Supporting Information

A structural investigation of novel thiophene functionalized BEDT-TTF donors for application as organic field effect transistors

Qiang Wang,[a] John D. Wallis,[b] Yiliang Wu[c] and Melanie Pilkington[a]*

[a] Department of Chemistry,
Brock University,
500 Glenridge Avenue, St Catharines, ON,
L2S 3A1, Canada.
Tel: +1 (905) 688 5550 ext. 3403
E-mail: mpilkington@brocku.ca

[b] School of Science and Technology,
Nottingham Trent University,
Clifton Lane, Nottingham, NG11 8NS, UK.

[c] Xerox Research Centre of Canada,
2660 Speakman Drive,
Mississauga, ON, L5K 2L1, Canada.

Contents

S-1 Preparation and configuration of the OFET device

Fig. 1 shows a schematic cross section of the organic thin-film field effect transistor (OTFTs) device configuration. An n-doped Si wafer with a 110 nm thermally grown silicon dioxide layer (capacitance of 32 nF/cm^2) was used as the substrate. Semiconductor films were deposited by spin coating 1 wt.% of chlorobenzene solution of the tested compound onto octyltrichlorosilane (OTS) modified or unmodified substrates, respectively, at 1000 rpm for 45 s. Gold source and drain electrodes were then deposited on top of the substrates by vacuum evaporation through a shadow mask with various channel lengths and widths, thus creating a series of transistors of various dimensions by bridging crystals as active channels over the drain-source electrodes.

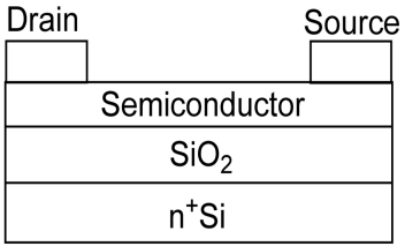

Fig.1. Schematic diagram of the configuration of an OTFT device.

S-2 Tables of bond lengths and angles for 1

Bond	Distance (Å)	Bond	Distance (Å)
S1-C1	1.809(5)	C9-C10	1.534(5)
S1-C3	1.751(4)	C9-C11	1.522(5)
S2-C2	1.798(5)	C11-C12	1.512(5)
S2-C4	1.748(4)	C13 -C14	1.437(5)
S3-C3	1.773(4)	C14-C15	1.395(5)
S3-C5	1.755(3)	C14-C15$^{\#}$	1.351(4)
S4-C4	1.770(4)	C15-C16	1.389(6)
S4-C5	1.755(3)	C15$^{\#}$-C16$^{\#}$	1.421(17)
S5-C6	1.754(3)	C16-C17	1.338(5)
S5-C7	1.769(3)	C16$^{\#}$-C17$^{\#}$	1.35(2)
S6-C6	1.747(3)	S6 -C8	1.761(3)
S7-C7	1.747(3)		
S7-C9	1.824(3)		
S8-C8	1.750(3)		
S8-C10	1.814(4)		
S9-C14	1.692(3)		
S9-C17	1.733(4)		
S9$^{\#}$-C14	1.641(5)		
S9$^{\#}$-C17$^{\#}$	1.698(14)		

Bond	Angle (°)	Bond	Angle (°)
C1-S1-C3	100.9(2)	S6-C8-C7	116.9(2)
C2-S2-C4	99.9(2)	S8 -C8-C7	128.9(2)
C3-S3-C5	92.59(16)	S6-C8-S8	113.97(15)
C4-S4-C5	92.18(16)	S7-C9-C11	112.2(2)
C6-S5-C7	93.48(14)	C10-C9-C11	113.5(2)
C6-S6-C8	94.09(14)	S7-C9-C10	110.3(2)
C7-S7-C9	99.59(14)	S8-C10-C9	115.1(2)
C8-S8-C10	101.51(15)	C9-C11-C12	113.7(2)
C14-S9-C17	92.02(16)	O1-C12-C11	111.3(3)
C14-S9$^{\#1}$-C17$^{\#1}$	99.3(7)	O1-C13-O2	124.5(3)
C12-O1-C13	116.0(3)	O1-C13-C14	111.0(3)
S1-C1-C2	114.7(4)	O2-C13-C14	124.5(3)
S2-C2-C1	114.4(4)	S9-C14-C13	122.4(3)
S1-C3-S3	115.3(2)	S9-C14-C15	107.2(2)
S1-C3-C4	128.7(3)	S9A-C14-C13	133.4(3)
S3-C3-C4	116.0(3)	C13-C14-C15$^{\#1}$	119.9(3
S2-C4-S4	114.3(2)	S9A-C14-C15$^{\#1}$	103.1(3)
S2-C4-C3	128.7(3)	C13-C14-C15	129.5(3)
S4-C4-C3	117.0(3)	C14-C15-C16	117.8(3)
S3-C5-C6	122.9(2)	C14-C15A-C16$^{\#1}$	119.6(3)
S4-C5-C6	124.0(2)	C15-C16-C17	108.0(4)
S3-C5-S4	112.91(17)	C15$^{\#1}$-C16$^{\#1}$-C17$^{\#1}$	109.7(14)
S5-C6-S6	114.39(18)	S9-C17-C16	114.1(3)
S5-C6-C5	123.2(2)	S9A-C17$^{\#1}$-C16$^{\#1}$	107.1(13)

S6-C6-C5	122.5(2)	S1-C1-H1$^{\#1}$	109.00
S5-C7-S7	114.47(14)	S1-C1-H1$^{\#2}$	109.00
S5-C7-C8	117.0(2)	C2 -C1-H1$^{\#1}$	109.00
S7-C7-C8	128.5(2)	C2-C1-H1$^{\#2}$	109.00

Symmetry transformations used to generate equivalent atoms:
#1 = x,y,1/2-z; #2 =1/2+x,-1/2+y,z

S-3 Tables of bond lengths and angles for 2

Bond	Length (Å)	Bond	Length (Å)
S1-C1	1.811(3)	C3-C4	1.342(3)
S1-C3	1.744(2)	C5 -C6	1.347(3)
S2-C2	1.804(3)	C7-C8	1.341(3)
S2-C4	1.746(2)	C9 -C10	1.521(3)
S3-C3	1.761(2)	C9-C11	1.515(3)
S3-C5	1.762(2)	C12-C13	1.465(4)
S4-C4	1.757(2)	C13-C14	1.406(4)
S4-C5	1.753(2)	C14-C15	1.415(4)
S5-C6	1.753(2)	C15-C16	1.361(4)
S5-C7	1.761(2)		
S6-C6	1.750(2)		
S6-C8	1.755(2)		
S7-C7	1.754(2)		
S7-C9	1.828(2)		
S8-C8	1.747(2)		
S8-C10	1.801(2)		
S9-C13	1.716(2)		
S9-C16	1.697(3)		
O1-C11	1.447(3)		
O1-C12	1.340(3)		
O2-C12	1.207(3)		
C1-C2	1.513(4)		

Bond	Angle(°)	Bond	Angle(°)
C1-S1-C3	103.91(11)	S6-C8-C7	117.85(16)
C2-S2-C4	98.61(11)	S8-C8-C7	126.38(16)
C3-S3-C5	94.12(10)	S7-C9-C10	113.66(15)
C4-S4-C5	94.23(10)	S7-C9-C11	109.14(15)
C6-S5-C7	95.09(10)	C10-C9-C11	112.51(18)
C6-S6-C8	94.90(10)	S8-C10-C9	112.61(15)
C7-S7-C9	103.84(10)	O1-C11-C9	105.76(17)
C8 -S8-C10	97.08(10)	O1-C12-O2	124.1(2)
C13-S9-C16	91.40(13)	O1-C12-C13	111.23(19)
C11-O1-C12	116.39(18)	O2-C12-C13	124.7(2)
S1-C1-C2	115.27(17)	S9-C13-C12	122.41(17)
S2-C2-C1	113.7(2)	S9-C13-C14	112.27(18)
S1-C3-S3	113.44(11)	C12-C13-C14	125.3(2)
S1-C3-C4	129.40(17)	C13-C14-C15	110.0(2)
S3-C3-C4	117.14(16)	C14-C15-C16	113.7(2)
S2-C4-S4	116.19(11)	S9-C16-C15	112.7(2)
S2-C4-C3	125.93(16)		
S4-C4-C3	117.53(16)		
S3-C5-S4	114.53(12)		
S3-C5-C6	122.53(16)		
S4-C5-C6	122.91(16)		
S5-C6-S6	114.91(11)		
S5-C6-C5	121.94(16)		
S6-C6-C5	123.14(16)		

S5	-C7	-S7	114.52(11)
S5	-C7	-C8	116.74(16)
S7	-C7	-C8	128.73(16)
S6	-C8	-S8	115.74(11)