Supplementary Information

Synthesis, optical and electrochemical properties of phenanthrodithiophene (fused-bibenzo[*c*]thiophene) derivative

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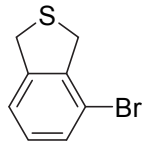
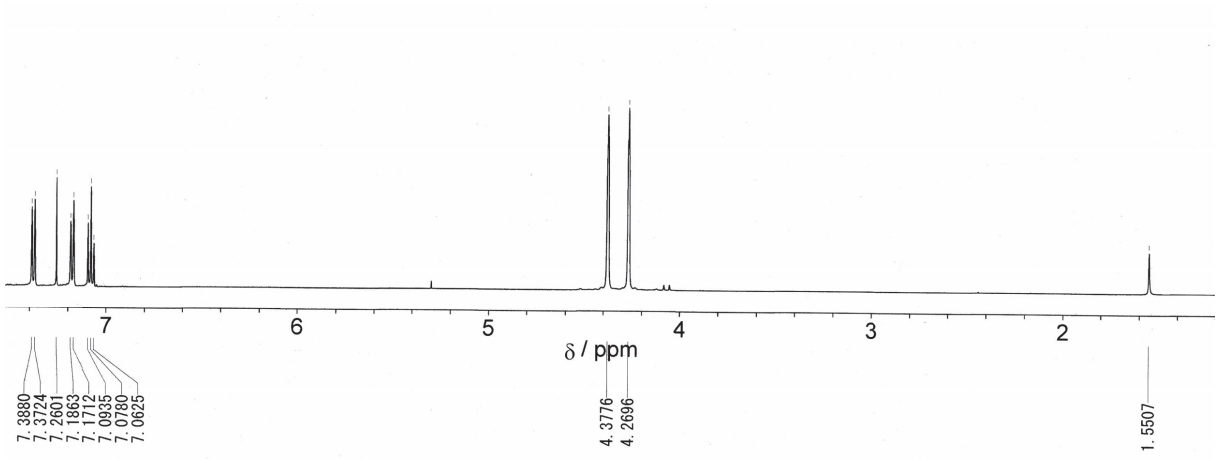
(a)



1



(b)

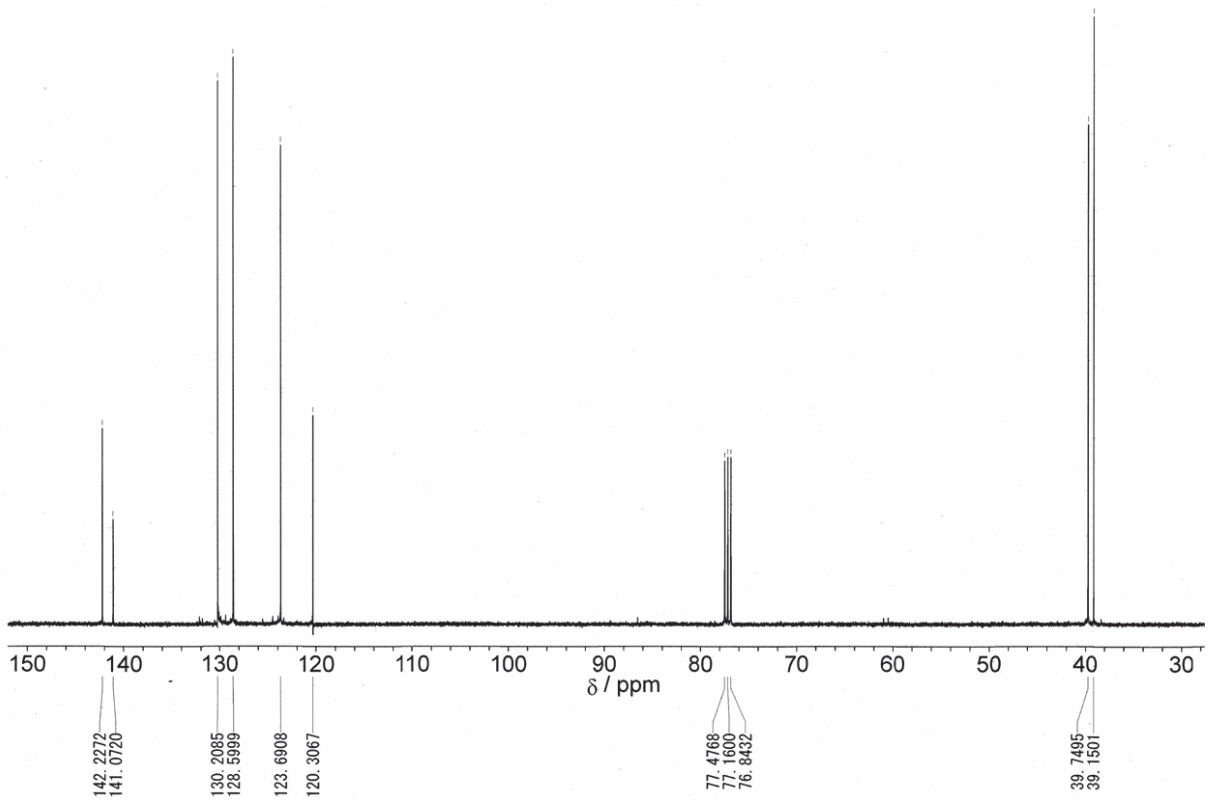
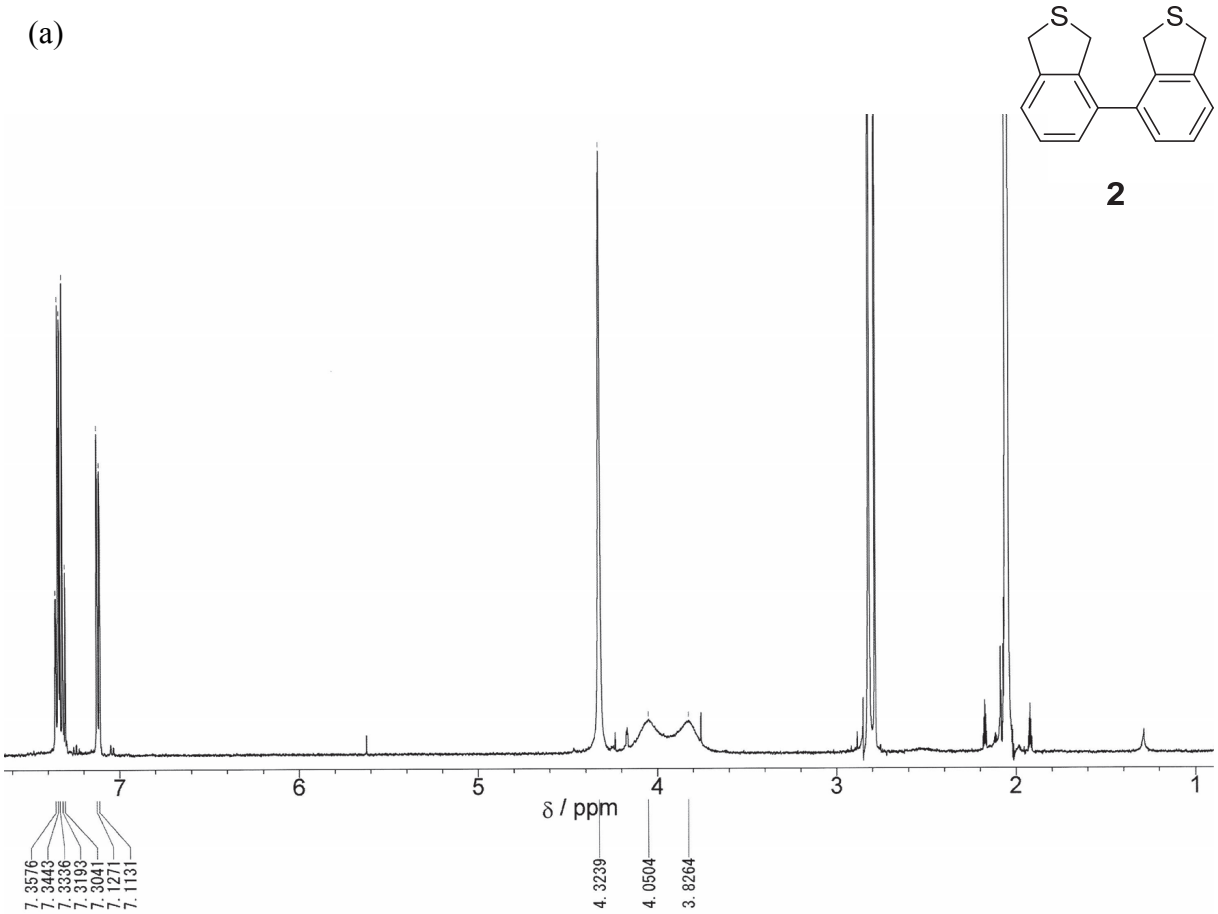


Fig. S1 (a) ^{1}H HMR (500 MHz) and (b) ^{13}C NMR (100 MHz) of **1** in $CDCl_3$.

(a)



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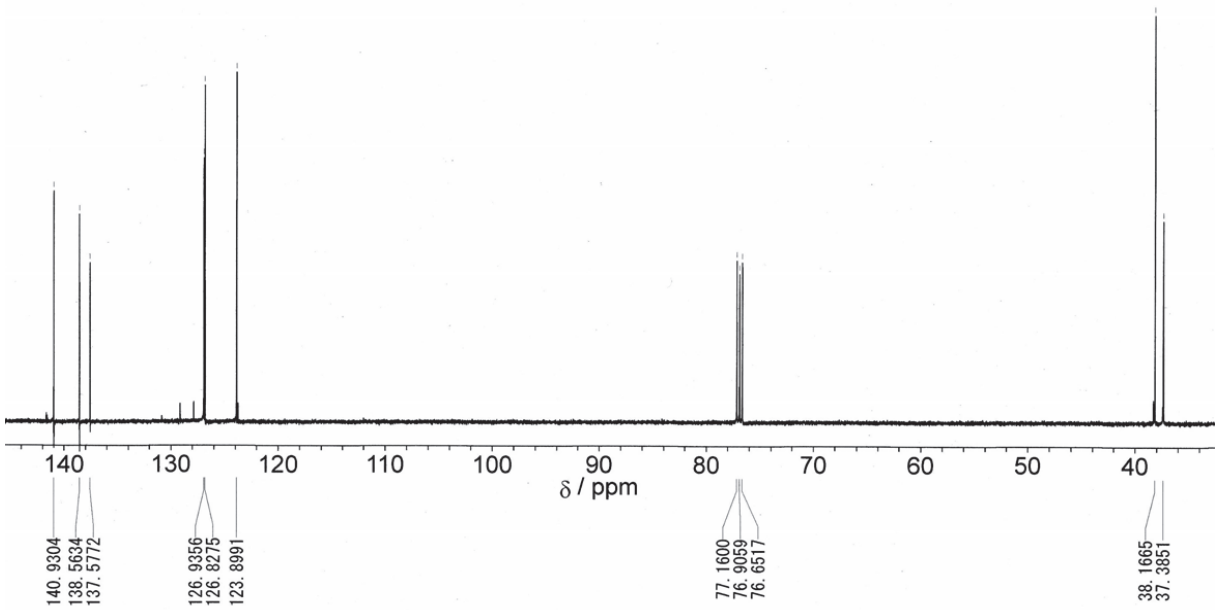
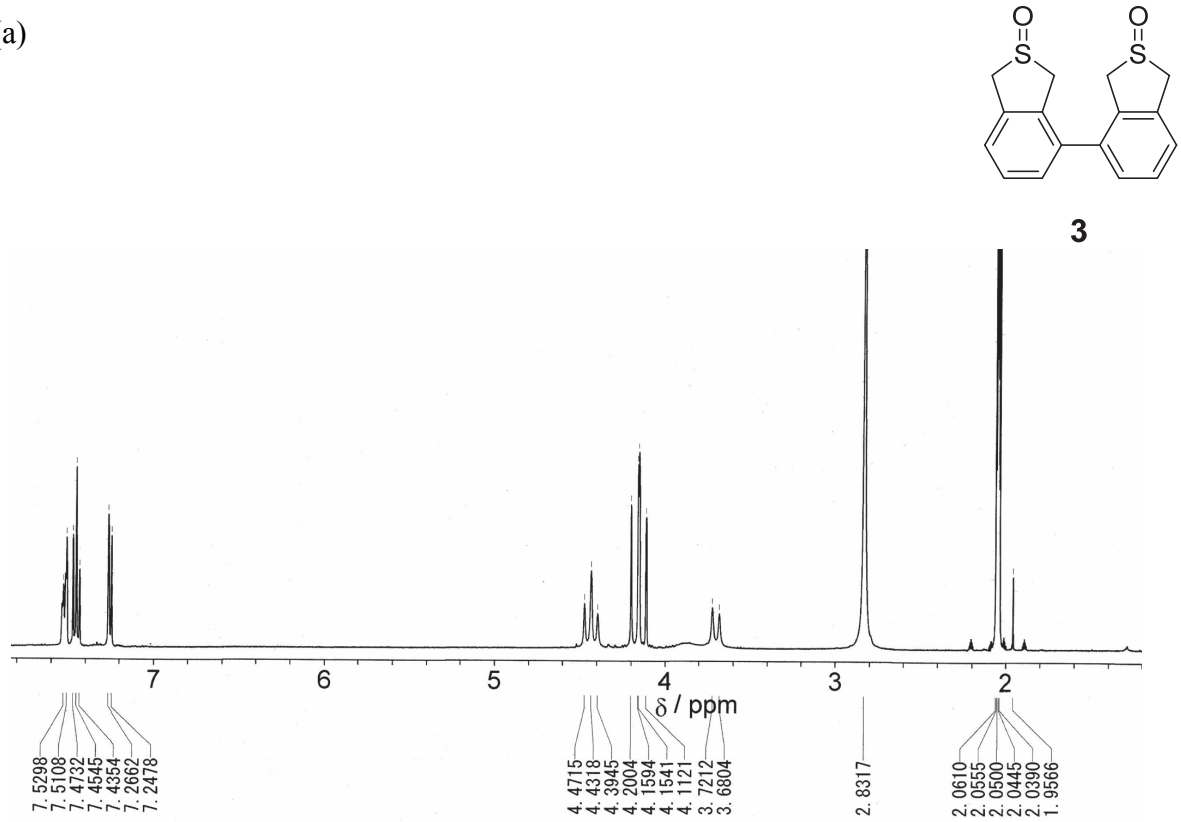


Fig. S2 (a) ^{1}H HMR (500 MHz) of **2** in acetone-d_6 and (b) ^{13}C NMR (125 MHz) of **2** in $CDCl_3$.

(a)



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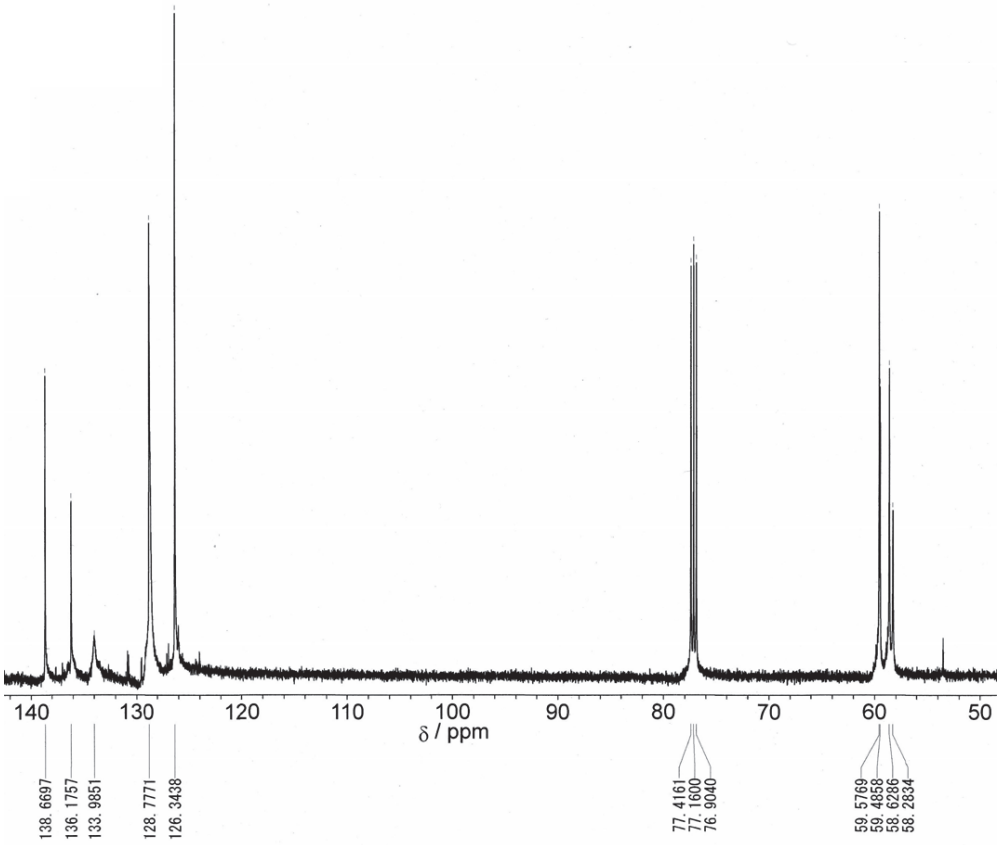
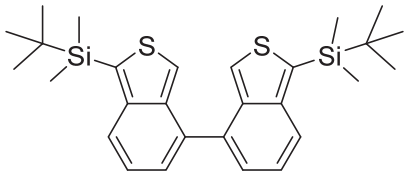
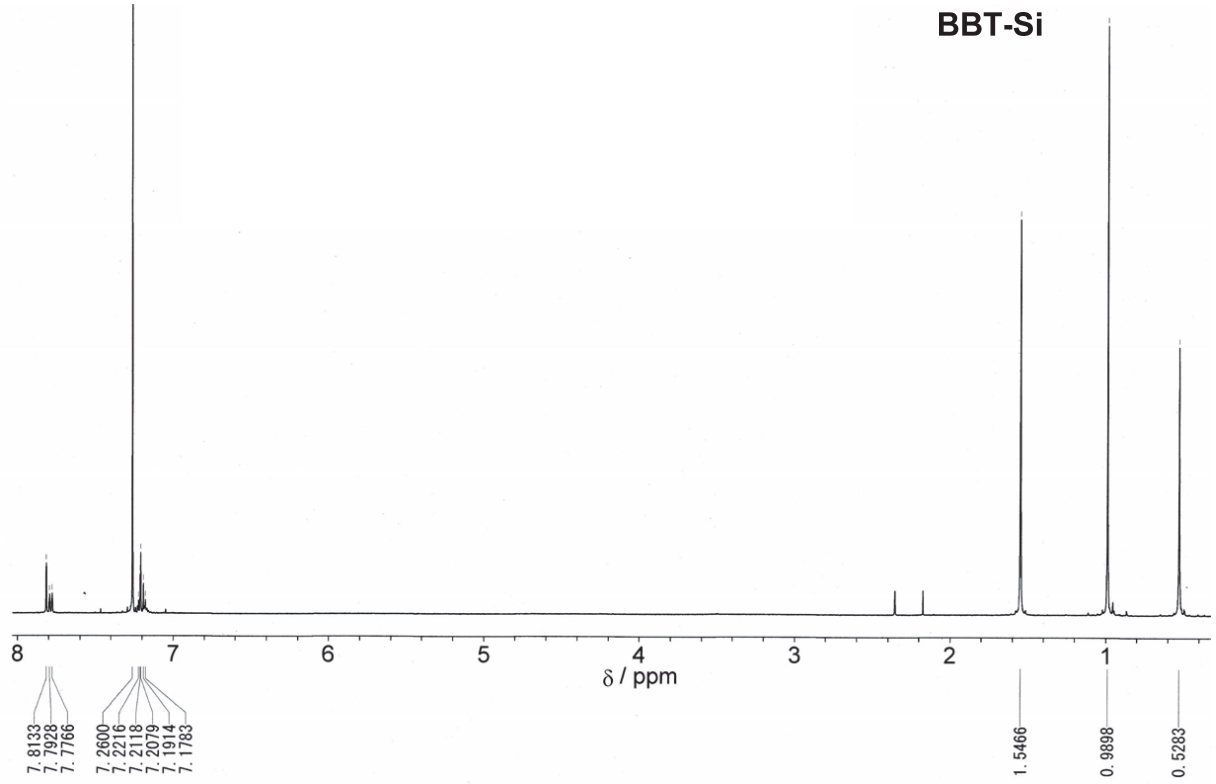


Fig. S3 (a) ^{1}H HMR (400 MHz) of **3** in acetone-d_6 and (b) ^{13}C NMR (125 MHz) of **3** in $CDCl_3$.

(a)





(b)

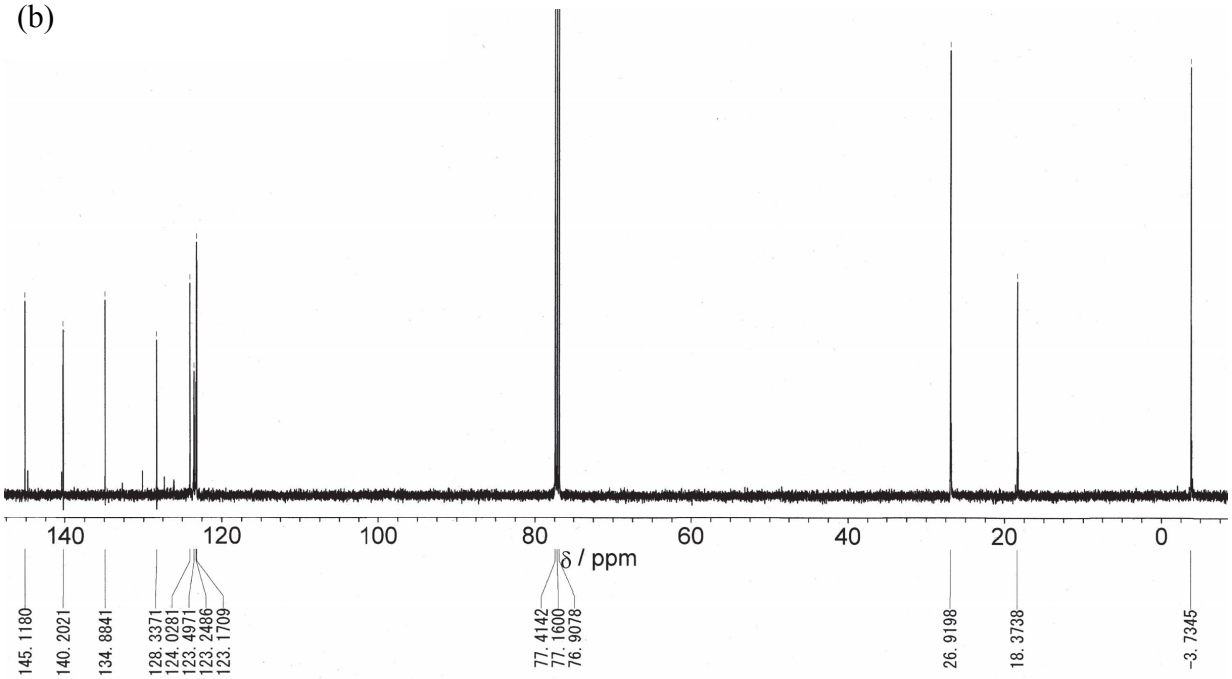


Fig. S4 (a) ^{1}H HMR (500 MHz) and (b) ^{13}C NMR (125 MHz) of **BBT-Si** in $CDCl_3$.

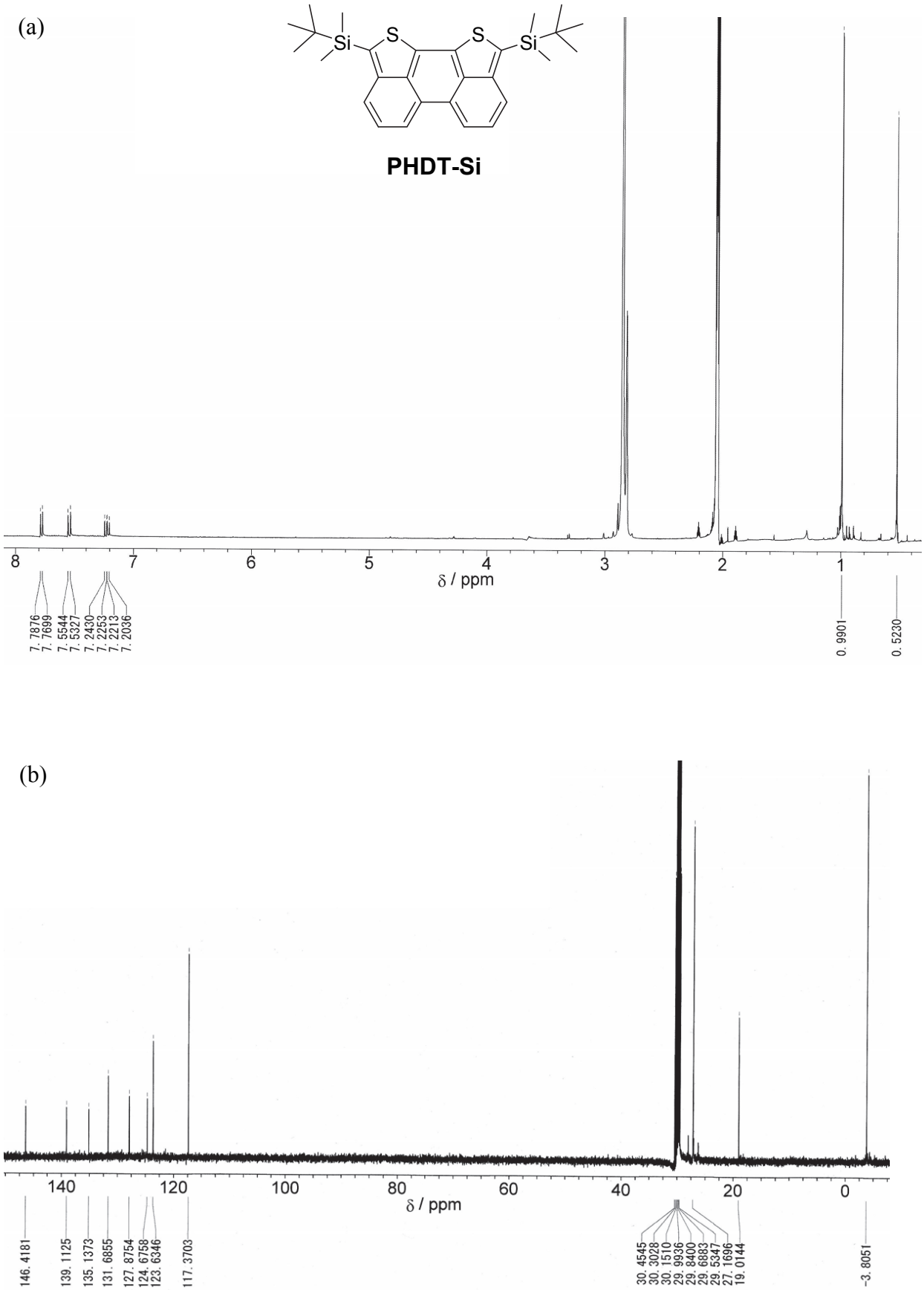
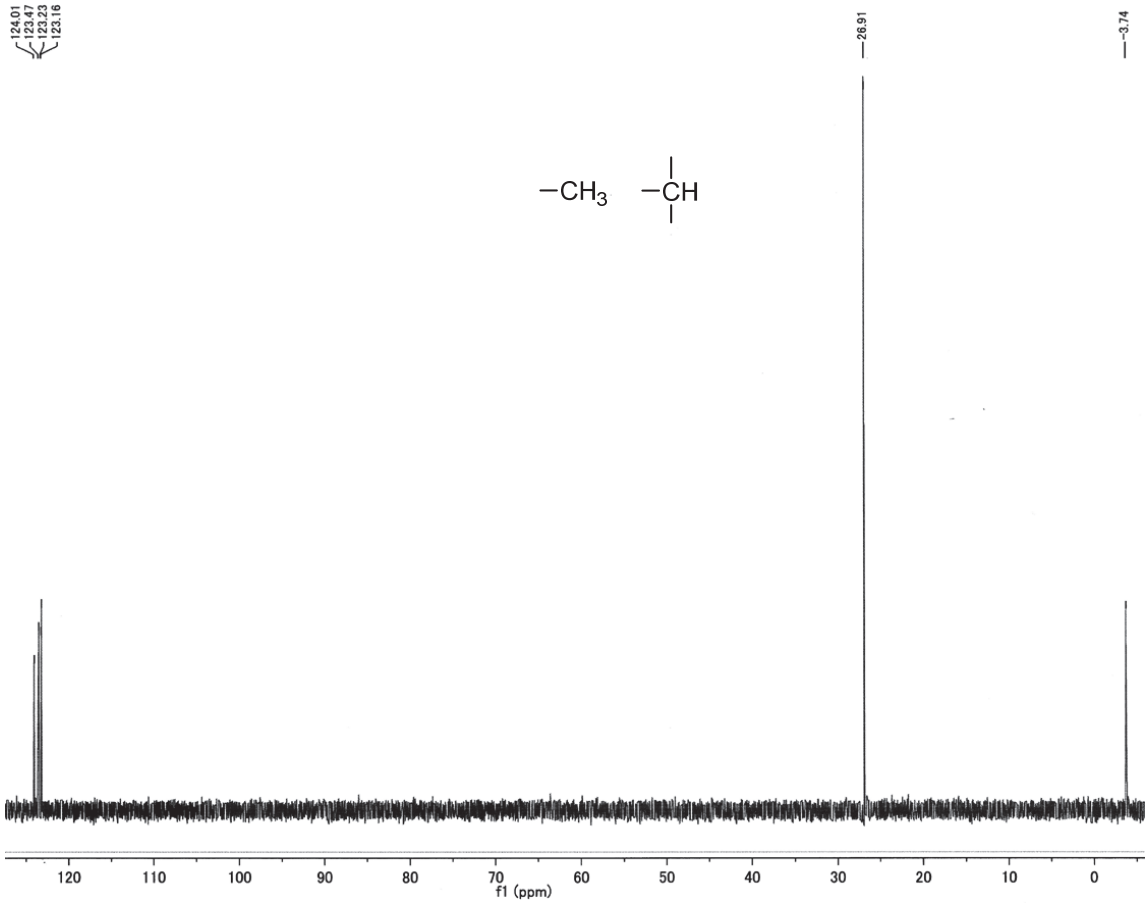


Fig. S5 (a) ^{1}H HMR (400 MHz) and (b) ^{13}C NMR (125 MHz) of **PHDT-Si** in acetone-d_6.

(a)



(b)

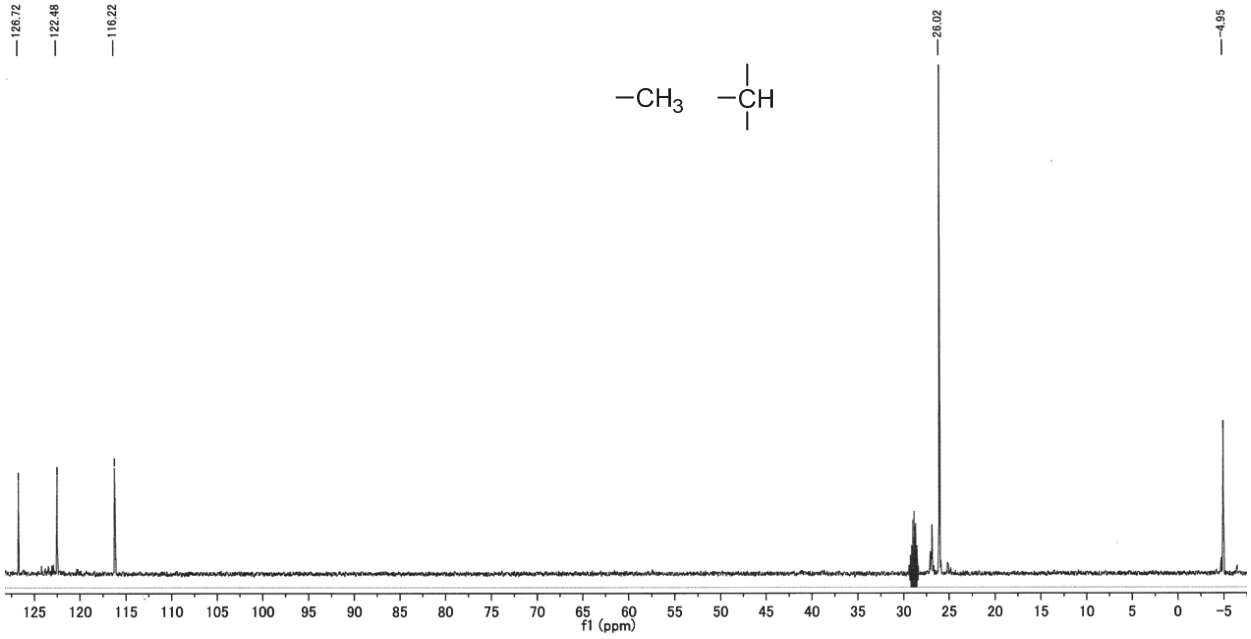


Fig. S6 DEPT ^{13}C HMR (125 MHz) of (a) **BBT-Si** in $CDCl_3$ and (b) **PHDT-Si** in acetone-d_6.

Table S1 Geometrical coordinates of the optimized **BBT-Si**.

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	0	-3.119904	0.395892	0.355748
2	C	0	-1.832771	-0.281924	0.309956
3	C	0	-0.657524	0.347009	0.865408
4	C	0	-0.801979	1.601556	1.415647
5	C	0	-2.062460	2.268648	1.464122
6	C	0	-3.195193	1.690831	0.957487
7	C	0	-4.163786	-0.331408	-0.234285
8	C	0	-1.925265	-1.509940	-0.329328
9	H	0	0.064485	2.089081	1.851744
10	H	0	-2.114484	3.251470	1.923589
11	H	0	-4.146148	2.211422	1.006525
12	H	0	-1.133078	-2.216509	-0.526412
13	C	0	1.832775	0.281938	0.309968
14	C	0	3.119918	-0.395866	0.355760
15	C	0	3.195208	-1.690795	0.957506
16	C	0	2.062473	-2.268612	1.464146
17	C	0	0.801990	-1.601534	1.415668
18	C	0	0.657527	-0.346993	0.865413
19	C	0	1.925251	1.509964	-0.329310
20	H	0	4.146155	-2.211400	1.006555
21	H	0	2.114510	-3.251433	1.923612
22	H	0	-0.064463	-2.089060	1.851787
23	H	0	1.133063	2.216531	-0.526390
24	S	0	3.526029	1.824933	-0.840725
25	S	0	-3.526045	-1.824913	-0.840733
26	C	0	4.163773	0.331455	-0.234311
27	Si	0	5.988232	-0.098846	-0.428639
28	Si	0	-5.988261	0.098832	-0.428621
29	C	0	6.859480	1.336833	-1.298770
30	H	0	6.787580	2.267207	-0.725881
31	H	0	7.924054	1.108499	-1.422209
32	H	0	6.446373	1.523858	-2.295447
33	C	0	6.770829	-0.365809	1.274067
34	H	0	6.272723	-1.162709	1.835356
35	H	0	7.828184	-0.637647	1.177072

36	H	0	6.713247	0.546255	1.877168
37	C	0	6.167327	-1.666893	-1.473716
38	H	0	5.644343	-2.518454	-1.026995
39	H	0	5.753646	-1.516590	-2.476320
40	H	0	7.222052	-1.943875	-1.584160
41	C	0	-6.167383	1.666906	-1.473655
42	H	0	-7.222122	1.943778	-1.584254
43	H	0	-5.644563	2.518516	-1.026837
44	H	0	-5.753533	1.516660	-2.476197
45	C	0	-6.770793	0.365618	1.274143
46	H	0	-6.272854	1.162696	1.835331
47	H	0	-7.828251	0.637109	1.177327
48	H	0	-6.712805	-0.546411	1.877258
49	C	0	-6.859432	-1.336818	-1.298877
50	H	0	-6.446313	-1.523714	-2.295572
51	H	0	-6.787500	-2.267252	-0.726091
52	H	0	-7.924016	-1.108511	-1.422291

Table S2 Geometrical coordinates of the optimized **PHDT-Si**.

Cartesian coordinates:

Center	Atomic	Atomic	Coordinates	(Angstroms)	
Number	Number	Type	X	Y	Z
1	C	0	2.820351	0.831615	0.000096
2	C	0	3.601599	2.027112	0.000205
3	C	0	2.966937	3.248929	0.000201
4	C	0	1.552089	3.370749	0.000112
5	C	0	0.735688	2.249685	0.000033
6	C	0	1.389442	0.975377	0.000033
7	C	0	0.712126	-0.249637	-0.000010
8	S	0	1.844820	-1.554342	-0.000047
9	C	0	-1.389440	0.975376	-0.000067
10	C	0	-0.735686	2.249685	-0.000059
11	C	0	-1.552087	3.370748	-0.000116
12	C	0	-2.966935	3.248929	-0.000189
13	C	0	-3.601597	2.027111	-0.000198
14	C	0	-2.820349	0.831614	-0.000116
15	S	0	-1.844819	-1.554342	-0.000057

16	C	0	-0.712123	-0.249637	-0.000032
17	H	0	4.685491	1.975331	0.000280
18	H	0	3.562973	4.157115	0.000276
19	H	0	1.117630	4.365300	0.000136
20	H	0	-1.117628	4.365299	-0.000124
21	H	0	-3.562971	4.157115	-0.000236
22	H	0	-4.685489	1.975330	-0.000247
23	C	0	3.244679	-0.509398	0.000075
24	C	0	-3.244677	-0.509400	-0.000080
25	Si	0	4.986306	-1.223925	-0.000051
26	Si	0	-4.986305	-1.223925	0.000097
27	C	0	4.871612	-3.111535	0.000468
28	H	0	4.350016	-3.490886	-0.884432
29	H	0	5.877247	-3.546706	0.000435
30	H	0	4.350338	-3.490271	0.885825
31	C	0	5.910914	-0.647761	1.548090
32	H	0	6.935633	-1.036656	1.556675
33	H	0	5.968887	0.443834	1.607192
34	H	0	5.410810	-0.999908	2.456169
35	C	0	5.910200	-0.648223	-1.548791
36	H	0	5.967756	0.443379	-1.608283
37	H	0	6.935048	-1.036764	-1.557726
38	H	0	5.409783	-1.000823	-2.456522
39	C	0	-4.871609	-3.111535	-0.000467
40	H	0	-5.877242	-3.546709	-0.000407
41	H	0	-4.350366	-3.490244	-0.885854
42	H	0	-4.349979	-3.490908	0.884403
43	C	0	-5.910978	-0.647733	-1.547996
44	H	0	-6.935704	-1.036610	-1.556523
45	H	0	-5.968935	0.443862	-1.607096
46	H	0	-5.410933	-0.999887	-2.456105
47	C	0	-5.910154	-0.648248	1.548875
48	H	0	-5.967667	0.443354	1.608404
49	H	0	-6.935016	-1.036751	1.557811
50	H	0	-5.409738	-1.000896	2.456588