Supplementary Information file

Aryl-substituted symmetrical and unsymmetrical benzothiadiazoles

Prabhat Gautam, Ramesh Maragani and Rajneesh Misra*

Department of Chemistry,
Indian Institute of Technology Indore,
Indore- 452017, India.

rajneeshmisra@iiti.ac.in

Table of Contents

I. Copies of ^{1}H NMR, ^{13}C NMR spectra and HRMS of BTDs 2, 3, 6, 8 and 9

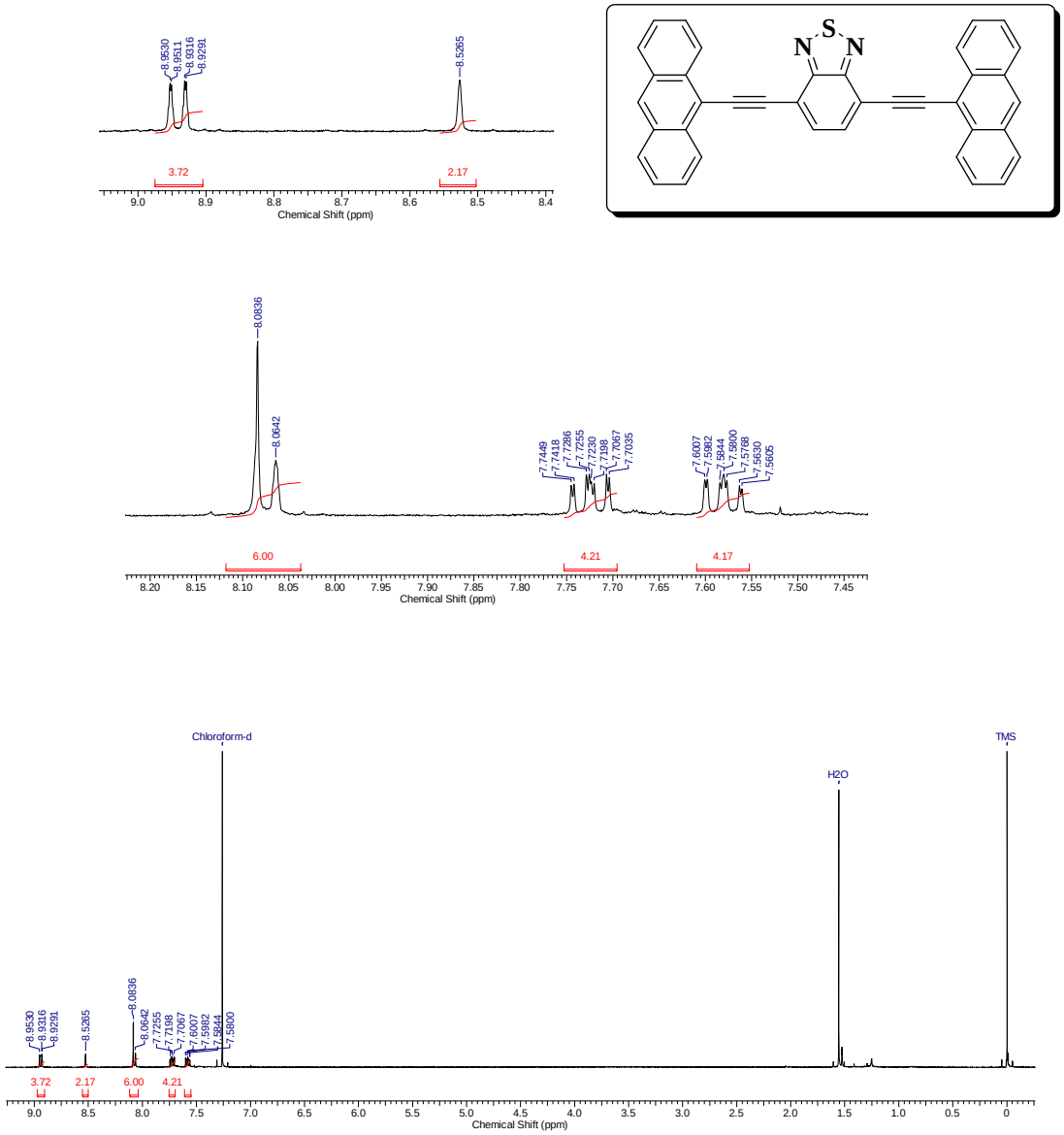


Figure S1. ^{1}H NMR spectrum of BTD **2**.

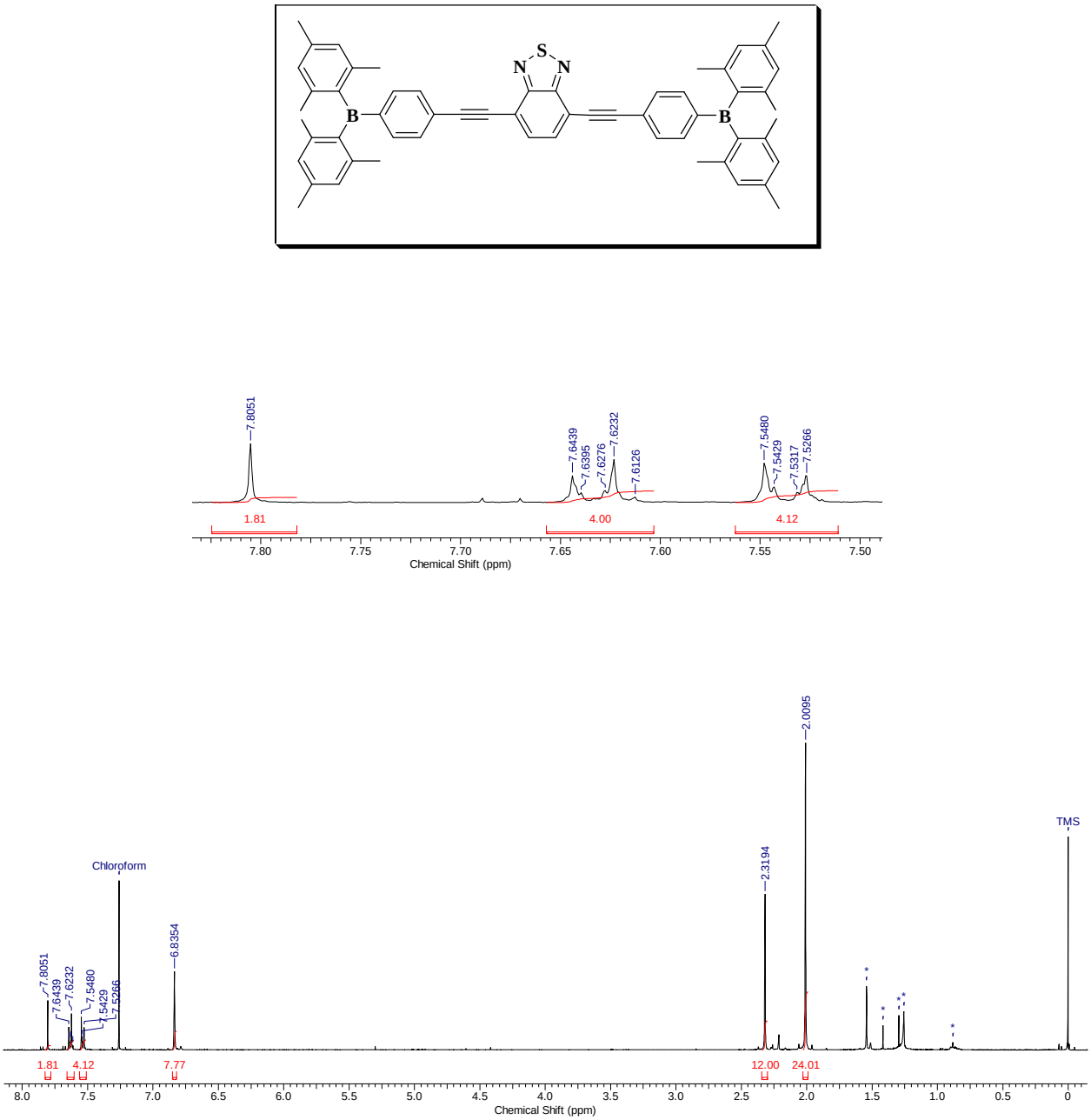
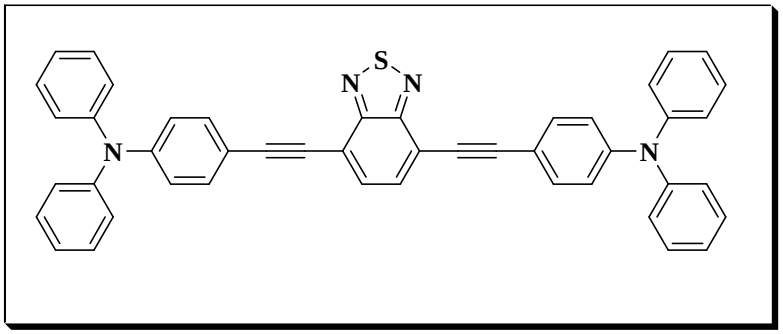
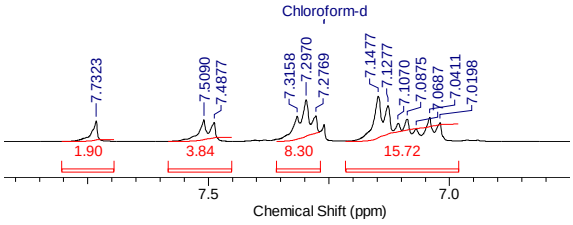


Figure S2. ^{1}H NMR spectrum of BTD **3**.





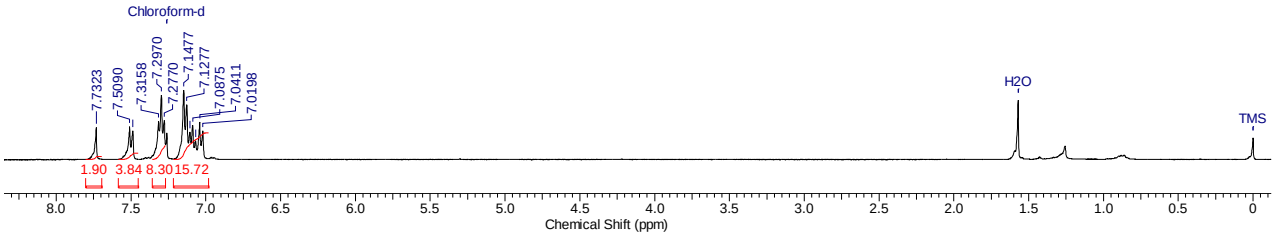


Figure S3. ^{1}H NMR spectrum of BTD **6**.

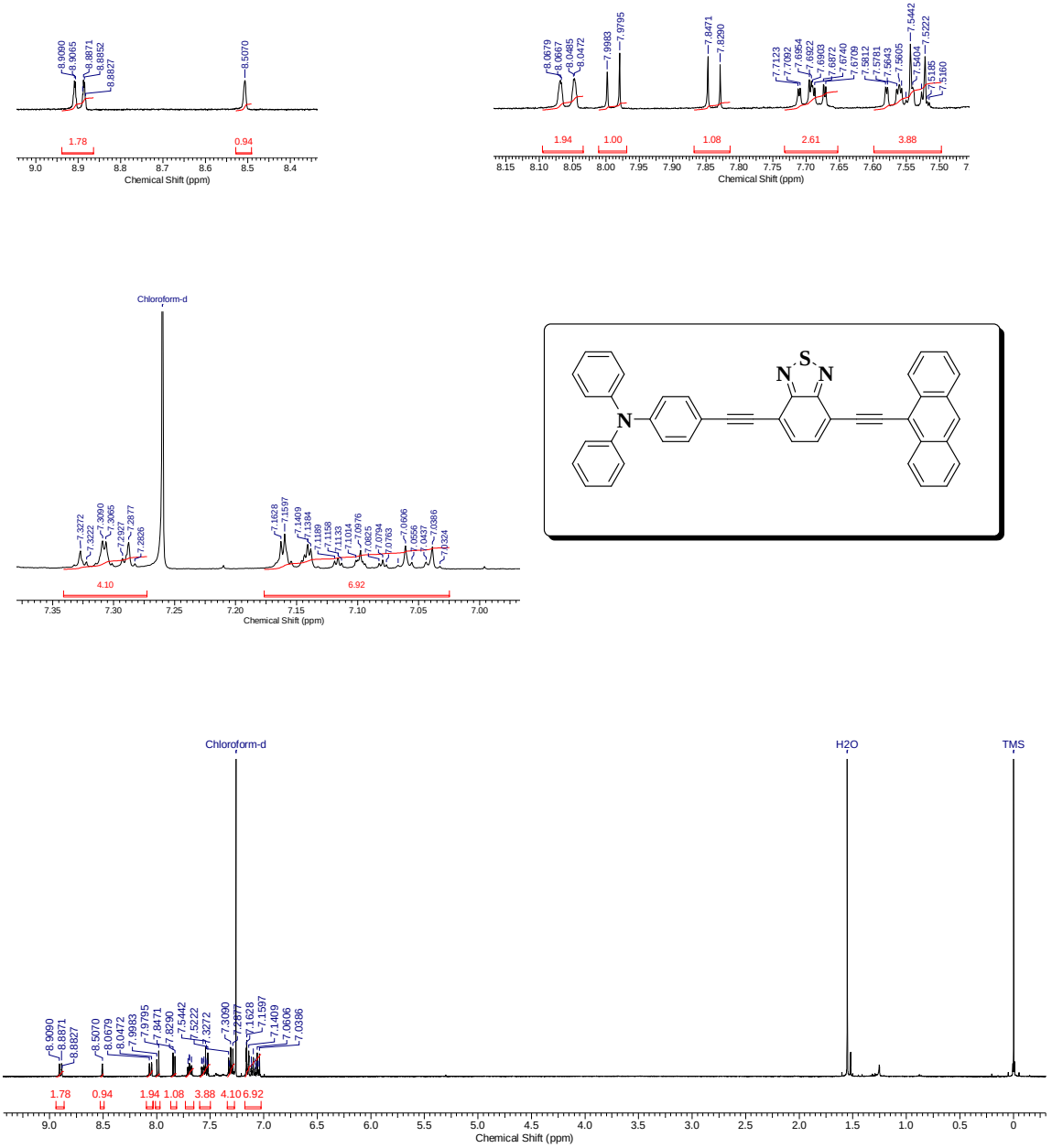


Figure S4. ^{1}H NMR spectrum of BTD **8**.

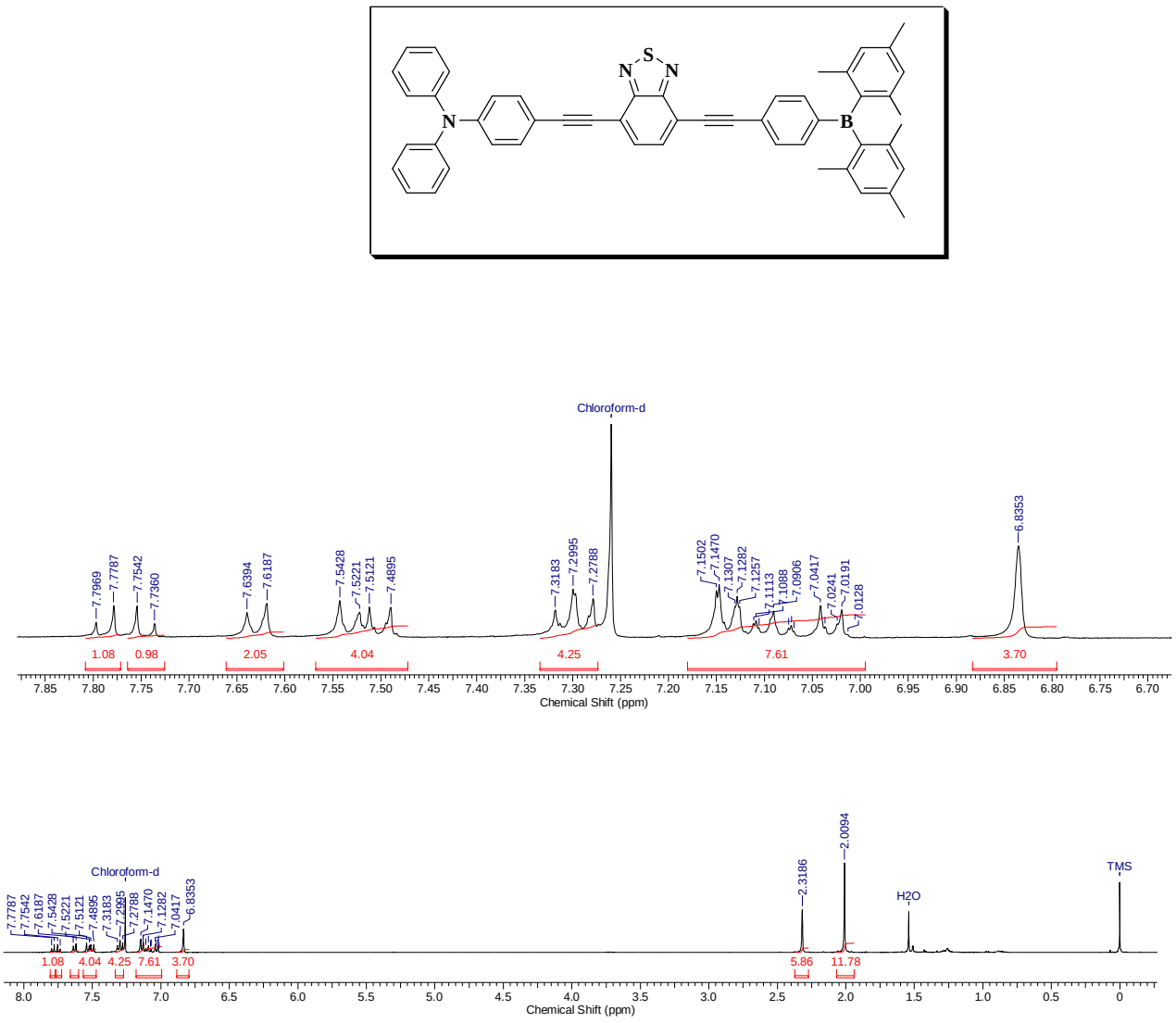


Figure S5. ^{1}H NMR spectrum of BTD **9**.

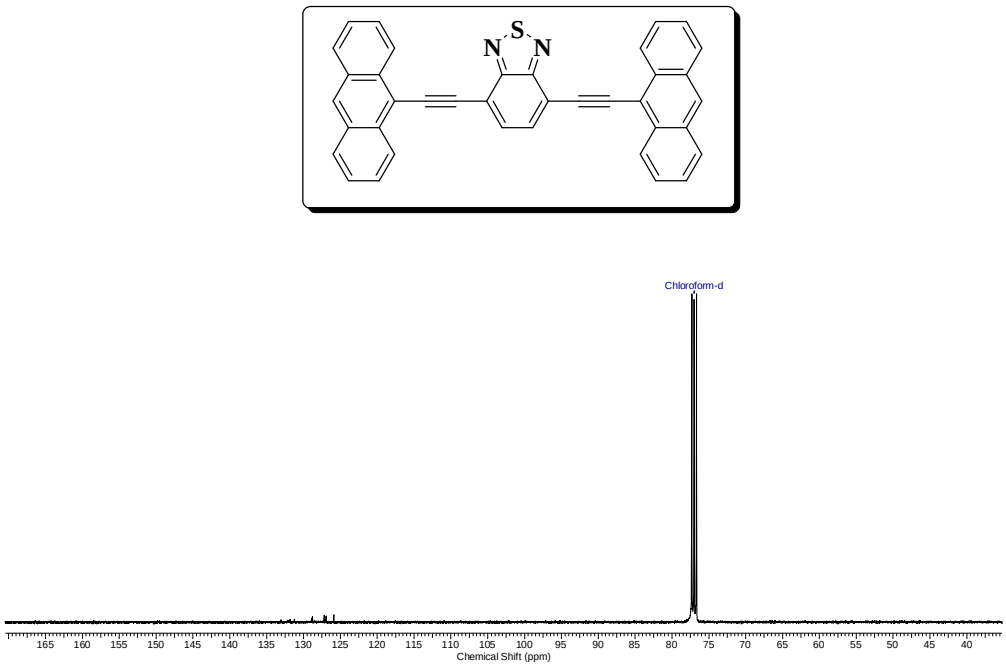


Figure S6. ^{13}C NMR spectrum of BTD **2** (precipitate formation at higher concentration resulted poor spectrum).

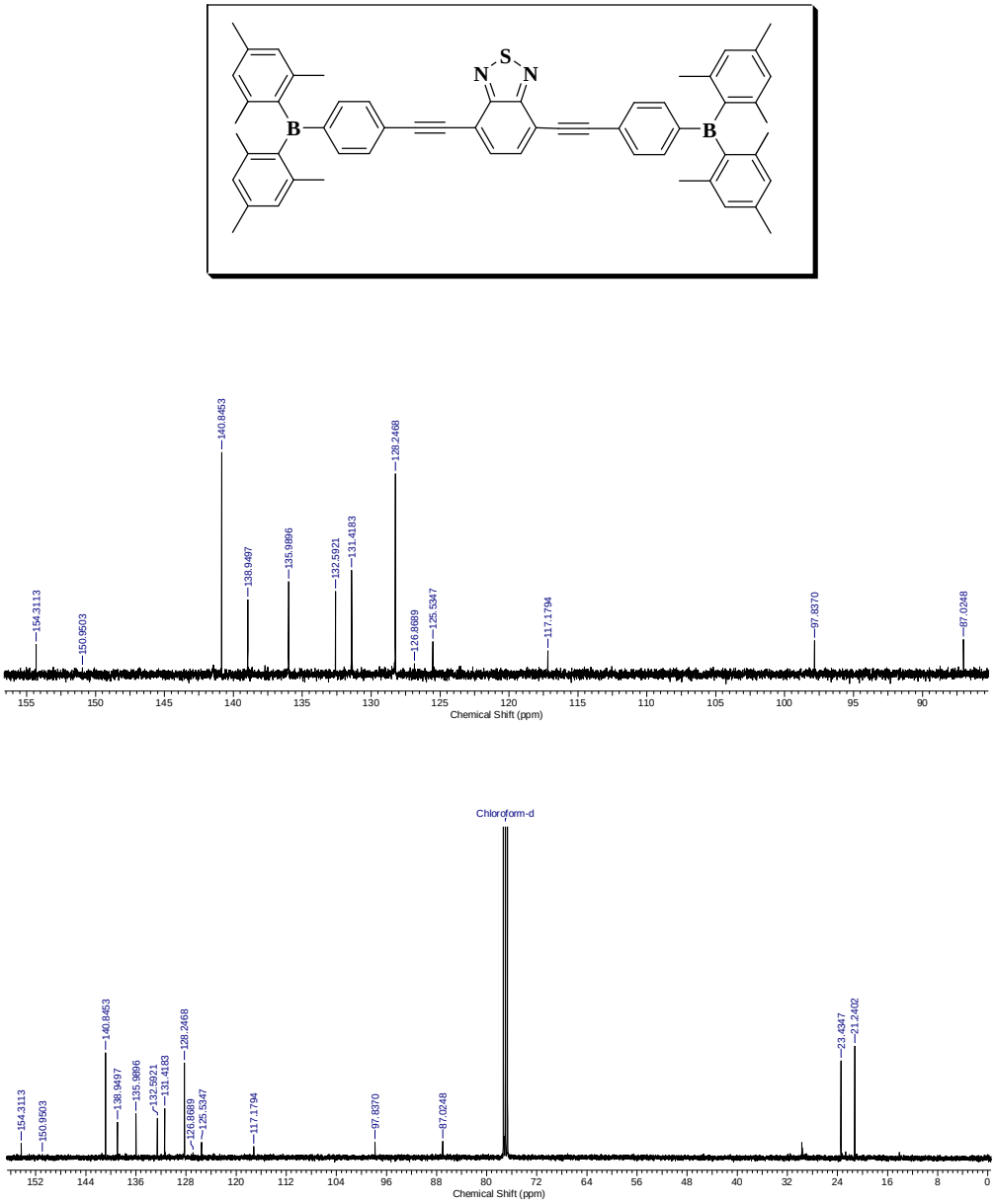


Figure S7. ^{13}C NMR spectrum of BTD **3**.

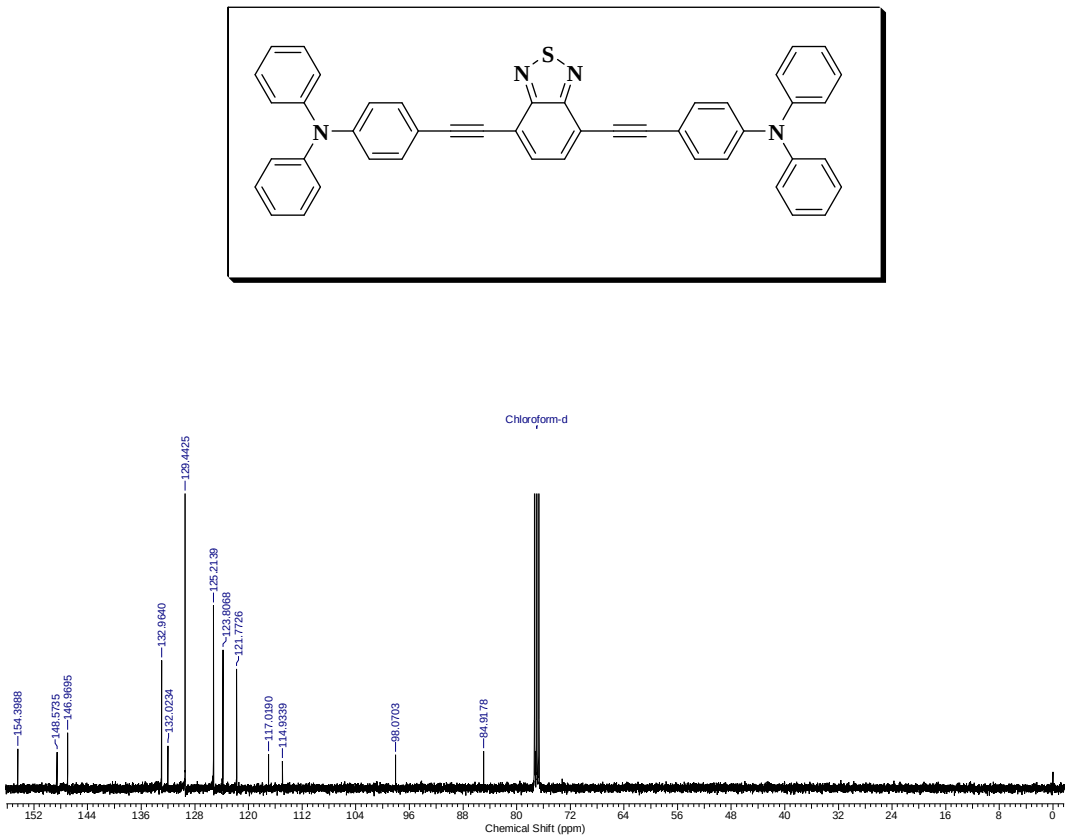


Figure S8. ^{13}C NMR spectrum of BTD **6**.

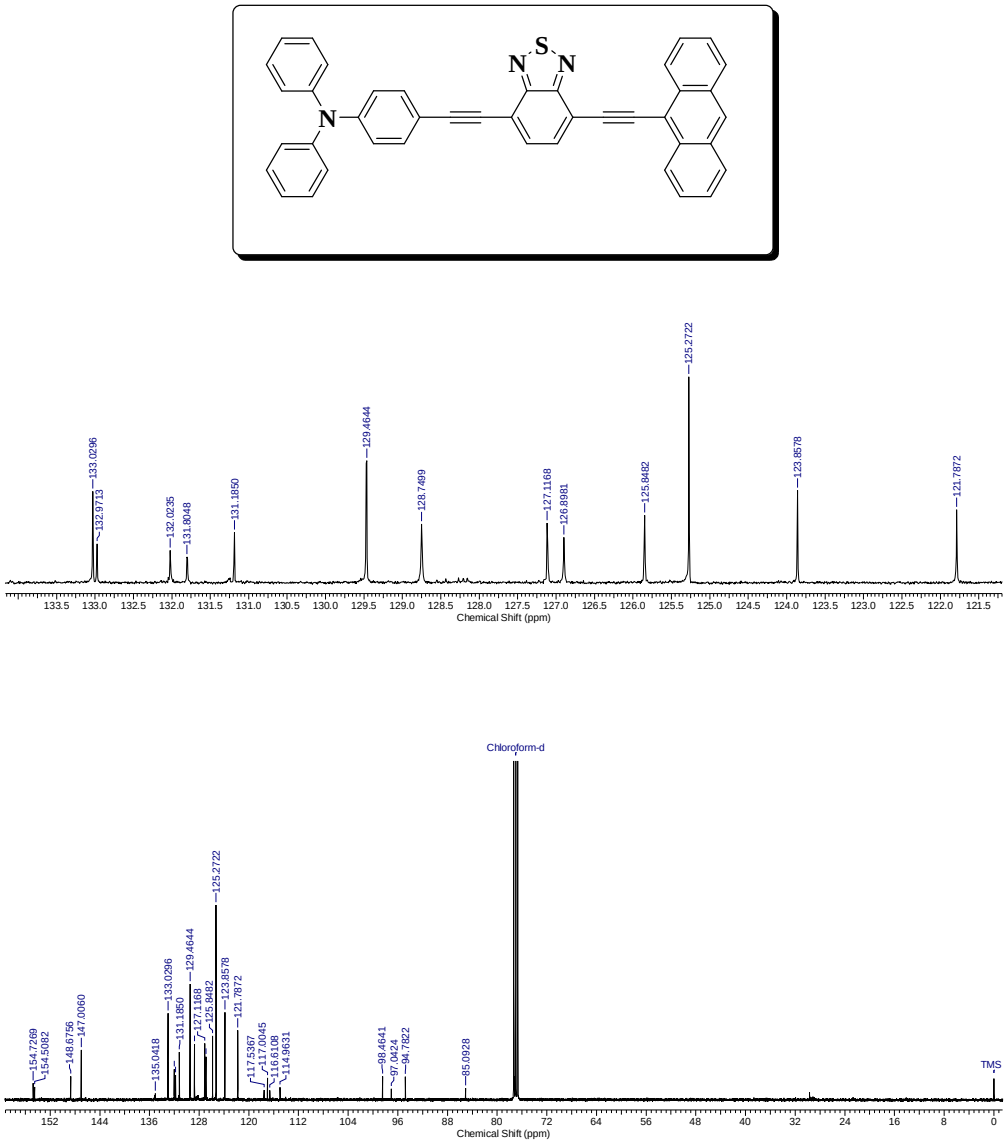


Figure S9. ^{13}C NMR spectrum of BTD **8**.

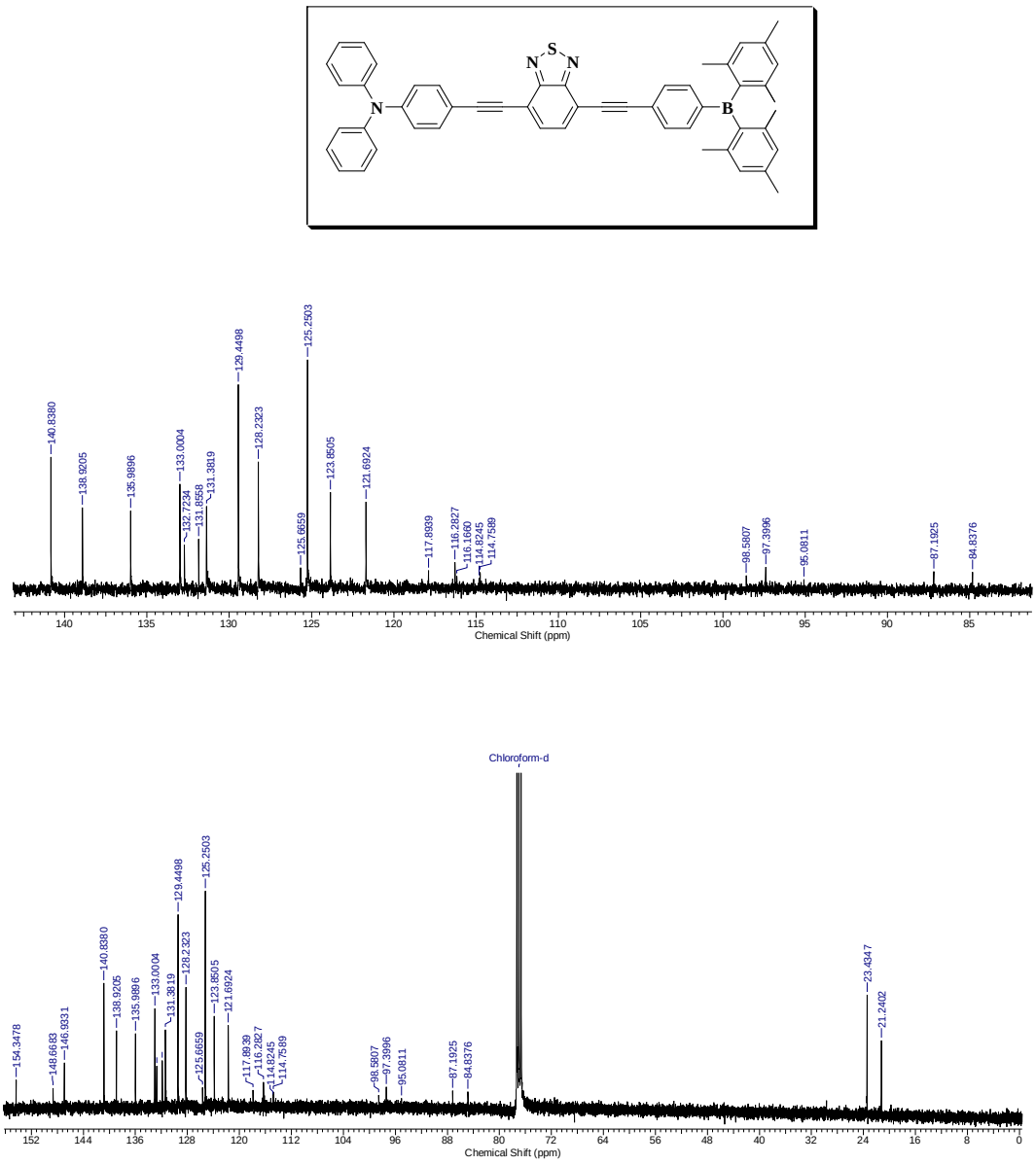
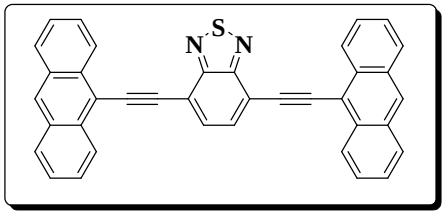


Figure S10. ^{13}C NMR spectrum of BTD **9**.



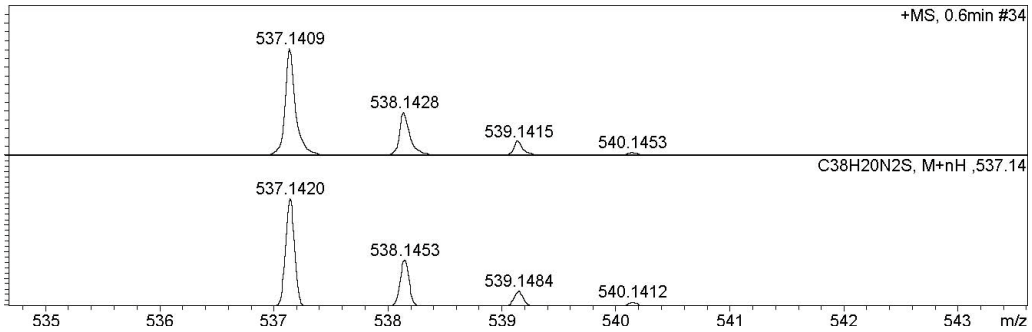


Figure S11. HRMS of BTD **2**.

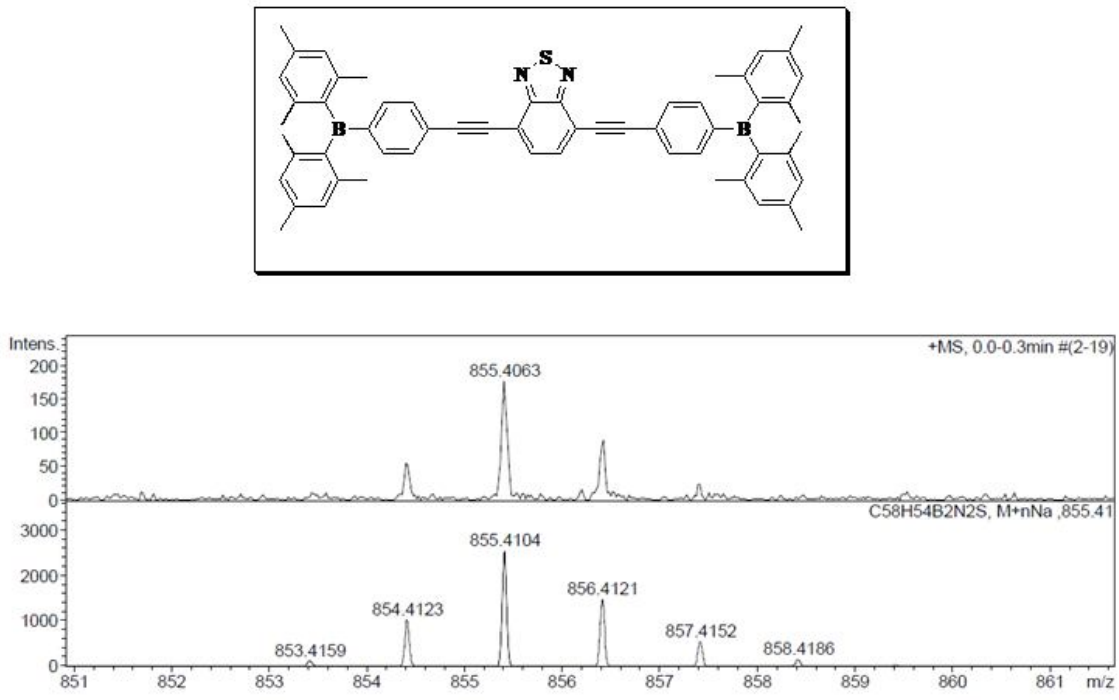


Figure S12. HRMS of BTD **3**.

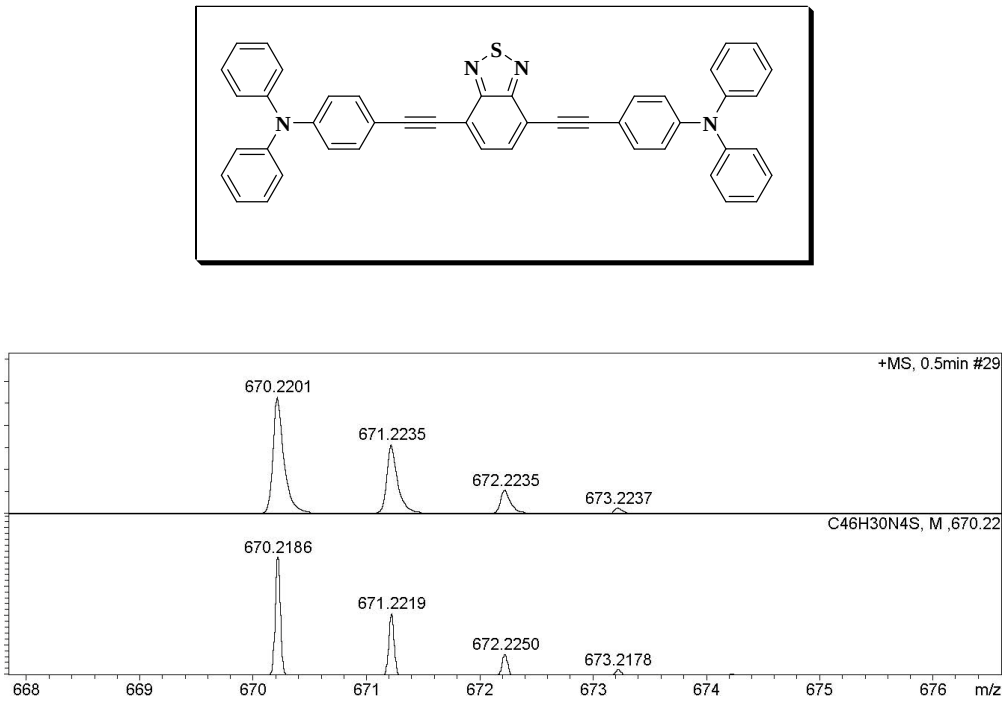


Figure S13. HRMS of BTD **6**.

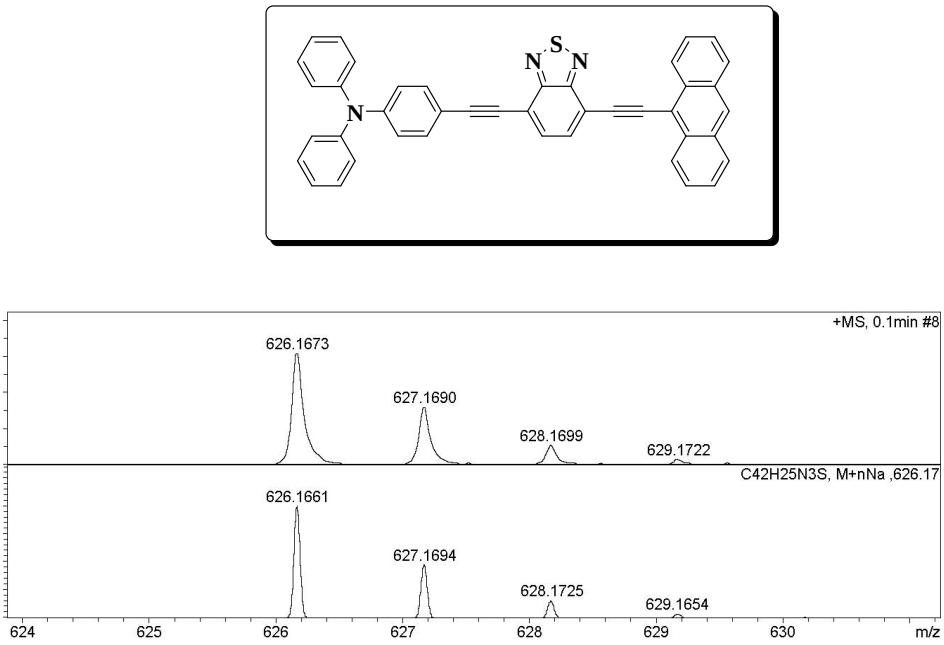


Figure S14. HRMS of BTD **8**.

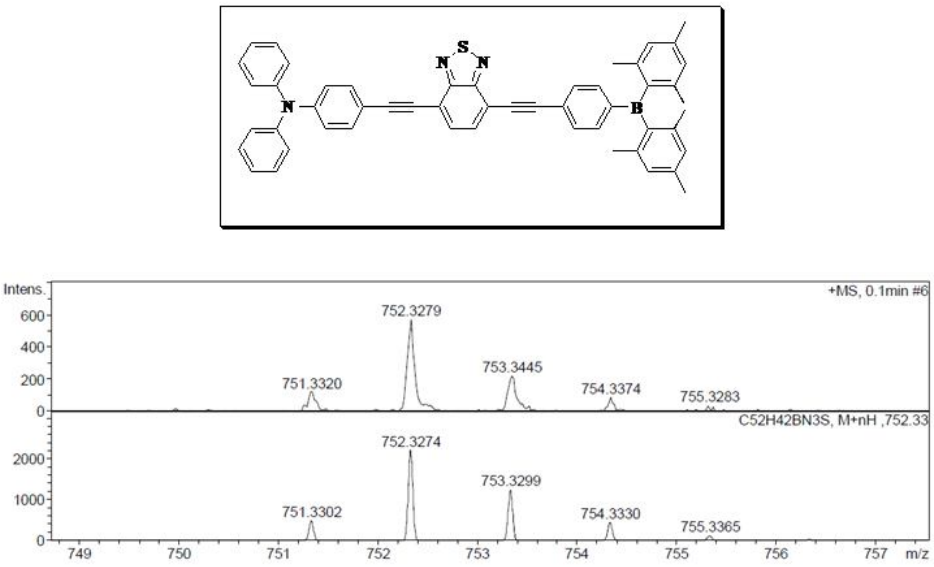


Figure S15. HRMS of BTD **9**.

II. Electrochemical Data for BTDs 2, 3, 6, 8 and 9

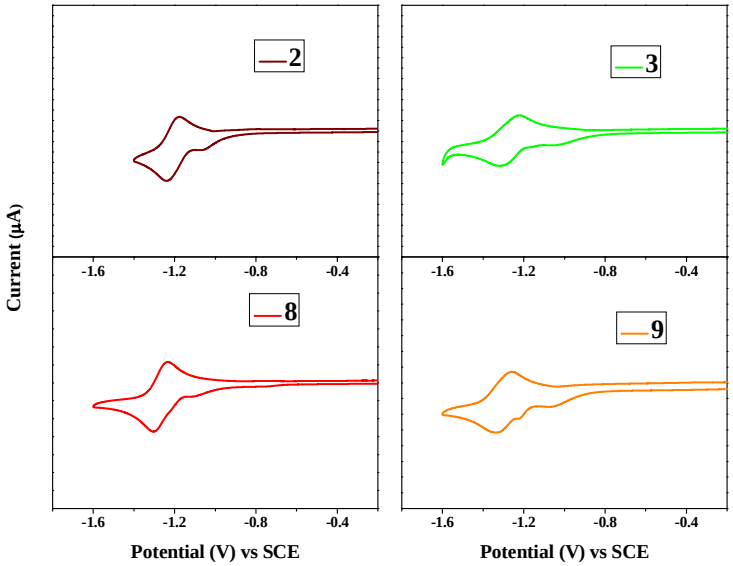


Figure S16. Cyclic voltammograms of benzothiadiazoles **2**, **3**, **8** and **9** at 0.01 M concentration in 0.1 M $TBAPF_6$ in dichloromethane recorded at a scan rate of 100 mV s^{-1}.

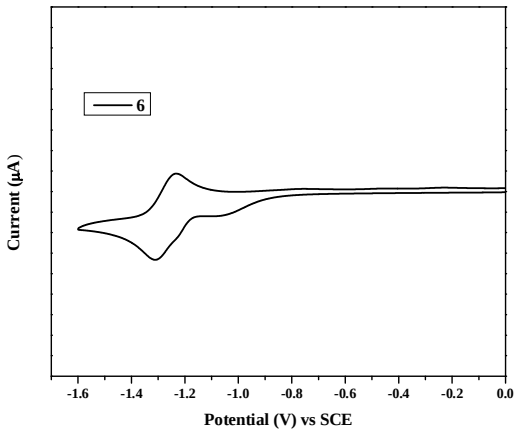


Figure S17. Cyclic voltammograms of benzothiadiazoles **6** at 0.01 M concentration in 0.1 M $TBAPF_6$ in dichloromethane recorded at a scan rate of 100 mV s^{-1}.

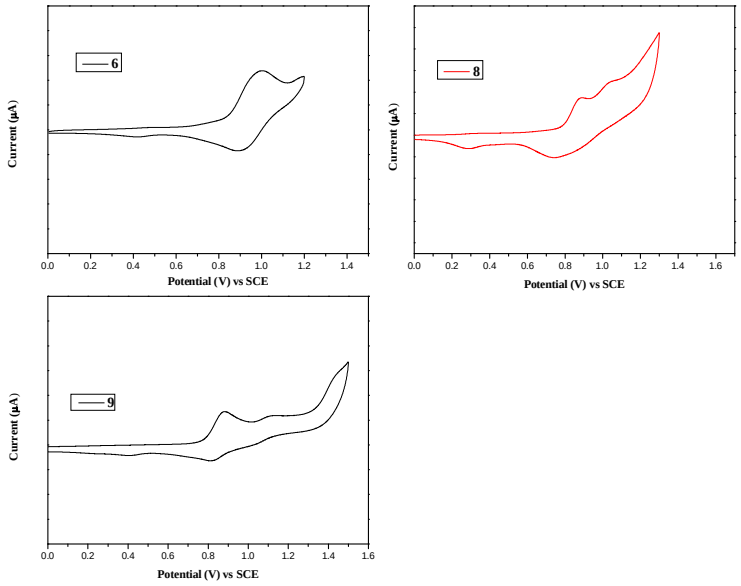


Figure S18. Cyclic voltammograms of benzothiadiazoles **6**, **8** and **9** at 0.01 M concentration in 0.1 M $TBAPF_6$ in dichloromethane recorded at a scan rate of 100 mV s^{-1}.

III. DFT Calculations for BTDs 2, 3, 6, 8 and 9

BTD 2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000096	-3.061788	-0.000267
2	7	0	-1.259315	-2.004503	-0.000353
3	7	0	1.259475	-2.004424	-0.000125
4	6	0	-0.724848	-0.780755	-0.000216
5	6	0	0.724923	-0.780725	-0.000186
6	6	0	1.462968	0.458544	-0.000145
7	6	0	0.706226	1.627054	-0.000090
8	1	0	1.225309	2.579784	-0.000011
9	6	0	-0.706301	1.627020	-0.000140
10	1	0	-1.225423	2.579726	-0.000125
11	6	0	-1.462970	0.458455	-0.000227
12	6	0	-2.873171	0.455056	-0.000284
13	6	0	-4.092484	0.415499	-0.000140
14	6	0	-5.505689	0.336450	-0.000046
15	6	0	-6.134931	-0.942810	-0.000098
16	6	0	-6.287828	1.527082	0.000128
17	6	0	-5.390330	-2.159884	-0.000345
18	6	0	-7.574337	-1.017219	0.000081
19	6	0	-7.725190	1.426332	0.000299
20	6	0	-5.700962	2.826592	0.000135
21	6	0	-6.030628	-3.374080	-0.000392
22	1	0	-4.306090	-2.111092	-0.000519
23	6	0	-8.200246	-2.302732	0.000044
24	6	0	-8.328217	0.162724	0.000286
25	6	0	-8.502546	2.626396	0.000470
26	1	0	-4.618975	2.904355	0.000000
27	6	0	-6.481036	3.955559	0.000291
28	6	0	-7.451855	-3.449927	-0.000184
29	1	0	-5.447198	-4.290220	-0.000599
30	1	0	-9.286190	-2.347983	0.000191
31	1	0	-9.413809	0.095651	0.000433
32	6	0	-7.900869	3.857054	0.000464
33	1	0	-9.585897	2.538939	0.000601
34	1	0	-6.013463	4.935953	0.000278
35	1	0	-7.938234	-4.421045	-0.000206
36	1	0	-8.502362	4.761290	0.000583
37	6	0	2.873159	0.455212	-0.000060
38	6	0	4.092473	0.415636	-0.000016
39	6	0	5.505663	0.336490	0.000025
40	6	0	6.287890	1.527078	-0.000093
41	6	0	6.134831	-0.942802	0.000215

42	6	0	5.701111	2.826622	-0.000246
43	6	0	7.725242	1.426235	-0.000051
44	6	0	7.574233	-1.017304	0.000250
45	6	0	5.390141	-2.159819	0.000386
46	6	0	6.481264	3.955542	-0.000347
47	1	0	4.619131	2.904465	-0.000277
48	6	0	8.502680	2.626241	-0.000163
49	6	0	8.328191	0.162584	0.000110
50	6	0	8.200050	-2.302865	0.000434
51	1	0	4.305904	-2.110948	0.000362
52	6	0	6.030352	-3.374062	0.000563
53	6	0	7.901084	3.856945	-0.000307
54	1	0	6.013745	4.935962	-0.000459
55	1	0	9.586024	2.538720	-0.000127
56	1	0	9.413779	0.095449	0.000135
57	6	0	7.451576	-3.450006	0.000580
58	1	0	9.285990	-2.348195	0.000448
59	1	0	5.446857	-4.290160	0.000686
60	1	0	8.502646	4.761135	-0.000383
61	1	0	7.937889	-4.421156	0.000712

Total energy (Sum of electronic and zero-point energies): = -1967.7056022 Hartree

BTD 3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.000023	-3.314817	0.000089
2	7	0	1.260385	-2.260548	-0.000857
3	7	0	-1.260397	-2.260509	0.000905
4	6	0	0.725107	-1.036942	-0.000545
5	6	0	-0.725082	-1.036919	0.000434
6	6	0	-1.461131	0.202452	0.000542
7	6	0	-0.707013	1.370805	0.000004
8	1	0	-1.227684	2.322610	0.000074
9	6	0	0.707109	1.370783	-0.000429
10	1	0	1.227810	2.322571	-0.000625
11	6	0	1.461191	0.202406	-0.000816
12	6	0	-2.874188	0.212977	0.001004
13	6	0	-4.091931	0.224353	0.001308
14	6	0	-5.512259	0.220717	0.001667
15	6	0	-6.237931	1.430854	-0.024350
16	6	0	-6.224066	-0.997974	0.027973

17	1	0	-5.696697	2.371733	-0.041352
18	6	0	-7.626631	1.412371	-0.038671
19	6	0	-7.612929	-0.994209	0.042700
20	1	0	-5.669944	-1.931115	0.044547
21	1	0	-8.167051	2.354298	-0.076015
22	6	0	-8.358477	0.204961	0.002112
23	1	0	-8.142919	-1.942044	0.079900
24	5	0	-9.930358	0.197059	0.001919
25	6	0	-10.695509	1.417430	-0.655505
26	6	0	-10.684465	-1.029976	0.659011
27	6	0	-10.436700	1.807475	-1.996521
28	6	0	-11.655165	2.168646	0.079233
29	6	0	-11.644345	-1.784163	-0.072233
30	6	0	-10.420393	-1.418791	1.999720
31	6	0	-11.121887	2.890203	-2.560645
32	6	0	-9.445289	1.079388	-2.886809
33	6	0	-12.295410	3.261160	-0.512113
34	6	0	-11.994027	1.847605	1.521190
35	6	0	-12.278424	-2.879312	0.521257
36	6	0	-11.995405	-1.460456	-1.510680
37	6	0	-11.099563	-2.503951	2.565910
38	6	0	-9.434263	-0.682833	2.889489
39	1	0	-10.921463	3.155659	-3.597057
40	6	0	-12.050932	3.637300	-1.836061
41	1	0	-9.734725	1.173733	-3.937974
42	1	0	-9.368915	0.014090	-2.657919
43	1	0	-8.436286	1.495070	-2.786494
44	1	0	-13.011624	3.831121	0.076608
45	1	0	-12.757896	2.532430	1.899962
46	1	0	-11.121128	1.940934	2.177617
47	1	0	-12.368654	0.826671	1.632381
48	1	0	-12.999974	-3.447627	-0.062489
49	6	0	-12.023829	-3.258292	1.842217
50	1	0	-11.125728	-1.543222	-2.172698
51	1	0	-12.380417	-0.442781	-1.616049
52	1	0	-12.754920	-2.151284	-1.887296
53	1	0	-10.899812	-2.764216	3.603779
54	1	0	-9.722039	-0.780414	3.940811
55	1	0	-9.366521	0.383204	2.661409
56	1	0	-8.422166	-1.090580	2.788066
57	6	0	-12.792683	4.791737	-2.466486
58	6	0	-12.713506	-4.452798	2.456453
59	1	0	-12.262106	5.178956	-3.341294
60	1	0	-12.927558	5.615520	-1.758089
61	1	0	-13.792903	4.486061	-2.798860
62	1	0	-12.184775	-5.383311	2.213246
63	1	0	-13.738106	-4.558463	2.085911
64	1	0	-12.751925	-4.376353	3.547161
65	6	0	2.874249	0.212902	-0.001253
66	6	0	4.091992	0.224260	-0.001509
67	6	0	5.512320	0.220614	-0.001818
68	6	0	6.237981	1.430756	0.024336
69	6	0	6.224139	-0.998066	-0.028166

70	1	0	5.696736	2.371627	0.041393
71	6	0	7.626681	1.412289	0.038725
72	6	0	7.613003	-0.994285	-0.042830
73	1	0	5.670033	-1.931215	-0.044817
74	1	0	8.167085	2.354220	0.076184
75	6	0	8.358541	0.204888	-0.002132
76	1	0	8.143003	-1.942113	-0.080068
77	5	0	9.930432	0.197016	-0.001872
78	6	0	10.695464	1.417445	0.655588
79	6	0	10.684579	-1.029986	-0.658959
80	6	0	10.436553	1.807469	1.996587
81	6	0	11.655073	2.168750	-0.079116
82	6	0	11.644422	-1.784201	0.072310
83	6	0	10.420595	-1.418731	-1.999704
84	6	0	11.121544	2.890326	2.560708
85	6	0	9.445251	1.079229	2.886875
86	6	0	12.295128	3.261377	0.512226
87	6	0	11.994062	1.847680	-1.521037
88	6	0	12.278534	-2.879325	-0.521185
89	6	0	11.995317	-1.460581	1.510814
90	6	0	11.099798	-2.503875	-2.565897
91	6	0	9.434533	-0.682729	-2.889514
92	1	0	10.921041	3.155776	3.597107
93	6	0	12.050507	3.637540	1.836143
94	1	0	9.734852	1.173351	3.938015
95	1	0	9.368812	0.013982	2.657783
96	1	0	8.436250	1.494980	2.786801
97	1	0	13.011311	3.831407	-0.076465
98	1	0	12.758104	2.532373	-1.899695
99	1	0	11.121256	1.941198	-2.177566
100	1	0	12.368505	0.826678	-1.632212
101	1	0	13.000064	-3.447655	0.062572
102	6	0	12.024015	-3.258245	-1.842180
103	1	0	11.125711	-1.544229	2.172830
104	1	0	12.379513	-0.442631	1.616444
105	1	0	12.755387	-2.150910	1.887224
106	1	0	10.900123	-2.764098	-3.603790
107	1	0	9.722373	-0.780293	-3.940820
108	1	0	9.366799	0.383304	-2.661416
109	1	0	8.422423	-1.090461	-2.788157
110	6	0	12.792049	4.792114	2.466562
111	6	0	12.713786	-4.452698	-2.456418
112	1	0	12.261400	5.179242	3.341367
113	1	0	12.926773	5.615919	1.758161
114	1	0	13.792325	4.486624	2.798939
115	1	0	12.185851	-5.383384	-2.212155
116	1	0	13.738811	-4.557557	-2.086811
117	1	0	12.751108	-4.376838	-3.547202

Total energy (Sum of electronic and zero-point energies): -2800.1012361 Hartree

BTD 6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000085	3.243683	0.000032
2	7	0	-1.260683	2.188499	0.000862
3	7	0	1.260805	2.188429	-0.001066
4	6	0	-0.725597	0.964879	0.000453
5	6	0	0.725653	0.964835	-0.000648
6	6	0	1.463441	-0.274122	-0.001156
7	6	0	0.706742	-1.441666	-0.000617
8	1	0	1.226681	-2.394008	-0.000990
9	6	0	-0.706811	-1.441618	0.000335
10	1	0	-1.226835	-2.393916	0.000657
11	6	0	-1.463460	-0.274035	0.000918
12	6	0	-2.875662	-0.282636	0.001806
13	6	0	-4.094115	-0.292315	0.002472
14	6	0	-5.512559	-0.282975	0.002927
15	6	0	-6.252310	-1.484485	0.003675
16	6	0	-6.227318	0.934154	0.002301
17	6	0	-7.639195	-1.471389	0.009814
18	1	0	-5.722748	-2.431836	0.014622
19	6	0	-7.614064	0.948912	-0.003785
20	1	0	-5.675782	1.868676	-0.008757
21	6	0	-8.347127	-0.253845	0.002864
22	1	0	-8.187059	-2.407068	0.024320
23	1	0	-8.142481	1.895713	-0.018363
24	7	0	-9.759461	-0.239821	0.002404
25	6	0	-10.490417	-1.243857	-0.695907
26	6	0	-10.471757	0.778203	0.699882
27	6	0	-10.117098	-1.625321	-1.994403
28	6	0	-11.600868	-1.857395	-0.095421
29	6	0	-11.572124	1.409789	0.099574
30	6	0	-10.090264	1.155385	1.997220
31	6	0	-10.835484	-2.610460	-2.669650
32	1	0	-9.265319	-1.146864	-2.466549
33	6	0	-12.323724	-2.828957	-0.785538
34	1	0	-11.890477	-1.567844	0.909383
35	6	0	-12.277197	2.394869	0.788886
36	1	0	-11.867892	1.123792	-0.904438
37	6	0	-10.790628	2.154042	2.671565
38	1	0	-9.246035	0.663504	2.469102
39	6	0	-11.943984	-3.215269	-2.072760
40	1	0	-10.534419	-2.894814	-3.673966
41	1	0	-13.180618	-3.295070	-0.307367
42	6	0	-11.889264	2.776788	2.074960

43	1	0	-13.126353	2.875079	0.310864
44	1	0	-10.483095	2.435251	3.674788
45	1	0	-12.505463	-3.977294	-2.604658
46	1	0	-12.436658	3.549534	2.606058
47	6	0	2.875649	-0.282740	-0.002089
48	6	0	4.094103	-0.292408	-0.002647
49	6	0	5.512546	-0.283057	-0.003037
50	6	0	6.252309	-1.484560	-0.003740
51	6	0	6.227296	0.934079	-0.002394
52	6	0	7.639193	-1.471453	-0.009816
53	1	0	5.722752	-2.431915	-0.014702
54	6	0	7.614040	0.948852	0.003755
55	1	0	5.675742	1.868592	0.008625
56	6	0	8.347110	-0.253901	-0.002839
57	1	0	8.187069	-2.407126	-0.024290
58	1	0	8.142451	1.895656	0.018339
59	7	0	9.759448	-0.239855	-0.002333
60	6	0	10.490413	-1.243867	0.695991
61	6	0	10.471730	0.778197	-0.699782
62	6	0	10.117066	-1.625371	1.994467
63	6	0	11.600932	-1.857332	0.095549
64	6	0	11.572047	1.409830	-0.099432
65	6	0	10.090263	1.155370	-1.997130
66	6	0	10.835473	-2.610483	2.669731
67	1	0	9.265244	-1.146963	2.466587
68	6	0	12.323809	-2.828866	0.785684
69	1	0	11.890577	-1.567747	-0.909235
70	6	0	12.277097	2.394945	-0.788719
71	1	0	11.867801	1.123841	0.904587
72	6	0	10.790599	2.154062	-2.671450
73	1	0	9.246067	0.663449	-2.469034
74	6	0	11.944030	-3.215224	2.072881
75	1	0	10.534379	-2.894865	3.674031
76	1	0	13.180754	-3.294920	0.307546
77	6	0	11.889188	2.776852	-2.074804
78	1	0	13.126217	2.875191	-0.310670
79	1	0	10.483084	2.435259	-3.674680
80	1	0	12.505525	-3.977232	2.604786
81	1	0	12.436563	3.549633	-2.605870

Total energy (Sum of electronic and zero-point energies): = -2388.0456938 Hartree

BTD 8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.001267	-2.925326	-0.762899
2	7	0	-3.250125	-1.885303	-0.507496
3	7	0	-0.730521	-1.907797	-0.539581
4	6	0	-2.701172	-0.698271	-0.237327
5	6	0	-1.251159	-0.711131	-0.255876
6	6	0	-0.499363	0.489539	0.015731
7	6	0	-1.243034	1.634206	0.287262
8	1	0	-0.712322	2.557151	0.496181
9	6	0	-2.656240	1.646340	0.306229
10	1	0	-3.164470	2.578785	0.528909
11	6	0	-3.425386	0.514505	0.054059
12	6	0	-4.836074	0.515098	0.076885
13	6	0	-6.054655	0.461284	0.087735
14	6	0	-7.466248	0.351707	0.089686
15	6	0	-8.068040	-0.904837	-0.212889
16	6	0	-8.273413	1.485450	0.391816
17	6	0	-7.297516	-2.066070	-0.519827
18	6	0	-9.505315	-1.014169	-0.210605
19	6	0	-9.708148	1.350743	0.388105
20	6	0	-7.714063	2.760037	0.701547
21	6	0	-7.911531	-3.259686	-0.806778
22	1	0	-6.214687	-1.992026	-0.522416
23	6	0	-10.103228	-2.276713	-0.515369
24	6	0	-10.284194	0.110442	0.088134
25	6	0	-10.510271	2.494468	0.693173
26	1	0	-6.634031	2.862254	0.705039
27	6	0	-8.517519	3.834544	0.989348
28	6	0	-9.330533	-3.369794	-0.805610
29	1	0	-7.308513	-4.133033	-1.037834
30	1	0	-11.187765	-2.348442	-0.511151
31	1	0	-11.367909	0.017707	0.087438
32	6	0	-9.934792	3.702634	0.985732
33	1	0	-11.591353	2.382244	0.687718
34	1	0	-8.070937	4.796778	1.222787
35	1	0	-9.795905	-4.323882	-1.035557
36	1	0	-10.555237	4.563777	1.215933
37	6	0	0.912033	0.478127	0.006604
38	6	0	2.130466	0.454982	0.003788
39	6	0	3.547057	0.389632	0.003265
40	6	0	4.337440	1.535101	0.235571
41	6	0	4.208215	-0.836797	-0.224326
42	6	0	5.722300	1.457633	0.251186

43	1	0	3.849290	2.486524	0.421376
44	6	0	5.592389	-0.913797	-0.219258
45	1	0	3.616494	-1.725784	-0.417095
46	6	0	6.376537	0.230994	0.024756
47	1	0	6.309850	2.347612	0.447442
48	1	0	6.079926	-1.864011	-0.407044
49	7	0	7.785729	0.146615	0.046112
50	6	0	8.584083	1.225006	-0.432608
51	6	0	8.427626	-1.014520	0.567570
52	6	0	8.264809	1.869277	-1.638477
53	6	0	9.709582	1.647986	0.291605
54	6	0	9.511799	-1.590160	-0.112793
55	6	0	7.990890	-1.590021	1.771132
56	6	0	9.052194	2.922545	-2.100343
57	1	0	7.401838	1.539207	-2.207453
58	6	0	10.500908	2.690481	-0.187501
59	1	0	9.958006	1.155105	1.225695
60	6	0	10.147468	-2.716364	0.407274
61	1	0	9.849428	-1.149789	-1.045214
62	6	0	8.621509	-2.726594	2.274077
63	1	0	7.158849	-1.143005	2.305187
64	6	0	10.175964	3.337070	-1.381893
65	1	0	8.792625	3.410697	-3.035477
66	1	0	11.368915	3.006291	0.384318
67	6	0	9.704668	-3.294087	1.599206
68	1	0	10.985161	-3.151105	-0.130662
69	1	0	8.272024	-3.161041	3.206382
70	1	0	10.791057	4.152977	-1.748984
71	1	0	10.198103	-4.175313	1.997666

Total energy (Sum of electronic and zero-point energies)= -2177.8756617 Hartree

BTD 9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.382761	-2.933747	-1.350807
2	7	0	2.638555	-1.972589	-0.903407
3	7	0	0.117446	-1.982267	-0.908501
4	6	0	2.098024	-0.865437	-0.388228
5	6	0	0.647417	-0.870843	-0.391105
6	6	0	-0.093432	0.249637	0.131260
7	6	0	0.657254	1.310968	0.625637
8	1	0	0.132676	2.171755	1.027123
9	6	0	2.070916	1.317775	0.626983

10	1	0	2.587136	2.183133	1.029047
11	6	0	2.831059	0.261290	0.134955
12	6	0	-1.506661	0.253544	0.133059
13	6	0	-2.724555	0.255010	0.133071
14	6	0	-4.144548	0.236389	0.121714
15	6	0	-4.888095	1.291126	0.693505
16	6	0	-4.839342	-0.843462	-0.465175
17	1	0	-4.360552	2.122778	1.150164
18	6	0	-6.276330	1.264262	0.662868
19	6	0	-6.227876	-0.863301	-0.463387
20	1	0	-4.271731	-1.655221	-0.908936
21	1	0	-6.830335	2.092273	1.096732
22	6	0	-6.991426	0.187937	0.091924
23	1	0	-6.744174	-1.709900	-0.907695
24	5	0	-8.561783	0.159998	0.075178
25	6	0	-9.350002	1.532616	0.149989
26	6	0	-9.296430	-1.240792	-0.017517
27	6	0	-9.111572	2.566403	-0.795079
28	6	0	-10.308116	1.779051	1.172081
29	6	0	-10.226167	-1.519671	-1.057288
30	6	0	-9.040781	-2.266016	0.932435
31	6	0	-9.816593	3.772895	-0.713470
32	6	0	-8.117530	2.422395	-1.933630
33	6	0	-10.969224	3.009252	1.235282
34	6	0	-10.620107	0.754198	2.243899
35	6	0	-10.841166	-2.772896	-1.134110
36	6	0	-10.561639	-0.502377	-2.129260
37	6	0	-9.700203	-3.496866	0.836453
38	6	0	-8.081424	-2.084929	2.095199
39	1	0	-9.630460	4.540849	-1.462215
40	6	0	-10.746538	4.020562	0.297108
41	1	0	-8.404731	3.059988	-2.775389
42	1	0	-8.040134	1.397853	-2.304502
43	1	0	-7.109345	2.720459	-1.624956
44	1	0	-11.684460	3.179597	2.037703
45	1	0	-11.405952	1.118921	2.911338
46	1	0	-9.744193	0.534689	2.865689
47	1	0	-10.952676	-0.194600	1.814945
48	1	0	-11.540047	-2.965223	-1.945851
49	6	0	-10.595654	-3.779013	-0.196169
50	1	0	-9.683697	-0.239054	-2.730738
51	1	0	-10.946026	0.427461	-1.702115
52	1	0	-11.315644	-0.897900	-2.815614
53	1	0	-9.506941	-4.255456	1.592781
54	1	0	-8.363011	-2.736202	2.928323
55	1	0	-8.054932	-1.059227	2.469998
56	1	0	-7.054900	-2.341374	1.810704
57	6	0	-11.510848	5.321539	0.357285
58	6	0	-11.262119	-5.129330	-0.308351
59	1	0	-10.963236	6.131299	-0.134235
60	1	0	-11.708125	5.622657	1.391002
61	1	0	-12.483060	5.234032	-0.144471
62	1	0	-10.686380	-5.802179	-0.956759

63	1	0	-12.265132	-5.046936	-0.738749
64	1	0	-11.349533	-5.615827	0.667788
65	6	0	4.242577	0.272824	0.137980
66	6	0	5.461168	0.281930	0.139243
67	6	0	6.879100	0.271804	0.131369
68	6	0	7.590074	-0.857511	-0.329004
69	6	0	7.621792	1.384473	0.580337
70	6	0	8.976416	-0.871499	-0.344476
71	1	0	7.035641	-1.718341	-0.688434
72	6	0	9.008378	1.368385	0.574626
73	1	0	7.094841	2.259098	0.948224
74	6	0	9.712926	0.240577	0.109407
75	1	0	9.502271	-1.744410	-0.715008
76	1	0	9.559084	2.229481	0.936622
77	7	0	11.124083	0.225521	0.098224
78	6	0	11.835742	-0.981380	0.359532
79	6	0	11.856360	1.417227	-0.175327
80	6	0	11.458279	-1.815651	1.423574
81	6	0	12.932457	-1.343316	-0.437970
82	6	0	12.970975	1.758568	0.606305
83	6	0	11.481147	2.256865	-1.235955
84	6	0	12.159251	-2.994188	1.673106
85	1	0	10.617517	-1.535308	2.049653
86	6	0	13.638399	-2.514742	-0.169343
87	1	0	13.225842	-0.702479	-1.262906
88	6	0	13.696581	2.915025	0.325407
89	1	0	13.262781	1.113323	1.428373
90	6	0	12.202298	3.420449	-1.497865
91	1	0	10.626588	1.991904	-1.849953
92	6	0	13.254606	-3.349207	0.882642
93	1	0	11.854902	-3.629732	2.499865
94	1	0	14.485052	-2.781619	-0.795492
95	6	0	13.315278	3.754916	-0.723181
96	1	0	14.557076	3.165963	0.939163
97	1	0	11.899853	4.060106	-2.322163
98	1	0	13.802669	-4.264456	1.084465
99	1	0	13.879069	4.658341	-0.934766

Total energy (Sum of electronic and zero-point energies): -2594.0734929 Hartree

IV. Scheme S1. Synthetic route to BTDs **6** and **7**