

10.1071/CH12325_AC

©CSIRO 2012

Australian Journal of Chemistry 2012, 65(12), 1674-1678

Supplementary Material

Synthesis, structure, physical properties, and displacement current measurement of an n-type organic semiconductor: 2:3, 5:6-bis(1,1-dicyanoethylene-2,2-dithiolate)-quinone

Jinchong Xiao,^{[a,b]†} Yasuo Azumal,^{[c]†} Yi Liu,^[a] Gang Li,^[a] Fengxia Wei,^[a] Ke Jie Tan,^[a] Christian Kloc,^[a] Hua, Zhang,^[a] Yutaka Majima,*^[c] and Qichun Zhang*^[a]

^a School of Materials Science and Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore. E-mail: qczechang@ntu.edu.sg.

^b Key Laboratory of Chemical Biology of Hebei Province, College of Chemistry and Environmental Science, Hebei University, Baoding 071002, P. R. China.

^c Materials and Structures Laboratory, Tokyo Institute of Technology, Nagatsuta-cho, Midori-ku, Yokohama 226-8503, Japan & CREST, Japan Science and Technology Agency, Nagatsuta-cho, Midori-ku, Yokohama 226-8503, Japan. E-mail: majima@msl.titech.ac.jp

Empirical formula	C ₁₄ N ₄ O ₂ S ₄
Formula weight	384.42
Crystal system	Triclinic
Space group	<i>P</i> 1̄
Unit cell dimensions	
a (Å)	6.8165(14)

Table S1.
Crystal
Data
and

Structure Refinements for Compound **1** (CCDC number: 844796).

b (Å)	7.6074(15)
c (Å)	8.0880(16)
alpha (deg.)	74.62(3)
beta (deg.)	72.21(3)
gamma (deg.)	72.70(3)
Volume(Å ³)	374.21(13)
Z	1
D _{cal} (g/cm ³)	1.706
μ(mm ⁻¹)	0.650
F(000)	192
Temperature(K)	293(2)
Final R indices [I>2σ(I)]	R _I = 0.0393, wR ₂ = 0.0829
R indices (all)	R _I = 0.0622, wR ₂ = 0.0933
Goodness-of-fit on F ²	1.076

$$R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|. \quad wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$$

Table S2. Selected Bond Lengths (Å) and angles (deg) for Compound **1** (CCDC number: 844796).

Bond distance			
O(1)-C(3)	1.210(4)	C(2)-C(1)#1	1.348(4)
S(1)-C(2)	1.726(3)	C(6)-C(5)	1.378(5)
S(1)-C(5)#1	1.731(4)	C(6)-C(4)	1.414(5)
S(2)-C(1)	1.725(3)	C(6)-C(7)	1.421(5)
S(2)-C(5)	1.733(3)	C(4)-N(1)	1.143(5)
C(3)-C(2)	1.472(5)	C(7)-N(2)	1.149(5)
C(3)-C(1)	1.478(4)		
Bond angle			
C(2)-S(1)-C(5)#1	94.32(17)	C(3)-C(1)-S(2)	119.9(2)
C(1)-S(2)-C(5)	94.00(16)	C(5)-C(6)-C(4)	121.1(3)
O(1)-C(3)-C(2)	122.5(3)	C(5)-C(6)-C(7)	119.9(3)
O(1)-C(3)-C(1)	122.6(3)	C(4)-C(6)-C(7)	119.0(3)
C(2)-C(3)-C(1)	114.9(3)	C(6)-C(5)-S(1)#1	121.6(3)
C(1)#1-C(2)-C(3)	123.0(3)	C(6)-C(5)-S(2)	121.9(3)
C(1)#1-C(2)-S(1)	117.2(3)	S(1)#1-C(5)-S(2)	116.5(2)
C(3)-C(2)-S(1)	119.8(3)	N(1)-C(4)-C(6)	177.5(4)
C(2)#1-C(1)-C(3)	122.2(3)	N(2)-C(7)-C(6)	177.9(4)
C(2)#1-C(1)-S(2)	117.9(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y-2,-z+1

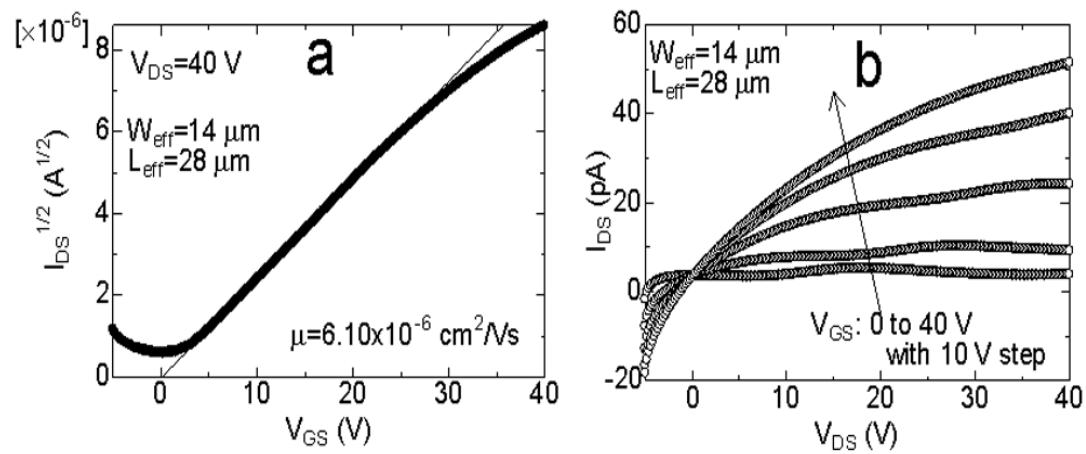


Figure S1 (a) Transfer curve and output curve of **BDQ**-based TFT transistors.

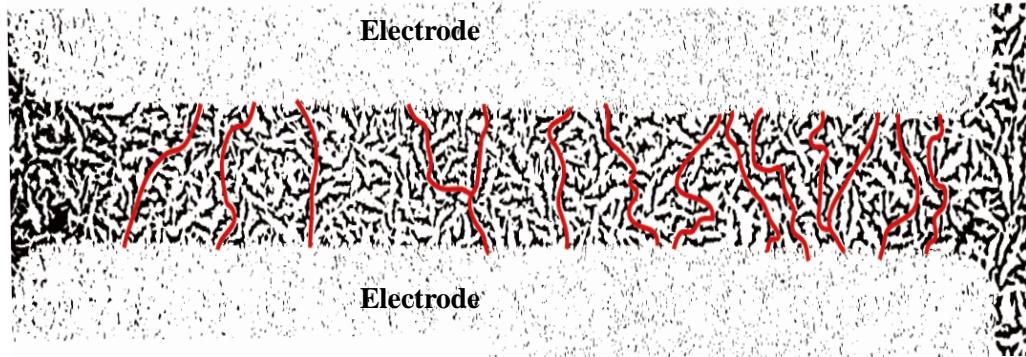


Figure S2. Optical microscope image of channel region (In channel region, white and black areas correspond to **BDQ** and SiO_2 , respectively)