Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Synthesis, optical and electrochemical properties of 1,1',3,3'-tetraaryl-4,4'-bibenzo[*c*]thiophene derivatives with same or different aryl substituents on the thiophene rings

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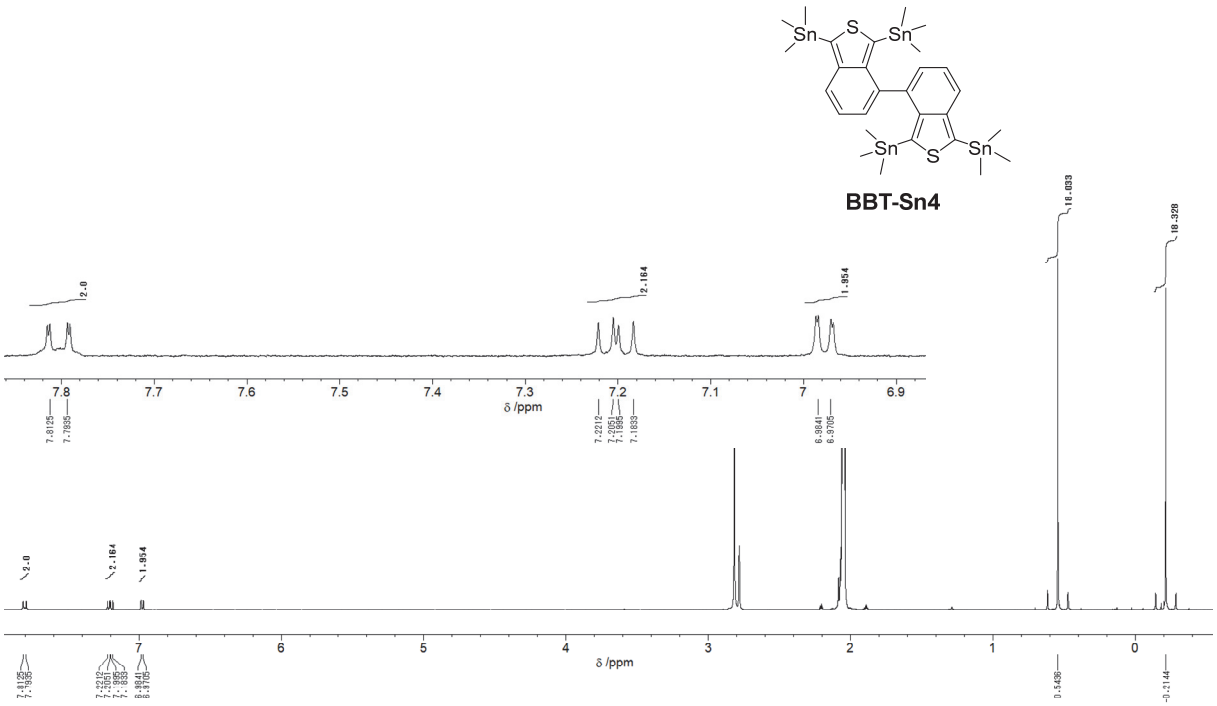

Fig. S1 ^{1}H NMR (400 MHz) spectrum of **BBT-Sn4** in acetone-d_6 at 23 ℃.

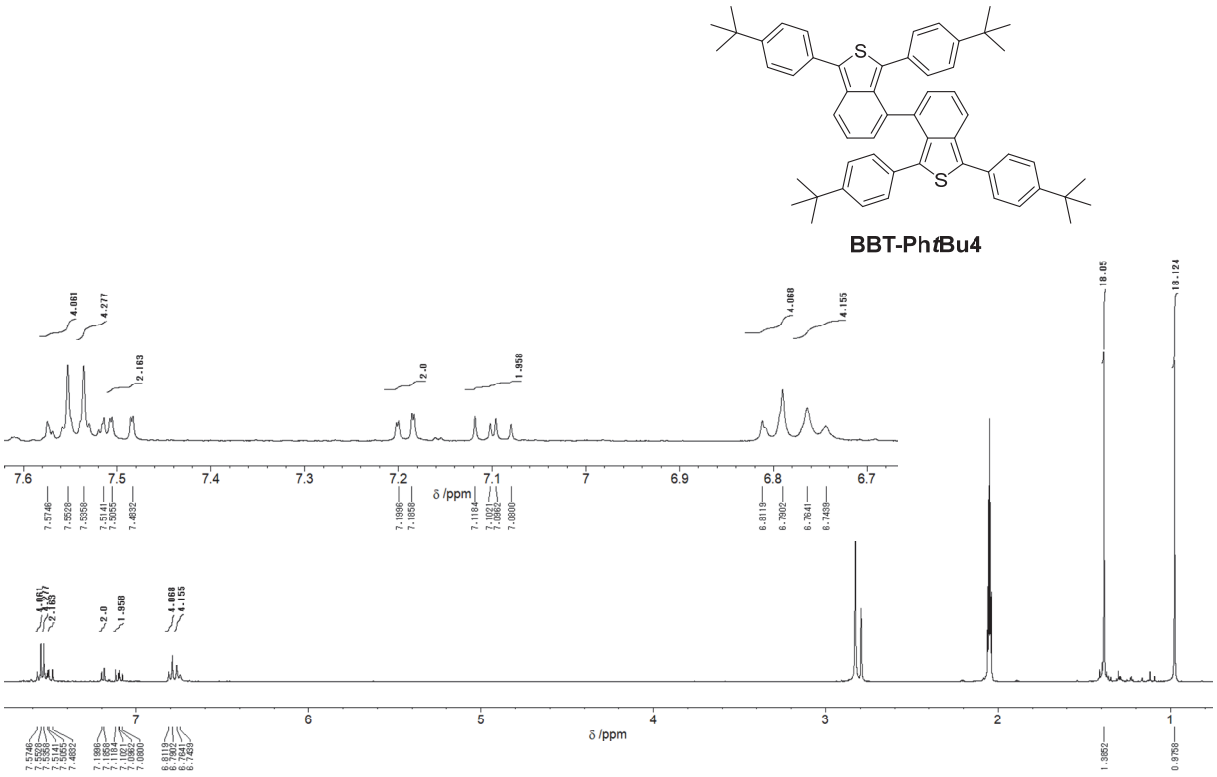

Fig. S2 ^{1}H NMR (400 MHz) spectrum of **BBT-Ph*t*Bu4** in acetone-d_6 at 23 ℃.

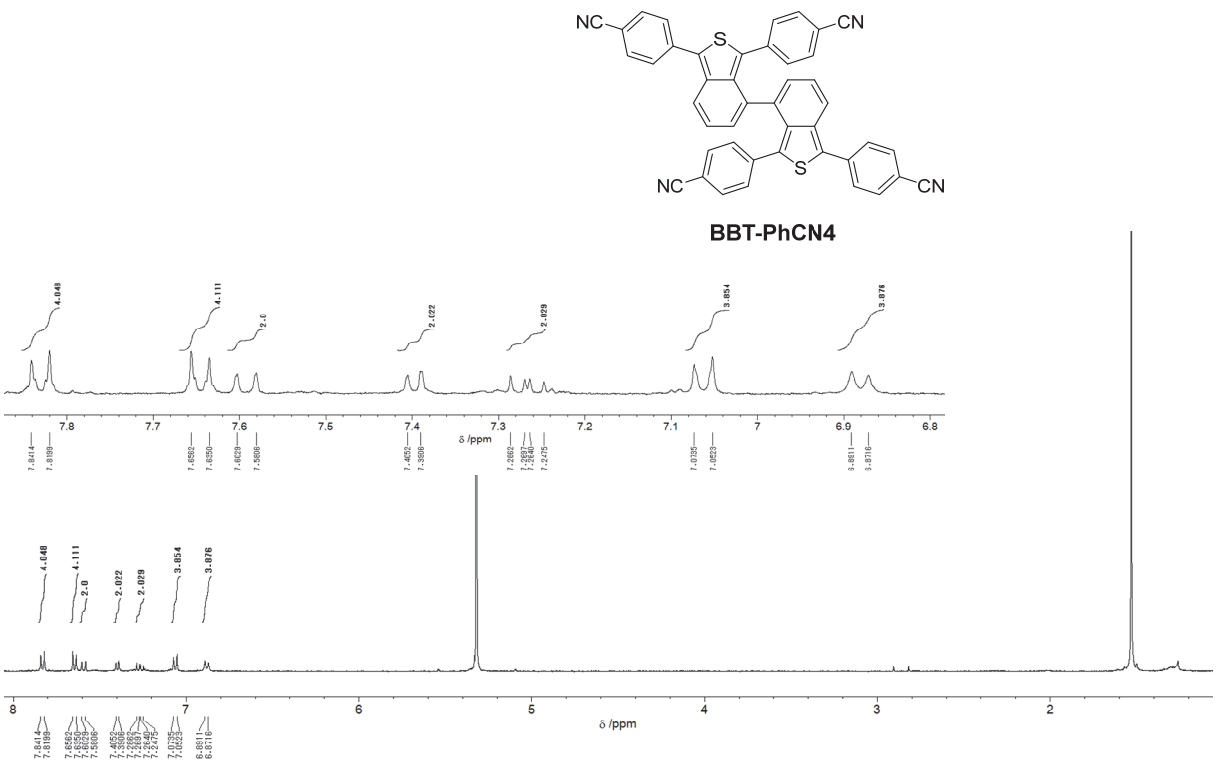

Fig. S3 ^{1}H NMR (400 MHz) spectrum of **BBT-PhCN4** in dichloromethane-d_2 at 23 ℃.

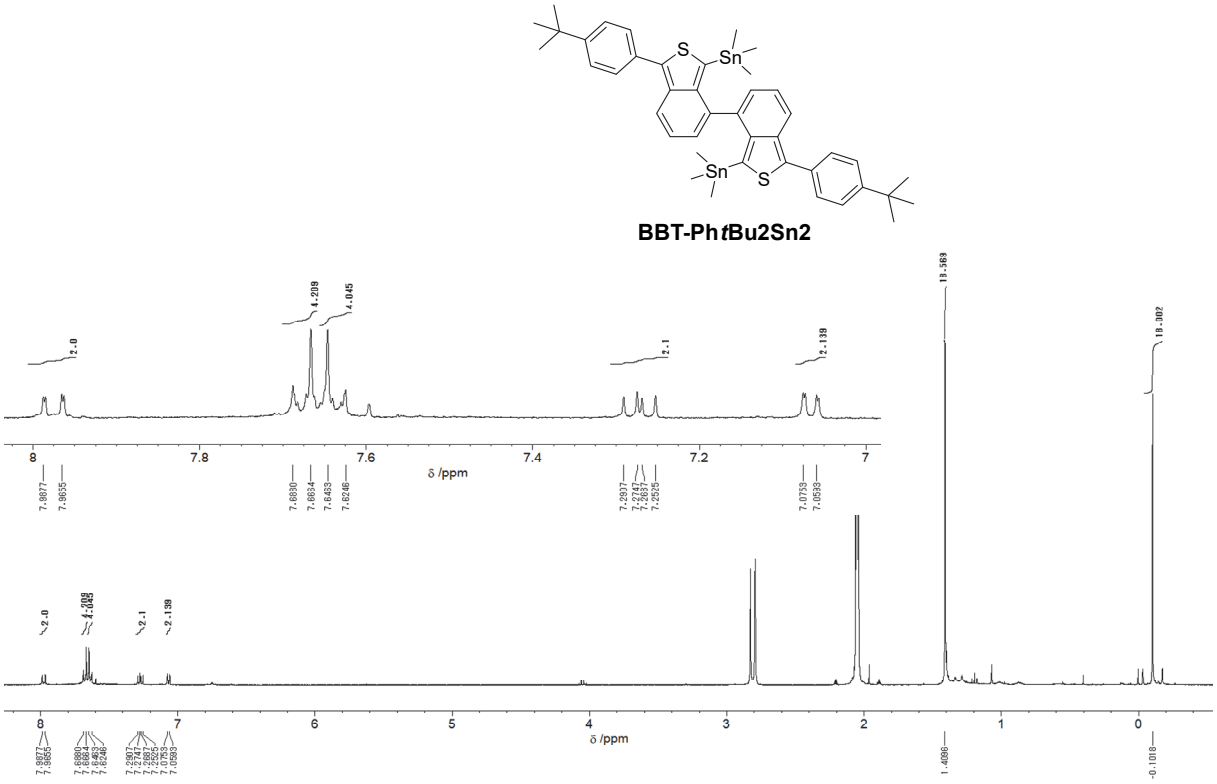

Fig. S4 ^{1}H NMR (400 MHz) spectrum of **BBT-Ph*t*Bu2Sn2** in acetone-d_6 at 23 ℃.

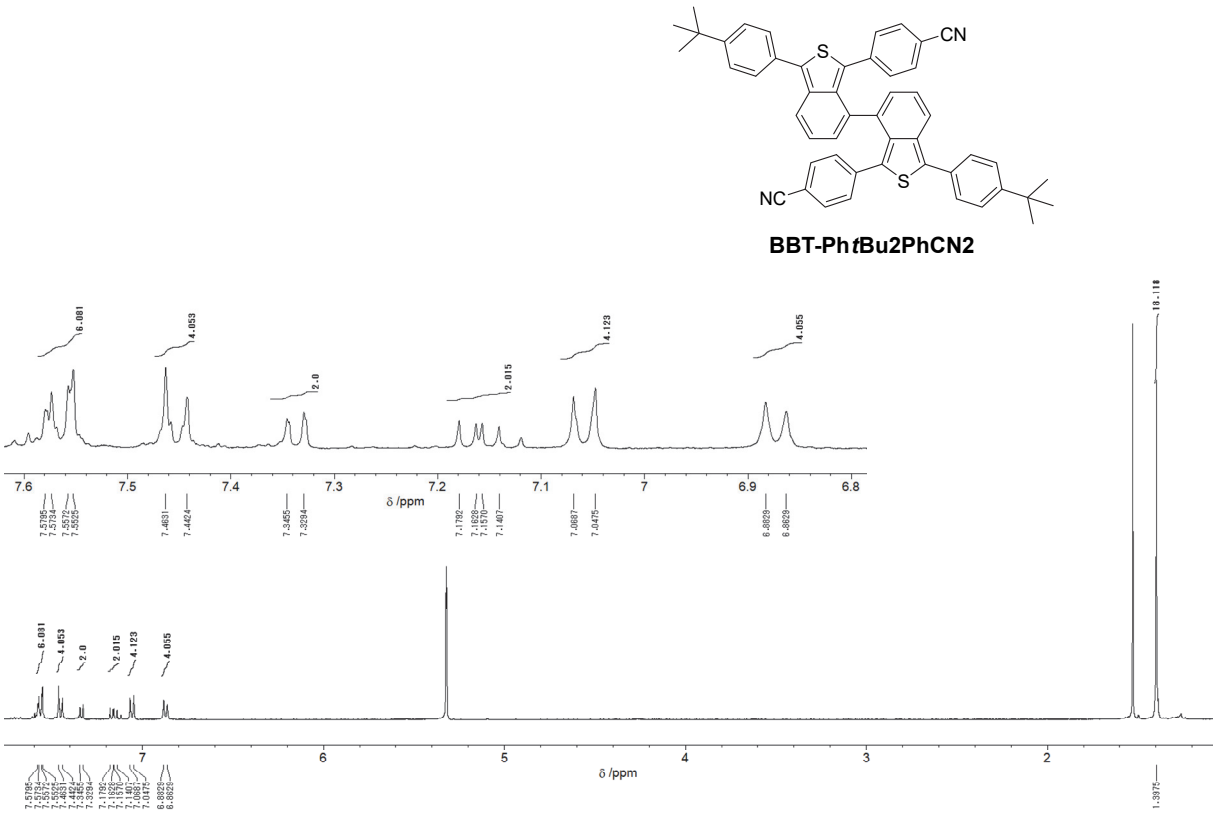

Fig. S5 ^{1}H NMR (400 MHz) spectrum of **BBT-Ph*t*Bu2PhCN2** in dichloromethane-d_2 at 23 °C.

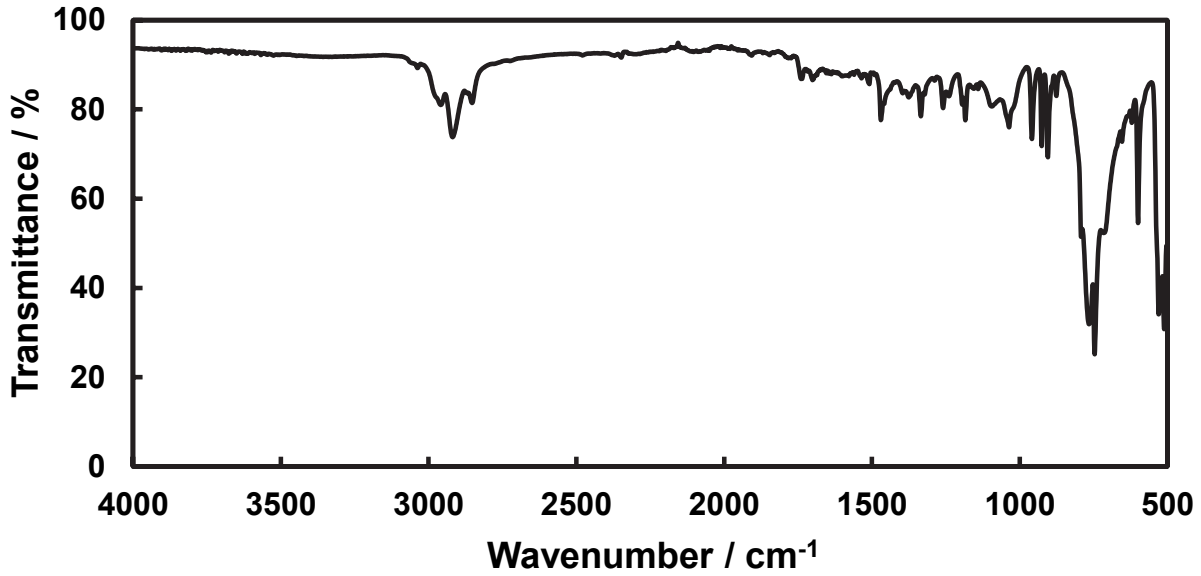

Fig. S6 FTIR spectrum of **BBT-Sn4**.

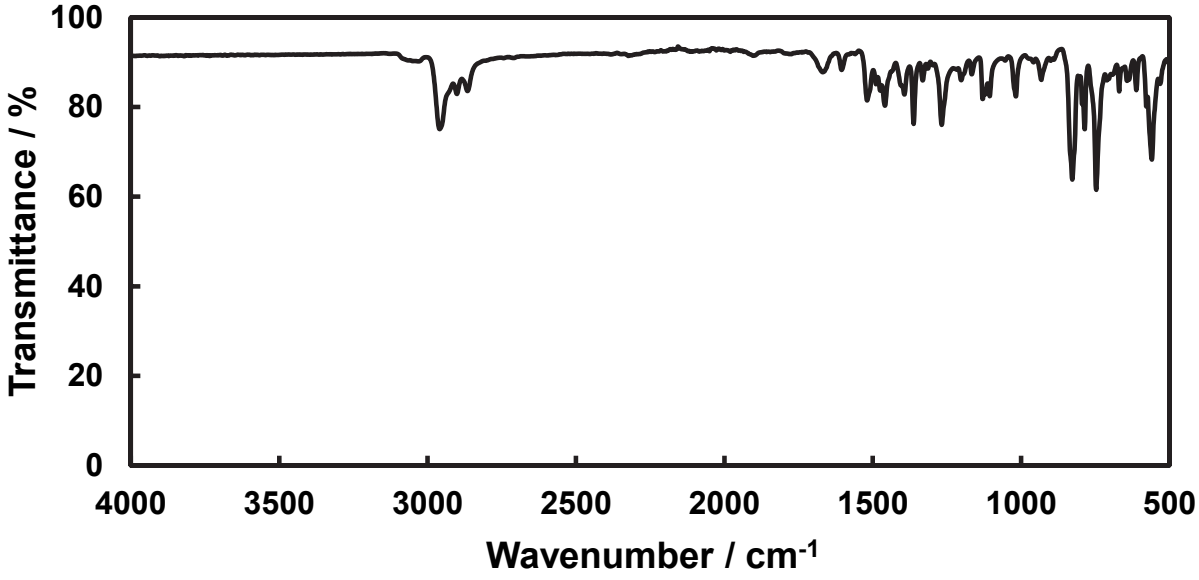

Fig. S7 FTIR spectrum of **BBT-Ph*t*Bu4**.

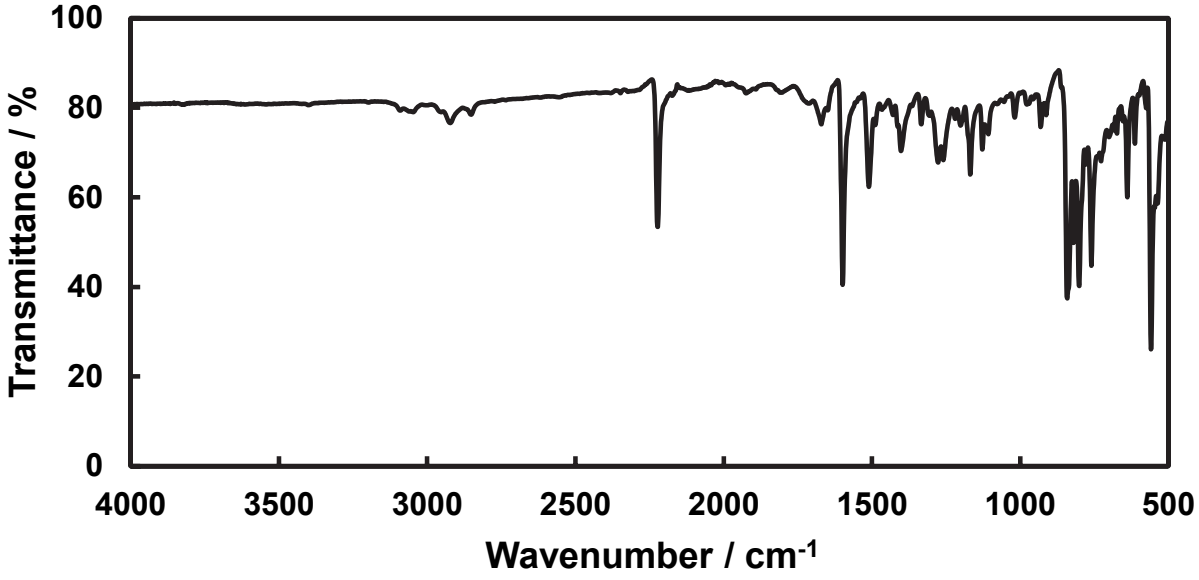

Fig. S8 FTIR spectrum of **BBT-PhCN4**.

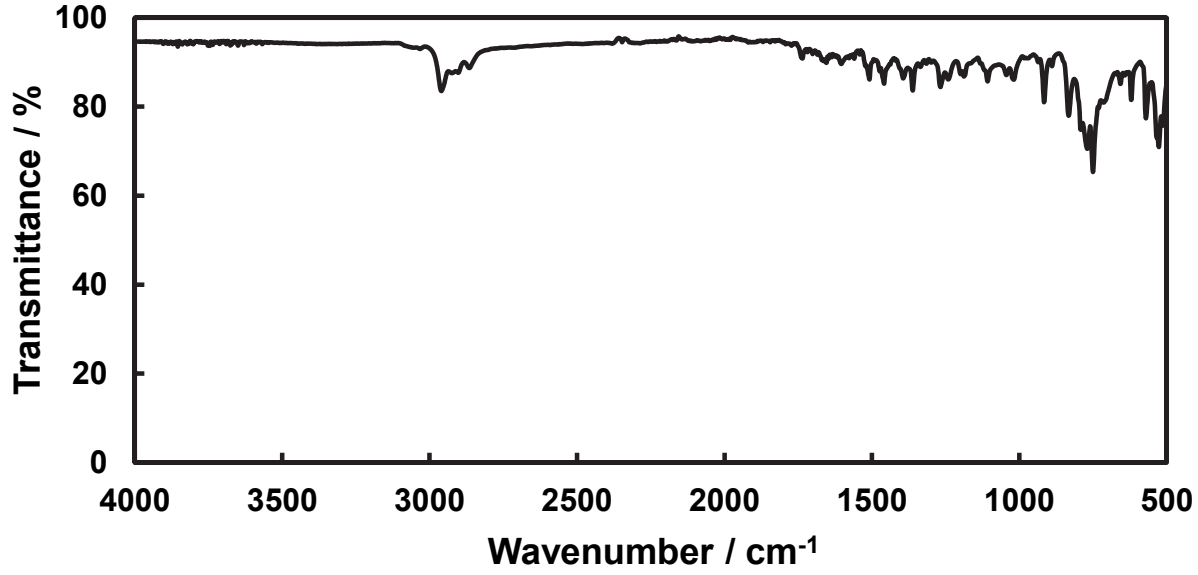

Fig. S9 FTIR spectrum of **BBT-Ph*t*Bu2Sn2**.

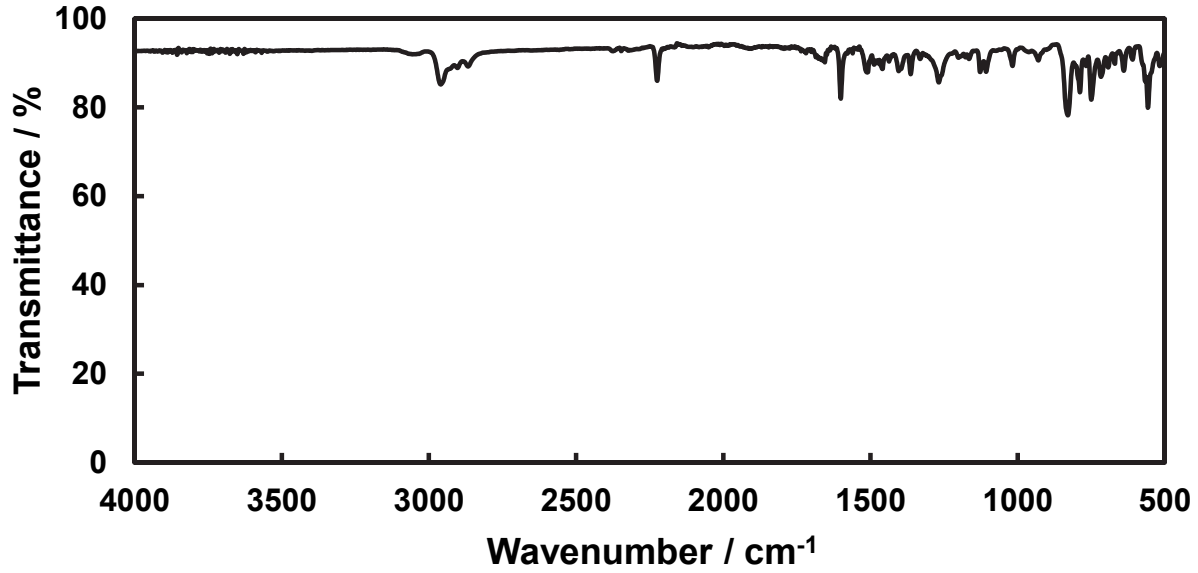

Fig. S10 FTIR spectrum of **BBT-Ph*t*Bu2PhCN2**.

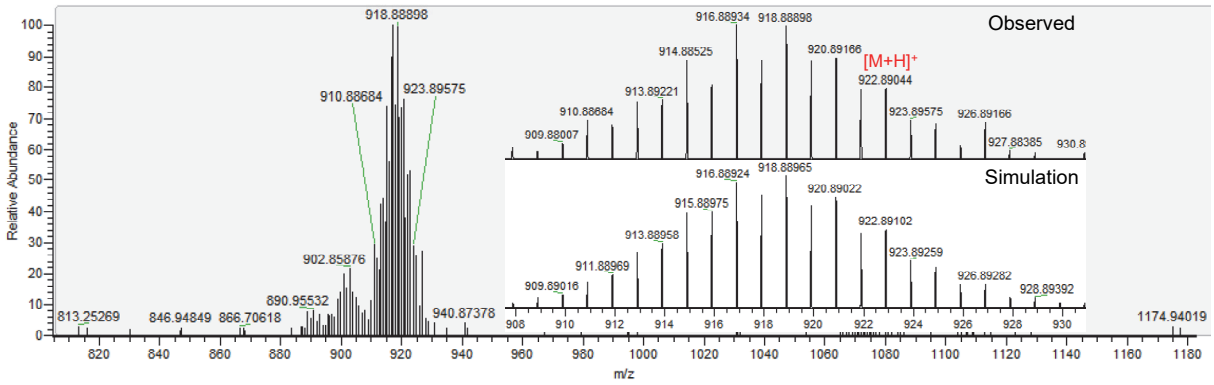

Fig. S11 HRMS (APCI) of **BBT-Sn4**.

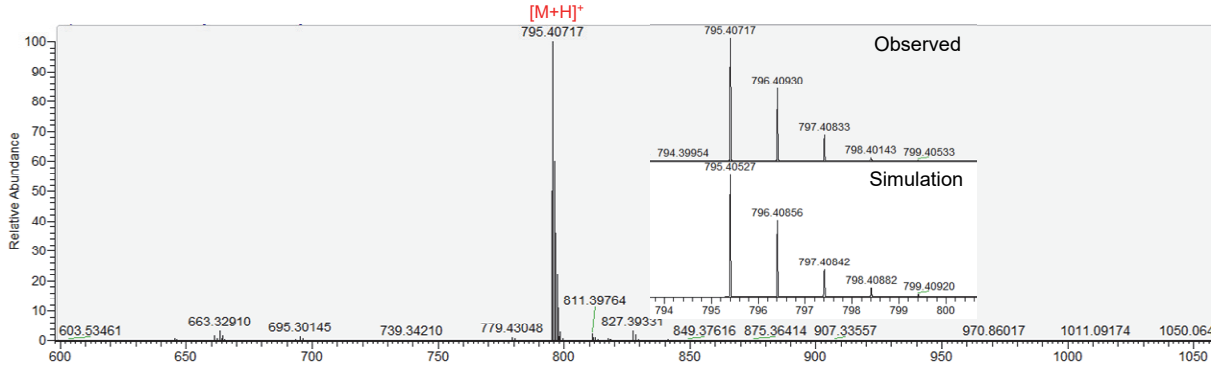

Fig. S12 HRMS (APCI) of **BBT-Ph*t*Bu4**.

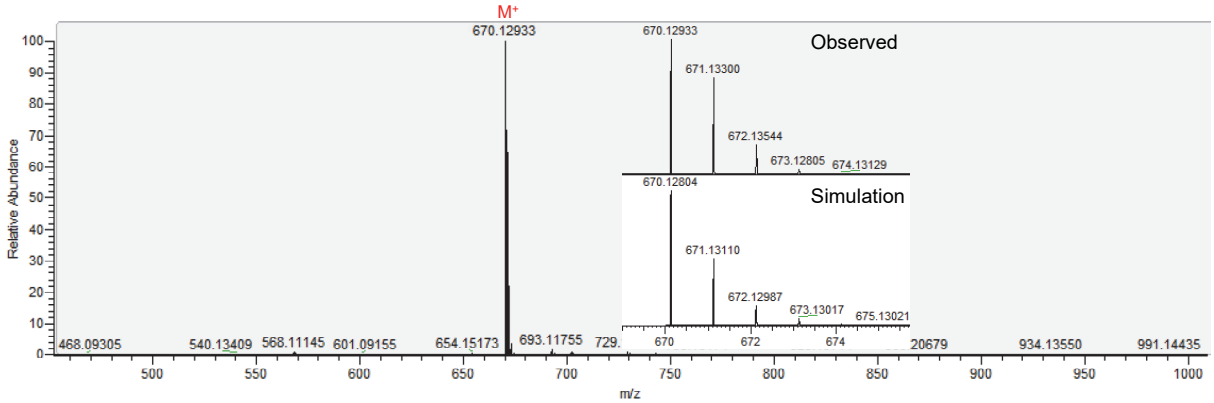

Fig. S13 HRMS (APCI) of **BBT-PhCN4**.

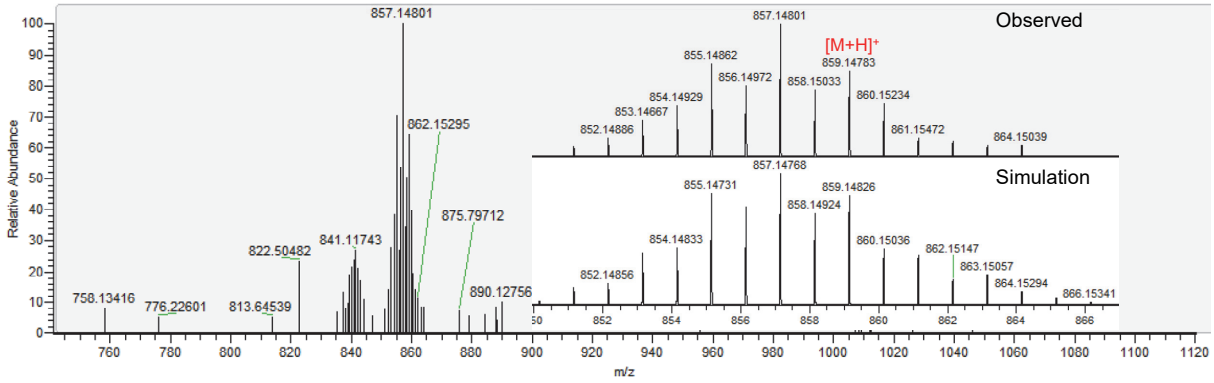

Fig. S14 HRMS (APCI) of **BBT-Ph*t*Bu2Sn2**.

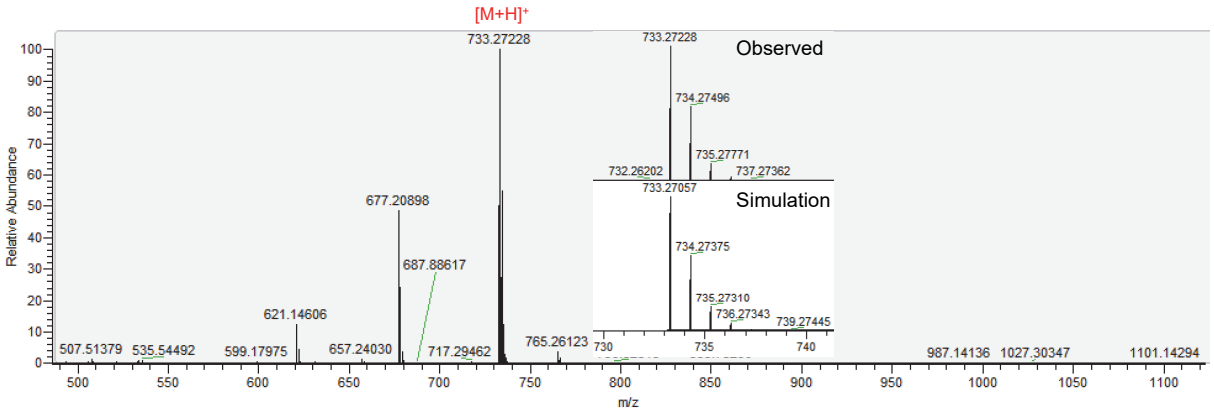

Fig. S15 HRMS (APCI) of **BBT-Ph*t*Bu2PhCN2**.

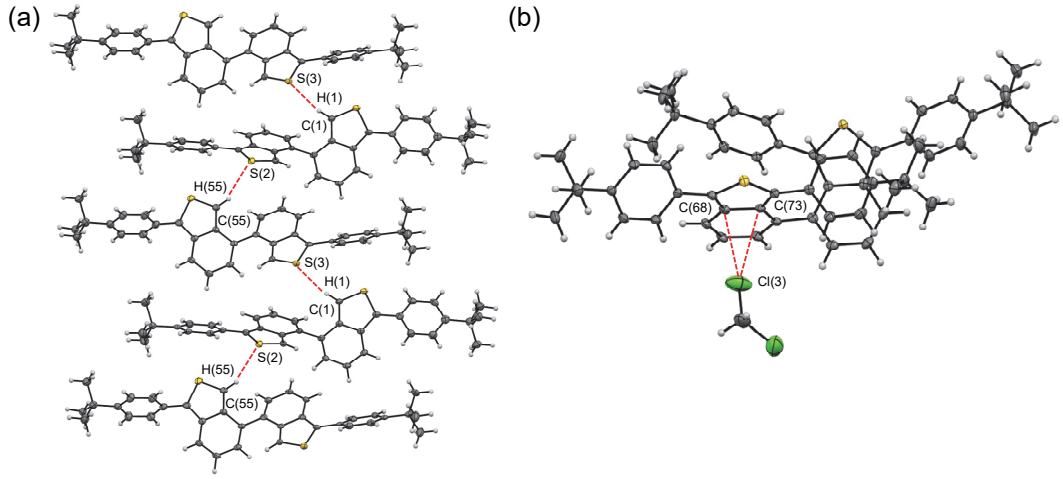

Fig. S16 (a) Intermolecular CH···S hydrogen bonding interactions (C(1)H(1)···S(3) angle = 162.85°, C(1)···S(3) distance = 3.833 Å, H(1)···S(3) distance = 2.915 Å and C(55)H(55)···S(2) angle = 153.77°, C(55)···S(2) distance = 3.668 Å, H(55)···S(2) distance = 2.792 Å) in the crystal structure of **BBT-Ph*t*Bu2** and (b) the short interatomic contacts (C(68)···Cl(3) distance = 3.362 Å and C(73)···Cl(3) distance = 3.397 Å) between the carbon atom of benzo[*c*]thiophene unit and the chlorine atom of CH_2Cl_2 were observed in the crystal structure of in the crystal structure of **BBT-Ph*t*Bu4**.

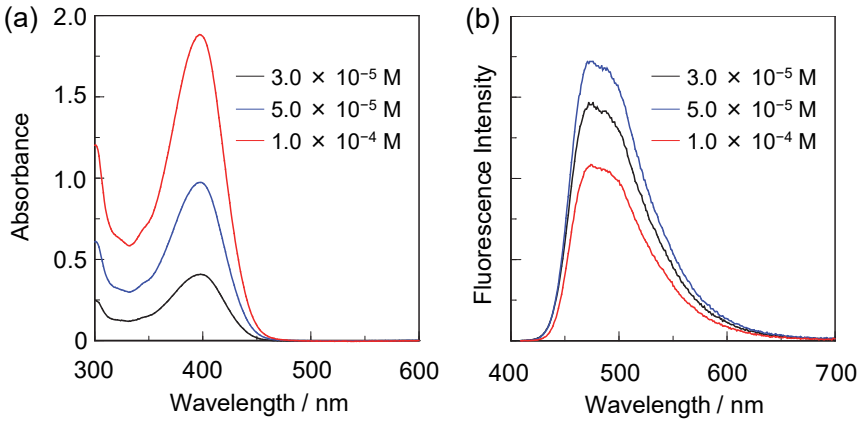

Fig. S17 (a) Photoabsorption and (b) fluorescence spectra (λ^{ex} = 399 nm) of **BBT-PhCN2** at various concentrations (3.0×10^{-5} M, 5.0×10^{-5} M, and 1.0×10^{-4} M) in toluene.

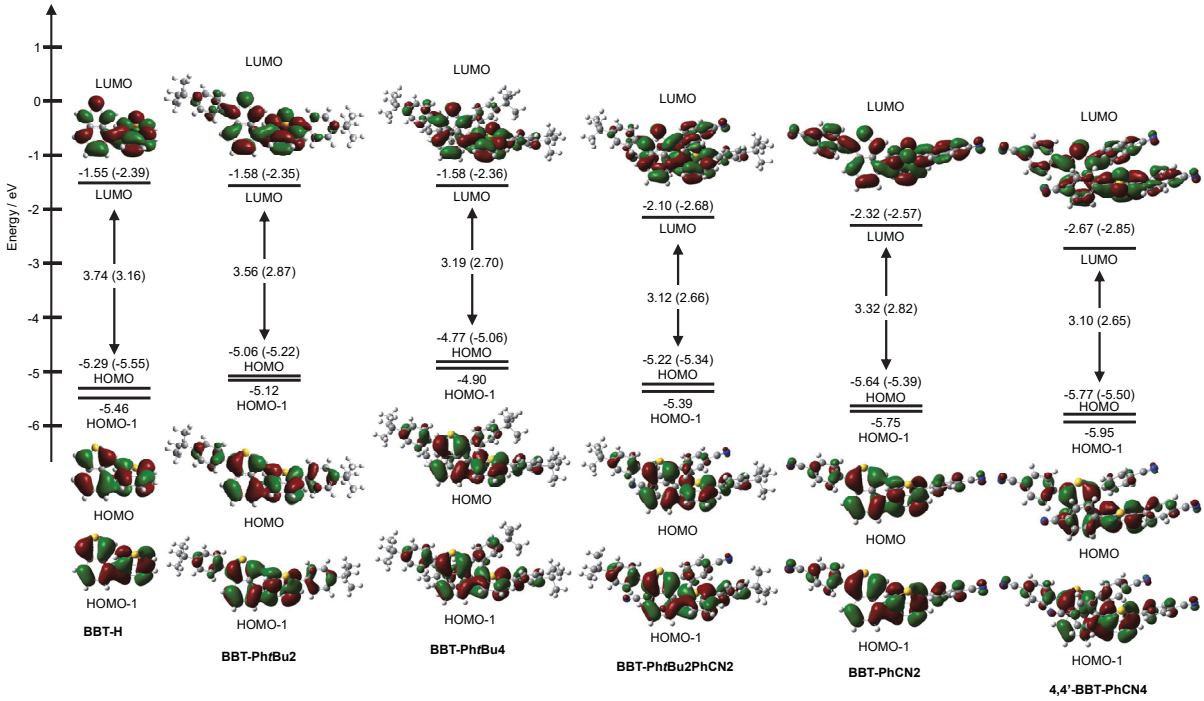

Fig. S18 Energy level diagram, HOMO, HOMO–1, and LUMO of **BBT-H**, **BBT-Ph*t*Bu2**, **BBT-Ph*t*Bu2**, **BBT-Ph*t*Bu2PhCN2**, **BBT-PhCN2**, and **BBT-PhCN4** derived from DFT calculations at the B3LYP/6-31G(d,p) level. For all the 4,4'-BBT derivatives the optimized geometries are a *syn-clinal* (*sc*) conformation. Numbers in parentheses are the experimental values (Table 1).

Table S1 Crystal data and structure refinement parameters for **BBT-Ph*t*Bu2** (CCDC 2248179) and **BBT-Ph*t*Bu4** (CCDC 2337948).

Compound	**BBT-Ph*t*Bu2**	**BBT-Ph*t*Bu4**
Molecular formula	$C_{36}H_{34}S_2$	$C_{57}H_{60}Cl_2S_2$
Formula weight	530.75	880.07
Number of reflection used for unit cell determination (2θ range/°)	51532 (3.606-50.7)	84132 (3.606-50.7)
Temperature/K	100	100
Crystal System	monoclinic	triclinic
Space group	$P2_1/n$	P-1
a/Å	10.3004(2)	14.4868(3)
b/Å	11.6368(3)	15.5221(5)
c/Å	47.0635(14)	22.5994(6)
α/°		75.521(2)
β/°	92.625(3)	80.754(2)
γ/°		84.376(2)
V/Å^3	5635.3(3)	4847.6(2)
Z	8	4
D_c/g cm^{-3}	1.251	1.206
F(000)	2256	1872
Radiation	Mo-Kα (λ = 0.71073 Å)	Mo-Kα (λ = 0.71073 Å)
Crystal size/mm^3	0.145×0.113×0.024	0.2×0.062×0.052
Range of induces *h*; *k*; *l*	-12, 12; -14, 14; -56, 56	-19, 19; -20, 20; -29, 29
Reflections collected (unique)	10317	23124
Reflection observed with $I_0>2\sigma I_0$	7324	16714
Number of parameters	697	1181
Final R indexes [$I_0>2\sigma I_0$]	R_1 = 0.0664, wR_2 =0.1488	R_1 = 0.0623, wR_2 =0.1496
Final R indexes [all data]	R_1 = 0.0994, wR_2 =0.1642	R_1 = 0.0922, wR_2 =0.1634
Goodness-of-fit on F^2	1.049	1.015
Max. Shift/Error in final cycle	0.00	0.00
Max. peak in final diff. map/e Å^{-3}	0.58	0.87
Min. peak in final diff. map/e Å^{-3}	-0.48	-1.33

Table S2 Geometrical coordinates of the optimized **BBT-H** by DFT at the B3LYP/6-31G(d,p) level.[1]

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	0	3.014613	0.092656	0.246587
2	C	0	3.469568	1.192933	1.038642
3	C	0	2.586725	2.181467	1.372708
4	C	0	1.21901	2.12832	0.956653
5	C	0	0.713504	1.089175	0.210163
6	C	0	1.622641	0.033794	-0.17567
7	S	0	2.781034	-2.035549	-1.172737
8	C	0	-1.622642	0.033794	0.17567
9	C	0	-0.713504	1.089175	-0.210163
10	C	0	-1.21901	2.128319	-0.956655
11	C	0	-2.586726	2.181466	-1.372709
12	C	0	-3.469569	1.192933	-1.038641
13	C	0	-3.014613	0.092656	-0.246585
14	S	0	-2.781033	-2.035551	1.172734
15	H	0	4.506637	1.23322	1.358132
16	H	0	2.916292	3.02579	1.971013
17	H	0	0.549238	2.927872	1.258602
18	H	0	-0.549238	2.927871	-1.258604
19	H	0	-2.916292	3.025789	-1.971014
20	H	0	-4.506638	1.23322	-1.35813
21	C	0	3.751548	-0.981598	-0.225472
22	H	0	4.800145	-1.191301	-0.070182
23	C	0	1.369808	-1.078593	-0.963293
24	H	0	0.437756	-1.375725	-1.419233
25	C	0	-1.369809	-1.078591	0.963295
26	H	0	-0.437757	-1.375723	1.419236
27	C	0	-3.751549	-0.981596	0.225475
28	H	0	-4.800146	-1.191299	0.070187

Table S3 Geometrical coordinates of the optimized **BBT-Ph*t*Bu2** by DFT at the B3LYP/6-31G(d,p) level.[1]

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	0	1.620738	1.023449	-0.238209

2	C	0	3.025876	1.083365	0.133791
3	C	0	3.480829	2.153026	0.966515
4	C	0	2.599335	3.125970	1.351629
5	C	0	1.227636	3.087165	0.953848
6	C	0	0.714470	2.062505	0.193584
7	C	0	1.336319	-0.081327	-1.024700
8	C	0	3.769099	0.014305	-0.378440
9	H	0	4.513994	2.178448	1.294241
10	H	0	2.936109	3.941171	1.985304
11	H	0	0.560206	3.875452	1.288908
12	C	0	-0.723119	2.057954	-0.192642
13	C	0	-1.620980	1.009232	0.233300
14	C	0	-1.244761	3.083294	-0.946208
15	C	0	-3.026897	1.060861	-0.136954
16	C	0	-1.327522	-0.098276	1.012655
17	C	0	-2.617111	3.114170	-1.342468
18	H	0	-0.583701	3.878787	-1.276837
19	C	0	-3.490857	2.132239	-0.962509
20	C	0	-3.761439	-0.016958	0.369271
21	H	0	-2.960676	3.930748	-1.970701
22	H	0	-4.524518	2.151998	-1.289170
23	S	0	2.735530	-1.032475	-1.302779
24	S	0	-2.719378	-1.061424	1.286306
25	C	0	-5.191529	-0.323611	0.241465
26	C	0	-5.642122	-1.634856	0.021131
27	C	0	-6.168773	0.683249	0.357653
28	C	0	-7.001455	-1.925985	-0.083290
29	H	0	-4.916929	-2.436052	-0.089229
30	C	0	-7.521328	0.384853	0.239351
31	H	0	-5.862729	1.701833	0.572165
32	C	0	-7.977949	-0.925731	0.015913
33	H	0	-7.291094	-2.955810	-0.257229
34	H	0	-8.237111	1.195472	0.340234
35	C	0	5.201196	-0.282539	-0.250771
36	C	0	6.170612	0.728347	-0.353774
37	C	0	5.659903	-1.596599	-0.041115
38	C	0	7.529954	0.440675	-0.233028
39	H	0	5.859547	1.747053	-0.560373
40	C	0	7.017124	-1.875039	0.064558

41	H	0	4.939188	-2.403175	0.058676
42	C	0	7.991545	-0.865298	-0.021292
43	H	0	8.234102	1.259752	-0.323341
44	H	0	7.320017	-2.904717	0.230199
45	C	0	-9.485922	-1.207807	-0.103694
46	C	0	-10.194232	-0.784326	1.205258
47	C	0	-10.068685	-0.397330	-1.285873
48	C	0	-9.783967	-2.698677	-0.350176
49	H	0	-9.806257	-1.347436	2.060215
50	H	0	-10.056906	0.280065	1.417014
51	H	0	-11.271276	-0.973248	1.133891
52	H	0	-9.591034	-0.681927	-2.229011
53	H	0	-11.144773	-0.581379	-1.380499
54	H	0	-9.926232	0.678901	-1.151312
55	H	0	-10.865229	-2.850065	-0.429325
56	H	0	-9.332181	-3.056357	-1.281161
57	H	0	-9.422617	-3.327826	0.469783
58	C	0	9.483081	-1.218948	0.113186
59	C	0	9.735187	-1.865939	1.496049
60	C	0	9.877491	-2.219551	-0.999142
61	C	0	10.390958	0.019082	-0.010132
62	H	0	9.471771	-1.176559	2.304760
63	H	0	9.148300	-2.779060	1.631881
64	H	0	10.792881	-2.130630	1.605747
65	H	0	9.716301	-1.785638	-1.991275
66	H	0	10.936574	-2.487300	-0.912821
67	H	0	9.295294	-3.143808	-0.940900
68	H	0	11.438677	-0.280433	0.094187
69	H	0	10.283797	0.508253	-0.983784
70	H	0	10.180459	0.758259	0.769674
71	H	0	0.386327	-0.369831	-1.448330
72	H	0	-0.374954	-0.382235	1.433564

Table S4 Geometrical coordinates of the optimized **BBT-PhCN2** by DFT at the B3LYP/6-31G(d,p) level.[1]

Cartesian coordinates:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	C	0	-0.249146	1.611493	0.866384

2	C	0	0.120699	3.016993	0.901592
3	C	0	0.865542	3.510639	2.017186
4	C	0	1.236605	2.647208	3.012357
5	C	0	0.903384	1.260144	2.958729
6	C	0	0.179881	0.721690	1.920006
7	C	0	-0.395896	3.738311	-0.183192
8	H	0	1.108075	4.564956	2.083962
9	H	0	1.795246	3.017025	3.866865
10	H	0	1.237068	0.607500	3.759591
11	C	0	-0.179881	-0.721690	1.920006
12	C	0	0.249146	-1.611493	0.866384
13	C	0	-0.903384	-1.260144	2.958729
14	C	0	-0.120699	-3.016993	0.901592
15	C	0	-1.236605	-2.647208	3.012357
16	H	0	-1.237068	-0.607500	3.759591
17	C	0	-0.865542	-3.510639	2.017186
18	C	0	0.395896	-3.738311	-0.183192
19	H	0	-1.795246	-3.017025	3.866865
20	H	0	-1.108075	-4.564956	2.083962
21	C	0	-0.236755	5.152114	-0.530686
22	C	0	-1.304628	5.890395	-1.080503
23	C	0	0.997236	5.809469	-0.347514
24	C	0	-1.153412	7.225749	-1.426795
25	H	0	-2.269605	5.412318	-1.215891
26	C	0	1.153170	7.148693	-0.679028
27	H	0	1.847973	5.252397	0.027988
28	C	0	0.077847	7.871746	-1.222424
29	H	0	-1.987123	7.780460	-1.843623
30	H	0	2.110349	7.638774	-0.536387
31	C	0	0.236755	-5.152114	-0.530686
32	C	0	1.304628	-5.890395	-1.080503
33	C	0	-0.997236	-5.809469	-0.347514
34	C	0	1.153412	-7.225749	-1.426795
35	H	0	2.269605	-5.412318	-1.215891
36	C	0	-1.153170	-7.148693	-0.679028
37	H	0	-1.847973	-5.252397	0.027988
38	C	0	-0.077847	-7.871746	-1.222424
39	H	0	1.987123	-7.780460	-1.843623
40	H	0	-2.110349	-7.638774	-0.536387

41	C	0	-0.236755	-9.252526	-1.568717
42	N	0	-0.366177	-10.374434	-1.849540
43	C	0	0.236755	9.252526	-1.568717
44	N	0	0.366177	10.374434	-1.849540
45	S	0	-1.338062	2.688549	-1.198553
46	S	0	1.338062	-2.688549	-1.198553
47	C	0	1.050890	-1.310846	-0.224295
48	C	0	-1.050890	1.310846	-0.224295
49	H	0	-1.470469	0.354420	-0.497486
50	H	0	1.470469	-0.354420	-0.497486

Table S5 Geometrical coordinates of the optimized **BBT-Ph*t*Bu4** by DFT at the B3LYP/6-31G(d,p) level.[1]

Cartesian coordinates:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	C	0	1.592273	-0.590026	1.476862
2	C	0	3.035406	-0.384420	1.566947
3	C	0	3.592213	0.316216	2.680315
4	C	0	2.763358	0.832492	3.635656
5	C	0	1.349921	0.710615	3.510727
6	C	0	0.744807	0.046072	2.465714
7	C	0	1.245417	-1.406157	0.392606
8	C	0	3.753410	-0.996249	0.534490
9	H	0	4.668591	0.405387	2.770665
10	H	0	3.175119	1.352954	4.495365
11	H	0	0.715873	1.178175	4.258200
12	C	0	-0.747129	-0.012962	2.465017
13	C	0	-1.593438	0.618414	1.472198
14	C	0	-1.353441	-0.672478	3.512532
15	C	0	-3.036693	0.413373	1.561663
16	C	0	-1.245349	1.429262	0.384365
17	C	0	-2.767016	-0.793701	3.636482
18	H	0	-0.720256	-1.136454	4.262962
19	C	0	-3.594798	-0.281817	2.677831
20	C	0	-3.753442	1.020312	0.525471
21	H	0	-3.179747	-1.310040	4.498208
22	H	0	-4.671278	-0.370282	2.767859
23	S	0	2.665217	-1.843059	-0.506021

24	S	0	-2.664068	1.861551	-0.518125
25	C	0	-5.196601	1.031188	0.256638
26	C	0	-5.841847	2.184844	-0.218381
27	C	0	-5.989162	-0.118707	0.438540
28	C	0	-7.208061	2.190841	-0.494919
29	H	0	-5.269231	3.097555	-0.355775
30	C	0	-7.353589	-0.099347	0.171785
31	H	0	-5.522772	-1.041763	0.764592
32	C	0	-8.003526	1.053119	-0.302672
33	H	0	-7.651296	3.111722	-0.855887
34	H	0	-7.919541	-1.013685	0.324848
35	C	0	5.196900	-1.008261	0.267667
36	C	0	5.989549	0.137971	0.444779
37	C	0	5.842246	-2.168625	-0.201468
38	C	0	7.359429	0.118880	0.182214
39	H	0	5.524298	1.063782	0.764666
40	C	0	7.205016	-2.174309	-0.472091
41	H	0	5.267966	-3.080705	-0.335884
42	C	0	8.005475	-1.034045	-0.283087
43	H	0	7.919721	1.034250	0.334365
44	H	0	7.655003	-3.096586	-0.827700
45	C	0	-9.515151	1.025215	-0.588674
46	C	0	-9.815789	-0.044569	-1.665506
47	C	0	-10.278185	0.671785	0.710115
48	C	0	-10.038479	2.380710	-1.099646
49	H	0	-9.293510	0.183524	-2.600285
50	H	0	-9.505440	-1.043476	-1.345302
51	H	0	-10.890493	-0.081542	-1.876488
52	H	0	-10.090328	1.417155	1.489710
53	H	0	-11.357331	0.640707	0.522072
54	H	0	-9.981035	-0.304620	1.103805
55	H	0	-11.114560	2.312773	-1.288901
56	H	0	-9.882504	3.180112	-0.367950
57	H	0	-9.557089	2.676281	-2.037543
58	C	0	9.513059	-1.090525	-0.585486
59	C	0	10.177158	-2.162534	0.311293
60	C	0	9.727177	-1.463458	-2.071811
61	C	0	10.212912	0.256065	-0.322654
62	H	0	10.048636	-1.920544	1.371274

63	H	0	9.750996	-3.155711	0.142129
64	H	0	11.251525	-2.221220	0.103510
65	H	0	9.273650	-0.717041	-2.731982
66	H	0	10.797437	-1.515288	-2.301450
67	H	0	9.287668	-2.435066	-2.315612
68	H	0	11.280114	0.167403	-0.549795
69	H	0	9.807636	1.055716	-0.951235
70	H	0	10.123430	0.564599	0.724043
71	C	0	0.019581	2.038287	-0.072895
72	C	0	0.805166	2.833536	0.779433
73	C	0	0.410985	1.950634	-1.417180
74	C	0	1.925542	3.502231	0.299663
75	H	0	0.519528	2.941903	1.819344
76	C	0	1.531693	2.632233	-1.892304
77	H	0	-0.170822	1.338900	-2.100218
78	C	0	2.314317	3.431634	-1.049941
79	H	0	2.495316	4.112310	0.994385
80	H	0	1.785524	2.530752	-2.941058
81	C	0	3.530590	4.233484	-1.547070
82	C	0	4.795226	3.805316	-0.766938
83	C	0	3.799576	4.018107	-3.048340
84	C	0	3.274134	5.741977	-1.314575
85	H	0	4.679865	3.958420	0.310309
86	H	0	5.017986	2.747135	-0.935130
87	H	0	5.661473	4.391143	-1.095166
88	H	0	2.954344	4.341420	-3.664557
89	H	0	4.672633	4.603690	-3.354094
90	H	0	4.009372	2.968326	-3.277615
91	H	0	4.129658	6.332514	-1.661697
92	H	0	2.386037	6.076502	-1.860479
93	H	0	3.119679	5.969500	-0.255777
94	C	0	-0.018872	-2.017513	-0.063291
95	C	0	-0.805310	-2.808975	0.791766
96	C	0	-0.408625	-1.936273	-1.408468
97	C	0	-1.924789	-3.480389	0.313669
98	H	0	-0.521023	-2.912328	1.832560
99	C	0	-1.528459	-2.620521	-1.881836
100	H	0	0.173817	-1.327513	-2.093619
101	C	0	-2.311789	-3.416381	-1.036777

102	H	0	-2.495192	-4.087457	1.010518
103	H	0	-1.780975	-2.524039	-2.931379
104	C	0	-3.526895	-4.221301	-1.531788
105	C	0	-4.792811	-3.790591	-0.755130
106	C	0	-3.794206	-4.012827	-3.034332
107	C	0	-3.269669	-5.728548	-1.292241
108	H	0	-4.678549	-3.938564	0.322962
109	H	0	-5.016327	-2.733425	-0.928607
110	H	0	-5.658146	-4.378707	-1.081670
111	H	0	-2.947962	-4.338262	-3.648034
112	H	0	-4.666458	-4.600397	-3.338556
113	H	0	-4.004508	-2.964242	-3.268556
114	H	0	-4.124385	-6.321211	-1.637720
115	H	0	-2.380721	-6.064892	-1.835638
116	H	0	-3.116266	-5.951251	-0.232267

Table S6 Geometrical coordinates of the optimized **BBT-PhCN4** by DFT at the B3LYP/6-31G(d,p) level.[1]

Cartesian coordinates:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	C	0	-1.539639	-0.631102	1.240043
2	C	0	-2.978142	-0.404041	1.232793
3	C	0	-3.600745	0.272017	2.326401
4	C	0	-2.829957	0.736247	3.355977
5	C	0	-1.410399	0.621165	3.310939
6	C	0	-0.745687	-0.002579	2.277711
7	C	0	-3.624360	-0.977256	0.132215
8	H	0	-4.678951	0.383654	2.343458
9	H	0	-3.292759	1.229505	4.205180
10	H	0	-0.822506	1.082759	4.098989
11	C	0	0.745633	0.002636	2.277721
12	C	0	1.539606	0.631141	1.240057
13	C	0	1.410324	-0.621121	3.310956
14	C	0	2.978103	0.404038	1.232815
15	C	0	2.829879	-0.736230	3.356007
16	H	0	0.822415	-1.082706	4.098998
17	C	0	3.600684	-0.272025	2.326433
18	C	0	3.624342	0.977217	0.132231

19	H	0	3.292663	-1.229497	4.205215
20	H	0	4.678887	-0.383690	2.343495
21	C	0	-5.040386	-0.927981	-0.250784
22	C	0	-5.699649	-2.073840	-0.737528
23	C	0	-5.765080	0.278005	-0.173546
24	C	0	-7.032314	-2.023425	-1.123244
25	H	0	-5.163850	-3.016223	-0.792330
26	C	0	-7.100490	0.335559	-0.551812
27	H	0	-5.267126	1.185007	0.149432
28	C	0	-7.747078	-0.817184	-1.028125
29	H	0	-7.530628	-2.914605	-1.489142
30	H	0	-7.640153	1.274879	-0.500572
31	C	0	5.040366	0.927883	-0.250772
32	C	0	5.699675	2.073711	-0.737523
33	C	0	5.765007	-0.278135	-0.173534
34	C	0	7.032336	2.023237	-1.123246
35	H	0	5.163916	3.016117	-0.792325
36	C	0	7.100412	-0.335749	-0.551810
37	H	0	5.267015	-1.185115	0.149450
38	C	0	7.747047	0.816965	-1.028129
39	H	0	7.530686	2.914393	-1.489149
40	H	0	7.640032	-1.275095	-0.500574
41	C	0	9.124771	0.765156	-1.419242
42	N	0	10.243932	0.728527	-1.735237
43	C	0	-9.124807	-0.765437	-1.419227
44	N	0	-10.243972	-0.728858	-1.735215
45	S	0	-2.483173	-1.834044	-0.841907
46	S	0	2.483187	1.834039	-0.841898
47	C	0	1.131691	1.440701	0.171327
48	C	0	-1.131694	-1.440658	0.171323
49	C	0	-0.170174	2.044934	-0.161084
50	C	0	-0.710766	1.934172	-1.455509
51	C	0	-0.876361	2.794901	0.797253
52	C	0	-1.936773	2.506905	-1.772283
53	H	0	-0.173282	1.370454	-2.211104
54	C	0	-2.105132	3.365117	0.493812
55	H	0	-0.451318	2.928997	1.784296
56	C	0	-2.651941	3.214180	-0.792035
58	H	0	-2.646019	3.931164	1.244194

59	C	0	0.170196	-2.044846	-0.161077
60	C	0	0.710788	-1.934083	-1.455501
61	C	0	0.876416	-2.794755	0.797280
62	C	0	1.936823	-2.506765	-1.772258
63	H	0	0.173278	-1.370407	-2.211109
64	C	0	2.105216	-3.364918	0.493857
65	H	0	0.451379	-2.928844	1.784327
66	C	0	2.652022	-3.213983	-0.791991
67	H	0	2.353327	-2.397076	-2.767635
68	H	0	2.646130	-3.930918	1.244255
69	C	0	3.945032	-3.756578	-1.087497
70	N	0	5.008344	-4.174920	-1.309005
71	C	0	-3.944918	3.756842	-1.087562
72	N	0	-5.008207	4.175235	-1.309085

Table S7 Geometrical coordinates of the optimized **BBT-Ph*t*Bu2PhCN2** by DFT at the B3LYP/6-31G(d,p) level.[1]

Cartesian coordinates:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	C	0	1.550349	-0.563683	1.416319
2	C	0	2.983587	-0.303729	1.408122
3	C	0	3.592276	0.392006	2.497156
4	C	0	2.813148	0.845869	3.524958
5	C	0	1.396289	0.698888	3.480319
6	C	0	0.744397	0.053836	2.451623
7	C	0	1.160528	-1.384754	0.350053
8	C	0	3.645714	-0.861971	0.310228
9	H	0	4.667761	0.528667	2.506683
10	H	0	3.264917	1.355738	4.370473
11	H	0	0.797570	1.153769	4.264362
12	C	0	-0.746325	0.029251	2.451237
13	C	0	-1.551694	0.622697	1.401510
14	C	0	-1.398796	-0.593116	3.493504
15	C	0	-2.984586	0.360810	1.397692
16	C	0	-1.161916	1.420103	0.317343
17	C	0	-2.815500	-0.741251	3.539646
18	H	0	-0.800465	-1.029609	4.288222
19	C	0	-3.593860	-0.311714	2.500871

20	C	0	-3.646386	0.893890	0.287354
21	H	0	-3.267568	-1.232957	4.395693
22	H	0	-4.669175	-0.450037	2.511732
23	S	0	2.524439	-1.741172	-0.665772
24	S	0	-2.525642	1.752331	-0.707057
25	C	0	-5.062649	0.798742	-0.091605
26	C	0	-5.770922	1.913168	-0.566769
27	C	0	-5.748831	-0.428382	-0.022963
28	C	0	-7.107553	1.808025	-0.948880
29	H	0	-5.275665	2.878573	-0.619809
30	C	0	-7.083035	-0.521133	-0.401108
31	H	0	-5.221871	-1.321700	0.295231
32	C	0	-7.800596	0.591927	-0.873123
33	H	0	-7.609646	2.700752	-1.303041
34	H	0	-7.564625	-1.492375	-0.343511
35	C	0	5.062465	-0.778538	-0.068986
36	C	0	5.755306	0.441617	-0.017547
37	C	0	5.765700	-1.907331	-0.528300
38	C	0	7.095513	0.524511	-0.393590
39	H	0	5.233661	1.343346	0.285396
40	C	0	7.099140	-1.812358	-0.907493
41	H	0	5.264132	-2.870067	-0.568394
42	C	0	7.803467	-0.596711	-0.847048
43	H	0	7.577070	1.493909	-0.345246
44	H	0	7.602670	-2.711348	-1.250138
45	C	0	-9.274858	0.438482	-1.285921
46	C	0	-9.379145	-0.584342	-2.442527
47	C	0	-10.096594	-0.069834	-0.077366
48	C	0	-9.890609	1.767806	-1.761096
49	H	0	-8.812758	-0.246424	-3.316367
50	H	0	-8.993655	-1.566590	-2.154937
51	H	0	-10.424959	-0.711518	-2.743706
52	H	0	-10.046753	0.638049	0.756461
53	H	0	-11.148832	-0.191174	-0.357661
54	H	0	-9.735471	-1.037295	0.283133
55	H	0	-10.937172	1.609491	-2.039886
56	H	0	-9.870652	2.530737	-0.975900
57	H	0	-9.373164	2.166385	-2.639834
58	C	0	9.280640	-0.539584	-1.273941

59	C	0	10.108269	-1.502075	-0.388983
60	C	0	9.404484	-0.971308	-2.754666
61	C	0	9.874974	0.874343	-1.133479
62	H	0	10.044687	-1.216716	0.666096
63	H	0	9.762930	-2.536420	-0.476559
64	H	0	11.163035	-1.477468	-0.684562
65	H	0	8.832949	-0.302785	-3.406456
66	H	0	10.452629	-0.941778	-3.072587
67	H	0	9.037181	-1.989240	-2.915093
68	H	0	10.924368	0.864670	-1.444715
69	H	0	9.351605	1.601937	-1.761916
70	H	0	9.841761	1.229702	-0.098448
71	C	0	0.117437	2.063543	-0.022689
72	C	0	0.811792	2.832687	0.930026
73	C	0	0.646423	1.979946	-1.324714
74	C	0	2.011897	3.453382	0.611888
75	H	0	0.397479	2.944000	1.924293
76	C	0	1.842326	2.604487	-1.656657
77	H	0	0.121820	1.397634	-2.075285
78	H	0	2.541049	4.035573	1.358389
79	H	0	2.247464	2.516869	-2.658953
80	C	0	-0.119186	-2.035084	0.024704
81	C	0	-0.812453	-2.783610	0.994485
82	C	0	-0.649772	-1.979006	-1.278108
83	C	0	-2.013381	-3.410137	0.691366
84	H	0	-0.396779	-2.873938	1.990314
85	C	0	-1.846635	-2.609582	-1.594953
86	H	0	-0.125938	-1.412964	-2.041545
87	C	0	-2.546242	-3.321100	-0.606287
88	H	0	-2.541848	-3.975918	1.450855
89	H	0	-2.253267	-2.542881	-2.598254
90	C	0	3.797183	3.951924	-1.003813
91	N	0	4.824619	4.439869	-1.251530
92	C	0	2.542834	3.337439	-0.684428
93	C	0	-3.802367	-3.939883	-0.909928
94	N	0	-4.831859	-4.430174	-1.144168

Ref. 1 M. J. Frisch , G. W. Trucks , H. B. Schlegel , G. E. Scuseria , M. A. Robb , J. R. Cheeseman , G. Scalmani , V. Barone , G. A. Petersson , H. Nakatsuji , X. Li , M. Caricato , A. V. Marenich , J. Bloino , B. G. Janesko , R. Gomperts , B. Mennucci , H. P. Hratchian , J. V. Ortiz , A. F. Izmaylov , J. L. Sonnenberg , D. Williams-Young , F. Ding , F. Lipparini , F. Egidi , J. Goings , B. Peng , A. Petrone , T. Henderson , D. Ranasinghe , V. G. Zakrzewski , J. Gao , N. Rega , G. Zheng , W. Liang , M. Hada , M. Ehara , K. Toyota , R. Fukuda , J. Hasegawa , M. Ishida , T. Nakajima , Y. Honda , O. Kitao , H. Nakai , T. Vreven , K. Throssell , J. A. Montgomery, Jr. , J. E. Peralta , F. Ogliaro , M. J. Bearpark , J. J. Heyd , E. N. Brothers , K. N. Kudin , V. N. Staroverov , T. A. Keith , R. Kobayashi , J. Normand , K. Raghavachari , A. P. Rendell , J. C. Burant , S. S. Iyengar , J. Tomasi , M. Cossi , J. M. Millam , M. Klene , C. Adamo , R. Cammi , J. W. Ochterski , R. L. Martin , K. Morokuma , O. Farkas , J. B. Foresman and D. J. Fox , *Gaussian 16, Revision B.01* , Gaussian, Inc., Wallingford CT, 2016.