Supporting Information

Dendritic Oligothiophene Bearing Perylene Bis(dicarboximide) Groups as an Active Material for Photovoltaic Device

Yutaka Ie, Toshihiko Uto, Nobuhiro Yamamoto, and Yoshio Aso*

The Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka 567-0047, Japan.

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General Information. Column chromatography was performed on silica gel, KANTO Chemical silica gel 60N (63–210 μm), or on aluminium oxide, MERCK aluminium oxide 90 standardized. TLC plates were visualized with UV light. Preparative gel-permeation chromatography (GPC) was performed on Japan Analytical Industry LC-908 equipped with JAI-GEL 3H/4H columns.

Melting points are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on a JEOL JMN-400 spectrometer in $CDCl_3$ with tetramethylsilane as an internal standard. Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m =

multiplet), coupling constant (Hz), and integration. Mass spectra were obtained on Shimadzu AXIMA-TOF. UV-visible spectra were recorded on Shimadzu UV-3100PC. Fluorescence spectra were recorded using a Fluoromax-2 spectrometer in the photo-counting mode equipped with a Hamamatsu R928 photomultiplier. The bandpass for the emission spectra was 1.0 nm. All spectra were obtained in spectrograde solvents. Cyclic voltammetry was carried out on a BAS ALC 620C voltammetric analyzer at a scan rate of 100 mV/s in *o*-dichlorobenzene/CH_3CN (9/1) containing 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as supporting electrolyte, using a platinum button as the working electrode, a platinum wire as the counter electrode, and a $Ag/AgNO_3$ as the reference electrode, respectively. Atomic force microscopy (AFM) measurements were carried out using Shimadzu SPM-9600.

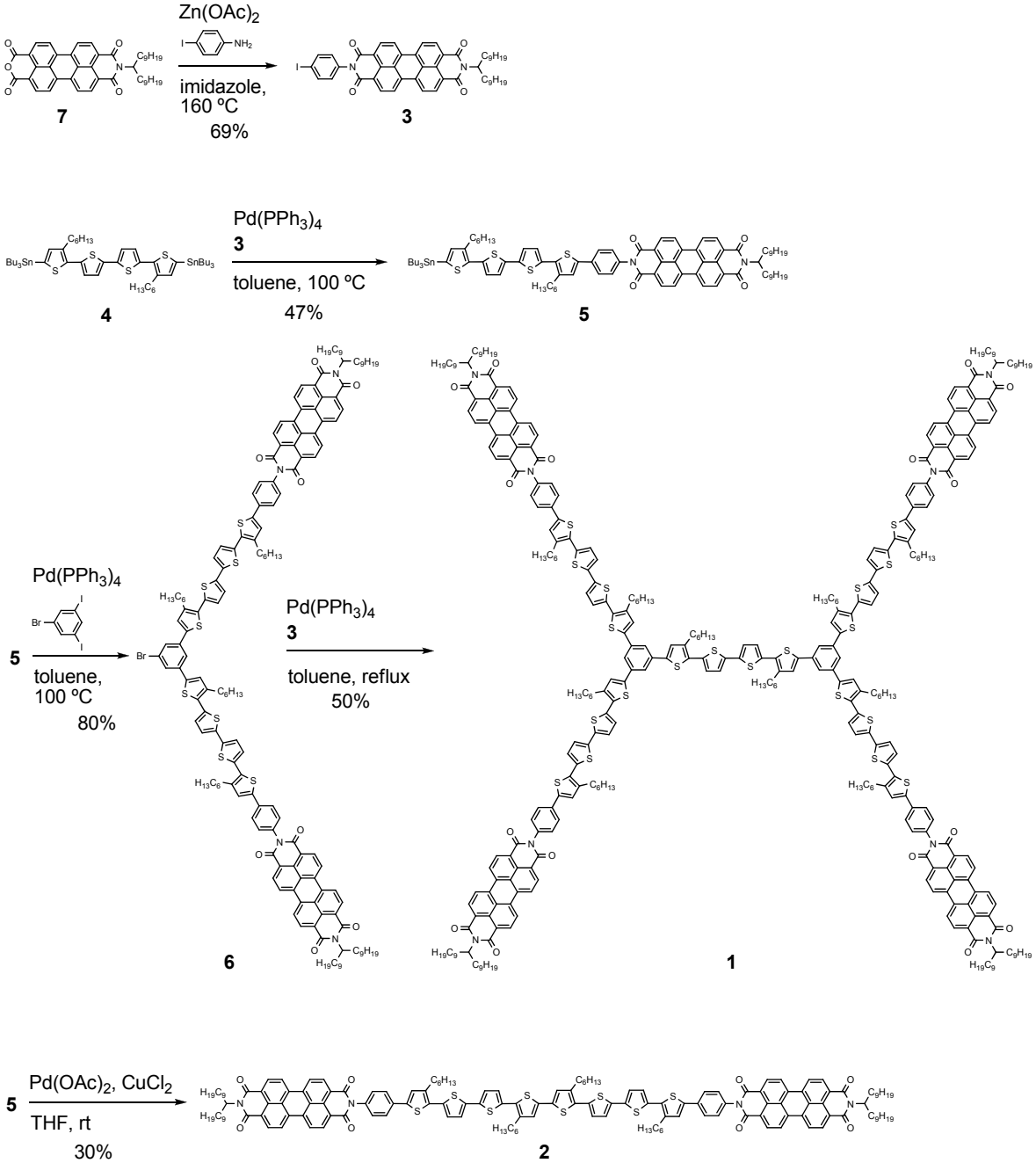
Elemental analyses were performed on Perkin Elmer LS-50B by the Elemental Analysis Section of Materials Analysis Center, ISIR, Osaka University.

Materials. All reactions were carried out under a nitrogen atmosphere. Solvents of the highest purity grade were used as received. Unless stated otherwise, all reagents were purchased from commercial sources and used without purification.

N-(10-Nonadecyl)-3,4,9,10-perylenetetracarboxylic acid 3,4-anhydride-9,10-imide (**7**)[1] and 5,5'''-bis(tri-*n*-butylstannyl)-3,3'''-dihexyl-2,2':5',2'':5'',2''':5''''-quaterthiophene (**4**)[2] were prepared by reported procedures, and ^1H NMR data of these compounds were in agreement with those previously reported.

Experimental Procedures

Scheme S1. Synthesis of **1** and **2**



Compound **3.**

Compound **7** (2.20 g, 3.35 mmol), 4-iodoaniline (2.93 mg, 13.3 mmol), $Zn(OAc)_2$ (460 mg, 2.51 mmol), and imidazole (25 g, 368 mmol) were placed in a flask and degassed with nitrogen. The mixture was stirred at 160 °C for 2 h. After cooling to room temperature, the reaction mixture was purified by column chromatography on silica gel (hexane:EtOAc=1:2 ~$CHCl_3$) to give **3** (2.02 g,

69%).

Red solid; Mp >300 °C; TLC R_f = 0.5 ($CHCl_3$); ^{1}H NMR ($CDCl_3$) δ 0.80–0.84 (m, 6H), 1.20–1.32 (m, 28H), 1.84–1.89 (m, 2H), 2.20–2.26 (m, 2H), 2.80–2.83 (m, 4H), 5.10–5.14 (m, 1H), 7.04–7.19 (m, 2H), 7.81–7.83 (m, 2H), 8.44–8.58 (m, 8H); ^{13}C NMR ($CDCl_3$) δ 14.1, 22.6, 27.0, 29.3, 29.5, 31.9, 32.4, 54.9, 76.7, 94.6, 122.9, 123.0, 123.3, 126.2, 126.5, 129.4, 129.7, 130.6, 131.8, 134.0, 134.8, 135.1, 138.6, 163.2; MS (MALDI-TOF, 1,8,9–trihydroxy-anthracene matrix) *m/z* 860.6 (M^+, calcd 858.3); Anal. Calcd for $C_{49}H_{51I}N_2O_4$: C, 68.53; H, 5.99; N, 3.26; Found: C, 68.63; H, 5.99; N, 3.11.

Compound **5**.

Compound **3** (800 mg, 0.93 mmol), **4** (2.0 g, 1.86 mmol), and tetrakis(triphenylphosphine)palladium(0) (54 mg, 0.046 mmol) were placed in a test tube, dissolved with toluene (18 mL), and degassed with nitrogen. The mixture was refluxed for 2 h. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on alumina (hexane/$CHCl_3$=5:1~1:1) to give **5** (590 mg, 42%).

Red solid; Mp 213–216 °C; TLC R_f = 0.5 (hexane–$CHCl_3$); ^{1}H NMR ($CDCl_3$) δ 0.81–0.93 (m, 21H), 1.10–1.14 (m, 6H), 1.20–1.42 (m, 46H), 1.50–1.61 (m, 6H), 1.60–1.74 (m, 4H), 1.85–1.88 (m, 2H), 2.23–2.27 (m, 2H), 2.80–2.83 (m, 4H), 5.15–5.22 (m, 1H), 6.97 (d, J = 3.9 Hz, 1H), 7.08 (d, J = 3.8 Hz, 1H), 7.14 (d, J = 3.9 Hz, 1H), 7.15 (d, J = 3.6 Hz, 1H), 7.22 (s, 1H), 7.38 (d, J = 8.5 Hz, 2H), 7.78 (d, J = 8.5 Hz, 2H), 8.63–8.75 (m, 8H); MS (MALDI-TOF, 1,8,9–trihydroxyanthracene matrix) *m/z* 1519.1 (M^+, calcd 1518.6); Anal. Calcd for $C_{160}H_{169}BrN_4O_8S_8$: C, 70.38; H, 7.30; N, 1.84; Found: C, 70.10; H, 7.33; N, 1.69.

Compound **6**.

Compound **5** (760 mg, 0.50 mmol), 3,5-diiodobromobenzene (89 mg, 0.22 mmol), and tetrakis(triphenylphosphine)palladium(0) (19 mg, 0.0165 mmol) were placed in a test tube, dissolved with toluene (7 mL), and degassed with nitrogen. The mixture was stirred at 100 ºC for 2 h. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel ($CHCl_3$) to give **6** (450 mg, 78%)

Dark-red solid; Mp 196–200 °C; TLC R_f = 0.4 ($CHCl_3$); ^{1}H NMR ($CDCl_3$) δ 0.81–0.85 (m, 12H), 0.91–0.94 (m, 12H), 1.20–1.44 (m, 80H), 1.68–1.74 (m, 8H), 1.85–1.93 (m, 4H), 2.23–2.26 (m, 4H), 2.78–2.83 (m, 8H), 5.15–5.22 (m, 2H), 7.09 (d, J = 3.9 Hz, 4H), 7.16 (d, J = 3.9 Hz, 2H), 7.17 (d, J

= 3.9 Hz, 2H), 7.17 (s, 2H), 7.21 (s, 2H), 7.36 (d, *J* = 8.6 Hz, 4H), 7.54-7.58 (m, 3H), 7.76 (d, *J* = 8.5 Hz, 4H), 8.58–8.72 (m, 16H); MS (MALDI-TOF, 1,8,9–trihydroxyanthracene matrix) *m/z* 2612.5 (M^+, calcd 2612.0) Anal. Calcd for $C_{160}H_{169}BrN_4O_8S_8$: C, 73.56; H, 6.52; N, 2.14; Found: C, 73.30; H, 6.52; N, 2.01.

Compound **1.**

Compound **6** (270 mg, 0.10 mmol), **3** (45 mg, 0.04 mmol), and tetrakis(triphenylphosphine)palladium(0) (4 mg, 0.004 mmol) were placed in a test tube, dissolved with toluene (3 mL), and degassed with nitrogen. The mixture was refluxed for 15 h. After removal of the solvent under reduced pressure, the residue was first separated by column chromatography on silica gel ($CHCl_3$), and then the fraction containing **2** was further purified by GPC ($CHCl_3$) to give pure **1** (110 mg, 45%).

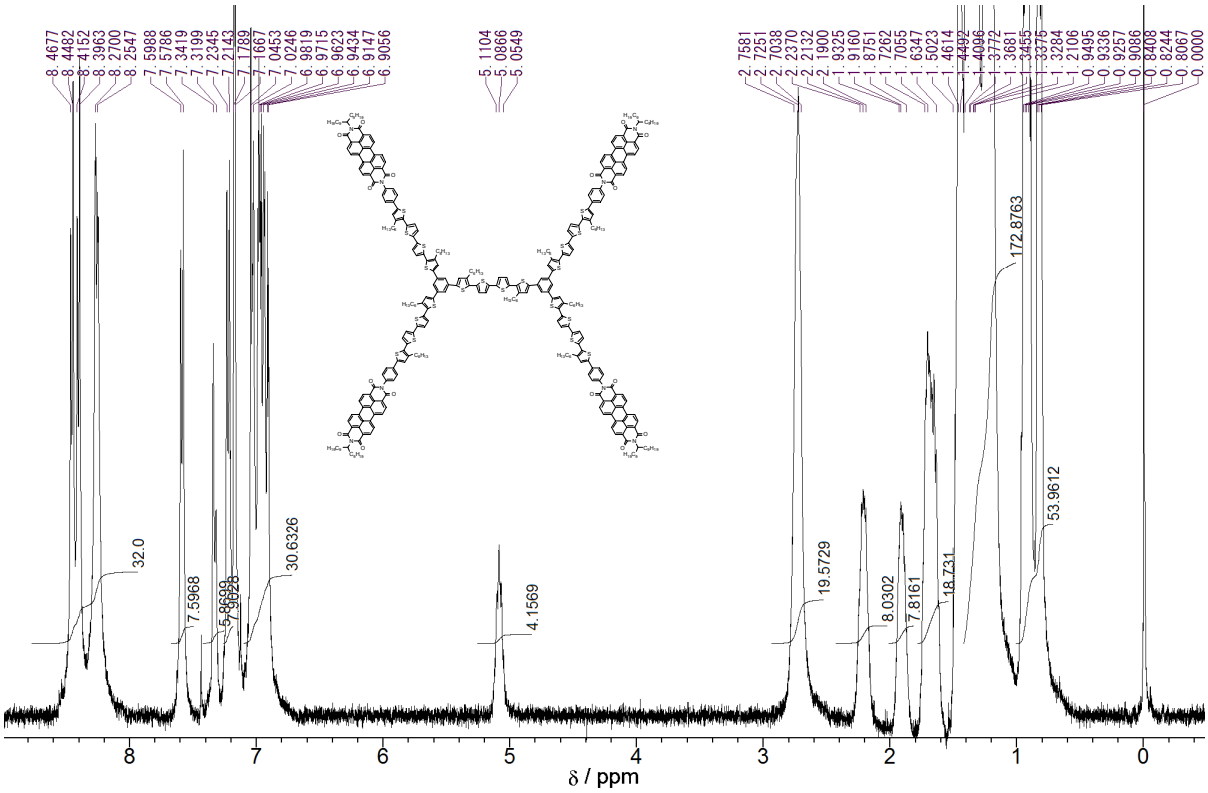
Dark-red solid; Mp 223–226 °C; TLC R_f = 0.1 ($CHCl_3$); ^{1}H NMR ($CDCl_3$) δ 0.81–0.95 (m, 54H), 1.21–1.41 (m, 172H), 1.63–1.73 (m, 20H), 1.88–1.93 (m, 8H), 2.19–2.14 (m, 8H), 2.70–2.76 (m, 20H), 5.05–5.11 (m, 4H), 6.91–7.04 (m, 30H), 7.21–7.23 (m, 8H), 7.32–7.34 (m, 6H), 7.58–7.60 (m, 8H), 8.26–8.47 (m, 32H); MS (MALDI-TOF, 1,8,9–trihydroxyanthracene matrix) *m/z* 5560.8 (M^+, calcd 5559.3); Anal. Calcd for $C_{348}H_{370}N_8O_{16}S_{20}$: C, 75.15; H, 6.71; N, 2.01. Found: C, 74.87; H, 6.66; N, 2.02.

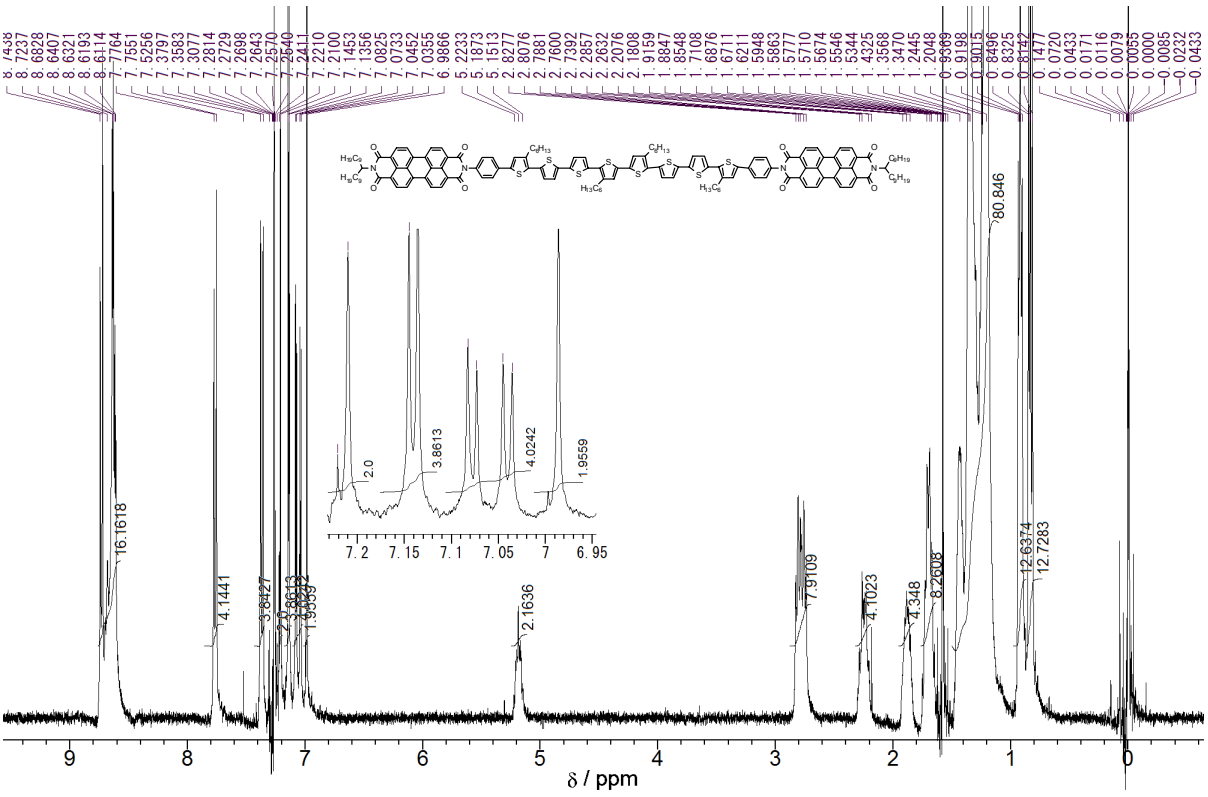
Compound **2**.

Compound **5** (200 mg, 0.13 mmol), $Pd(OAc)_2$ (3.00 mg, 0.013 mmol), and $CuCl_2$ (36 mg, 0.26 mmol) were placed in a test tube, dissolved with toluene (3 mL), and degassed with nitrogen. The mixture was stirred at room temperature for 15 min. After removal of the solvent under reduced pressure, the residue was first separated by column chromatography on silica gel ($CHCl_3$), and then the fraction containing **2** was further purified by GPC ($CHCl_3$) to give pure **2** (50 mg, 30%).

Dark-red solid; Mp 207–209 °C; TLC R_f = 0.5 ($CHCl_3$); ^{1}H NMR ($CDCl_3$) δ 0.81–0.85 (m, 12H), 0.90–0.94 (m, 12H), 1.21–1.53 (m, 80H), 1.67–1.71 (m, 8H), 1.85–1.91 (m, 4H), 2.21–2.29 (m, 4H), 2.74–2.83 (m, 8H), 5.15–5.22 (m, 2H), 6.99 (s, 2H), 7.04 (d, *J* = 3.9 Hz, 2H), 7.08 (d, *J* = 3.9 Hz, 2H), 7.14 (d, 4H), 7.22 (s, 2H), 7.36 (d, *J* = 8.5 Hz, 4H), 7.76 (d, *J* = 8.5 Hz, 4H), 8.61–8.74 (m, 16H); MS (MALDI-TOF, 1,8,9–trihydroxyanthracene matrix) *m/z* 2458.7 (M^+, calcd 2456.1); Anal. Calcd for $C_{154}H_{166}N_4O_8S_8$: C, 75.27; H, 6.81; N, 2.28; Found: C, 74.89; H, 6.60; N, 2.15.

Representative NMR Spectra





Computational Details

All calculations were conducted using Gaussian 03 program. The geometry was optimized with the restricted Becke Hybrid (B3LYP) at 6-31 G(d, p) level.

Optimized structure of **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.640003	0.242961	-1.164872
2	6	0	2.011008	-0.964980	-0.936351
3	6	0	0.600849	-0.874151	-0.884674
4	6	0	0.117119	0.406144	-1.071683
5	16	0	1.447736	1.521105	-1.345747
6	1	0	2.555607	-1.889631	-0.782460
7	1	0	-0.045208	-1.721951	-0.686894
8	6	0	-1.248413	0.871087	-1.067388
9	6	0	-1.730194	2.163192	-0.987182
10	16	0	-2.583722	-0.266180	-1.177535
11	6	0	-3.141958	2.247436	-0.990779
12	1	0	-1.080876	3.026919	-0.899574
13	6	0	-3.773855	1.022410	-1.074449
14	1	0	-3.684338	3.182372	-0.907195
15	6	0	-5.186443	0.723356	-1.088163
16	6	0	-5.819106	-0.491772	-0.915328
17	16	0	-6.374241	1.986780	-1.360966
18	6	0	-7.231384	-0.412808	-0.983897
19	1	0	-5.280489	-1.411321	-0.715932
20	6	0	-7.709843	0.859578	-1.207995
21	1	0	-7.883179	-1.265210	-0.832315
22	6	0	4.051854	0.529352	-1.263625
23	6	0	4.698511	1.748604	-1.223528
24	16	0	5.219436	-0.764296	-1.473874
25	6	0	6.106649	1.650017	-1.341827
26	1	0	4.174111	2.686932	-1.082071
27	6	0	6.567490	0.358310	-1.472997
28	1	0	6.768835	2.506317	-1.289437
29	6	0	7.951036	-0.112106	-1.601084
30	6	0	8.330909	-1.386233	-1.152968
31	6	0	8.929257	0.732285	-2.149279
32	6	0	9.658907	-1.828651	-1.260909
33	1	0	7.598616	-2.022651	-0.668075
34	6	0	10.265844	0.319756	-2.257968
35	1	0	8.648444	1.721960	-2.491098
36	6	0	10.616164	-0.965624	-1.815160
37	1	0	11.634918	-1.315560	-1.948494
38	6	0	-9.103554	1.301600	-1.320727
39	6	0	-9.486059	2.607262	-0.981388
40	6	0	-10.086158	0.401268	-1.765018
41	6	0	-10.824673	3.021658	-1.083220
42	1	0	-8.746859	3.294899	-0.584774
43	6	0	-11.433137	0.781060	-1.850853
44	1	0	-9.789256	-0.591439	-2.085625
45	6	0	-11.788404	2.095736	-1.507105
46	1	0	-12.828231	2.397882	-1.571377
47	6	0	-11.194182	4.394757	-0.723867
48	6	0	-10.421190	5.533845	-0.777420
49	16	0	-12.796677	4.782433	-0.124397
50	6	0	-11.098478	6.708038	-0.365308
51	1	0	-9.400247	5.532321	-1.141154
52	6	0	-12.407347	6.488257	0.015453
53	1	0	-10.646322	7.693442	-0.373108
54	6	0	-13.393428	7.432665	0.485494
55	6	0	-14.757401	7.266876	0.623644
56	16	0	-12.925784	9.047841	0.996211
57	6	0	-15.426327	8.413816	1.109657
58	1	0	-15.266321	6.347689	0.356413
59	6	0	-14.589776	9.485413	1.354394
60	1	0	-16.499982	8.464204	1.250803
61	6	0	-12.462469	-0.155926	-2.313003
62	6	0	-13.662162	0.120672	-2.931555
63	16	0	-12.280044	-1.887928	-2.101684
64	6	0	-14.422502	-1.030598	-3.252082
65	1	0	-13.972996	1.127458	-3.185125
66	6	0	-13.817677	-2.215387	-2.882345
67	1	0	-15.375805	-0.993537	-3.767166
68	6	0	-14.288226	-3.570131	-3.051596
69	6	0	-13.586051	-4.754670	-2.950662
70	16	0	-15.971827	-3.895624	-3.435824
71	6	0	-14.373817	-5.907031	-3.176585
72	1	0	-12.525072	-4.790130	-2.730874
73	6	0	-15.697923	-5.631977	-3.458894
74	1	0	-13.981230	-6.916447	-3.129210
75	6	0	-16.775555	-6.547074	-3.744843
76	6	0	-18.130446	-6.295977	-3.841569

77	16	0	-16.455632	-8.251524	-4.032735
78	6	0	-18.906210	-7.444391	-4.122248
79	1	0	-18.557034	-5.310461	-3.692605
80	6	0	-18.164076	-8.602248	-4.248187
81	1	0	-19.986704	-7.428081	-4.208886
82	6	0	-18.612033	-9.947049	-4.521966
83	6	0	-17.912610	-11.133721	-4.424189
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88	1	0	-18.291703	-13.286143	-4.716137
89	6	0	-14.922059	10.802695	1.839842
90	6	0	-14.171407	11.961639	1.809044
91	16	0	-16.472765	11.106811	2.608554
92	6	0	-14.828565	13.082490	2.368452
93	1	0	-13.182194	12.007888	1.367854
94	6	0	-16.096714	12.807418	2.841140
95	1	0	-14.392775	14.074609	2.401711
96	6	0	-17.054816	13.693927	3.458180
97	6	0	-18.394903	13.479929	3.713637
98	16	0	-16.582027	15.288126	4.021216
99	6	0	-19.037436	14.576413	4.337422
100	1	0	-18.907407	12.566100	3.434709
101	6	0	-18.208389	15.652391	4.570390
102	1	0	-20.094715	14.589782	4.574842
103	6	0	10.018855	-3.173058	-0.799176
104	6	0	9.226158	-4.298098	-0.735810
105	16	0	11.630927	-3.537624	-0.211568
106	6	0	9.895268	-5.444926	-0.242726
107	1	0	8.196110	-4.308338	-1.072695
108	6	0	11.217486	-5.217583	0.084137
109	1	0	9.427762	-6.419215	-0.155114
110	6	0	11.260517	1.218526	-2.853440
111	6	0	11.068625	2.214428	-3.785949
112	16	0	12.954086	1.131574	-2.404774
113	6	0	12.256440	2.891614	-4.155901
114	1	0	10.101153	2.427309	-4.225627
115	6	0	13.384214	2.425719	-3.509700
116	1	0	12.289094	3.680619	-4.898791
117	6	0	12.196371	-6.139413	0.610865
118	6	0	13.567203	-5.998325	0.699030
119	16	0	11.703910	-7.689087	1.276949
120	6	0	14.221213	-7.115040	1.269639
121	1	0	14.090652	-5.120646	0.337089
122	6	0	13.365733	-8.137619	1.630605
123	1	0	15.296774	-7.180999	1.388306
124	6	0	13.673221	-9.415150	2.226449
125	6	0	12.885795	-10.546268	2.317365
126	16	0	15.229596	-9.698629	2.991622
127	6	0	13.518381	-11.631560	2.967205
128	1	0	11.886663	-10.599773	1.900020
129	6	0	14.804125	-11.356357	3.389280
130	1	0	13.053060	-12.601576	3.100491
131	6	0	15.740704	-12.214187	4.076465
132	6	0	17.100531	-12.053366	4.254051
133	16	0	15.201718	-13.690076	4.858568
134	6	0	17.705450	-13.100281	4.991366
135	1	0	17.651850	-11.216642	3.839930
136	6	0	16.826620	-14.083856	5.391099
137	1	0	18.769558	-13.149089	5.190957
138	6	0	14.753077	2.868238	-3.635084
139	6	0	15.912104	2.245722	-3.215845
140	16	0	15.133685	4.403857	-4.399754
141	6	0	17.089848	2.968910	-3.516029
142	1	0	15.913801	1.278078	-2.726998
143	6	0	16.859680	4.162052	-4.173018
144	1	0	18.086021	2.611808	-3.280699
145	6	0	17.809189	5.141972	-4.641297
146	6	0	17.616254	6.193027	-5.516566
147	16	0	19.477806	5.112907	-4.090190
148	6	0	18.783391	6.952597	-5.763206
149	1	0	16.661856	6.394123	-5.989878
150	6	0	19.896842	6.501109	-5.082422
151	1	0	18.815071	7.795072	-6.444708
152	6	0	21.245115	7.017687	-5.097302
153	6	0	22.411571	6.419867	-4.663071
154	16	0	21.585951	8.624482	-5.715392
155	6	0	23.562362	7.226655	-4.835774
156	1	0	22.440578	5.414741	-4.257568
157	6	0	23.305047	8.455160	-5.405655
158	1	0	24.562737	6.896173	-4.581887
159	6	0	24.248791	9.527203	-5.730801
160	6	0	23.974685	10.474821	-6.733635
161	6	0	25.469043	9.633090	-5.036797
162	6	0	24.878942	11.488779	-7.028780
163	1	0	23.052160	10.407135	-7.301781
164	6	0	26.382050	10.635066	-5.342534
165	1	0	25.693038	8.936827	-4.235705
166	6	0	26.086340	11.567738	-6.336641
167	1	0	24.655986	12.209681	-7.807532
168	1	0	27.315442	10.709150	-4.795553

169	6	0	-21.029962	-12.917618	-5.548699
170	6	0	-22.391812	-12.609194	-5.379093
171	6	0	-20.698688	-14.159282	-6.123398
172	6	0	-23.383036	-13.503944	-5.767054
173	1	0	-22.678100	-11.668203	-4.919769
174	6	0	-21.687504	-15.061494	-6.496468
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176	6	0	-23.031702	-14.733544	-6.321200
177	1	0	-24.429336	-13.256508	-5.624978
178	1	0	-21.419471	-16.013440	-6.941766
179	6	0	-18.541500	16.940357	5.183860
180	6	0	-17.825156	18.112680	4.882440
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182	6	0	-18.162500	19.328729	5.467014
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184	6	0	-19.956983	18.248941	6.670121
185	1	0	-20.155249	16.136874	6.374476
186	6	0	-19.232626	19.398958	6.356950
187	1	0	-17.607339	20.227142	5.220401
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192	6	0	16.576155	-17.593891	6.781070
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194	6	0	18.491525	-16.497315	7.761968
195	1	0	18.822235	-14.465940	7.169374
196	6	0	17.675056	-17.621211	7.637975
197	1	0	15.949102	-18.473049	6.681004
198	1	0	19.336736	-16.518679	8.441199
199	7	0	-19.596969	20.662461	6.956132
200	6	0	-20.204590	21.628339	6.124996
201	6	0	-19.331802	20.834465	8.331874
202	6	0	-20.598076	22.904291	6.770659
203	8	0	-20.392952	21.408267	4.939397
204	6	0	-19.735203	22.131765	8.927102
205	8	0	-18.800847	19.950471	8.984701
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214	6	0	-21.391872	25.365891	7.940400
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223	6	0	-21.950172	28.076863	10.554587
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250	6	0	-26.574155	-17.934237	-5.159253
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263	6	0	-28.645391	-19.923896	-11.017181
264	6	0	-29.648338	-20.793091	-6.341008
265	6	0	-30.121090	-21.259447	-9.055207
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268	6	0	-30.633381	-21.706150	-6.731666
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273	1	0	-31.221763	-22.241015	-5.994433
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293	6	0	19.490598	-23.440196	8.615920
294	1	0	19.349929	-22.258175	6.806284
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297	1	0	17.486497	-19.099805	12.408231
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329	8	0	26.653307	13.578760	-4.593669
330	6	0	28.616508	13.682034	-8.197885
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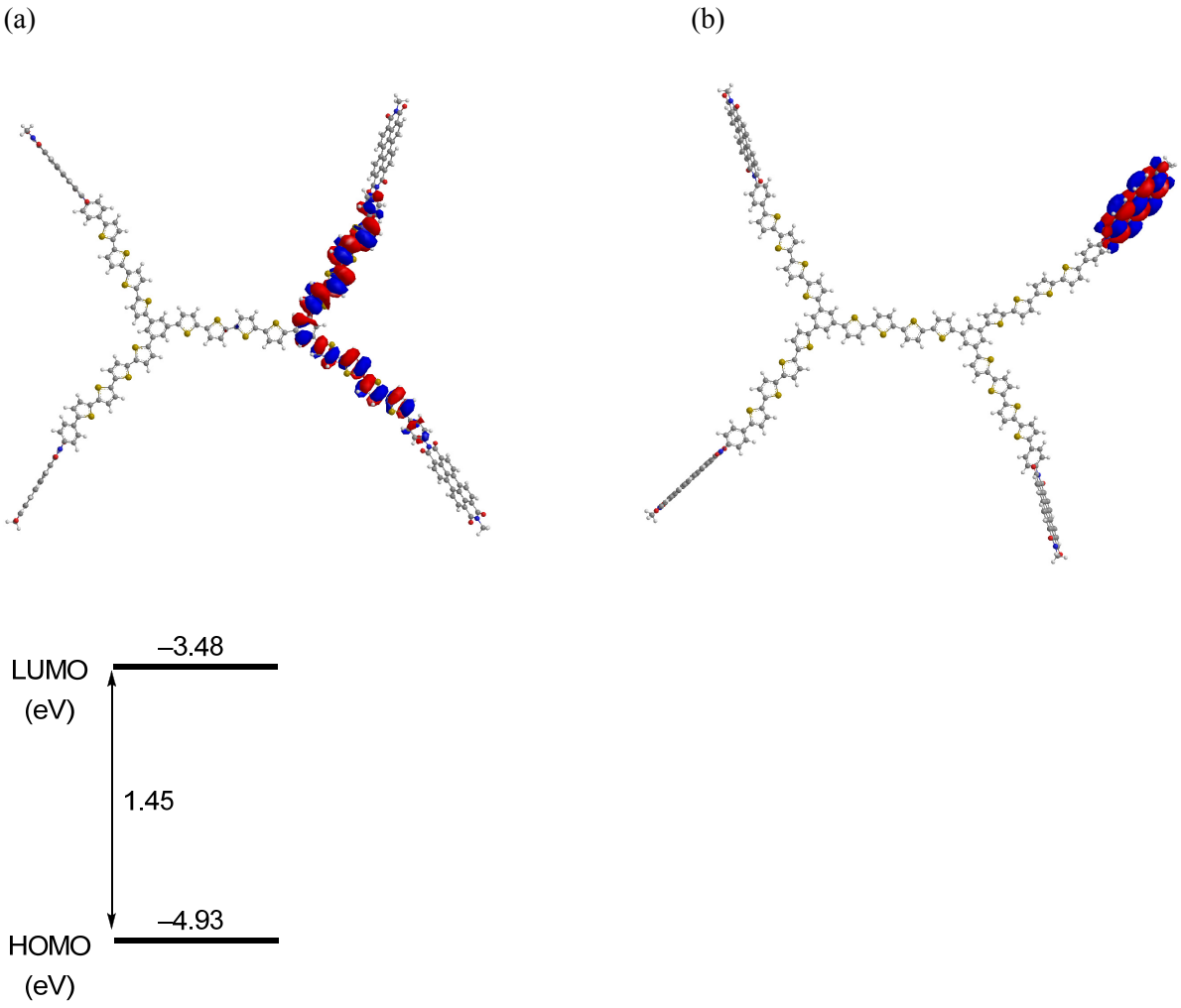
334	6	0	29.270364	13.695237	-9.417855
335	6	0	29.328966	16.733890	-5.385690
336	1	0	27.911767	15.670032	-4.140330
337	6	0	29.781065	15.763377	-7.568109
338	6	0	30.170774	14.719328	-9.728563
339	1	0	29.067695	12.897271	-10.123574
340	6	0	30.011410	16.794139	-6.602330
341	1	0	29.483092	17.499319	-4.635249
342	6	0	30.444394	15.757787	-8.836284
343	1	0	30.658542	14.688281	-10.694906
344	6	0	30.953616	17.877010	-6.922151
345	6	0	31.386618	16.840584	-9.156249
346	6	0	31.615571	17.871930	-8.191050
347	6	0	31.226964	18.915749	-6.030006
348	6	0	32.068855	16.901554	-10.372974
349	6	0	32.529745	18.925502	-8.502563
350	6	0	32.123356	19.943118	-6.342949
351	1	0	30.740855	18.945497	-5.062772
352	6	0	32.962117	17.936411	-10.669406

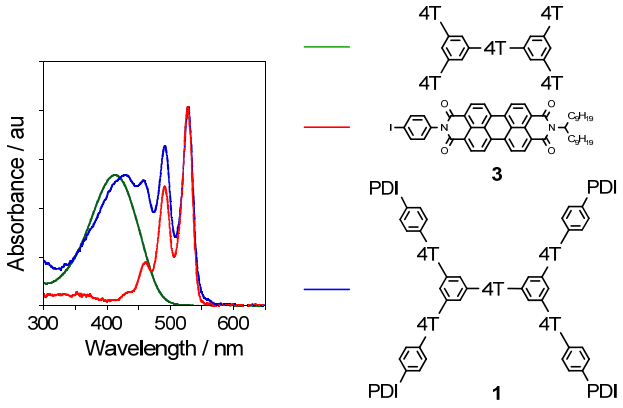
353	1	0	31.915810	16.135581	-11.123123
354	6	0	33.197852	18.944539	-9.750919
355	6	0	32.773125	19.957448	-7.564514
356	1	0	32.324436	20.742684	-5.638466
357	1	0	33.483334	17.967455	-11.619766
358	6	0	34.150416	20.028938	-10.095776
359	6	0	33.718196	21.056911	-7.873703
360	7	0	34.346955	21.022609	-9.124518
361	8	0	34.737255	20.062217	-11.169213
362	8	0	33.955224	21.965508	-7.088642
363	6	0	35.278117	22.118343	-9.416191
364	1	0	35.671749	21.960359	-10.416855
365	1	0	36.085914	22.123222	-8.681433
366	1	0	34.753868	23.073971	-9.353716

Fig. S1 Caluculated HOMO (a) and LUMO (b) of **1**.



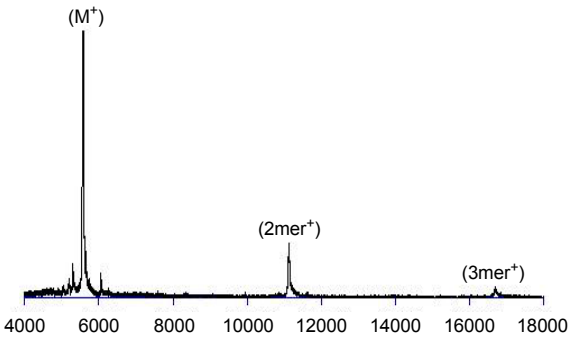
UV-vis Absorption Spectra

Fig. S2 UV-vis spectra of dendritic oligothiophene, **1**, and **3** in $CHCl_3$.



MALDI-TOF mass

Fig. S3 MALDI-TOF mass spectrum of **1**.



Device Fabrication

Photovoltaic cells with the structure of ITO/active layer (**1** or **2**)/Al were fabricated. ITO-coated glass substrates were first cleaned by successive ultrasonications in toluene, acetone, H_2O, and *i*-PrOH. ITO-coated glass substrates were then activated by ozone treatment for 1 h. The active layers were prepared by spin-coating the 1.0 wt% chloroform solution at 1500 rpm for 2 min. The substrates were dried at room temperature for 20 min in ambient air condition and then stored under vacuum (1.0×10^{-3} Pa). An Al electrode (100 nm) was deposited through a shadow mask to define the active area of the devices (0.5×1.0 mm^2).

The thickness of active layer was determined by Otsuka Electronics Co., Ltd. FE-3000 reflective film thickness monitor. Monochromic light was produced by a MORITEX MME-250 light source and a Jasco CT-10 monochromator. The current–voltage characteristics of photovoltaic cells were measured by using a KEITHLEY 2400 semiconductor parameter analyzer. All the photovoltaic properties were evaluated in ambient air condition at room temperature and are summarized in Table S1.

Table S1. Photovoltaic performances of **1** and **2** as active layers[a]

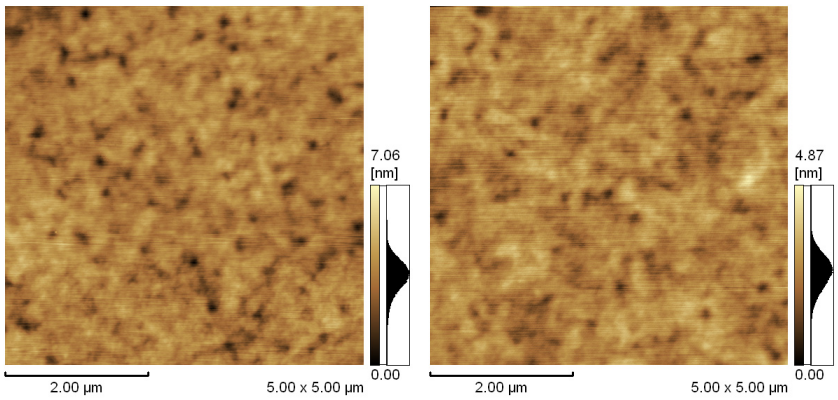
run	compd	J_{sc} /nA m^{-2}	λ_{inc} /nm	IPCE /%	$V_{oc.}$ /V	*FF*	η /%
1	**1**	204	470	5.5	0.46	0.27	0.25
2	**1**	185	470	5.0	0.45	0.28	0.24
3	**1**	163	470	4.4	0.46	0.27	0.21
4	**2**	25	460	0.67	0.22	0.26	0.014
5	**2**	17	460	0.45	0.24	0.25	0.010
6	**2**	29	460	0.76	0.13	0.21	0.008

[a] Upon illumination with 10-μW cm^{-2} monochromatic light.

AFM Images

Fig. S4 AFM images of the spin-coated films of **1** (a) and **2** (b).

(a) (b)



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(1) Wescott, L. D.; Mattern, D. L. *J. Org. Chem.* **2003**, *68*, 10058–10066.

(2) Sato, M.-A.; Fukui, K. *Synth. Met.* **2007**, *157*, 619–626.