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Supplementary Information

Sigma-spacer Regulated Thiophenyl Triazine Conjugates: Synthesis, Crystal, Electronic and Luminescent Properties

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1. Crystal date and structure of **TTC**s.

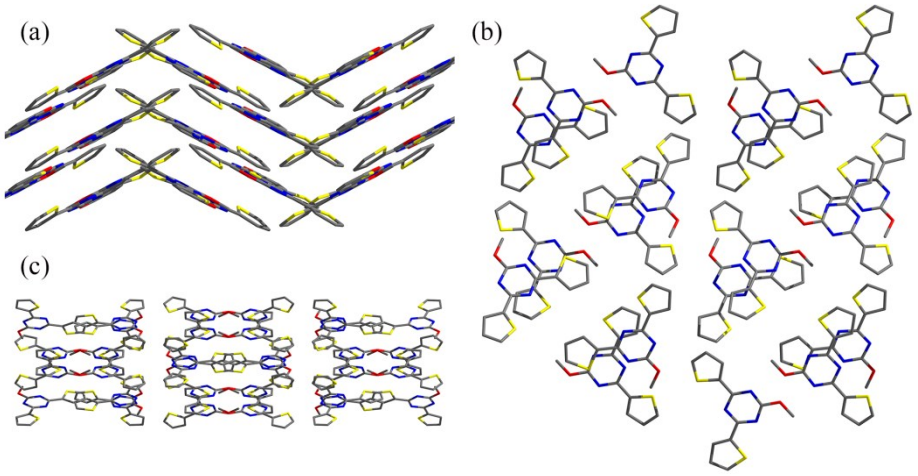


Figure S1. Cristal structure of **2a** (a/b/c) view along the **a/b/c** axis

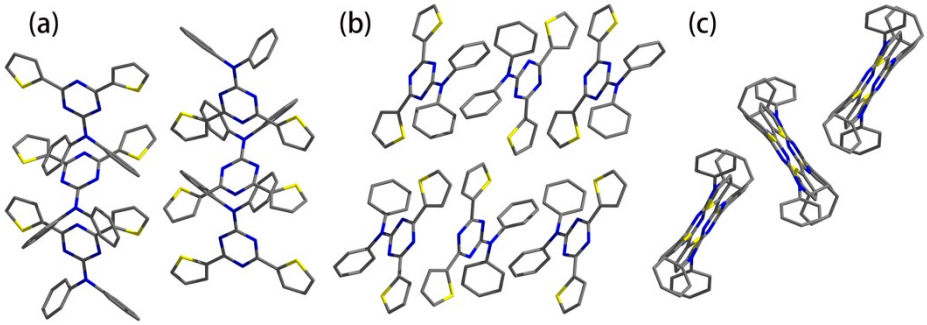


Figure.S2 Cristal structure of **2d** (a/b/c) view along the **a/b/c** axis

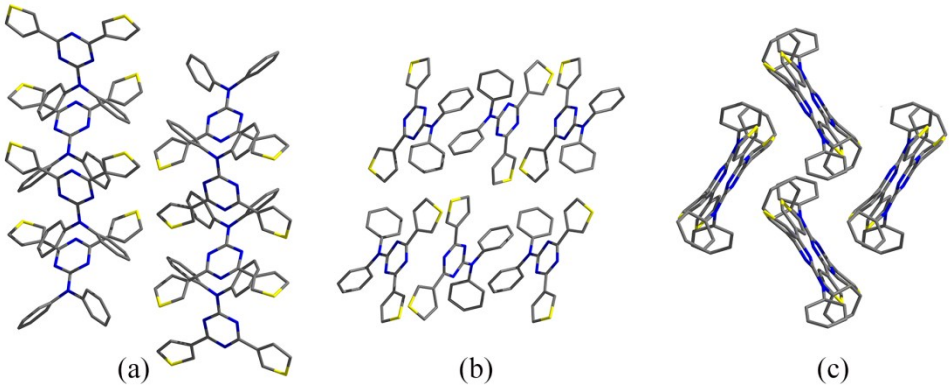


Figure.S3 Cristal structure of **3d** (a/b/c) view along the **a/b/c** axis

Table S1. Crystal data and structure refinement

Compound	**2a**	**2d**	**3d**
CCDC	1435751	1430748	1430747
Empirical formula	$(C_{12}H_9N_3OS_2)_2$	$C_{23}H_{16}N_4S_2$	$C_{23}H_{16}N_4S_2$
Formula weight	550.68	412.52	412.52
Temperature/K	293(2)	100(2) K	298(2)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	C2/c	$P2_1/c$	$P2_1/c$
a/Å	30.6659(15)	11.0590(6)	11.0027(13)
b/Å	7.7991(4)	9.0657(5)	9.2037(10)
c/Å	21.6105(11)	20.5704(11)	20.727(3)
α/°	90	90	90
β/°	97.152(2)	103.800(2)	104.570(4)
γ/°	90	90	90
Volume/Å^3	5128.3(4)	2002.81(19)	2031.4(4)
Z	8	4	4
ρ_{calc}g/cm^3	1.426	1.368	1.349
μ/mm^{-1}	0.405	0.283	0.279
F(000)	2272.0	856.0	856.0
Radiation	Mo-Kα (λ = 0.71073)	Mo-Kα (λ = 0.71073)	Mo-Kα (λ = 0.71073)
Θ range for data collection/°	2.696 to 26.430	2.36 to 27.56	2.03 to 27.51
Index ranges (h, k, lmax)	38, 9, 26	14, 11, 26	14, 11, 26
Reflections collected	71086	54220	71435
Data/restraints/parameters	5237 / 0 / 385	4622 / 10 / 300	4657 / 0 / 262
Goodness-of-fit on F^2	1.077	1.094	1.043
Final R indexes [I>=2σ (I)]	R1 = 0.0422 wR2 = 0.1024	R1 = 0.0311 wR2 = 0.0860	R1 = 0.0657 wR2 = 0.1986
Final R indexes [all data]	R1 = 0.0601 wR2 = 0.1126	R1 = 0.0357 wR2 = 0.0892	R1 = 0.0895 wR2 = 0.2125
Largest diff. peak/hole / e Å^{-3}	0.218 / -0.296	0.336 / -0.287	0.604 / -0.508

2. Copies of thermal properties chart of **TTC**s by **DSC.**

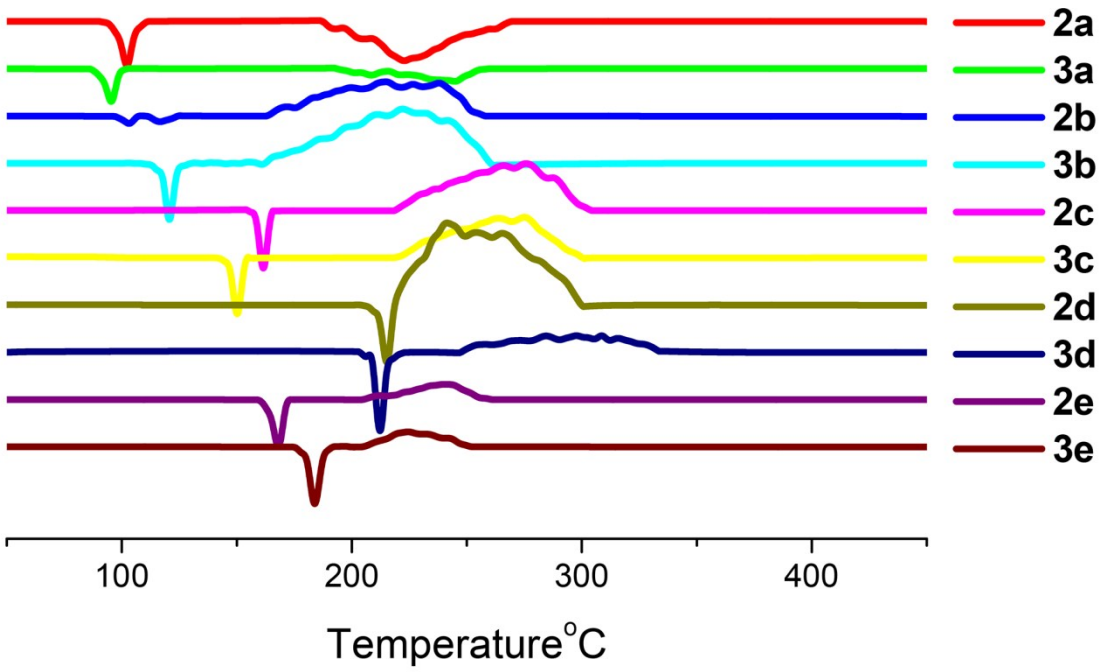
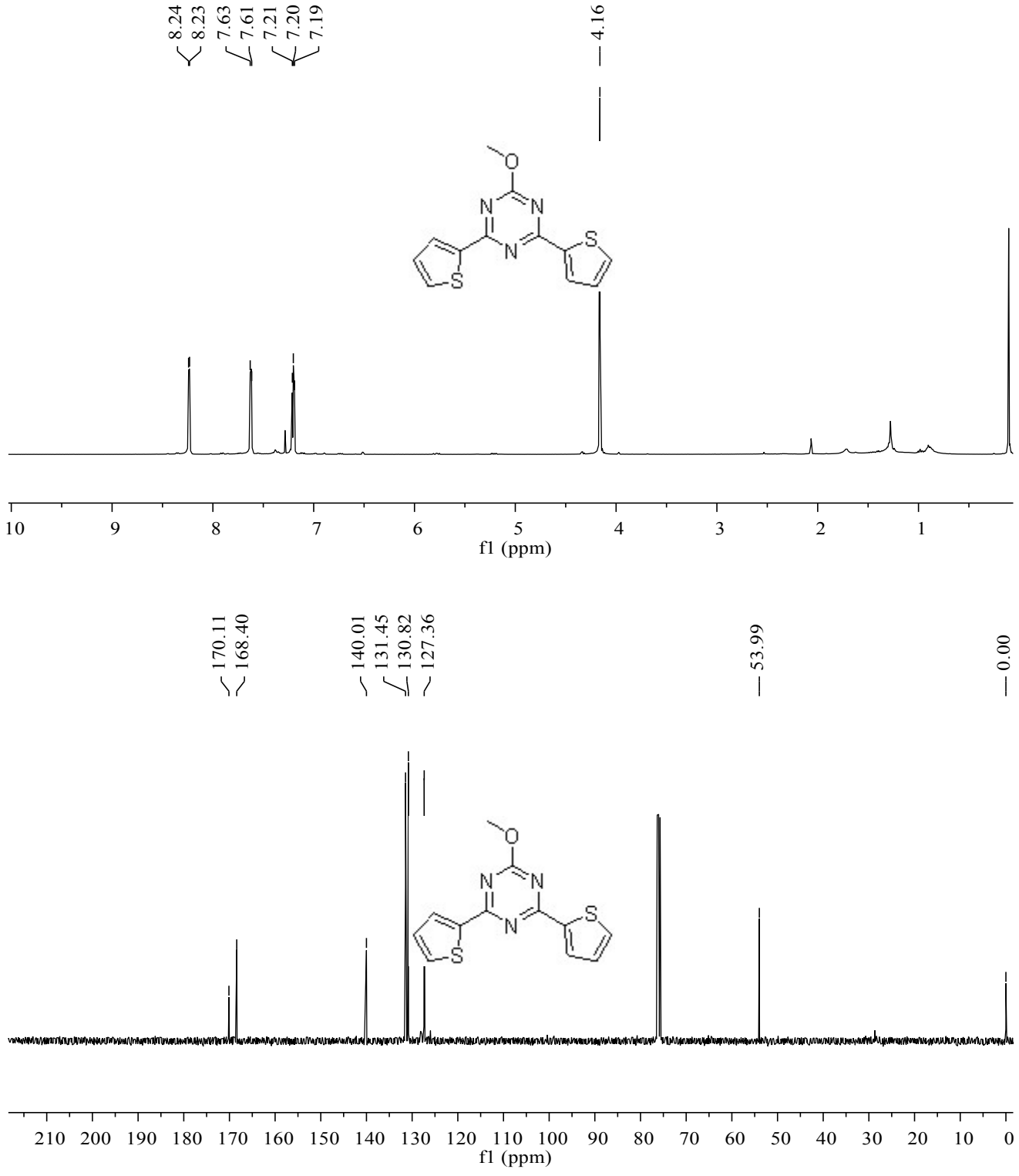
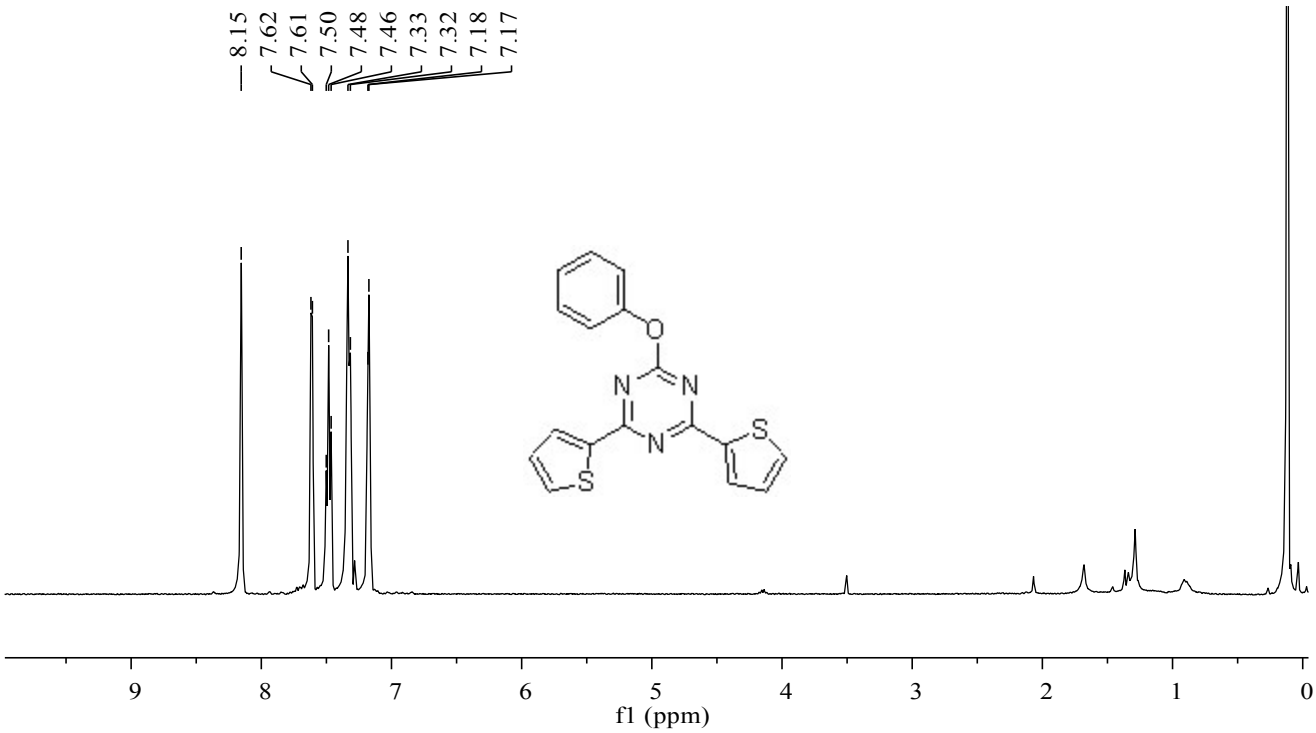


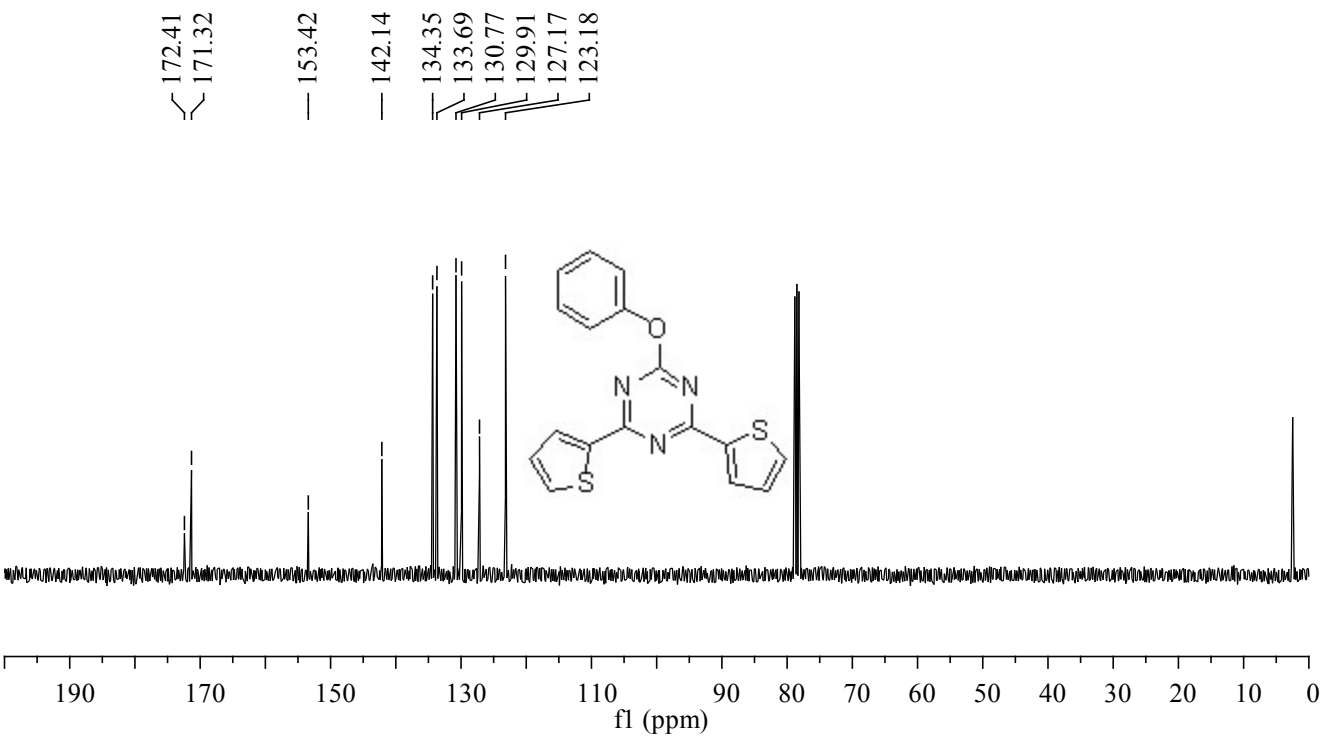
Fig.S4 thermal properties chart of **TTC**s by **DSC**

3. Copies of ^{1}H and $^{13}C\{^{1}H\}$ **NMR** Charts for **TTC**s.

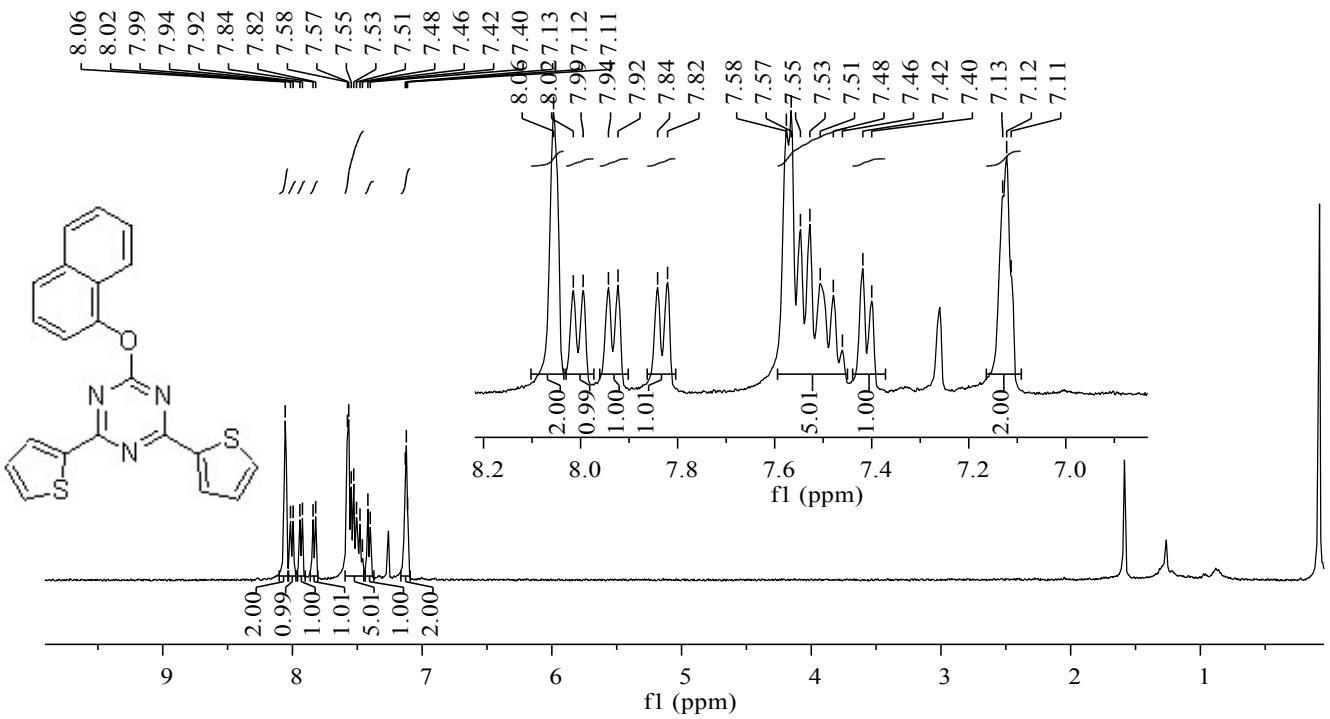


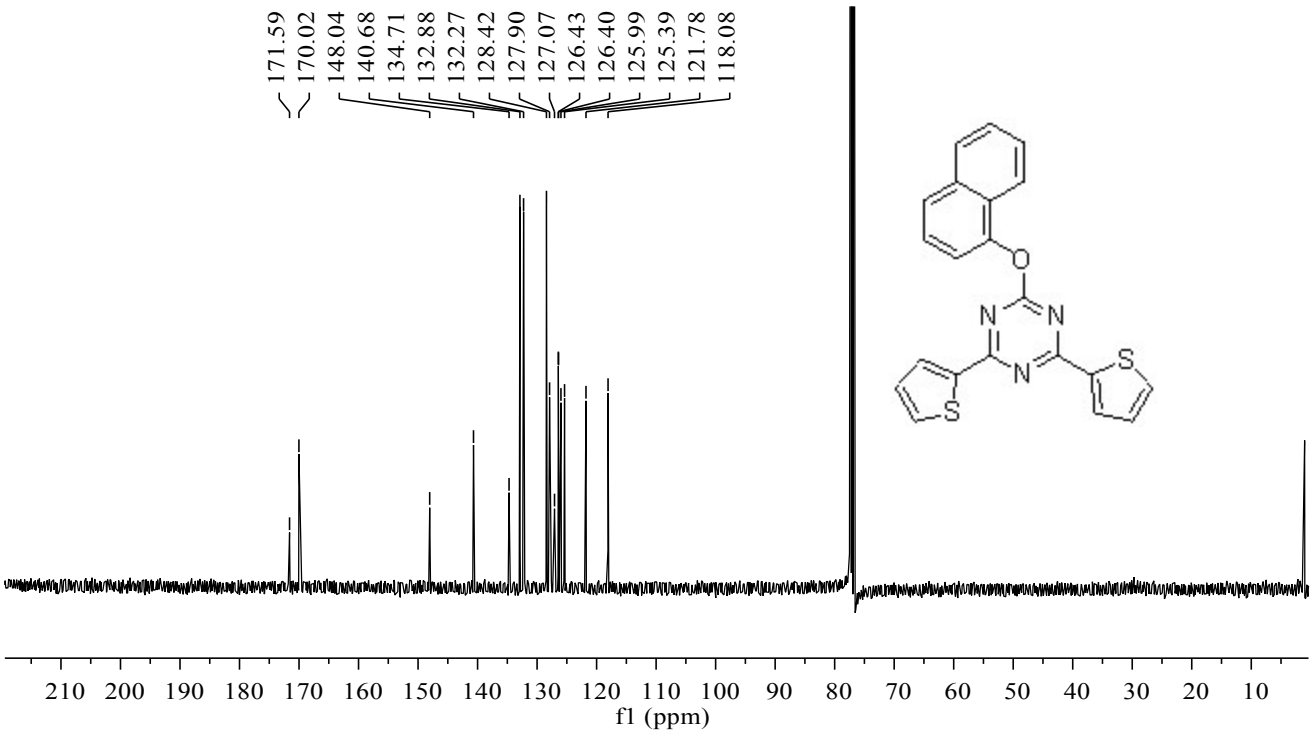
^{1}H **NMR** (400 MHz) and $^{13}C\{^{1}H\}$ **NMR** (101 MHz) spectra of **2a** ($CDCl_3$)



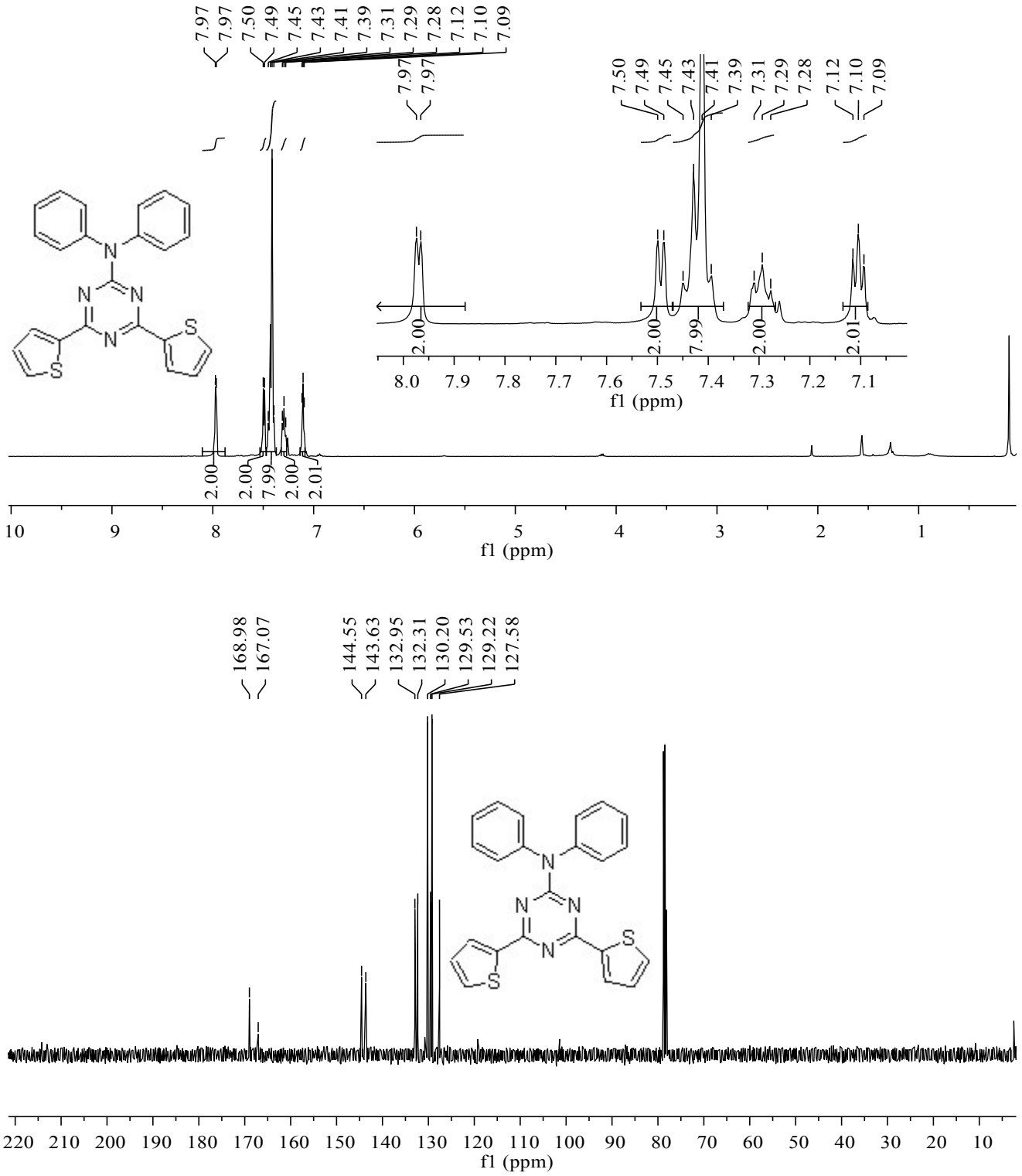


^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **2b** ($CDCl_3$)

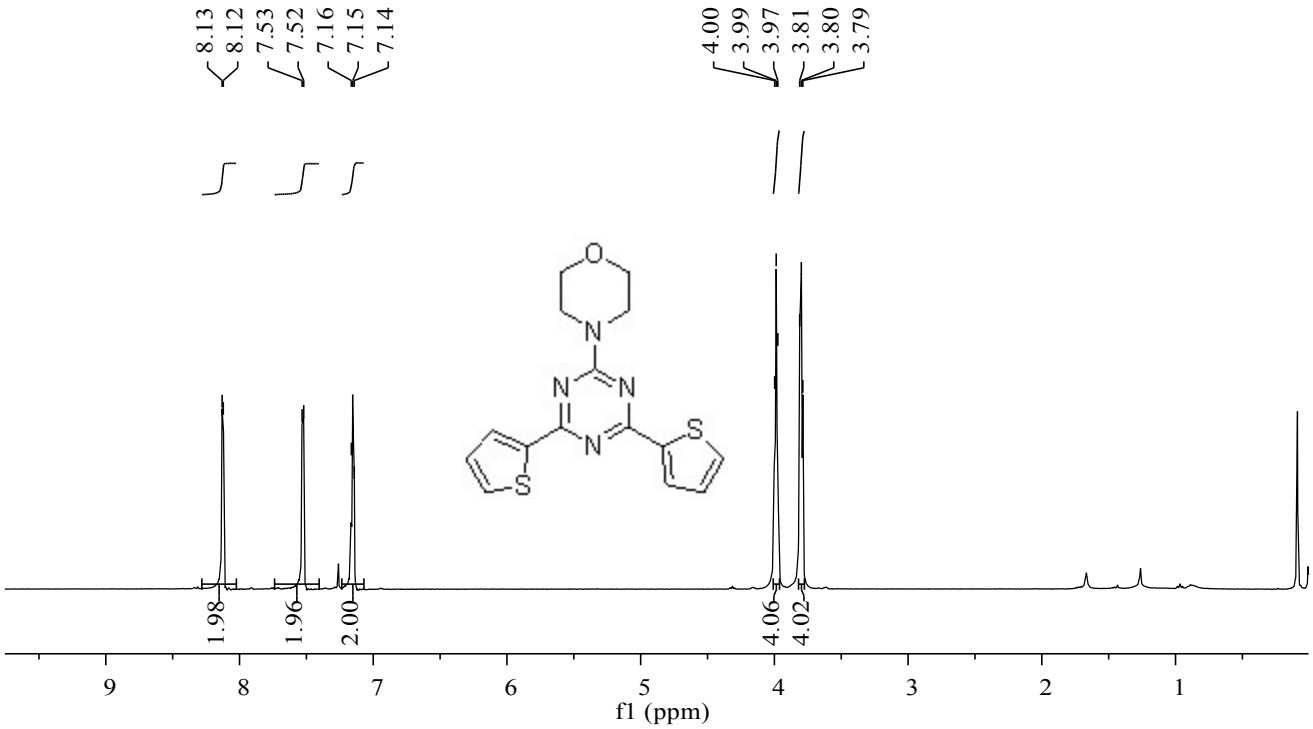


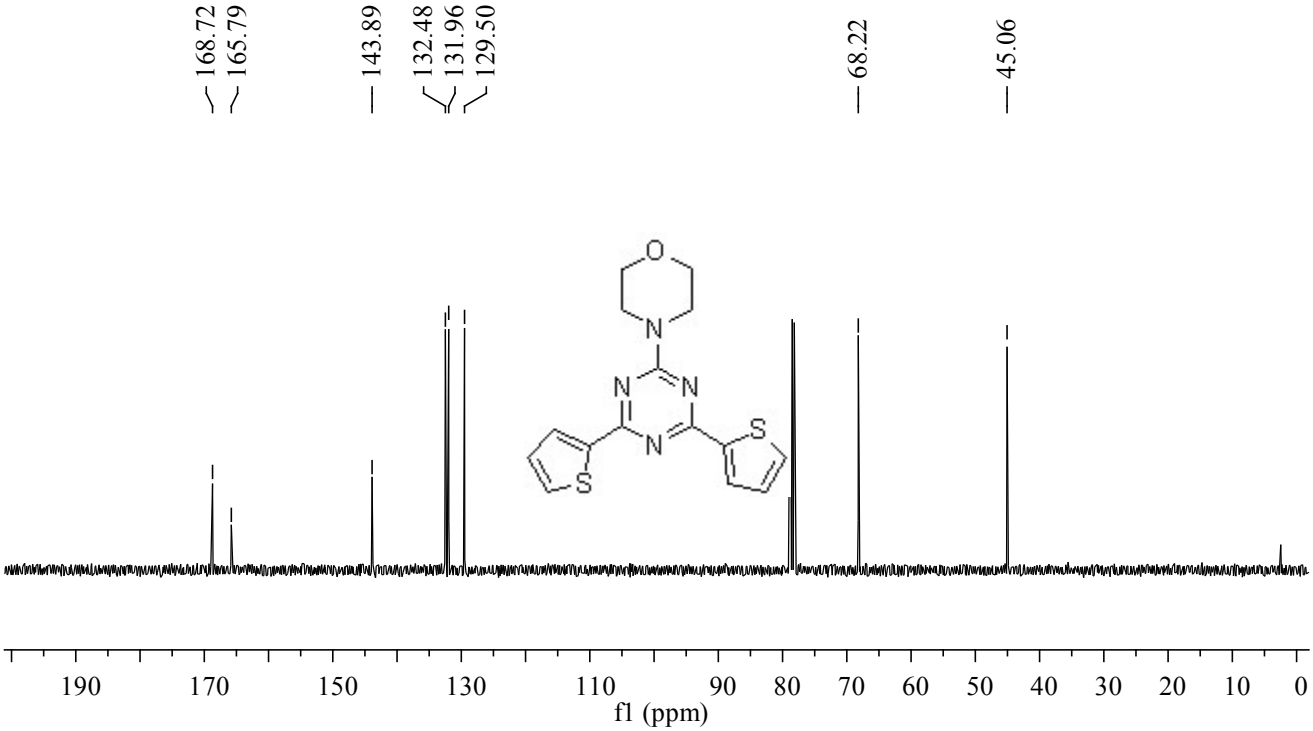


^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **2c** ($CDCl_3$)

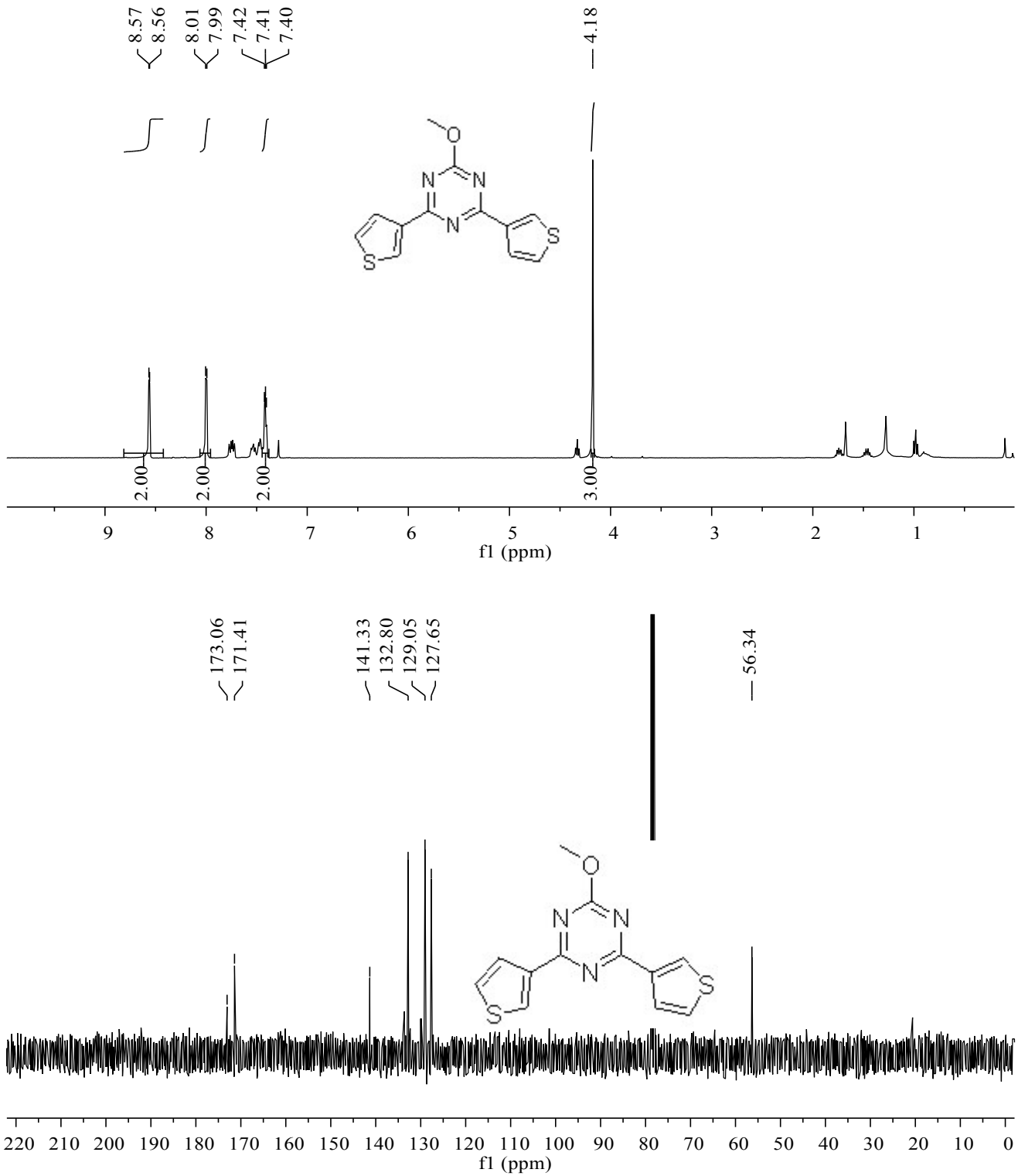


^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **2d** ($CDCl_3$)

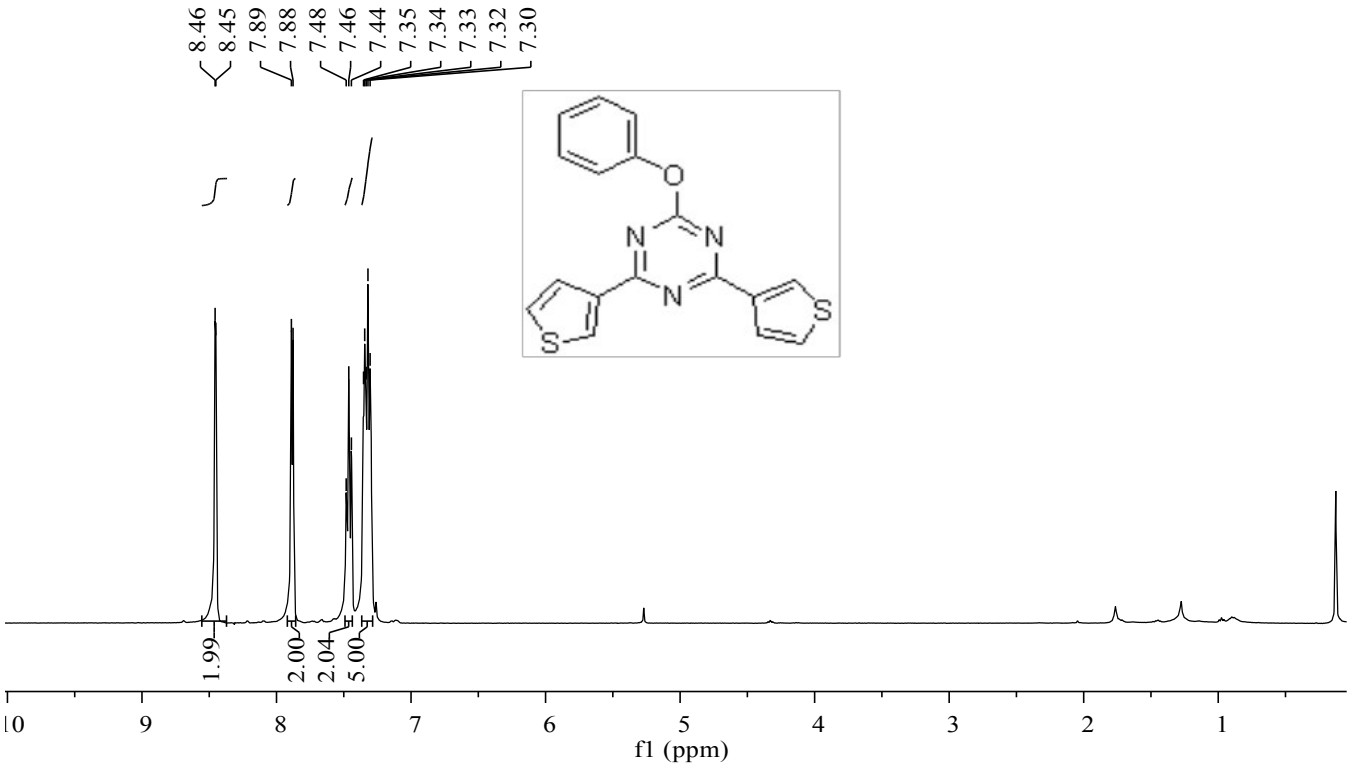


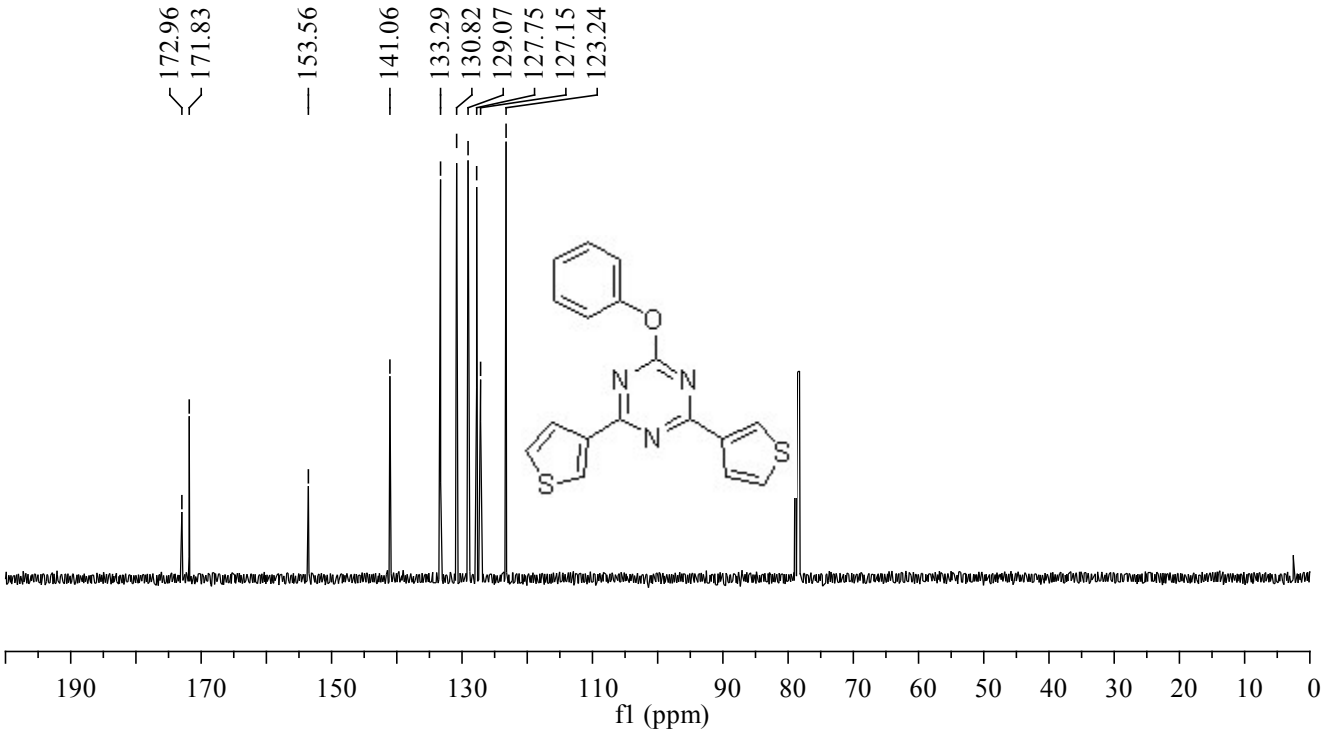


^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **2e** ($CDCl_3$)

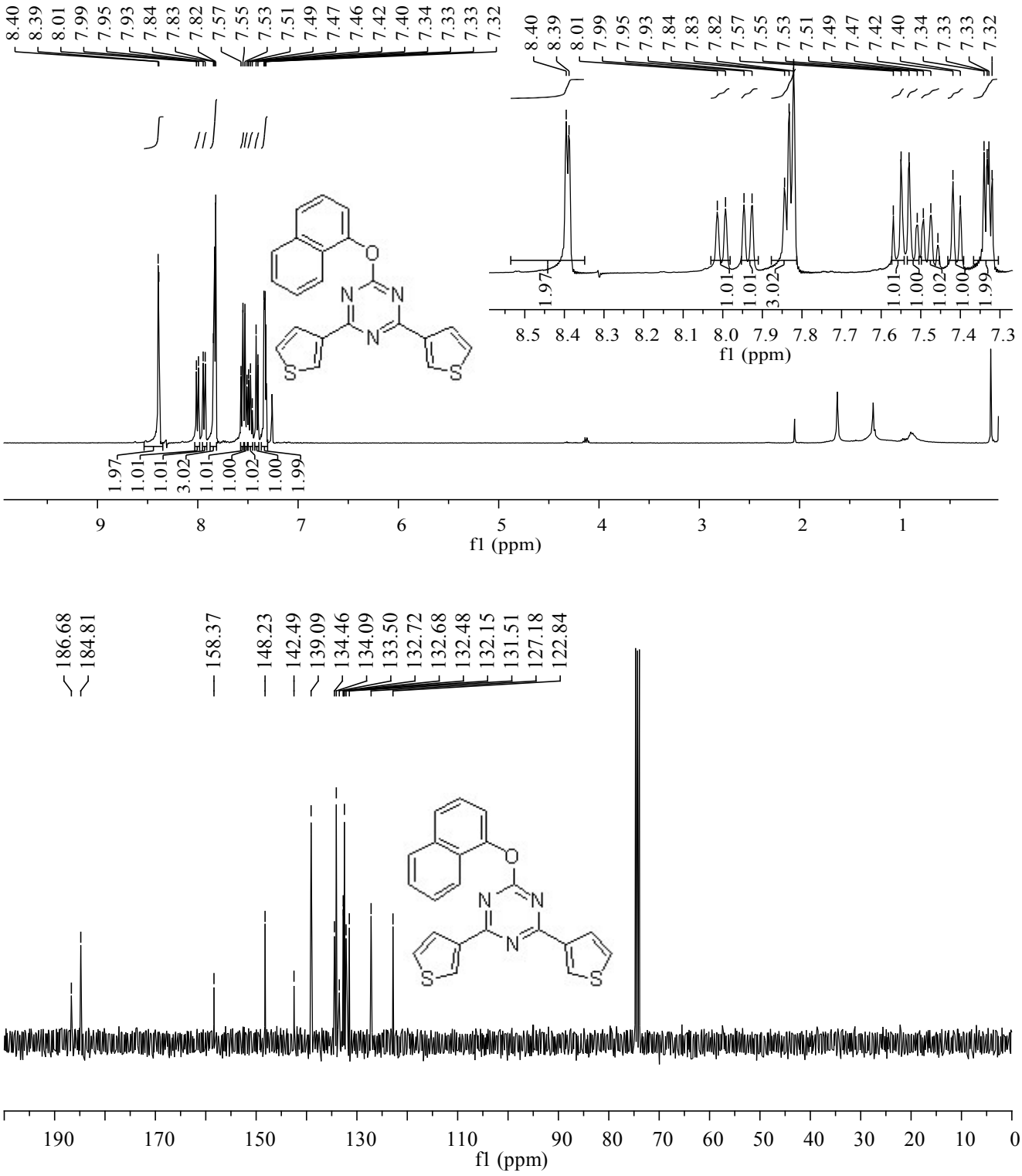


^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **3a** ($CDCl_3$)

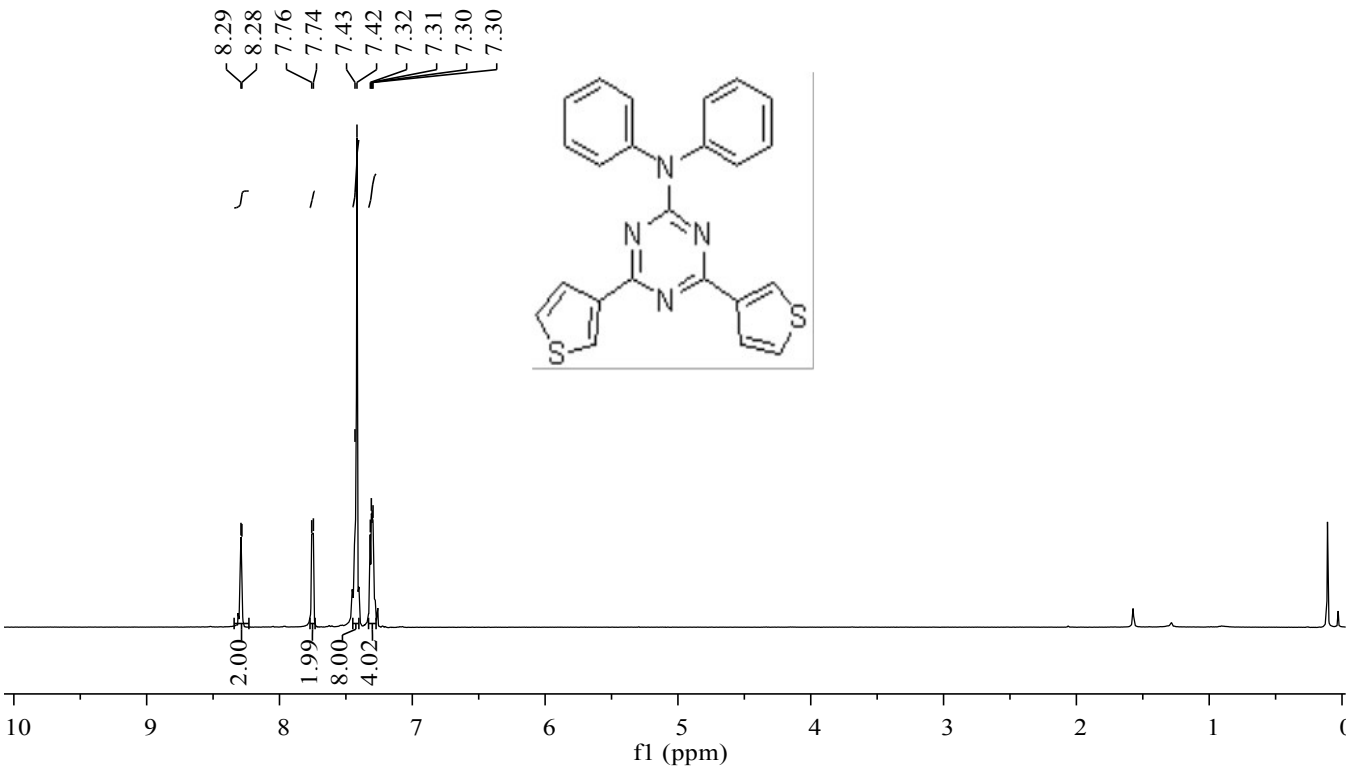


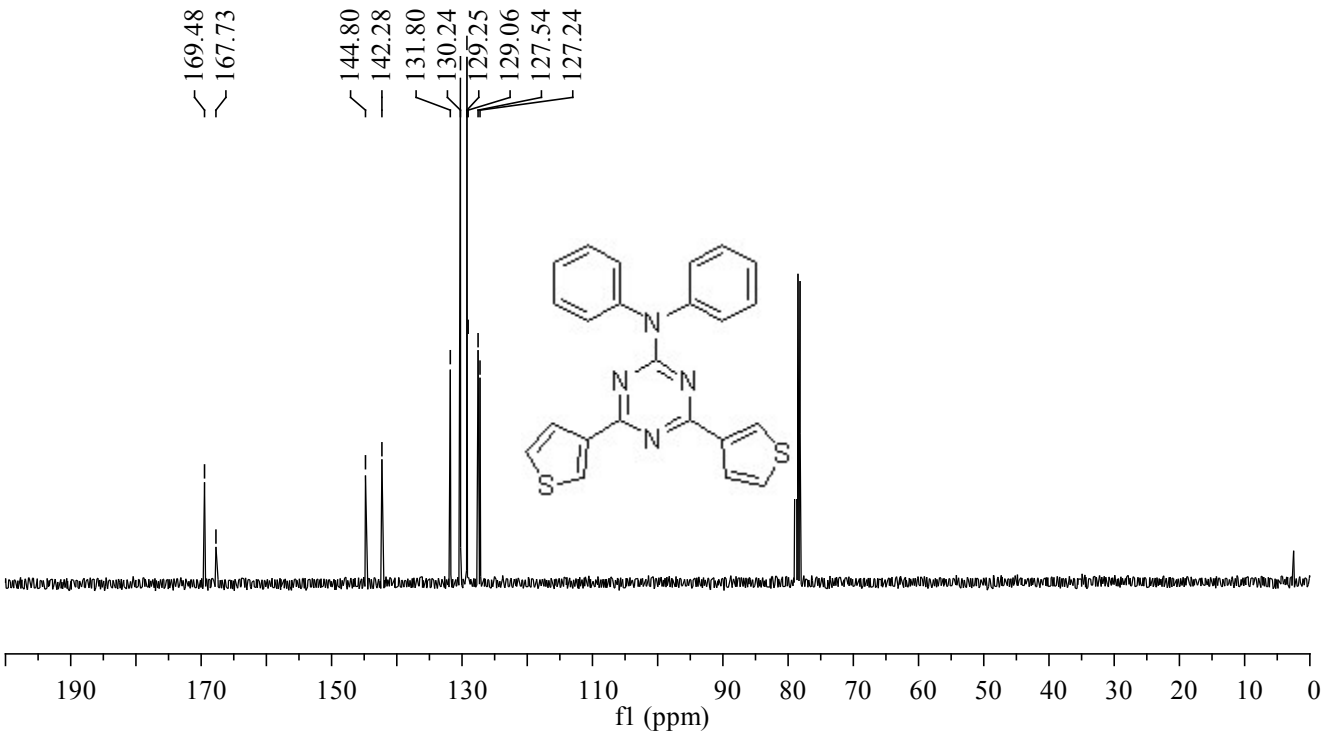


^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **3b** ($CDCl_3$)

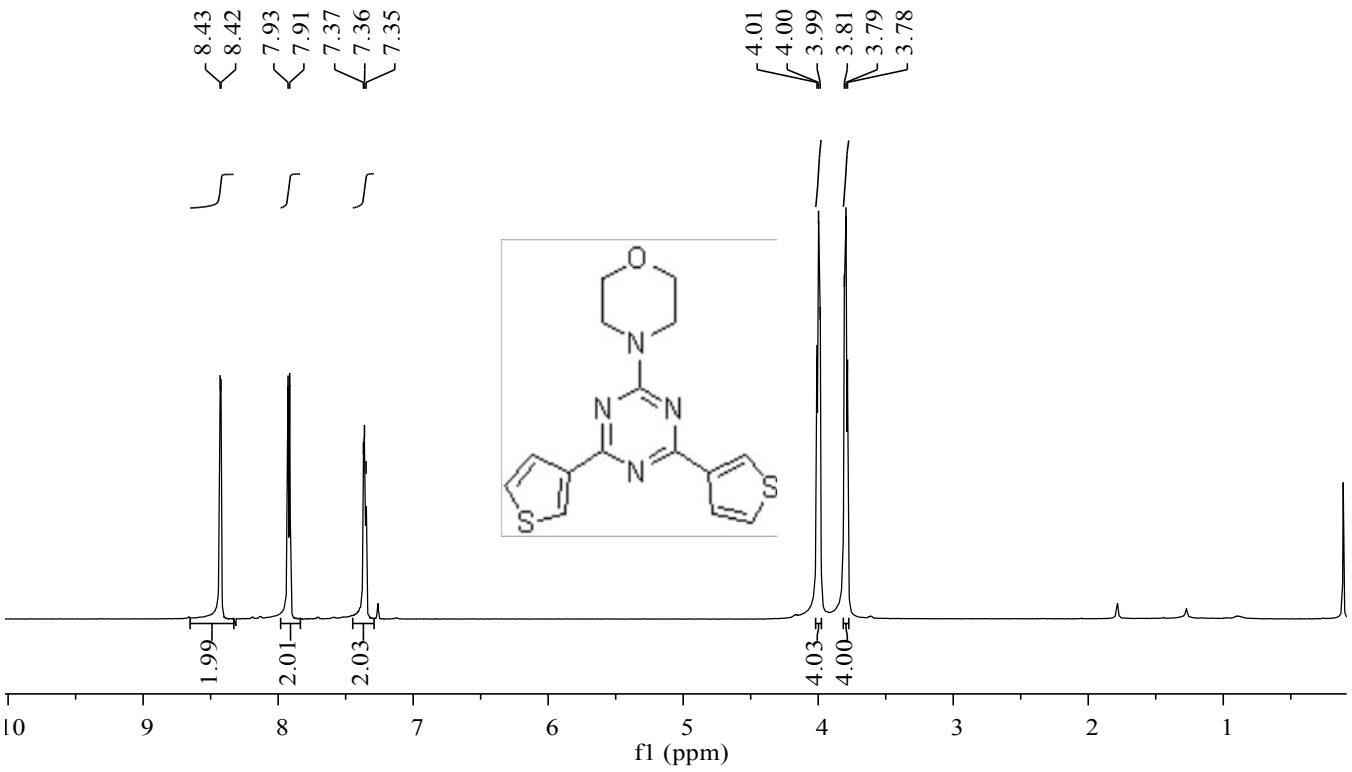


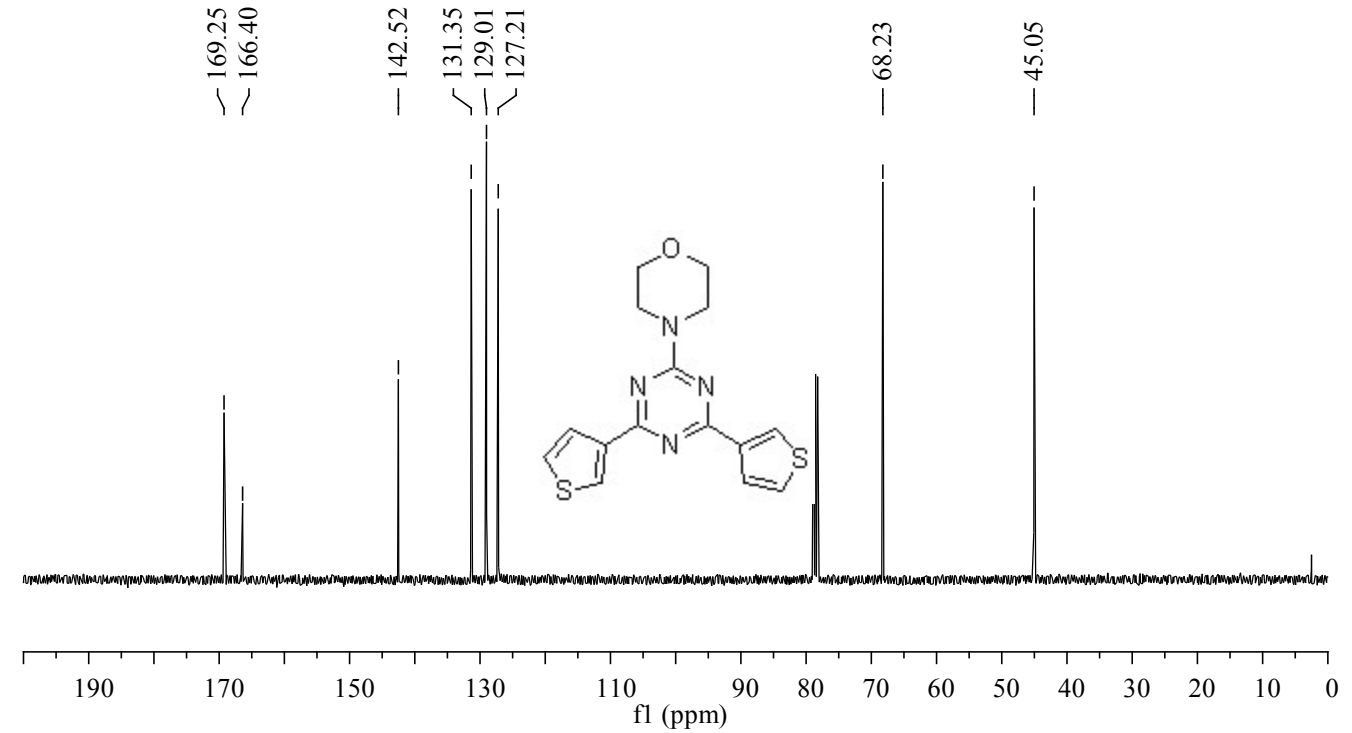
^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **3c** ($CDCl_3$)



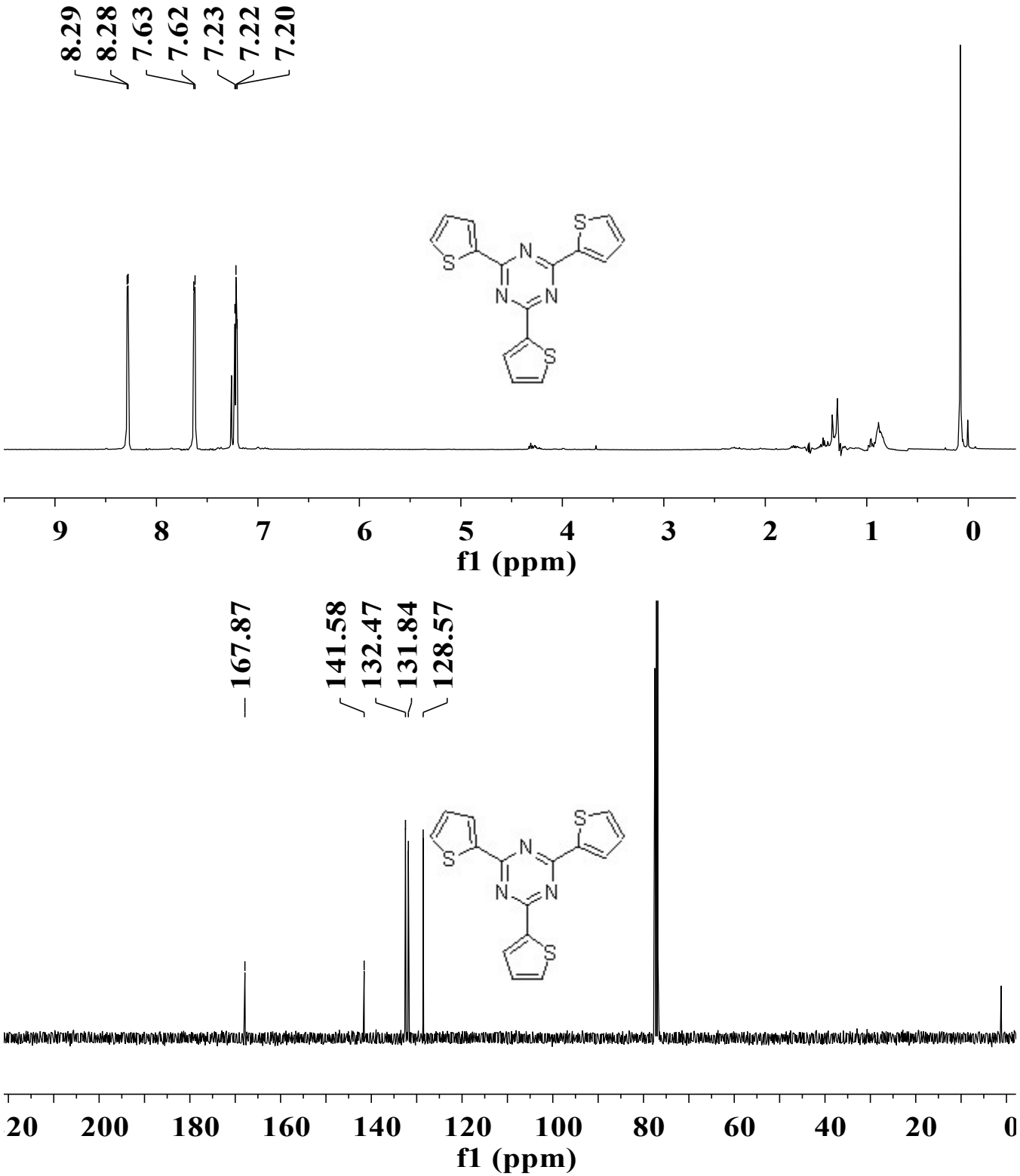


^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **3d** ($CDCl_3$)

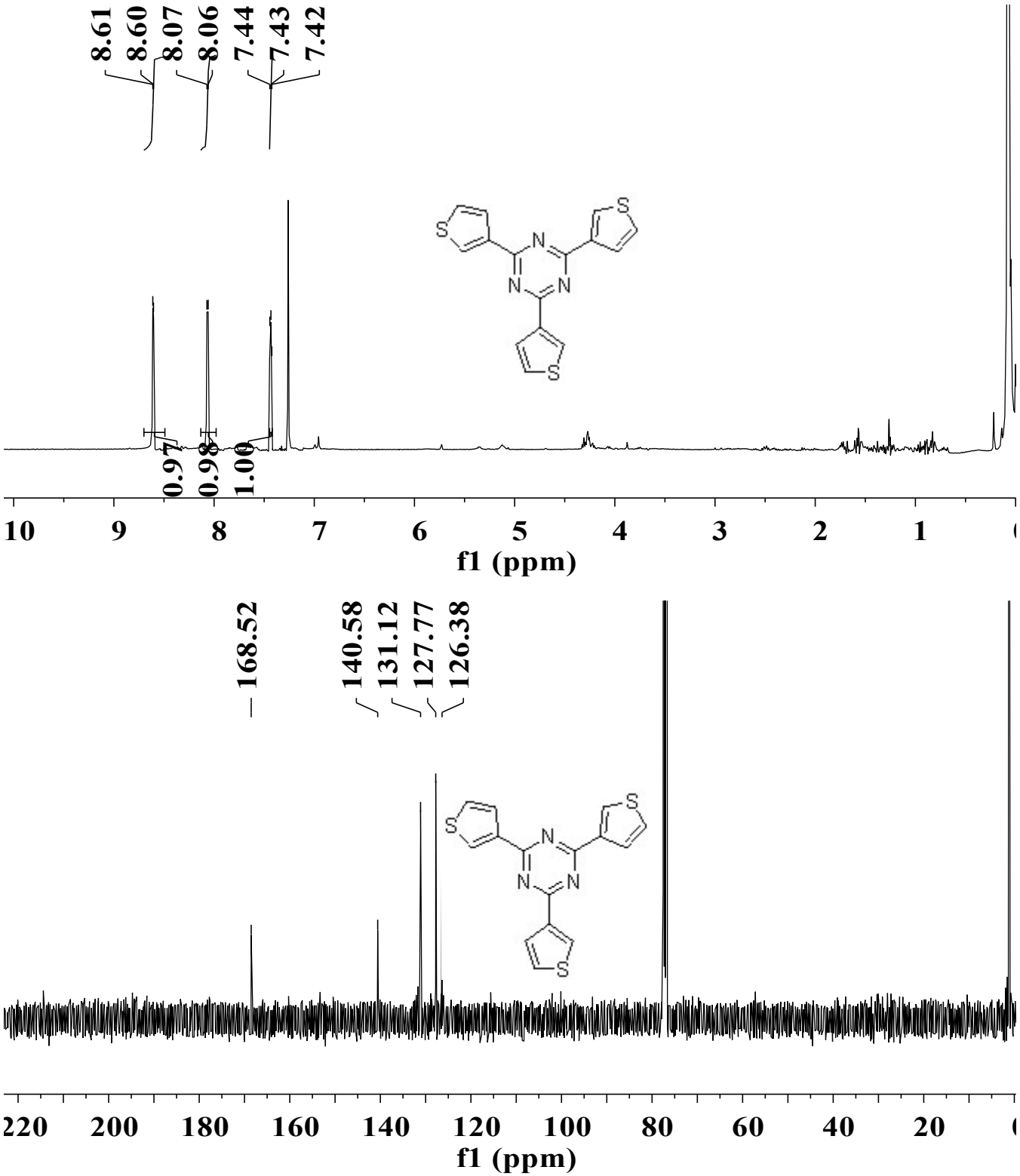




^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **3e** ($CDCl_3$)



^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **4a** ($CDCl_3$)



^{1}H **NMR** (400 MHz) and ^{13}C{^{1}H} **NMR** (101 MHz) spectra of **5a** ($CDCl_3$)

4. Table of energy of computed HOMO, LUMO, E_g , E_T and E (absolute energies).

Energy/eV	**2a**	**2b**	**2c**	**2d**	**2e**
HOMO	-6.68	-6.69	-5.94	-5.95	-6.32
LUMO	-2.46	-2.52	-2.54	-2.21	-2.45
E_g	4.21	4.17	3.40	3.73	4.07
E_T	2.39	2.35	2.35	2.30	2.33
E	-19652.16637	-24868.71814	-29048.9058	-30614.49003	-24334.18125
Energy/eV	**3a**	**3b**	**3c**	**3d**	**3e**
HOMO	-6.82	-6.81	-6.05	-6.01	-6.38
LUMO	-2.29	-2.27	-2.29	-2.03	-1.96
E_g	4.54	4.55	3.77	3.98	4.42
E_T	2.42	2.29	1.20	1.86	2.21
E	-19652.18356	-24868.72932	-29048.91563	-30614.50618	-24334.15388

5. Tables of atom coordinates of **TTC**s.

Table of atom coordinates of **2a**

Tag	Symbol	X	Y	Z
1	N	-1.231689	1.519223	-0.000093
2	C	-1.140193	0.160955	-0.000295
3	N	0.044652	-0.526115	-0.000612
4	C	1.173514	0.228611	-0.000371
5	N	1.175434	1.598844	-0.000184
6	C	-0.04745	2.177429	-0.000222
7	O	-0.141986	3.534257	-0.000477
8	C	2.458211	-0.453646	-0.000202
9	C	-2.371826	-0.60911	-0.000108
10	C	-2.506986	-1.987812	-0.000371
11	C	-3.872183	-2.42927	-0.000062
12	C	-4.777933	-1.385606	0.000486
13	S	-3.980234	0.215018	0.000626
14	C	3.72151	0.112251	0.000689
15	C	4.783965	-0.85302	0.001126
16	C	4.329801	-2.157598	0.000465
17	S	2.543643	-2.258785	-0.000656
18	C	1.101324	4.321823	0.000015
19	H	-1.645774	-2.645285	-0.00078
20	H	-4.165458	-3.473137	-0.00023
21	H	-5.857895	-1.437069	0.000816
22	H	3.866658	1.185918	0.001118
23	H	5.835422	-0.588178	0.001956
24	H	4.910702	-3.069419	0.000549
25	H	0.761412	5.358385	-0.001186
26	H	1.692708	4.101398	0.894103
27	H	1.694265	4.099908	-0.89273

Table of atom coordinates of **2b**

Tag	Symbol	X	Y	Z
1	N	0.828689	-1.659257	0.017499
2	C	1.802438	-0.701451	0.0053
3	N	1.555061	0.640744	-0.02739
4	C	0.243796	1.007555	-0.042197
5	N	-0.792046	0.115263	-0.027183
6	C	-0.436356	-1.186797	-0.002474
7	O	-1.394399	-2.164211	-0.017127
8	C	-0.073153	2.424745	-0.075309
9	C	3.185652	-1.145102	0.02851
10	C	-2.796841	-1.908537	0.028694
11	C	-3.569981	-2.657799	-0.869661
12	C	-4.971761	-2.547267	-0.820085
13	C	-5.582475	-1.699704	0.124501
14	C	-4.784865	-0.964316	1.023485
15	C	-3.382252	-1.065717	0.986543
16	H	-3.073532	-3.310852	-1.580642
17	H	-5.580506	-3.121824	-1.513505
18	H	-6.665485	-1.614982	0.162067
19	H	-5.251575	-0.311392	1.756651
20	H	-2.76611	-0.494099	1.6706
21	C	0.815455	3.487072	-0.086127
22	C	0.174206	4.770254	-0.118898
23	C	-1.204778	4.686369	-0.133196
24	S	-1.78834	2.995527	-0.108839
25	C	3.652335	-2.448195	0.062232
26	C	5.084069	-2.543656	0.079626
27	C	5.709853	-1.312087	0.058931
28	S	4.54545	0.045662	0.016223
29	H	1.887889	3.332989	-0.070917
30	H	0.714019	5.710471	-0.131772
31	H	-1.92468	5.492593	-0.158857
32	H	2.975557	-3.294396	0.073745
33	H	5.622144	-3.484578	0.106357
34	H	6.769734	-1.098715	0.065412

Table of atom coordinates of **2c**

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	0.937669	-1.508243	0.362039	21	C	1.315063	5.079404	-0.569595
2	C	2.181884	-0.989773	0.143259	22	S	0.172997	3.740798	-0.248855
3	N	2.432302	0.336546	-0.061519	23	C	3.270442	-3.283507	0.308389
4	C	1.349735	1.161856	-0.031817	24	C	4.563169	-3.902714	0.240162
5	N	0.072595	0.727695	0.193279	25	C	5.584446	-3.001367	0.009588
6	C	-0.064556	-0.602051	0.374879	26	S	4.99136	-1.319845	-0.137376
7	O	-1.300509	-1.152212	0.57891	27	H	3.701736	2.691914	-0.521961
8	C	1.560467	2.582131	-0.251309	28	H	3.458279	5.311226	-0.857556
9	C	3.304899	-1.9112	0.128585	29	H	0.933898	6.086493	-0.667311
10	C	-2.517203	-0.420574	0.681453	30	H	2.340021	-3.810594	0.482571
11	C	-3.623875	-1.01339	-0.004232	31	H	4.724944	-4.968282	0.357956
12	C	-4.913838	-0.38649	0.135601	32	H	6.642832	-3.198674	-0.086983
13	C	-5.041009	0.784958	0.946131	33	C	-6.033785	-0.96151	-0.544352
14	C	-3.936103	1.315584	1.596717	34	C	-5.884642	-2.100474	-1.323936
15	C	-2.652587	0.707587	1.472252	35	C	-4.603984	-2.718537	-1.455819
16	H	-6.017367	1.253769	1.046855	36	C	-3.495149	-2.188053	-0.808479
17	H	-4.036056	2.204703	2.213509	37	H	-7.008647	-0.489276	-0.439412
18	H	-1.795454	1.136301	1.975918	38	H	-6.742289	-2.529155	-1.836829
19	C	2.762155	3.229892	-0.484385	39	H	-4.500936	-3.611806	-2.06685
20	C	2.623809	4.64664	-0.665169	40	H	-2.520581	-2.65663	-0.895618

Table of atom coordinates of **2d**

Tag	Symbol	X	Y	Z
1	N	0.020804	1.156333	-0.067937
2	C	-1.31572	1.395583	-0.069491
3	N	-2.272745	0.422394	-0.001702
4	C	-1.801996	-0.855297	0.069313
5	N	-0.484359	-1.192222	0.071904
6	C	0.398254	-0.154642	0.00239
7	N	1.752994	-0.447166	0.003372
8	C	-2.773853	-1.937625	0.152259
9	C	-1.763283	2.778763	-0.150884
10	C	2.225769	-1.81421	-0.105567
11	C	2.753402	0.597533	0.118358
12	C	3.799015	0.650997	-0.824223
13	C	4.804351	1.626842	-0.702966
14	C	4.768387	2.555049	0.355081
15	C	3.719887	2.497735	1.294395
16	C	2.71732	1.519607	1.182729
17	C	3.133879	-2.30391	0.853388
18	C	3.639285	-3.611482	0.739365
19	C	3.238356	-4.436778	-0.328558
20	C	2.329797	-3.942209	-1.285591
21	C	1.82743	-2.633982	-1.18012
22	C	-3.066482	3.24482	-0.161576
23	C	-3.164289	4.674559	-0.251173
24	C	-1.93365	5.298989	-0.30884
25	S	-0.573861	4.136034	-0.256219
26	C	-2.52254	-3.295047	0.245796
27	C	-3.71251	-4.096192	0.314529
28	C	-4.872845	-3.348188	0.273649
29	S	-4.547936	-1.592285	0.147274
30	H	3.82232	-0.064049	-1.641679
31	H	5.607528	1.664037	-1.434879
32	H	5.544059	3.311412	0.446215
33	H	3.684067	3.210367	2.114702
34	H	1.907235	1.48086	1.903507
35	H	3.440182	-1.665582	1.677296
36	H	4.338782	-3.983487	1.484009
37	H	3.627973	-5.448082	-0.415239
38	H	2.018298	-4.570885	-2.116326
39	H	1.125525	-2.254643	-1.915804
40	H	-3.912233	2.569841	-0.106357
41	H	-4.106449	5.211058	-0.272021
42	H	-1.721565	6.356761	-0.380562
43	H	-1.511873	-3.685476	0.266458
44	H	-3.703504	-5.177816	0.391902
45	H	-5.896219	-3.695153	0.308878

Table of atom coordinates of **2e**

Tag	Symbol	X	Y	Z
1	N	1.206305	0.433073	-0.204755
2	C	1.152978	-0.915189	-0.062168
3	N	-0.00065	-1.643405	0.01429
4	C	-1.153752	-0.914337	-0.062083
5	N	-1.206083	0.43398	-0.204565
6	C	0.000351	1.081818	-0.274405
7	N	0.000824	2.438512	-0.420699
8	C	-2.416096	-1.639966	0.015038
9	C	2.414795	-1.641717	0.015
10	C	2.600986	-3.004472	0.161675
11	C	3.98244	-3.396676	0.201262
12	C	4.852264	-2.330945	0.084367
13	S	3.994645	-0.767925	-0.083041
14	C	-2.603254	-3.002587	0.161686
15	C	-3.984991	-3.393835	0.201142
16	C	-4.854074	-2.32751	0.084177
17	S	-3.995349	-0.765082	-0.083117
18	C	-1.242837	3.230338	-0.506927
19	C	-1.208267	4.352087	0.546733
20	O	0.00228	5.166111	0.409744
21	C	1.212135	4.350941	0.545952
22	C	1.245017	3.229427	-0.507852
23	H	1.76344	-3.68733	0.236946
24	H	4.311225	-4.42414	0.311514
25	H	5.933305	-2.343586	0.083298
26	H	-1.766193	-3.68603	0.236991
27	H	-4.314491	-4.421073	0.311349
28	H	-5.935129	-2.339399	0.083003
29	H	-2.0954	2.566763	-0.352388
30	H	-1.312412	3.674696	-1.510745
31	H	-1.252214	3.919334	1.559426
32	H	-2.045159	5.042738	0.409071
33	H	2.049614	5.040747	0.407925
34	H	1.256238	3.917938	1.55844
35	H	1.314049	3.673945	-1.511551
36	H	2.097201	2.565257	-0.354158

Table of atom coordinates of **3a**

Tag	Symbol	X	Y	Z
1	N	1.151969	1.7543	-0.0001
2	C	1.237426	0.396857	-0.000014
3	N	0.150551	-0.436912	0.000129
4	C	-1.06808	0.161551	0.000054
5	N	-1.24382	1.519637	-0.000028
6	C	-0.10885	2.252774	-0.000008
7	O	-0.190278	3.610928	0.000188
8	C	-2.262005	-0.69277	0.000014
9	C	2.577354	-0.20005	-0.000045
10	C	3.797171	0.583851	-0.000723
11	C	4.934655	-0.18056	-0.000645
12	S	4.54937	-1.945414	0.00032
13	C	2.807926	-1.563834	0.000554
14	C	-3.554169	-0.19986	-0.000133
15	S	-4.767836	-1.506137	-0.000205
16	C	-3.444337	-2.733569	-0.000049
17	C	-2.208079	-2.141589	0.000073
18	C	-1.524988	4.231424	0.000341
19	H	3.781757	1.666707	-0.001238
20	H	5.968346	0.132895	-0.001123
21	H	2.070834	-2.352383	0.001156
22	H	-3.860501	0.835228	-0.000227
23	H	-3.69878	-3.783344	0.000025
24	H	-1.269633	-2.68132	0.000213
25	H	-1.322244	5.303284	0.001228
26	H	-2.083483	3.936563	-0.893436
27	H	-2.083655	3.93523	0.893541

Table of atom coordinates of **3b**

Tag	Symbol	X	Y	Z
1	N	0.782	-1.647345	-0.010555
2	C	1.705632	-0.64311	-0.007975
3	N	1.384243	0.684255	-0.027737
4	C	0.058225	0.98467	-0.046179
5	N	-0.929899	0.03853	-0.045474
6	C	-0.506148	-1.241108	-0.03155
7	O	-1.416759	-2.265371	-0.059913
8	C	-0.353413	2.392431	-0.069369
9	C	3.120816	-1.026405	0.01826
10	C	3.57059	-2.404701	0.042239
11	C	4.935021	-2.530877	0.065591
12	S	5.751583	-0.919821	0.058867
13	C	4.161554	-0.115154	0.023668
14	C	0.538742	3.449422	-0.057918
15	S	-0.293547	5.025062	-0.0924
16	C	-1.889241	4.180427	-0.123362
17	C	-1.739115	2.81808	-0.107128
18	C	-2.825117	-2.050157	0.010631
19	C	-3.593829	-2.667494	-0.985115
20	C	-4.997108	-2.5832	-0.911662
21	C	-5.611386	-1.892739	0.150881
22	C	-4.817062	-1.28844	1.14622
23	C	-3.414047	-1.366268	1.085416
24	H	2.874917	-3.234619	0.041183
25	H	5.537869	-3.426915	0.086302
26	H	4.089697	0.96179	0.009042
27	H	1.616571	3.395848	-0.03188
28	H	-2.795634	4.767173	-0.153617
29	H	-2.558256	2.109939	-0.125198
30	H	-3.095647	-3.201263	-1.788509
31	H	-5.604101	-3.057129	-1.678742
32	H	-6.695098	-1.830297	0.206657
33	H	-5.287197	-0.761655	1.97282
34	H	-2.79672	-0.904096	1.84826

Table of atom coordinates of **3c**

Tag	Symbol	X	Y	Z
1	N	0.886818	-1.503215	0.377536
2	C	2.103839	-0.930498	0.149681
3	N	2.288338	0.409277	-0.041253
4	C	1.173496	1.186	0.008349
5	N	-0.081168	0.691483	0.239655
6	C	-0.154671	-0.643037	0.410384
7	O	-1.366197	-1.247372	0.624089
8	C	-2.594085	-0.539213	0.761028
9	C	-3.675813	-1.0373	-0.029284
10	C	-4.967573	-0.420238	0.138567
11	C	-5.119738	0.645934	1.079578
12	C	-4.03795	1.084061	1.831804
13	C	-2.754347	0.483947	1.678824
14	H	-6.097398	1.106648	1.201501
15	H	-4.159227	1.889588	2.55107
16	H	-1.913848	0.832836	2.267553
17	C	-6.064248	-0.899786	-0.645427
18	C	-5.891581	-1.939672	-1.548776
19	C	-4.60987	-2.549982	-1.706504
20	C	-3.523074	-2.110155	-0.962104
21	H	-7.040003	-0.434944	-0.520113
22	H	-6.731699	-2.29687	-2.139238
23	H	-4.489552	-3.366691	-2.413847
24	H	-2.548731	-2.575657	-1.068273
25	C	1.303455	2.632968	-0.194137
26	C	2.513498	3.267933	-0.408806
27	S	2.316314	5.026907	-0.615721
28	C	0.532261	4.851478	-0.399302
29	C	0.175706	3.544595	-0.19017
30	H	3.491494	2.813569	-0.45669
31	H	-0.093624	5.730414	-0.449202
32	H	-0.840792	3.202225	-0.041023
33	C	3.271825	-1.816127	0.109204
34	C	3.189635	-3.250676	0.304052
35	C	4.404324	-3.880338	0.225334
36	S	5.740076	-2.70922	-0.100407
37	C	4.562121	-1.371779	-0.117236
38	H	2.247666	-3.750607	0.492409
39	H	4.637635	-4.929796	0.3299
40	H	4.884251	-0.356221	-0.290638

Table of atom coordinates of **3d**

Tag	Symbol	X	Y	Z
1	S	4.106878	4.262655	-0.181894
2	S	4.178197	-4.203255	0.186684
3	N	-1.889739	-0.018614	-0.00174
4	N	0.131404	1.196776	-0.066046
5	N	2.225586	0.014096	0.002232
6	N	0.151496	-1.205052	0.065198
7	C	-2.453604	2.112185	1.153974
8	H	-1.69838	1.900913	1.904056
9	C	-3.227649	3.282551	1.234802
10	H	-3.07292	3.972186	2.061385
11	C	-4.204757	3.559867	0.258116
12	H	-4.804343	4.463791	0.325665
13	C	-4.400166	2.657869	-0.80532
14	H	-5.150002	2.863553	-1.565123
15	C	-3.622738	1.489089	-0.894242
16	H	-3.76885	0.792039	-1.714732
17	C	-2.647662	1.216071	0.084789
18	C	-3.661077	-1.498875	0.856769
19	H	-3.843467	-0.777649	1.648262
20	C	-4.436305	-2.668696	0.768981
21	H	-5.21974	-2.849668	1.500486
22	C	-4.196478	-3.603586	-0.256188
23	H	-4.794919	-4.508719	-0.322849
24	C	-3.176437	-3.356434	-1.196325
25	H	-2.98707	-4.070672	-1.99401
26	C	-2.403527	-2.185295	-1.117792
27	H	-1.616504	-1.998384	-1.840382
28	C	-2.642369	-1.255667	-0.085746
29	C	-0.503207	-0.009656	-0.001119
30	C	1.508735	-1.145365	0.062027
31	C	1.489109	1.160641	-0.060093
32	C	2.239866	-2.419362	0.125468
33	C	1.586168	-3.710795	0.213688
34	H	0.507736	-3.805743	0.246608
35	C	2.462929	-4.76376	0.256004
36	H	2.257107	-5.82204	0.32443
37	C	3.619045	-2.510804	0.102349
38	H	4.327418	-1.698848	0.039818
39	C	2.198961	2.446598	-0.125054
40	C	1.523976	3.726136	-0.225164
41	H	0.444354	3.802556	-0.265345
42	C	2.38303	4.793851	-0.267418
43	H	2.159139	5.847868	-0.343253
44	C	3.575899	2.561179	-0.092352
45	H	4.297542	1.761518	-0.020092

Table of atom coordinates of **3e**

Tag	Symbol	X	Y	Z
1	N	0.700392	-1.20992	-0.228434
2	C	-0.649442	-1.154765	-0.099049
3	N	-1.368496	0.003044	-0.029711
4	C	-0.644049	1.157464	-0.09904
5	N	0.706023	1.206285	-0.228436
6	C	1.349586	-0.00332	-0.289987
7	N	2.710247	-0.006387	-0.419088
8	C	-1.371075	2.43497	-0.028917
9	C	-1.382573	-2.428762	-0.02894
10	C	-0.747046	-3.729715	-0.101075
11	C	-1.629169	-4.775757	-0.01392
12	S	-3.328882	-4.19597	0.165967
13	C	-2.755274	-2.507011	0.113401
14	C	-2.743474	2.519759	0.112729
15	S	-3.308989	4.211444	0.165449
16	C	-1.606425	4.783109	-0.013293
17	C	-0.729281	3.732863	-0.100295
18	C	3.50603	1.234367	-0.500579
19	C	4.620607	1.199382	0.560722
20	O	5.433686	-0.01212	0.429595
21	C	4.615398	-1.220082	0.561035
22	C	3.500659	-1.250563	-0.500263
23	H	0.323791	-3.841549	-0.214301
24	H	-1.433842	-5.837873	-0.039709
25	H	-3.451377	-1.68568	0.18925
26	H	-3.443532	1.70174	0.187979
27	H	-1.405932	5.844272	-0.038666
28	H	0.342125	3.839707	-0.212986
29	H	2.842797	2.087723	-0.350568
30	H	3.957662	1.303499	-1.501323
31	H	4.180988	1.24414	1.570396
32	H	5.313551	2.035114	0.427427
33	H	5.304738	-2.058813	0.427912
34	H	4.175622	-1.262703	1.570733
35	H	3.952033	-1.321902	-1.500972
36	H	2.833824	-2.101083	-0.350074