Tuning of the HOMO-LUMO Gap of Donor-Substituted Symmetrical and Unsymmetrical Benzothiadiazoles

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I. Copies of ^{1}H NMR Spectra of the New Compounds

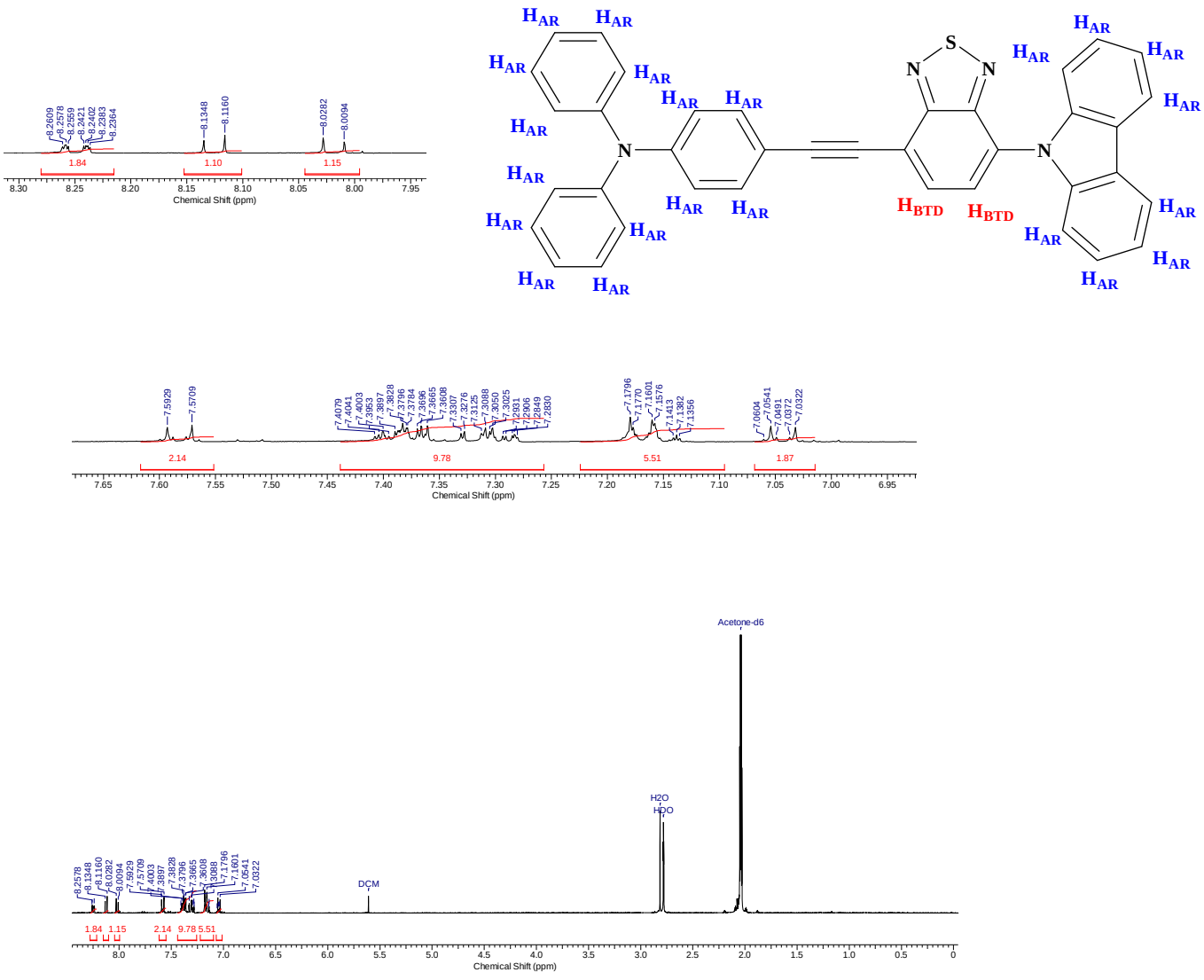

Figure S1. ^{1}H NMR spectra of BTD **5**

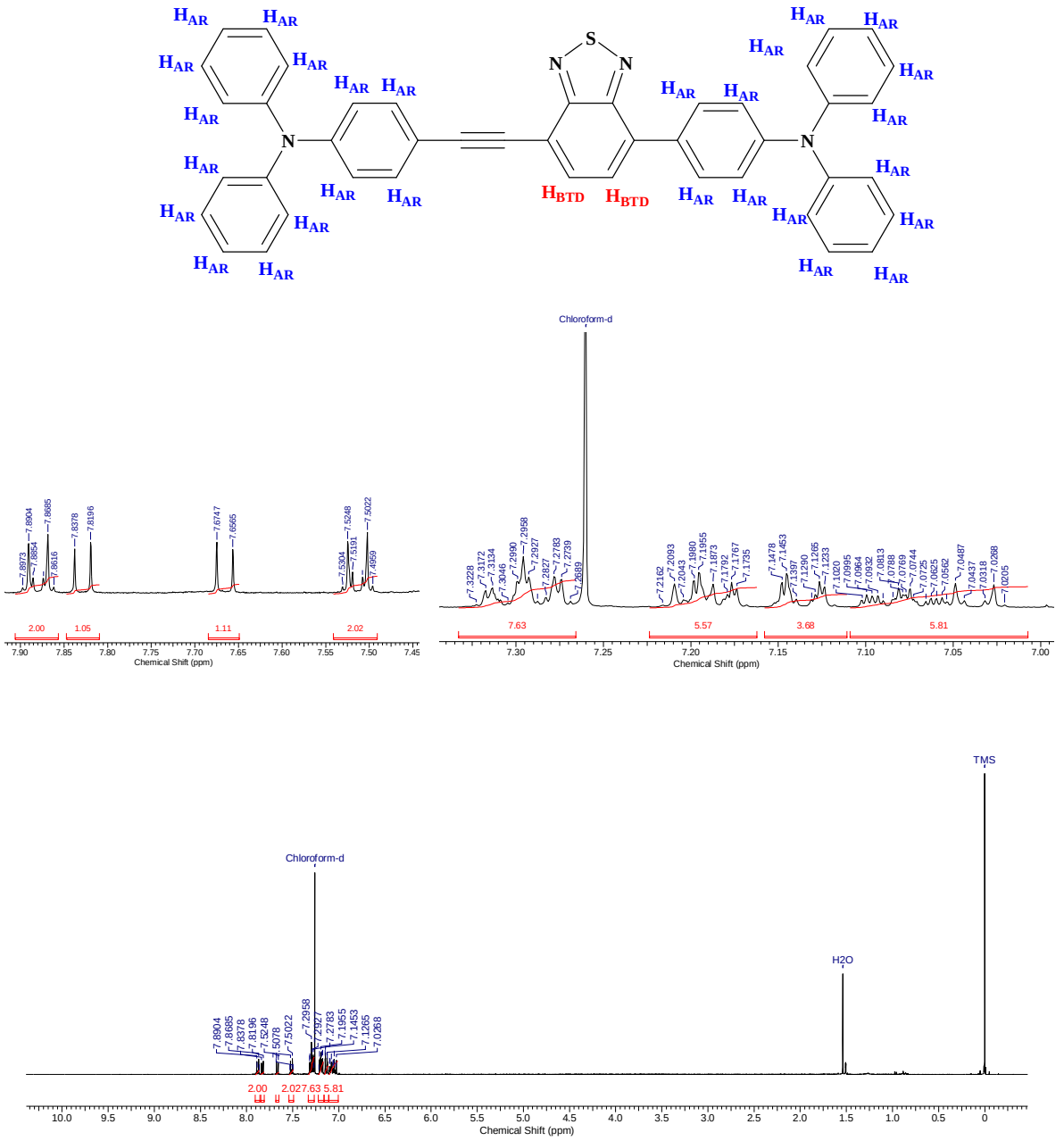

Figure S2. ^{1}H NMR spectra of BTD **6**

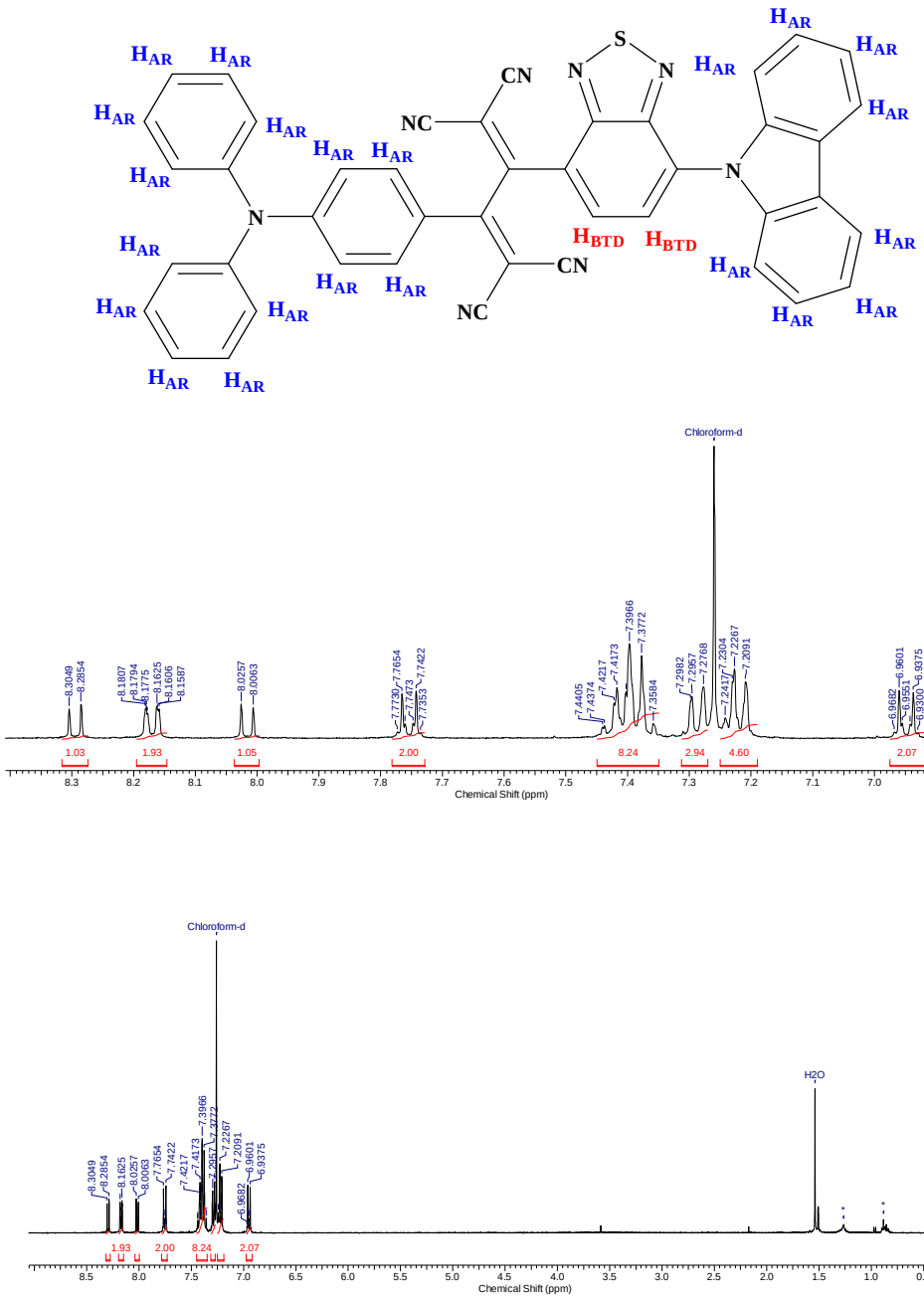

Figure S3. ^{1}H NMR spectra of BTD **7**

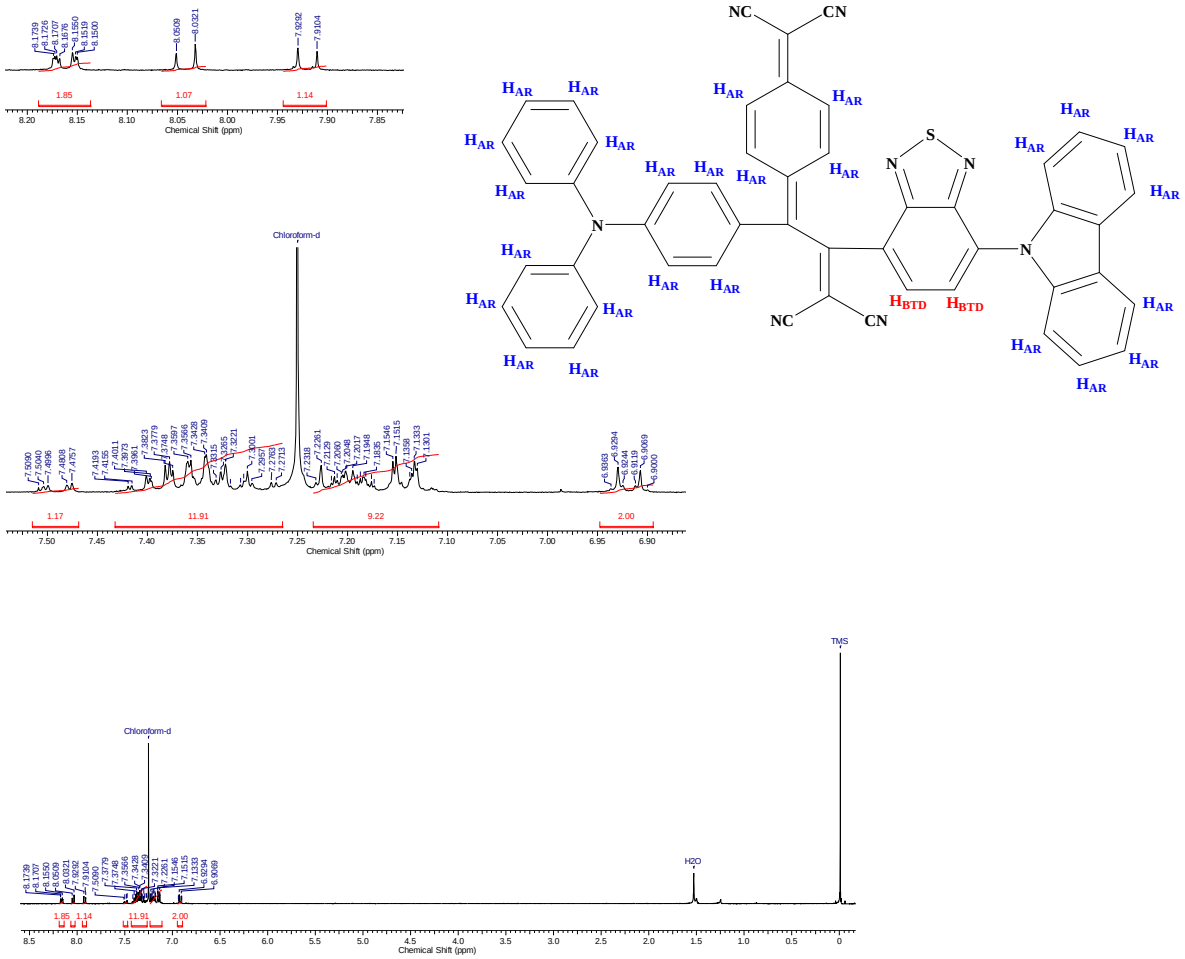

Figure S4. ^{1}H NMR spectra of BTD **8**

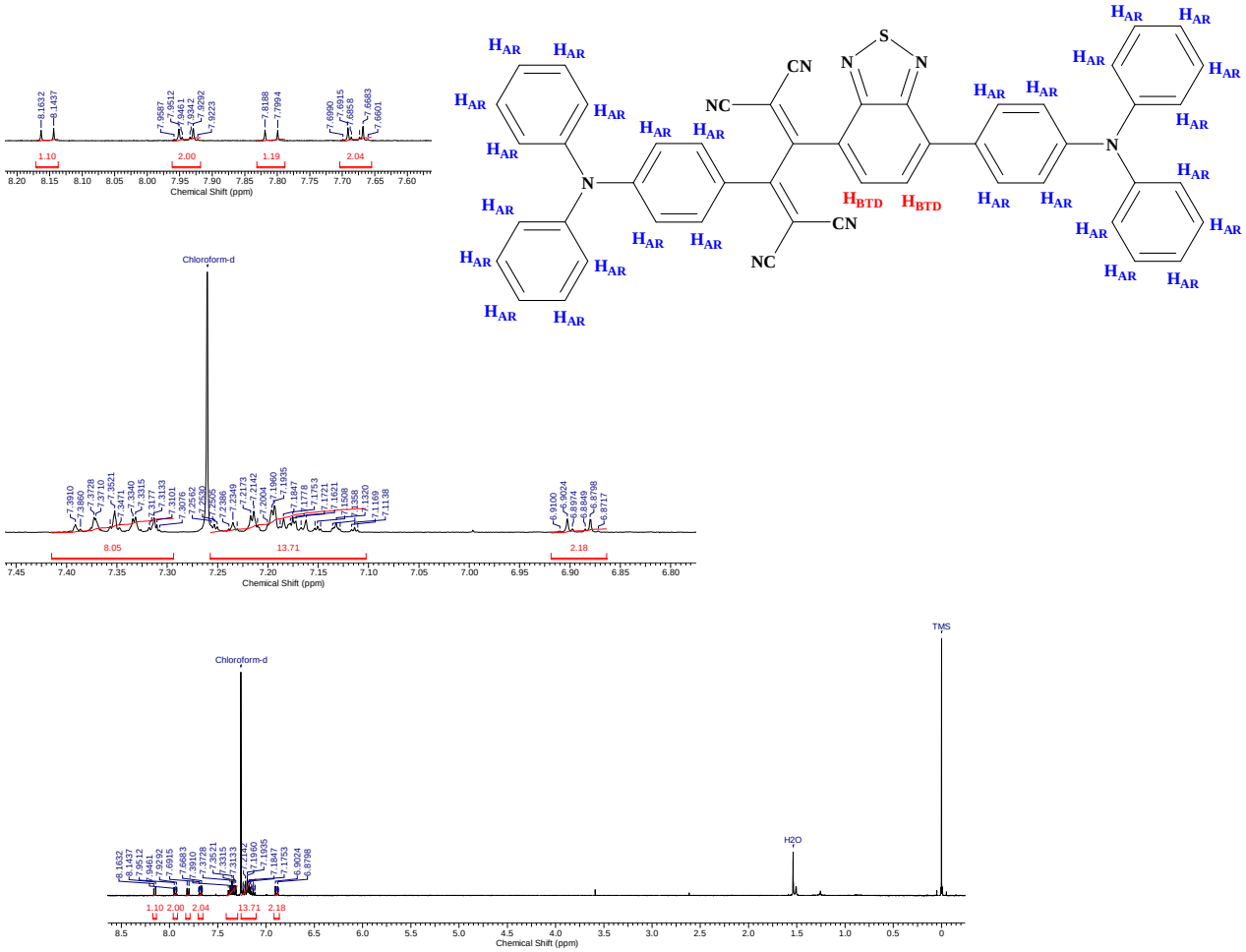

Figure S5. ^{1}H NMR spectra of BTD **9**

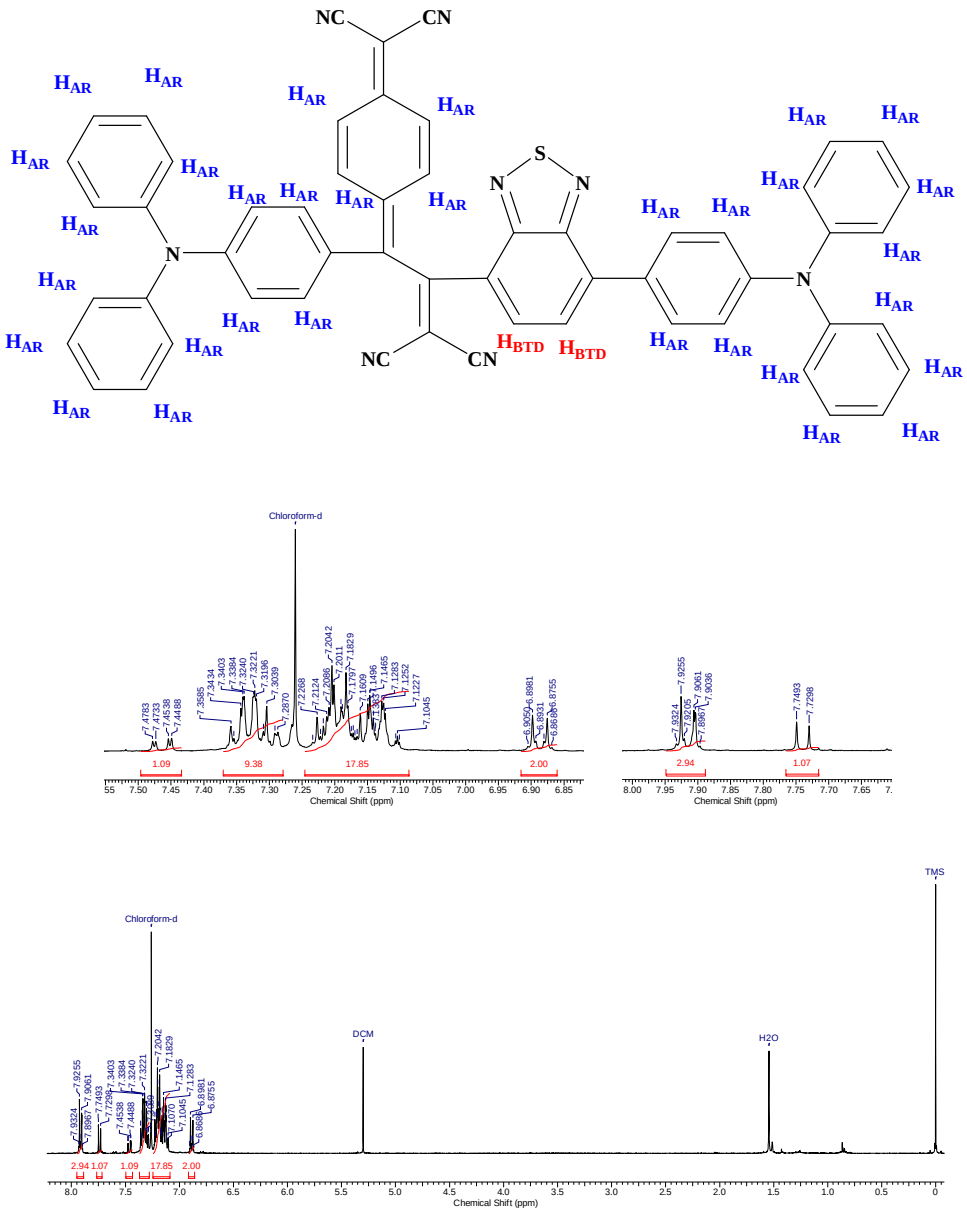

Figure S6. ^{1}H NMR spectra of BTD **10**

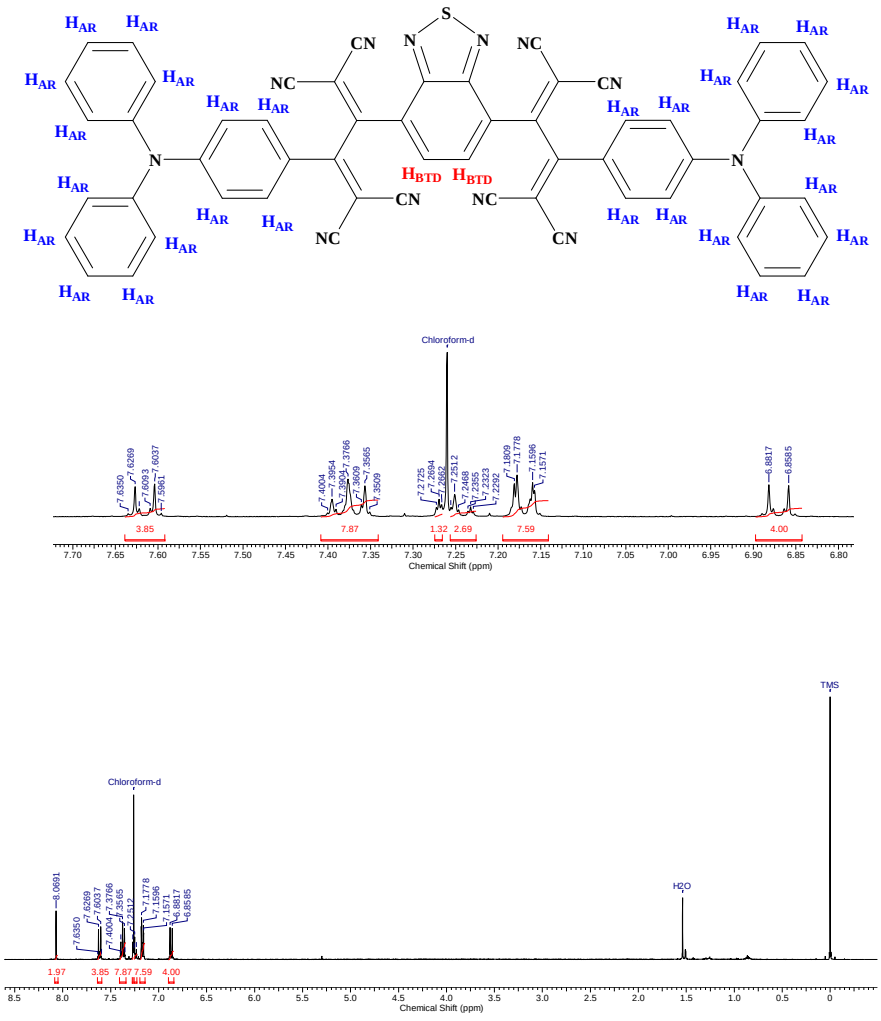

Figure S7. ^{1}H NMR spectra of BTD **11**

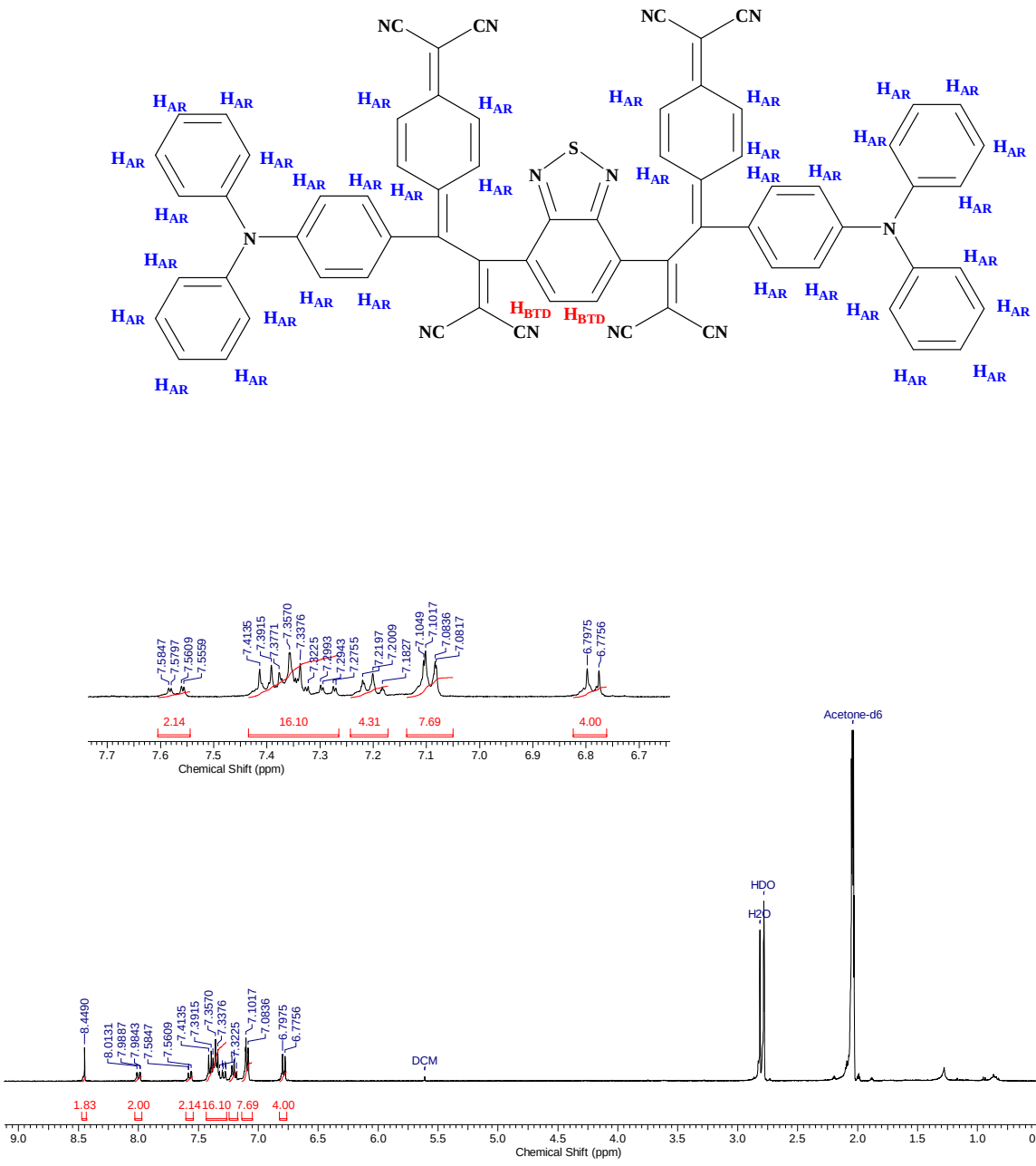

Figure S8. ^{1}H NMR spectra of BTD **12**

Copies of ^{13}C NMR Spectra of the New Compounds

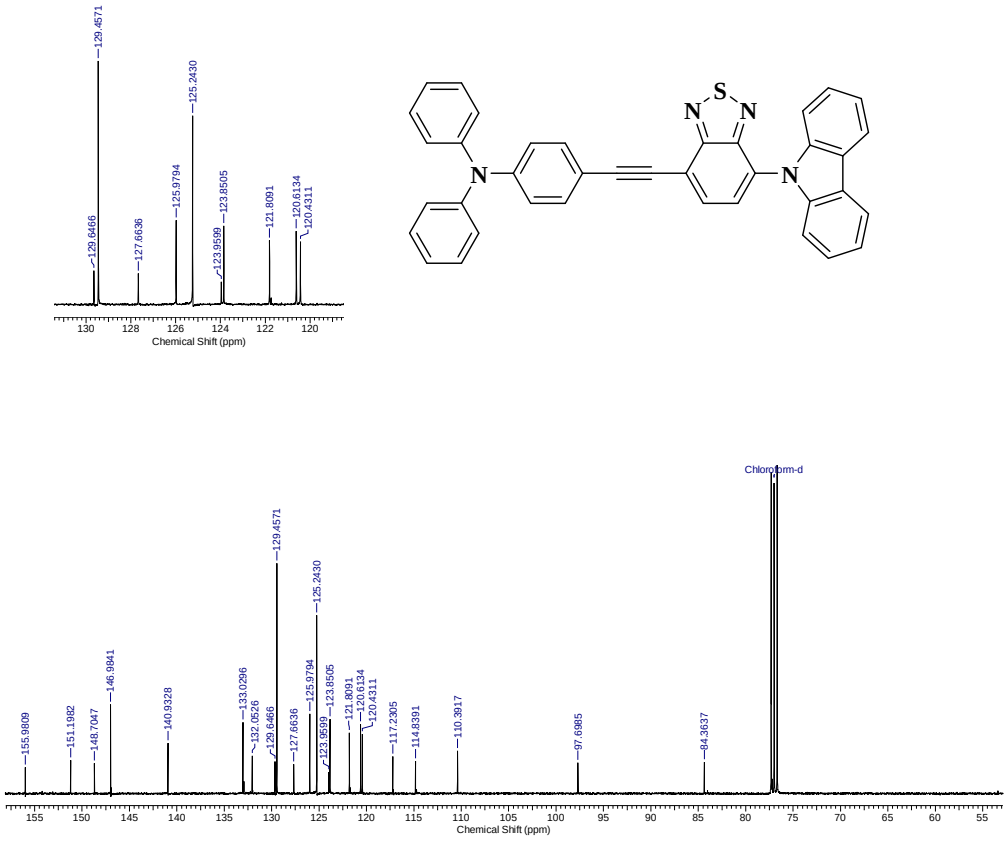

Figure S9. ^{13}C NMR spectra of BTD **5**

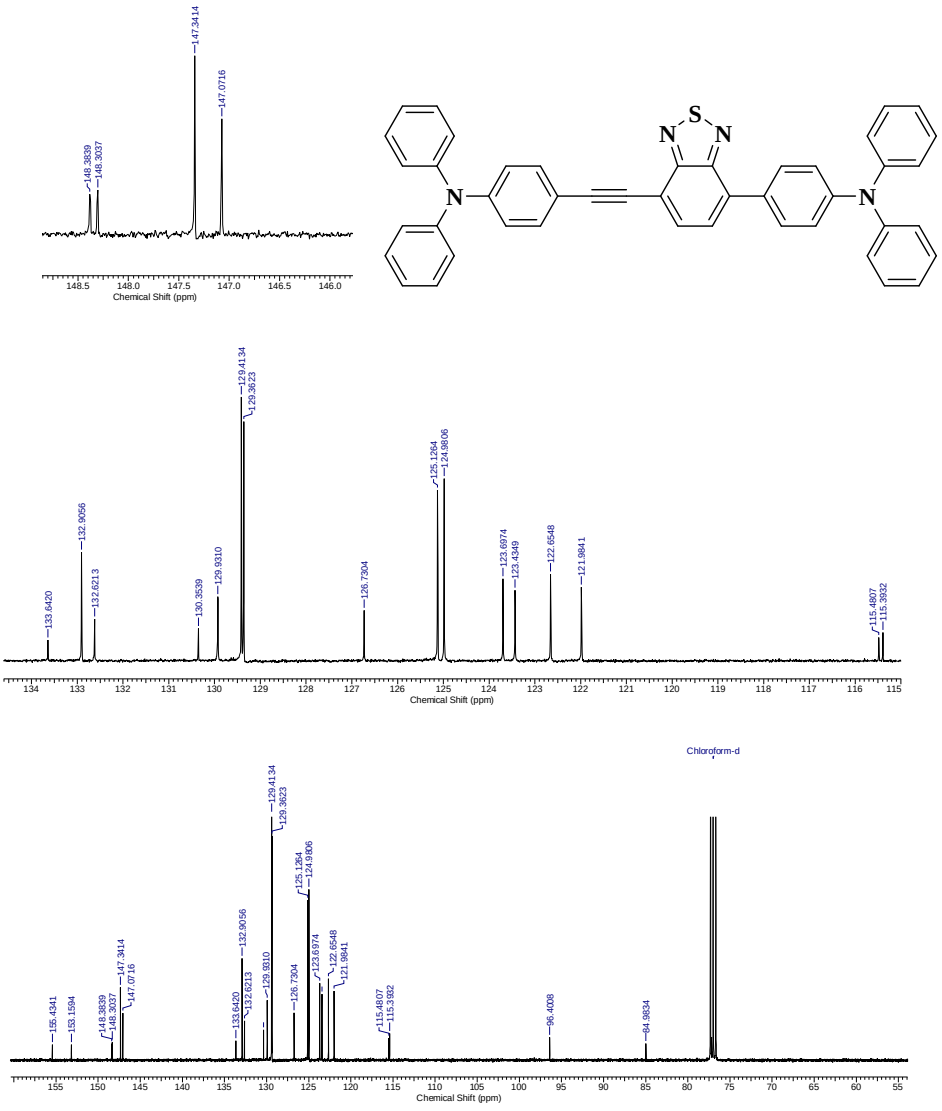

Figure S10. ^{13}C NMR spectra of BTD **6**

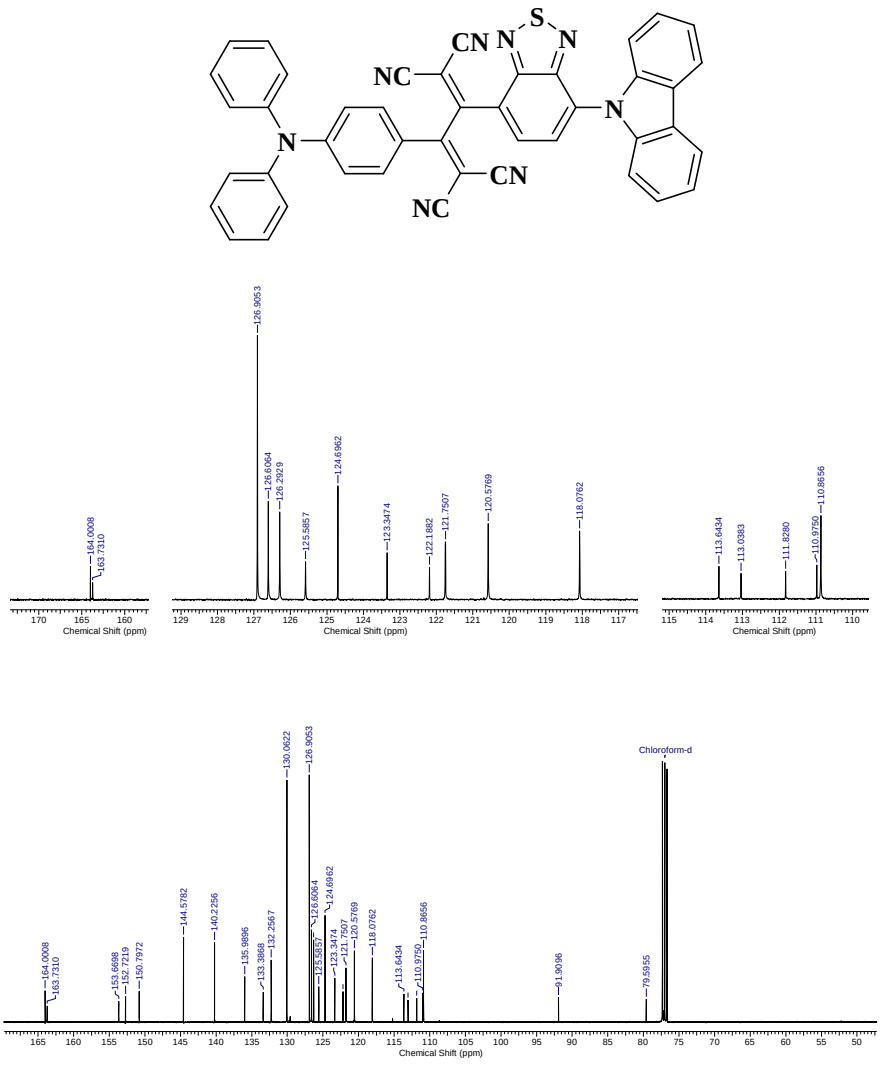

Figure S11. ^{13}C NMR spectra of BTD **7**

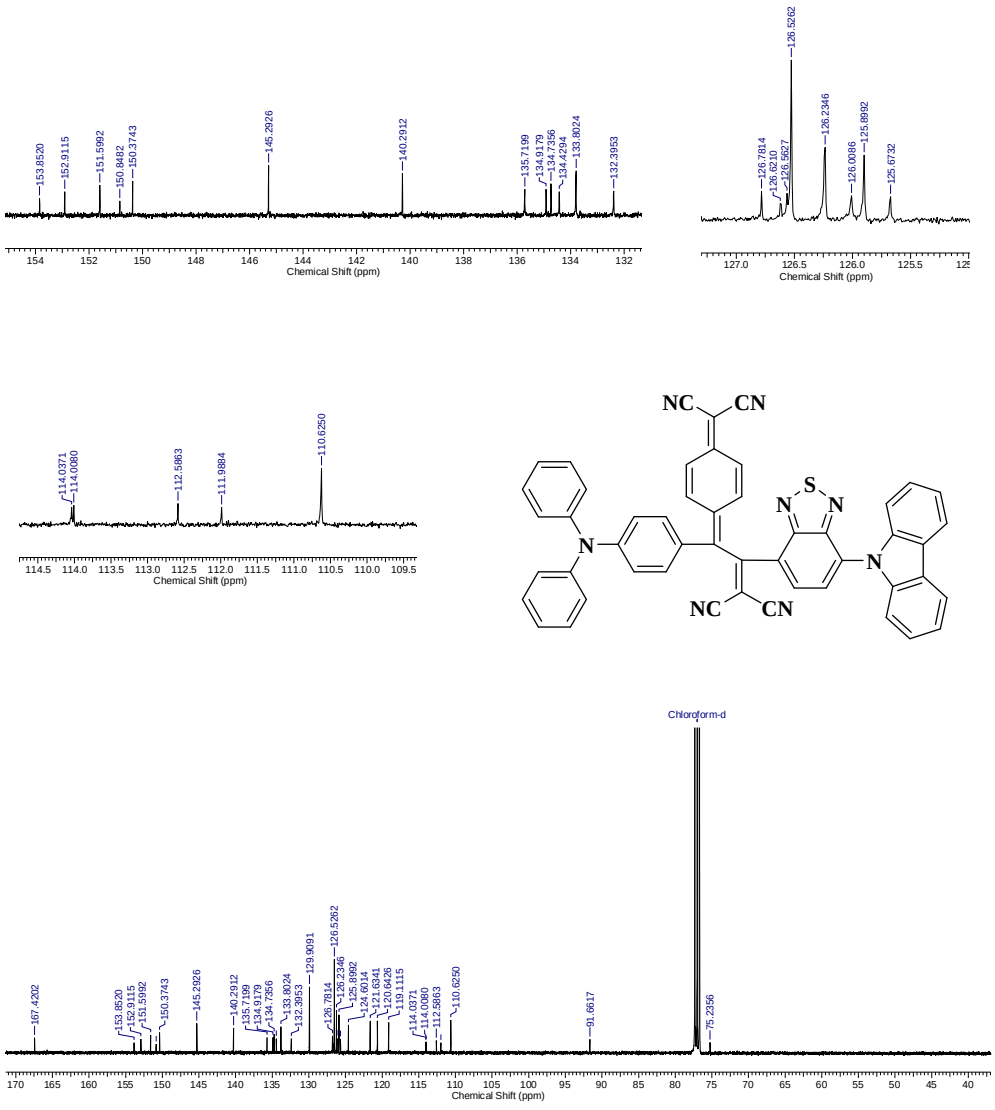

Figure S12. ^{13}C NMR spectra of BTD **8**

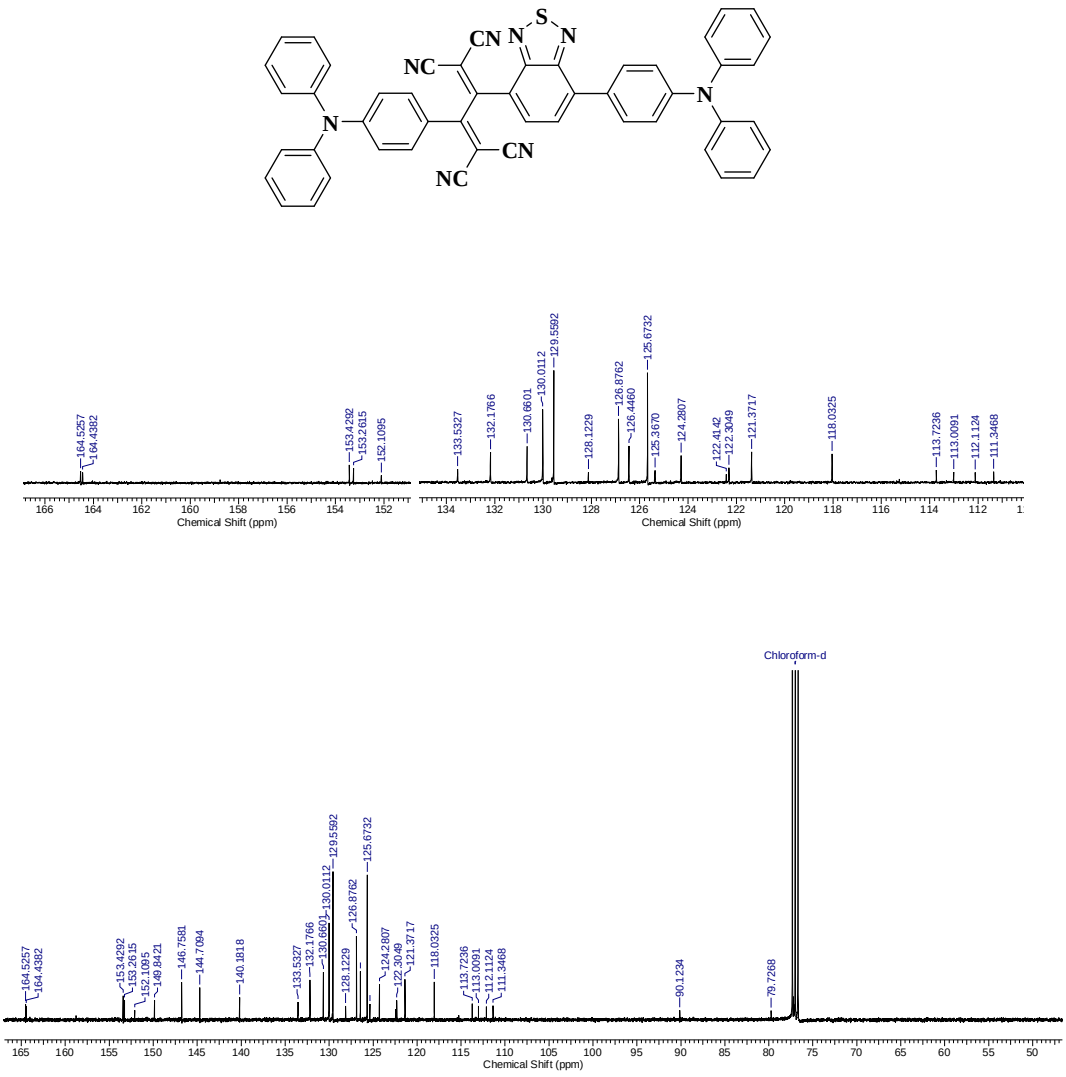

Figure S13. ^{13}C NMR spectra of BTD **9**

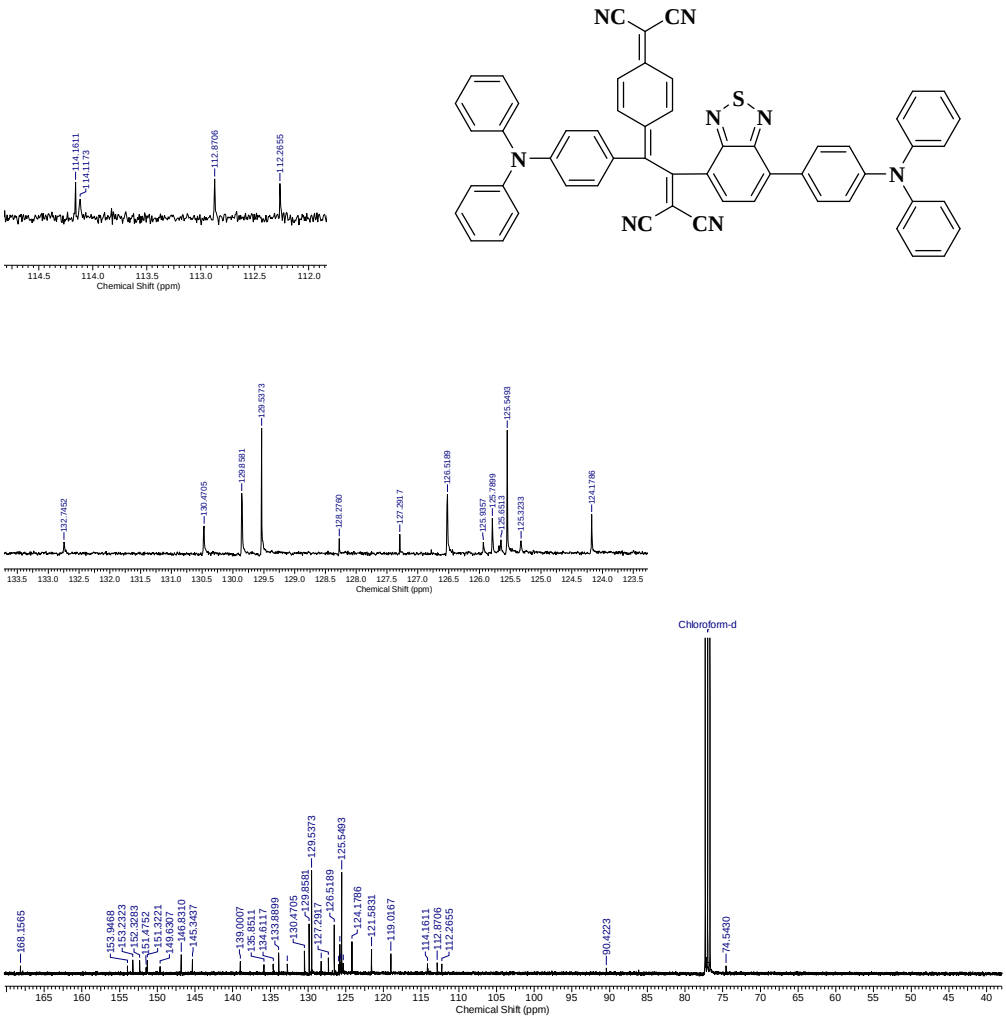

Figure S14. ^{13}C NMR spectra of BTD **10**

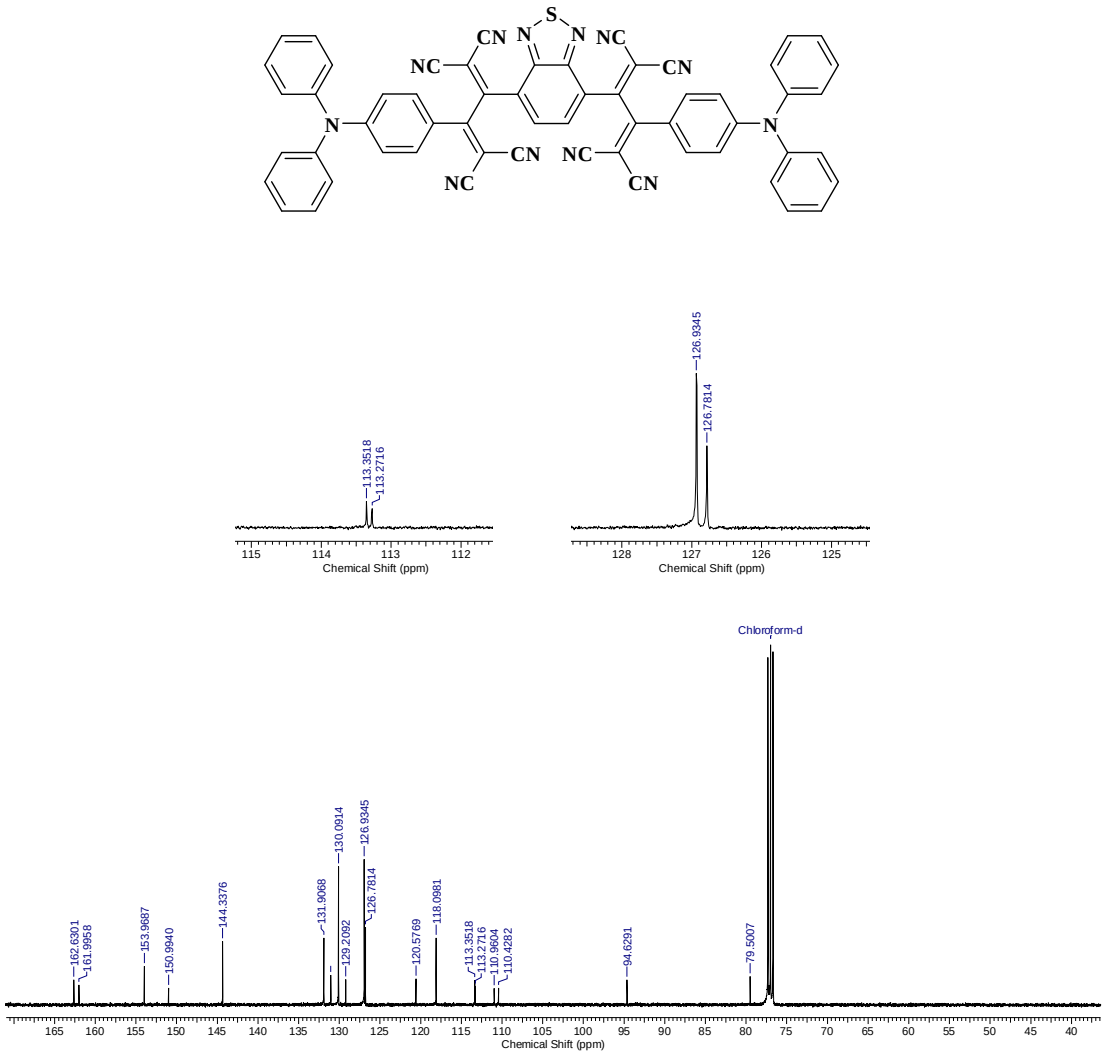

Figure S15. ^{13}C NMR spectra of BTD **11**

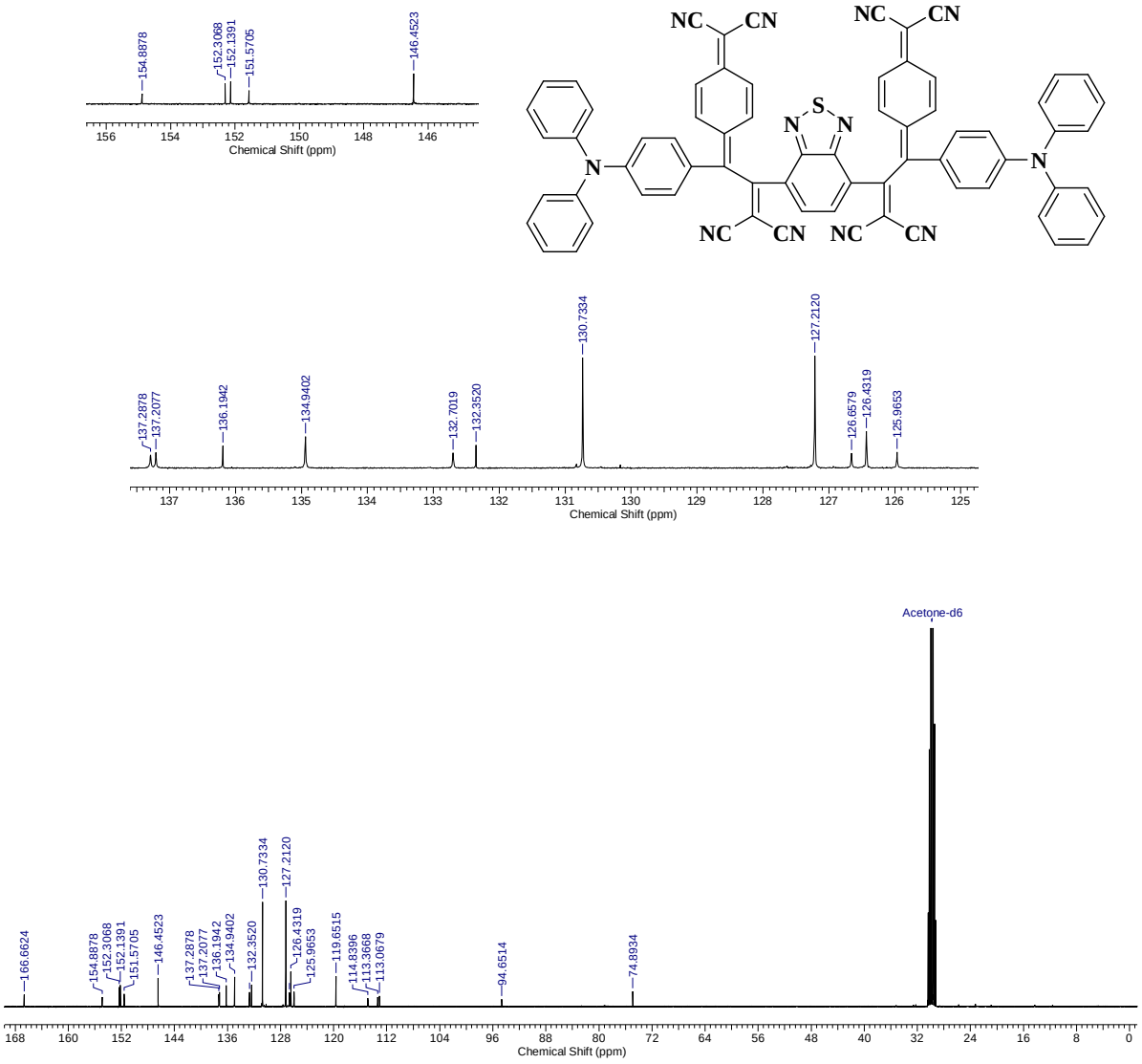

Figure S16. ^{13}C NMR spectra of BTD **12**

Copies of HRMS of new compounds.

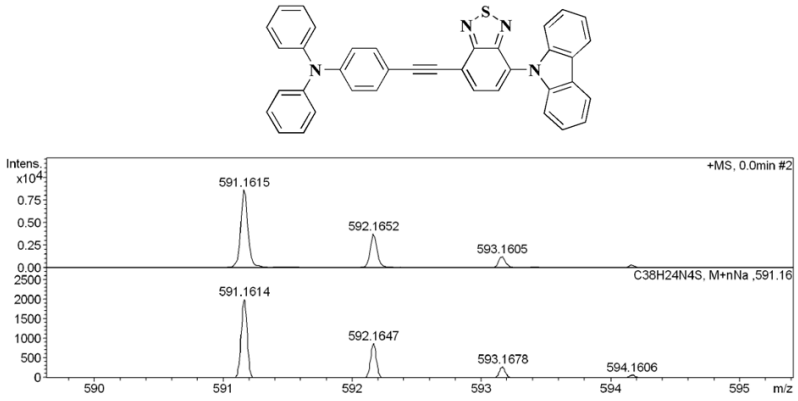

Figure S17. HRMS spectra of BTD **5**

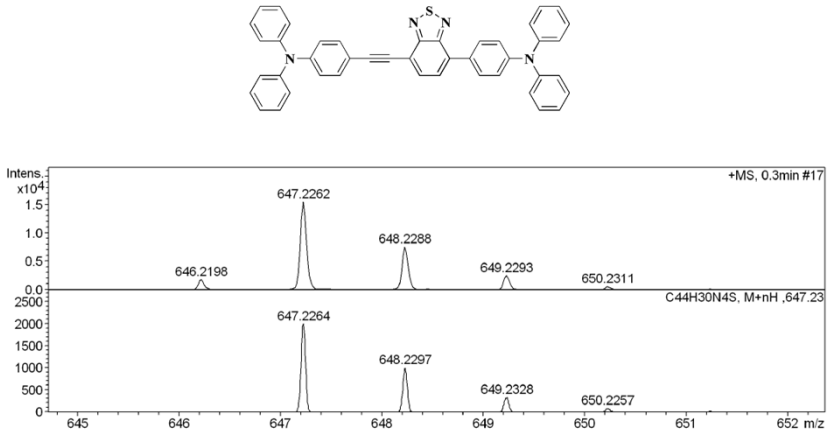

Figure S18. HRMS spectra of BTD **6**

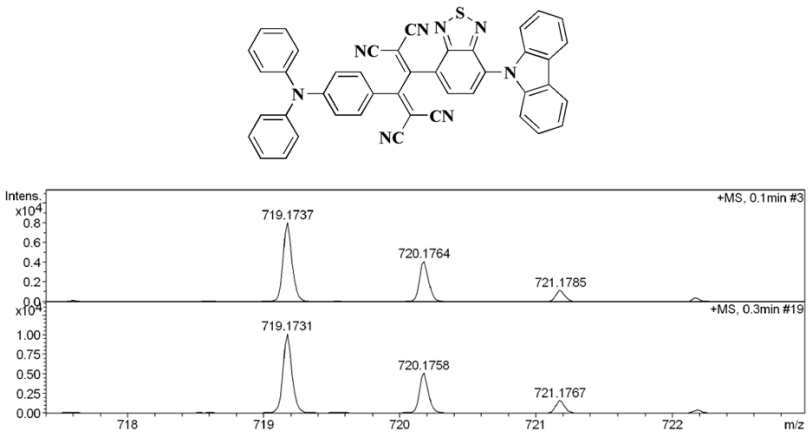

Figure S19. HRMS spectra of BTD **7**

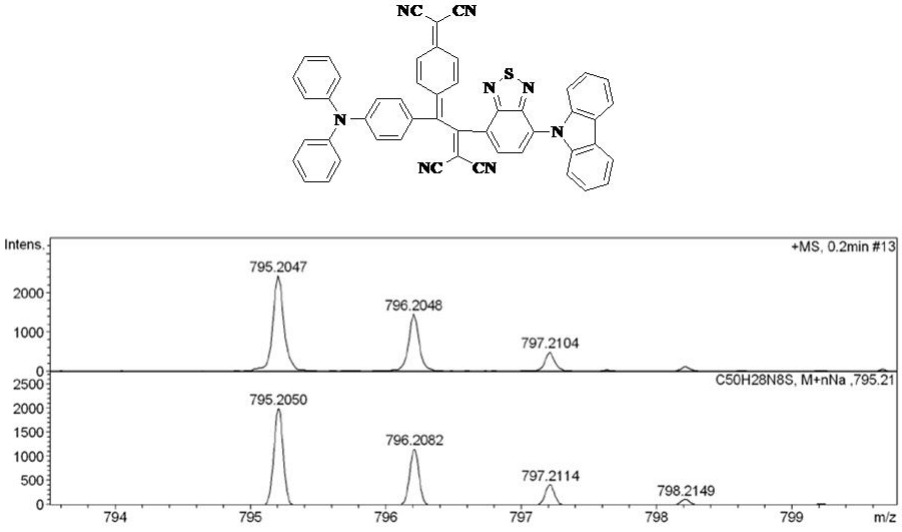

Figure S20. HRMS spectra of BTD **8**

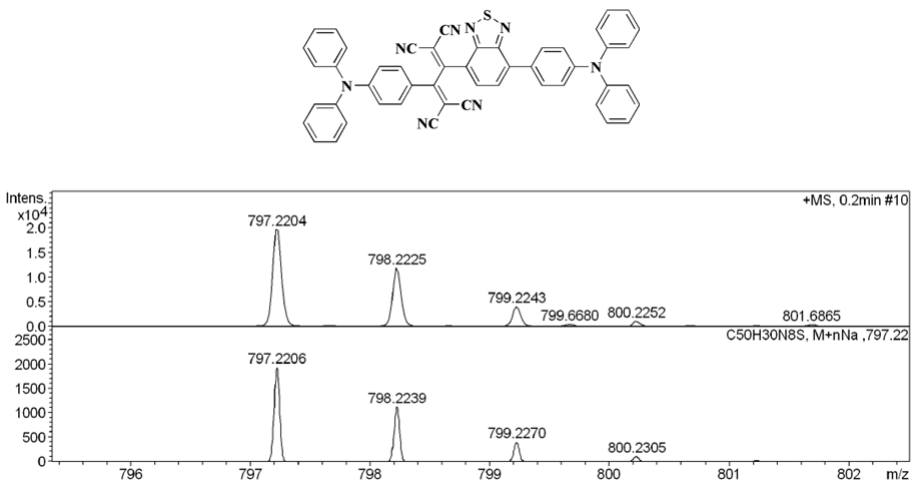

Figure S21. HRMS spectra of BTD **9**

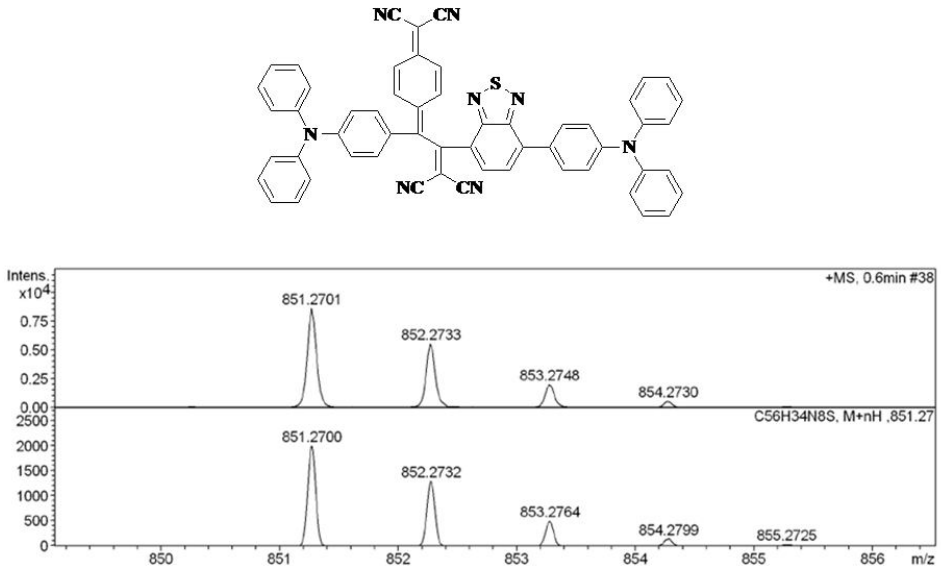

Figure S22. HRMS spectra of BTD **10**

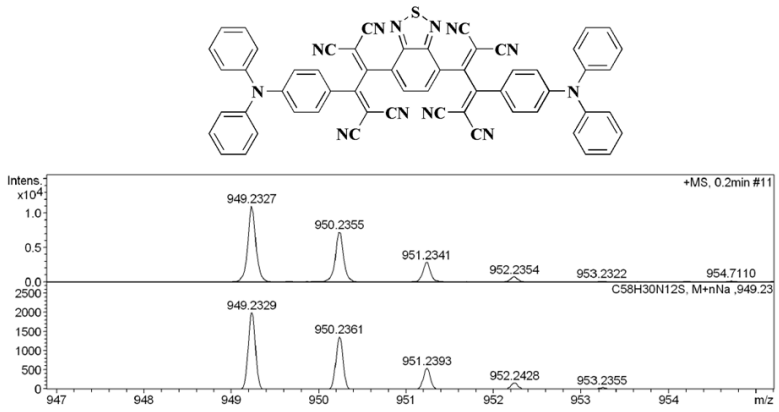

Figure S23. HRMS spectra of BTD **11**

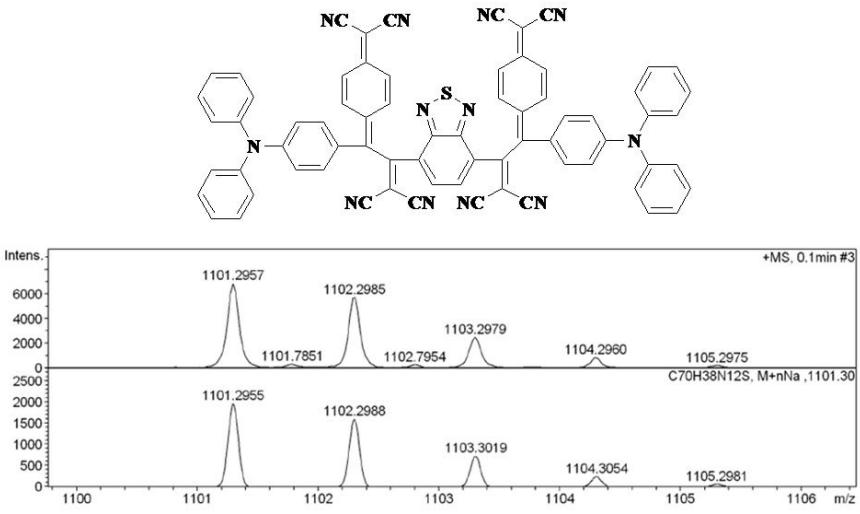

Figure S24. HRMS spectra of BTD **12**

II. Emission Data for BTD 5 and 6

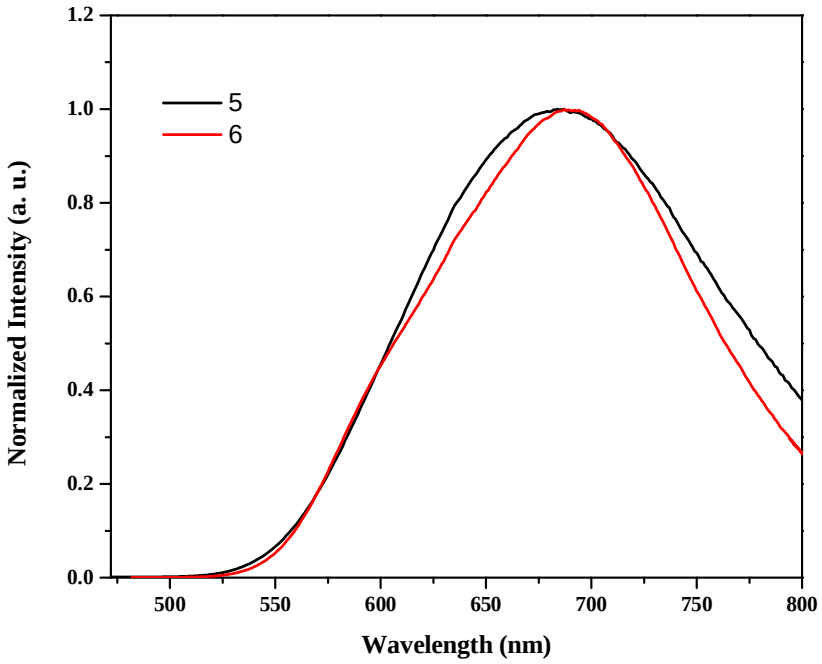

Figure S25. Emission spectra of BTD **5** and **6** at 0.1 absorption, excited at 462 nm and 473 nm respectively in dichloromethane (recorded at T = 293 K).

III. Electrochemical Data for BTD 5–12

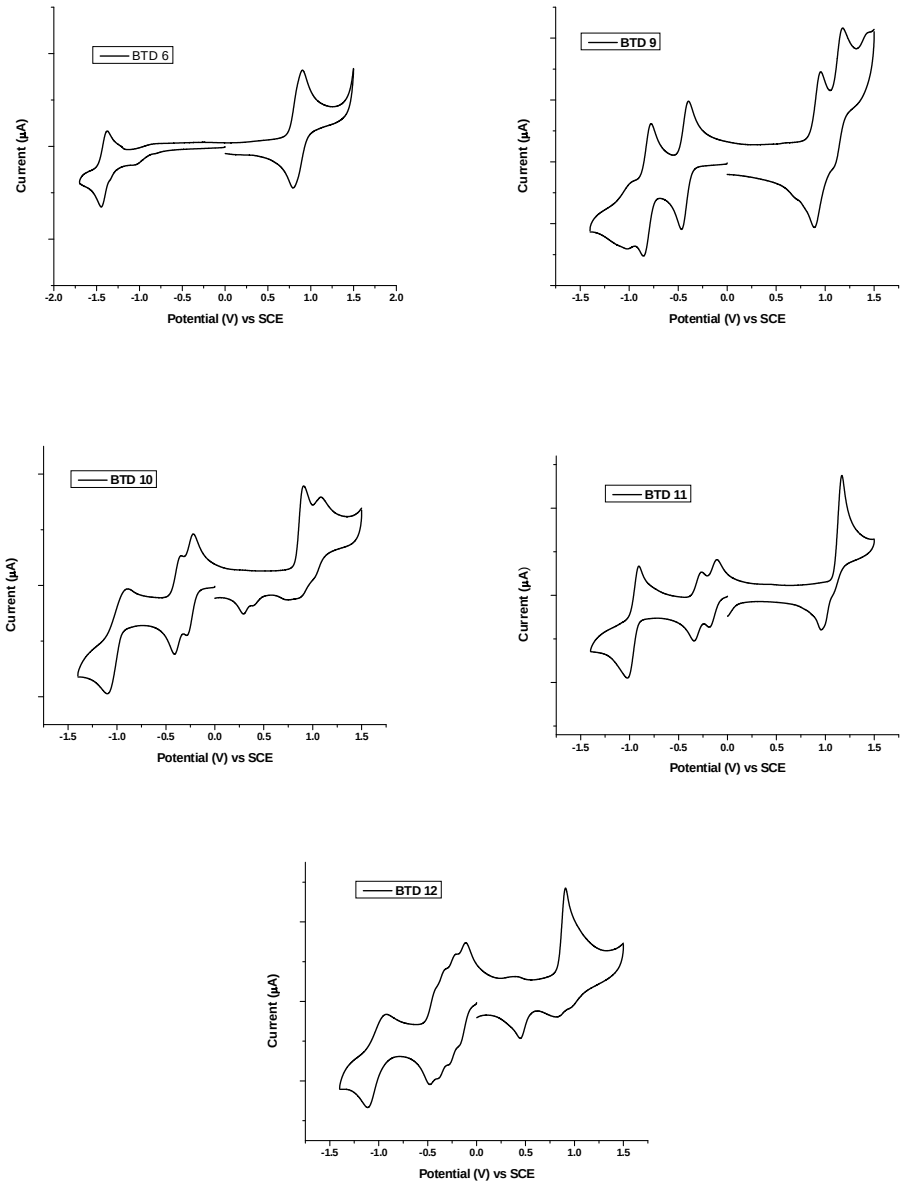

Figure S26. Cyclic voltammogram of benzothiadiazoles **6, 9, 10, 11** and **12** at 0.01 M concentration in 0.1 M $TBAPF_6$ in dichloromethane recorded at 100 mVs^{-1} scan speed.

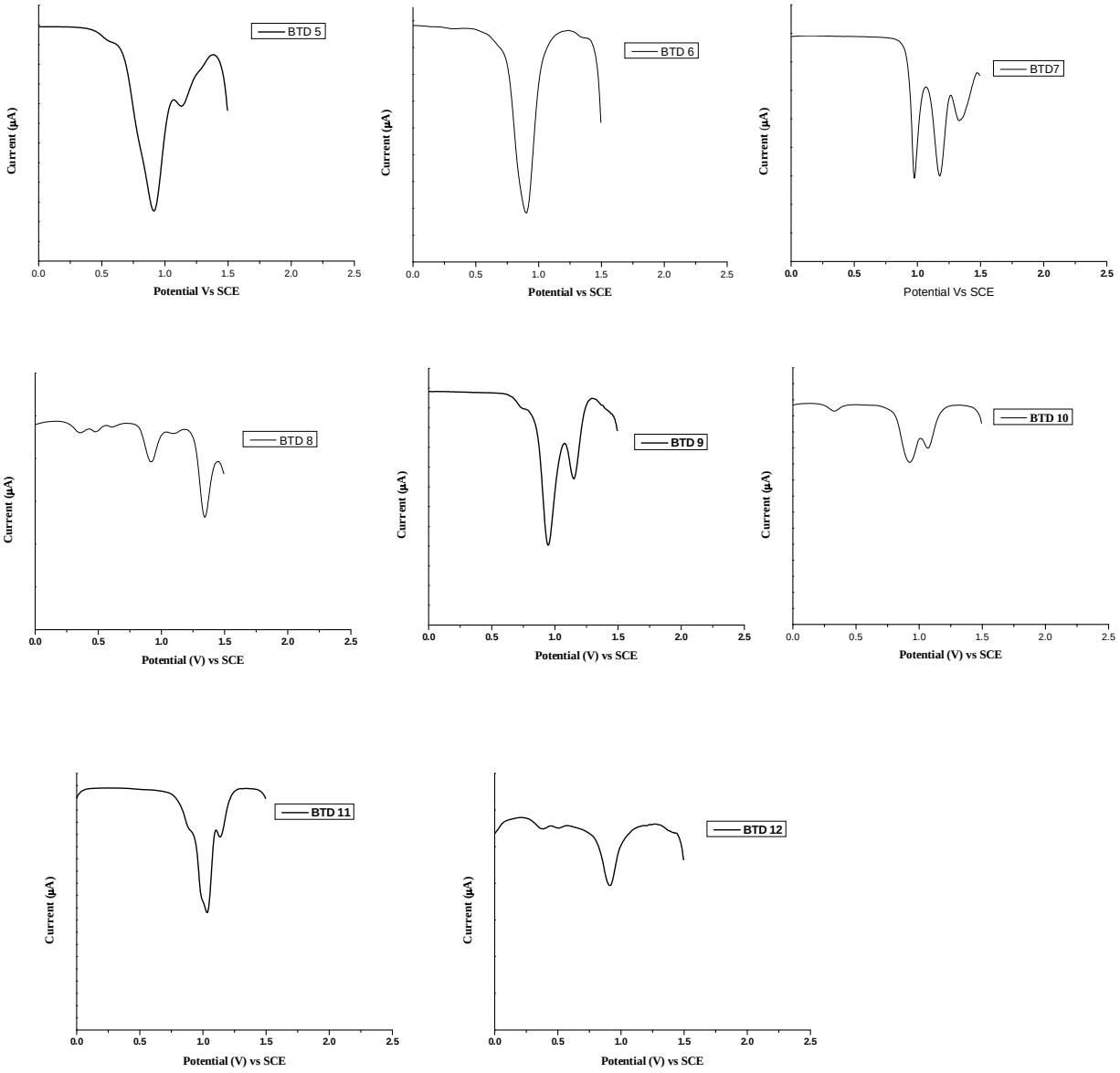

Figure S27. Differential pulse voltammogram of benzothiadiazoles **5–12** at 0.01 M concentration in 0.1 M $TBAPF_6$ in dichloromethane (representing the oxidation waves).

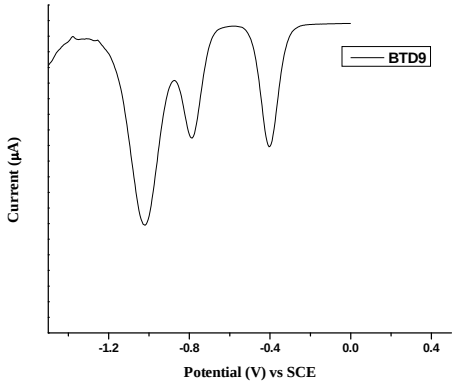

Figure S28. Differential pulse voltammogram of benzothiadiazoles **9** at 0.01 M concentration in 0.1 M $TBAPF_6$ in dichloromethane (representing the reduction waves).

VI. Thermogravimetric analysis data

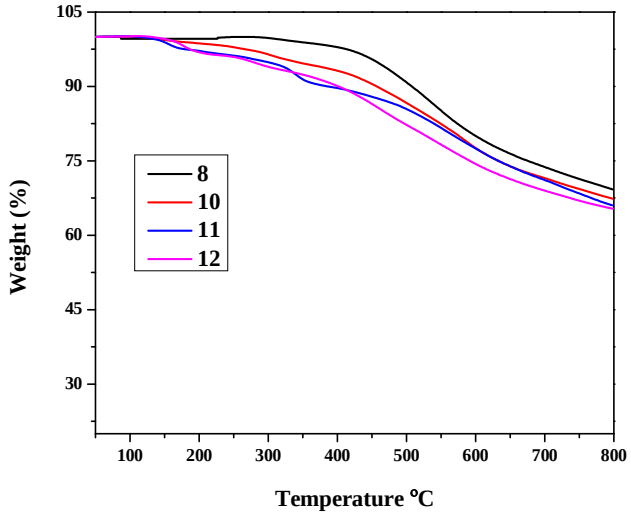

Figure S29. TGA plots of benzothiadiazoles **8**, **10–12** at a heating rate of 10 °C min^{-1}, under a nitrogen atmosphere.

V. DFT calculation

BTD 5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.100464	-2.560943	1.882939
2	7	0	1.834397	-1.723688	1.255785
3	7	0	4.354132	-1.708279	1.251759
4	6	0	2.359056	-0.737493	0.523950
5	6	0	3.811946	-0.731068	0.517622
6	6	0	4.525840	0.272654	-0.218918
7	6	0	3.773680	1.216178	-0.888742
8	1	0	4.290338	1.982642	-1.457265
9	6	0	2.354690	1.219432	-0.872577
10	1	0	1.830465	1.991040	-1.426129
11	6	0	1.610008	0.265394	-0.192576
12	6	0	0.196662	0.260138	-0.186219
13	6	0	-1.021331	0.251346	-0.181504
14	6	0	-2.439646	0.220732	-0.161918
15	6	0	-3.202970	1.159489	-0.887404
16	6	0	-3.128930	-0.756323	0.587884
17	6	0	-4.589202	1.120435	-0.870422
18	1	0	-2.692846	1.912707	-1.479392
19	6	0	-4.514889	-0.789103	0.616041
20	1	0	-2.558406	-1.480242	1.160659
21	6	0	-5.272427	0.146844	-0.115449
22	1	0	-5.155836	1.842668	-1.447451
23	1	0	-5.023765	-1.539551	1.210705
24	7	0	-6.683205	0.109976	-0.092635
25	6	0	-7.438156	1.317499	-0.151293
26	6	0	-7.372126	-1.135310	-0.012269
27	6	0	-7.076516	2.423597	0.633844
28	6	0	-8.561139	1.410242	-0.988031
29	6	0	-8.463308	-1.285347	0.857543
30	6	0	-6.977294	-2.221753	-0.808744
31	6	0	-7.818582	3.601668	0.569820
32	1	0	-6.215200	2.352978	1.289947
33	6	0	-9.307411	2.586615	-1.031890
34	1	0	-8.842853	0.558472	-1.598239
35	6	0	-9.146348	-2.498576	0.922511
36	1	0	-8.770045	-0.448949	1.476913
37	6	0	-7.655286	-3.436534	-0.723539
38	1	0	-6.140330	-2.107388	-1.489668
39	6	0	-8.939361	3.689977	-0.258900
40	1	0	-7.526175	4.449074	1.183414
41	1	0	-10.174018	2.643411	-1.684493

42	6	0	-8.744965	-3.581942	0.137937
43	1	0	-9.988997	-2.599624	1.600615
44	1	0	-7.337598	-4.268305	-1.345867
45	1	0	-9.519385	4.606828	-0.300811
46	1	0	-9.275241	-4.527552	0.196374
47	7	0	5.936140	0.313654	-0.221128
48	6	0	6.715752	1.405569	0.189621
49	6	0	6.795941	-0.694985	-0.681185
50	6	0	6.314648	2.625585	0.739181
51	6	0	8.084337	1.088508	0.000824
52	6	0	6.487423	-1.940935	-1.230967
53	6	0	8.134543	-0.246997	-0.558783
54	6	0	7.309360	3.537977	1.086952
55	1	0	5.266514	2.855612	0.896487
56	6	0	9.063333	2.022700	0.358261
57	6	0	7.546727	-2.748178	-1.639278
58	1	0	5.461394	-2.274660	-1.332764
59	6	0	9.181359	-1.077781	-0.976003
60	6	0	8.670458	3.244994	0.896979
61	1	0	7.022779	4.493869	1.515834
62	1	0	10.116385	1.793787	0.220578
63	6	0	8.881598	-2.326630	-1.511985
64	1	0	7.333023	-3.723997	-2.065751
65	1	0	10.212742	-0.748082	-0.887481
66	1	0	9.420702	3.978253	1.176996
67	1	0	9.683853	-2.981228	-1.838933

Total energy (Sum of electronic and zero-point energies): -2079.647759 Hartree

BTD 6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.013314	-3.249917	-0.799663
2	7	0	0.214365	-2.182481	-0.574504
3	7	0	-2.300746	-2.259153	-0.558551
4	6	0	-0.354167	-1.006097	-0.300663
5	6	0	-1.809311	-1.043478	-0.286137
6	6	0	-2.582130	0.144750	-0.020198
7	6	0	-1.840111	1.291877	0.218545
8	1	0	-2.366826	2.209892	0.458737
9	6	0	-0.424134	1.336874	0.204538
10	1	0	0.068913	2.281092	0.411684
11	6	0	0.359279	0.219141	-0.044569

12	6	0	1.772452	0.254558	-0.043342
13	6	0	2.990225	0.279059	-0.035356
14	6	0	4.409409	0.274419	-0.022429
15	6	0	5.145980	1.456055	0.203680
16	6	0	5.126468	-0.923416	-0.229876
17	6	0	6.533078	1.440420	0.232866
18	1	0	4.614257	2.386826	0.373938
19	6	0	6.513170	-0.938340	-0.212705
20	1	0	4.576849	-1.840168	-0.417227
21	6	0	7.242875	0.242368	0.025147
22	1	0	7.078939	2.357741	0.424142
23	1	0	7.044375	-1.867829	-0.385684
24	7	0	8.655783	0.222508	0.058173
25	6	0	9.405150	1.323626	-0.446089
26	6	0	9.345179	-0.893545	0.614016
27	6	0	9.060899	1.920574	-1.669406
28	6	0	10.505535	1.819648	0.270632
29	6	0	10.469391	-1.427516	-0.035175
30	6	0	8.915532	-1.468005	1.820907
31	6	0	9.798846	2.998148	-2.155994
32	1	0	8.216995	1.534930	-2.231917
33	6	0	11.248041	2.886276	-0.232864
34	1	0	10.772541	1.363609	1.218203
35	6	0	11.150856	-2.509920	0.518625
36	1	0	10.802017	-0.989183	-0.970308
37	6	0	9.592809	-2.561447	2.357508
38	1	0	8.052018	-1.053997	2.330990
39	6	0	10.898029	3.485173	-1.444986
40	1	0	9.520202	3.448974	-3.104321
41	1	0	12.096963	3.258478	0.333707
42	6	0	10.715598	-3.086591	1.713862
43	1	0	12.019037	-2.912047	0.004094
44	1	0	9.247703	-2.995149	3.291835
45	1	0	11.474681	4.320145	-1.831150
46	1	0	11.244858	-3.934179	2.138487
47	6	0	-4.057623	0.159339	-0.009005
48	6	0	-4.763085	1.308071	-0.417962
49	6	0	-4.819911	-0.940737	0.429040
50	6	0	-6.150048	1.363885	-0.389002
51	1	0	-4.216244	2.160279	-0.810246
52	6	0	-6.207106	-0.886911	0.478065
53	1	0	-4.317001	-1.843642	0.751940
54	6	0	-6.900078	0.265433	0.067962
55	1	0	-6.662219	2.254611	-0.736337
56	1	0	-6.764412	-1.743262	0.842071
57	7	0	-8.313536	0.315162	0.103937
58	6	0	-8.982604	1.525297	0.440807
59	6	0	-9.080635	-0.843340	-0.208976
60	6	0	-8.531606	2.317792	1.508894
61	6	0	-10.109849	1.939353	-0.286869
62	6	0	-10.191073	-1.191821	0.576169
63	6	0	-8.743325	-1.647201	-1.309601
64	6	0	-9.190338	3.503093	1.830673

65	1	0	-7.666688	1.998413	2.080795
66	6	0	-10.772513	3.116994	0.054151
67	1	0	-10.460611	1.333525	-1.115751
68	6	0	-10.949739	-2.317171	0.259017
69	1	0	-10.453429	-0.576469	1.430452
70	6	0	-9.497432	-2.780640	-1.608009
71	1	0	-7.890517	-1.379502	-1.924630
72	6	0	-10.315988	3.908724	1.110131
73	1	0	-8.828709	4.104268	2.660229
74	1	0	-11.643171	3.422825	-0.519193
75	6	0	-10.606547	-3.120832	-0.830351
76	1	0	-11.805976	-2.573227	0.876741
77	1	0	-9.222805	-3.392386	-2.462733
78	1	0	-10.830804	4.828997	1.368821
79	1	0	-11.195671	-4.000782	-1.070160

Total energy (Sum of electronic and zero-point energies): -2311.8903622 Hartree

BTD 7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	4.592399	-2.626093	1.916482
2	7	0	4.978535	-1.202413	1.201795
3	7	0	3.049003	-2.804810	1.387215
4	6	0	3.899867	-0.816108	0.513199
5	6	0	2.785683	-1.736992	0.626638
6	6	0	1.533569	-1.454800	-0.007238
7	6	0	1.441495	-0.279214	-0.723000
8	1	0	0.512250	-0.027303	-1.222867
9	6	0	2.537726	0.617454	-0.855445
10	1	0	2.407105	1.512823	-1.452793
11	6	0	3.763660	0.386648	-0.263289
12	6	0	0.428814	-2.417016	0.122545
13	6	0	-1.047407	-2.452911	0.187232
14	6	0	-0.214629	-2.994043	1.372457
15	6	0	-0.349989	-3.222460	-0.931233
16	6	0	-0.152631	-4.391503	1.779624
17	6	0	-0.180866	-2.100708	2.521697
18	6	0	-0.317711	-4.673582	-1.068463
19	6	0	-0.426661	-2.569188	-2.231464
20	7	0	-0.125474	-5.481366	2.177695
21	7	0	-0.159420	-1.384211	3.434368

22	7	0	-0.299803	-5.817097	-1.266934
23	7	0	-0.476441	-2.048065	-3.267197
24	7	0	4.817655	1.308139	-0.372981
25	6	0	4.719227	2.686134	-0.101876
26	6	0	6.114765	1.043501	-0.853188
27	6	0	3.648448	3.415671	0.419161
28	6	0	5.962961	3.297269	-0.392397
29	6	0	6.666097	-0.152845	-1.315001
30	6	0	6.846145	2.255172	-0.876788
31	6	0	3.834548	4.781721	0.627081
32	1	0	2.704559	2.941430	0.664151
33	6	0	6.124469	4.670094	-0.175149
34	6	0	7.980795	-0.124309	-1.775525
35	1	0	6.100417	-1.076616	-1.314143
36	6	0	8.165884	2.258074	-1.342938
37	6	0	5.056459	5.406971	0.329786
38	1	0	3.015982	5.370337	1.030595
39	1	0	7.073277	5.152008	-0.392819
40	6	0	8.728467	1.065126	-1.786512
41	1	0	8.433469	-1.043718	-2.134811
42	1	0	8.738149	3.181034	-1.364611
43	1	0	5.168832	6.473067	0.501355
44	1	0	9.751177	1.052004	-2.150573
45	6	0	-2.213230	-1.557623	0.119770
46	6	0	-2.179020	-0.252500	0.637891
47	6	0	-3.406466	-2.018423	-0.458814
48	6	0	-3.298449	0.565525	0.574907
49	1	0	-1.268672	0.132512	1.085569
50	6	0	-4.530304	-1.207095	-0.520137
51	1	0	-3.460110	-3.029228	-0.852983
52	6	0	-4.499755	0.104597	-0.002994
53	1	0	-3.245479	1.574097	0.967575
54	1	0	-5.443008	-1.588045	-0.962666
55	7	0	-5.633487	0.929725	-0.064349
56	6	0	-6.597974	0.770038	-1.107451
57	6	0	-7.963212	0.700400	-0.796000
58	6	0	-6.192871	0.703172	-2.448728
59	6	0	-8.906764	0.568452	-1.813766
60	1	0	-8.276515	0.752083	0.241668
61	6	0	-7.142075	0.553497	-3.458867
62	1	0	-5.137334	0.768190	-2.692811
63	6	0	-8.502217	0.489370	-3.147991
64	1	0	-9.961527	0.515788	-1.559950
65	1	0	-6.816025	0.501700	-4.493614
66	1	0	-9.239119	0.380398	-3.937805
67	6	0	-5.856276	1.945675	0.915501
68	6	0	-6.226180	3.237451	0.514238
69	6	0	-5.730486	1.659214	2.283134
70	6	0	-6.467553	4.224199	1.468948
71	1	0	-6.324732	3.459289	-0.543360
72	6	0	-5.955767	2.657208	3.230101
73	1	0	-5.457445	0.657019	2.597206
74	6	0	-6.328641	3.942194	2.829569

75	1	0	-6.754333	5.220616	1.145357
76	1	0	-5.853769	2.422955	4.285743
77	1	0	-6.511172	4.714710	3.570251

Total energy (Sum of electronic and zero-point energies): -2527.1551482 Hartree

BTD 8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	4.811031	1.858566	-2.343127
2	7	0	5.199734	0.673745	-1.278419
3	7	0	3.173805	1.833103	-2.218447
4	6	0	4.046294	0.208262	-0.789153
5	6	0	2.879517	0.881361	-1.326078
6	6	0	1.560740	0.536004	-0.887593
7	6	0	1.461607	-0.454487	0.066366
8	1	0	0.481262	-0.762119	0.416439
9	6	0	2.601080	-1.123646	0.595703
10	1	0	2.450760	-1.909425	1.327820
11	6	0	3.888658	-0.828548	0.195189
12	6	0	0.411848	1.259481	-1.456632
13	6	0	-1.050613	1.181325	-1.545277
14	6	0	-0.208743	1.099804	-2.842441
15	6	0	-0.194942	2.083951	-3.916036
16	6	0	-0.086716	-0.245213	-3.386750
17	7	0	-0.202666	2.826081	-4.809584
18	7	0	0.015092	-1.317946	-3.818993
19	6	0	-2.199029	0.374800	-1.088531
20	6	0	-2.157472	-1.026823	-0.994308
21	6	0	-3.397267	1.026540	-0.755147
22	6	0	-3.268232	-1.746646	-0.573770
23	1	0	-1.250081	-1.564252	-1.248940
24	6	0	-4.514195	0.313151	-0.342078
25	1	0	-3.457801	2.108002	-0.833895
26	6	0	-4.472568	-1.092408	-0.241858
27	1	0	-3.206429	-2.825815	-0.496104
28	1	0	-5.429561	0.841299	-0.102433
29	7	0	-5.598162	-1.820424	0.177379
30	6	0	-6.560761	-1.235554	1.057082
31	6	0	-7.928207	-1.323171	0.759606
32	6	0	-6.152546	-0.588888	2.233145
33	6	0	-8.869622	-0.773506	1.628591
34	1	0	-8.244421	-1.823745	-0.149786

35	6	0	-7.099681	-0.026449	3.087718
36	1	0	-5.095300	-0.530880	2.471437
37	6	0	-8.461687	-0.118716	2.792688
38	1	0	-9.925963	-0.848006	1.387116
39	1	0	-6.770879	0.472579	3.994701
40	1	0	-9.197266	0.313893	3.463813
41	6	0	-5.813810	-3.160474	-0.268989
42	6	0	-6.171729	-4.156032	0.651565
43	6	0	-5.692898	-3.490510	-1.627272
44	6	0	-6.405938	-5.459670	0.216835
45	1	0	-6.266828	-3.900992	1.701991
46	6	0	-5.911070	-4.800830	-2.050303
47	1	0	-5.428811	-2.719836	-2.344174
48	6	0	-6.271779	-5.790510	-1.133215
49	1	0	-6.683237	-6.221374	0.939803
50	1	0	-5.812867	-5.043817	-3.104331
51	1	0	-6.448329	-6.808130	-1.467819
52	6	0	-0.432626	2.440695	-0.902426
53	6	0	-0.443680	3.799322	-1.490024
54	6	0	-0.536535	2.418105	0.575718
55	6	0	-0.536408	4.911673	-0.730159
56	1	0	-0.368382	3.912573	-2.561911
57	6	0	-0.629300	3.534977	1.322574
58	1	0	-0.538061	1.448438	1.062285
59	1	0	-0.536532	5.887463	-1.205121
60	1	0	-0.702161	3.463652	2.402896
61	6	0	-0.636143	4.852589	0.714432
62	6	0	-0.734200	5.999247	1.486031
63	6	0	-0.835196	5.935167	2.909213
64	6	0	-0.742130	7.301263	0.899654
65	7	0	-0.918408	5.863316	4.068839
66	7	0	-0.748910	8.358637	0.411390
67	7	0	5.000565	-1.480003	0.754232
68	6	0	5.997394	-2.184465	0.052213
69	6	0	5.253773	-1.611474	2.132464
70	6	0	6.135168	-2.400091	-1.320021
71	6	0	6.893468	-2.755935	0.987186
72	6	0	4.564795	-1.068488	3.219080
73	6	0	6.426318	-2.385635	2.308291
74	6	0	7.209246	-3.177496	-1.748115
75	1	0	5.438516	-1.977920	-2.034091
76	6	0	7.965449	-3.532531	0.532302
77	6	0	5.058488	-1.329731	4.496596
78	1	0	3.679880	-0.457004	3.081190
79	6	0	6.901576	-2.633738	3.600752
80	6	0	8.120131	-3.735799	-0.835599
81	1	0	7.340526	-3.355267	-2.811338
82	1	0	8.660913	-3.975948	1.239113
83	6	0	6.211884	-2.107402	4.689788
84	1	0	4.539345	-0.918696	5.357351
85	1	0	7.800483	-3.224844	3.750525
86	1	0	8.947125	-4.335687	-1.202852
87	1	0	6.570000	-2.293878	5.697536

Total energy (Sum of electronic and zero-point energies): -2758.1914218 Hartree

BTD 9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.209860	4.639350	1.075221
2	7	0	-2.994969	3.243980	0.721141
3	7	0	-0.687429	4.232585	0.613712
4	6	0	-2.086066	2.398116	0.220125
5	6	0	-0.754506	2.975273	0.165405
6	6	0	0.355239	2.213636	-0.318688
7	6	0	0.095941	0.921002	-0.724259
8	1	0	0.905090	0.307820	-1.107767
9	6	0	-1.208669	0.361578	-0.680011
10	1	0	-1.332454	-0.648617	-1.054720
11	6	0	-2.324807	1.043436	-0.218176
12	6	0	1.681864	2.841708	-0.387373
13	6	0	3.115724	2.496816	-0.309148
14	6	0	2.510554	3.488289	0.711039
15	6	0	2.598841	3.160278	-1.582718
16	6	0	2.839404	4.905100	0.793833
17	6	0	2.294767	2.912360	2.030752
18	6	0	2.948719	4.499111	-2.041042
19	6	0	2.441238	2.241659	-2.702581
20	7	0	3.120659	6.021832	0.938399
21	7	0	2.129096	2.448136	3.081409
22	7	0	3.228418	5.532250	-2.490401
23	7	0	2.307822	1.512641	-3.595651
24	6	0	4.007965	1.336496	-0.153902
25	6	0	3.658141	0.229475	0.636320
26	6	0	5.257755	1.337217	-0.792765
27	6	0	4.528202	-0.842900	0.779060
28	1	0	2.695414	0.200040	1.136097
29	6	0	6.134176	0.271046	-0.648587
30	1	0	5.553610	2.189185	-1.398243
31	6	0	5.786455	-0.842845	0.142505
32	1	0	4.232948	-1.693922	1.381488
33	1	0	7.098259	0.298900	-1.142386
34	7	0	6.669695	-1.925329	0.290412
35	6	0	7.599230	-2.254607	-0.743903
36	6	0	8.948251	-2.474896	-0.431274
37	6	0	7.171155	-2.380092	-2.073962
38	6	0	9.851877	-2.819127	-1.435517
39	1	0	9.279366	-2.376603	0.597430

40	6	0	8.085162	-2.707257	-3.074587
41	1	0	6.125560	-2.219901	-2.316797
42	6	0	9.427566	-2.932218	-2.761146
43	1	0	10.894218	-2.987420	-1.180601
44	1	0	7.741721	-2.800054	-4.100830
45	1	0	10.135080	-3.193948	-3.541956
46	6	0	6.671799	-2.712705	1.482096
47	6	0	6.696990	-4.112493	1.398132
48	6	0	6.670024	-2.099656	2.744203
49	6	0	6.722427	-4.882999	2.559582
50	1	0	6.699404	-4.587724	0.422618
51	6	0	6.676987	-2.878595	3.900289
52	1	0	6.662859	-1.016741	2.813720
53	6	0	6.707119	-4.272271	3.815367
54	1	0	6.742517	-5.966152	2.480459
55	1	0	6.673897	-2.391172	4.870912
56	1	0	6.720361	-4.875466	4.717978
57	6	0	-3.654025	0.410026	-0.171573
58	6	0	-3.776312	-0.974079	0.062280
59	6	0	-4.842774	1.135408	-0.382665
60	6	0	-5.011415	-1.604752	0.081775
61	1	0	-2.889581	-1.561167	0.281584
62	6	0	-6.081490	0.509242	-0.384796
63	1	0	-4.793522	2.200792	-0.569739
64	6	0	-6.193025	-0.874408	-0.151181
65	1	0	-5.071024	-2.666218	0.294433
66	1	0	-6.975062	1.092465	-0.576887
67	7	0	-7.450423	-1.510650	-0.141943
68	6	0	-7.584892	-2.855961	-0.594603
69	6	0	-8.610290	-0.817895	0.315597
70	6	0	-6.967649	-3.273990	-1.783930
71	6	0	-8.350186	-3.775005	0.139520
72	6	0	-9.806868	-0.886336	-0.413878
73	6	0	-8.573678	-0.072790	1.504420
74	6	0	-7.104998	-4.590897	-2.219499
75	1	0	-6.384783	-2.563371	-2.360670
76	6	0	-8.496581	-5.085051	-0.313412
77	1	0	-8.826860	-3.455432	1.060341
78	6	0	-10.945393	-0.225033	0.043754
79	1	0	-9.837184	-1.458601	-1.335304
80	6	0	-9.712411	0.599645	1.944796
81	1	0	-7.652702	-0.023876	2.076094
82	6	0	-7.872115	-5.502590	-1.490729
83	1	0	-6.622104	-4.899844	-3.142231
84	1	0	-9.092358	-5.785246	0.265200
85	6	0	-10.904750	0.524589	1.221295
86	1	0	-11.864822	-0.287002	-0.531407
87	1	0	-9.669159	1.172949	2.866434
88	1	0	-7.983398	-6.525489	-1.837237
89	1	0	-11.791657	1.043768	1.571451

Total energy (Sum of electronic and zero-point energies): -2759.3997905 Hartree

BTD 10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	2.460377	3.949407	-2.337874
2	7	0	3.274975	2.697289	-1.660458
3	7	0	0.915078	3.459114	-2.072831
4	6	0	2.358928	1.839955	-1.193669
5	6	0	0.997914	2.284703	-1.439650
6	6	0	-0.121927	1.492296	-1.032932
7	6	0	0.163193	0.298277	-0.405402
8	1	0	-0.651917	-0.341784	-0.081392
9	6	0	1.493735	-0.133357	-0.155368
10	1	0	1.624967	-1.069218	0.376953
11	6	0	2.619782	0.584824	-0.528470
12	6	0	-1.480424	1.995955	-1.287097
13	6	0	-2.879781	1.556052	-1.265433
14	6	0	-2.253512	2.012482	-2.604971
15	6	0	-2.637191	3.191467	-3.369279
16	6	0	-1.905685	0.919427	-3.501815
17	7	0	-2.956930	4.096240	-4.023884
18	7	0	-1.627119	0.047751	-4.216371
19	6	0	-3.727582	0.391663	-0.941161
20	6	0	-3.361274	-0.929539	-1.249933
21	6	0	-4.966288	0.607198	-0.316330
22	6	0	-4.197628	-1.993114	-0.935953
23	1	0	-2.413456	-1.133543	-1.736580
24	6	0	-5.810977	-0.450361	-0.006638
25	1	0	-5.277312	1.620813	-0.081398
26	6	0	-5.442250	-1.776128	-0.310390
27	1	0	-3.886288	-3.004126	-1.171600
28	1	0	-6.766425	-0.253444	0.465350
29	7	0	-6.290416	-2.852540	0.002881
30	6	0	-7.185858	-2.776828	1.113556
31	6	0	-8.531572	-3.138774	0.957064
32	6	0	-6.727727	-2.360239	2.372418
33	6	0	-9.401429	-3.086248	2.045213
34	1	0	-8.886561	-3.460599	-0.016528
35	6	0	-7.608455	-2.293541	3.451021
36	1	0	-5.683987	-2.090983	2.498697
37	6	0	-8.947382	-2.658980	3.294802
38	1	0	-10.441437	-3.369264	1.910920
39	1	0	-7.241799	-1.968124	4.420286
40	1	0	-9.629050	-2.612527	4.138511
41	6	0	-6.286729	-4.042133	-0.787564
42	6	0	-6.254933	-5.297959	-0.163923
43	6	0	-6.335313	-3.971225	-2.188056
44	6	0	-6.274580	-6.461530	-0.931376
45	1	0	-6.218048	-5.353922	0.919131
46	6	0	-6.336098	-5.139920	-2.948031

47	1	0	-6.371555	-3.001646	-2.674155
48	6	0	-6.309865	-6.389915	-2.325525
49	1	0	-6.250453	-7.427748	-0.435680
50	1	0	-6.372293	-5.070795	-4.031375
51	1	0	-6.318497	-7.297920	-2.920641
52	6	0	3.979831	0.080060	-0.270953
53	6	0	4.234829	-1.305890	-0.261242
54	6	0	5.065410	0.935790	-0.000214
55	6	0	5.496572	-1.815100	0.007132
56	1	0	3.439522	-1.999194	-0.517953
57	6	0	6.327678	0.434767	0.286452
58	1	0	4.913250	2.007791	0.005686
59	6	0	6.571656	-0.951662	0.294723
60	1	0	5.662933	-2.886017	-0.022939
61	1	0	7.135944	1.120472	0.514407
62	7	0	7.855629	-1.460783	0.571749
63	6	0	8.013535	-2.716145	1.228859
64	6	0	9.022190	-0.732978	0.190310
65	6	0	7.250328	-3.028601	2.364780
66	6	0	8.948555	-3.648818	0.754459
67	6	0	10.082348	-0.575929	1.095740
68	6	0	9.129902	-0.180384	-1.095126
69	6	0	7.412668	-4.257671	3.001820
70	1	0	6.535672	-2.304892	2.742956
71	6	0	9.116208	-4.868207	1.408442
72	1	0	9.539500	-3.411142	-0.123914
73	6	0	11.229717	0.119167	0.717092
74	1	0	10.000717	-1.000623	2.090916
75	6	0	10.273786	0.528231	-1.458907
76	1	0	8.316157	-0.308919	-1.801343
77	6	0	8.347412	-5.182582	2.531134
78	1	0	6.815525	-4.485335	3.880287
79	1	0	9.843724	-5.580298	1.029435
80	6	0	11.330634	0.679130	-0.558302
81	1	0	12.042718	0.233556	1.428363
82	1	0	10.343466	0.951303	-2.456945
83	1	0	8.476538	-6.135808	3.034578
84	1	0	12.222955	1.225773	-0.847647
85	6	0	-2.483070	2.744188	-0.363724
86	6	0	-2.906761	4.148575	-0.557428
87	6	0	-2.346662	2.341796	1.055617
88	6	0	-3.143229	4.979029	0.481175
89	1	0	-3.026543	4.531391	-1.560717
90	6	0	-2.586295	3.179109	2.083041
91	1	0	-2.037780	1.321761	1.257832
92	1	0	-3.448349	6.002975	0.290870
93	1	0	-2.469892	2.834820	3.105465
94	6	0	-3.002416	4.550704	1.858299
95	6	0	-3.252773	5.408446	2.917992
96	6	0	-3.115710	4.980699	4.273592
97	6	0	-3.662392	6.760376	2.710140
98	7	0	-3.000511	4.614814	5.373545
99	7	0	-3.997310	7.861408	2.530526

Total energy (Sum of electronic and zero-point energies): -2990.4359033 Hartree

BTD 11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.025744	-2.250719	-2.267089
2	7	0	-2.320749	-1.857950	-0.703650
3	7	0	-0.389674	-2.353001	-2.232789
4	6	0	-1.132525	-1.801441	-0.094344
5	6	0	-0.019615	-2.080111	-0.977320
6	6	0	1.327594	-2.024704	-0.494027
7	6	0	1.511632	-1.702117	0.834297
8	1	0	2.514563	-1.640085	1.241369
9	6	0	0.414509	-1.453994	1.708002
10	1	0	0.630783	-1.219905	2.745774
11	6	0	-0.897784	-1.498090	1.285099
12	6	0	2.434427	-2.316215	-1.420110
13	6	0	3.817184	-1.873273	-1.711646
14	6	0	2.721963	-1.743150	-2.796602
15	6	0	3.581093	-3.335642	-1.347084
16	6	0	2.686203	-2.499772	-4.041532
17	6	0	2.242794	-0.381617	-2.988044
18	6	0	3.739913	-4.470462	-2.249387
19	6	0	3.988325	-3.678776	0.009571
20	7	0	2.652649	-3.032266	-5.072158
21	7	0	1.863415	0.704661	-3.138959
22	7	0	3.901141	-5.419557	-2.897655
23	7	0	4.300371	-3.955470	1.092512
24	6	0	4.837779	-0.941165	-1.210077
25	6	0	4.500657	0.316686	-0.682494
26	6	0	6.193459	-1.302331	-1.271087
27	6	0	5.485448	1.181800	-0.228137
28	1	0	3.461055	0.620293	-0.615421
29	6	0	7.182700	-0.439968	-0.821985
30	1	0	6.478039	-2.264024	-1.688399
31	6	0	6.848955	0.823137	-0.289313
32	1	0	5.201689	2.140675	0.188984
33	1	0	8.222706	-0.736281	-0.888681
34	7	0	7.844023	1.697534	0.169343
35	6	0	9.085823	1.198110	0.672316
36	6	0	10.294970	1.748891	0.225036
37	6	0	9.107044	0.174157	1.630759
38	6	0	11.506175	1.280748	0.732441

39	1	0	10.277534	2.542138	-0.515253
40	6	0	10.323535	-0.299699	2.119949
41	1	0	8.171642	-0.244779	1.987677
42	6	0	11.527548	0.252448	1.677071
43	1	0	12.436572	1.715329	0.378651
44	1	0	10.327492	-1.093506	2.861215
45	1	0	12.472715	-0.113865	2.065860
46	6	0	7.642106	3.113013	0.149294
47	6	0	7.928591	3.878185	1.288533
48	6	0	7.178338	3.750129	-1.011072
49	6	0	7.754015	5.261120	1.263329
50	1	0	8.287724	3.384581	2.185724
51	6	0	6.989745	5.131401	-1.021641
52	1	0	6.967688	3.160443	-1.897473
53	6	0	7.279612	5.893645	0.112202
54	1	0	7.979104	5.843707	2.151911
55	1	0	6.628372	5.613486	-1.925293
56	1	0	7.138464	6.970000	0.098103
57	6	0	-1.989823	-1.241684	2.242182
58	6	0	-3.364580	-0.710804	2.360423
59	6	0	-2.210554	-0.026401	3.134981
60	6	0	-3.097766	-2.142732	2.811157
61	6	0	-4.491620	-0.161341	1.593662
62	6	0	-2.057050	-0.006183	4.584137
63	6	0	-1.768741	1.228293	2.543474
64	6	0	-3.137024	-2.608900	4.193723
65	6	0	-3.594672	-3.178265	1.912999
66	6	0	-4.309706	0.692699	0.493988
67	6	0	-5.800448	-0.463562	2.000929
68	7	0	-1.906060	0.095084	5.730822
69	7	0	-1.406925	2.227106	2.075978
70	7	0	-3.199871	-3.055892	5.263112
71	7	0	-3.994684	-4.043445	1.251760
72	6	0	-5.401159	1.226498	-0.174501
73	1	0	-3.310597	0.927535	0.144402
74	6	0	-6.896376	0.070328	1.338253
75	1	0	-5.964429	-1.111389	2.857348
76	6	0	-6.718727	0.931052	0.235825
77	1	0	-5.239410	1.870006	-1.031180
78	1	0	-7.896867	-0.169470	1.677808
79	7	0	-7.821239	1.477332	-0.438723
80	6	0	-9.075247	0.791701	-0.467636
81	6	0	-7.725877	2.743632	-1.094449
82	6	0	-10.257470	1.477854	-0.155731
83	6	0	-9.138656	-0.562950	-0.826306
84	6	0	-8.220874	2.897103	-2.397414
85	6	0	-7.159496	3.846748	-0.438401
86	6	0	-11.483561	0.816195	-0.204848
87	1	0	-10.208160	2.525926	0.121102
88	6	0	-10.367215	-1.221327	-0.855508
89	1	0	-8.225769	-1.092500	-1.079598
90	6	0	-8.149549	4.136887	-3.030830
91	1	0	-8.660395	2.044243	-2.904293

92	6	0	-7.076137	5.078340	-1.086232
93	1	0	-6.787273	3.733739	0.574662
94	6	0	-11.544895	-0.535795	-0.549066
95	1	0	-12.392631	1.358410	0.038728
96	1	0	-10.403452	-2.270659	-1.133468
97	6	0	-7.573003	5.231181	-2.382473
98	1	0	-8.536320	4.243279	-4.040203
99	1	0	-6.633867	5.924381	-0.568287
100	1	0	-12.500696	-1.049788	-0.580114
101	1	0	-7.513060	6.193565	-2.881397

Total energy (Sum of electronic and zero-point energies): -3283.0554384 Hartree

BTD 12

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.945826	0.937522	-2.871535
2	7	0	2.331070	0.781023	-1.282727
3	7	0	0.313842	0.832943	-2.776291
4	6	0	1.179108	0.640315	-0.616685
5	6	0	0.016485	0.666536	-1.483512
6	6	0	-1.305805	0.499768	-0.957726
7	6	0	-1.411916	0.309205	0.402767
8	1	0	-2.386932	0.143631	0.848481
9	6	0	-0.273210	0.297805	1.257507
10	1	0	-0.436930	0.143048	2.319584
11	6	0	1.019545	0.458639	0.798460
12	6	0	-2.447361	0.540230	-1.887326
13	6	0	-3.848457	0.109481	-1.985472
14	6	0	-2.802481	-0.472821	-2.968652
15	6	0	-2.761703	-0.249057	-4.407761
16	6	0	-2.390140	-1.834640	-2.658356
17	7	0	-2.734224	-0.129536	-5.562733
18	7	0	-2.055640	-2.919098	-2.413815
19	6	0	-4.901523	-0.556487	-1.196373
20	6	0	-4.630297	-1.605613	-0.301241
21	6	0	-6.236071	-0.150225	-1.357897
22	6	0	-5.653229	-2.219868	0.408491
23	1	0	-3.611353	-1.947860	-0.153254

24	6	0	-7.265088	-0.765016	-0.658241
25	1	0	-6.471538	0.650047	-2.053431
26	6	0	-6.995011	-1.817070	0.241614
27	1	0	-5.415714	-3.017648	1.102263
28	1	0	-8.287170	-0.439974	-0.812383
29	7	0	-8.028645	-2.446784	0.950773
30	6	0	-9.242305	-1.754461	1.252700
31	6	0	-10.478838	-2.356814	0.981017
32	6	0	-9.210901	-0.481690	1.841551
33	6	0	-11.664055	-1.693728	1.295851
34	1	0	-10.502770	-3.342128	0.527020
35	6	0	-10.400919	0.181784	2.137136
36	1	0	-8.254675	-0.019533	2.065162
37	6	0	-11.632099	-0.421111	1.869866
38	1	0	-12.615773	-2.170783	1.080700
39	1	0	-10.363988	1.167369	2.592096
40	1	0	-12.556841	0.095156	2.108473
41	6	0	-7.906021	-3.808505	1.370224
42	6	0	-8.219494	-4.164836	2.689406
43	6	0	-7.494722	-4.799865	0.467251
44	6	0	-8.122788	-5.494888	3.095989
45	1	0	-8.539455	-3.397343	3.386748
46	6	0	-7.383557	-6.124615	0.887208
47	1	0	-7.263165	-4.528094	-0.557584
48	6	0	-7.699729	-6.479440	2.200506
49	1	0	-8.368602	-5.759069	4.120416
50	1	0	-7.061926	-6.883209	0.179638
51	1	0	-7.618813	-7.513210	2.522088
52	6	0	2.130451	0.417698	1.769830
53	6	0	3.526570	-0.001070	1.966923
54	6	0	2.405555	-0.702443	2.771204
55	6	0	4.682424	-0.578215	1.257987
56	6	0	2.205436	-0.640540	4.213411
57	6	0	2.069725	-2.031189	2.277869
58	6	0	4.546234	-1.488912	0.197973
59	6	0	5.976260	-0.235051	1.681642
60	7	0	2.028233	-0.648740	5.361672
61	7	0	1.792347	-3.090900	1.893414
62	6	0	5.663985	-2.037275	-0.415215
63	1	0	3.560650	-1.758868	-0.164486
64	6	0	7.098644	-0.784833	1.077963
65	1	0	6.103872	0.460585	2.506102
66	6	0	6.964494	-1.702214	0.015734
67	1	0	5.535283	-2.726185	-1.241798
68	1	0	8.086237	-0.514140	1.432367
69	7	0	8.094143	-2.266155	-0.599665
70	6	0	9.335332	-1.559710	-0.640323
71	6	0	8.035007	-3.569705	-1.182315
72	6	0	10.524674	-2.207428	-0.276679
73	6	0	9.381852	-0.222707	-1.062807
74	6	0	8.566153	-3.790916	-2.461188
75	6	0	7.467308	-4.641923	-0.477837
76	6	0	11.739275	-1.525904	-0.337460

77	1	0	10.489927	-3.241903	0.049020
78	6	0	10.598539	0.456667	-1.103557
79	1	0	8.464359	0.276529	-1.357492
80	6	0	8.529844	-5.066469	-3.022469
81	1	0	9.006476	-2.962223	-3.006097
82	6	0	7.418799	-5.910190	-1.054495
83	1	0	7.066170	-4.476390	0.516804
84	6	0	11.782942	-0.190968	-0.745121
85	1	0	12.653450	-2.038987	-0.053237
86	1	0	10.620957	1.491853	-1.431696
87	6	0	7.952202	-6.130366	-2.326310
88	1	0	8.944724	-5.225081	-4.013683
89	1	0	6.974739	-6.731443	-0.499528
90	1	0	12.729807	0.338638	-0.785119
91	1	0	7.919382	-7.120943	-2.769434
92	6	0	3.184240	1.473097	2.243724
93	6	0	3.140679	2.111541	3.580268
94	6	0	3.655539	2.364817	1.157418
95	6	0	3.482414	3.403269	3.771443
96	1	0	2.820619	1.534723	4.436034
97	6	0	3.995994	3.652035	1.366019
98	1	0	3.723887	1.936730	0.163734
99	1	0	3.430895	3.829944	4.768094
100	1	0	4.339094	4.262900	0.537263
101	6	0	3.927283	4.252902	2.683875
102	6	0	4.278364	5.576383	2.894324
103	6	0	4.218419	6.171913	4.190924
104	6	0	4.721923	6.410709	1.823349
105	7	0	5.083383	7.076385	0.938581
106	7	0	4.165798	6.645247	5.253774
107	6	0	-3.546635	1.614627	-2.130290
108	6	0	-3.894282	2.373308	-0.904900
109	6	0	-3.660633	2.400034	-3.381148
110	6	0	-4.273460	3.665284	-0.923977
111	1	0	-3.847808	1.846428	0.041852
112	6	0	-4.039595	3.695608	-3.386333
113	1	0	-3.426711	1.928087	-4.324461
114	1	0	-4.520633	4.174096	0.002055
115	1	0	-4.104532	4.231716	-4.327686
116	6	0	-4.369372	4.407622	-2.167460
117	6	0	-4.762948	5.735223	-2.183191
118	6	0	-5.092470	6.430920	-0.979959
119	6	0	-4.863883	6.474079	-3.401245
120	7	0	-5.359699	6.980578	0.011472
121	7	0	-4.943838	7.066014	-4.400956

Total energy (Sum of electronic and zero-point energies): -3745.1304756 Hartree

TD-DFT Data of BTD 7

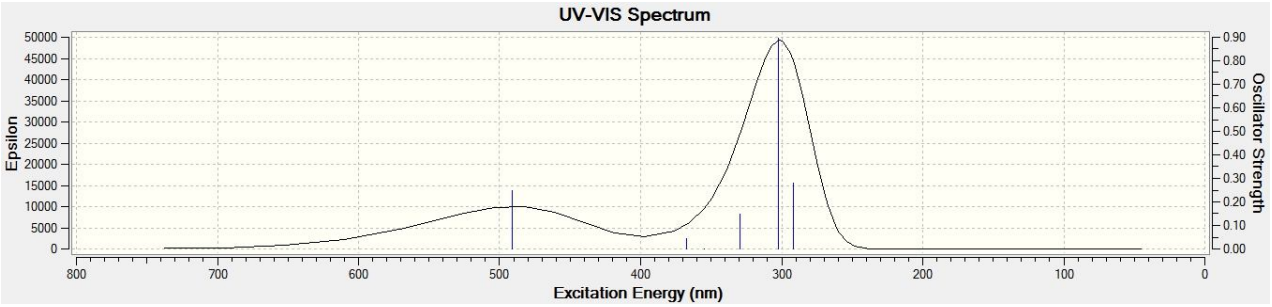

Fig S30. Simulated UV-visible optical absorption spectra of BTD 7 at the TDDFT/CAM-B3LYP/6-31G** level for C, N, H, and S in dichloromethane.

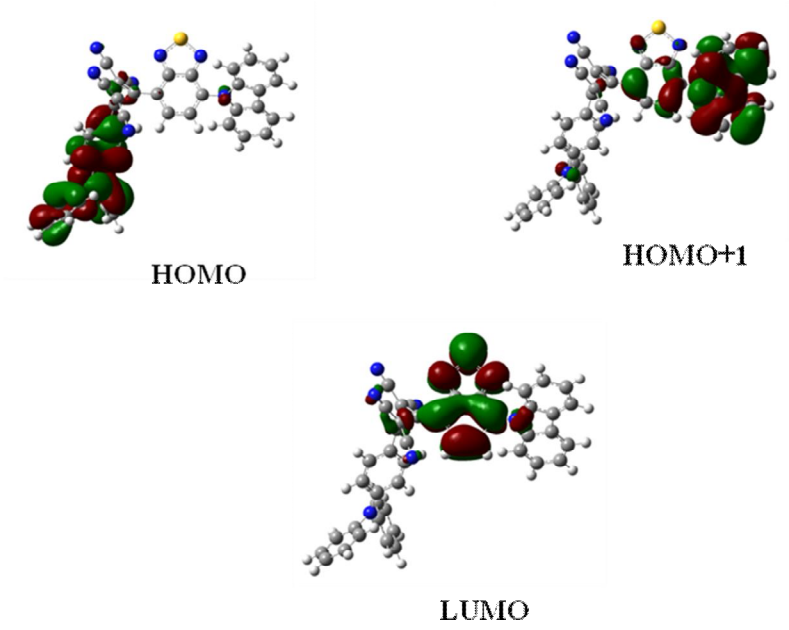

Fig S31. Frontier molecular orbitals of BTD 7 at the TDDFT/CAM-B3LYP/6-31G** level for C, N, H, and S in dichloromethane

Chart 1. Excitation energies and oscillator strengths:

```
 Excited State   1:      Singlet-A      2.5254 eV  490.95 nm
f=0.2481  <S**2>=0.000
     179 ->181         0.66788
     180 ->181        -0.17618
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-
particle RhoCI density.

 Excited State   2:      Singlet-A      3.3764 eV  367.21 nm
f=0.0451  <S**2>=0.000
     177 ->181        -0.16496
     179 ->181        -0.19166
     180 ->181        -0.64967

 Excited State   3:      Singlet-A      3.4931 eV  354.94 nm
f=0.0007  <S**2>=0.000
     178 ->181         0.69689

 Excited State   4:      Singlet-A      3.7605 eV  329.70 nm
f=0.1491  <S**2>=0.000
     172 ->181        -0.13477
     176 ->181         0.23279
     177 ->181         0.60248
     180 ->181        -0.17312

 Excited State   5:      Singlet-A      4.1010 eV  302.32 nm
f=0.8975  <S**2>=0.000
     180 ->182         0.45291
     180 ->183        -0.26889
     180 ->184        -0.35794
     180 ->185         0.13485
     180 ->187         0.12912
     180 ->195         0.10082

 Excited State   6:      Singlet-A      4.2506 eV  291.68 nm
f=0.2806  <S**2>=0.000
     170 ->181         0.65393
     174 ->181        -0.12256
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	4.508267	-2.510826	2.063596
2	7	0	4.923280	-1.101329	1.259405
3	7	0	2.951120	-2.683322	1.475133
4	6	0	3.865657	-0.758237	0.534917
5	6	0	2.738169	-1.662153	0.655805
6	6	0	1.539009	-1.396389	-0.060104
7	6	0	1.457246	-0.248080	-0.866009
8	1	0	0.547397	-0.045151	-1.418347
9	6	0	2.517551	0.631932	-0.975965
10	1	0	2.445203	1.491573	-1.630288
11	6	0	3.730315	0.385655	-0.293620
12	6	0	0.445976	-2.351908	0.063192
13	6	0	-1.021119	-2.427288	0.146960
14	6	0	-0.170814	-2.929831	1.313839
15	6	0	-0.332162	-3.193308	-0.963272
16	6	0	-0.058324	-4.319028	1.736075
17	6	0	-0.146275	-2.030238	2.457177
18	6	0	-0.270184	-4.643811	-1.072161
19	6	0	-0.442309	-2.573264	-2.273779
20	7	0	0.020583	-5.400839	2.130351
21	7	0	-0.144889	-1.322500	3.368566
22	7	0	-0.216725	-5.787043	-1.224575
23	7	0	-0.525098	-2.087592	-3.317522
24	7	0	4.791346	1.288063	-0.428725
25	6	0	4.690670	2.667693	-0.229484
26	6	0	6.095437	0.984996	-0.803591
27	6	0	3.590488	3.398989	0.206816
28	6	0	5.942522	3.262593	-0.487087
29	6	0	6.633610	-0.252684	-1.152584
30	6	0	6.848984	2.178819	-0.856279
31	6	0	3.757401	4.775465	0.338701
32	1	0	2.649613	2.920195	0.444840
33	6	0	6.090880	4.626762	-0.339943
34	6	0	7.972047	-0.277261	-1.531511
35	1	0	6.038623	-1.154301	-1.125049
36	6	0	8.173163	2.132825	-1.238188
37	6	0	4.982411	5.380113	0.067470
38	1	0	2.921696	5.380921	0.669483
39	1	0	7.043738	5.109074	-0.526753
40	6	0	8.731437	0.890193	-1.568645
41	1	0	8.428006	-1.221846	-1.803913
42	1	0	8.771423	3.035294	-1.293366
43	1	0	5.085175	6.452799	0.185439
44	1	0	9.772112	0.839949	-1.867973
45	6	0	-2.199480	-1.549986	0.094610
46	6	0	-2.131327	-0.218041	0.509749
47	6	0	-3.418835	-2.050761	-0.366100
48	6	0	-3.251788	0.591921	0.466665

49	1	0	-1.190444	0.197946	0.853749
50	6	0	-4.543385	-1.247029	-0.406813
51	1	0	-3.492766	-3.085583	-0.684308
52	6	0	-4.480820	0.091487	0.010444
53	1	0	-3.174967	1.626272	0.777213
54	1	0	-5.482076	-1.657828	-0.756601
55	7	0	-5.615716	0.909137	-0.030645
56	6	0	-6.647695	0.680278	-0.985088
57	6	0	-7.981380	0.649622	-0.575693
58	6	0	-6.339459	0.508358	-2.335866
59	6	0	-8.992167	0.452868	-1.508085
60	1	0	-8.219659	0.782922	0.473822
61	6	0	-7.354160	0.293689	-3.259758
62	1	0	-5.304158	0.543539	-2.656941
63	6	0	-8.684185	0.268948	-2.852127
64	1	0	-10.025721	0.432313	-1.178347
65	1	0	-7.102623	0.159560	-4.306701
66	1	0	-9.474952	0.109066	-3.577144
67	6	0	-5.767474	1.993417	0.880299
68	6	0	-6.134792	3.254223	0.408317
69	6	0	-5.572918	1.802142	2.249500
70	6	0	-6.308194	4.307752	1.297013
71	1	0	-6.285148	3.401784	-0.655488
72	6	0	-5.730007	2.864730	3.130125
73	1	0	-5.298758	0.819987	2.618732
74	6	0	-6.101933	4.120260	2.659872
75	1	0	-6.595556	5.283292	0.918675
76	1	0	-5.574594	2.704780	4.192007
77	1	0	-6.231875	4.946049	3.351043

Total energy (Sum of electronic and zero-point energies): -2526.064
 5628 Hartree