
C	3.75277800	1.98410400	-0.31781400
S	2.90026000	-0.43282400	-0.12764300
C	2.34397700	2.09970000	-0.21820100
H	4.40649000	2.84105200	-0.42353100
C	1.71590800	0.86430600	-0.11766800
C	0.30408900	0.60928300	-0.02114500
C	-0.30250800	-0.60237000	0.01031100
H	-0.31351400	1.50135800	0.03376000
H	0.31510200	-1.49435700	-0.04579100
C	-1.71426500	-0.85750700	0.10669400
C	-2.34292400	-2.09342500	0.19701400
S	-2.89793500	0.44004900	0.12914400
C	-3.75151200	-1.97806200	0.29764800
C	-4.23276900	-0.68666800	0.28755100
H	-4.40528300	-2.83581300	0.39617000
C	-5.61817100	-0.26406500	0.32076500
C	-6.22041500	0.85972000	0.86759500
S	-6.80381000	-1.32588200	-0.40584400
C	-7.62772100	0.83849600	0.70950200
C	-8.13152700	-0.26776400	0.05504700
H	-8.27043400	1.61781200	1.08866100
C	-9.52398000	-0.56809600	-0.24350200

C	-10.61671800	0.30957400	0.13212000
C	-9.93127800	-1.70846300	-0.90611900
C	-11.99777300	-0.02740500	-0.18303900
C	-11.28607000	-2.02739300	-1.21013600
C	-12.32776600	-1.22542100	-0.86961900
H	-13.34955200	-1.48309100	-1.10781300
N	-10.50706500	1.46912800	0.77639900
N	-12.87832500	0.88270600	0.23140300
S	-12.02190900	2.07245300	0.96283800
F	-9.02801400	-2.61620900	-1.31865400
F	-11.48951000	-3.18080800	-1.86147000
C	1.63413000	3.42866600	-0.28785900
H	0.72492100	3.40723100	0.32102900
H	2.27822400	4.19281100	0.16048000
C	1.27370800	3.85485600	-1.72495900
H	2.18637900	3.87264800	-2.33220400
H	0.62592700	3.09272800	-2.17330800
C	0.58550800	5.22215600	-1.79285300
H	1.23841900	5.97842900	-1.34047000
H	-0.32386300	5.20061800	-1.17974900
C	5.53120600	-1.97494400	-1.60462000
H	4.57420100	-1.63147900	-2.00550200
H	6.14505700	-2.25383600	-2.46846500
C	5.30142200	-3.22709300	-0.73586400
H	6.26366600	-3.57310600	-0.34049000
H	4.69454200	-2.95681900	0.13587900
C	4.62055900	-4.36731000	-1.50023700
H	5.22792800	-4.62903600	-2.37534800
H	3.65945200	-4.01421600	-1.89292700
C	4.39592300	-5.61644300	-0.64366400
H	3.90812400	-6.40994700	-1.21625300
H	5.34355200	-6.01354300	-0.26688600
H	3.76440800	-5.39464500	0.22225600
C	-5.52577900	1.99037300	1.58499700
H	-4.56808100	1.65062400	1.98739400
C	-1.63372000	-3.42333300	0.25465900
H	-0.72482100	-3.39695900	-0.35449400
H	-2.27842700	-4.18315400	-0.20009200
C	-1.27295400	-3.86231700	1.68781400
H	-2.18539200	-3.88500400	2.29524900
H	-0.62463500	-3.10451100	2.14266000
C	-0.58541000	-5.23050100	1.74348900
H	0.32371200	-5.20409300	1.13021100
H	-1.23890100	-5.98247600	1.28483000
H	-6.13787600	2.27727600	2.44741700
C	-5.29761800	3.23465300	0.70451700

H	-4.69212500	2.95681400	-0.16578600
H	-6.26065200	3.57686200	0.30778700
C	-4.61587700	4.38175200	1.45775200
H	-5.22186400	4.65077100	2.33160700
H	-3.65395900	4.03246500	1.85184500
C	-4.39326700	5.62357100	0.59009000
H	-3.90514600	6.42229000	1.15510600
H	-3.76288600	5.39474800	-0.27482100
H	-5.34171500	6.01680300	0.21130700
C	-0.22707600	-5.66560400	3.16723800
H	-1.12022900	-5.73795300	3.79546500
H	0.26297700	-6.64289400	3.17357300
H	0.45229900	-4.95000900	3.64037400
C	0.22749000	5.64470100	-3.22045900
H	-0.26354700	6.62140400	-3.23538400
H	1.12086900	5.71258700	-3.84885500
H	-0.45092900	4.92439300	-3.68777700

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