Machine Learning, Divergent Syntheses, and X-ray Analyses of Dithienobenzothiazole-based Semiconductors Controlled by S•••N and S•••S Interactions

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Abstract: Inspired by the previous machine-learning study that the number of hydrogen-bonding acceptor (N_{HBA}) is important index for the hole mobility of organic semiconductors, we synthesized seven dithienobenzothiazole (DBT) derivatives 1a-g $(N_{\text{HBA}} = 5)$ by one-step functionalization from a common precursor. X-ray single-crystal structural analyses confirmed that the molecular arrangements of 1b (the diethyl and ethylthienyl derivative) and 1c (the di(n-propyl) and n-propylthienyl derivative) in the crystal are classified into brickwork structures with multidirectional intermolecular charge-transfer integrals, as a result of incorporation of multiple hydrogen-bond acceptors. The solution-processed top-gate bottom-contact devices of 1b and 1c had hole mobilities of 0.16 and 0.029 cm² V⁻¹s⁻¹, respectively.

Introduction

Organic semiconductors (OSCs)^[1,2] are employed in various electronic applications including organic light-emitting diodes,[3] organic photovoltaic cells,^[4] and organic field-effect transistors (OFETs).^[5-10] The results of a large number of papers show that the performance of OSCs is controlled by solid-state packing governed by intermolecular interactions, exemplified by $\pi^{\bullet\bullet\bullet\pi}$ interaction,^[11] CH····π interaction,^[12] S····S contact,^[13] and S····N contact^[14] to construct brickwork,^[15] herringbone,^[1,16-20] and slipped-*π*-stacked crystal structures.^[21] Actually, some linearlyfused *π*-electronic systems exhibit high charge-carrier mobilities as a result of their close-packed crystalline structures.^[22-25] For dialkylated dinaphtho[2,1-b:2',1'-f]thieno[3,2example, 1)^[26] b]thiophenes (S-DNTTs, Figure and 2.7-

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diphenyl[1]benzothieno[3,2-b][1]benzothiophene (DPh-BTBT)[27] are known to be high performance OSC materials. However, these types of materials form a columnar crystal structure, whose semiconductor characteristics suffered from a lattice defect.^[28,29] In this respect, organic semiconductor molecules possessing annulated p-conjugated planes enable various multidirectional intermolecular interactions.



Figure 1. Chemical structures of S-DNTTs, DPh-BTBT, and 1a-g with the DBT core.

It is believed that the adoption of materials informatics (MI) and cheminformatics (CI) assisted by machine learning are important for the development of high-performance optoelectronic materials.^[30-32] However, MI and CI often outputs molecular structures that have difficulty in synthesis or air-stability. On the other hand, if the importance is output from the decision tree, as in the "Random Forest Algorithm", it can be a useful tool for molecular design, utilizing the results of machine learning to the knowledge of organic chemists. Previous MI study revealed that the most important factor of in the molecular structure of organic semiconductors is the number of hydrogen-bonding acceptor (N_{HBA}), *i.e.* the number of O, N, S, and other HBA atoms in the molecule.^[33] Because semiconductor molecules have multiple hydrogens, a high NHBA value bring about a tightly-packed crystal structure owing to strong O ····H, N ····H, and S ····H hydrogenbonding. The tight packing provides strong intermolecular interaction between the adjacent two molecules, required for an efficient hole transportation.

In this work, we studied the performance of the parent (1a, Figure 1) and its alkyl and aryl derivatives (1b-1g) with a dithieno[2',3':3,4;3",2":5,6]benzo[1,2-d]thiazole (DBT) core as novel p-type OFET materials, in which the thienyl-DBT moiety has an N_{HBA} value of 5. To make efficient assessment of the effect of substituents on molecular alignment in the crystal, seven DBT derivatives 1a-g were divergently synthesized using a validated coupling reaction to one common synthetic intermediate. Below,

we describe the diversity of semiconductor properties based on the crystal properties of each derivative.

Results and Discussion

Synthesis. According to procedures shown in Scheme 1, a common intermediate for divergent syntheses of 1a-g, 5,8dibromo-2-(5-bromothiophen-2-yl)dithieno[2',3':3,4;3",2":5,6]benzo[1.2-d]thiazole (5). was prepared from 2.4.5tribromothiazole $^{[34]}\left(2\right) .$ The Stille cross-coupling reaction of 2 and 2-(tri(*n*-butyl)stannyl)thiophene^[35] with a palladium catalyst provided 2,4,5-tris(thiophen-2-yl)thiazole (3) in 80% yield.[36] Reaction of 3 with N-bromosuccinimide (NBS) afforded tribromide 4 in 86% yield.^[37] Although photochemical cyclization reactions^{[38-} ^{40]} were not applicable to this system, the Scholl cyclization reaction of 4 in the presence of FeCl₃ gave 5 in 91% yield.^[37] Various functionalization of 5 complete the divergent synthesis of DBTs 1a-g (Table 1). Reductive debromination of 5 with NaBH₄ and a palladium catalyst gave 1a in 70% yield (run 1).[41] Linear alkyl groups were successively introduced by using Negishi coupling reactions deploying the corresponding 1-bromoalkane (runs 2-5).^[42] Phenyl and 4-isopropylphenyl groups also substituted for the Br atoms in 5 by Suzuki-Miyaura crosscoupling reaction to give 1f and 1g in moderate yields, respectively (runs 6 and 7).[43]



Scheme 1. Divergent synthesis of DBTs 1a–g using a common synthetic intermediate 5 available from 2 via three steps in good yields.

Table 1. Divergent Syntheses of DBTs 1a-g from 5 ^a							
run	reagent, additive, catalyst, solvent	product (R), yield / %					
1	NaBH ₄ , TMEDA, PdCl ₂ (dppf)•CH ₂ Cl ₂ , THF	1a (H), 70					
2	EtZnCl, ^b PdCl ₂ (dppf)•CH ₂ Cl ₂ , THF	1b (Et), 32					
3	<i>n</i> PrZnCl, ^b PdCl ₂ (dppf)•CH ₂ Cl ₂ , THF	1c (<i>n</i> Pr), 38					
4	nBuZnCl, ^b PdCl ₂ (dppf)•CH ₂ Cl ₂ , THF	1d (<i>n</i> Bu), 55					
5	<i>n</i> PeZnCl, ^b PdCl ₂ (dppf)•CH ₂ Cl ₂ , THF	1e (<i>n</i> Pe), 53					
6	PhB(OH) ₂ , Pd(PPh ₃) ₄ , DMF	1f (Ph), 66					
7	4-iPrC ₆ H ₄ B(OH) ₂ , Pd(PPh ₃) ₄ , DMF	1g (4-iPrC ₆ H ₄), 76					



Theoretical Calculation. The optimized geometries and the HOMO and the lowest unoccupied molecular orbital (LUMO) of DBTs 1a were calculated based on density functional theory (DFT) using the B3LYP hybrid functional and the 6-31+G(d,p) basis set (Figure 2). The thienyl groups of 1a is co-planar with the DBT core. The intramolecular distance between the S atom of thienyl group and the N atom of the DBT core in 1a (3.08 Å) is shorter than the sum of its van der Waals (vdW) radii (3.35 Å), suggesting that an S•••N contact exists between them. This is also the case with other DBTs 1b-g (For the detail, see the Supporting Information). As described later, the S•••N contacts are also confirmed in crystal. The HOMO energy level (EH,DFT) of 1a is calculated to be -5.44 eV, which is a good fit with Au with a work function of ca. 5 eV, suggesting that DBTs 1a-g are suitable for p-type semiconductors used in contact with Au. Note that $E_{H,DFT}$ values of 1b-g are up to ca. -5.1 eV higher compared to 1a (Figure 3, Table 2) due to substitution of electron-donating alkyl or alkyl-substituted aryl groups. As discussed later, the HOMO energy level (EH,CV) obtained from cyclic voltammetry (CV) data seems to be slightly lower than the calculated values $E_{H,DFT}$.



Figure 2. Optimized geometries of **1a** (H), **1b** (Et), and **1g** (4-iPrC₆H₄) obtained by DFT calculation [B3LYP/6-31+G(d,p)].



Figure 3. The HOMO and LUMO with those energy levels of 1a (H), 1b (Et), and 1g (4-iPrC₆H₄) obtained by DFT calculation [B3LYP/6-31+G(d,p)].

 Table 2. Energy Levels of the HOMO and LUMO of 1a-g Obtained

 by DFT Calculations [B3LYP/6-31+G(d,p)]

substrates (R)	E _{H,DFT} / eV	$E_{L,DFT}^{a}$ / eV
1a (H)	-5.45	-1.88
1b (Et)	-5.18	-1.70
1c (<i>n</i> Pr)	-5.15	-1.88
1d (<i>n</i> Bu)	-5.14	-1.88
1e (<i>n</i> Pe)	-5.35	-1.87
1f (Ph)	-5.17	-2.27
1g (4-iPrC ₆ H ₄)	-5.05	-2.18

^aThe LUMO energy level.

Basic Physical Properties. First described are thermal stability and solubility in toluene, one of the common solvents used for thin-film deposition of solution-processed OFETs. The melting point of **1a** was 242–242.5 °C and solubility into toluene is 2.5 g L⁻¹ (Table 3). Probably, the introduction of alkyl groups may have reduced the intermolecular interaction in crystal, resulting in lower mp (71–133 °C for **1b–d**) and high solubility (43–55 g L⁻¹). On the other hand, the introduction of aryl groups may have increased π – π interaction, resulting in high mp (274–293 °C for **1f** and **1g**) and low solubility (0.32–1.9 g L⁻¹). From the viewpoint of ease of handling such as thermal stability and solubility, alkyl derivatives are suitable for solution-processed OFET.

The parent and alkyl derivatives **1a–e** exhibited absorption bands at *ca*. 290–300 and *ca*. 375–390 nm region, while the aryl derivatives **1f** and **1g** showed absorption bands at longer wavelengths region at *ca*. 350 and 420 nm in aerated CH_2Cl_2 solution (Figure 4a and Table 3). These absorption band did not change after 24 h in air, indicating that **1a–g** have atmospheric stability.

A CV study of **1a** in a CH₂Cl₂ solution containing $nBu_4N^+PF_6^-$ (0.1 M) did not give any clear oxidation wave. On the other hand, those of **1b–g** gave each reversible waves with one-electron oxidation peak (E^{OX}_p) at *ca.* +0.65 to +0.85 V (Figure 4b), indicating that these p-type semiconductor materials are electrochemically stable under these one-electron oxidation conditions. The peak potential difference between the oneelectron oxidation wave (E^{OX}_p) and the reduction wave (E^{RED}_p) is not 0.059 V as expected from the Nernst equation. This phenomenon may indicate some geometrical (but not chemical) changes of $1b-g^{++}$ generated by oxidation.

The experimental HOMO energy levels ($E_{H,CV}$) of **1a–g** calculated by using these oxidation potentials vs ferrocene are in the range of -5.43 to -5.64 eV. Although these values are slightly lower than the work function of Au, a carrier injection from Au electrode to **1a–g** is expected to be possible.

Table 3. Basic Physical Properties of 1a-g

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substratos (P)	mp	Solubility ^a	λ_{\max}^{b}	$E^{OX}_{1/2}$	$E_{\rm H,CV}^{d}$			
substrates (R)	°C	g L ^{_1}	nm	V	eV			
1a (H)	242	2.5	291, 374	e	e			
1b (Et)	133	45	299, 387	+0.75	-5.55			
1c (<i>n</i> Pr)	88	43	299, 387	+0.77	-5.57			
1d (<i>n</i> Bu)	94	48	299, 387	+0.84	-5.64			
1e (<i>n</i> Pe)	71	54	298, 387	+0.78	-5.58			
1f (Ph)	290	0.32	347, 418	+0.75	-5.55			
1g (4_iPrC_0H_()	274	1.9	351, 423	+0.63	-5.43			

^aIn toluene at room temperature. ^bIn a CH₂Cl₂ solution containing **1** (1.0 × 10⁻⁵ M). ^c $E^{OX}_{1/2} = E^{OX}_{p} - 0.03$ V vs Fc/Fc⁺. In a CH₂Cl₂ solution containing **1** (1.0 × 10⁻³ M) and *n*Bu₄N⁺PF₆⁻ (0.1 M). Scan rate: 0.1 V s⁻¹. Reference electrode: Ag/Ag⁺; working and counter electrodes: Pt. ^d $E_{H,CV}$ = - (4.8 eV + 1e^{*} E^{OX}). ^eNot available.



Figure 4. (a) Absorption spectra of **1a–g** in CH₂Cl₂. (b) Cyclic voltammograms of **1a**, **1b**, and **1g** in a CH₂Cl₂ solution containing **1** (1.0×10^{-3} M) and *n*Bu₄N⁺PF₆⁻ (0.1 M). Scan rate: 0.1 Vs⁻¹. Reference electrode: Ag/Ag⁺, working and counter electrodes: Pt.

X-Ray Crystallographic Analysis. We successfully prepared single crystals of **1a–e** and **1g** by recrystallization from appropriate solvents, and conducted X-ray crystallographic analyses (Figure 5). The S atom of the thienyl group of **1b–e** and **1g** is on the side of the N atom of the DBT core. The dihedral angles between the thienyl groups and the DBT core are in the range of 0.4–9.2°. The intramolecular distances between the S atom of thienyl group and the N atom in **1b–e** and **1g** (2.95–3.09 Å) are shorter than the sum of the *vdW* radii (3.35 Å) of S and N atoms. These findings are in line with the results obtained by DFT calculation studies described above, indicating that an intramolecular S•••N contact takes place to increase molecular planarity of **1b–e** and **1g**.

On the other hand, the intermolecular distance between the S atoms of the thienyl groups in two adjacent molecules (1d) and those between the S atoms of the thienyl and thieno groups (1a and 1c) are in the range of 3.48–3.57 Å. The distances are shorter than the sum of the *vdW* radii of the two S atoms (3.6 Å), suggesting that these S···S contacts significantly control the whole crystal structures of these DBTs. The packing diagram of the crystals of 1b and 1c were into the brickwork structure. These packing structures are analogous with that of high-mobility semiconductors.^[15–17] The crystals of 1c–e and 1g were classified into some slipped p-stacking structures. These structures are often found in asymmetric semiconductor materials where

remarkable steric repulsion and dipole moment relaxation takes place.^[44] Introduction of even one or two bulky substituent tends to reduce intermolecular interactions. Therefore, it is desirable to introduce small substituents such as Et and *n*Pr groups, even if they are three or four, to maintain strong intermolecular interactions.

To evaluate the degree of intermolecular interactions required for semiconductor properties, the intermolecular charge-transfer integrals (t) between a variety of two adjacent molecules in crystal were calculated by CAM-B3LYP/6-31G(d) level of theory (Figure 5).[45] Compounds 1a-c possessing herringbone and brickwork structures provide high t values for multiple pairs, and therefore enable multidirectional conduction. However, t values of 1d, 1e, and 1g are low for the adjacent columns. These results indicate that among **1a–g**, the materials for which high μ_h values are expected for 1b and 1c. A molecule of 1b in the crystal has four S····H contacts with neighboring molecules (Figure 6a) to form a tight packing structure. Moreover, a molecule of 1c in the crystal have two S····H two S····S, and two N····H contacts with neighboring molecules (Figure 6b) to form a more tight packing structure. These contacts involve N_{HBA} proposed by machine learning.



Figure 5. Packing structures of the crystal **1a** (a), **1b** (b), **1c** (c), **1d** (d), **1e** (e), and **1g** (f) with *t* values in meV calculated at the CAM-B3LYP/6-31G(d) level of theory using X-ray coordinate data.



Figure 6. Representation of the major contacts observed between neighboring molecules of 1b (a) and 1c (b) in the crystal. Red: S•••H, pink: S•••S, green: N•••H.

Thin-Film Properties. To estimate solution-processed OFET characteristics, thin-film properties of **1a–g** were investigated. Films of **1b** and the others were prepared by using its 0.5 wt% CHCl₃ solution and 1 wt% solutions, respectively, by spin coating on glass substrates. Analyses based on polarized optical microscope measurement suggested that the thin films of **1b–e** were polycrystalline (Figure 7). Unfortunately, thin films of **1a, 1f**, and **1g** could not be formed probably due to the low solubility.

Based on the results of out-of-plane X-ray diffraction (XRD) measurements, molecules of **1b–e** in the thin film have edge-on orientation against the glass substrate (Figure 8). A grating constant *d* of 8.0 Å for **1b**, perpendicular to the glass substrate, was shorter than the molecular length of 16.6 Å. The out-of-plane XRD pattern of the thin film of **1b** contains characteristic peaks at 5.5 and 11.1°, which is similar to those (5.6, 11.2°) observed in the X-ray crystallographic analysis of single crystal shown above. Therefore, the thin-film of **1b** contains a molecular packing displayed in Figure 5b, which is expected to exhibit a high hole mobility. However, the out-of-plane XRD patterns of the thin films of **1c–d** were different from those of the single crystals, suggesting that different polymorphs are formed in the thin films.

Since *t* values of **1b** and **1c** are high in multiple directions in the calculation, we fabricated top-gate bottom-contact OFETs of them by using spin-coat method.^[46] As a result of evaluation, the OFET devices of **1b** and **1c** were found to exhibit p-type conduction with hole mobilities (μ _h) of 0.16 and 0.029 cm² V⁻¹s⁻¹, respectively, in the saturation regions (Figure S6). The difference in μ _h between **1b** and **1c** was due to those of molecular orientation in the thin film. Improvement of hole mobilities of the OFETs is possible by optimizing thin-film fabrication processes or by modifying OFET structures.



Figure 7. Photographs of crystalline thin films of 1b (a) and 1c (b) observed with polarized optical microscopy.



Figure 8. XRD patterns of out-of-plane thin-film and single crystal of 1b (a) and 1c (b).

Conclusion

Based on the MI proposal of incorporating the index N_{HBA} into molecular design, we synthesized seven DBTs **1a–g** (N_{HBA} = 5), by one-step functionalization of a common easily-synthesized intermediate. DFT calculations for the packing structure suggest that various multi-directional intermolecular interactions and therefore high hole mobility are possible, because there are not only multiple hydrogen-bondings but also S•••S and S•••N contacts because they have one N atom in addition to S atoms in the DBT core.

In fact, the findings of X-ray crystallographic analysis show that these DBTs exhibit multiple intermolecular and intramolecular interactions, such as hydrogen bondings and S•••N and S•••S contacts, leading to herringbone (**1a**) and brickwork packing structures (**1b** and **1c**). These contacts involve N_{HBA} proposed by machine learning. Calculations based on X-ray packing diagram showed that **1b** and **1c** exhibit reasonable transfer integral values *t* for neighboring molecules in multiple directions. In particular, solution-processed top-gate bottom-contact OFETs using **1b** and **1c** yielded mobilities μ_{h} of 10^{-1} to 10^{-2} cm²V⁻¹s⁻¹, giving good results for the first trial based on the DBTs core. MI approaches have the potential to simplify complex molecular structures and enable new molecular designs required for organic semiconductors.

Experimental Section Preparation of Materials

Procedures for preparation of **2–5** and **1a,c,d,e,g** (Scheme 2) and physical data of all materials are given in the supporting information. Those of **1b and 1f** are as follows.

5,8-Diethyl-2-(5-ethyllthiophen-2-yl)dithieno-

[2',3':3,4;3",2":5,6]benzo[1,2-d]thiazole (1b): To a 25-mL round-bottom flask, 1-bromoethane (0.9 mL, 12 mmol), Mg (0.320 g, 12.0 mmol), and THF (3.0 mL) were added and stirred for 30 minutes at room temperature. To the prepared colorless solution of EtMgBr was added ZnCl₂ in THF (1.0 M, 12 mL, 12.0 mmol) at 0 °C. After stirring at room temperature for 1 h, 5 (0.340 g, 0.601 mmol) and PdCl₂(dppf)·CH₂Cl₂ (0.060 mmol) were successively added at room temperature. The resulting brown suspension was stirred at 65 °C for 18 h. After cooling to room temperature, the reaction was guenched with 10 mL of water. The resultant mixture was extracted with CHCl₃ (20 mL \times 3), and the organic layer was washed with brine, and dried over anhydrous Na₂SO₄. The combined organic layer was concentrated under reduced pressure to give residual brown solid. Column chromatography [silica gel, *n*-hexane/CHCl₃= 5 (v/v)] followed by recrystallization from CHCl₃-MeOH to give 1b (0.079 g, 0.191 mmol, y. 32%) as light green needles. mp 133–133.5 °C; ¹H NMR (400 MHz, CDCl₃) δ_{ppm} 1.38 (t, J = 7.2 Hz, 3H), 1.45 (t, J = 7.2 Hz, 3H), 1.46 (t, J = 7.2 Hz, 3H), 2.91 (q, J = 7.2 Hz, 2H), 3.03 (q, J = 7.2 Hz, 2H), 3.06 (q, J = 7.2 Hz, 2H), 6.83 (d, J = 4.0 Hz, 1H), 7.34 (s, 2H),7.50 (d, J = 4.0 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ_{ppm} 15.68, 15.77 (1C +1C), 23.80, 24.17, 24.20, 118.40, 118.81, 123.40, 124.57, 127.81, 127.91, 129.45, 132.89, 134.01, 134.61, 145.55, 147.79, 148.28, 151.91, 159.40; IR (ATR, neat) v/cm⁻¹ 667, 792, 824, 891, 948, 1339, 1377, 1433, 1447, 1489; LR-Mass (ASAP) m/z 414 ([M+H]⁺); Anal. Calcd for C₂₁H₁₉NS₄: C, 60.98; H, 4.65; N, 3.39; S, 31.00; Found: C, 60.85; H, 4.63; N, 3.35.

5,8-Diphenyl-2-(5-phenylthiophen-2-yl)dithieno-

[2',3':3,4;3",2":5,6]benzo[1,2-d]thiazole (1f): To a 25-mL round-

bottom flask, 5 (0.170 g, 0.300 mmol), phenylboronic acid (0.146 g, 1.2 mmol), K₃PO4•xH₂O (2.00 g), and DMF (6 mL) were added the mixture was purged by argon by 30 min of bubbling. To a 100mL round-bottom flask, Pd(PPh₃)₄ (0.035 g, 0.030 mmol) and the solution were added and stirred for 19 h at 100 °C. After cooling to room temperature, the reaction was quenched with 10 mL of water. The resulting precipitate was filtered and washed several times with hot MeOH. The organic layer was concentrated under reduced pressure to give residual black solid that was subjected to column chromatography [silica gel, n-hexane/toluene = 3 (v/v)]. The obtained solid was subjected to recrystallization from toluene to give 1f (0.110g, 0.20 mmol, y. 66%) as a yellow solid. dp 290-302 °C; ¹H NMR (400 MHz, CDCl₃) δ_{ppm} 7.38 (m, 4H), 7.47 (m, 6H), 7.69 (d, J = 4.0 Hz, 1H), 7.72 (AA'BB'C, J = 7.6 Hz, 2H), 7.80 (AA'BB'C, J = 7.2 Hz, 2H), 7.86 (AA'BB'C, J = 7.2 Hz, 2H), 8.00 (s, 1H), 8.01 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ_{ppm} (unobservable probably due to low solubility); LR-Mass (ASAP) m/z (unobservable probably due to low volatility); IR (ATR, neat) v / cm⁻¹ 688, 754; Anal. Calcd for C₃₃H₁₉NS₄: C, 71.06; H, 3.43; N, 2.51; Found: C, 71.07; H, 3.70; N, 2.50.

Fabrication of OFET

The glass substrate with deposited the gold electrode was ultrasonically cleaned with acetone and 2-propanol for 10 min, followed by UV-ozone treatment (UV Ozone Cleaner Filgen UV253) for 1 h. The thin films were prepared on the substrates using the solution of **1b** (0.5 wt% in CHCl₃) or **1c** (1.0 wt% in toluene) by spin-coat method at 500 rpm for 5 s, followed by 2000 rpm for 60 s (Spincoater: Kyowa Riken K359S1). The films were dried at room temperature for 1 h in a glove box. The CYTOP layer was spin-coated onto the substrates at 500 rpm for 5 s, followed by 4000 rpm for 60 s, and dried under vacuum for 24 h. After drying, Al electrodes were deposited using ULVAC Kikou VPC-260F to fabricate a top-gate bottom-contact OFET. OFETs characteristics were evaluated using a Keithley 6430 or Keithley 2400 source meter.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords: Divergent synthesis • Organic semiconductor • Organic field-effect transistor• Crystal structure • Materials Informatics

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Entry for the Table of Contents



We designed seven dithienobenzothiazole (DBT) derivatives by considering previous machine-learning study indicating that the number of hydrogen-bonding acceptor (N_{HBA}) is important index for the hole mobility of organic semiconductors. The solution-processed top-gate bottom-contact devices of DBTs exhibit hole mobilities of up to 0.16 cm² V⁻¹s⁻¹.

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5.5×5.0 cm (max. width × height) or 11.5×2.5 cm