Electronic Supplementary Information

Antiaromatic planar cyclooctatetraene: a strategy for ambipolar semiconductors in field effect transistors

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Contents

General

^{1}H and ^{13}C NMR spectra were recorded on JEOL JNM-270, LA-400, L-500, or Bruker AV500 instruments. Chemical shifts are reported in ppm with reference to tetramethylsilane, using the signal of internal tetramethylsilane or the solvents. Mass spectra were recorded on a SHIMADZU GC-MS QP2020 or an AXIMA-CFR instrument for EI or LDI-TOF method, respectively. Only the more intense or structurally diagnostic mass spectral fragment ion peaks are reported. Electronic absorption spectra were recorded on a SHIMADZU UV-Vis-NIR scanning spectrophotometer (Model UV-3101-PC). Cyclic voltammetry (CV) was performed on a BAS-ALS620B electrochemical analyzer using a standard three-electrode cell consisting of Pt wire and glassy-carbon working electrodes, a Pt wire counter electrode, and a $Ag/AgNO_3$ reference electrode under nitrogen atmosphere. The potentials were calibrated with ferrocene as an external standard. Preparative gel-permeation chromatography (GPC) was performed with a JAI LC-08 chromatograph equipped with JAIGEL 1H and 2H columns. Elemental analyses were performed at the microanalysis laboratory of Tokyo Metropolitan University.

Commercially available reagents were used as received. Solvents were distilled from relevant drying agents prior to use.

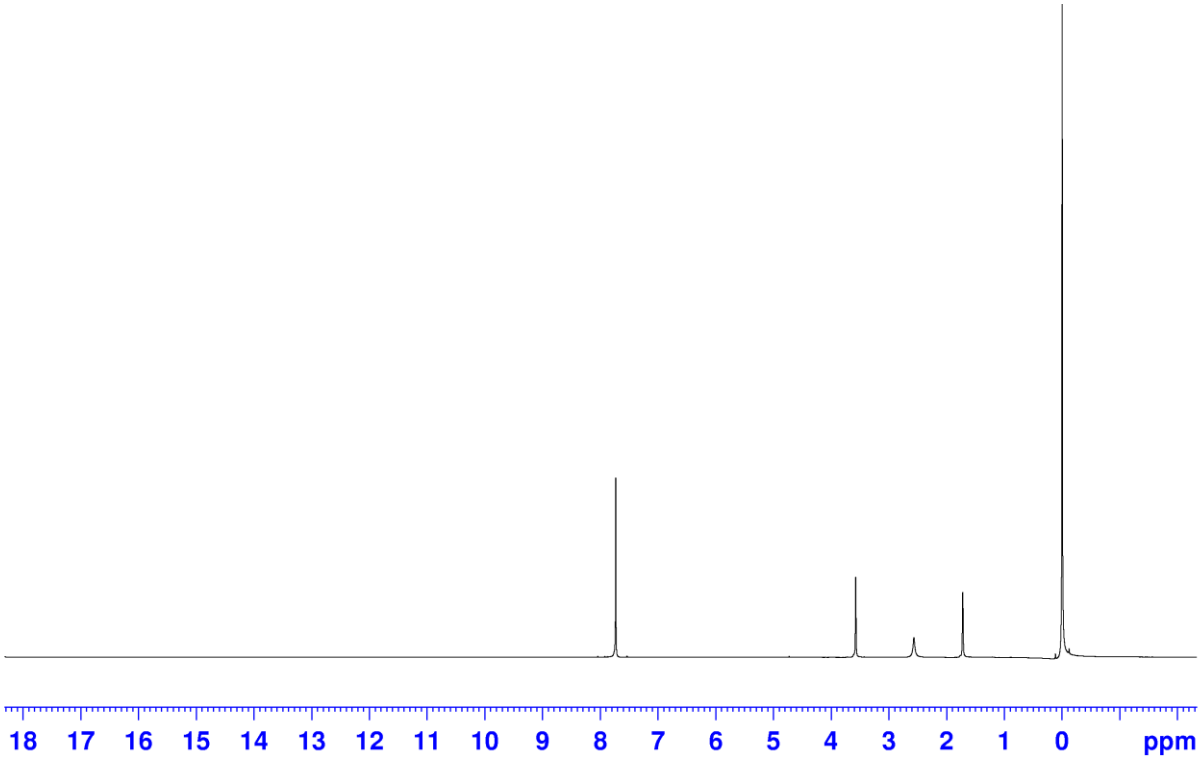
Computational methods

DFT calculations were performed with the Gaussian 03 program.[1] All geometry optimizations were carried out at the B3LYP/6–31G(d,p) basis set. For **1a**, the optimized structure with D_2 symmetry was found to be the minimum. Thus, the geometry optimizations of **1b** and **1c** were also conducted with D_2 symmetry.

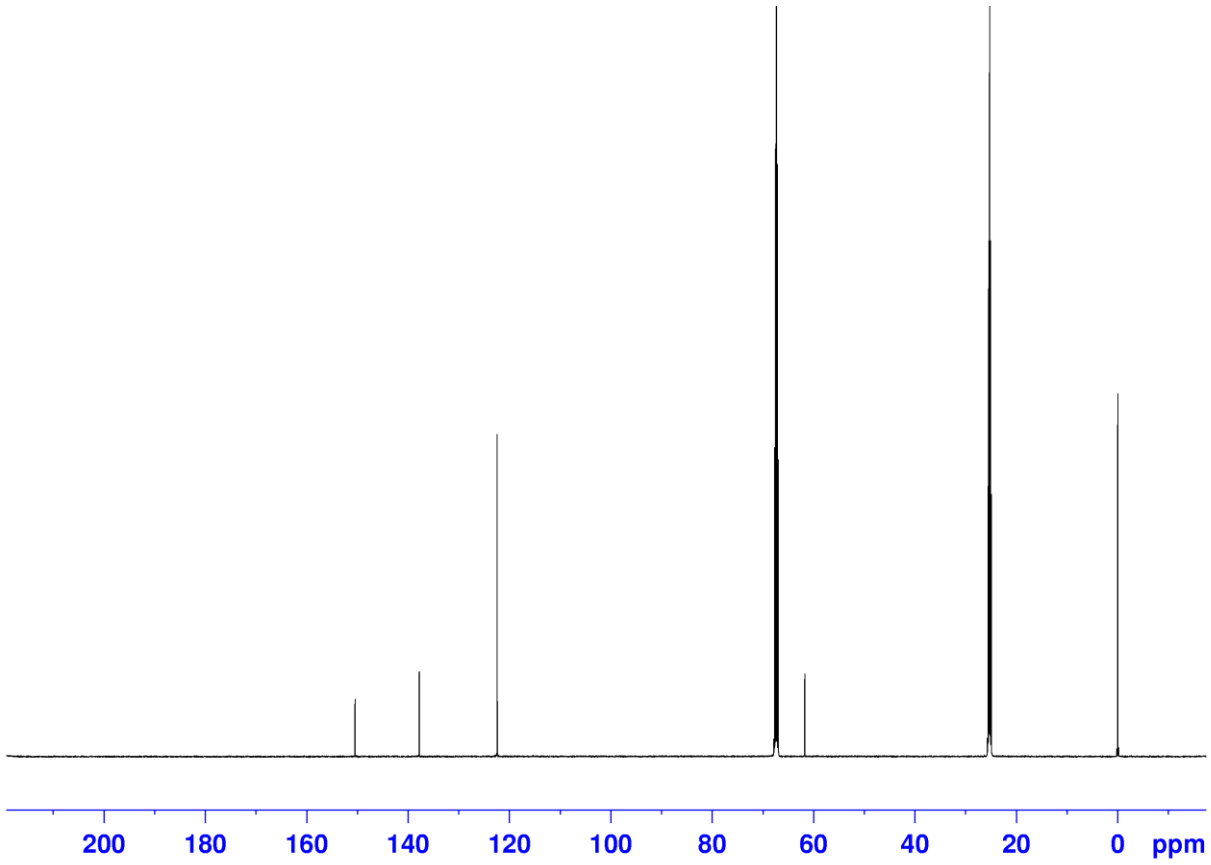
Synthesis

Synthesis of 3. To a solution of **2** (1.70 g, 5.00 mmol) in anhydrous THF (225 ml) was added iodine monochloride (1.0 M in CH_2Cl_2, 10.3 ml) at -78˚C, and the mixture was stirred at the same temperature for 2 h and at room temperature for 12 h. Then $Na_2S_2O_3$ aq. was added, and the organic layer was separated. The aqueous layer was extracted with CH_2Cl_2. The combined organic layer was dried over $MgSO_4$. After filtration and evaporation, the crude product was purified by recrystallization from chloroform to give **3** (1.81 g, 4.05 mmol, 81%) as pale yellow solid: m.p. > 300 ˚C; ^{1}H NMR (THF-d_8, 500 MHz) δ 7.74 (s, 2H) ; ^{13}C NMR (THF-d_8, 500 MHz): δ 150.5, 137.8, 122.5, 61.8; MS(EI) *m/z* = 448 [M^+]. Anal. Calcd. for $C_8H_2I_2S_3$: C, 21.44; H, 0.45. Found: C,21.39 ; H, 0.15.

^{1}H NMR spectrum of **3**

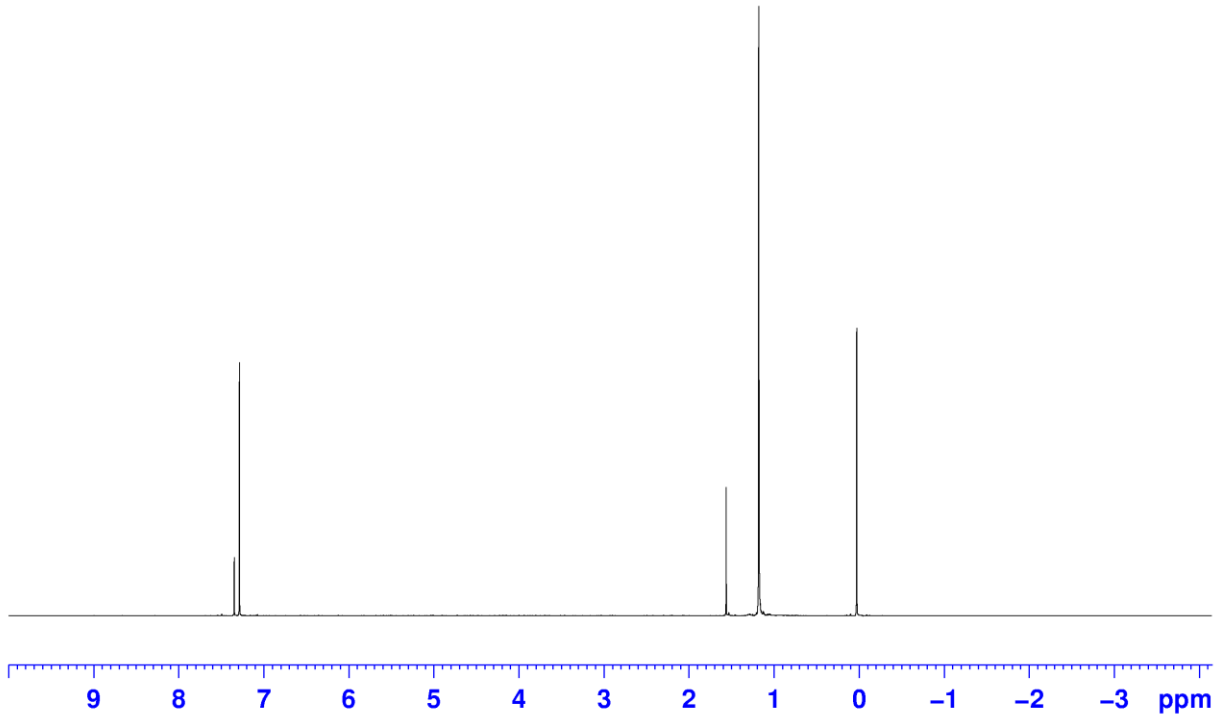


^{13}C NMR spectrum of **3**

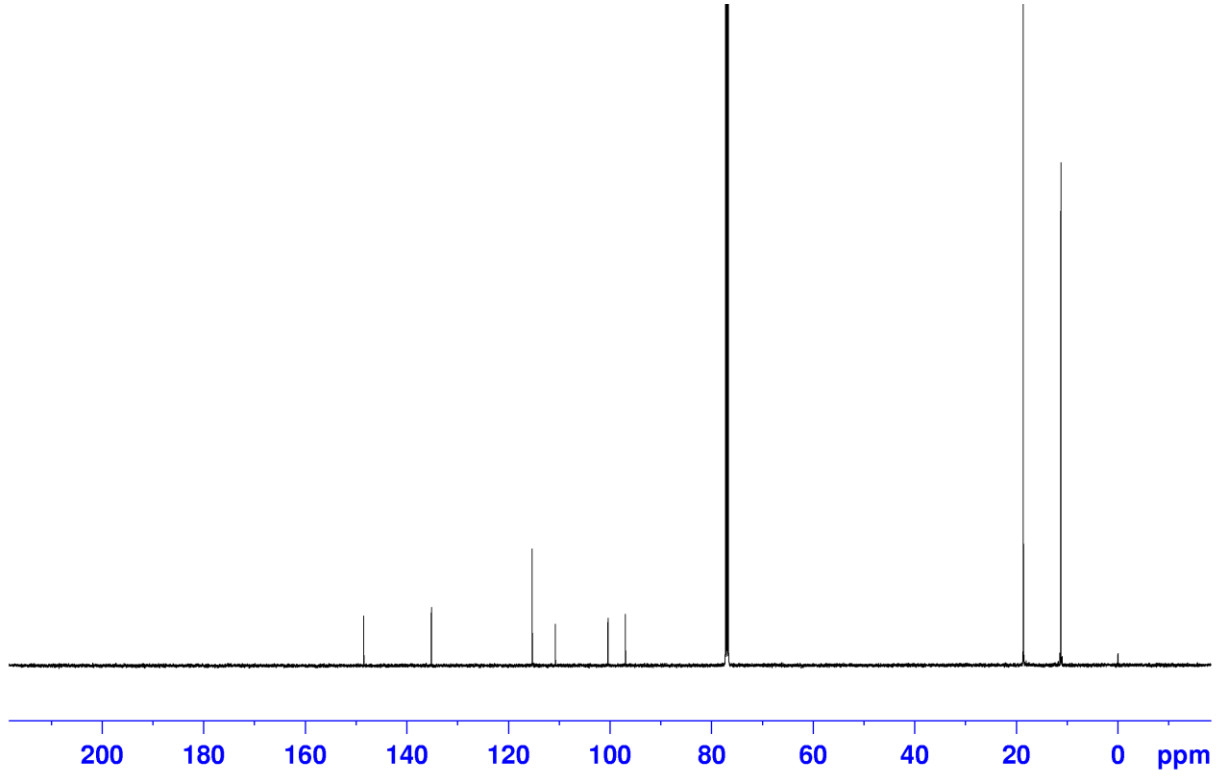


Synthesis of 4. To a stirred solution of **3** (1.0 mmol), $Pd(PPh_3)_4$ (0.1 mmol) and triisopropylsilylacetylene (3.0 mmol) were dissolved in toluene (10ml) and Et_3N (2ml). The solution was degassed under N_2 for 15min. CuI (0.15 mmol) was added and the mixture was stirred at 70 ˚C for 12 h. The solution was allowed to cool to room temperature, and the precipitate was filtered off over Celite. The filtrate was concentrated in vacuo, purified by silica gel column chromatography using hexane and AcOEt as a mixed eluent to give **4** as white solid (507 mg, 0.911 mmol, 91%); m.p. 125.1–126.3 ˚C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.32 (s, 2H), 1.15 (m, 21H); ^{13}C NMR ($CDCl_3$, 500 MHz) δ 148.5, 135.2, 115.4, 110.8, 100.4, 97.0, 18.7, 11.2; MS(EI) *m/z* = 557 [M^+]. Anal. Calcd. for $C_{30}H_{44}S_3Si_2$: C, 64.69; H, 7.96. Found: C, 64.78; H, 8.21.

^{1}H NMR spectrum of **4**

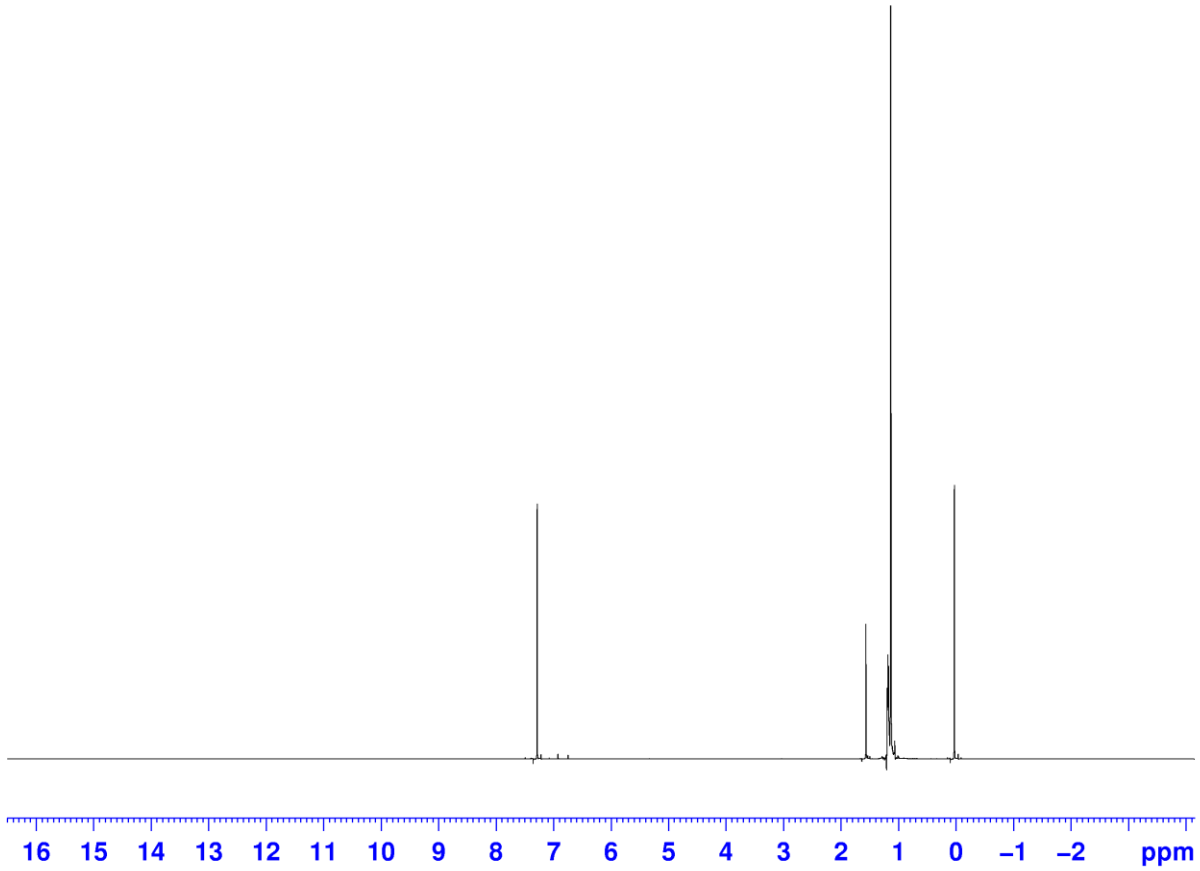


^{13}C NMR spectrum of **4**

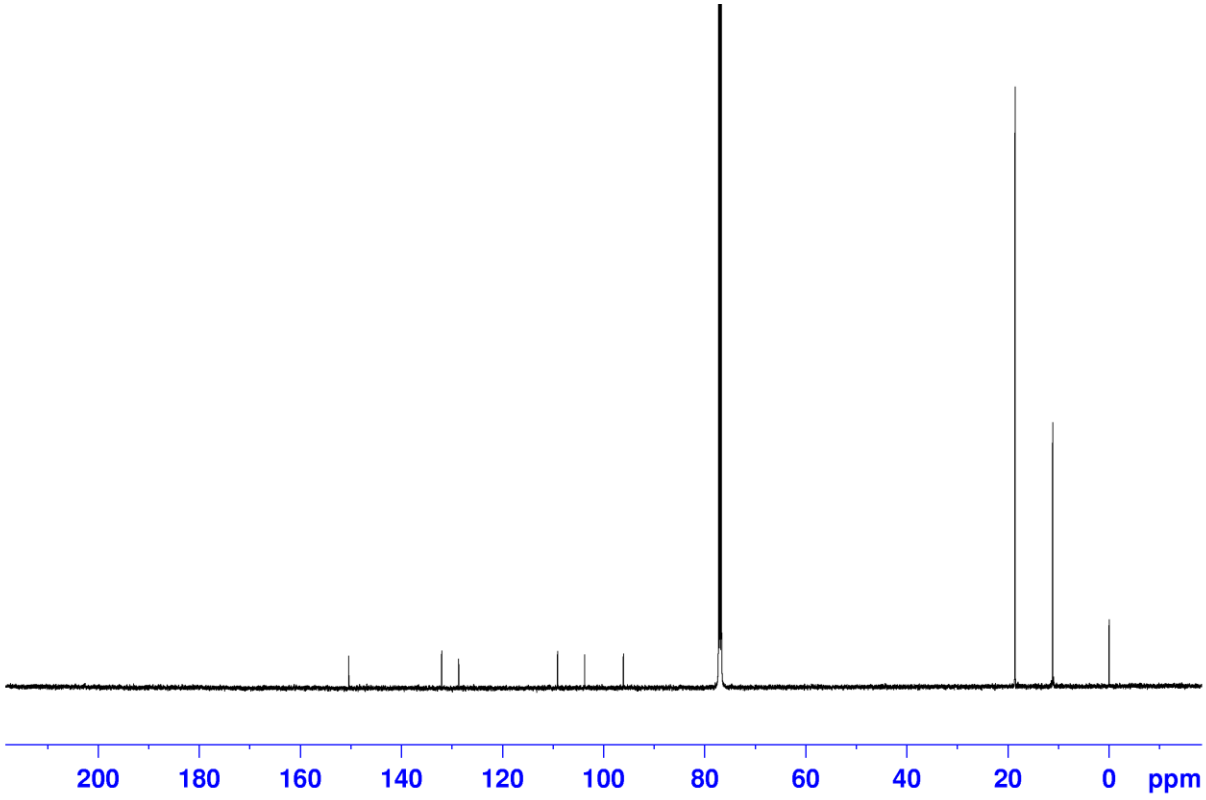


Synthesis of 1c. To a solution of **4** (217 mg, 0.389 mmol) in anhydrous THF (5 ml) was added *n*-BuLi (1.58 M in hexane) (0.54 ml, 0.856 mmol) at 0 ˚C, and the mixture was stirred at room temperature for 1 h. Then, dry $CuCl_2$ (157 mg, 1.17 mmol) was added in one portion at 0 ˚C. The reaction mixture was stirred at room temperature for 12 h. The reaction mixture was passed through an alumina short column using toluene as eluent to remove a solid residue. After evaporation, the residue was separated by preparative GPC eluted with toluene to give **1c** (134 mg, 0.120 mmol, 62%) as blue crystals: m.p. > 300 ˚C; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 1.19 – 1.13 (m); ^{13}C NMR ($CDCl_3$, 500 MHz): δ 150.5, 132.1, 128.7, 109.2, 103.8, 96.1, 18.6, 11.2; MS(LDI) *m/z* = 1110 [M^+]. Anal. Calcd. for $C_{60}H_{84}S_6Si_4$: C, 64.92; H, 7.63. Found: C, 64.72; H, 7.75.

^{1}H NMR spectrum of **1c**



^{13}C NMR spectrum of **1c**



X-ray crystallography of 1c. X-ray data were taken on a Bruker Smart APEX diffractometer equipped with a CCD area detector with graphite-monochromated $Mo_{k\alpha}$. radiation (λ = 0.71073 Å). The structure was solved by direct methods (SHELXTL) and refined by the full-matrix least-squares method on F^2 (SHELXL-97). Non-hydrogen atoms were refined anisotropically, and Hydrogen atoms were placed using AFIX instructions. **1c**: $C_{60}H_{84}S_6Si_4$, M = 1109.99; triclinic, space group P-1; a = 14.7404(14), b = 15.0150(15), c = 15.4645(15), α = 71.010(2), β = 87.452(2), γ = 74.597(2), V = 3116.9(5) Å^3; Dc (Z = 2) = 1.183 g cm^{-3}; T = 123 K, 13390 collected reflections, 8889 reflections with $I > 2\sigma(I)$, R_1 = 0.042, wR_2 = 0.115, GOF = 1.053.

FET Device Preparation

Fabrication of thin film FET devices. OFETs with a top-contact configuration were fabricated on highly n-doped silicon wafer with a thermally oxidized 200 nm thick SiO_2 as gate dielectric layer. The dielectric layer modified with octadecanylltrichlorosilane (OTS) self-assembled monolayer (SAM) was obtained by immersing the substrate in OTS solution. Thin films (50 nm thick) of **1a** were vacuum-deposited on the bare or OTS treated SiO_2/Si substrates at room temperature, followed by the shadow mask deposition of Au as the source and drain electrodes. All of the measurements were performed under ambient atmosphere at room temperature.

Field-effect mobility (μ) was calculated in the saturation regime (V_d = –40 V) of the I_d using the following equation:

$$\mu = 2L\, I_d / (W\, C_i\, (V_g - V_{th})^2)$$

where μ is the field-effect mobility, I_d is the source-drain current, V_g is the gate voltage, and V_{th} is the threshold voltage. The channel length (L) and width (W) are 0.05 and 5 mm, respectively. The capacitances of the gate dielectric layer (Ci) are 15 nF cm^{-2}.

Fabrication of single crystal FET devices. The top-contact type single crystal FET devices were prepared by the crystal-lamination technique. As substrates for the crystal-lamination, we used n^+-doped Si wafer with 210 nm thick thermally grown SiO_2, which was covered with a thin film (ca. 300 nm) of polystyrene (PS). Shiny, thin and defect-free single crystals were carefully selected and laminated on top of the substrates. Source and drain electrodes were painted at both ends of the long axis of the crystals with a water-based solution of colloidal graphite. The electrical properties of the FET devices were measured by using an Agilent 4155C semiconductor parameter analyzer under vacuum at room temperature.

Field-effect mobility (μ) was calculated in the saturation regime of the drain current (I_d) using the same equation shown above.

Ref.

1. Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

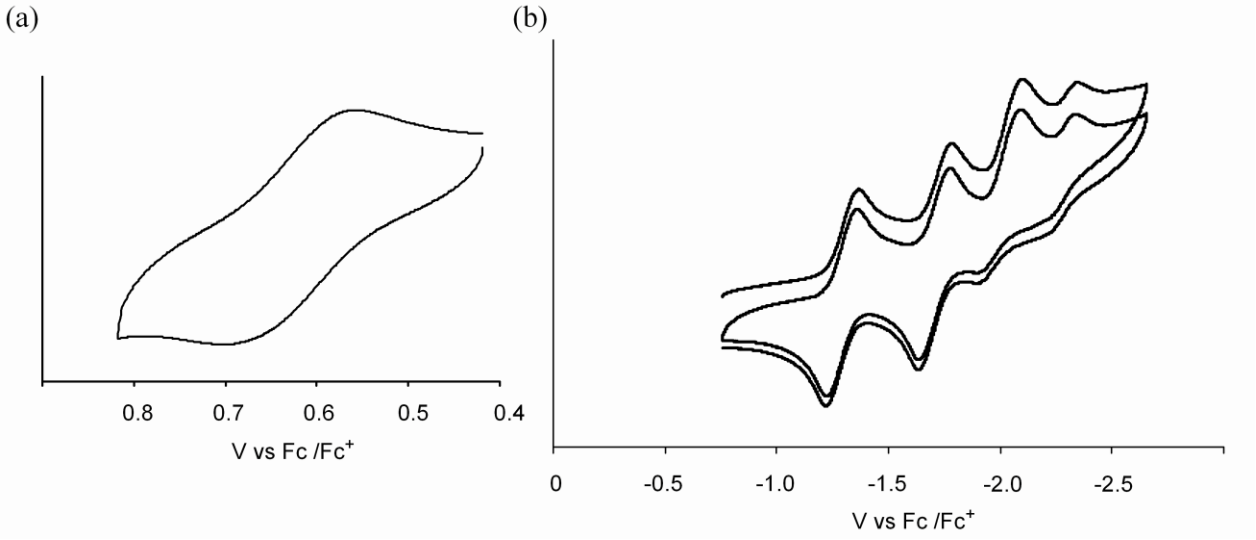


Figure S1. Cyclic Voltammograms of **1c**. (a) anodic region observed in CH_2Cl_2 and (b) cathodic region in THF.

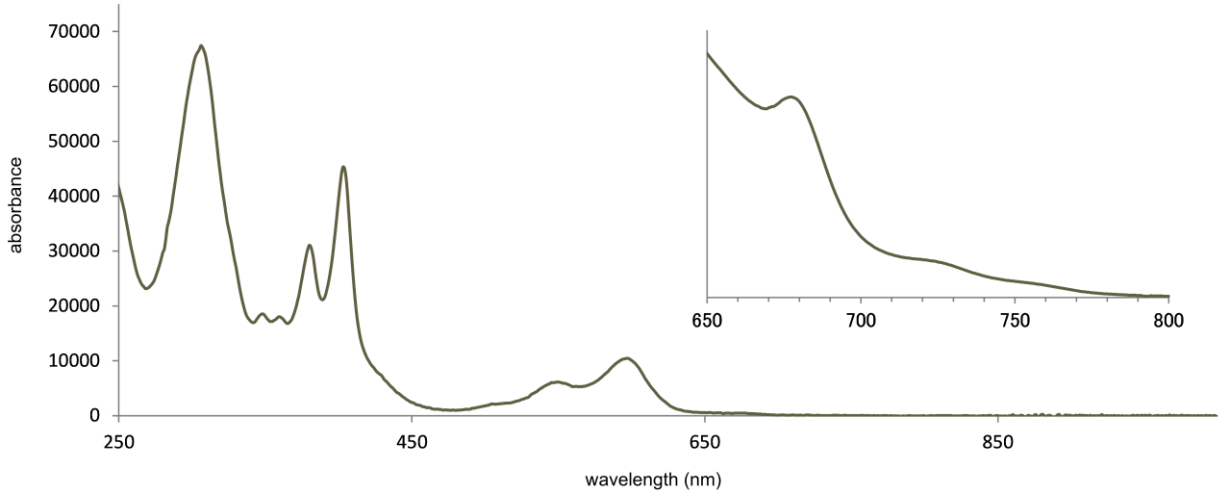
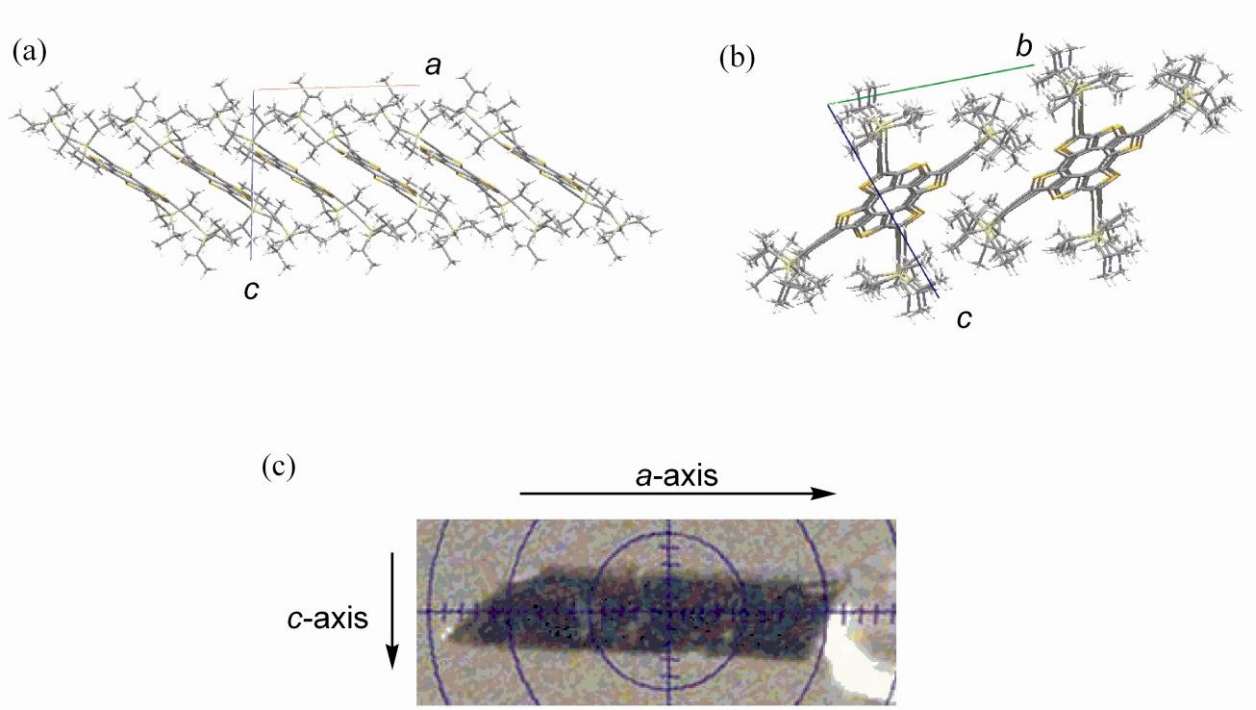


Figure S2. UV-vis-NIR spectra of **1c**.



(d)

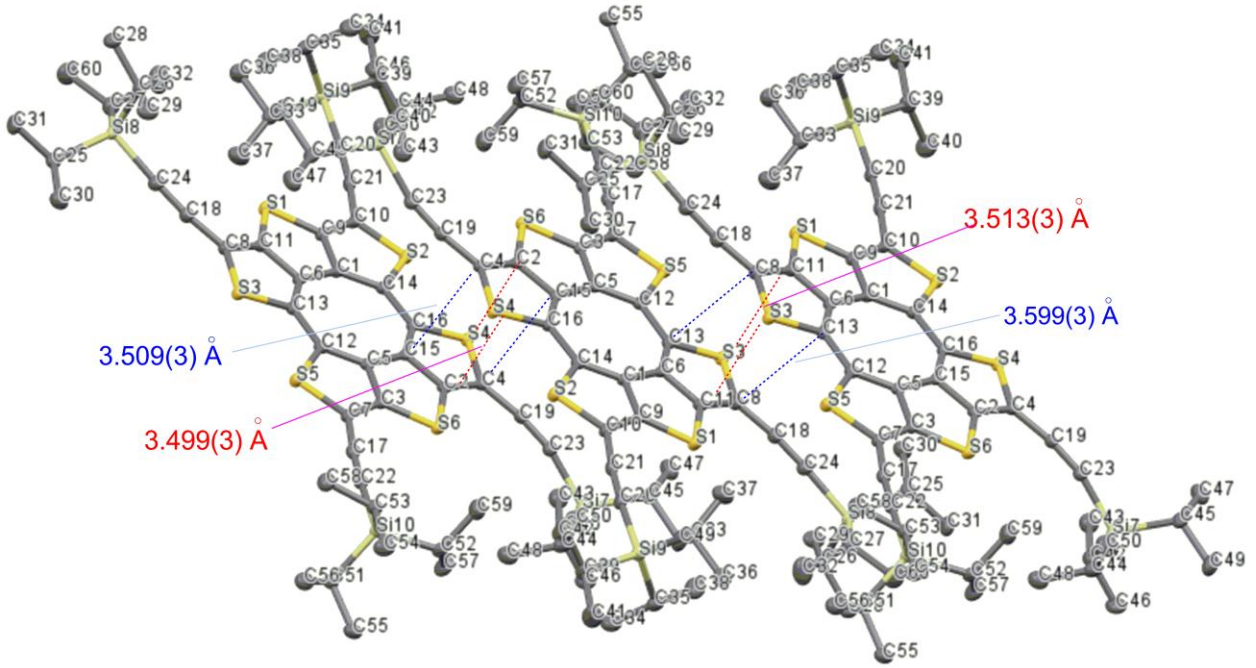


Figure S3. Packing structure in (a) a-c plane and (b) a-b plane and (c) top view of a single crystal of **1c**. (d) Intermolecular short contacts with atom labels (symmetry code: 2-X, -Y, 1-Z (left); 1-X, -Y, 1-Z (right)) are also shown.

(a) (b)

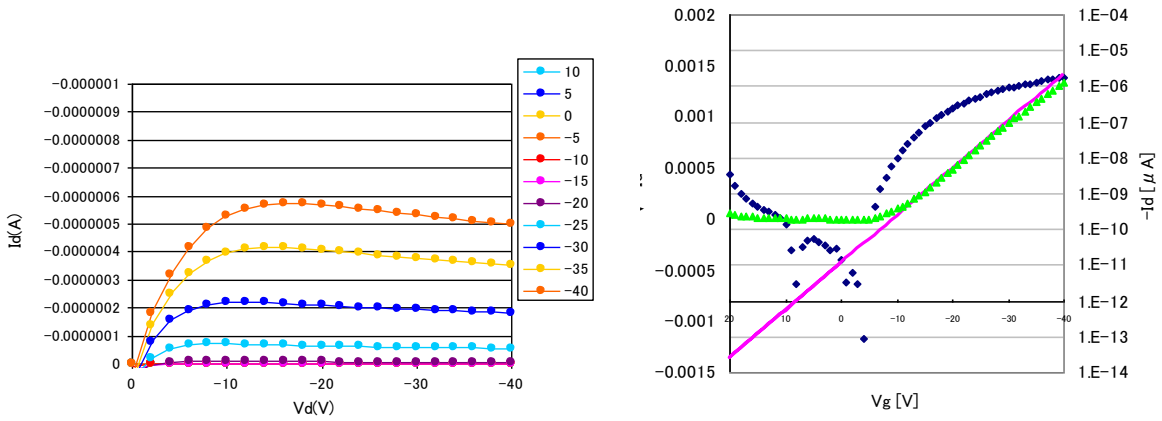


Figure S4. (a) Output characteristic and (b) transfer characteristic at -40 V for **1a**-based thin film transistor vaccum-deposited on OTS-treated Si/SiO_2 substrate.

(a) (b)

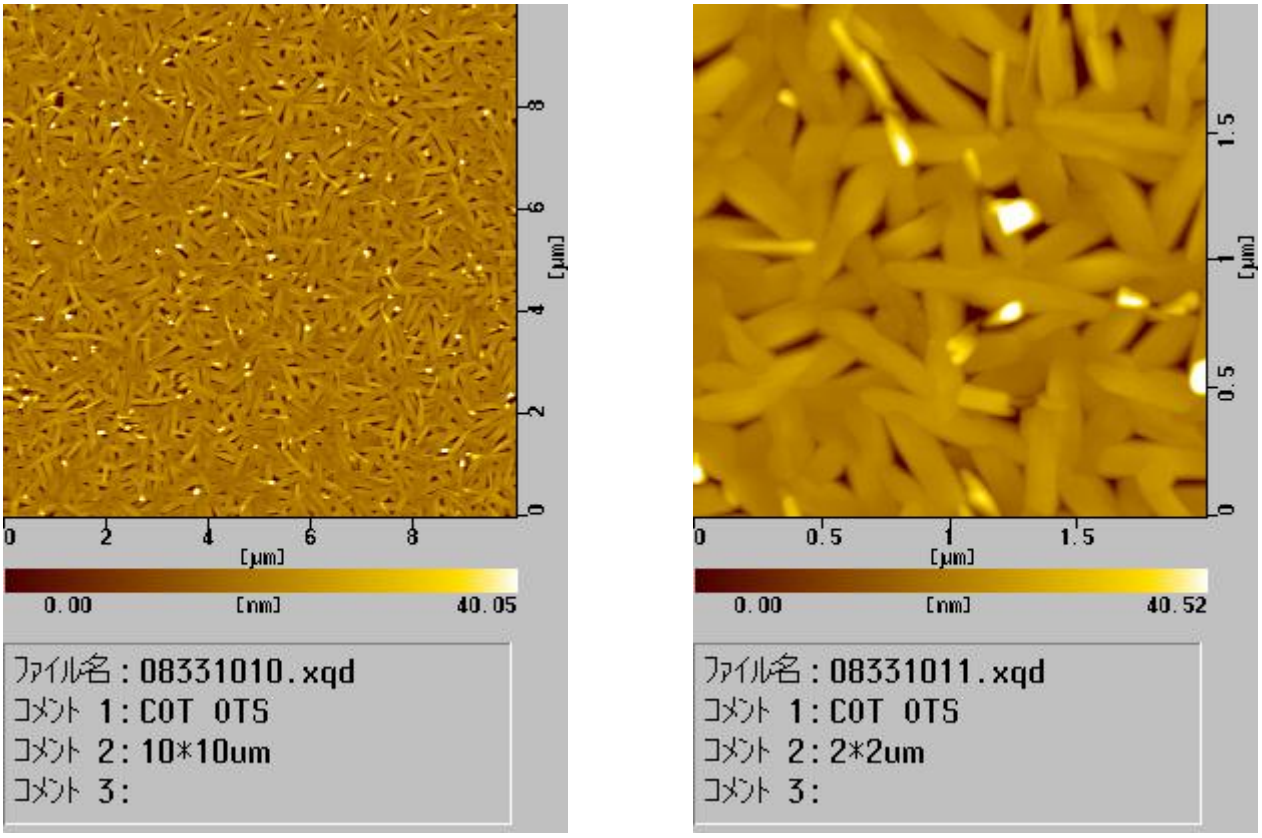


Figure S5 AFM images of vacuum-deposited films of **1a** on the OTS-treated Si/SiO_2 substrate ((a) 10 × 10 μm and (b) 2 × 2 μm).

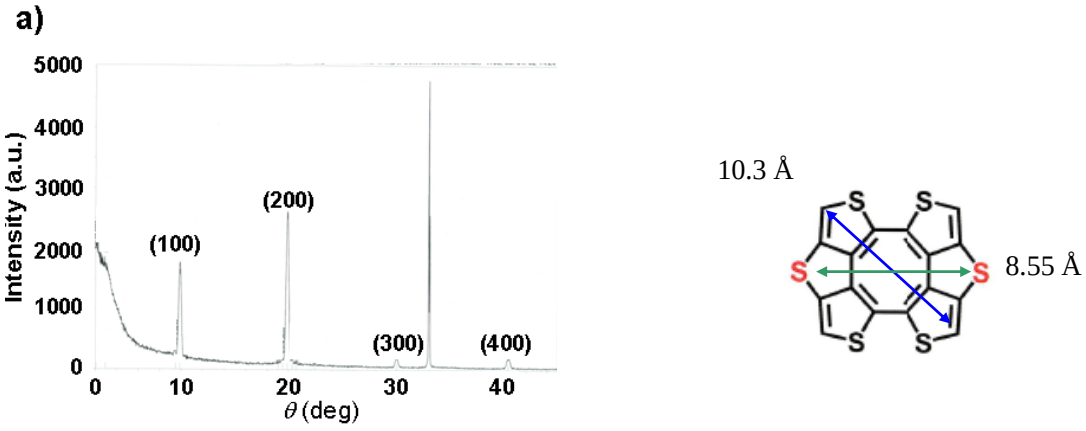


Figure S6. XRD patterns of vacuum-deposited films of **1a** on OTS-treated Si/SiO_2 substrate.

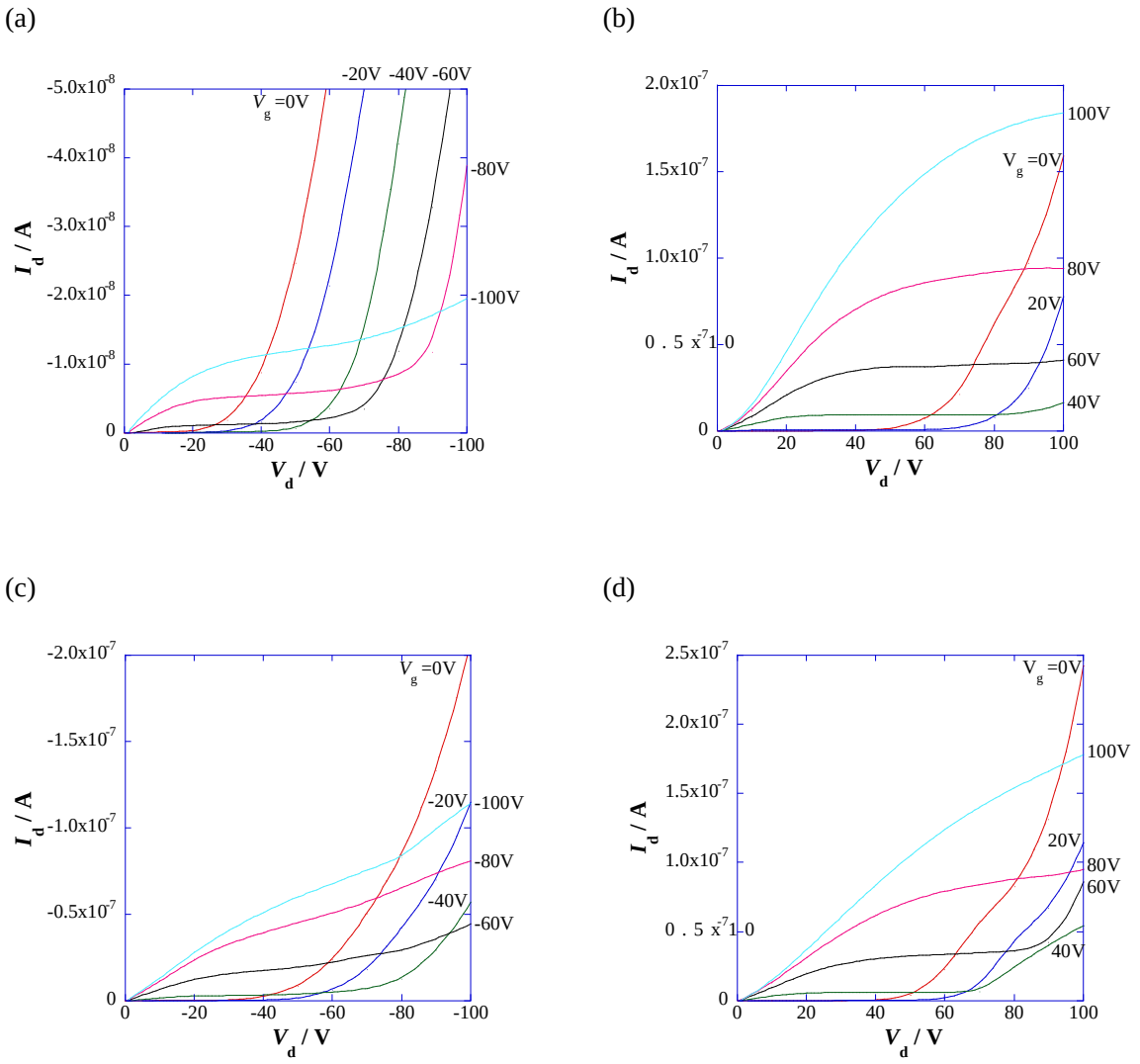


Figure S7 Output curves of another **1c**-based single crystal FET devise with carbon source and drain electrodes under (a) negative and (b) positive biased conditions (μ_h = 0.12 cm^2 V^{-1} s^{-1}, I_{on}/I_{off} = 5, V_{th} = –32 V, μ_e = 0.072 cm^2 V^{-1} s^{-1}, I_{on}/I_{off} = 10, V_{th} = 3 V) and (c) (d) same measurements after storage under ambient conditions for one month (μ_h = 0.34 cm^2 V^{-1} s^{-1}, I_{on}/I_{off} = 10, V_{th} = –18 V, μ_e = 0.059 cm^2 V^{-1} s^{-1}, I_{on}/I_{off} = 10, V_{th} = 5 V).

Table S1. Cartesian coordinate of optimized geometry of **1b** at the RB3LYP/6-31G(d,p) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	0.000000	-4.262742
2	6	0	-0.036492	0.730075	-1.665496
3	6	0	-0.048420	1.751785	-0.725185
4	16	0	-0.184623	3.299137	-1.546787
5	6	0	-0.174304	2.615284	-3.150101
6	6	0	-0.088384	1.250629	-3.007914
7	6	0	0.036492	-0.730075	-1.665496
8	6	0	0.048420	-1.751785	-0.725185
9	16	0	0.184623	-3.299137	-1.546787
10	6	0	0.174304	-2.615284	-3.150101
11	6	0	0.088384	-1.250629	-3.007914
12	16	0	0.000000	0.000000	4.262742
13	6	0	-0.036492	-0.730075	1.665496
14	6	0	-0.048420	-1.751785	0.725185
15	16	0	-0.184623	-3.299137	1.546787
16	6	0	-0.174304	-2.615284	3.150101
17	6	0	-0.088384	-1.250629	3.007914
18	6	0	0.036492	0.730075	1.665496
19	6	0	0.048420	1.751785	0.725185
20	16	0	0.184623	3.299137	1.546787
21	6	0	0.174304	2.615284	3.150101
22	6	0	0.088384	1.250629	3.007914
23	14	0	0.287376	-3.687832	-4.701317
24	14	0	-0.287376	3.687832	-4.701317
25	14	0	-0.287376	-3.687832	4.701317
26	14	0	0.287376	3.687832	4.701317
27	6	0	-1.251151	-3.398587	-5.760494
28	1	0	-1.364700	-2.343453	-6.029454
29	1	0	-1.194976	-3.975932	-6.690370
30	1	0	-2.158241	-3.704101	-5.229084
31	6	0	0.382532	-5.498414	-4.171291

32	1	0	1.263952	-5.696981	-3.552712
33	1	0	-0.502450	-5.804438	-3.603816
34	1	0	0.447456	-6.145046	-5.053456
35	6	0	1.842034	-3.207281	-5.662764
36	1	0	1.916989	-3.781405	-6.593332
37	1	0	1.842283	-2.144491	-5.925559
38	1	0	2.743888	-3.402511	-5.073574
39	6	0	-1.842034	3.207281	-5.662764
40	1	0	-1.916989	3.781405	-6.593332
41	1	0	-1.842283	2.144491	-5.925559
42	1	0	-2.743888	3.402511	-5.073574
43	6	0	1.251151	3.398587	-5.760494
44	1	0	1.364700	2.343453	-6.029454
45	1	0	1.194976	3.975932	-6.690370
46	1	0	2.158241	3.704101	-5.229084
47	6	0	-0.382532	5.498414	-4.171291
48	1	0	-1.263952	5.696981	-3.552712
49	1	0	0.502450	5.804438	-3.603816
50	1	0	-0.447456	6.145046	-5.053456
51	6	0	0.382532	5.498414	4.171291
52	1	0	1.263952	5.696981	3.552712
53	1	0	-0.502450	5.804438	3.603816
54	1	0	0.447456	6.145046	5.053456
55	6	0	1.842034	3.207281	5.662764
56	1	0	1.916989	3.781405	6.593332
57	1	0	1.842283	2.144491	5.925559
58	1	0	2.743888	3.402511	5.073574
59	6	0	-1.251151	3.398587	5.760494
60	1	0	-1.364700	2.343453	6.029454
61	1	0	-1.194976	3.975932	6.690370
62	1	0	-2.158241	3.704101	5.229084
63	6	0	1.251151	-3.398587	5.760494
64	1	0	1.364700	-2.343453	6.029454
65	1	0	1.194976	-3.975932	6.690370
66	1	0	2.158241	-3.704101	5.229084
67	6	0	-0.382532	-5.498414	4.171291

68	1	0	-1.263952	-5.696981	3.552712
69	1	0	0.502450	-5.804438	3.603816
70	1	0	-0.447456	-6.145046	5.053456
71	6	0	-1.842034	-3.207281	5.662764
72	1	0	-1.916989	-3.781405	6.593332
73	1	0	-1.842283	-2.144491	5.925559
74	1	0	-2.743888	-3.402511	5.073574

HF= -4636.0009968 hartree

Table S2. Cartesian coordinate of optimized geometry of **1c** at the RB3LYP/6-31G(d,p) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	0.000000	-4.261668
2	6	0	-0.043893	0.730289	-1.659484
3	6	0	-0.057976	1.758903	-0.722007
4	16	0	-0.217011	3.312818	-1.534262
5	6	0	-0.199342	2.597639	-3.134074
6	6	0	-0.291930	3.371732	-4.299495
7	6	0	-0.379049	4.041066	-5.321158
8	6	0	-0.101413	1.228967	-3.002915
9	6	0	0.043893	-0.730289	-1.659484
10	6	0	0.057976	-1.758903	-0.722007
11	16	0	0.217011	-3.312818	-1.534262
12	6	0	0.199342	-2.597639	-3.134074
13	6	0	0.291930	-3.371732	-4.299495
14	6	0	0.379049	-4.041066	-5.321158
15	6	0	0.101413	-1.228967	-3.002915
16	16	0	0.000000	0.000000	4.261668
17	6	0	-0.043893	-0.730289	1.659484
18	6	0	-0.057976	-1.758903	0.722007
19	16	0	-0.217011	-3.312818	1.534262
20	6	0	-0.199342	-2.597639	3.134074
21	6	0	-0.291930	-3.371732	4.299495

22	6	0	-0.379049	-4.041066	5.321158
23	6	0	-0.101413	-1.228967	3.002915
24	6	0	0.043893	0.730289	1.659484
25	6	0	0.057976	1.758903	0.722007
26	16	0	0.217011	3.312818	1.534262
27	6	0	0.199342	2.597639	3.134074
28	6	0	0.291930	3.371732	4.299495
29	6	0	0.379049	4.041066	5.321158
30	6	0	0.101413	1.228967	3.002915
31	14	0	-0.549213	5.054049	-6.859862
32	14	0	0.549213	5.054049	6.859862
33	14	0	-0.549213	-5.054049	6.859862
34	14	0	0.549213	-5.054049	-6.859862
35	6	0	0.885350	4.536105	-8.021845
36	1	0	1.781503	4.817478	-7.448645
37	6	0	-2.332416	4.761767	-7.503576
38	1	0	-2.951250	5.002901	-6.626080
39	6	0	-0.343596	6.889765	-6.351743
40	1	0	-0.463228	7.470605	-7.279235
41	6	0	0.343596	6.889765	6.351743
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43	6	0	2.332416	4.761767	7.503576
44	1	0	2.951250	5.002901	6.626080
45	6	0	-0.885350	4.536105	8.021845
46	1	0	-1.781503	4.817478	7.448645
47	6	0	0.885350	-4.536105	8.021845
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49	6	0	-2.332416	-4.761767	7.503576
50	1	0	-2.951250	-5.002901	6.626080
51	6	0	-0.343596	-6.889765	6.351743
52	1	0	-0.463228	-7.470605	7.279235
53	6	0	0.343596	-6.889765	-6.351743
54	1	0	0.463228	-7.470605	-7.279235
55	6	0	-0.885350	-4.536105	-8.021845
56	1	0	-1.781503	-4.817478	-7.448645
57	6	0	2.332416	-4.761767	-7.503576

58	1	0	2.951250	-5.002901	-6.626080
59	6	0	-1.437900	-7.348500	5.368847
60	1	0	-1.393600	-6.779804	4.433152
61	1	0	-1.312363	-8.408188	5.113669
62	1	0	-2.444955	-7.228366	5.781069
63	6	0	1.055544	-7.195459	5.784684
64	1	0	1.141183	-8.254811	5.512081
65	1	0	1.254960	-6.608392	4.880994
66	1	0	1.852451	-6.978093	6.503023
67	6	0	0.919005	-5.327852	9.343720
68	1	0	1.833620	-5.103488	9.906805
69	1	0	0.073602	-5.067120	9.989829
70	1	0	0.891608	-6.411279	9.184913
71	6	0	0.981519	-3.021526	8.283063
72	1	0	0.988506	-2.446630	7.352071
73	1	0	0.144678	-2.660968	8.890147
74	1	0	1.902959	-2.782157	8.828651
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76	1	0	-3.708567	-3.163733	8.067661
77	1	0	-2.109977	-3.001226	8.792140
78	1	0	-2.349148	-2.602494	7.085395
79	6	0	-2.753163	-5.718259	8.636636
80	1	0	-2.186614	-5.531920	9.555359
81	1	0	-3.814243	-5.582815	8.881005
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83	6	0	-1.437900	7.348500	-5.368847
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87	6	0	1.055544	7.195459	-5.784684
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92	1	0	1.833620	5.103488	-9.906805
93	1	0	0.073602	5.067120	-9.989829

94	1	0	0.891608	6.411279	-9.184913
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