SUPPLEMENTARY DATA FOR

Synthesis, Characterization, and Optical Properties of Novel 1,3-Dithiole Donor-Based Chromophores

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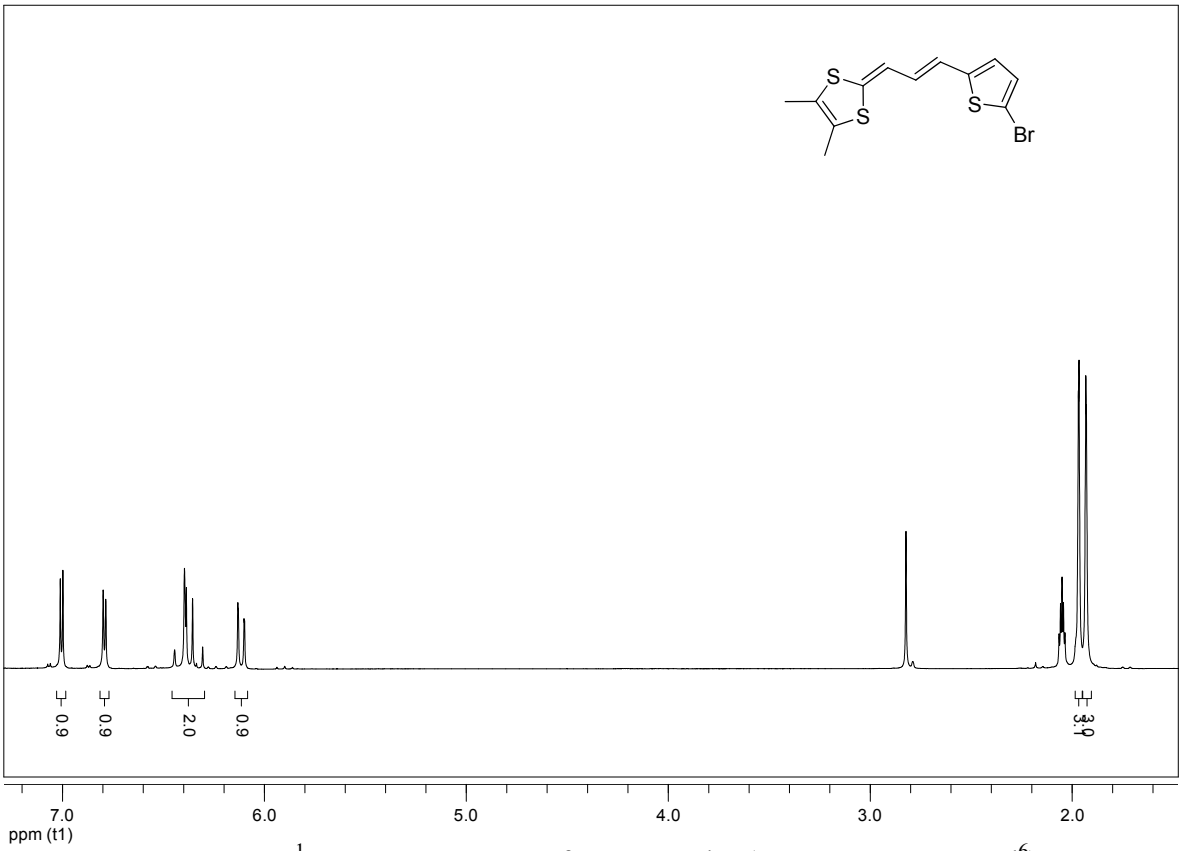

Figure S-1: ^{1}H NMR spectrum of compound **5** (300 MHz, acetone-d^{6}).

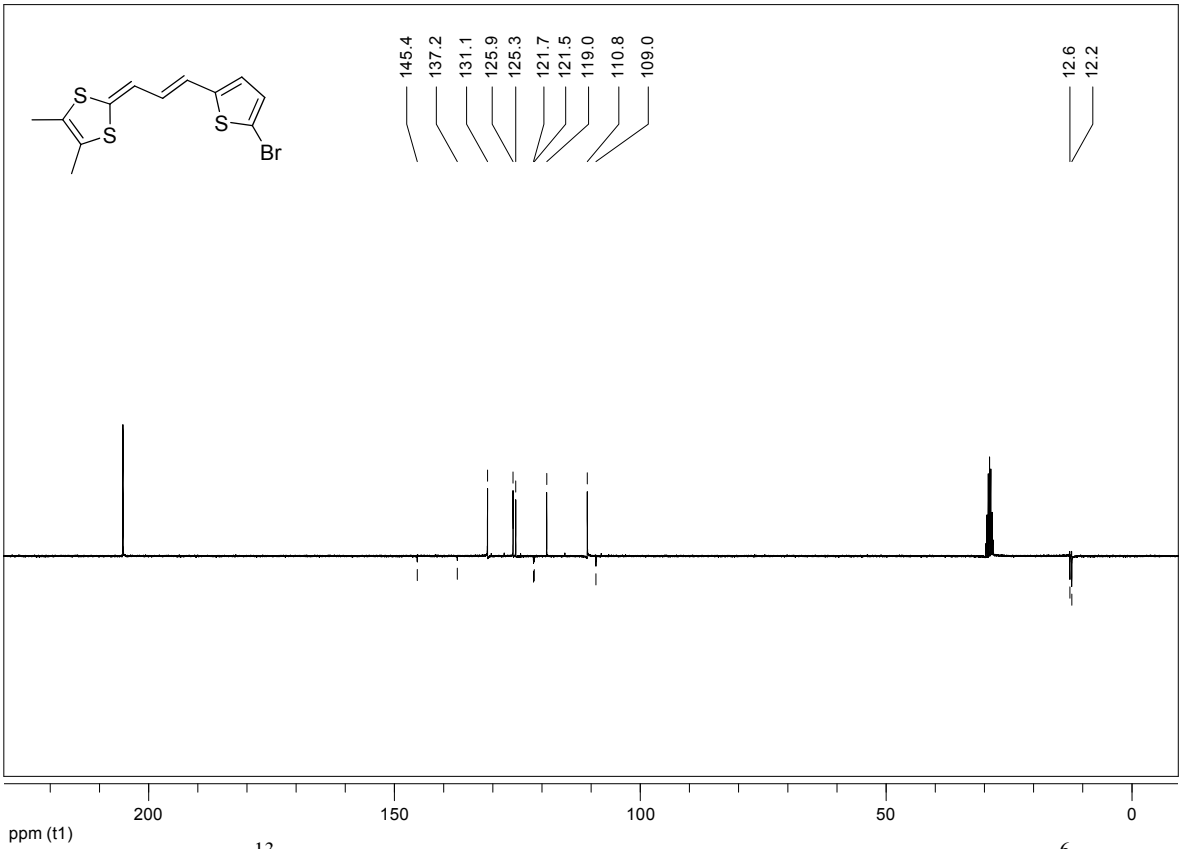

Figure S-2: ^{13}C NMR (APT) spectrum of compound **5** (75 MHz, acetone-d^{6}).

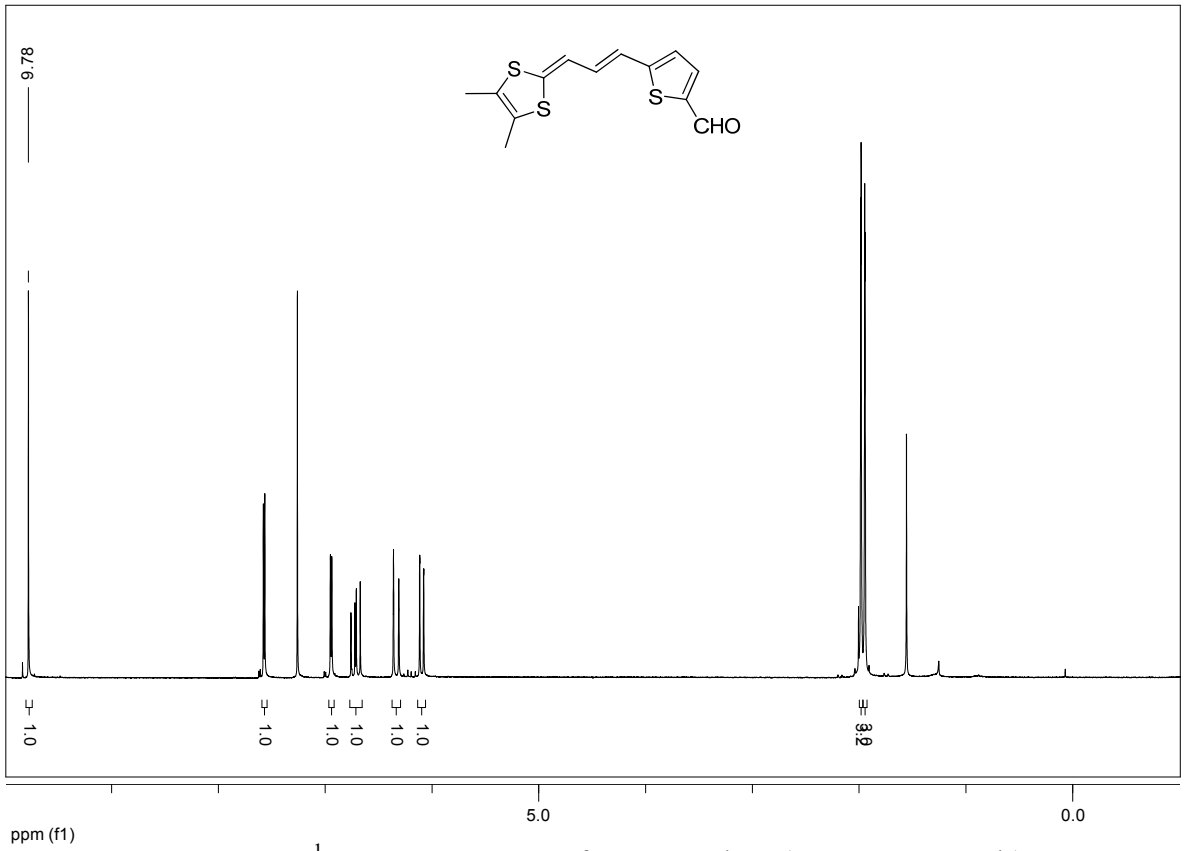

Figure S-3: ^{1}H NMR spectrum of compound **8b** (300 MHz, $CDCl_3$).

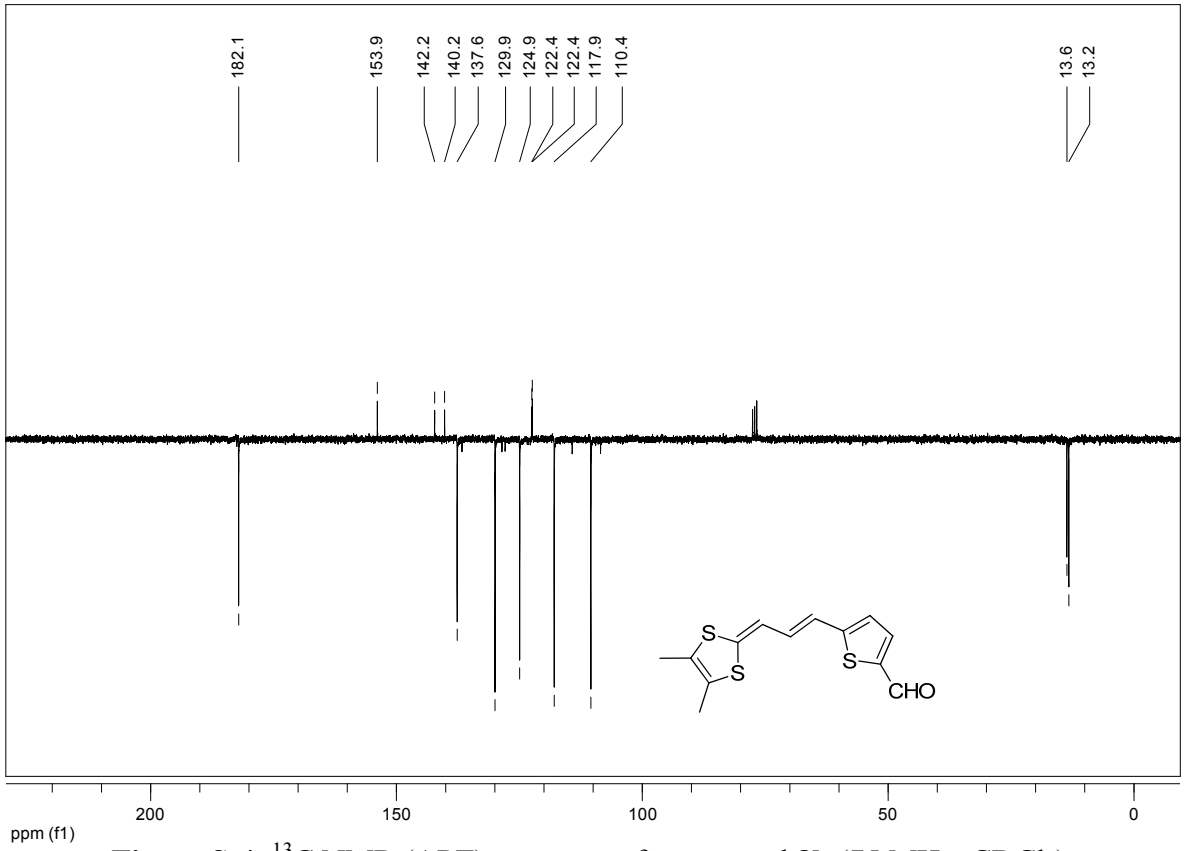

Figure S-4: ^{13}C NMR (APT) spectrum of compound **8b** (75 MHz, $CDCl_3$).

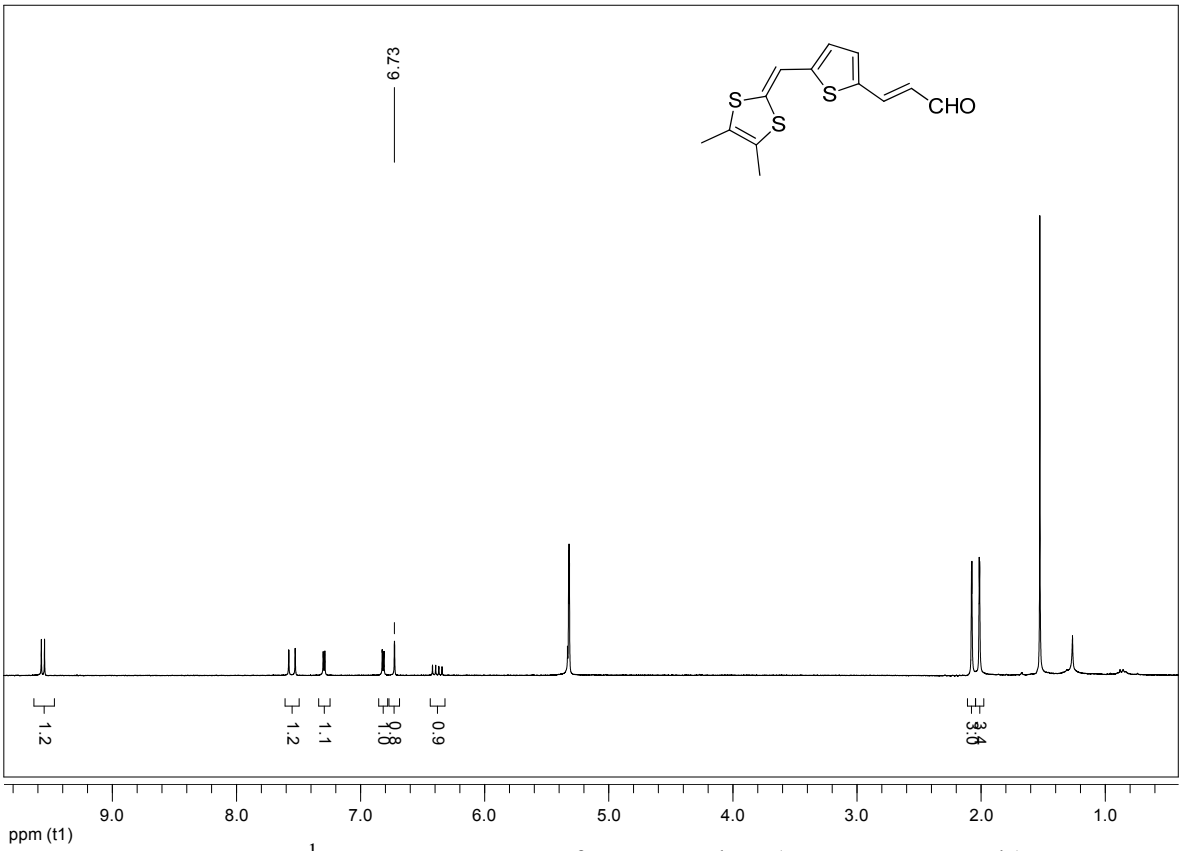

Figure S-5: ^{1}H NMR spectrum of compound **8c** (300 MHz, CD_2Cl_2).

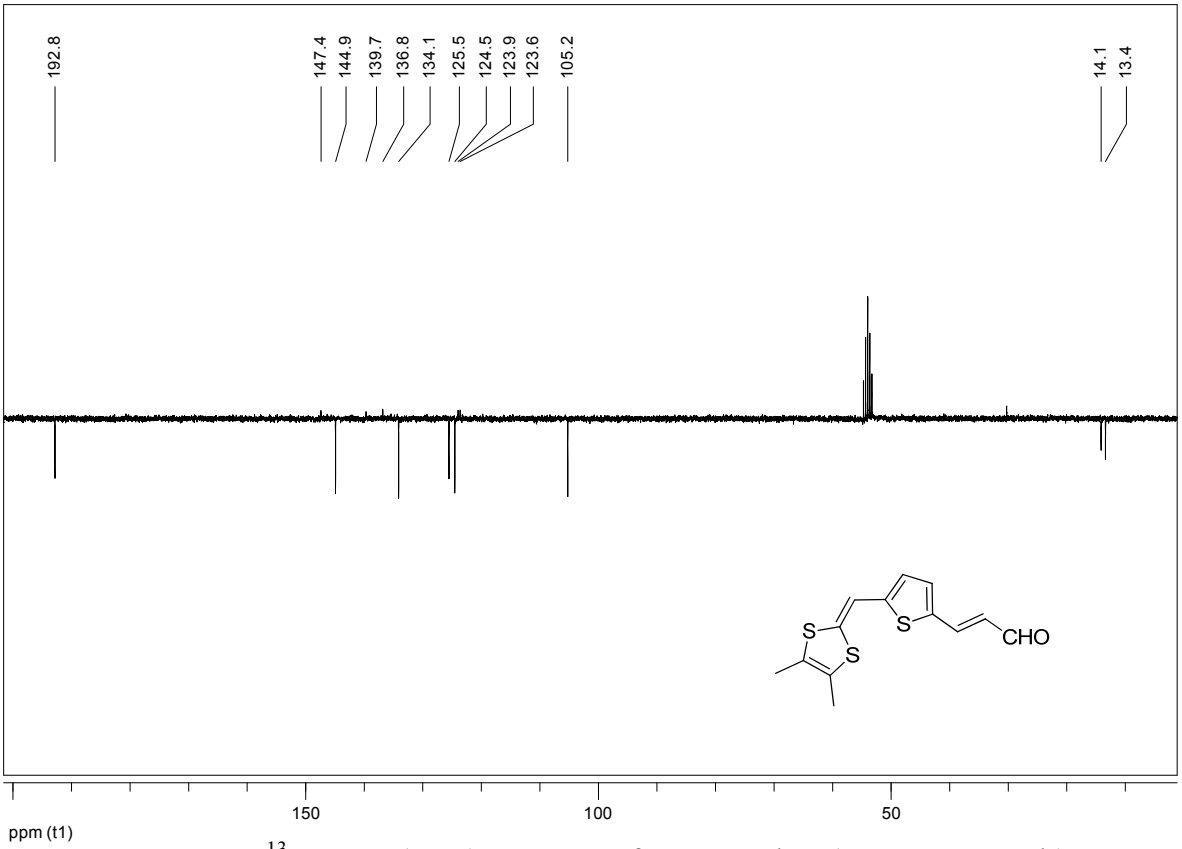

Figure S-6: ^{13}C NMR (APT) spectrum of compound **8c** (75 MHz, CD_2Cl_2).

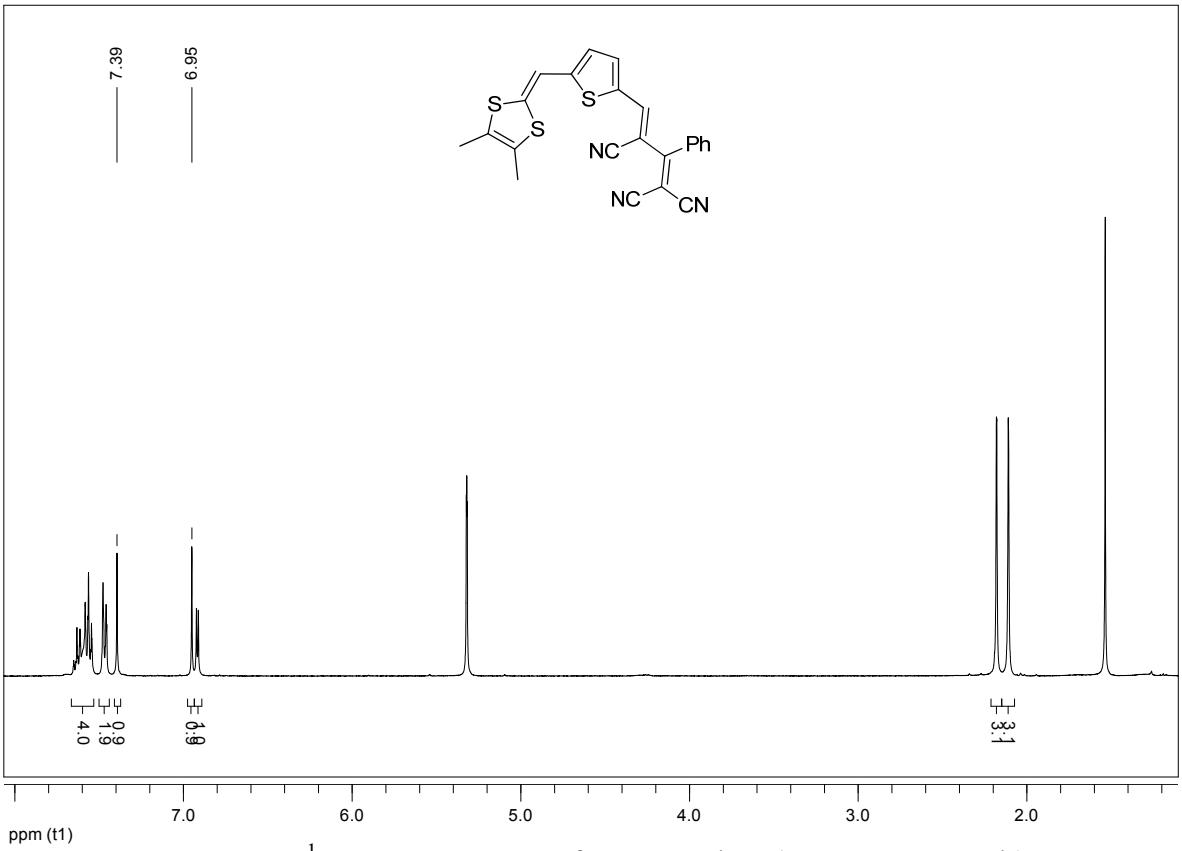

Figure S-7: ^{1}H NMR spectrum of compound **9a** (400 MHz, CD_2Cl_2).

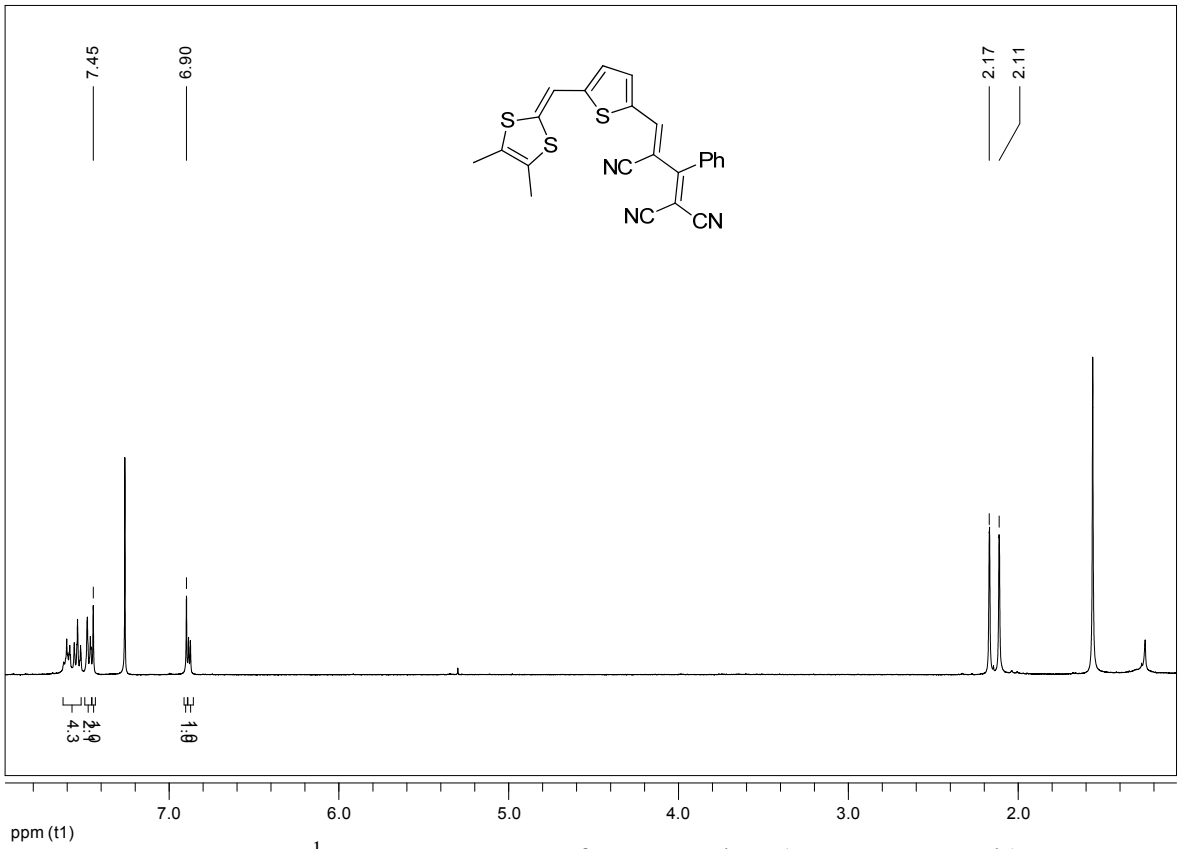

Figure S-8: ^{1}H NMR spectrum of compound **9a** (400 MHz, $CDCl_3$).

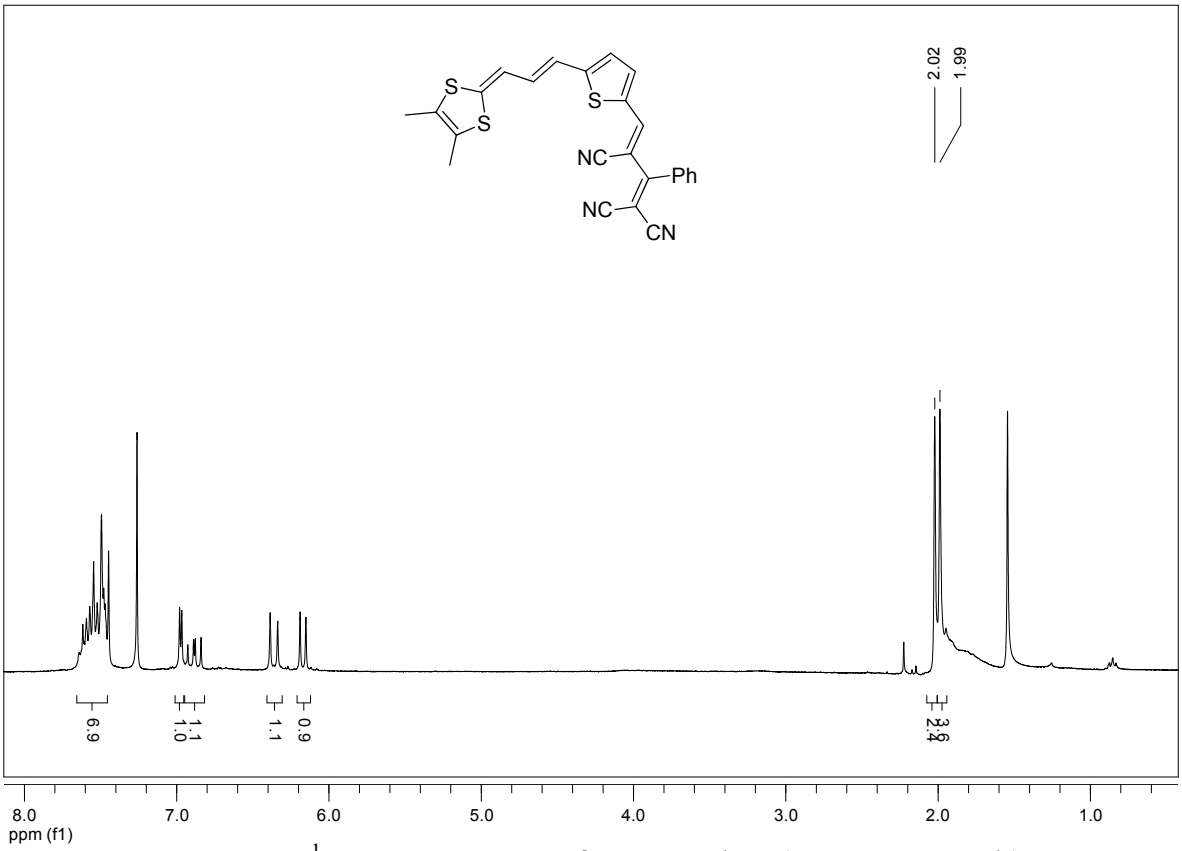

Figure S-9: ^{1}H NMR spectrum of compound **9b** (300 MHz, $CDCl_3$).

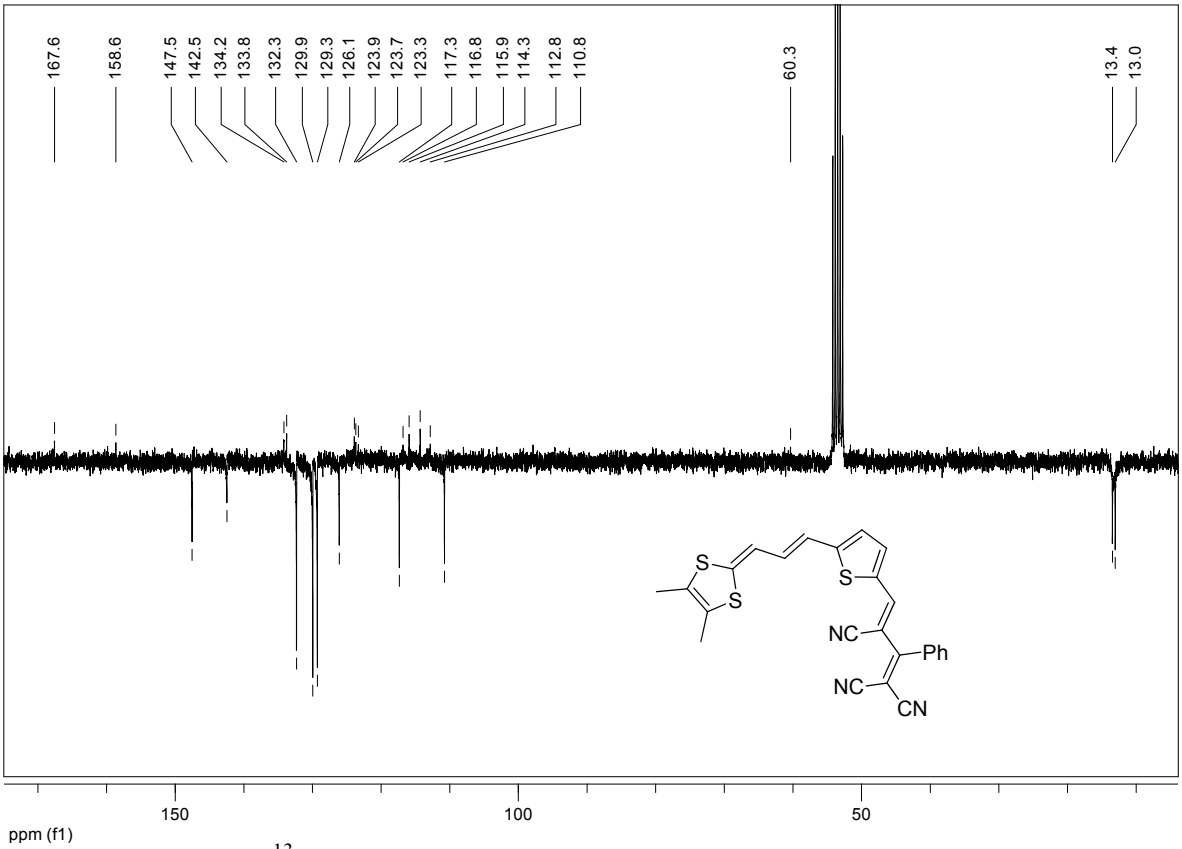

Figure S-10: ^{13}C NMR (APT) spectrum of compound **9b** (75 MHz, CD_2Cl_2).

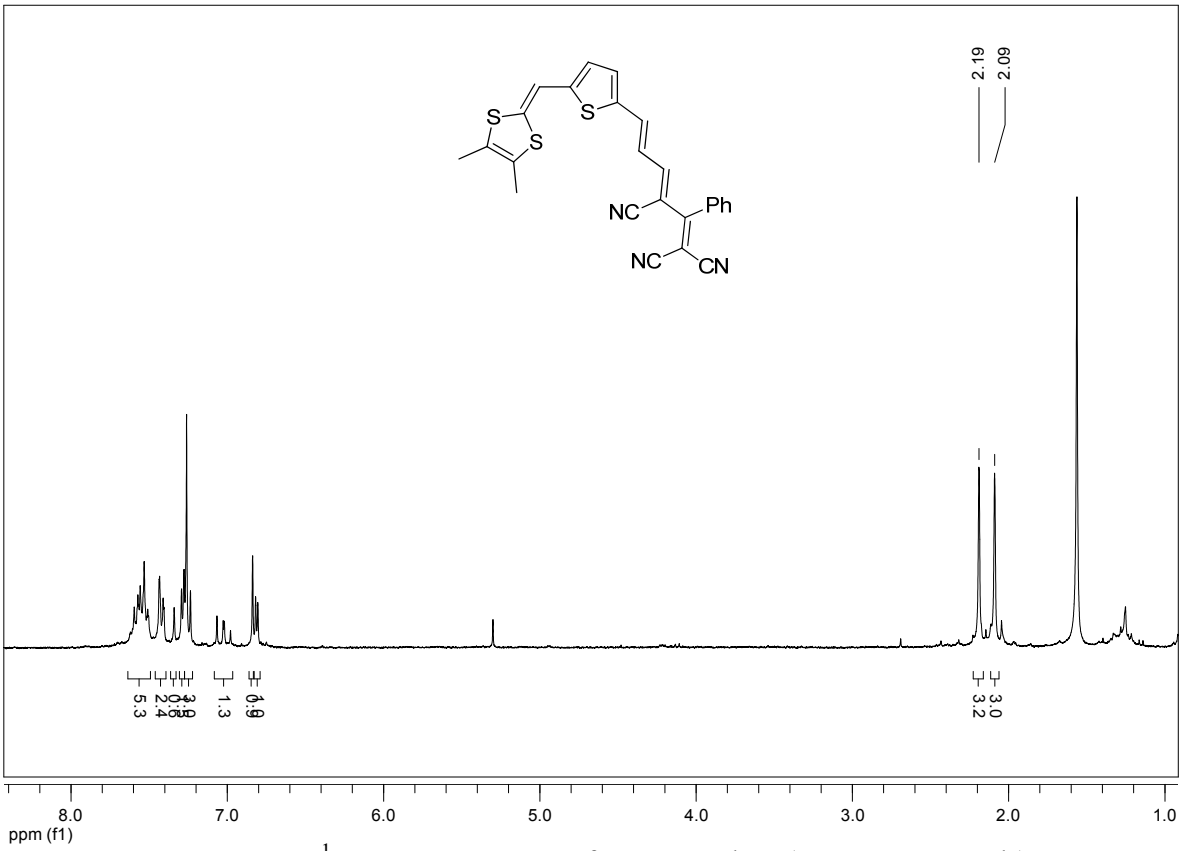

Figure S-11: ^{1}H NMR spectrum of compound **9c** (300 MHz, $CDCl_3$).

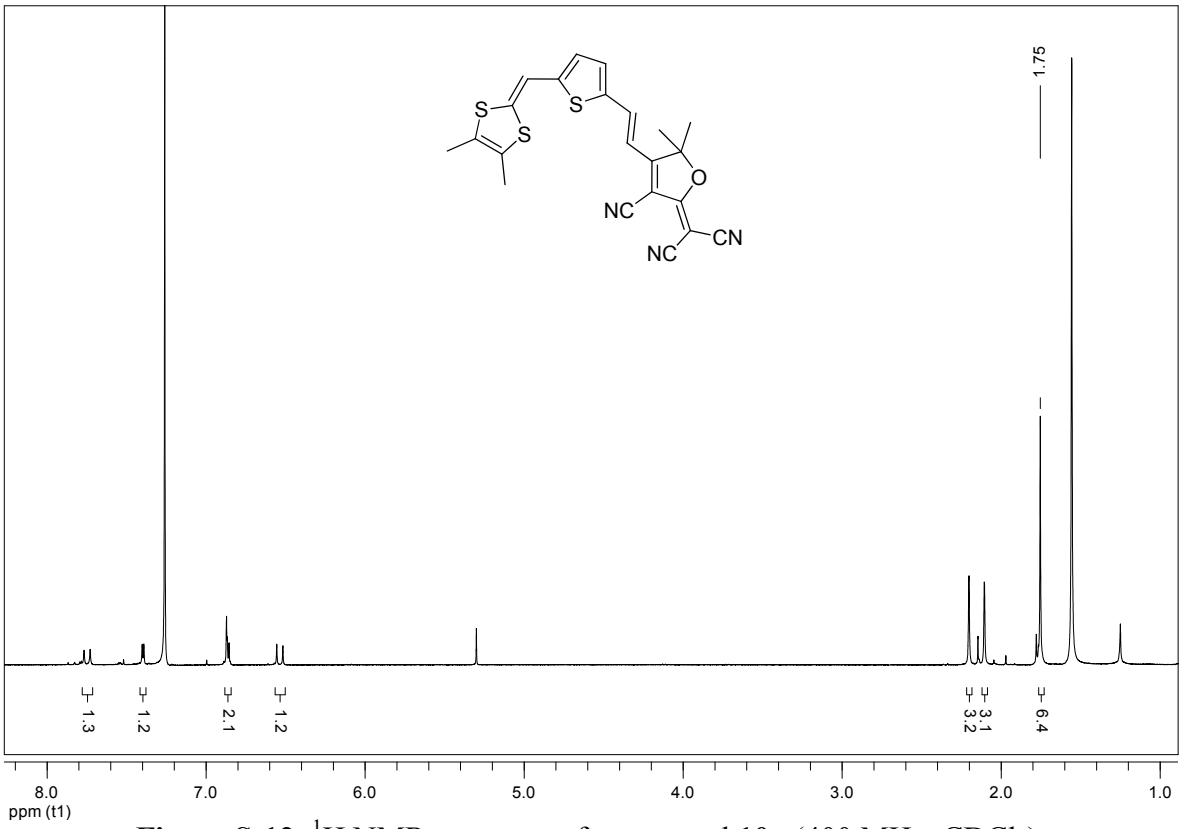

Figure S-12: ^{1}H NMR spectrum of compound **10a** (400 MHz, $CDCl_3$).

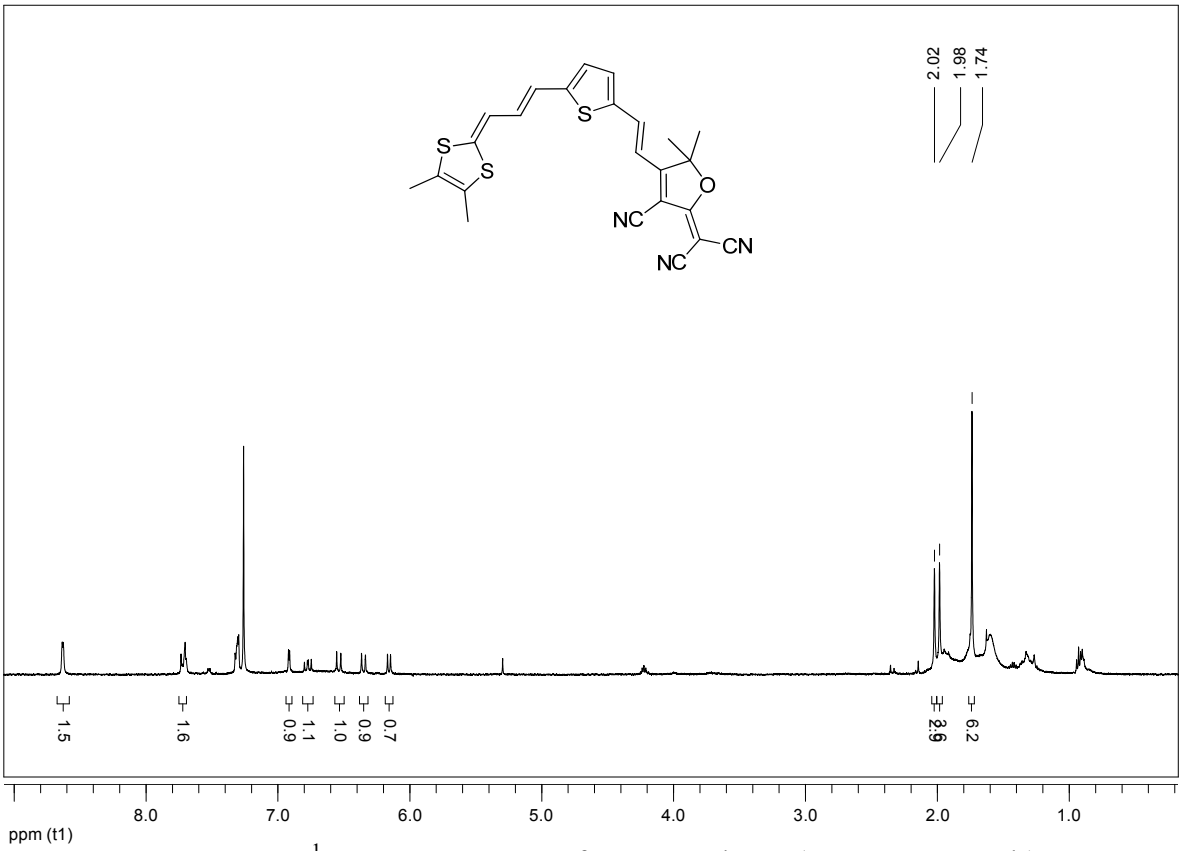

Figure S-13: ^{1}H NMR spectrum of compound **10b** (500 MHz, $CDCl_3$).

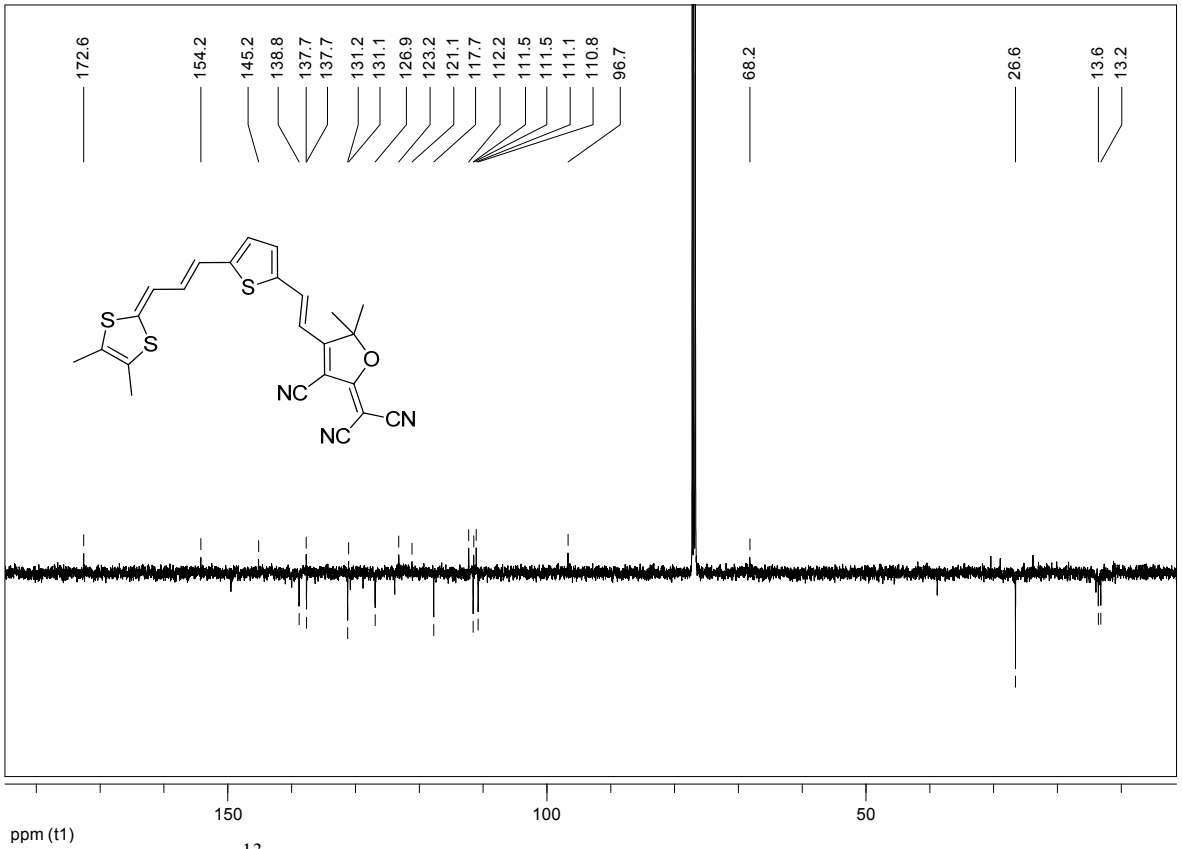

Figure S-14: ^{13}C NMR (APT) spectrum of compound **10b** (125.77 MHz, $CDCl_3$).

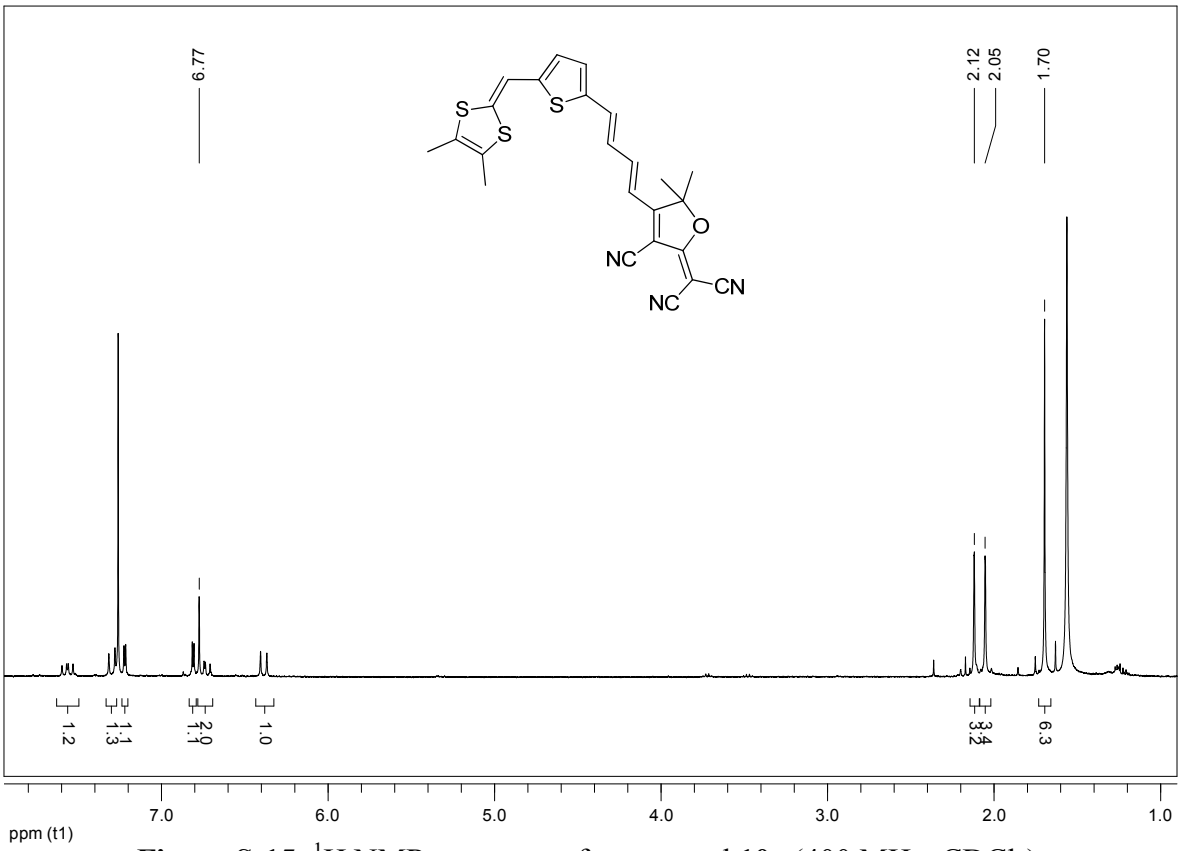

Figure S-15: ^{1}H NMR spectrum of compound **10c** (400 MHz, $CDCl_3$).

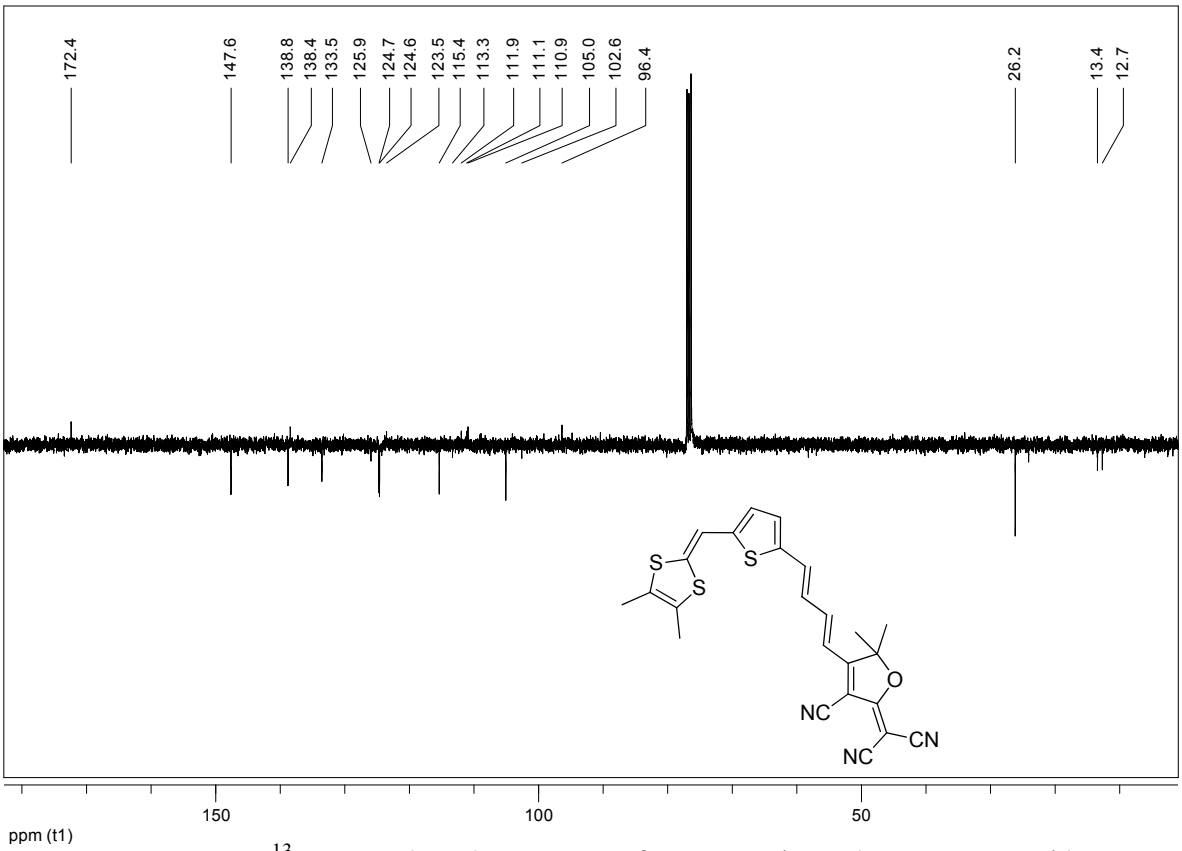

Figure S-16: ^{13}C NMR (APT) spectrum of compound **10c** (75 MHz, $CDCl_3$).

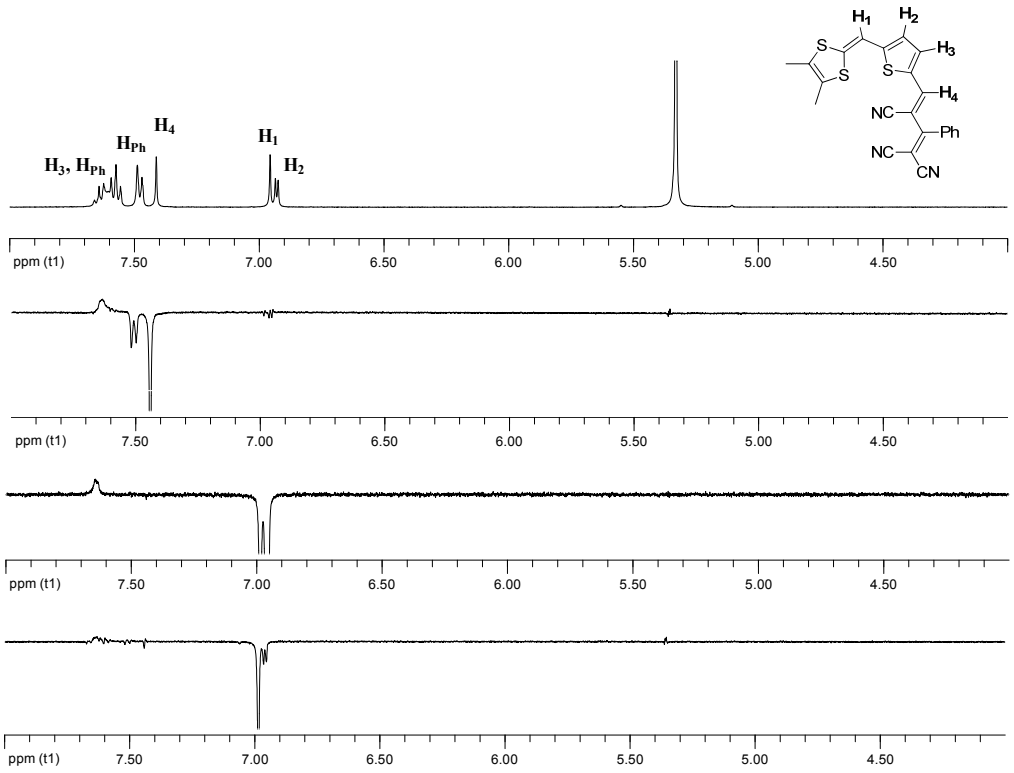

Figure S-17: nOe experiment of compound **9a**.

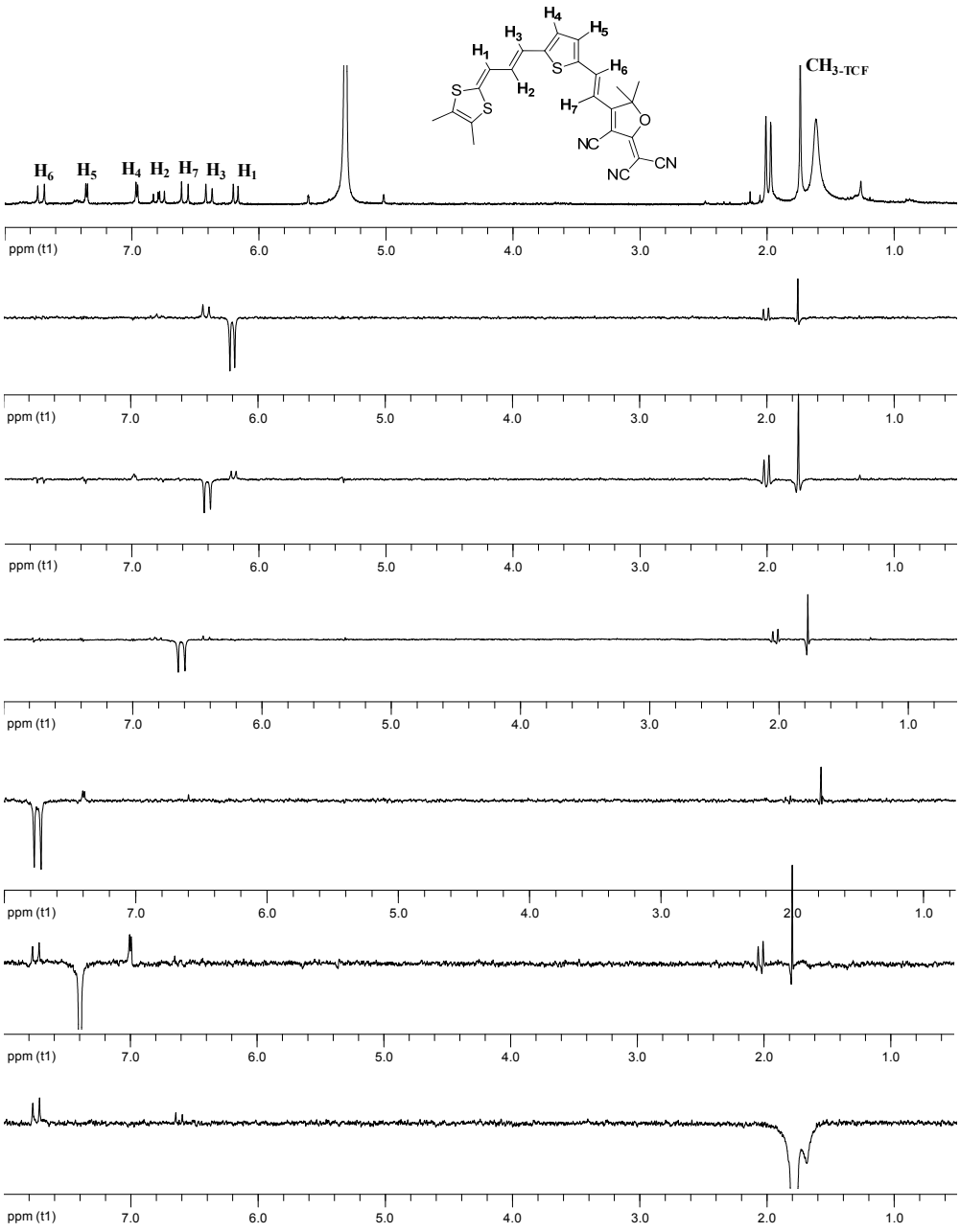

Figure S-18: nOe experiment of compound **10b** (300 MHz, CD_2Cl_2).

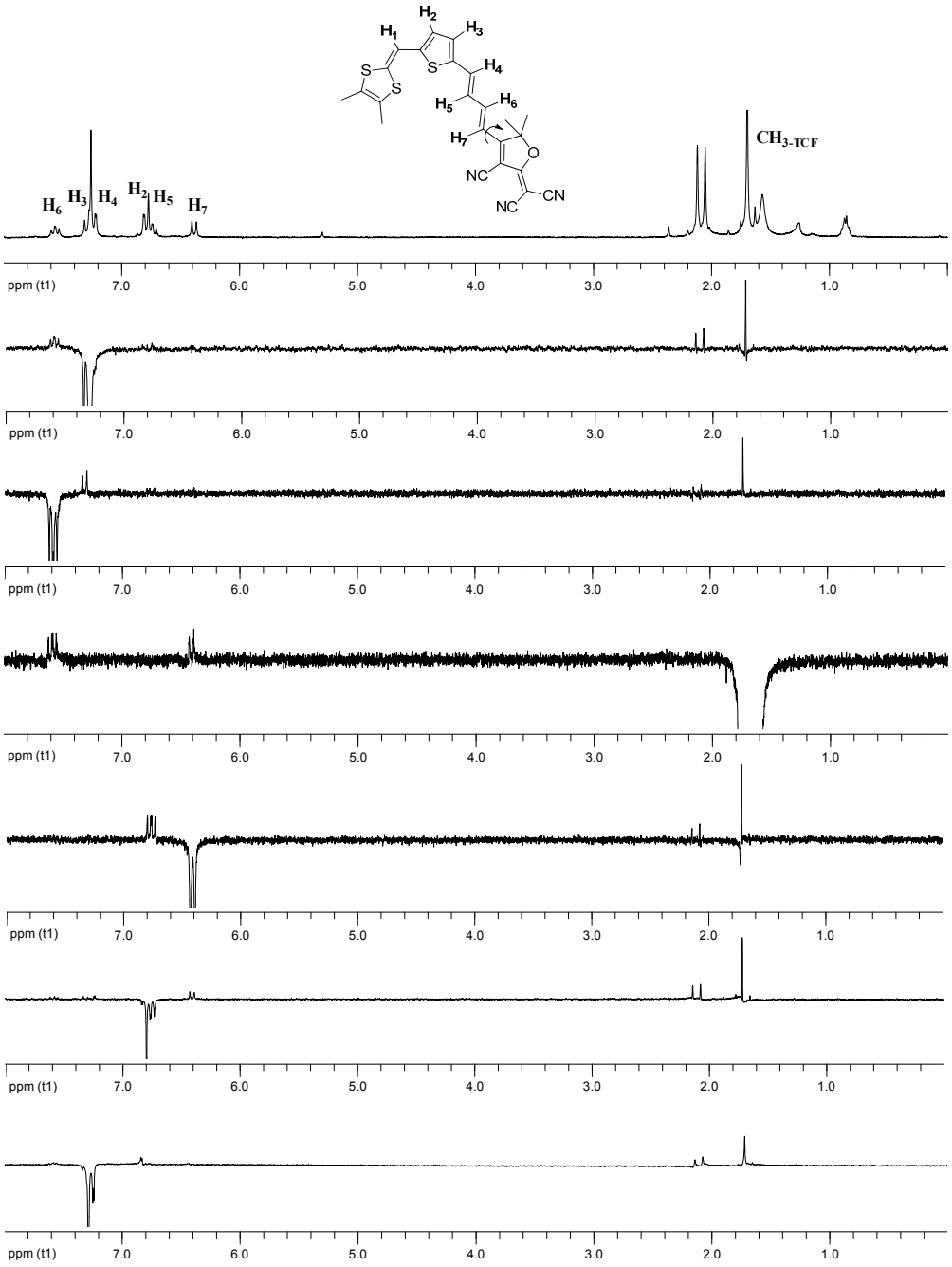

Figure S-19: nOe experiment of compound **10c** (400 MHz, $CDCl_3$).

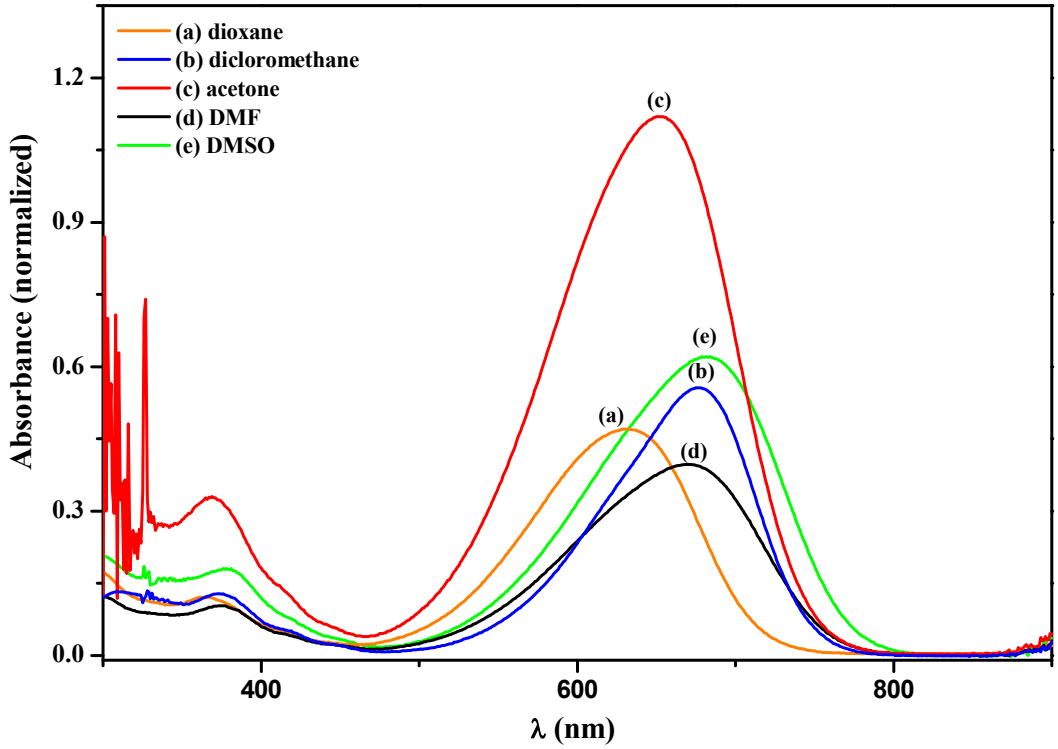

Figure S-20: Normalized UV-vis absorption of compound **9a** (10^{-5} M).

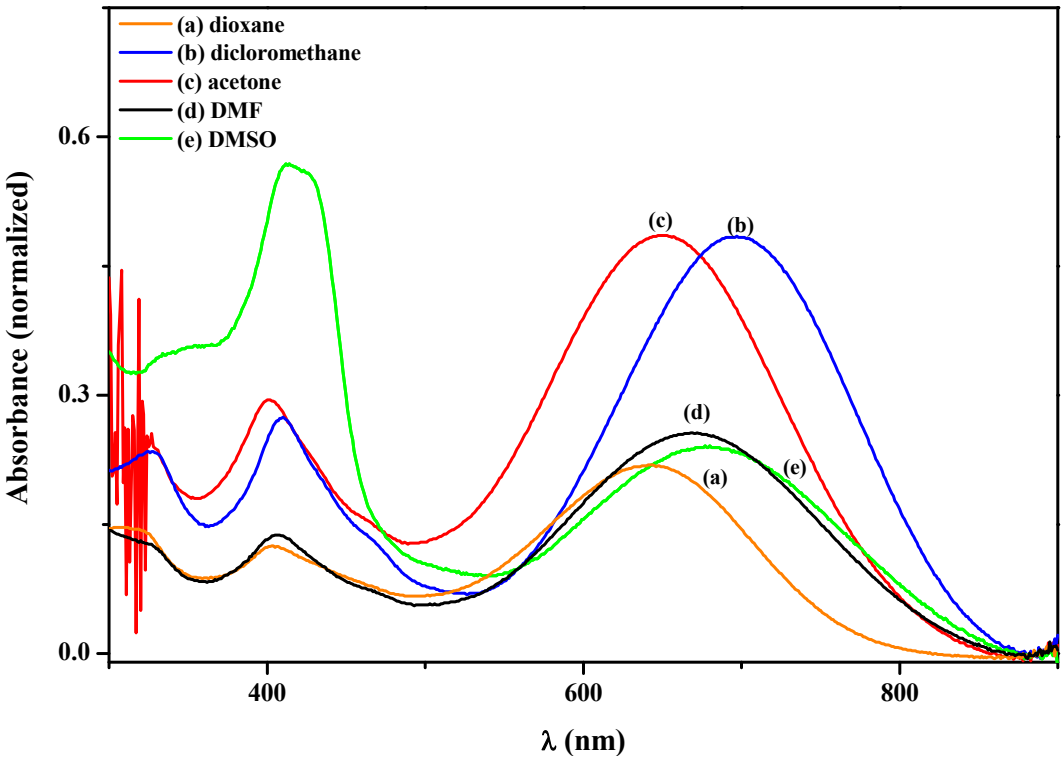

Figure S-21: Normalized UV-vis absorption of compound **9b** (10^{-5} M).

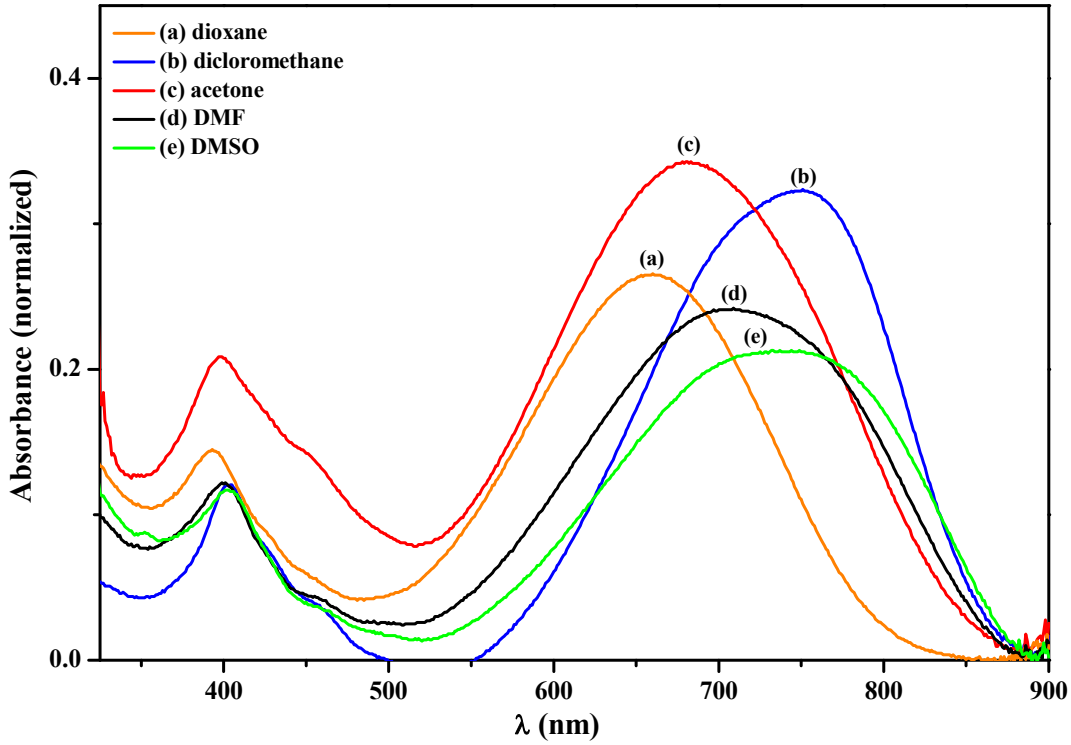

Figure S-22: Normalized UV-vis absorption of compound **9c** (10^{-5} M).

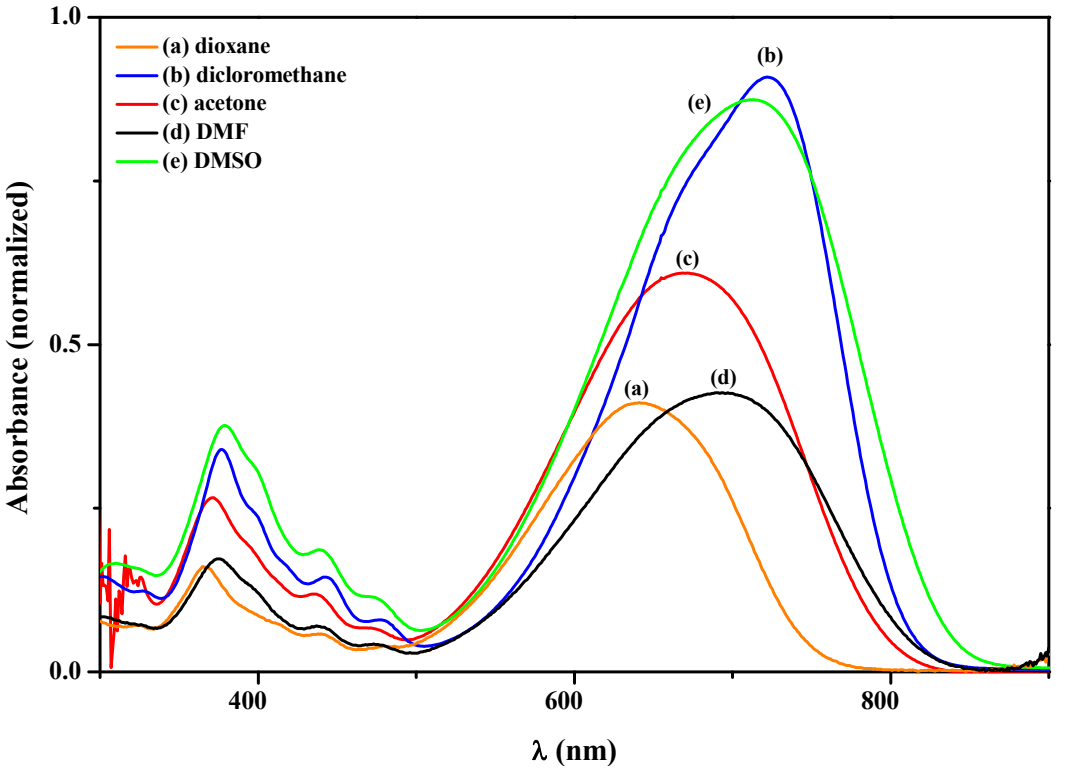

Figure S-23: Normalized UV-vis absorption of compound **10a** (10^{-5} M).

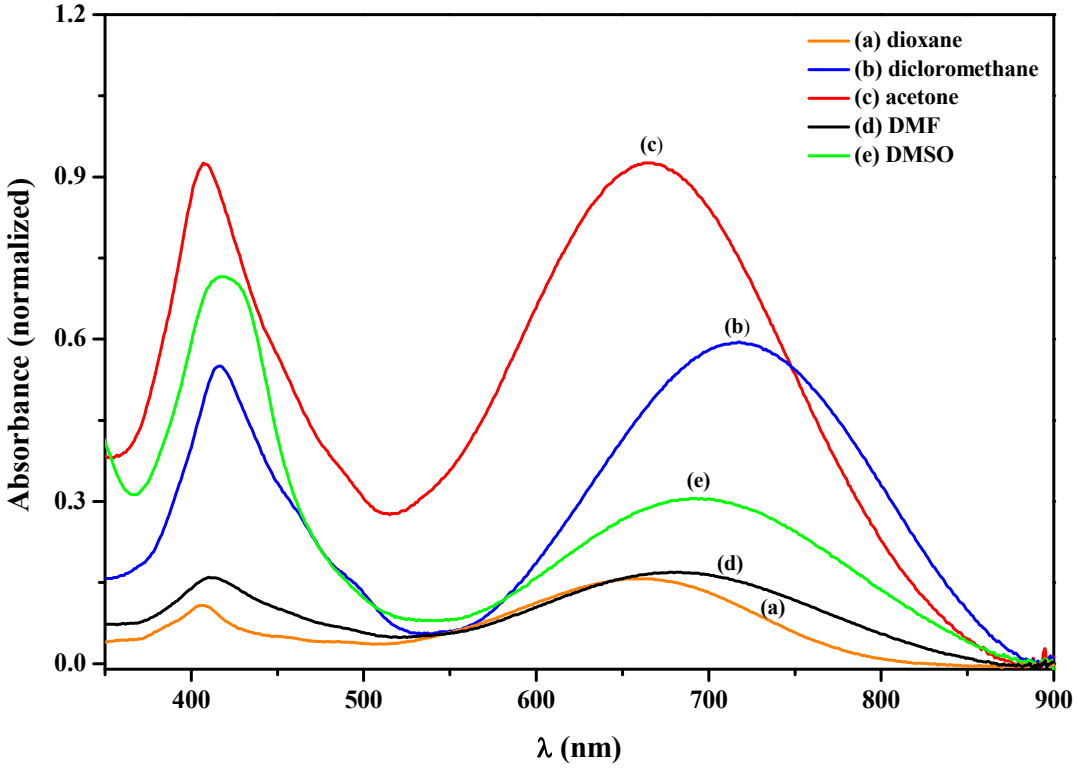

Figure S-24: Normalized UV-vis absorption of compound **10b** (10^{-5} M).

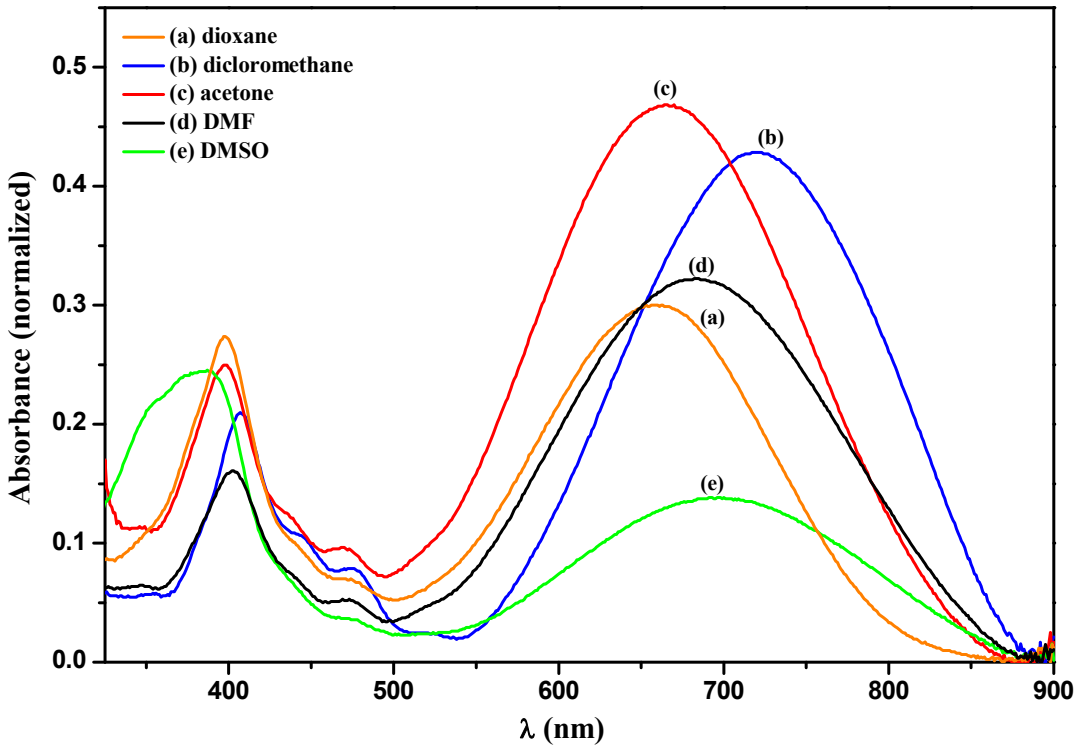

Figure S-25: Normalized UV-vis absorption of compound **10c** (10^{-5} M).

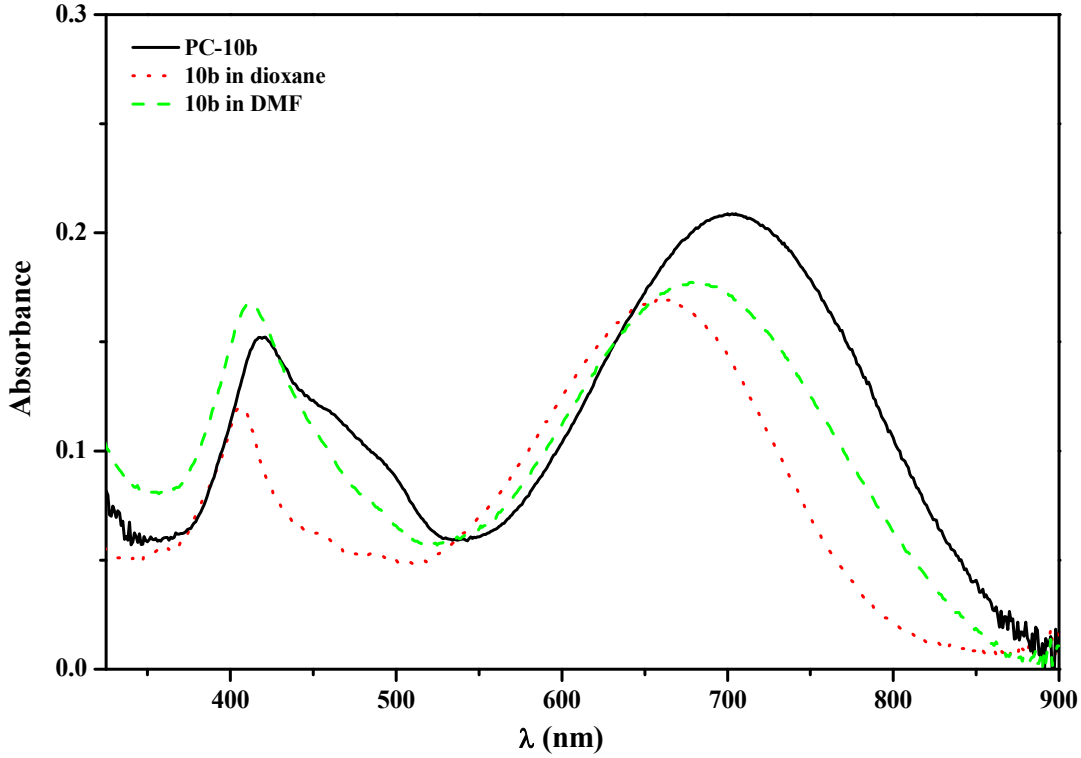

Figure S-26: UV-vis absorption of compound **10b** in dioxane and DMF solutions (10^{-5} M) and of a thin film of polycarbonate with the same compound embedded in.

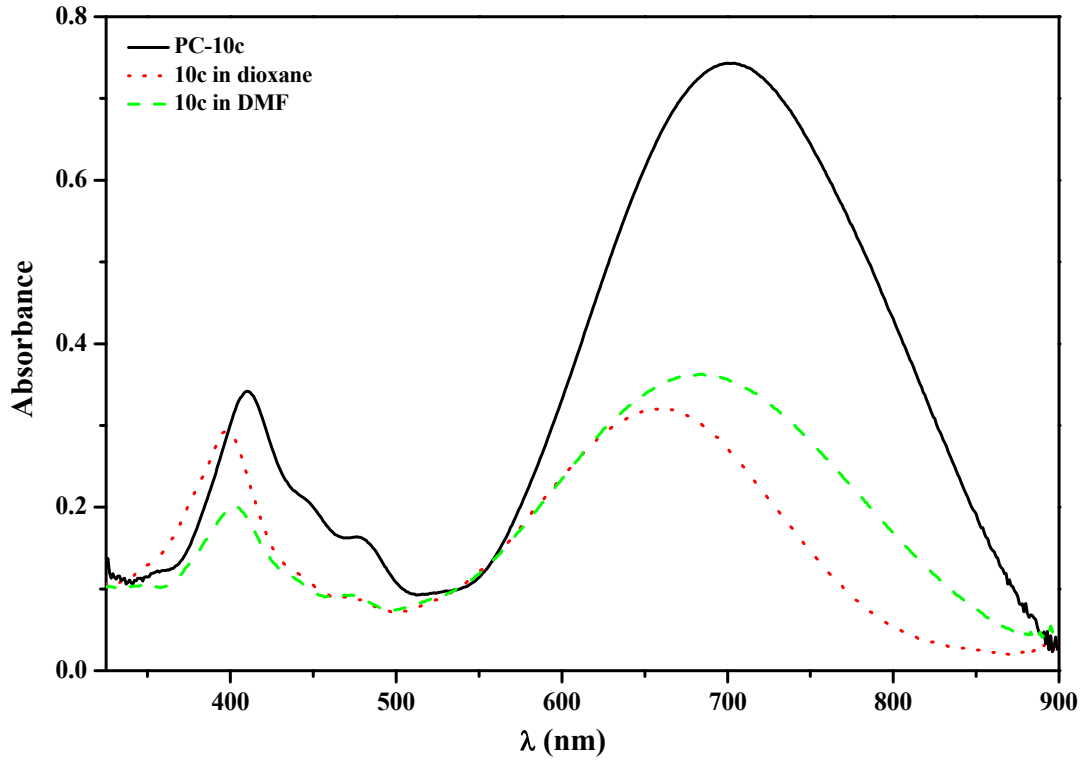

Figure S-27: UV-vis absorption of compound **10c** in dioxane and DMF solutions (10^{-5} M) and of a thin film of polycarbonate with the same compound embedded in.

Computational Procedures.

All theoretical calculations were performed by using the Gaussian 09[7] program. The gas phase molecular geometries were optimized using the B3P86[8] functional and the 6-31G*[9] basis set. The same model chemistry (B3P86/6-31G*) was used for TD-DFT calculations and the excited state dipole moments were calculated by using the CI density. Molecular hyperpolarizabilities were calculated by the Coupled Perturbed Hartree Fock method (CPHF) using the HF/6-31G* model. The default G09 parameters were used in every calculation.

Calculations in DMF solution were performed using a Polarizable Continuum Model (PCM), TD-DFT calculations used the equilibrium PCM solvation (EqSolv) and the 6-311+G(2d,p) basis set on geometries optimized using PCM, the same functional and the 6-31G* basis set. CIS calculations used the 6-311+G(2d,p) basis set on PCM-HF/6-31G* geometries.

Cartesian coordinates and energies of optimized geometries used in theoretical calculations (gas phase, B3P86/6-31G*)

9a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.384222	-1.913537	-0.496821
2	1	0	-3.815936	-2.882273	-0.738836
3	6	0	-1.964920	-1.873745	-0.545018
4	6	0	-1.149644	-2.965020	-0.871606
5	16	0	-0.999980	-0.467478	-0.201002
6	6	0	0.204700	-2.666954	-0.840029
7	1	0	-1.558286	-3.938039	-1.120113
8	6	0	0.492061	-1.342551	-0.490268
9	1	0	0.991527	-3.380270	-1.063033
10	6	0	1.800095	-0.827597	-0.398755
11	6	0	2.262874	0.440628	-0.095198
12	1	0	2.569031	-1.563424	-0.622973
13	6	0	3.690911	0.718608	-0.058143
14	6	0	4.604386	-0.403771	0.256791
15	6	0	4.366454	-1.207621	1.381710
16	6	0	5.715607	-0.677240	-0.551017

17	6	0	5.230272	-2.248808	1.698124
18	1	0	3.511022	-0.996294	2.016421
19	6	0	6.569121	-1.729762	-0.239511
20	1	0	5.900757	-0.069815	-1.431318
21	6	0	6.331571	-2.514188	0.886438
22	1	0	5.045231	-2.852059	2.582086
23	1	0	7.422959	-1.934790	-0.878220
24	1	0	7.004075	-3.331130	1.131790
25	6	0	4.215531	1.974842	-0.290857
26	6	0	5.592563	2.275115	-0.062981
27	7	0	6.703540	2.570905	0.119601
28	6	0	3.459749	3.067222	-0.810440
29	7	0	2.904168	3.974923	-1.281538
30	6	0	1.333223	1.470778	0.227905
31	7	0	0.543252	2.264793	0.548098
32	6	0	-4.265066	-0.912919	-0.190304
33	16	0	-3.848462	0.730434	0.230749
34	6	0	-6.485754	0.422897	0.265874
35	6	0	-5.495780	1.314996	0.461057
36	16	0	-5.993224	-1.202554	-0.190940
37	6	0	-7.960565	0.644286	0.390536
38	1	0	-8.180643	1.674795	0.674896
39	1	0	-8.472066	0.440636	-0.557035
40	1	0	-8.396341	-0.014476	1.150282
41	6	0	-5.612243	2.754773	0.850984
42	1	0	-6.656436	3.045498	0.980359
43	1	0	-5.088171	2.951686	1.792944
44	1	0	-5.172318	3.406592	0.087885

E(RB3P86) = -2248.23248110 A.U.

9b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.581016	-1.655136	-0.278662
2	1	0	-4.955401	-2.661395	-0.456502
3	6	0	-0.850784	-2.303760	-0.545354
4	6	0	0.076656	-3.316353	-0.802166
5	16	0	-0.046812	-0.791565	-0.239277
6	6	0	1.395346	-2.878175	-0.754192
7	1	0	-0.223045	-4.336001	-1.017055
8	6	0	1.533645	-1.518751	-0.457728
9	1	0	2.256949	-3.514567	-0.928380
10	6	0	2.783740	-0.872977	-0.363327
11	6	0	3.110301	0.445468	-0.103397
12	1	0	3.626695	-1.536185	-0.542668
13	6	0	4.502511	0.868226	-0.052207
14	6	0	5.519558	-0.142093	0.319055
15	6	0	5.343232	-0.930664	1.465981
16	6	0	6.671211	-0.320976	-0.458199
17	6	0	6.306339	-1.862055	1.834224
18	1	0	4.456335	-0.791750	2.077035
19	6	0	7.625397	-1.264462	-0.094477
20	1	0	6.810111	0.273659	-1.355540
21	6	0	7.448010	-2.032807	1.053416
22	1	0	6.166946	-2.453096	2.734644
23	1	0	8.510343	-1.397056	-0.709536
24	1	0	8.198572	-2.763874	1.339885
25	6	0	4.901363	2.162258	-0.324101
26	6	0	6.235379	2.610591	-0.083448
27	7	0	7.306094	3.026263	0.105884
28	6	0	4.051270	3.152183	-0.900249
29	7	0	3.420294	3.982366	-1.417071
30	6	0	2.076556	1.389629	0.162061
31	7	0	1.206249	2.113972	0.435246

32	6	0	-5.503557	-0.670398	-0.057373
33	16	0	-5.119077	1.013252	0.240448
34	6	0	-7.750697	0.658699	0.281382
35	6	0	-6.779273	1.581003	0.414794
36	16	0	-7.224747	-0.990514	-0.047959
37	6	0	-9.230224	0.859327	0.378681
38	1	0	-9.473803	1.903528	0.582907
39	1	0	-9.729848	0.574001	-0.554186
40	1	0	-9.659421	0.250788	1.182918
41	6	0	-6.929669	3.043393	0.692953
42	1	0	-7.981042	3.322040	0.785078
43	1	0	-6.424453	3.321748	1.624804
44	1	0	-6.491357	3.644772	-0.111589
45	6	0	-3.176253	-1.461689	-0.293260
46	6	0	-2.267379	-2.453558	-0.525587
47	1	0	-2.805369	-0.452963	-0.106122
48	1	0	-2.630434	-3.462152	-0.718400

E(RB3P86) = -2325.89144161 A.U.

9c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.685492	-1.878313	-0.341407
2	1	0	-5.323260	-2.745673	-0.497921
3	6	0	-3.293448	-2.154413	-0.426722
4	6	0	-2.743450	-3.412498	-0.688536
5	16	0	-2.025759	-0.975709	-0.221627
6	6	0	-1.351106	-3.417805	-0.721328
7	1	0	-3.362382	-4.288217	-0.848985
8	6	0	-0.775623	-2.170628	-0.487018
9	1	0	-0.750454	-4.301322	-0.911129
10	6	0	2.571076	-0.454562	-0.225139
11	6	0	3.229498	0.747988	-0.028676
12	1	0	3.190318	-1.329018	-0.410868
13	6	0	4.677862	0.836657	-0.039274
14	6	0	5.446004	-0.388830	0.282013
15	6	0	5.158311	-1.116026	1.446322
16	6	0	6.470677	-0.835116	-0.561995
17	6	0	5.890672	-2.253389	1.764484
18	1	0	4.371189	-0.770656	2.110104
19	6	0	7.191384	-1.981854	-0.247824
20	1	0	6.692609	-0.287013	-1.472298
21	6	0	6.906546	-2.690507	0.916673
22	1	0	5.670387	-2.797008	2.678578
23	1	0	7.978847	-2.320002	-0.914627
24	1	0	7.476073	-3.581696	1.164271
25	6	0	5.359438	2.003703	-0.326952
26	6	0	6.772178	2.115897	-0.155263
27	7	0	7.919783	2.259788	-0.022812
28	6	0	4.744294	3.178550	-0.851691
29	7	0	4.310122	4.148136	-1.327098
30	6	0	2.426698	1.901633	0.224638
31	7	0	1.699334	2.773315	0.482179
32	6	0	-5.319785	-0.693623	-0.095449
33	16	0	-4.547020	0.849410	0.189421
34	6	0	-7.186054	1.122063	0.296249
35	6	0	-6.022768	1.791790	0.401839
36	16	0	-7.070437	-0.601051	-0.039084
37	6	0	-8.573963	1.665676	0.429691
38	1	0	-8.558335	2.736407	0.640565
39	1	0	-9.148409	1.512494	-0.490959
40	1	0	-9.115361	1.170775	1.243947
41	6	0	-5.815463	3.247437	0.678612
42	1	0	-6.768667	3.767492	0.790022

43	1	0	-5.240634	3.396229	1.599691
44	1	0	-5.262579	3.729068	-0.135759
45	6	0	0.604426	-1.865045	-0.458103
46	6	0	1.173318	-0.638530	-0.226145
47	1	0	1.265157	-2.712304	-0.643429
48	1	0	0.540905	0.227820	-0.040417

E(RB3P86) = -2325.89372412 A.U.

10a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.208412	-1.774496	-0.000173
2	1	0	4.879305	-2.630913	-0.000172
3	6	0	2.828696	-2.115139	-0.000088
4	6	0	2.328364	-3.420340	-0.000004
5	16	0	1.515403	-0.968104	-0.000077
6	6	0	0.937304	-3.484973	0.000072
7	1	0	2.981013	-4.286142	0.000002
8	6	0	0.313401	-2.239292	0.000048
9	1	0	0.372394	-4.411573	0.000144
10	6	0	-1.079946	-1.991886	0.000110
11	6	0	-1.686033	-0.763118	0.000084
12	1	0	-1.690331	-2.892214	0.000195
13	1	0	-1.056905	0.126022	0.000021
14	6	0	-3.077571	-0.510070	0.000154
15	6	0	-4.205261	-1.521859	0.000229
16	6	0	-3.649450	0.749388	0.000175
17	6	0	-5.080960	0.606963	0.000295
18	6	0	-6.087042	1.547156	0.000343
19	6	0	-7.443581	1.122320	0.000493
20	7	0	-8.555732	0.778439	0.000616
21	6	0	-5.823214	2.941832	0.000252
22	7	0	-5.648124	4.092907	0.000179
23	6	0	-2.901429	1.950217	0.000103
24	7	0	-2.195769	2.875916	0.000089
25	6	0	-4.269857	-2.361218	-1.271891
26	1	0	-3.421486	-3.047278	-1.335319
27	1	0	-5.194040	-2.945725	-1.273120
28	1	0	-4.261225	-1.717123	-2.155039
29	6	0	-4.269544	-2.361343	1.272280
30	1	0	-5.193707	-2.945879	1.273658
31	1	0	-3.421133	-3.047379	1.335443
32	1	0	-4.260732	-1.717335	2.155490
33	6	0	4.796919	-0.541141	-0.000252
34	16	0	3.967176	0.997865	-0.000273
35	6	0	6.594155	1.382384	-0.000416
36	6	0	5.406677	2.017342	-0.000379
37	16	0	6.542144	-0.376021	-0.000356
38	6	0	7.961465	1.990685	-0.000496
39	1	0	7.907461	3.080757	-0.000593
40	1	0	8.530652	1.682393	0.883792
41	1	0	8.530620	1.682233	-0.884750
42	6	0	5.145775	3.490458	-0.000391
43	1	0	6.079546	4.055727	-0.000653
44	1	0	4.570819	3.789774	-0.883942
45	1	0	4.571252	3.789867	0.883411
46	8	0	-5.400674	-0.692389	0.000405

E(RB3P86) = -2286.63647841 A.U.

10b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.132006	-1.435737	0.000041
2	1	0	5.715431	-2.354355	0.000061
3	6	0	1.629424	-2.899908	0.000090
4	6	0	0.934763	-4.108923	0.000134
5	16	0	0.512718	-1.560396	0.000046
6	6	0	-0.452582	-3.956379	0.000137
7	1	0	1.444202	-5.066133	0.000166
8	6	0	-0.872823	-2.629242	0.000092
9	1	0	-1.155398	-4.783283	0.000170
10	6	0	-2.212855	-2.171316	0.000085
11	6	0	-2.617124	-0.862468	0.000034
12	1	0	-2.955372	-2.966158	0.000121
13	1	0	-1.853558	-0.085674	-0.000016
14	6	0	-3.949933	-0.388260	0.000029
15	6	0	-5.227379	-1.202385	0.000095
16	6	0	-4.308268	0.947518	-0.000052
17	6	0	-5.743734	1.041215	-0.000063
18	6	0	-6.582704	2.133087	-0.000142
19	6	0	-7.990388	1.935072	-0.000131
20	7	0	-9.143694	1.776919	-0.000122
21	6	0	-6.095713	3.466362	-0.000237
22	7	0	-5.737020	4.574030	-0.000316
23	6	0	-3.375525	2.011270	-0.000131
24	7	0	-2.530745	2.811967	-0.000194
25	6	0	-5.430181	-2.019667	-1.271815
26	1	0	-4.708003	-2.837385	-1.336244
27	1	0	-6.438612	-2.442571	-1.272341
28	1	0	-5.315336	-1.386491	-2.155442
29	6	0	-5.430188	-2.019463	1.272136
30	1	0	-6.438624	-2.442354	1.272733
31	1	0	-4.708023	-2.837181	1.336693
32	1	0	-5.315331	-1.386149	2.155662
33	6	0	5.819179	-0.253743	0.000015
34	16	0	5.078486	1.334913	-0.000016
35	6	0	7.723970	1.563970	-0.000015
36	6	0	6.575903	2.266700	-0.000027
37	16	0	7.568715	-0.191429	0.000011
38	6	0	9.124888	2.089275	-0.000013
39	1	0	9.137112	3.180742	-0.000066
40	1	0	9.674888	1.747190	0.884139
41	1	0	9.674924	1.747103	-0.884109
42	6	0	6.404784	3.752941	-0.000038
43	1	0	7.370330	4.262163	-0.000139
44	1	0	5.848730	4.086022	-0.883743
45	1	0	5.848894	4.086055	0.883758
46	6	0	3.718479	-1.552330	0.000047
47	6	0	3.044578	-2.739277	0.000080
48	1	0	3.138461	-0.628316	0.000026
49	1	0	3.615507	-3.666769	0.000105
50	8	0	-6.271272	-0.188267	0.000017

E(RB3P86) = -2364.29582397 A.U.

10c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.484802	-1.587410	-0.000903
2	1	0	6.261867	-2.348866	-0.001013
3	6	0	4.161142	-2.108462	-0.000675
4	6	0	3.838477	-3.466674	-0.000595

5	16	0	2.704907	-1.147758	-0.000455
6	6	0	2.466791	-3.717240	-0.000368
7	1	0	4.600368	-4.238228	-0.000702
8	6	0	1.682439	-2.567493	-0.000266
9	1	0	2.030801	-4.710864	-0.000275
10	6	0	-1.923374	-1.410890	0.000301
11	6	0	-2.709280	-0.286817	0.000413
12	1	0	-2.386150	-2.396274	0.000411
13	1	0	-2.208632	0.680294	0.000330
14	6	0	-4.122681	-0.233997	0.000658
15	6	0	-5.094870	-1.395290	0.000782
16	6	0	-4.867945	0.931457	0.000833
17	6	0	-6.264602	0.587113	0.001092
18	6	0	-7.394389	1.374537	0.001320
19	6	0	-8.676377	0.760372	0.001592
20	7	0	-9.728069	0.261256	0.001815
21	6	0	-7.333152	2.792593	0.001310
22	7	0	-7.326313	3.956888	0.001309
23	6	0	-4.299176	2.226834	0.000765
24	7	0	-3.734363	3.244566	0.000741
25	6	0	-5.039620	-2.236023	-1.270915
26	1	0	-4.101532	-2.793065	-1.334252
27	1	0	-5.870533	-2.946924	-1.270698
28	1	0	-5.124300	-1.598339	-2.154725
29	6	0	-5.038992	-2.236258	1.272295
30	1	0	-5.869887	-2.947181	1.272337
31	1	0	-4.100857	-2.793288	1.335080
32	1	0	-5.123268	-1.598743	2.156266
33	6	0	5.907579	-0.289428	-0.001002
34	16	0	4.883530	1.130156	-0.000864
35	6	0	7.438612	1.853939	-0.001295
36	6	0	6.178793	2.328307	-0.001097
37	16	0	7.617986	0.103776	-0.001297
38	6	0	8.714427	2.636101	-0.001503
39	1	0	8.518496	3.709811	-0.001542
40	1	0	9.319262	2.404833	0.882655
41	1	0	9.319043	2.404726	-0.885782
42	6	0	5.728085	3.754881	-0.001025
43	1	0	6.579439	4.438010	-0.001367
44	1	0	5.119008	3.976739	-0.884721
45	1	0	5.119623	3.976846	0.883070
46	6	0	0.267402	-2.503533	-0.000030
47	6	0	-0.508611	-1.375728	0.000060
48	1	0	-0.233073	-3.472246	0.000098
49	1	0	-0.032590	-0.395669	-0.000052
50	8	0	-6.396439	-0.744336	0.001153

E(RB3P86) = -2364.29569888 A.U.

11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.065534	1.117190	-0.389797
2	6	0	7.677783	-0.040067	-0.075658
3	16	0	5.302008	1.105107	-0.377338
4	6	0	5.105905	-0.573026	0.083706
5	16	0	6.629046	-1.402753	0.304346
6	6	0	3.902980	-1.202313	0.261058
7	6	0	2.635606	-0.595298	0.096240
8	1	0	3.926491	-2.251278	0.549389
9	6	0	1.439500	-1.240038	0.275388
10	1	0	2.605544	0.455721	-0.195043
11	6	0	0.186701	-0.608698	0.098863
12	1	0	1.443676	-2.290099	0.565505
13	6	0	-1.028228	-1.225795	0.266380

14	1	0	0.195362	0.442616	-0.193425
15	6	0	-2.247601	-0.545153	0.068399
16	1	0	-1.058716	-2.274779	0.554630
17	6	0	-3.512850	-1.096211	0.181261
18	1	0	-2.192884	0.502839	-0.216819
19	6	0	-4.711188	-0.308008	-0.041638
20	6	0	-3.600421	-2.469878	0.561973
21	6	0	-5.919501	-0.862457	-0.417053
22	6	0	-4.617936	1.157978	0.152261
23	7	0	-3.582004	-3.572662	0.934168
24	6	0	-7.122476	-0.094752	-0.457836
25	6	0	-6.081930	-2.216766	-0.833827
26	6	0	-4.088559	1.678949	1.341895
27	6	0	-5.060882	2.042326	-0.839322
28	7	0	-8.130391	0.486396	-0.497247
29	7	0	-6.269859	-3.294376	-1.231228
30	6	0	-4.020643	3.052863	1.539258
31	6	0	-4.976804	3.416429	-0.644533
32	1	0	-3.750824	0.998564	2.118056
33	1	0	-5.460558	1.649082	-1.768824
34	6	0	-4.461826	3.924445	0.545426
35	1	0	-3.625957	3.443510	2.472660
36	1	0	-5.317985	4.090641	-1.424354
37	1	0	-4.405172	4.998254	0.699137
38	6	0	9.146919	-0.315841	-0.008500
39	1	0	9.442468	-0.637636	0.996559
40	1	0	9.431172	-1.110965	-0.707074
41	1	0	9.727825	0.573357	-0.259813
42	6	0	7.696293	2.424747	-0.751087
43	1	0	7.400815	3.212823	-0.049076
44	1	0	8.785478	2.354932	-0.736123
45	1	0	7.393917	2.745501	-1.754513

E(RB3P86) = -1850.96261387 A.U.

12

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-8.490526	-0.112850	-0.000106
2	6	0	-7.919349	1.105554	-0.000147
3	16	0	-6.160656	1.151273	-0.000084
4	6	0	-5.904940	-0.582147	0.000010
5	16	0	-7.399537	-1.492528	0.000003
6	6	0	-4.679235	-1.192468	0.000078
7	6	0	-3.435983	-0.516402	0.000084
8	6	0	-2.213636	-1.135588	0.000148
9	6	0	-0.987571	-0.429104	0.000151
10	6	0	0.254666	-1.009703	0.000205
11	6	0	1.456422	-0.263294	0.000199
12	6	0	2.707829	-0.825924	0.000228
13	6	0	3.945498	-0.141578	0.000209
14	6	0	5.186848	-0.752177	0.000089
15	6	0	4.175626	1.355642	0.000252
16	8	0	5.626203	1.473169	0.000034
17	6	0	6.202924	0.265855	-0.000038
18	6	0	7.577300	0.177960	-0.000229
19	6	0	8.260414	-1.066222	-0.000337
20	7	0	8.858509	-2.065167	-0.000429
21	6	0	8.355014	1.367820	-0.000326
22	7	0	8.995280	2.340078	-0.000406
23	6	0	3.693056	2.046416	1.271935
24	6	0	3.692615	2.046518	-1.271205
25	1	0	-4.663660	-2.280521	0.000129
26	1	0	-3.448777	0.574641	0.000032
27	1	0	-2.174181	-2.224504	0.000197

28	1	0	-1.044456	0.660807	0.000100
29	1	0	0.330982	-2.096423	0.000250
30	1	0	1.351915	0.820432	0.000141
31	1	0	2.776083	-1.912796	0.000222
32	1	0	4.092604	1.542666	2.155959
33	1	0	4.038719	3.083908	1.273275
34	1	0	2.601969	2.040289	1.333444
35	1	0	2.601505	2.040344	-1.332349
36	1	0	4.038236	3.084024	-1.272555
37	1	0	4.091893	1.542869	-2.155409
38	6	0	5.372557	-2.154623	0.000013
39	7	0	5.418602	-3.317646	-0.000033
40	6	0	-9.956800	-0.407037	-0.000148
41	1	0	-10.247482	-0.986085	-0.884212
42	1	0	-10.247551	-0.985994	0.883953
43	1	0	-10.534039	0.520343	-0.000218
44	6	0	-8.634715	2.426812	-0.000242
45	1	0	-9.267721	2.533510	-0.887264
46	1	0	-9.267779	2.533607	0.886726
47	1	0	-7.929618	3.262005	-0.000265

E(RB3P86) = -1889.36358206 A.U.