Supporting Information for

Preparation, Structure and Redox Behavior of Bis(diarylmethylene)dihydrothiophene and Its π-Extended Analogues

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1. Selected bond length and torsion angle of molecular structure 1 and 2

Table S1 Selected bond lengths and torsion angles of **1a,b** and **2b** determined by X-ray analyses.

	1a	**1b**	**2b**
d(C_A-C_B), Å^{-1}	1.370(3)	1.366(5)	1.367(4)
d(C_A'-C_B'), Å^{-1}	1.366(3)	1.374(5)	1.367(4)
d(C_B-C_C), Å^{-1}	1.447(3)	1.446(4)	1.501(3)
d(C_B'-C_C'), Å^{-1}	1.446(3)	1.439(5)	1.501(3)
d(C_C-C_C'), Å^{-1}	1.335(3)	1.337(5)	———
d(C_c-C_d), Å^{-1}	———	———	1.38553(2)
d(C_C'-C_D'), Å^{-1}	———	———	1.38553(2)
d(C_D-C_D'), Å^{-1}	———	———	1.436(3)
torsion (thiophene-Ar_1), deg	26.627(67)	37.338(118)	48.496(83)
torsion (thiophene-Ar_2), deg	59.758(62)	57.540(109)	53.003(83)
torsion (thiophene-Ar_3), deg	29.251(65)	34.475(115)	53.003(83)
torsion (thiophene-Ar_4), deg	60.584(63)	49.011(109)	48.496(83)

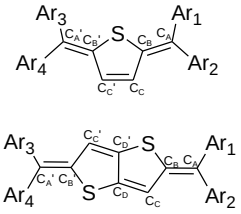
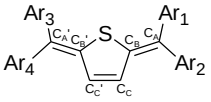


Table S2 Selected bond lengths and torsion angles of optimized structures of **1**.

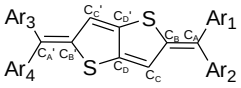
	1a	**1b**	**1c**
d(C_A-C_B), Å^{-1}	1.371	1.372	1.372
d(C_A'-C_B'), Å^{-1}	1.371	1.372	1.372
d(C_B-C_C), Å^{-1}	1.449	1.447	1.448
d(C_B'-C_C'), Å^{-1}	1.449	1.447	1.448
d(C_C-C_C'), Å^{-1}	1.355	1.356	1.355
torsion (thiophene-Ar_1), deg	50.14	49.63	49.81
torsion (thiophene-Ar_2), deg	52.22	51.71	51.98
torsion (thiophene-Ar_3), deg	50.13	49.63	49.81
torsion (thiophene-Ar_4), deg	52.22	51.71	51.98



a: Optimized at the B3LYP/6-31G* level of theory.

Table S3 Selected bond lengths and torsion angles of optimized structures of **2**.

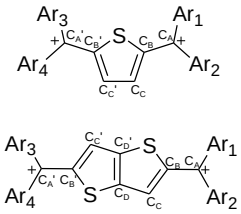
	2a	**2b**	**2c**
$d(C_A\text{-}C_B)$, $Å^{-1}$	1.372	1.373	1.373
$d(C_A\text{'}\text{-}C_B\text{'})$, $Å^{-1}$	1.372	1.373	1.373
$d(C_B\text{-}C_C)$, $Å^{-1}$	1.448	1.447	1.447
$d(C_B\text{'}\text{-}C_C\text{'})$, $Å^{-1}$	1.448	1.447	1.447
$d(C_c\text{-}C_d)$, $Å^{-1}$	1.361	1.361	1.361
$d(C_C\text{'}\text{-}C_D\text{'})$, $Å^{-1}$	1.361	1.361	1.361
$d(C_D\text{-}C_D\text{'})$, $Å^{-1}$	1.443	1.443	1.442
torsion (thiophene-Ar_1), deg	54.27	53.78	54.01
torsion (thiophene-Ar_2), deg	50.49	50.20	50.31
torsion (thiophene-Ar_3), deg	50.54	50.20	50.31
torsion (thiophene-Ar_4), deg	54.20	53.78	54.01



a: Optimized at the B3LYP/6-31G* level of theory.

Table S4 Selected bond lengths and torsion angles of optimized structures of $\mathbf{1}^{2+}$ and $\mathbf{2}^{2+}$.[a]

	1a	**1b**	**2a**	**2b**
$d(C_A\text{-}C_B)$, $Å^{-1}$	1.449	1.454	1.440	1.446
$d(C_A\text{'}\text{-}C_B\text{'})$, $Å^{-1}$	1.449	1.454	1.440	1.447
$d(C_B\text{-}C_C)$, $Å^{-1}$	1.400	1.396	1.399	1.394
$d(C_B\text{'}\text{-}C_C\text{'})$, $Å^{-1}$	1.400	1.396	1.399	1.394
$d(C_C\text{-}C_C\text{'})$, $Å^{-1}$	1.399	1.402	———	———
$d(C_c\text{-}C_d)$, $Å^{-1}$	———	———	1.404	1.406
$d(C_C\text{'}\text{-}C_D\text{'})$, $Å^{-1}$	———	———	1.404	1.406
$d(C_D\text{-}C_D\text{'})$, $Å^{-1}$	———	———	1.413	1.409
torsion (thiophene-Ar_1), deg	56.43	57.44	56.61	57.28
torsion (thiophene-Ar_2), deg	56.44	54.87	53.67	54.25
torsion (thiophene-Ar_3), deg	53.99	57.44	53.67	54.25
torsion (thiophene-Ar_4), deg	54.00	54.87	56.62	57.28



a: Optimized at the B3LYP/6-31G* level of theory.

2. Cyclic voltammograms of 1b and 2b

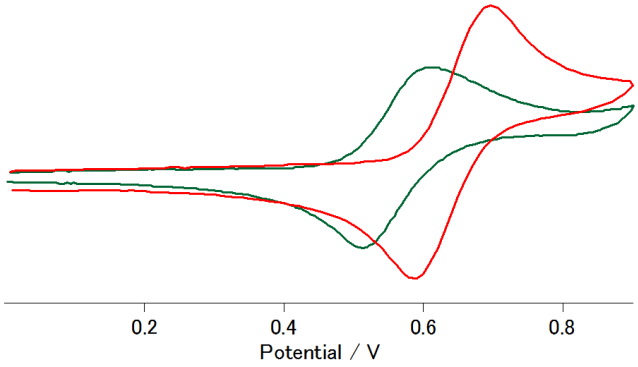


Figure S1 Cyclic voltammograms of **1b** (red) and **2b**(green) (CH_2Cl_2, vs Ag/AgCl).

3. ORTEP drawing of 1a,b and 2a,b

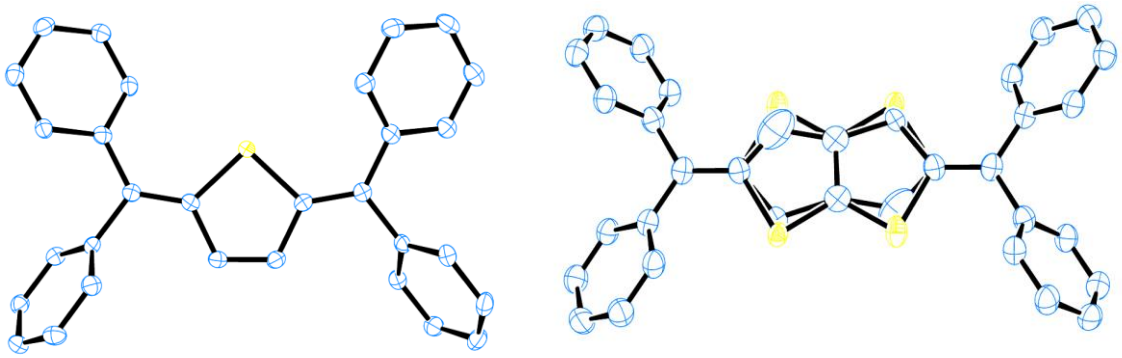


Figure S2 ORTEP drawings of **1a** (left) and **2a** (right).

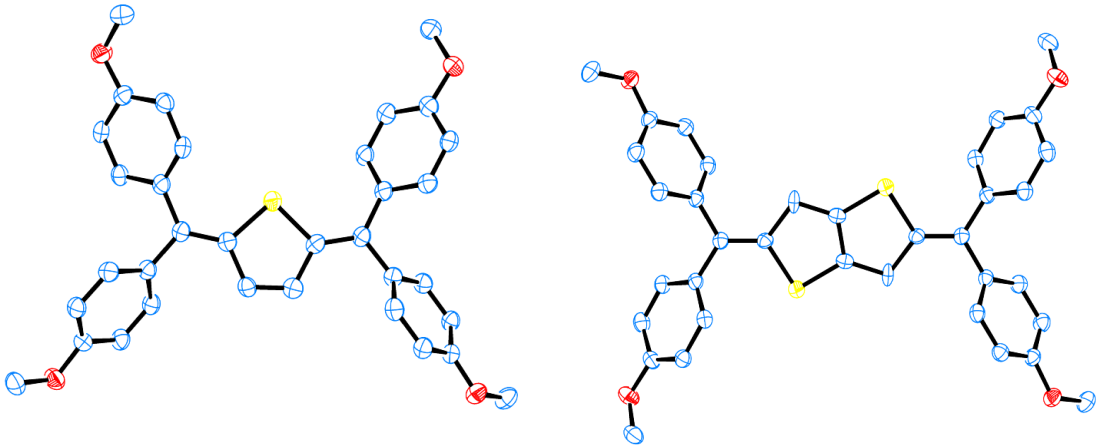


Figure S3 ORTEP drawings of **2b** (left) and **2b** (right).

4. Fluorescence of thienoquinoid 1in the solid state

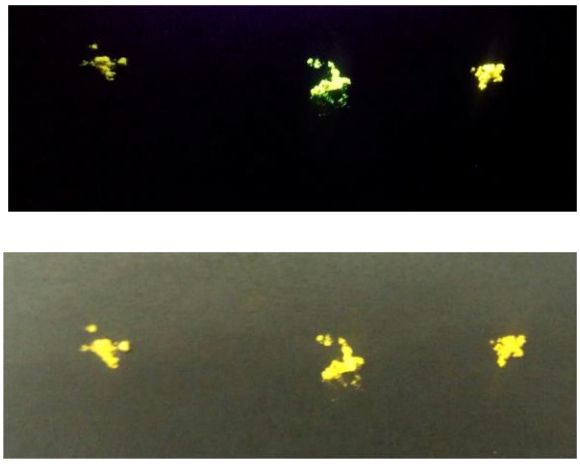
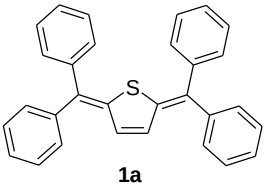


Figure S4 Photos of **1a** (left), **1b** (center) and **1c** (right) in the solid state with irradiation of 365 nm light (top) and without irradiation of UV-light. (bottom)

5. ^{1}H and ^{13}C NMR spectra of compounds 1-4



1a

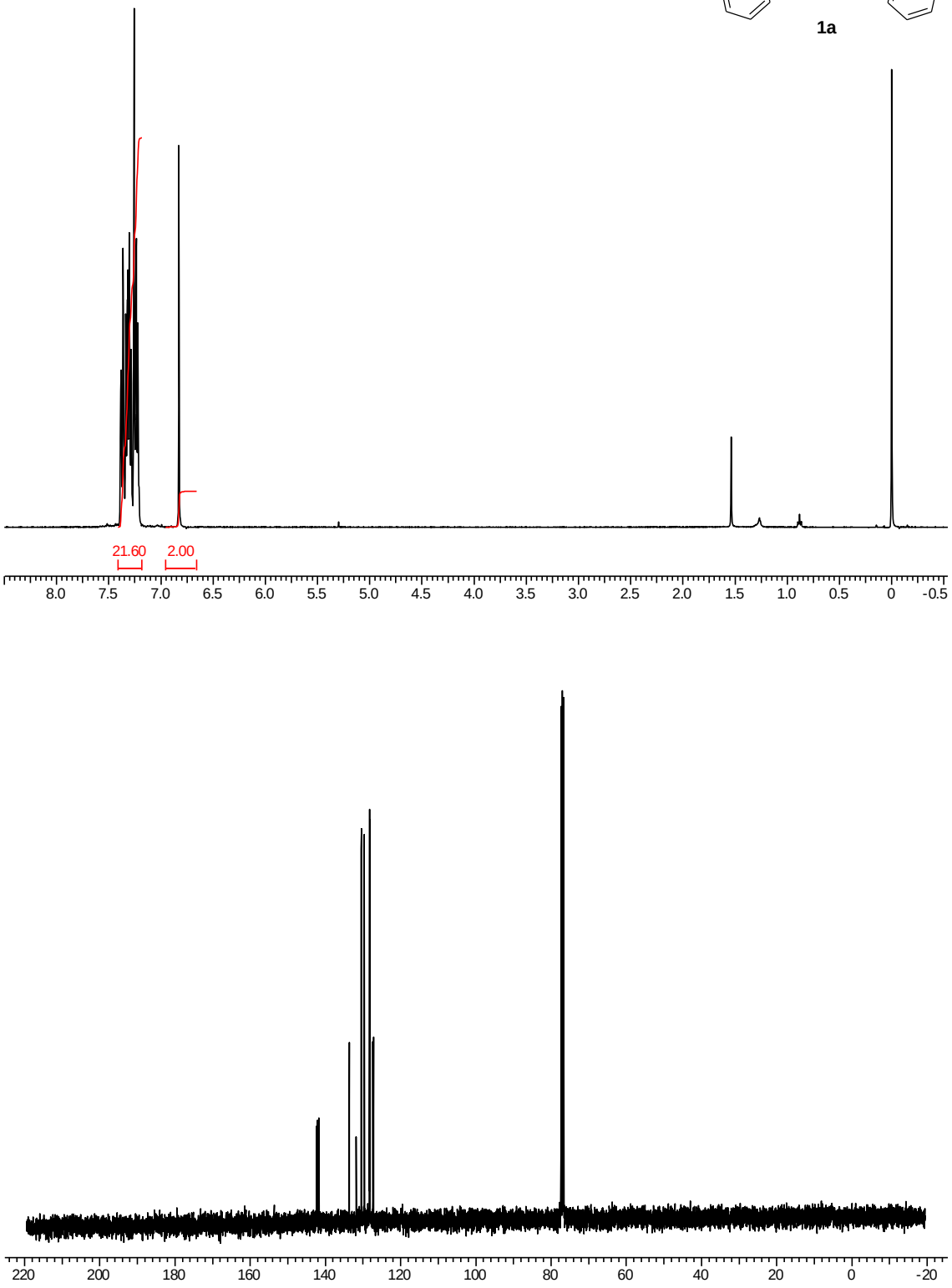


Figure S5 ^{1}H(top) and ^{13}C(bottom) NMR spectra of **1a** in $CDCl_3$.

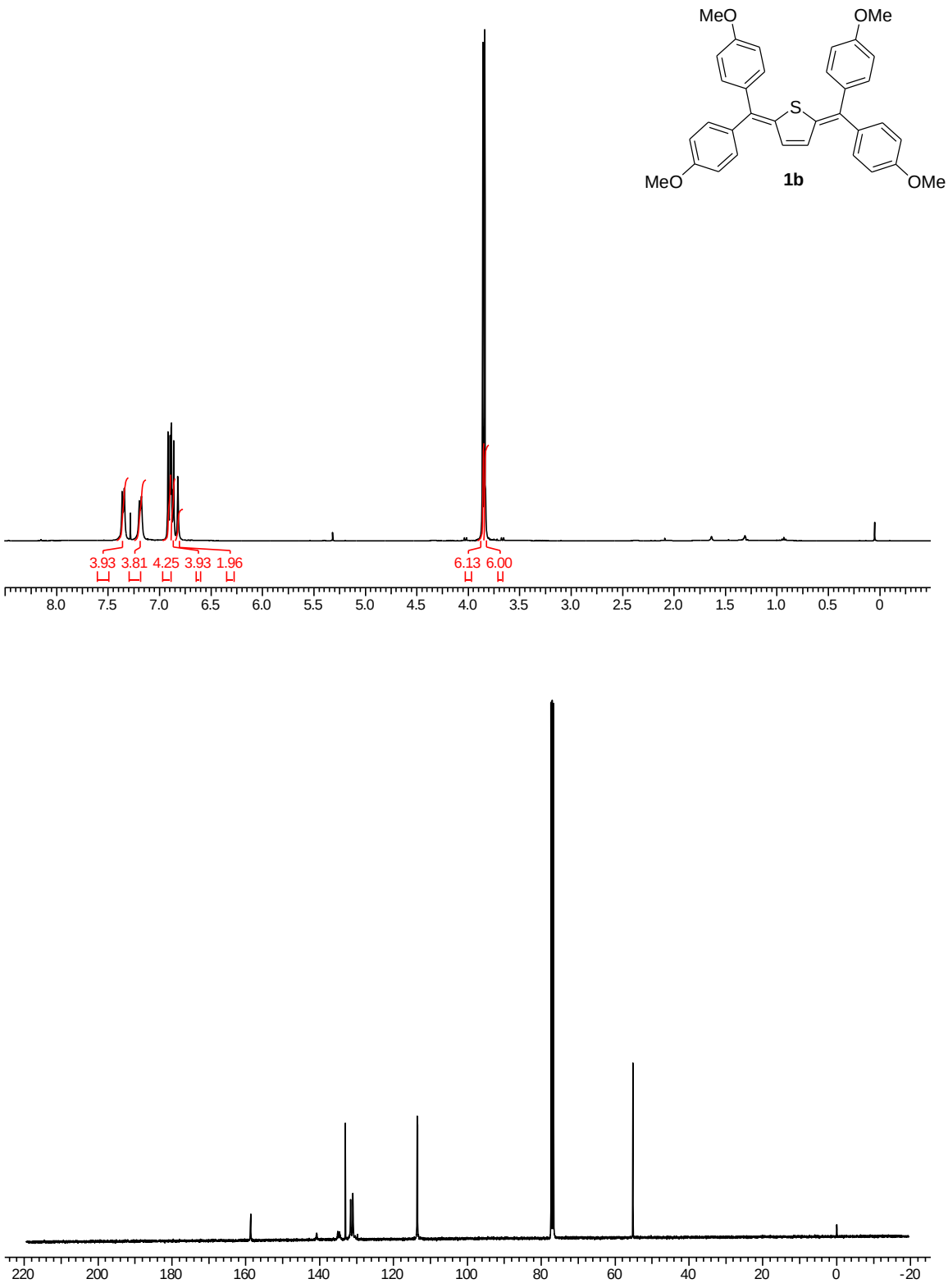


Figure S6 ^{1}H(top) and ^{13}C(bottom) NMR spectra of **1b** in $CDCl_3$.

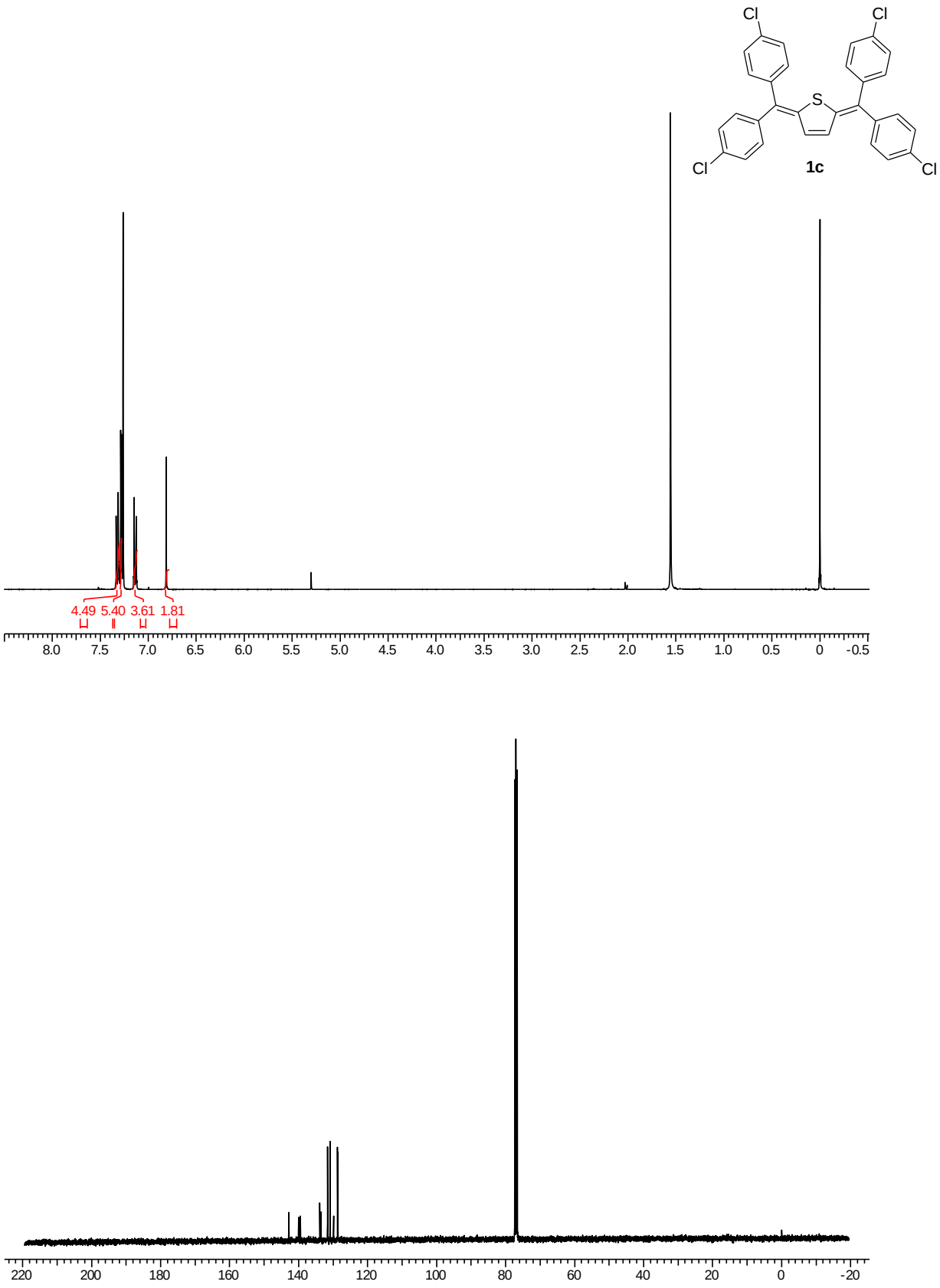


Figure S7 ^{1}H(top) and ^{13}C(bottom) NMR spectra of **1c** in $CDCl_3$.

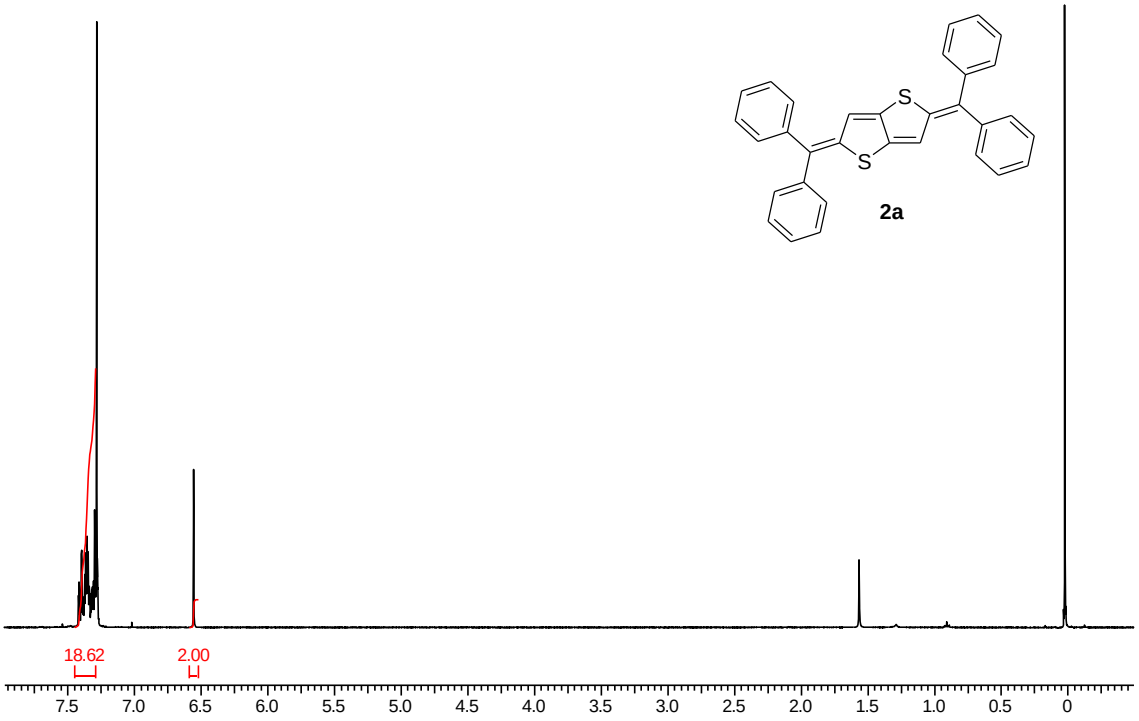


Figure S8 ^{1}H NMR spectra of **2a** in $CDCl_3$.

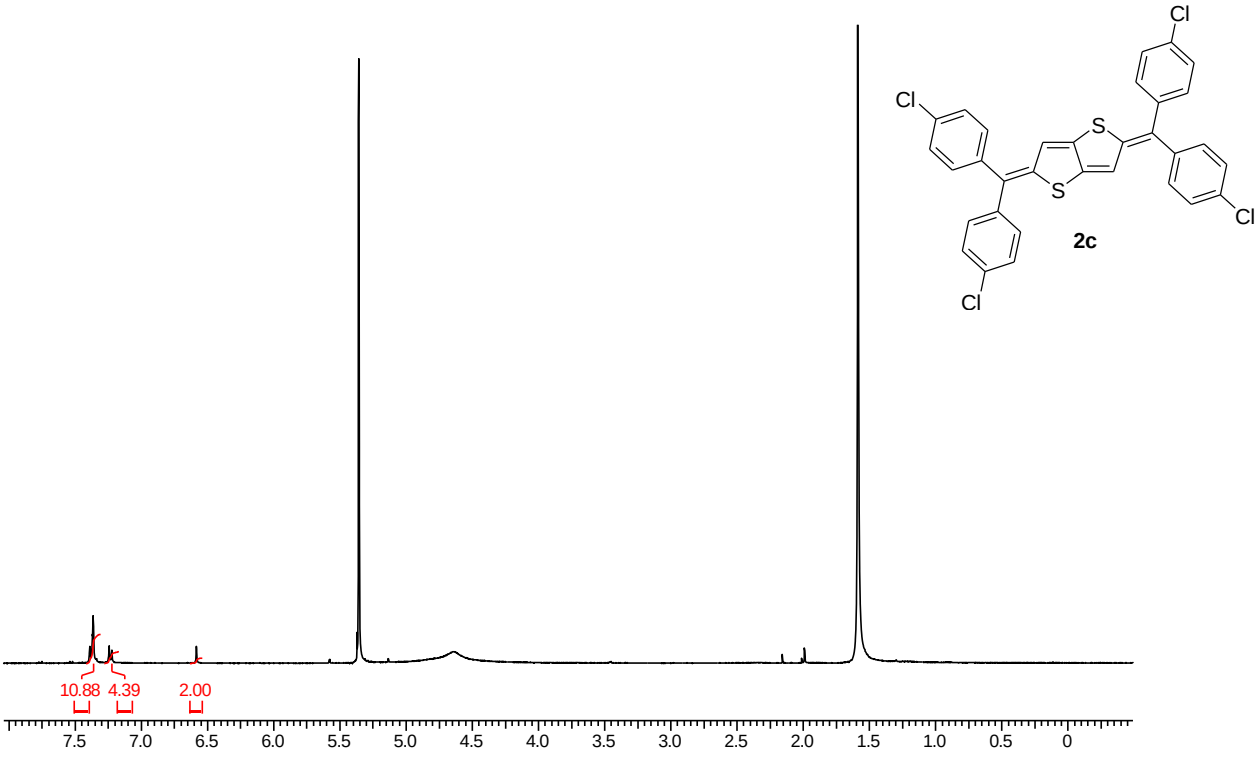


Figure S9 ^{1}H NMR spectra of **2c** in CD_2Cl_2.

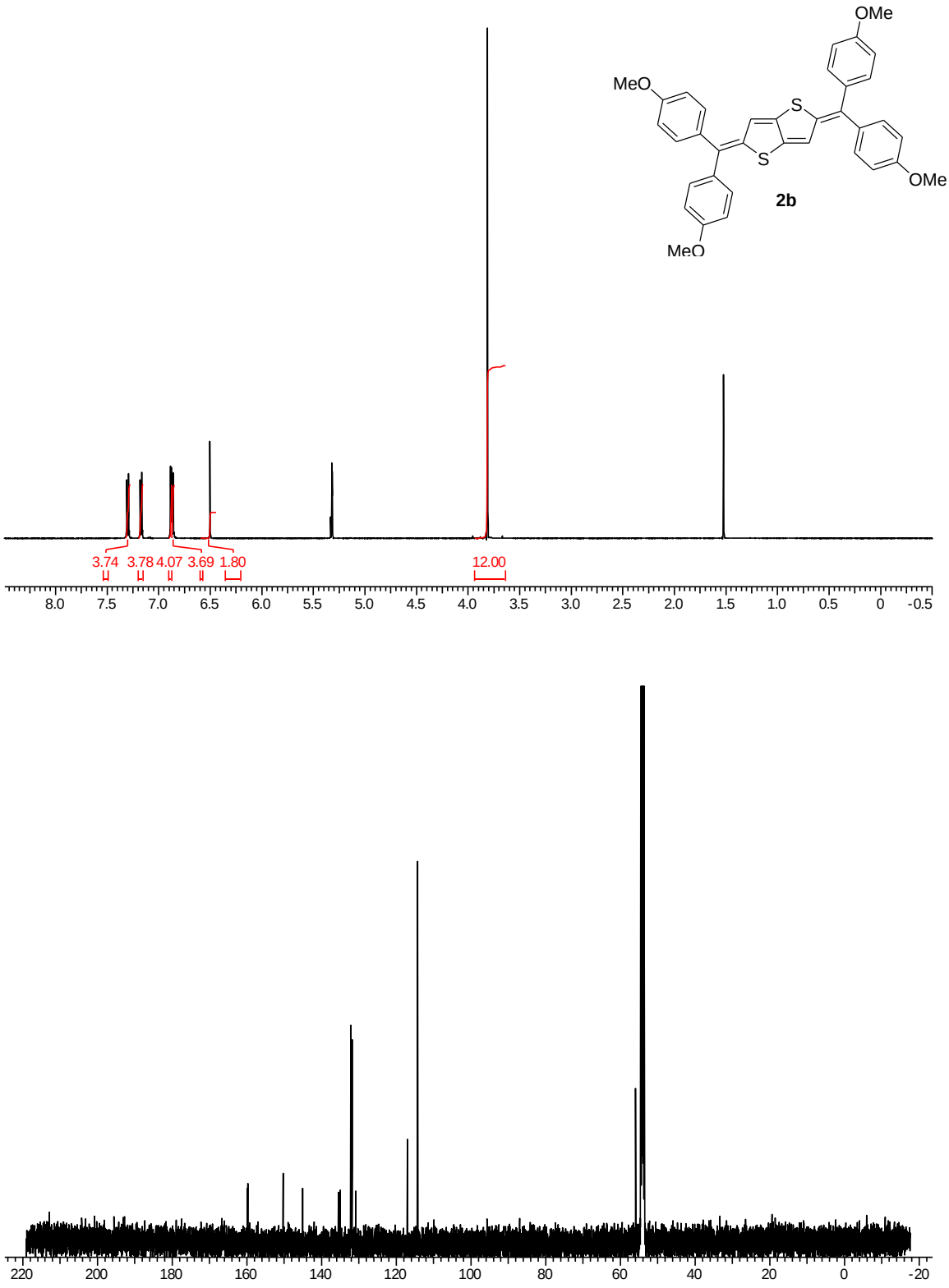


Figure S10 ^{1}H(top) and ^{13}C(bottom) NMR spectra of **2b** in CD_2Cl_2.

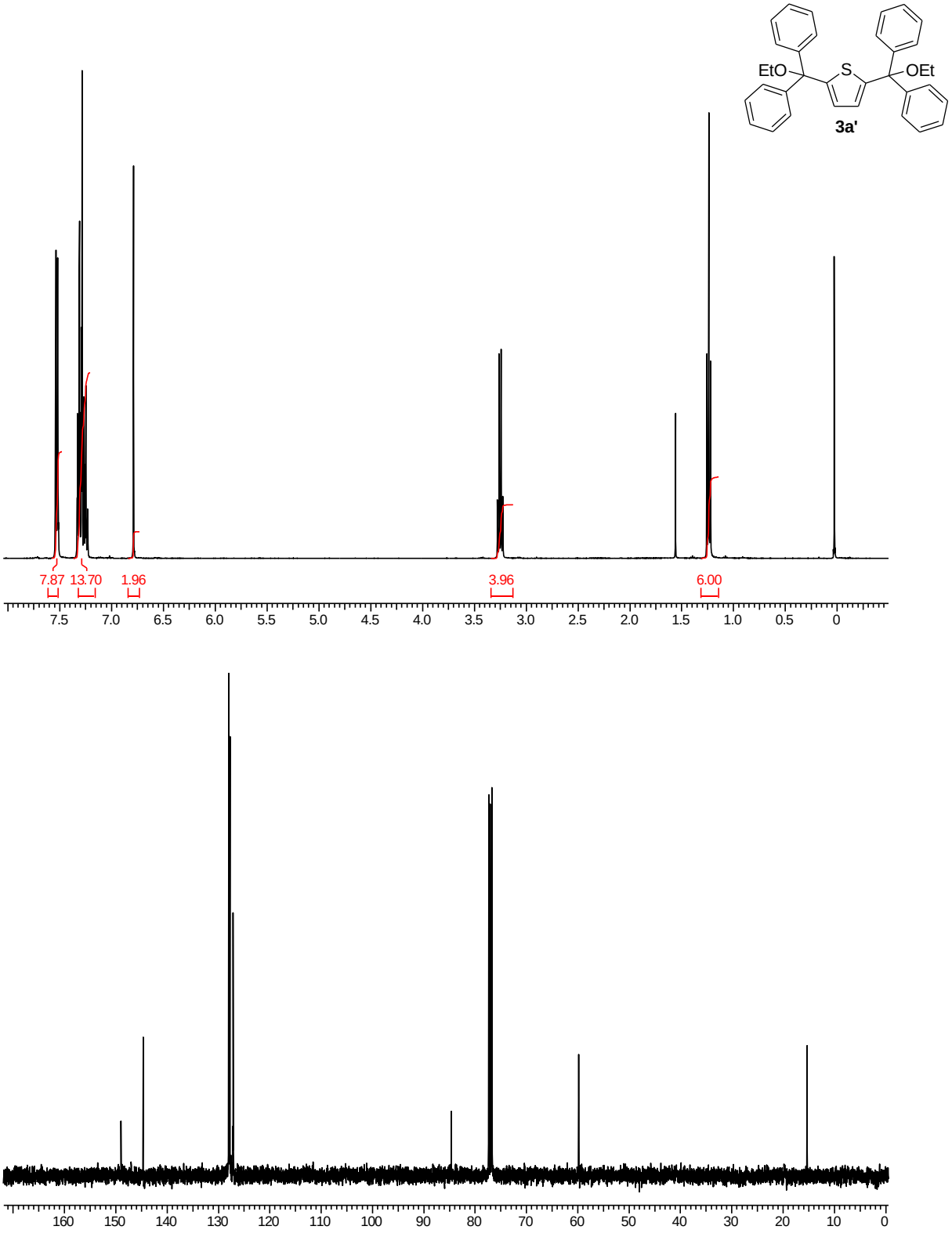


Figure S11 ^{1}H(top) and ^{13}C(bottom) NMR spectra of **3a'** in $CDCl_3$.

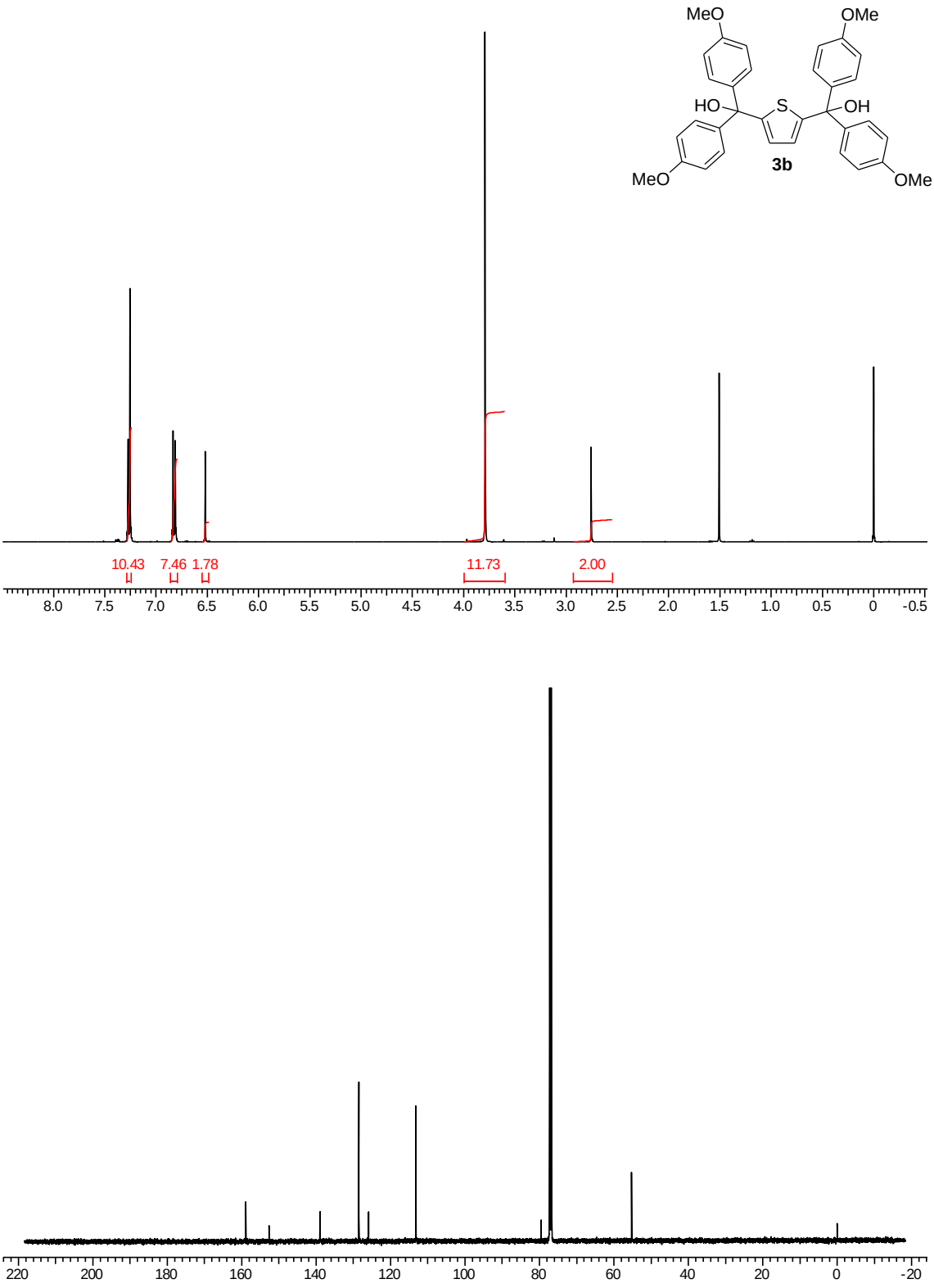


Figure S12 ^{1}H(top) and ^{13}C(bottom) NMR spectra of **3b** in $CDCl_3$.

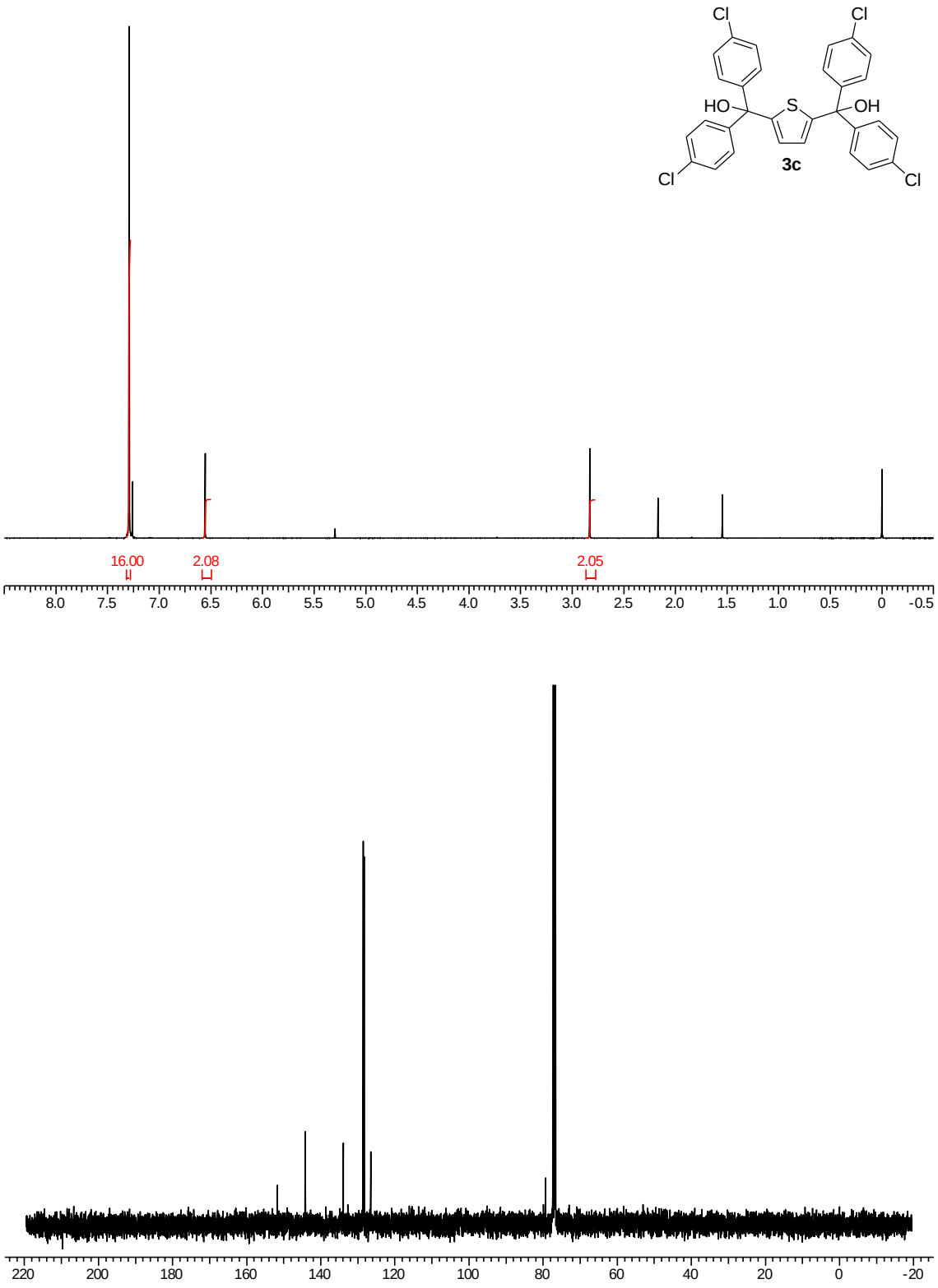


Figure S13 ^{1}H(top) and ^{13}C(bottom) NMR spectra of **3c** in $CDCl_3$.

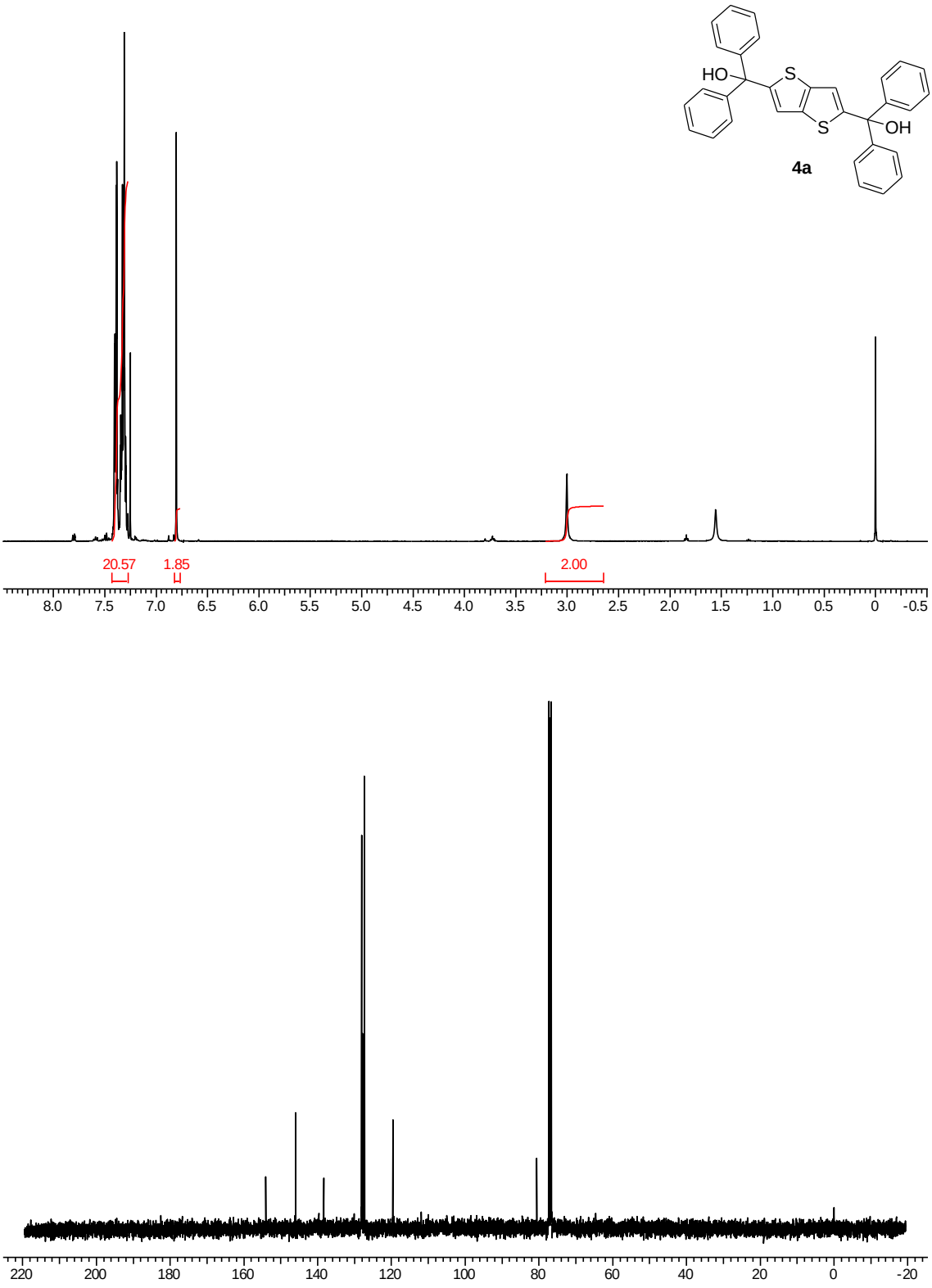


Figure S14 ^{1}H(top) and ^{13}C(bottom) NMR spectra of **4a** in $CDCl_3$.

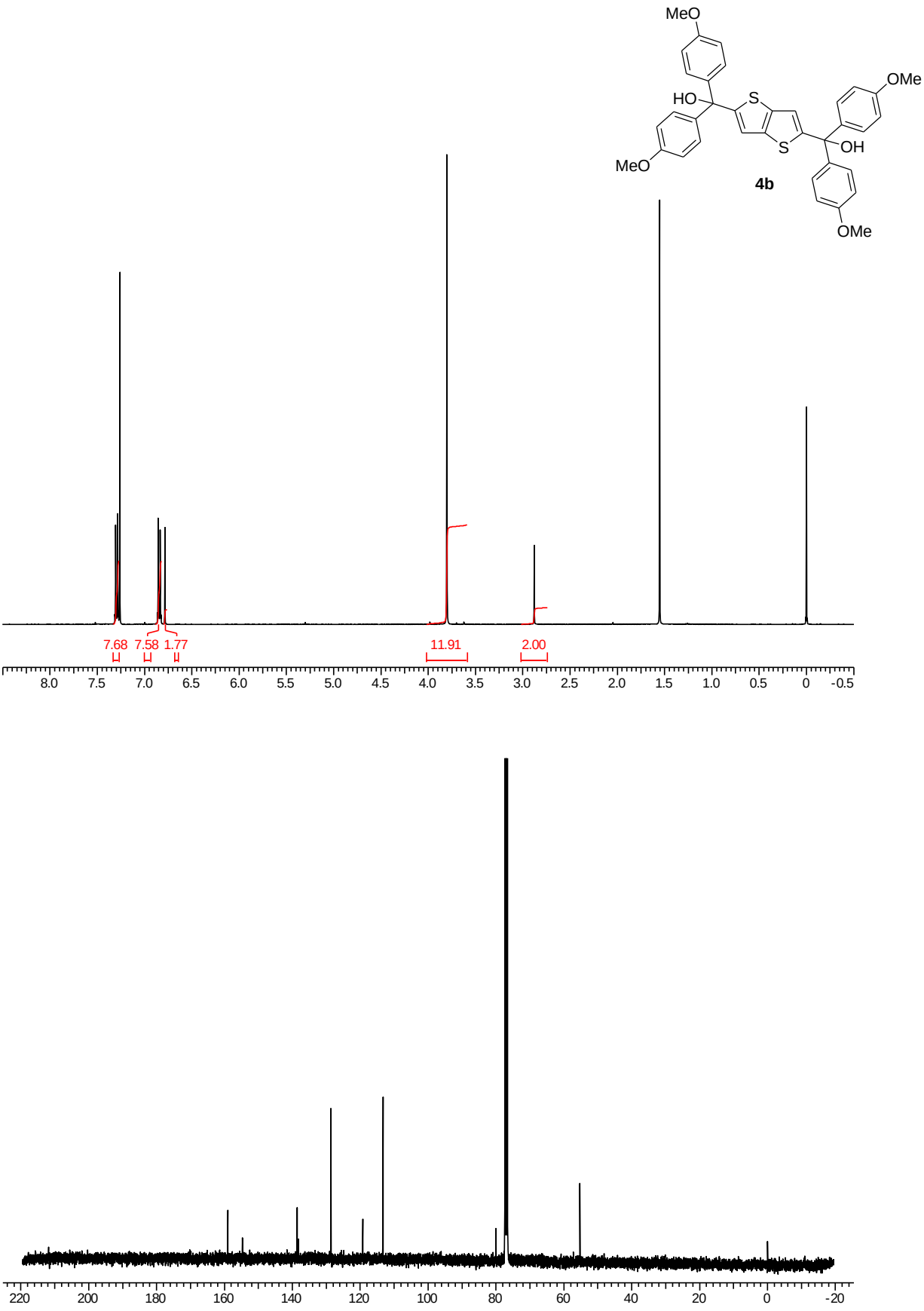


Figure S15 ^{1}H(top) and ^{13}C(bottom) NMR spectra of **4b** in $CDCl_3$.

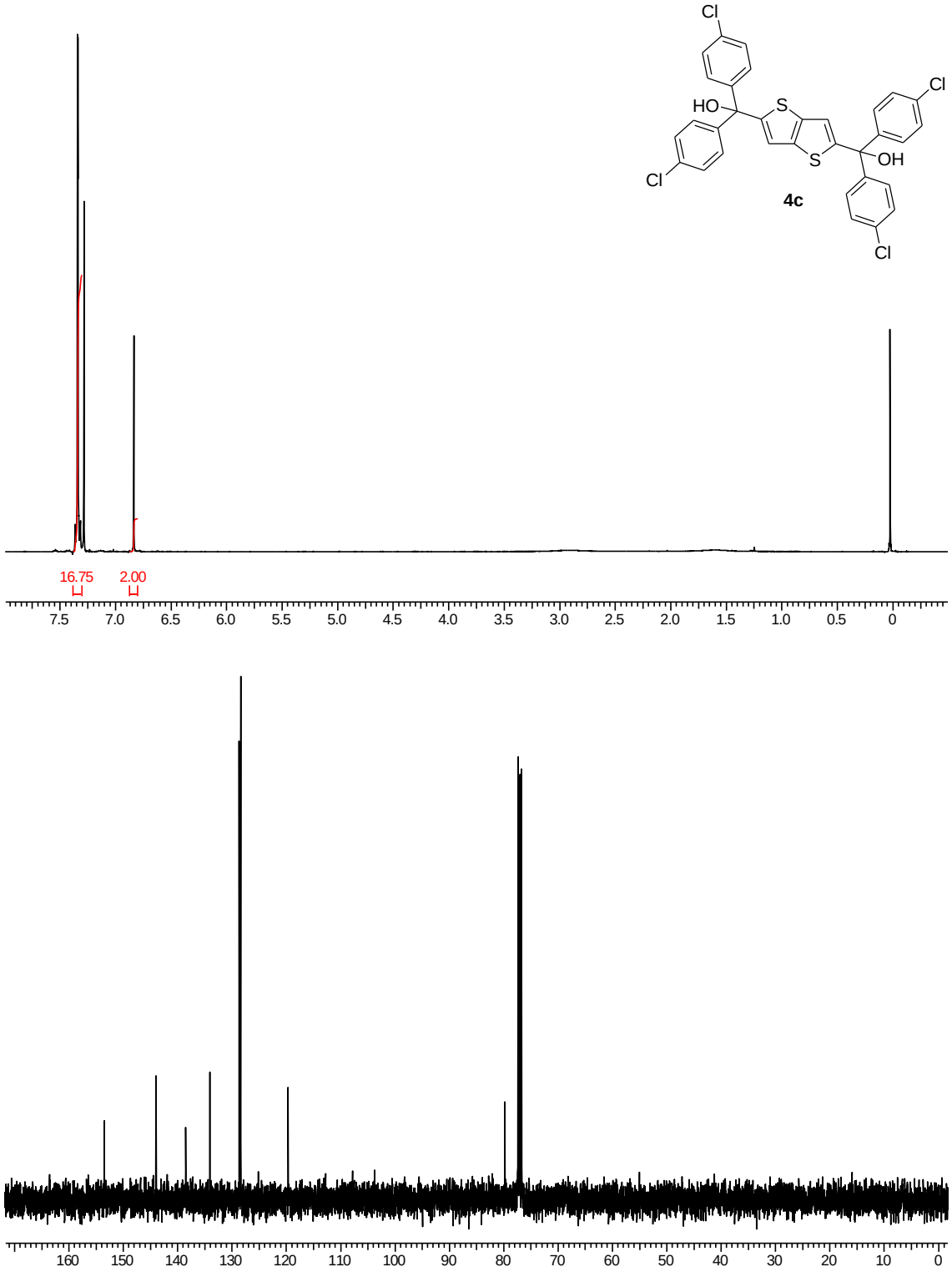


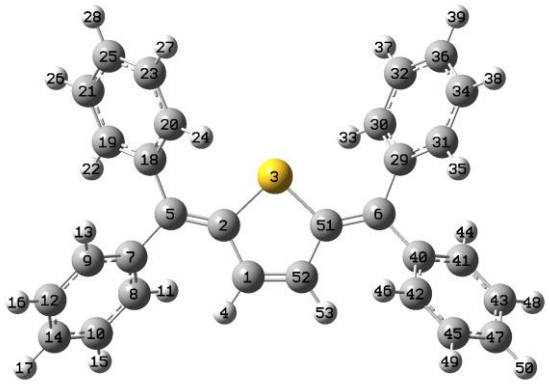
Figure S16 ^{1}H(top) and ^{13}C(bottom) NMR spectra of **4c** in $CDCl_3$.

6. Cartesian coordinates for optimized structures

Cartesian coordinates of the optimized structure of **1a**

E(RB3LYP) = -1554.61409639 a.u.

Number of imaginary frequency: 0



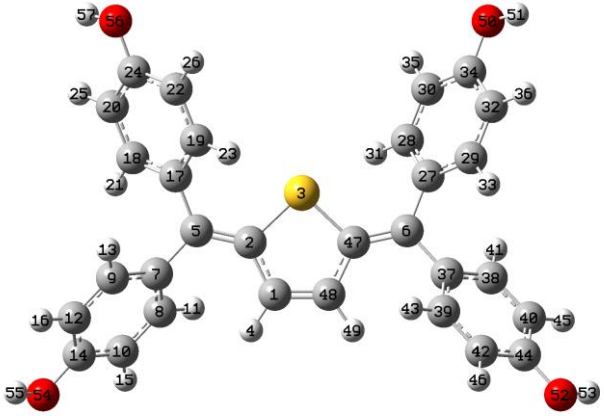
Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	−0.676750	−1.765630	0.031655
2	C	−1.297204	−0.456743	0.051413
3	S	0.000014	0.779776	0.000067
4	H	−1.273526	−2.668354	0.074665
5	C	−2.637729	−0.170159	0.064360
6	C	2.637746	−0.170127	−0.064263
7	C	−3.644856	−1.255390	−0.099817
8	C	−3.561534	−2.191892	−1.146355
9	C	−4.738112	−1.345395	0.782448
10	C	−4.519848	−3.195759	−1.289612
11	H	−2.749264	−2.114512	−1.863230
12	C	−5.692363	−2.350299	0.641538
13	H	−4.827921	−0.623041	1.588663
14	C	−5.586509	−3.282528	−0.393980
15	H	−4.437549	−3.903584	−2.110459
16	H	−6.521177	−2.406662	1.342517
17	H	−6.333878	−4.063399	−0.506180
18	C	−3.165297	1.209936	0.217531

19	C	−4.224671	1.652685	−0.598866
20	C	−2.656255	2.101802	1.179523
21	C	−4.733441	2.943090	−0.477357
22	H	−4.640141	0.976406	−1.340001
23	C	−3.171503	3.391780	1.304789
24	H	−1.867058	1.773494	1.848154
25	C	−4.208140	3.820401	0.474800
26	H	−5.542460	3.265249	−1.127880
27	H	−2.765693	4.059274	2.060457
28	H	−4.608206	4.826063	0.572611
29	C	3.165219	1.209991	−0.217507
30	C	2.655925	2.101846	−1.179374
31	C	4.224705	1.652796	0.598714
32	C	3.171064	3.391861	−1.304711
33	H	1.866604	1.773504	−1.847845
34	C	4.733367	2.943237	0.477134
35	H	4.640352	0.976532	1.339763
36	C	4.207833	3.820531	−0.474912
37	H	2.765058	4.059347	−2.060280
38	H	5.542484	3.265439	1.127514
39	H	4.607812	4.826222	−0.572776
40	C	3.644949	−1.255305	0.099840
41	C	4.738093	−1.345294	−0.782567
42	C	3.561844	−2.191735	1.146460
43	C	5.692426	−2.350129	−0.641726
44	H	4.827745	−0.622984	−1.588838
45	C	4.520243	−3.195531	1.289648
46	H	2.749682	−2.114348	1.863457
47	C	5.586778	−3.282297	0.393867
48	H	6.521146	−2.406484	−1.342818
49	H	4.438111	−3.903300	2.110561
50	H	6.334214	−4.063111	0.506014
51	C	1.297228	−0.456744	−0.051254
52	C	0.676774	−1.765633	−0.031513
53	H	1.273543	−2.668359	−0.074568

Cartesian coordinates of the optimized structure of **1b**

E(RB3LYP) = -1855.48036394 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	−0.677124	−1.817800	0.036151
2	C	−1.298307	−0.510885	0.058862
3	S	−0.000001	0.725768	0.000000
4	H	−1.272420	−2.721431	0.084464
5	C	−2.640021	−0.222842	0.075930
6	C	2.640022	−0.222843	−0.075938
7	C	−3.644825	−1.305208	−0.105161
8	C	−3.556309	−2.242465	−1.152897
9	C	−4.750716	−1.404767	0.758391
10	C	−4.505083	−3.246443	−1.318614
11	H	−2.736788	−2.167176	−1.861448
12	C	−5.704933	−2.406403	0.605756
13	H	−4.856823	−0.689949	1.569118
14	C	−5.583981	−3.335956	−0.433595
15	H	−4.433031	−3.958857	−2.134576
16	H	−6.544758	−2.468663	1.296287
17	C	−3.165686	1.153179	0.249583
18	C	−4.241041	1.606515	−0.537886
19	C	−2.645142	2.046661	1.207172

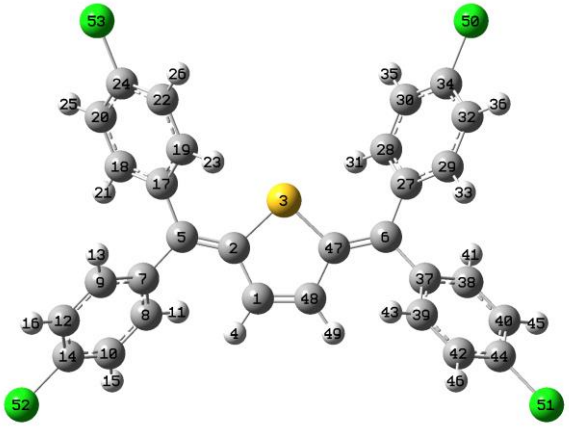
20	C	−4.753416	2.892409	−0.399647
21	H	−4.674080	0.941094	−1.278506
22	C	−3.153251	3.331822	1.359374
23	H	−1.841278	1.720557	1.858939
24	C	−4.208757	3.764063	0.550277
25	H	−5.576966	3.221423	−1.031676
26	H	−2.750170	4.009232	2.105624
27	C	3.165698	1.153174	−0.249588
28	C	2.645167	2.046664	−1.207177
29	C	4.241056	1.606500	0.537885
30	C	3.153287	3.331821	−1.359374
31	H	1.841303	1.720568	−1.858949
32	C	4.753443	2.892389	0.399651
33	H	4.674088	0.941074	1.278505
34	C	4.208794	3.764051	−0.550272
35	H	2.750214	4.009236	−2.105624
36	H	5.576993	3.221394	1.031683
37	C	3.644816	−1.305218	0.105157
38	C	4.750712	−1.404786	−0.758388
39	C	3.556274	−2.242484	1.152882
40	C	5.704917	−2.406433	−0.605748
41	H	4.856834	−0.689967	−1.569111
42	C	4.505036	−3.246473	1.318603
43	H	2.736742	−2.167194	1.861420
44	C	5.583945	−3.335990	0.433599
45	H	6.544748	−2.468701	−1.296271
46	H	4.432963	−3.958895	2.134556
47	C	1.298307	−0.510882	−0.058869
48	C	0.677128	−1.817799	−0.036139
49	H	1.272428	−2.721428	−0.084437
50	O	4.671669	5.036599	−0.737511
51	H	5.392231	5.204091	−0.110263
52	O	6.489928	−4.339840	0.637652
53	H	7.181011	−4.281478	−0.040297
54	O	−6.489981	−4.339792	−0.637649

55	H	−7.181073	−4.281407	0.040290
56	O	−4.671621	5.036615	0.737521
57	H	−5.392183	5.204115	0.110275

Cartesian coordinates of the optimized structure of **1c**

E(RB3LYP) = -3392.99837715 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	−0.676708	−1.872315	0.035874
2	C	−1.295890	−0.563440	0.059497
3	S	−0.000004	0.672467	−0.000053
4	H	−1.272006	−2.775709	0.084533
5	C	−2.636566	−0.274922	0.081187
6	C	2.636558	−0.274932	−0.081222
7	C	−3.645115	−1.356674	−0.084973
8	C	−3.564599	−2.292842	−1.131522
9	C	−4.740819	−1.447444	0.793844
10	C	−4.519987	−3.296699	−1.284017
11	H	−2.754155	−2.220690	−1.850529
12	C	−5.700481	−2.446330	0.657011
13	H	−4.835050	−0.729820	1.603394
14	C	−5.580645	−3.369132	−0.382892

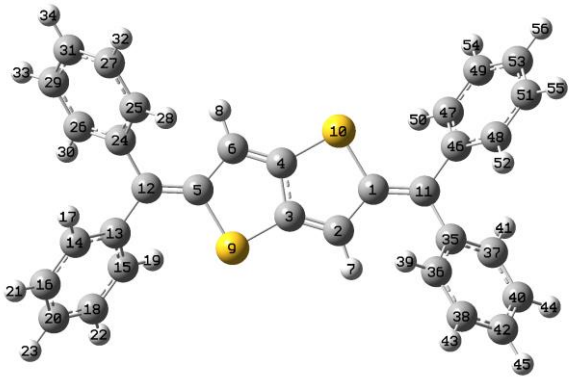
15	H	−4.449719	−4.006991	−2.101066
16	H	−6.532872	−2.512348	1.349592
17	C	−3.160914	1.103821	0.244858
18	C	−4.231028	1.551528	−0.554284
19	C	−2.640191	1.995072	1.200876
20	C	−4.742817	2.839206	−0.428729
21	H	−4.660246	0.882552	−1.293796
22	C	−3.146865	3.285557	1.342284
23	H	−1.842928	1.670185	1.861152
24	C	−4.193379	3.701142	0.521155
25	H	−5.558349	3.174395	−1.060705
26	H	−2.740032	3.958452	2.089577
27	C	3.160916	1.103808	−0.244877
28	C	2.640228	1.995062	−1.200913
29	C	4.231004	1.551514	0.554301
30	C	3.146908	3.285547	−1.342301
31	H	1.842991	1.670178	−1.861221
32	C	4.742799	2.839192	0.428766
33	H	4.660195	0.882538	1.293829
34	C	4.193395	3.701130	−0.521135
35	H	2.740103	3.958443	−2.089608
36	H	5.558310	3.174378	1.060771
37	C	3.645103	−1.356685	0.084965
38	C	4.740795	−1.447491	−0.793865
39	C	3.564609	−2.292808	1.131556
40	C	5.700456	−2.446375	−0.657010
41	H	4.835015	−0.729900	−1.603444
42	C	4.519996	−3.296663	1.284073
43	H	2.754186	−2.220619	1.850584
44	C	5.580636	−3.369137	0.382931
45	H	6.532835	−2.512423	−1.349603
46	H	4.449744	−4.006919	2.101155
47	C	1.295879	−0.563445	−0.059576
48	C	0.676684	−1.872317	−0.036024
49	H	1.271974	−2.775714	−0.084720

50	Cl	4.837392	5.326959	−0.690915
51	Cl	6.790481	−4.630407	0.566355
52	Cl	−6.790489	−4.630408	−0.566286
53	Cl	−4.837367	5.326973	0.690959

Cartesian coordinates of the optimized structure of **2a**

E(RB3LYP) = -2029.01097276 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	2.344803	0.007919	−0.076644
2	C	1.413226	−1.100413	−0.084486
3	C	0.108632	−0.713234	−0.068078
4	C	−0.108632	0.712881	−0.068027
5	C	−2.344819	−0.008261	−0.076648
6	C	−1.413227	1.100059	−0.084449
7	H	1.759119	−2.124790	−0.127508
8	H	−1.759093	2.124447	−0.127446
9	S	−1.423632	−1.569265	−0.088866
10	S	1.423646	1.568895	−0.088696
11	C	3.714913	−0.041319	−0.035637
12	C	−3.714940	0.041074	−0.035604
13	C	−4.562250	−1.167039	−0.212158
14	C	−5.629750	−1.414808	0.672465

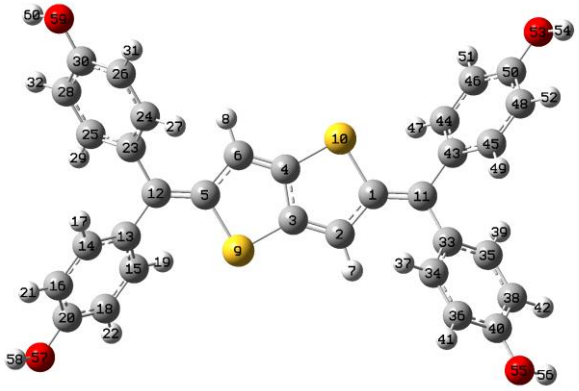
15	C	−4.351701	−2.074910	−1.266445
16	C	−6.435084	−2.541225	0.525809
17	H	−5.815968	−0.718728	1.484965
18	C	−5.162953	−3.199750	−1.415384
19	H	−3.561166	−1.883368	−1.985191
20	C	−6.204206	−3.440840	−0.518147
21	H	−7.245138	−2.718183	1.228556
22	H	−4.985555	−3.882758	−2.241986
23	H	−6.835518	−4.317595	−0.634841
24	C	−4.420992	1.326737	0.210266
25	C	−4.034686	2.199475	1.244774
26	C	−5.532404	1.685675	−0.576619
27	C	−4.716705	3.395594	1.466896
28	H	−3.207926	1.922239	1.892023
29	C	−6.209902	2.882513	−0.356800
30	H	−5.855122	1.019641	−1.371467
31	C	−5.804002	3.745202	0.664633
32	H	−4.403866	4.049174	2.277093
33	H	−7.057326	3.143326	−0.985508
34	H	−6.336064	4.676583	0.838494
35	C	4.421257	−1.326745	0.210230
36	C	4.034424	−2.200163	1.244011
37	C	5.533513	−1.684863	−0.575839
38	C	4.716729	−3.396094	1.466151
39	H	3.207046	−1.923535	1.890725
40	C	6.211315	−2.881529	−0.355986
41	H	5.856644	−1.018351	−1.370113
42	C	5.804878	−3.744873	0.664667
43	H	4.403479	−4.050184	2.275777
44	H	7.059398	−3.141693	−0.984073
45	H	6.337180	−4.676112	0.838555
46	C	4.561958	1.167068	−0.212142
47	C	4.352049	2.074048	−1.267330
48	C	5.628498	1.415843	0.673299
49	C	5.163047	3.199048	−1.416369

50	H	3.562175	1.881657	−1.986574
51	C	6.433584	2.542449	0.526547
52	H	5.814191	0.720408	1.486476
53	C	6.203371	3.441162	−0.518316
54	H	4.986223	3.881387	−2.243647
55	H	7.242911	2.720252	1.229918
56	H	6.834498	4.318041	−0.635085

Cartesian coordinates of the optimized structure of **2b**

E(RB3LYP) = -2329.87747421 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	2.346220	0.007073	−0.083644
2	C	1.414629	−1.099726	−0.089737
3	C	0.109085	−0.712504	−0.070691
4	C	−0.109085	0.712464	−0.070770
5	C	−2.346220	−0.007115	−0.083663
6	C	−1.414629	1.099684	−0.089869
7	H	1.759360	−2.124492	−0.136280
8	H	−1.759360	2.124444	−0.136524
9	S	−1.424005	−1.568168	−0.091203
10	S	1.424005	1.568126	−0.091361
11	C	3.718029	−0.040578	−0.045406

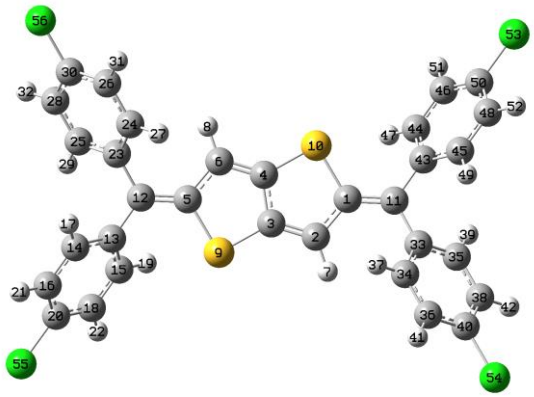
12	C	−3.718029	0.040549	−0.045433
13	C	−4.561955	−1.163402	−0.247642
14	C	−5.647249	−1.424203	0.609492
15	C	−4.340639	−2.067359	−1.305925
16	C	−6.454131	−2.544776	0.440423
17	H	−5.852880	−0.740821	1.427828
18	C	−5.143716	−3.187611	−1.488437
19	H	−3.537189	−1.875520	−2.009871
20	C	−6.203328	−3.435436	−0.609867
21	H	−7.279156	−2.730017	1.126522
22	H	−4.971305	−3.873487	−2.311883
23	C	−4.422610	1.320373	0.221660
24	C	−4.029365	2.191431	1.257520
25	C	−5.545858	1.690382	−0.541151
26	C	−4.702200	3.382678	1.506078
27	H	−3.192916	1.915259	1.892397
28	C	−6.225109	2.881580	−0.304809
29	H	−5.884054	1.036413	−1.339345
30	C	−5.803454	3.736849	0.719780
31	H	−4.397584	4.042209	2.312695
32	H	−7.083609	3.149776	−0.918794
33	C	4.422632	−1.320356	0.221830
34	C	4.029387	−2.191322	1.257768
35	C	5.545908	−1.690413	−0.540918
36	C	4.702246	−3.382528	1.506459
37	H	3.192920	−1.915108	1.892604
38	C	6.225184	−2.881569	−0.304441
39	H	5.884106	−1.036515	−1.339169
40	C	5.803528	−3.736749	0.720222
41	H	4.397630	−4.041985	2.313136
42	H	7.083706	−3.149803	−0.918379
43	C	4.561932	1.163368	−0.247759
44	C	4.340620	2.067166	−1.306177
45	C	5.647194	1.424319	0.609368
46	C	5.143673	3.187413	−1.488829

47	H	3.537189	1.875206	−2.010113
48	C	6.454053	2.544889	0.440159
49	H	5.852820	0.741059	1.427808
50	C	6.203255	3.435390	−0.610268
51	H	4.971265	3.873168	−2.312377
52	H	7.279055	2.730251	1.126253
53	O	6.962014	4.550181	−0.832200
54	H	7.652799	4.601531	−0.153283
55	O	6.431234	−4.917272	1.004154
56	H	7.171805	−5.035566	0.389128
57	O	−6.962109	−4.550239	−0.831659
58	H	−7.652931	−4.601459	−0.152769
59	O	−6.431136	4.917417	1.003581
60	H	−7.171688	5.035672	0.388525

Cartesian coordinates of the optimized structure of **2c**

E(RB3LYP) = -3867.39486092 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	2.343033	0.005600	−0.102412
2	C	1.411911	−1.102224	−0.109809
3	C	0.107490	−0.713154	−0.093335
4	C	−0.107502	0.713034	−0.093347

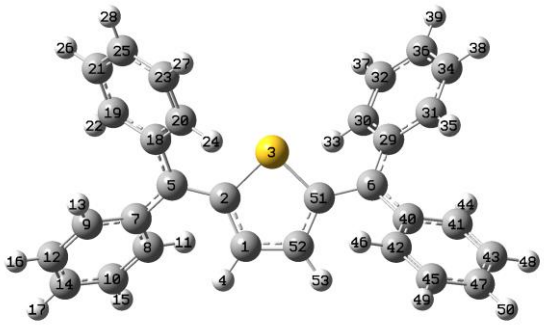
5	C	−2.343045	−0.005722	−0.102562
6	C	−1.411923	1.102103	−0.109899
7	H	1.755406	−2.127314	−0.155853
8	H	−1.755421	2.127192	−0.155954
9	S	−1.425044	−1.567038	−0.113131
10	S	1.425033	1.566916	−0.113062
11	C	3.714118	−0.044582	−0.062025
12	C	−3.714129	0.044491	−0.062232
13	C	−4.561521	−1.160565	−0.248984
14	C	−5.636891	−1.411871	0.624801
15	C	−4.347169	−2.066324	−1.304028
16	C	−6.447663	−2.532524	0.474162
17	H	−5.831842	−0.723065	1.441038
18	C	−5.154631	−3.190100	−1.470262
19	H	−3.552635	−1.878760	−2.018953
20	C	−6.197892	−3.418263	−0.574838
21	H	−7.264384	−2.721052	1.162830
22	H	−4.983215	−3.875329	−2.293640
23	C	−4.418984	1.326976	0.194622
24	C	−4.027127	2.196759	1.229155
25	C	−5.538212	1.690471	−0.578809
26	C	−4.703470	3.391284	1.469582
27	H	−3.195606	1.922500	1.871003
28	C	−6.220862	2.882039	−0.353014
29	H	−5.870732	1.032892	−1.376255
30	C	−5.795294	3.728553	0.671392
31	H	−4.395511	4.047310	2.276921
32	H	−7.073693	3.155089	−0.965485
33	C	4.419041	−1.327012	0.194885
34	C	4.027216	−2.196805	1.229426
35	C	5.538338	−1.690437	−0.578482
36	C	4.703638	−3.391273	1.469903
37	H	3.195667	−1.922588	1.871255
38	C	6.221067	−2.881949	−0.352637
39	H	5.870846	−1.032849	−1.375925

40	C	5.795518	−3.728480	0.671762
41	H	4.395700	−4.047303	2.277247
42	H	7.073947	−3.154942	−0.965064
43	C	4.561447	1.160520	−0.248810
44	C	4.347119	2.066156	−1.303961
45	C	5.636713	1.411990	0.625052
46	C	5.154515	3.189976	−1.470236
47	H	3.552651	1.878466	−2.018928
48	C	6.447417	2.532688	0.474374
49	H	5.831637	0.723278	1.441375
50	C	6.197678	3.418300	−0.574740
51	H	4.983123	3.875113	−2.293695
52	H	7.264060	2.721348	1.163099
53	Cl	7.220488	4.832642	−0.775996
54	Cl	6.65565	−5.231646	0.968177
55	Cl	−7.220785	−4.83255	−0.776044
56	Cl	−6.655324	5.231792	0.96774

Cartesian coordinates of the optimized structure of **1a**$^{2+}$

E(RB3LYP) = -1554.07219041 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	−0.698984	−1.802669	0.026473
2	C	−1.252845	−0.517002	0.065893
3	S	0.000006	0.701627	0.000524
4	H	−1.300890	−2.702077	0.074730

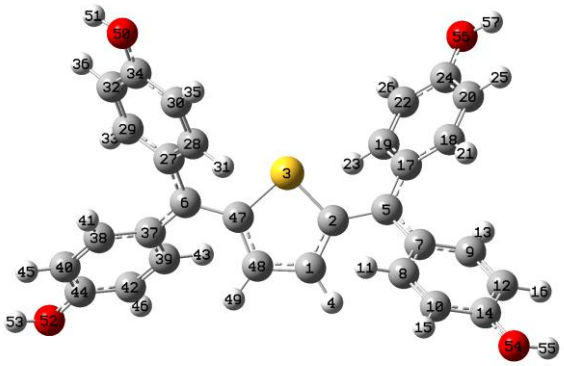
5	C	−2.659960	−0.175336	0.126655
6	C	2.659985	−0.175188	−0.126528
7	C	−3.617394	−1.068759	−0.481271
8	C	−3.297275	−1.825022	−1.645517
9	C	−4.917877	−1.211436	0.084884
10	C	−4.237251	−2.666120	−2.217182
11	H	−2.335226	−1.688248	−2.127166
12	C	−5.839319	−2.079240	−0.479508
13	H	−5.161853	−0.685901	1.001407
14	C	−5.505764	−2.801963	−1.632856
15	H	−3.997157	−3.210898	−3.124563
16	H	−6.814844	−2.205723	−0.021186
17	H	−6.234663	−3.472444	−2.078552
18	C	−3.096589	1.037434	0.781494
19	C	−4.224011	1.749487	0.281401
20	C	−2.428501	1.543939	1.932195
21	C	−4.646234	2.918890	0.894707
22	H	−4.713794	1.405774	−0.622980
23	C	−2.881149	2.695573	2.555782
24	H	−1.609736	0.983974	2.370452
25	C	−3.982514	3.390388	2.034810
26	H	−5.486238	3.471349	0.486169
27	H	−2.390968	3.052495	3.455818
28	H	−4.324193	4.299745	2.520340
29	C	3.096380	1.037575	−0.781546
30	C	2.428126	1.543856	−1.932251
31	C	4.223740	1.749851	−0.281630
32	C	2.880555	2.695487	−2.556003
33	H	1.609418	0.983717	−2.370391
34	C	4.645746	2.919245	−0.895103
35	H	4.713644	1.406318	0.622754
36	C	3.981863	3.390520	−2.035201
37	H	2.390250	3.052234	−3.456041
38	H	5.485703	3.471871	−0.486696
39	H	4.323370	4.299871	−2.520863

40	C	3.617615	−1.068518	0.481226
41	C	4.917942	−1.211236	−0.085276
42	C	3.297822	−1.824684	1.645624
43	C	5.839552	−2.078971	0.478949
44	H	5.161656	−0.685799	−1.001923
45	C	4.237967	−2.665712	2.217114
46	H	2.335897	−1.687888	2.127514
47	C	5.506324	−2.801586	1.632460
48	H	6.814952	−2.205486	0.020370
49	H	3.998126	−3.210412	3.124610
50	H	6.235355	−3.472015	2.078020
51	C	1.252907	−0.516928	−0.065330
52	C	0.699143	−1.802624	−0.025550
53	H	1.301108	−2.701998	−0.073708

Cartesian coordinates of the optimized structure of **1b**$^{2+}$

E(RB3LYP) = -1854.98261743 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	0.005129	0.701178	−1.848642
2	C	−0.008092	1.257774	−0.568352
3	S	0.000000	0.000000	0.648991
4	H	−0.013128	1.303351	−2.749191
5	C	0.000000	2.671237	−0.225737
6	C	0.000000	−2.671237	−0.225737

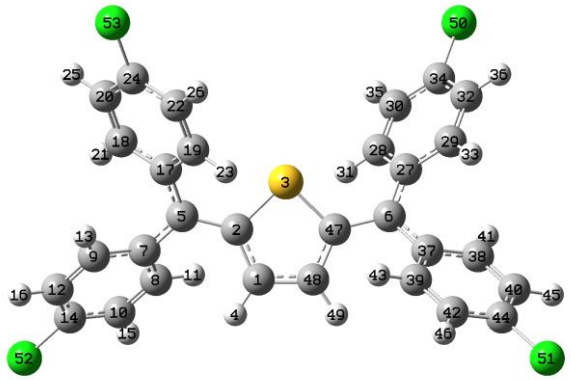
7	C	0.703770	3.580174	−1.089976
8	C	1.863712	3.181525	−1.822609
9	C	0.253564	4.924814	−1.252606
10	C	2.534982	4.061855	−2.637785
11	H	2.261391	2.181882	−1.687548
12	C	0.903553	5.804343	−2.091497
13	H	−0.657697	5.243460	−0.758853
14	C	2.057927	5.384610	−2.788407
15	H	3.438141	3.773919	−3.164946
16	H	0.517984	6.810433	−2.234597
17	C	−0.684574	3.140556	0.951084
18	C	−0.187590	4.258217	1.683663
19	C	−1.879179	2.519947	1.426767
20	C	−0.825985	4.717759	2.816396
21	H	0.747382	4.717467	1.382137
22	C	−2.539429	2.993293	2.536842
23	H	−2.318158	1.703369	0.864575
24	C	−2.015491	4.094579	3.251197
25	H	−0.406030	5.544482	3.383385
26	H	−3.469939	2.551139	2.876072
27	C	0.684574	−3.140556	0.951084
28	C	1.879179	−2.519947	1.426767
29	C	0.187590	−4.258217	1.683663
30	C	2.539429	−2.993293	2.536842
31	H	2.318158	−1.703369	0.864575
32	C	0.825985	−4.717759	2.816396
33	H	−0.747382	−4.717467	1.382137
34	C	2.015491	−4.094579	3.251197
35	H	3.469939	−2.551139	2.876072
36	H	0.406030	−5.544482	3.383385
37	C	−0.703770	−3.580174	−1.089976
38	C	−0.253564	−4.924814	−1.252606
39	C	−1.863712	−3.181525	−1.822609
40	C	−0.903553	−5.804343	−2.091497
41	H	0.657697	−5.243460	−0.758853

42	C	−2.534982	−4.061855	−2.637785
43	H	−2.261391	−2.181882	−1.687548
44	C	−2.057927	−5.384610	−2.788407
45	H	−0.517984	−6.810433	−2.234597
46	H	−3.438141	−3.773919	−3.164946
47	C	0.008092	−1.257774	−0.568352
48	C	−0.005129	−0.701178	−1.848642
49	H	0.013128	−1.303351	−2.749191
50	O	2.696778	−4.485052	4.328630
51	H	2.287527	−5.257112	4.757635
52	O	−2.746084	−6.175907	−3.609587
53	H	−2.367861	−7.071903	−3.654973
54	O	2.746084	6.175907	−3.609587
55	H	2.367861	7.071903	−3.654973
56	O	−2.696778	4.485052	4.32863
57	H	−2.287527	5.257112	4.757635

Cartesian coordinates of the optimized structure of **1c**$^{2+}$

E(RB3LYP) = -3392.44094565 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	−0.698507	−1.911995	0.043950
2	C	−1.252972	−0.628057	0.096223
3	S	0.000000	0.590168	0.000334

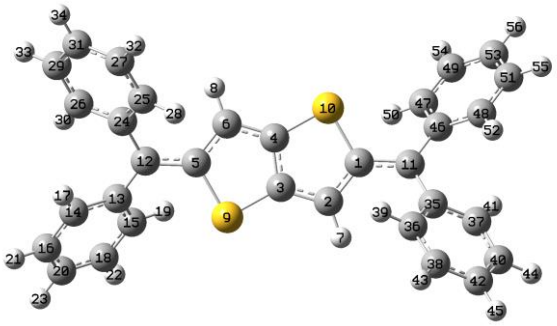
4	H	−1.297610	−2.812471	0.107403
5	C	−2.659302	−0.285923	0.190114
6	C	2.659313	−0.285787	−0.189954
7	C	−3.628177	−1.169743	−0.410008
8	C	−3.331029	−1.922386	−1.583131
9	C	−4.924438	−1.315962	0.165889
10	C	−4.273295	−2.754491	−2.154966
11	H	−2.374532	−1.793225	−2.077456
12	C	−5.859159	−2.171156	−0.385683
13	H	−5.161824	−0.799094	1.089080
14	C	−5.538550	−2.887176	−1.552565
15	H	−4.054418	−3.295237	−3.069202
16	H	−6.829723	−2.304901	0.079476
17	C	−3.079376	0.916869	0.870850
18	C	−4.222112	1.638198	0.420270
19	C	−2.380303	1.415262	2.006902
20	C	−4.631516	2.796730	1.053819
21	H	−4.743933	1.310883	−0.472243
22	C	−2.806950	2.553909	2.663417
23	H	−1.544668	0.857301	2.414414
24	C	−3.928573	3.253159	2.181932
25	H	−5.480623	3.360172	0.682679
26	H	−2.295723	2.905336	3.552871
27	C	3.079228	0.917003	−0.870792
28	C	2.379937	1.415361	−2.006724
29	C	4.222043	1.638352	−0.420444
30	C	2.806443	2.554004	−2.663337
31	H	1.544237	0.857378	−2.414073
32	C	4.631311	2.796879	−1.054089
33	H	4.744044	1.311050	0.471970
34	C	3.928146	3.253280	−2.182075
35	H	2.295045	2.905407	−3.552703
36	H	5.480483	3.360336	−0.683123
37	C	3.628322	−1.169531	0.410059
38	C	4.924579	−1.315539	−0.165901

39	C	3.331307	−1.922308	1.583127
40	C	5.859425	−2.170664	0.385566
41	H	5.161867	−0.798557	−1.089053
42	C	4.273698	−2.754342	2.154859
43	H	2.374804	−1.793316	2.077487
44	C	5.538947	−2.886820	1.552401
45	H	6.829989	−2.304251	−0.079639
46	H	4.054920	−3.295194	3.069057
47	C	1.253019	−0.627989	−0.095799
48	C	0.698646	−1.911955	−0.043268
49	H	1.297808	−2.812401	−0.106621
50	Cl	4.443638	4.684682	−2.984796
51	Cl	6.704334	−3.938668	2.251586
52	Cl	−6.703781	−3.939110	−2.251880
53	Cl	−4.444236	4.684568	2.984530

Cartesian coordinates of the optimized structure of **2a**$^{2+}$

E(RB3LYP) = -2028.48919082 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	2.303045	0.000986	−0.063844
2	C	1.437075	−1.097163	−0.051283
3	C	0.090403	−0.700454	−0.069499
4	C	−0.090406	0.700446	−0.069559

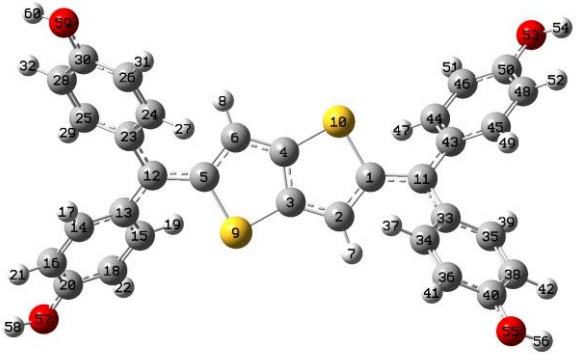
5	C	−2.303052	−0.000991	−0.063899
6	C	−1.437079	1.097157	−0.051409
7	H	1.786853	−2.121608	−0.075373
8	H	−1.786855	2.121600	−0.075593
9	S	−1.424473	−1.545943	−0.093356
10	S	1.424469	1.545935	−0.093448
11	C	3.741795	−0.045269	−0.025693
12	C	−3.741803	0.045268	−0.025771
13	C	−4.536262	−1.015000	−0.610365
14	C	−5.765662	−1.396618	−0.004336
15	C	−4.123631	−1.687725	−1.793931
16	C	−6.530380	−2.418064	−0.547295
17	H	−6.073380	−0.923360	0.921545
18	C	−4.913393	−2.684561	−2.345405
19	H	−3.224737	−1.369217	−2.309983
20	C	−6.110749	−3.059131	−1.719747
21	H	−7.450105	−2.723532	−0.058917
22	H	−4.609532	−3.166646	−3.268997
23	H	−6.718227	−3.850396	−2.148975
24	C	−4.388764	1.169249	0.618978
25	C	−3.821387	1.798344	1.761793
26	C	−5.623669	1.664084	0.113635
27	C	−4.466379	2.864073	2.369898
28	H	−2.915699	1.395274	2.201968
29	C	−6.243694	2.750318	0.712426
30	H	−6.049338	1.224050	−0.781438
31	C	−5.672083	3.347976	1.843158
32	H	−4.045144	3.314068	3.263196
33	H	−7.168755	3.139913	0.299780
34	H	−6.168578	4.189171	2.317790
35	C	4.388752	−1.169213	0.619119
36	C	3.821280	−1.798362	1.761856
37	C	5.623758	−1.663945	0.113923
38	C	4.466277	−2.864051	2.370027
39	H	2.915505	−1.395367	2.201921

40	C	6.243788	−2.750142	0.712774
41	H	6.049511	−1.223857	−0.781085
42	C	5.672081	−3.347859	1.843427
43	H	4.044965	−3.314091	3.263267
44	H	7.168931	−3.139661	0.300239
45	H	6.168580	−4.189023	2.318110
46	C	4.536260	1.014967	−0.610330
47	C	4.123553	1.687755	−1.793834
48	C	5.765748	1.396478	−0.004415
49	C	4.913328	2.684553	−2.345357
50	H	3.224580	1.369327	−2.309798
51	C	6.530480	2.417890	−0.547418
52	H	6.073533	0.923158	0.921413
53	C	6.110772	3.059023	−1.719808
54	H	4.609404	3.166689	−3.268903
55	H	7.450277	2.723277	−0.059127
56	H	6.71826	3.850259	−2.149073

Cartesian coordinates of the optimized structure of **2b**$^{2+}$

E(RB3LYP) = -2329.39567978 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	2.306227	−0.002673	−0.070673
2	C	1.440572	−1.095831	−0.058613
3	C	0.091511	−0.698422	−0.071703

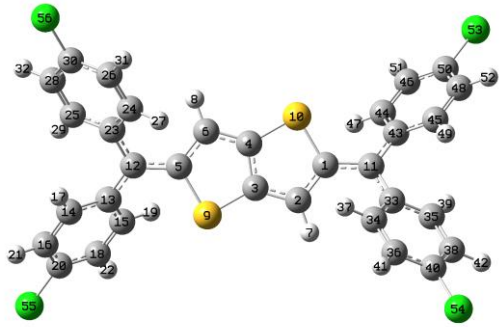
4	C	−0.091565	0.698376	−0.071907
5	C	−2.306290	0.002632	−0.070773
6	C	−1.440628	1.095788	−0.058991
7	H	1.788613	−2.120972	−0.082897
8	H	−1.788662	2.120922	−0.083581
9	S	−1.426432	−1.541232	−0.090948
10	S	1.426376	1.541186	−0.091309
11	C	3.752046	−0.045396	−0.033150
12	C	−3.752113	0.045379	−0.033245
13	C	−4.533902	−0.983449	−0.672833
14	C	−5.784592	−1.389717	−0.124522
15	C	−4.098325	−1.627171	−1.869658
16	C	−6.541268	−2.380184	−0.715706
17	H	−6.120111	−0.956162	0.811119
18	C	−4.863288	−2.592869	−2.482738
19	H	−3.179628	−1.305125	−2.346736
20	C	−6.091024	−2.988235	−1.906634
21	H	−7.471897	−2.704500	−0.257248
22	H	−4.554303	−3.055782	−3.413662
23	C	−4.392559	1.133536	0.662865
24	C	−3.808506	1.741605	1.814134
25	C	−5.645242	1.643857	0.213608
26	C	−4.434494	2.773049	2.476081
27	H	−2.883486	1.342728	2.215539
28	C	−6.264310	2.696805	0.854521
29	H	−6.091940	1.239174	−0.687885
30	C	−5.668107	3.268756	1.998569
31	H	−4.012954	3.210495	3.374668
32	H	−7.198747	3.097887	0.470463
33	C	4.392540	−1.133426	0.663094
34	C	3.808192	−1.741847	1.814027
35	C	5.645627	−1.643193	0.214348
36	C	4.434265	−2.773147	2.476117
37	H	2.882833	−1.343371	2.215051
38	C	6.264791	−2.696004	0.855394

39	H	6.092611	−1.238168	−0.686853
40	C	5.668276	−3.268336	1.999090
41	H	4.012482	−3.210869	3.374456
42	H	7.199562	−3.096672	0.471718
43	C	4.533818	0.983332	−0.672899
44	C	4.097838	1.627443	−1.869365
45	C	5.784926	1.389044	−0.125140
46	C	4.862806	2.593026	−2.482621
47	H	3.178774	1.305813	−2.346023
48	C	6.541620	2.379401	−0.716487
49	H	6.120802	0.955119	0.810203
50	C	6.090961	2.987867	−1.907048
51	H	4.553497	3.056247	−3.413284
52	H	7.472598	2.703298	−0.258444
53	O	6.769446	3.944649	−2.543643
54	H	7.607537	4.15246	−2.094717
55	O	6.210091	−4.280504	2.679444
56	H	7.064899	−4.552559	2.301974
57	O	−6.769517	−3.945102	−2.543091
58	H	−7.607311	−4.153289	−2.093785
59	O	−6.209853	4.281036	2.678812
60	H	−7.06439	4.553459	2.300992

Cartesian coordinates of the optimized structure of **2c**$^{2+}$

E(RB3LYP) = -3866.85761072 a.u.

Number of imaginary frequency: 0



Atom Number	Element	Cartesian coordinates		
		X	Y	Z
1	C	2.304550	−0.003510	−0.082403
2	C	1.436289	−1.099112	−0.070555
3	C	0.089955	−0.700121	−0.085993
4	C	−0.089954	0.700112	−0.086037
5	C	−2.304549	0.003501	−0.082508
6	C	−1.436289	1.099104	−0.070683
7	H	1.783075	−2.124598	−0.097581
8	H	−1.783073	2.124588	−0.097782
9	S	−1.427202	−1.542649	−0.107123
10	S	1.427204	1.542639	−0.107143
11	C	3.744797	−0.050740	−0.045197
12	C	−3.744799	0.050735	−0.045362
13	C	−4.538232	−1.000095	−0.644291
14	C	−5.776170	−1.386169	−0.057649
15	C	−4.121733	−1.669633	−1.828797
16	C	−6.543252	−2.396736	−0.607865
17	H	−6.096296	−0.923361	0.869305
18	C	−4.902526	−2.656835	−2.400852
19	H	−3.215806	−1.357440	−2.336071
20	C	−6.110019	−3.029373	−1.784760
21	H	−7.467424	−2.710360	−0.135038
22	H	−4.599643	−3.136464	−3.325087
23	C	−4.389902	1.166088	0.612400
24	C	−3.819443	1.791741	1.755980
25	C	−5.630132	1.667365	0.125256
26	C	−4.454262	2.848327	2.382262
27	H	−2.907896	1.393646	2.188157
28	C	−6.252401	2.744141	0.729992
29	H	−6.066750	1.239074	−0.770265
30	C	−5.668128	3.332414	1.864148
31	H	−4.034804	3.295873	3.276598
32	H	−7.179029	3.142944	0.331910
33	C	4.389879	−1.166060	0.612640

34	C	3.819358	−1.791691	1.756202
35	C	5.630152	−1.667323	0.125594
36	C	4.454159	−2.848245	2.382557
37	H	2.907772	−1.393604	2.188306
38	C	6.252405	−2.744067	0.730402
39	H	6.066821	−1.239047	−0.769909
40	C	5.668070	−3.332320	1.864537
41	H	4.034652	−3.295774	3.276879
42	H	7.179069	−3.142861	0.332394
43	C	4.538251	1.000063	−0.644145
44	C	4.121765	1.669584	−1.828665
45	C	5.776195	1.386126	−0.057509
46	C	4.902577	2.656759	−2.400740
47	H	3.215831	1.357399	−2.335931
48	C	6.543297	2.396667	−0.607745
49	H	6.096312	0.923327	0.869454
50	C	6.110077	3.029287	−1.784654
51	H	4.599704	3.136375	−3.324985
52	H	7.467474	2.710282	−0.134923
53	Cl	7.070175	4.276710	−2.483290
54	Cl	6.449569	−4.660817	2.632673
55	Cl	−7.070093	−4.276829	−2.483371
56	Cl	−6.449648	4.660951	2.632192