Supporting Information

Synthesis Of Novel Derivatives Of Thiophene-Carbazole, Their Electronic Properties And Computational Studies

Damit E. F.,[1] Nordin N.,[1] Ariffin A.*[,1] and Sulaiman K.[2]

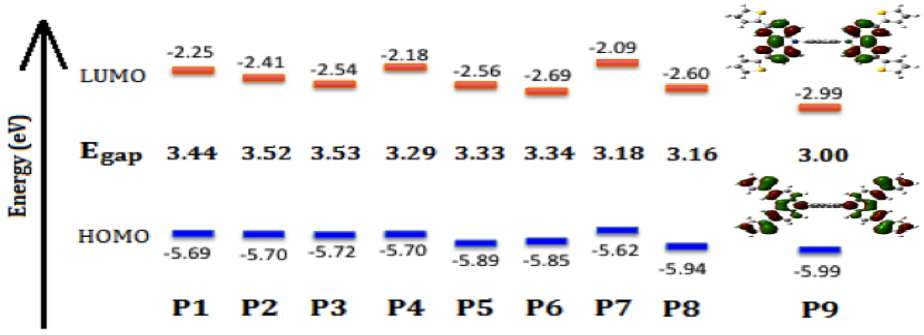
[1]*Chemistry Department, Science Faculty, University of Malaya,*

50603, Kuala Lumpur, Malaysia

[2]*Physic Department, Science Faculty, University of Malaya,*

50603, Kuala Lumpur, Malaysia

E-mail: azhar70@um.edu.my



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1. ^{1}H NMR and ^{13}C spectra in $CDCl_3$ solution.

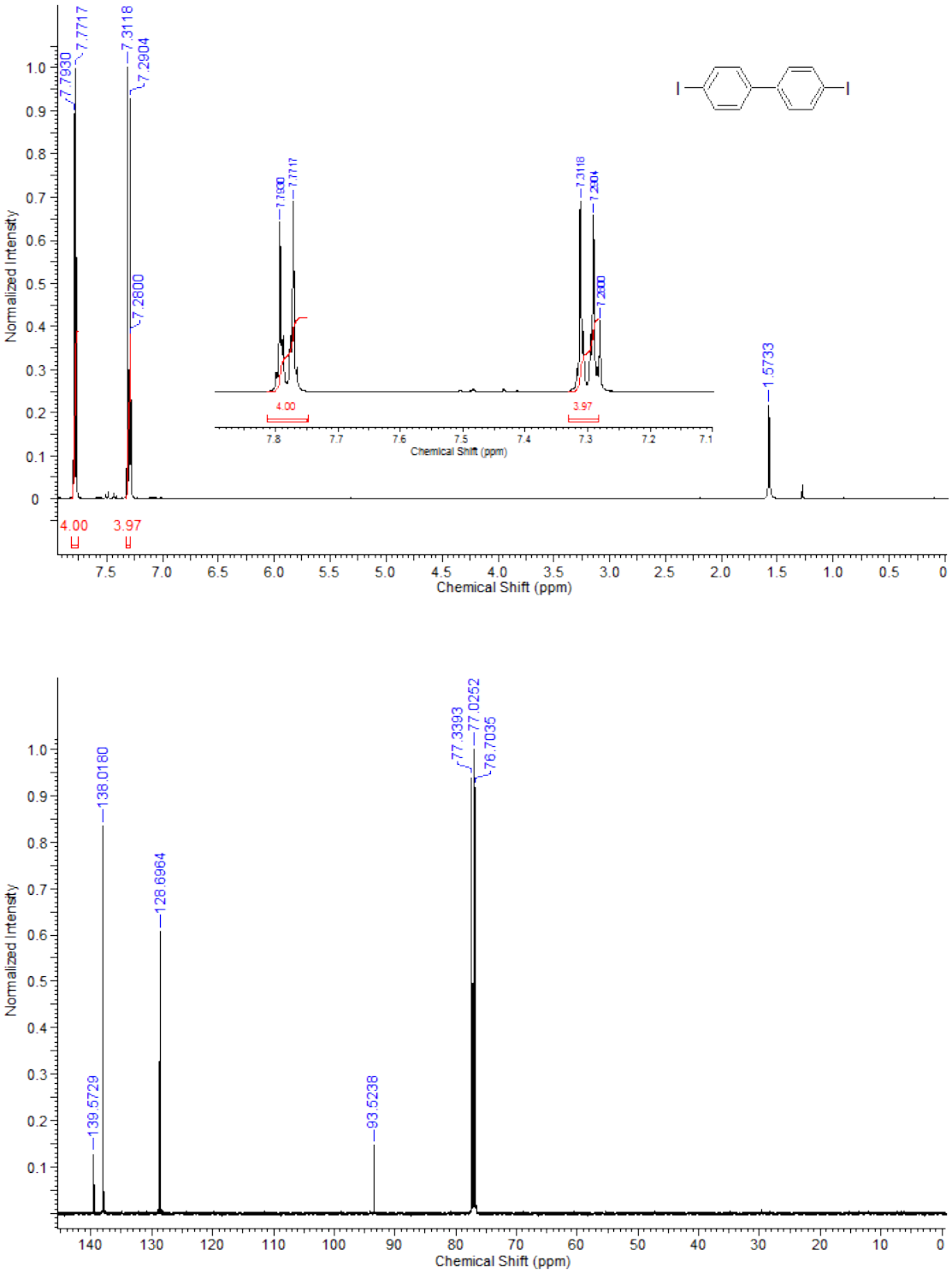

Figure S1. ^{1}H NMR and ^{13}C NMR of 4,4-diiodobiphenyl (2) in $CDCl_3$.

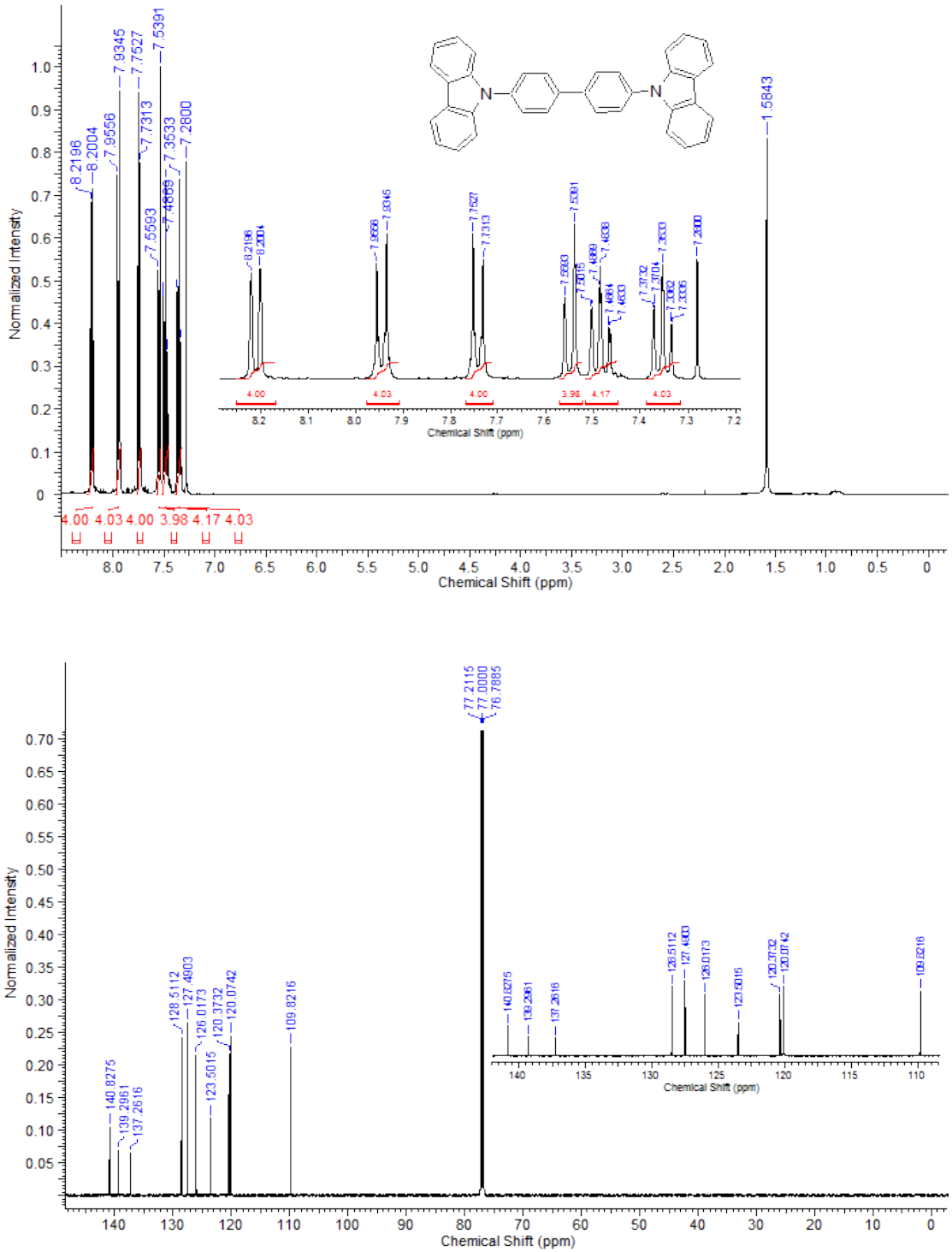

Figure S2. ^{1}H NMR and ^{13}C NMR of 4,4'-Di(9H-carbazol-9-yl)-1,1'-biphenyl (P1) in $CDCl_3$.

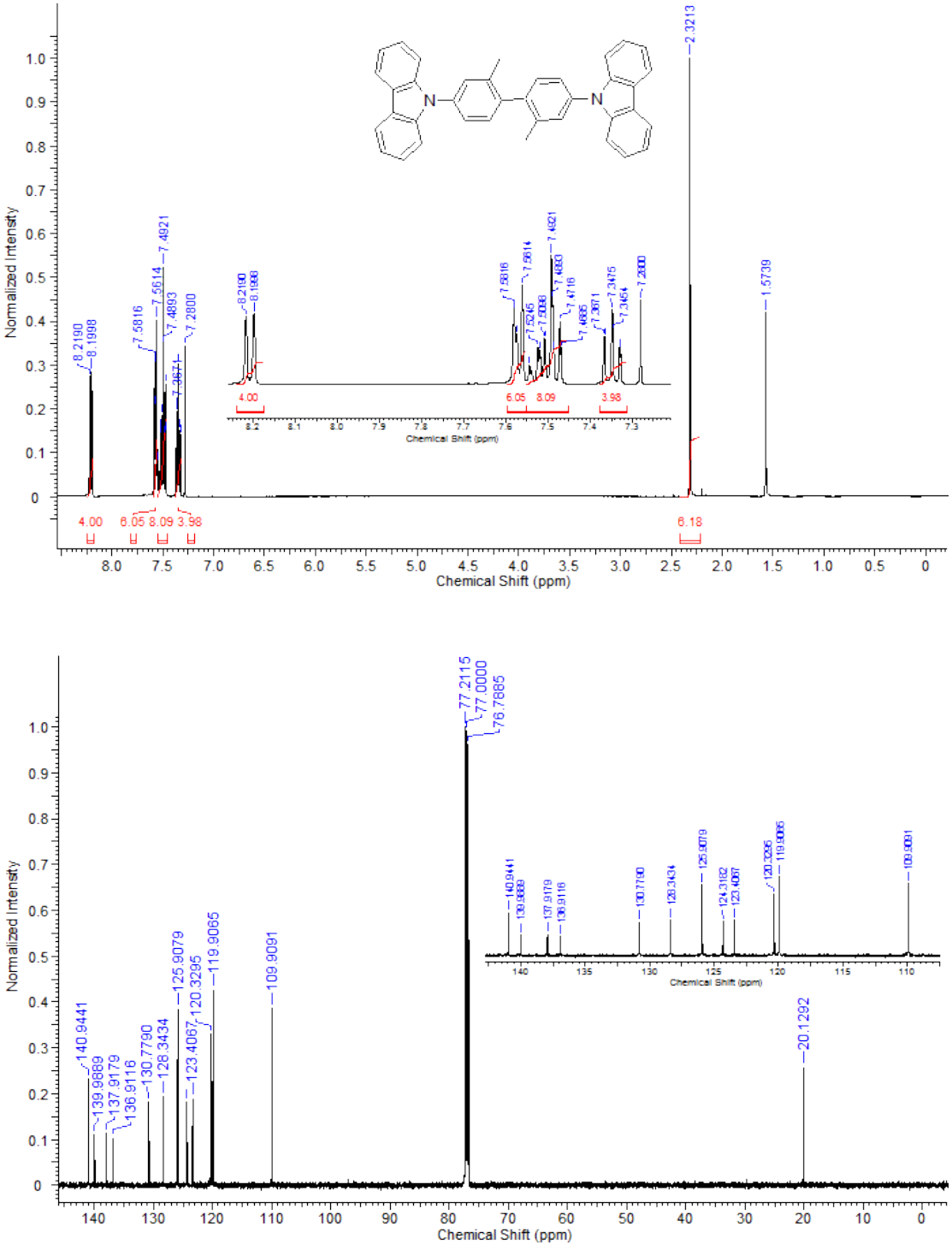

Figure S3. ^{1}H NMR and ^{13}C NMR of 9,9'-(2,2'-dimethyl-[1,1'-biphenyl]-4,4'-diyl)bis(9H-carbazole) (P2) in $CDCl_3$.

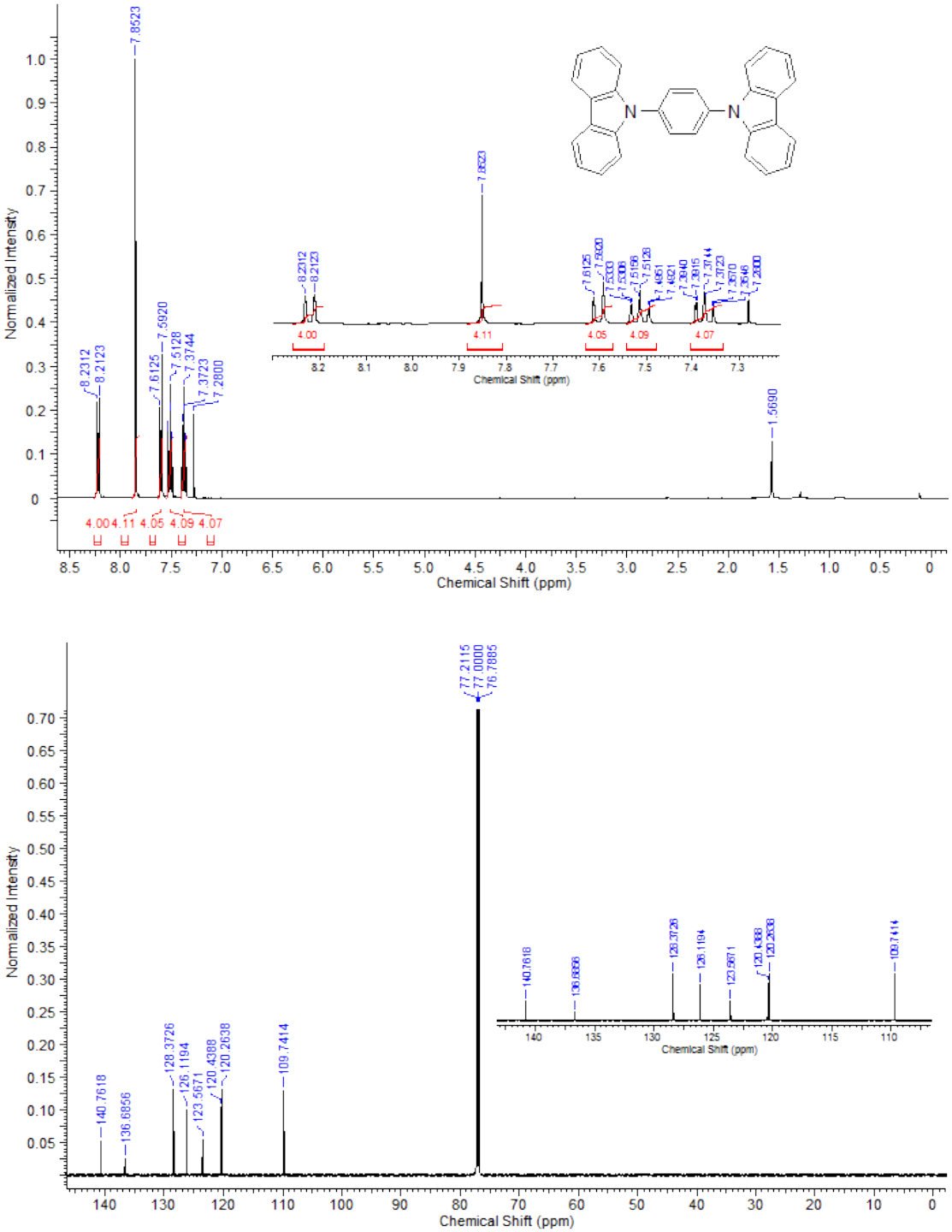

Figure S4. ^{1}H NMR and ^{13}C NMR of 1,4-di(9H-carbazol-9-yl)benzene (P3) in $CDCl_3$.

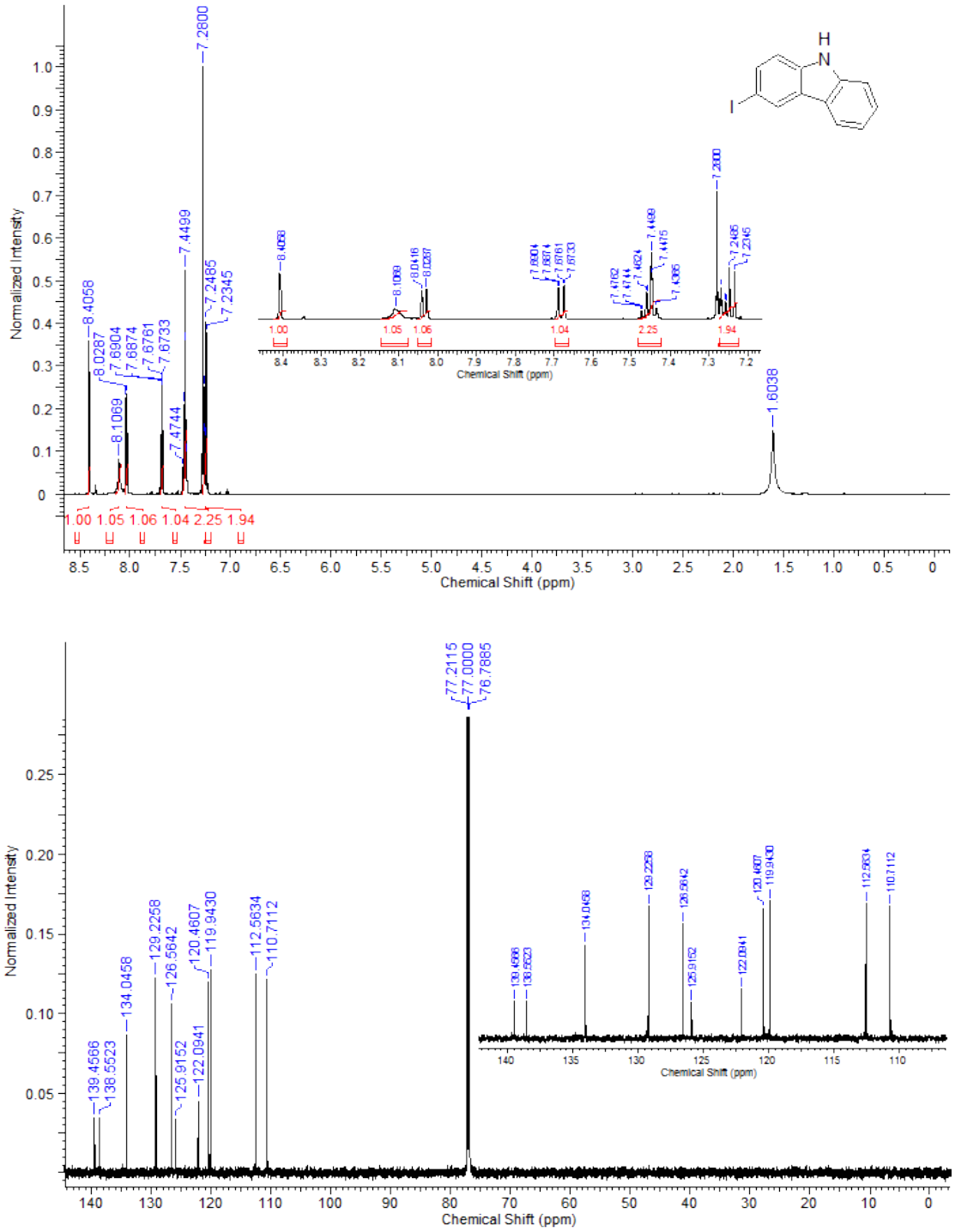

Figure S5. ^{1}H NMR and ^{13}C NMR of 3-Diiodocarbazole (5) in $CDCl_3$.

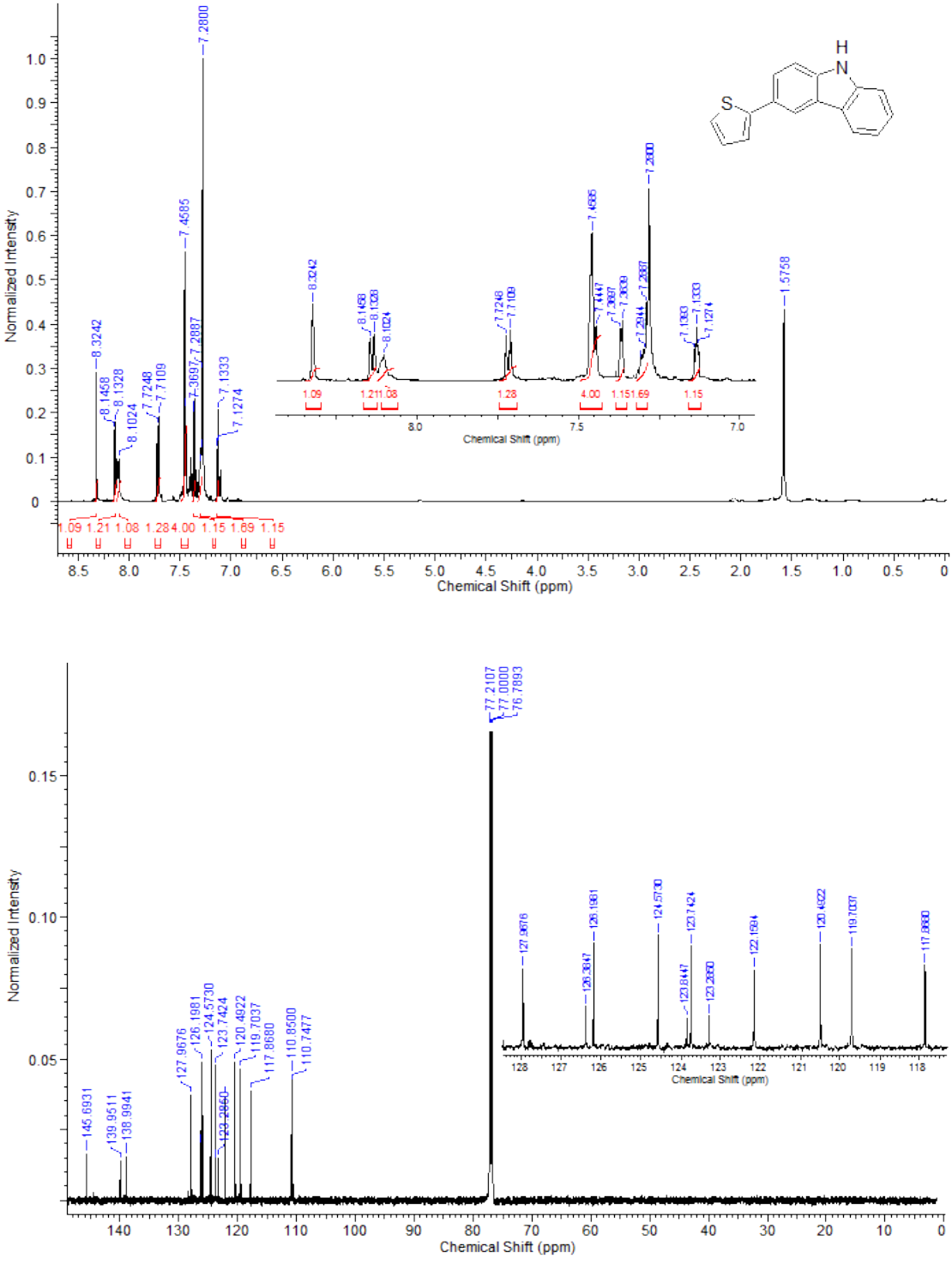

Figure S6. ^{1}H NMR and ^{13}C NMR of 3-(Thiophen-2-yl)carbazole (7) in $CDCl_3$.

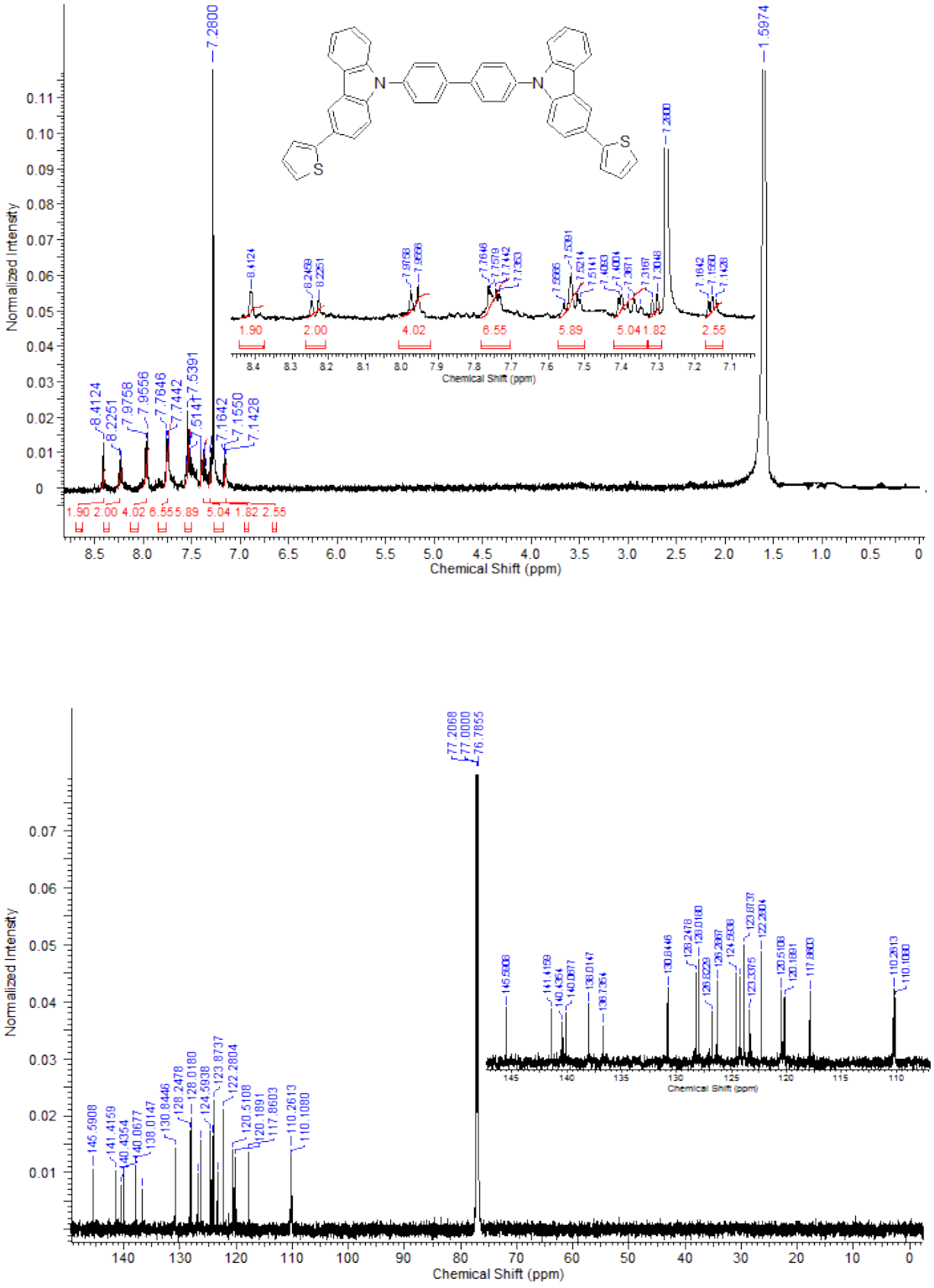

Figure S7. ^{1}H NMR and ^{13}C NMR of compound P4 in $CDCl_3$.

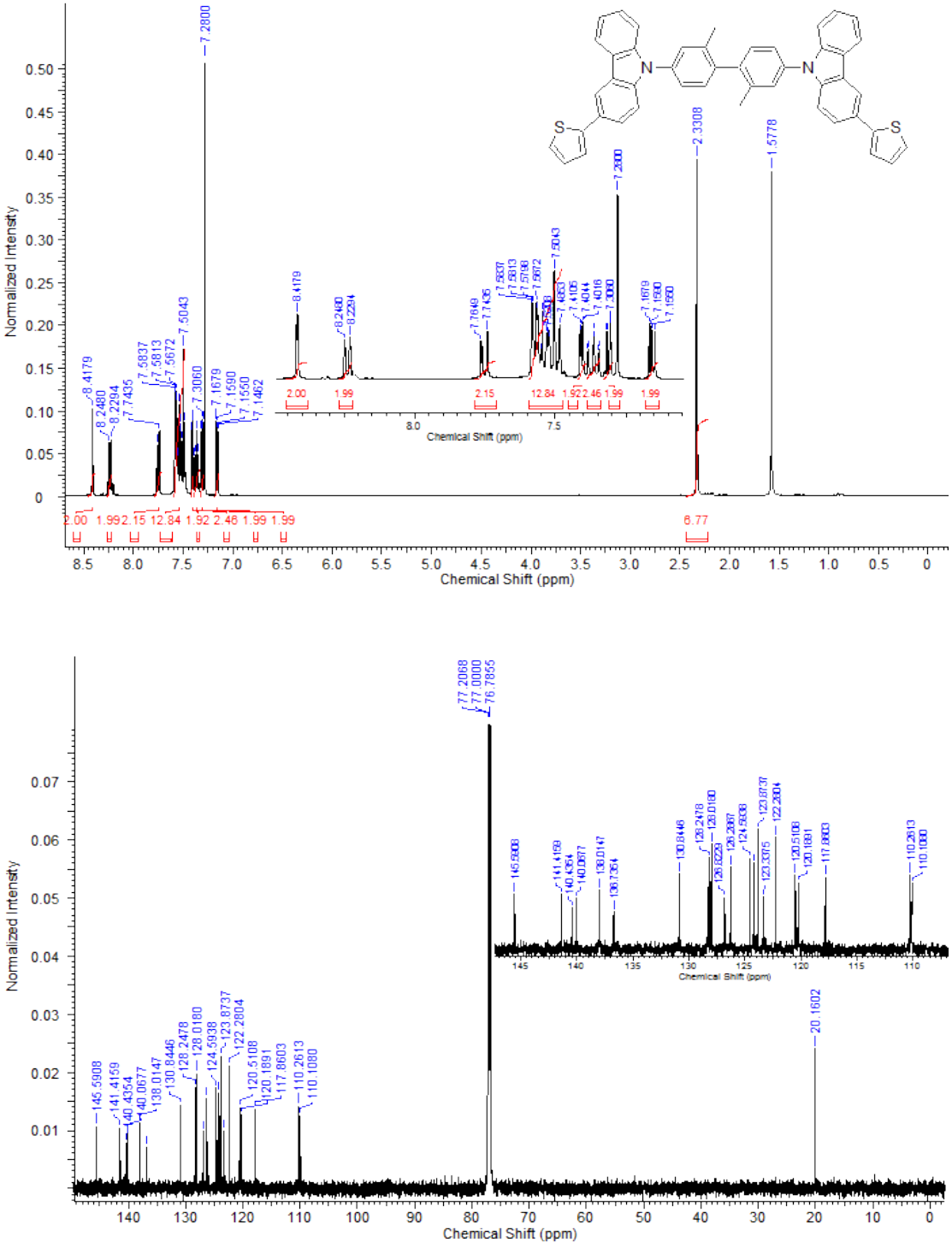

Figure S8. ^{1}H NMR and ^{13}C NMR of compound P5 in $CDCl_3$.

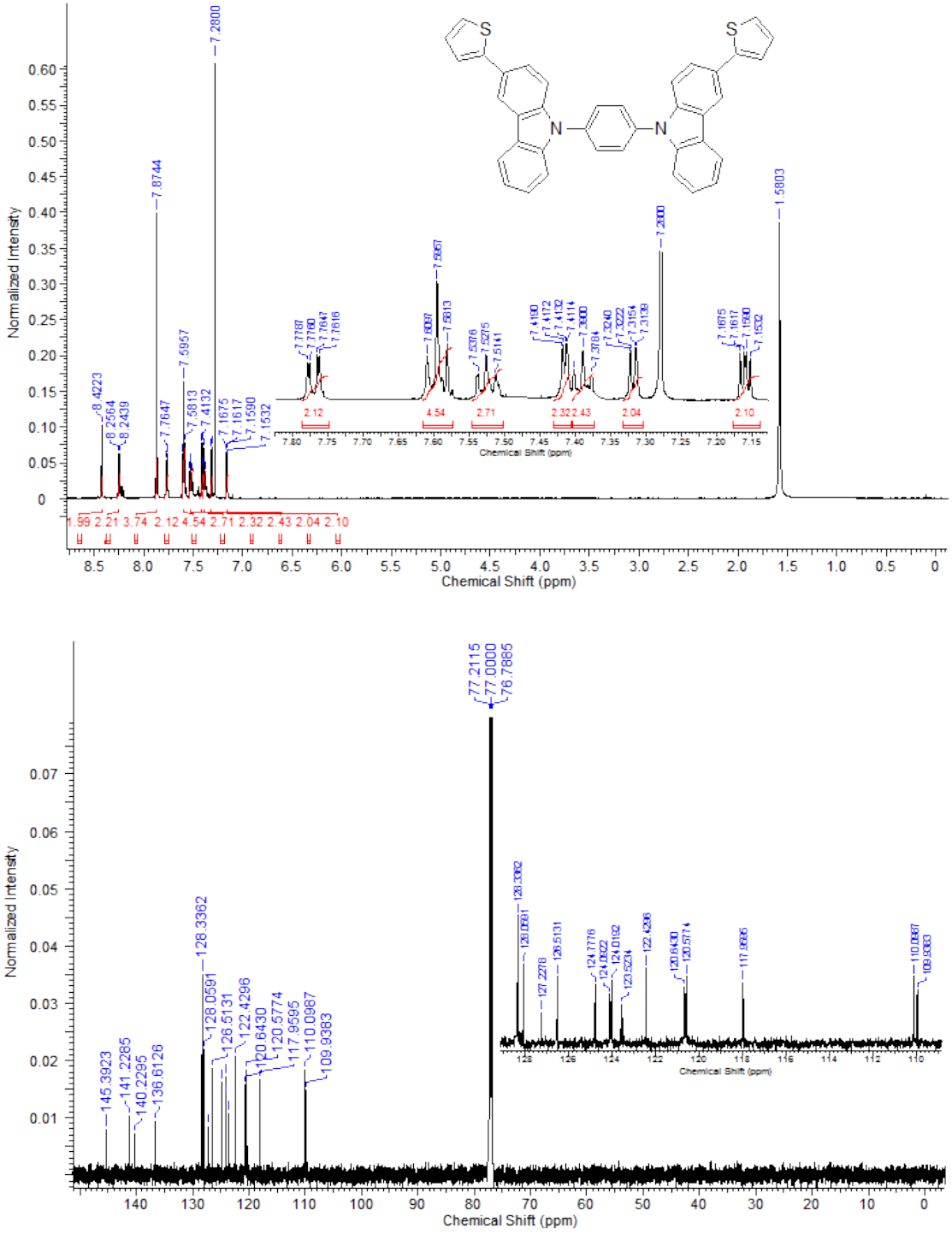

Figure S9. ^{1}H NMR and ^{13}C NMR of compound P6 in $CDCl_3$.

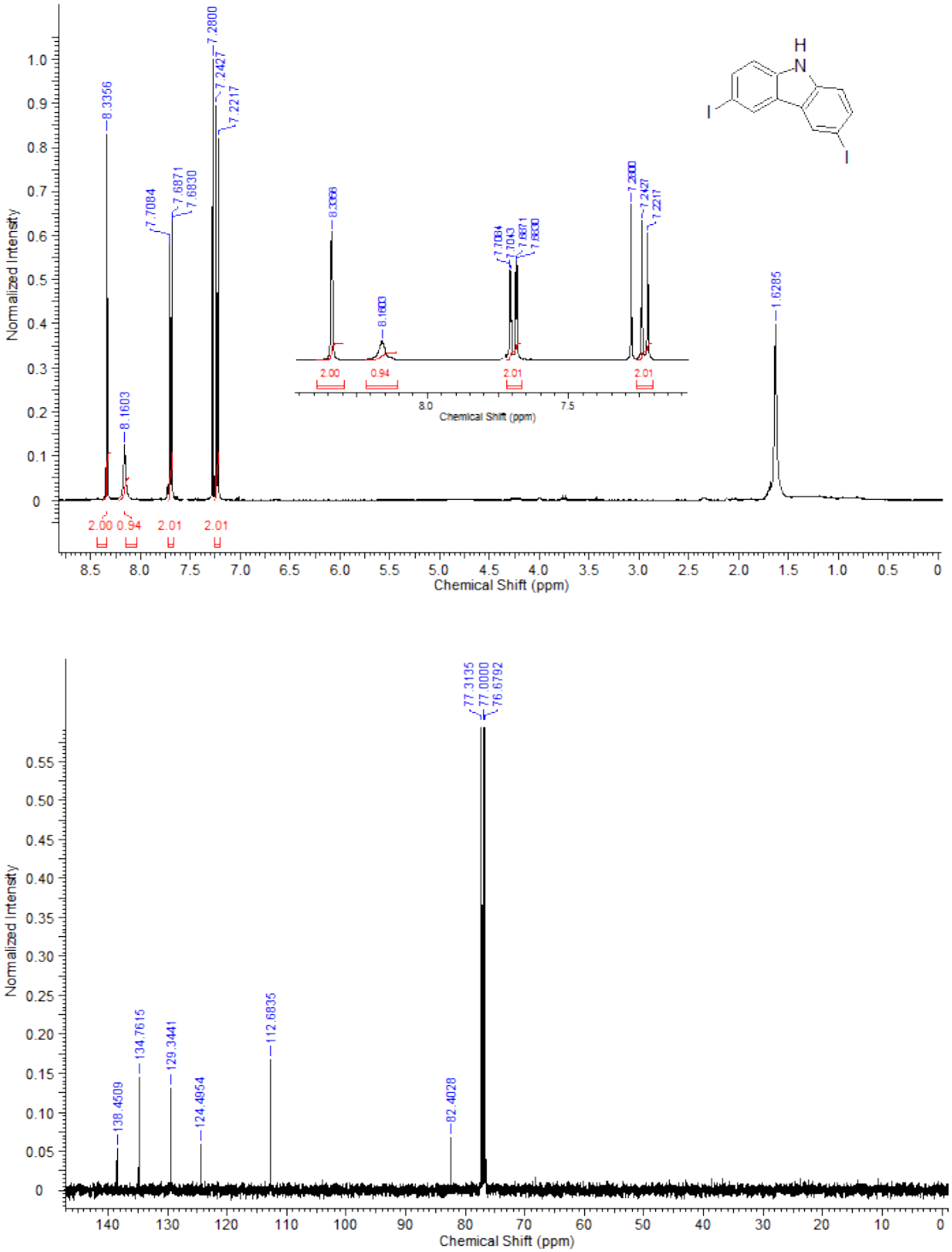

Figure S10. ^{1}H NMR and ^{13}C NMR of 3,6-Diiodocarbazole (8) in $CDCl_3$.

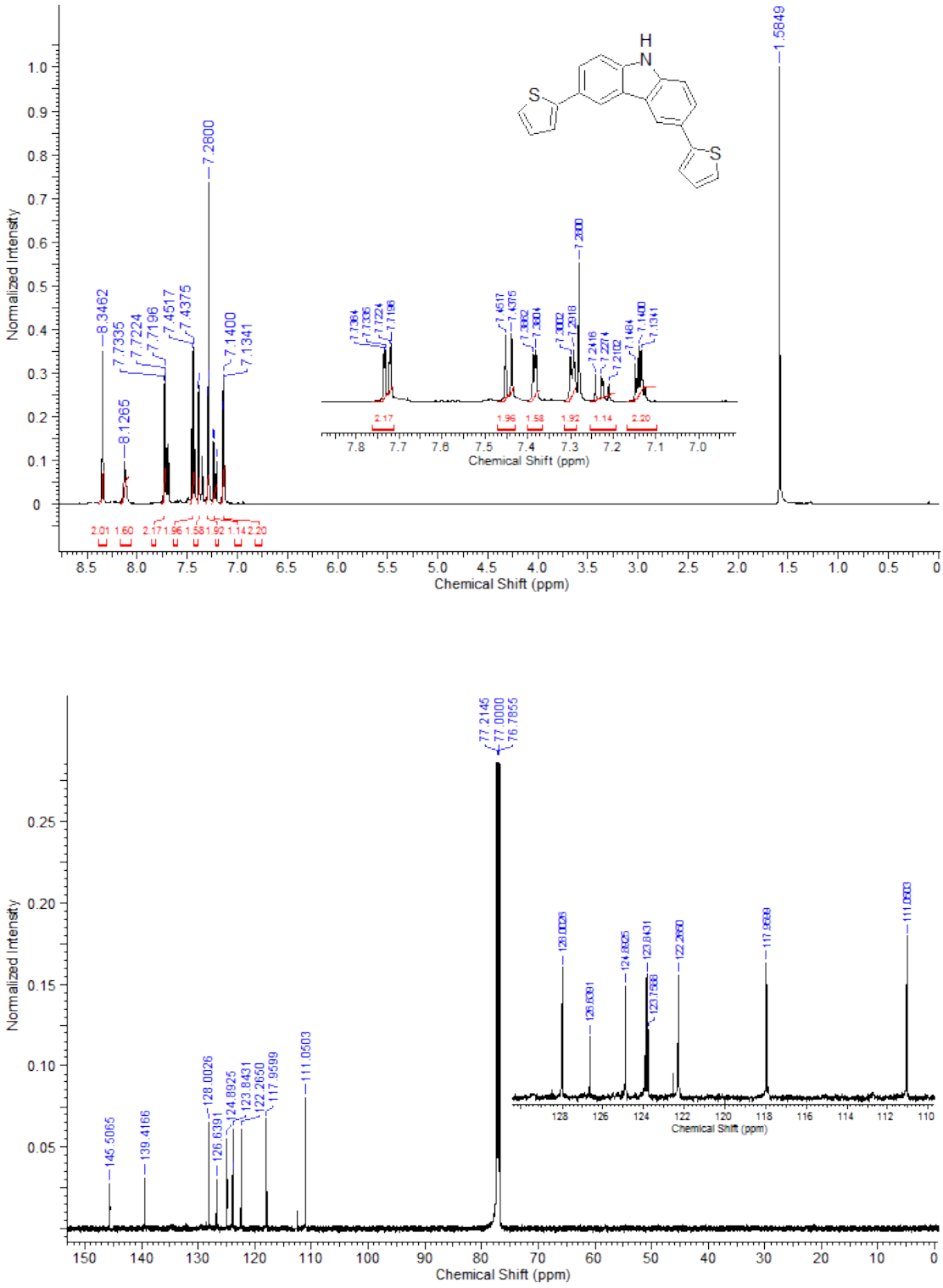

Figure S11. ^{1}H NMR and ^{13}C NMR of 3,6-Di(thiophen-2-yl)-9H-carbazole (9) in $CDCl_3$.

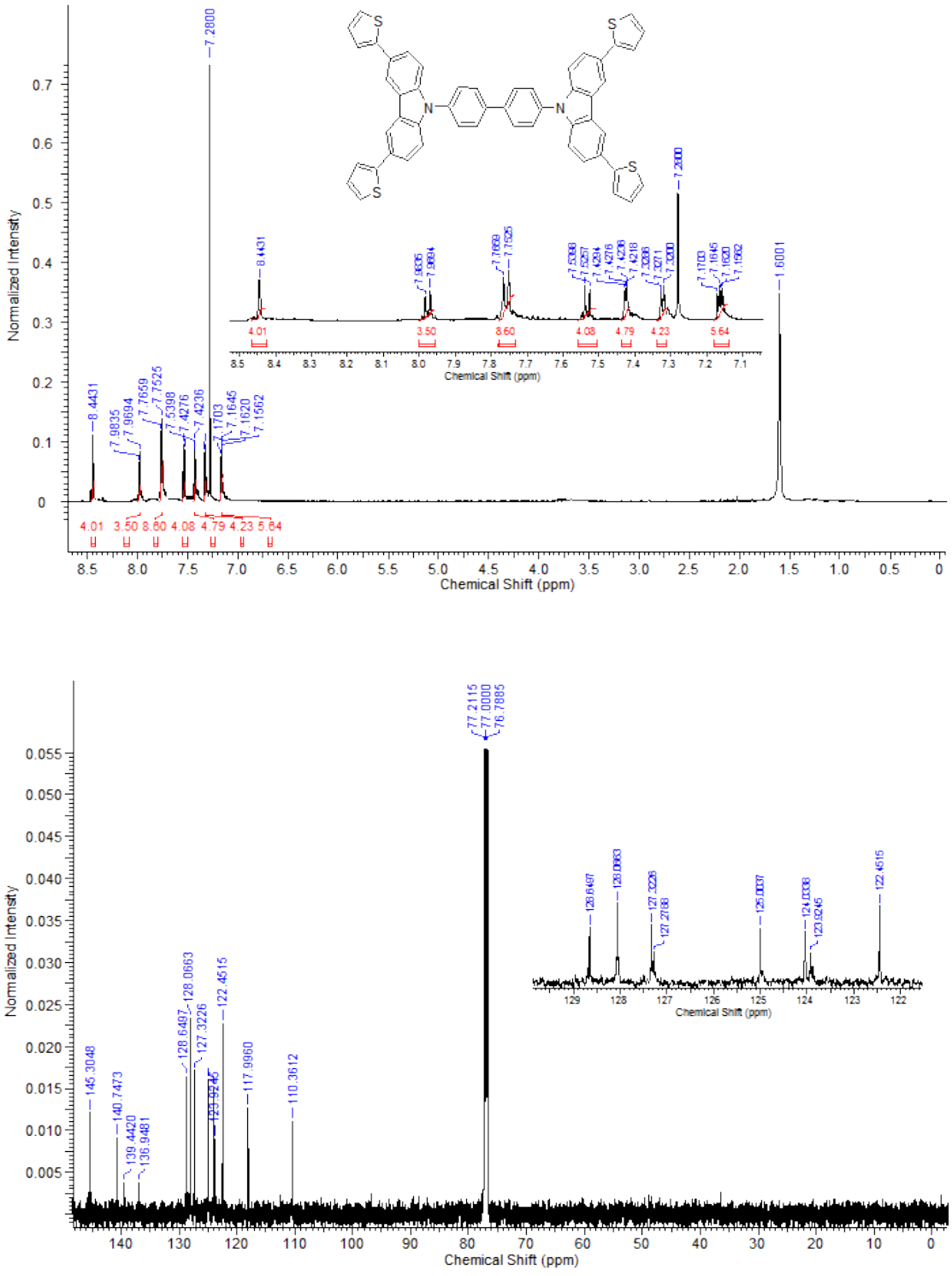

Figure S12. ^{1}H NMR and ^{13}C NMR of compound P7 in $CDCl_3$.

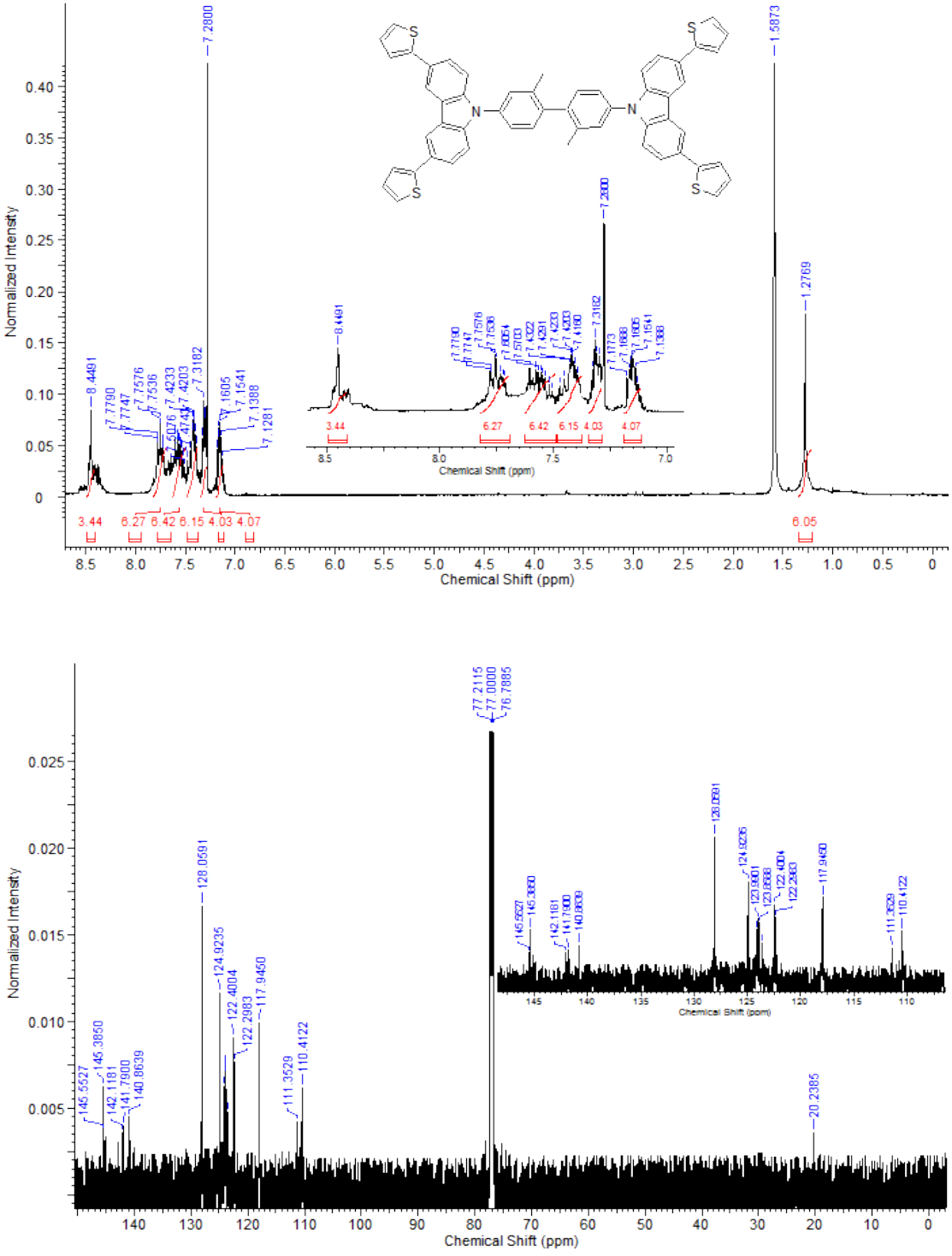

Figure S13. ^{1}H NMR and ^{13}C NMR of compound P8 in $CDCl_3$.

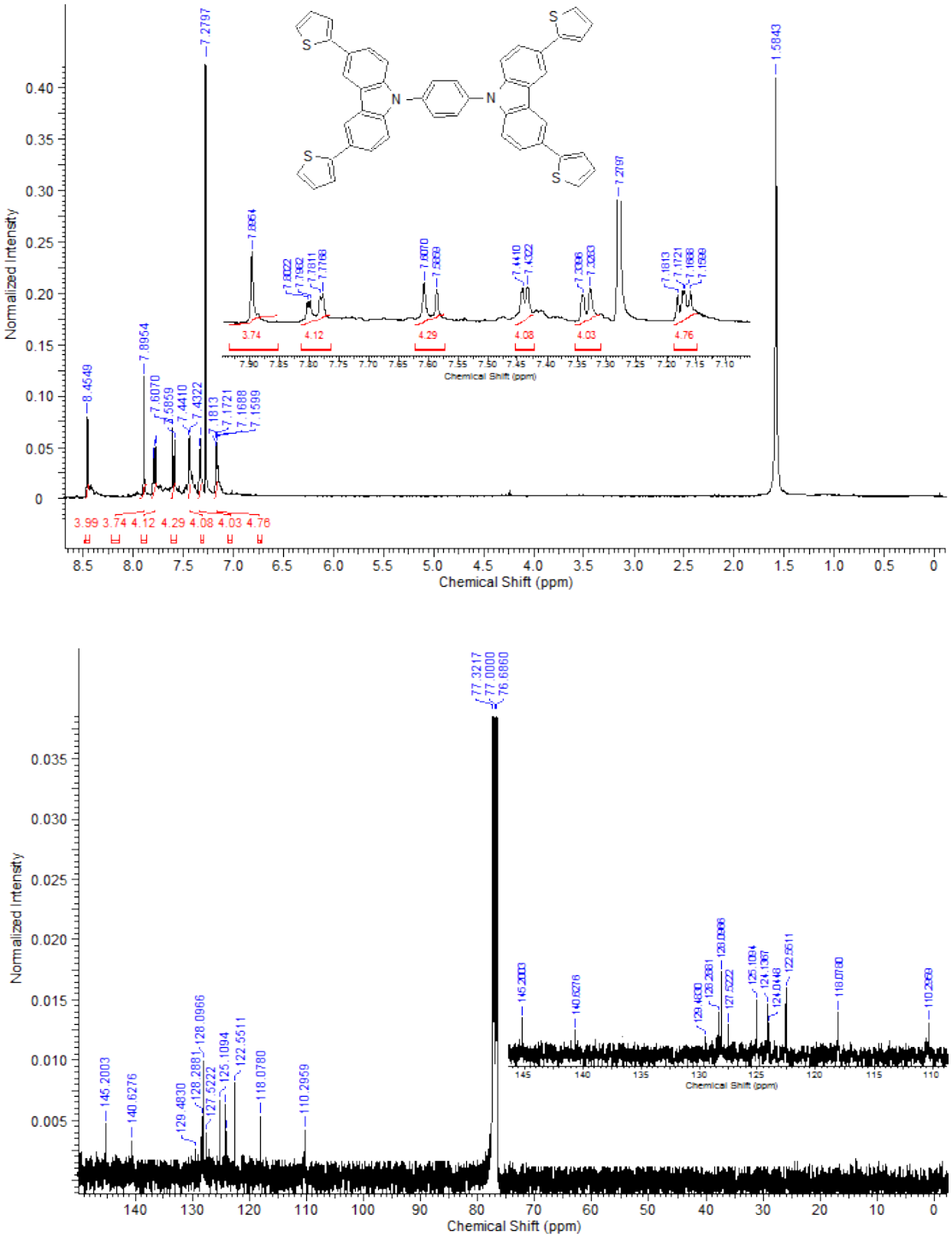

Figure S14. ^{1}H NMR and ^{13}C NMR of compound P9 in $CDCl_3$.

Table S1. Cartesian Coordinates (Å) of the Optimized Structure of **P1** at the B3LYP/6-31G Level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.748746	-0.534047	-0.179529
2	6	0	-1.147023	-0.533634	-1.523127
3	6	0	-2.509763	-0.534835	-1.850017
4	6	0	-3.474265	-0.536522	-0.833307
5	6	0	-3.075978	-0.535940	0.510316
6	6	0	-1.713216	-0.534640	0.837202
7	6	0	0.748786	-0.534085	0.179642
8	6	0	1.713227	-0.534301	-0.837114
9	6	0	3.075994	-0.535665	-0.510271
10	6	0	3.474323	-0.536661	0.833337
11	6	0	2.509853	-0.535357	1.850080
12	6	0	1.147098	-0.534117	1.523230
13	1	0	-0.410627	-0.532473	-2.299418
14	1	0	-2.813830	-0.534542	-2.875900
15	1	0	-3.812359	-0.536554	1.286612
16	1	0	-1.409117	-0.534195	1.863080
17	1	0	1.409096	-0.533519	-1.862984
18	1	0	3.812350	-0.536006	-1.286590
19	1	0	2.813951	-0.535390	2.875953
20	1	0	0.410721	-0.533267	2.299540
21	6	0	-5.428642	0.853641	-1.207783
22	6	0	-5.695543	-1.159096	-0.078686
23	6	0	-5.237362	1.786259	-2.162077
24	6	0	-6.183180	1.117967	-0.084522
25	6	0	-5.801484	-2.468245	0.224568
26	6	0	-6.357316	-0.195485	0.652310
27	6	0	-5.750962	3.080035	-1.932980
28	1	0	-4.706476	1.554561	-3.061729
29	6	0	-6.662531	2.339750	0.210017
30	6	0	-6.533380	-2.821552	1.377665
31	1	0	-5.338985	-3.215398	-0.385964
32	6	0	-7.034248	-0.464408	1.783135
33	6	0	-6.445977	3.364386	-0.730858
34	1	0	-5.613050	3.847695	-2.665490
35	1	0	-7.193932	2.523993	1.120273
36	6	0	-7.132365	-1.813400	2.173808
37	1	0	-6.633666	-3.850626	1.653064
38	1	0	-7.486632	0.315562	2.359235
39	1	0	-6.808098	4.353166	-0.540910
40	1	0	-7.660449	-2.076946	3.066319
41	6	0	5.428681	0.853489	1.207873
42	6	0	5.695558	-1.159111	0.078517
43	6	0	5.237442	1.785998	2.162280

44	6	0	6.183137	1.117960	0.084585
45	6	0	5.801508	-2.468223	-0.224891
46	6	0	6.357259	-0.195404	-0.652408
47	6	0	5.750994	3.079814	1.933287
48	1	0	4.706626	1.554187	3.061941
49	6	0	6.662439	2.339787	-0.209852
50	6	0	6.533335	-2.821387	-1.378072
51	1	0	5.339061	-3.215452	0.385588
52	6	0	7.034121	-0.464186	-1.783313
53	6	0	6.445921	3.364314	0.731148
54	1	0	5.613110	3.847391	2.665887
55	1	0	7.193774	2.524143	-1.120126
56	6	0	7.132246	-1.813134	-2.174140
57	1	0	6.633627	-3.850430	-1.653589
58	1	0	7.486448	0.315859	-2.359360
59	1	0	6.808005	4.353122	0.541283
60	1	0	7.660279	-2.076570	-3.066716
61	7	0	4.903804	-0.539233	1.176261
62	7	0	-4.903731	-0.539067	-1.176306

Rotational constants (GHZ): 0.2265247 0.0357328 0.0343215
The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -1495.69665403 A.U. after 15 cycles
Convg = 0.3793D-08 -V/T = 2.0028

Table S2. Cartesian Coordinates (Å) of the Optimized Structure of **P2** at the B3LYP/6-31G Level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.760189	0.935433	-0.786051
2	6	0	-7.111119	0.676383	-0.502148
3	6	0	-8.104007	1.376576	-1.180557
4	6	0	-7.737061	2.319788	-2.127112
5	6	0	-6.386433	2.565580	-2.397701
6	6	0	-5.381575	1.879703	-1.733806
7	1	0	-9.141615	1.190929	-0.975613
8	1	0	-8.491672	2.867453	-2.657991
9	1	0	-6.122209	3.300408	-3.134262

10	1	0	-4.348034	2.072702	-1.944965
11	6	0	-7.132477	-0.353319	0.524166
12	6	0	-8.153548	-1.013048	1.201249
13	6	0	-5.793347	-0.666128	0.810121
14	6	0	-7.826092	-1.969963	2.148579
15	1	0	-9.182585	-0.785948	0.994841
16	6	0	-5.454346	-1.624434	1.758770
17	6	0	-6.486814	-2.269371	2.421391
18	1	0	-8.602829	-2.486665	2.678586
19	1	0	-4.429639	-1.857671	1.972385
20	1	0	-6.253313	-3.013541	3.158975
21	7	0	-4.963217	0.118164	0.012464
22	6	0	-3.540299	0.089167	0.012753
23	6	0	-2.823051	0.921287	0.857740
24	6	0	-2.864532	-0.774500	-0.838775
25	6	0	-1.436352	0.876230	0.841714
26	1	0	-3.344127	1.591439	1.513653
27	6	0	-1.472966	-0.829203	-0.865939
28	1	0	-3.437724	-1.408503	-1.488473
29	6	0	-0.749822	0.010619	-0.006523
30	1	0	-0.878273	1.521498	1.493875
31	6	0	0.749820	0.010616	0.006526
32	6	0	1.436340	0.876226	-0.841724
33	6	0	1.472974	-0.829209	0.865927
34	6	0	2.823036	0.921294	-0.857763
35	1	0	0.878241	1.521465	-1.493895
36	6	0	2.864541	-0.774488	0.838756
37	6	0	3.540295	0.089185	-0.012774
38	1	0	3.344102	1.591444	-1.513685
39	1	0	3.437742	-1.408492	1.488448
40	7	0	4.963215	0.118196	-0.012492
41	6	0	5.760183	0.935461	0.786032
42	6	0	5.381565	1.879742	1.733773
43	6	0	7.111115	0.676416	0.502129
44	6	0	6.386419	2.565626	2.397667
45	1	0	4.348022	2.072737	1.944929
46	6	0	8.103998	1.376639	1.180515
47	6	0	7.737048	2.319840	2.127078
48	1	0	6.122190	3.300453	3.134228
49	1	0	9.141608	1.190988	0.975579
50	1	0	8.491655	2.867510	2.657956
51	6	0	5.793349	-0.666111	-0.810132
52	6	0	7.132479	-0.353336	-0.524135
53	6	0	5.454354	-1.624443	-1.758755
54	6	0	8.153554	-1.013107	-1.201171
55	6	0	6.486825	-2.269435	-2.421317
56	1	0	4.429647	-1.857677	-1.972377
57	6	0	7.826102	-1.970045	-2.148479
58	1	0	9.182589	-0.786011	-0.994754

59	1	0	6.253329	-3.013631	-3.158876
60	1	0	8.602842	-2.486776	-2.678454
61	6	0	0.777928	-1.776632	1.817464
62	1	0	0.173656	-1.238866	2.539072
63	1	0	0.117868	-2.457639	1.292789
64	1	0	1.501713	-2.368117	2.363352
65	6	0	-0.777899	-1.776613	-1.817472
66	1	0	-0.173474	-1.238850	-2.538952
67	1	0	-0.117987	-2.457747	-1.292775
68	1	0	-1.501679	-2.367970	-2.363508

Rotational constants (GHZ): 0.2433396 0.0297766 0.0297603
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RHF) = -1563.73833966 A.U. after 7 cycles
Convg = 0.1857D-08 -V/T = 1.9990

Table S3. Cartesian Coordinates (Å) of the Optimized Structure of **P3** at the B3LYP/6-31G Level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.957853	-2.983205	0.588175
2	6	0	-4.059674	-3.400737	-0.424567
3	6	0	-3.264617	-2.450082	-1.098513
4	6	0	-3.388561	-1.154426	-0.744642
5	6	0	-4.329374	-0.754243	0.178550
6	6	0	-5.086493	-1.613632	0.884052
7	1	0	-5.538526	-3.705540	1.122926
8	1	0	-3.981970	-4.437814	-0.676231
9	1	0	-2.578196	-2.748952	-1.862968
10	1	0	-5.765307	-1.268698	1.635805
11	6	0	-3.388448	1.154002	-0.745609
12	6	0	-3.264348	2.449348	-1.100578
13	6	0	-4.059377	3.400649	-0.427526
14	6	0	-4.957662	2.984060	0.585508
15	6	0	-5.086417	1.614753	0.882579
16	6	0	-4.329325	0.754690	0.177881
17	1	0	-2.577823	2.747504	-1.865228
18	1	0	-3.981574	4.437503	-0.680094
19	1	0	-5.538326	3.706899	1.119583

20	1	0	-5.765303	1.270526	1.634584
21	6	0	-1.261784	-0.000310	-0.609892
22	6	0	-0.102716	-0.000258	-1.397619
23	6	0	-1.159089	-0.000242	0.787746
24	6	0	1.159041	-0.000207	-0.787736
25	1	0	-0.181125	-0.000260	-2.464747
26	6	0	0.102674	-0.000275	1.397632
27	1	0	-2.044045	-0.000184	1.389216
28	6	0	1.261757	-0.000301	0.609905
29	1	0	2.043981	-0.000115	-1.389214
30	1	0	0.1 81077	-0.000282	2.464755
31	6	0	3.388497	1.153983	0.745633
32	6	0	3.388577	-1.154421	0.744634
33	6	0	3.264575	2.449277	1.100802
34	6	0	4.329217	0.754705	-0.178046
35	6	0	3.264743	-2.450055	1.098625
36	6	0	4.329285	-0.754251	-0.178692
37	6	0	4.059565	3.400606	0.427750
38	1	0	2.578221	2.747373	1.865625
39	6	0	5.086165	1.614827	-0.882871
40	6	0	4.059826	-3.400718	0.424726
41	1	0	2.578393	-2.748902	1.863153
42	6	0	5.086339	-1.613682	-0.884247
43	6	0	4.957575	2.984110	-0.585565
44	1	0	3.981942	4.437416	0.680532
45	1	0	5.764815	1.270672	-1.635130
46	6	0	4.957858	-2.983238	-0.588167
47	1	0	3.982254	-4.437768	0.676546
48	1	0	5.764992	-1.268798	-1.636173
49	1	0	5.538154	3.707003	-1.119664
50	1	0	5.538541	-3.705600	-1.122878
51	7	0	2.585273	-0.000456	1.249752
52	7	0	-2.585259	-0.000451	-1.249748

Rotational constants (GHZ): 0.2566061 0.0828358 0.0678497
The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -1265.00446024 A.U. after 16 cycles
Convg = 0.2418D-08 -V/T = 2.0040

Table S4. Cartesian Coordinates (Å) of the Optimized Structure of **P4** at the B3LYP/6-31G Level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.674232	0.208832	-0.368298
2	6	0	-0.703266	0.227122	-1.769826
3	6	0	-1.931442	0.231513	-2.445057
4	6	0	-3.129918	0.215380	-1.719220
5	6	0	-3.100707	0.197314	-0.318527
6	6	0	-1.873417	0.195199	0.357103
7	6	0	0.675044	0.203981	0.374052
8	6	0	1.873548	0.202699	-0.352266
9	6	0	3.101281	0.196078	0.322519
10	6	0	3.131209	0.194033	1.723369
11	6	0	1.933357	0.196596	2.450196
12	6	0	0.704747	0.200462	1.775543
13	1	0	0.212072	0.237600	-2.324145
14	1	0	-1.954086	0.246777	-3.514449
15	1	0	-4.015959	0.185419	0.235172
16	1	0	-1.852069	0.182699	1.426675
17	1	0	1.851286	0.206410	-1.422119
18	1	0	4.016297	0.193065	-0.231890
19	1	0	1.956624	0.195467	3.519762
20	1	0	-0.210424	0.201042	2.330254
21	6	0	-4.929741	1.609088	-2.564594
22	6	0	-5.465068	-0.429612	-1.587771
23	6	0	-4.505161	2.563696	-3.416326
24	6	0	-5.953549	1.845875	-1.671330
25	6	0	-5.635943	-1.745888	-1.352768
26	6	0	-6.302215	0.515141	-1.033291
27	6	0	-5.072454	3.850357	-3.301966
28	1	0	-3.756649	2.354052	-4.151323
29	6	0	-6.503819	3.059680	-1.486237
30	6	0	-6.638797	-2.128283	-0.437802
31	1	0	-5.025296	-2.477040	-1.839426
32	6	0	-7.247508	0.217662	-0.123398
33	6	0	-6.058851	4.105549	-2.316978
34	1	0	-4.755730	4.634728	-3.956917
35	1	0	-7.255528	3.222308	-0.742087
36	6	0	-7.431430	-1.140602	0.198385
37	1	0	-6.799018	-3.163819	-0.221627
38	1	0	-7.841350	0.982314	0.332601
39	1	0	-6.466479	5.088741	-2.207959
40	6	0	4.928167	1.580607	2.581379
41	6	0	5.465802	-0.446897	1.582539
42	6	0	4.502213	2.526037	3.442746
43	6	0	5.950984	1.827991	1.689930

44	6	0	5.637672	-1.760195	1.333017
45	6	0	6.301163	0.504686	1.037552
46	6	0	5.067704	3.814736	3.341488
47	1	0	3.753856	2.307925	4.175473
48	6	0	6.499474	3.044359	1.517078
49	6	0	6.640510	-2.131713	0.413651
50	1	0	5.027591	-2.497189	1.811581
51	6	0	7.246292	0.218182	0.123746
52	6	0	6.053503	4.081250	2.358707
53	1	0	4.749955	4.592130	4.004697
54	1	0	7.250592	3.215462	0.774220
55	6	0	7.431971	-1.136577	-0.212216
56	1	0	6.801481	-3.164681	0.186241
57	1	0	7.838330	0.988803	-0.324808
58	1	0	6.460249	5.065937	2.259568
59	7	0	-4.419034	0.217264	-2.425979
60	7	0	4.420248	0.189343	2.428839
61	6	0	-8.493748	-1.551800	1.234208
62	6	0	-9.306117	-0.684817	1.894694
63	16	0	-8.831867	-3.219415	1.726051
64	6	0	-10.394896	-1.418679	2.722230
65	1	0	-9.213203	0.379724	1.840708
66	6	0	-10.300523	-2.770108	2.608377
67	1	0	-11.140283	-0.918935	3.304914
68	1	0	-11.016273	-3.465469	2.994416
69	6	0	8.494805	-1.536435	-1.251940
70	6	0	9.305876	-0.662460	-1.905404
71	16	0	8.835327	-3.199263	-1.758290
72	6	0	10.395572	-1.387778	-2.739525
73	1	0	9.211472	0.401479	-1.842530
74	6	0	10.303293	-2.740420	-2.636830
75	1	0	11.140093	-0.882131	-3.318209
76	1	0	11.020270	-3.431276	-3.028606

Rotational constants (GHZ): 0.1001811 0.0172505 0.0170990
The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -2599.25394643 A.U. after 16 cycles
Convg = 0.4623D-08 -V/T = 2.0025

Table S5. Cartesian Coordinates (Å) of the Optimized Structure of **P5** at the B3LYP/6-31G Level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.678321	0.168565	-0.368335
2	6	0	-0.754971	0.179132	-1.782821
3	6	0	-1.998617	0.184107	-2.421386
4	6	0	-3.182983	0.179300	-1.675959
5	6	0	-3.119537	0.169575	-0.276900
6	6	0	-1.880456	0.164165	0.366821
7	6	0	0.678239	0.167911	0.368650
8	6	0	1.880400	0.164905	-0.366548
9	6	0	3.119492	0.169157	0.277156
10	6	0	3.182944	0.176276	1.676228
11	6	0	1.998579	0.179687	2.421691
12	6	0	0.754876	0.175861	1.783176
13	1	0	-2.046559	0.191910	-3.494405
14	1	0	-4.023358	0.166564	0.302044
15	1	0	-1.825994	0.156963	1.450498
16	1	0	1.825944	0.159719	-1.450270
17	1	0	4.023322	0.167233	-0.301806
18	1	0	2.046581	0.185493	3.494709
19	6	0	-4.969870	1.570654	-2.545556
20	6	0	-5.524139	-0.438644	-1.548417
21	6	0	-4.520089	2.514643	-3.412900
22	6	0	-6.016787	1.830088	-1.673786
23	6	0	-5.701222	-1.761275	-1.288836
24	6	0	-6.379110	0.523710	-1.024584
25	6	0	-5.084276	3.805054	-3.334330
26	1	0	-3.753815	2.289870	-4.131525
27	6	0	-6.562321	3.068242	-1.537193
28	6	0	-6.722642	-2.125794	-0.390619
29	1	0	-5.077955	-2.506352	-1.747923
30	6	0	-7.350146	0.224376	-0.124274
31	6	0	-6.086566	4.087205	-2.382648
32	1	0	-4.747543	4.577204	-4.000629
33	1	0	-7.334405	3.261846	-0.815709
34	6	0	-7.535010	-1.132168	0.212801
35	1	0	-6.885258	-3.161798	-0.160073
36	1	0	-7.961572	0.992671	0.310299
37	1	0	-6.489645	5.080129	-2.307853
38	6	0	4.969808	1.566078	2.548302
39	6	0	5.524093	-0.441423	1.547535
40	6	0	4.520015	2.508508	3.417327
41	6	0	6.016713	1.827083	1.676982
42	6	0	5.701180	-1.763587	1.285564
43	6	0	6.379054	0.521878	1.025455

44	6	0	5.084196	3.799062	3.341064
45	1	0	3.753756	2.282444	4.135556
46	6	0	6.562238	3.065480	1.542609
47	6	0	6.722618	-2.126481	0.386717
48	1	0	5.077877	-2.509484	1.743297
49	6	0	7.350118	0.224169	0.124633
50	6	0	6.086473	4.082924	2.389885
51	1	0	4.747467	4.570017	4.008753
52	1	0	7.334308	3.260387	0.821457
53	6	0	7.535035	-1.131779	-0.214848
54	1	0	6.885214	-3.162064	0.154293
55	1	0	7.961546	0.993246	-0.308558
56	1	0	6.489548	5.075992	2.316858
57	6	0	-8.605138	-1.529126	1.213912
58	6	0	-9.449890	-0.668174	1.851968
59	16	0	-8.924229	-3.199417	1.696323
60	6	0	-10.517851	-1.394820	2.647967
61	1	0	-9.378517	0.400862	1.792469
62	6	0	-10.398474	-2.746488	2.553788
63	1	0	-11.283717	-0.896549	3.211815
64	1	0	-11.106456	-3.455649	2.937290
65	6	0	8.605245	-1.526917	-1.216582
66	6	0	9.450035	-0.664799	-1.853033
67	16	0	8.924406	-3.196314	-1.701974
68	6	0	10.518059	-1.390000	-2.650268
69	1	0	9.378655	0.404130	-1.791619
70	6	0	10.398691	-2.741833	-2.558524
71	1	0	11.283954	-0.890711	-3.213169
72	1	0	11.106694	-3.450303	-2.943253
73	6	0	-0.509322	0.180965	2.644830
74	1	0	-1.286272	0.687516	2.081843
75	1	0	-0.814891	-0.832156	2.846432
76	1	0	-0.324620	0.689173	3.576771
77	6	0	0.509237	0.185875	-2.644315
78	1	0	1.286092	0.691415	-2.080273
79	1	0	0.814844	-0.826860	-2.847743
80	1	0	0.324613	0.695798	-3.575326
81	7	0	4.470409	0.180369	2.375119
82	7	0	-4.470449	0.184642	-2.374868

Rotational constants (GHZ): 0.097534 0.0168097 0.0167615
The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -2678.37684898 A.U. after 38 cycles

Convg = 0.6124D-09 -V/T = 2.0035

Table S6. Cartesian Coordinates (Å) of the Optimized Structure of **P6** at the B3LYP/6-31G Level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.956566	5.054733	0.658180
2	6	0	1.806972	5.040143	-0.157397
3	6	0	1.468627	3.884916	-0.890501
4	6	0	2.286013	2.793329	-0.776508
5	6	0	3.444458	2.841066	-0.051202
6	6	0	3.795793	3.928184	0.707191
7	1	0	3.193311	5.930844	1.238849
8	1	0	1.182757	5.915795	-0.219929
9	1	0	0.590640	3.862342	-1.514869
10	1	0	4.685900	3.925017	1.314673
11	6	0	3.392698	0.830916	-1.168892
12	6	0	3.846979	-0.333058	-1.734109
13	6	0	5.105395	-0.812156	-1.328153
14	6	0	5.869910	-0.104204	-0.371197
15	6	0	5.383670	1.116932	0.147252
16	6	0	4.169128	1.558401	-0.306918
17	1	0	3.259087	-0.868778	-2.460839
18	1	0	5.488161	-1.726377	-1.749255
19	1	0	5.949855	1.682616	0.867117
20	6	0	1.024034	0.720904	-0.672193
21	6	0	-0.076085	0.241622	-1.391468
22	6	0	1.106973	0.489239	0.707735
23	6	0	-1.090332	-0.465487	-0.737686
24	1	0	-0.138817	0.419553	-2.452060
25	6	0	0.093056	-0.217900	1.361900
26	1	0	1.950603	0.855251	1.267211
27	6	0	-1.006859	-0.696995	0.642074
28	1	0	-1.934073	-0.832113	-1.296718
29	1	0	0.155824	-0.396131	2.422467
30	6	0	-2.269488	-2.772115	0.747567
31	6	0	-3.373424	-0.807050	1.134120
32	6	0	-1.454126	-3.863213	0.866671
33	6	0	-3.427078	-2.818608	0.020105
34	6	0	-3.824672	0.361561	1.699482
35	6	0	-4.149193	-1.537899	0.270715
36	6	0	-1.793826	-5.022116	0.134526
37	1	0	-0.577438	-3.839983	1.492838
38	6	0	-3.779494	-3.908392	-0.738127

39	6	0	-5.081924	0.842750	1.289834
40	1	0	-3.236871	0.896096	2.426952
41	6	0	-5.363921	-1.095683	-0.188503
42	6	0	-2.941852	-5.036155	-0.683424
43	1	0	-1.171428	-5.898775	0.200335
44	1	0	-4.667902	-3.904915	-1.347991
45	6	0	-5.846221	0.132631	0.330724
46	1	0	-5.464615	1.757979	1.708923
47	1	0	-5.930654	-1.661491	-0.907501
48	1	0	-3.178699	-5.913342	-1.262480
49	6	0	7.197804	-0.648256	0.087133
50	6	0	8.022544	-0.060371	1.007888
51	16	0	7.879273	-2.167379	-0.503059
52	6	0	9.183890	-0.935223	1.371337
53	1	0	7.858532	0.913543	1.433911
54	6	0	9.164416	-2.120804	0.700564
55	1	0	9.939813	-0.656514	2.085382
56	1	0	9.831292	-2.945532	0.879595
57	6	0	-7.165080	0.677118	-0.127696
58	6	0	-7.996343	0.075422	-1.040678
59	16	0	-7.855744	2.191320	0.469522
60	6	0	-9.312368	0.776879	-1.154430
61	1	0	-7.742238	-0.804445	-1.604612
62	6	0	-9.391134	1.861570	-0.330314
63	1	0	-10.104867	0.454515	-1.807803
64	1	0	-10.277050	2.448368	-0.163183
65	7	0	-2.058305	-1.436646	1.354266
66	7	0	2.073933	1.460594	-1.386843

Rotational constants (GHZ): 0.1381161 0.0305733 0.0262602
The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -2368.45122171 A.U. after 129 cycles
Convg = 0.1583D-06 -V/T = 2.0076

Table S7. Cartesian Coordinates (Å) of the Optimized Structure of **P7** at the B3LYP/6-31G Level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.697700	0.004877	0.049145
2	6	0	-1.475186	0.008933	-1.162052
3	6	0	-2.860027	0.008259	-1.152082
4	6	0	-3.576047	0.003008	0.064175
5	6	0	-2.847426	-0.001068	1.272822
6	6	0	-1.462456	0.000166	1.268408
7	6	0	0.743875	0.005177	0.041421
8	6	0	1.512968	-0.008288	-1.181159
9	6	0	2.894029	-0.008885	-1.191907
10	6	0	3.616265	0.004645	0.025451
11	6	0	2.907675	0.018441	1.250789
12	6	0	1.526502	0.018578	1.255407
13	1	0	-0.976220	0.015686	-2.123973
14	1	0	-3.410283	0.012543	-2.088709
15	1	0	-3.387962	-0.006134	2.215118
16	1	0	-0.953326	-0.005836	2.224997
17	1	0	1.000834	-0.021355	-2.135272
18	1	0	3.428890	-0.020521	-2.137909
19	1	0	3.453020	0.029596	2.190800
20	1	0	1.024978	0.031925	2.215190
21	6	0	-5.835723	1.132713	0.088055
22	6	0	-5.833013	-1.131958	0.051935
23	6	0	-5.482158	2.485970	0.102199
24	6	0	-7.201936	0.725414	0.079981
25	6	0	-5.476151	-2.484133	0.023908
26	6	0	-7.200195	-0.727900	0.056582
27	6	0	-6.505778	3.429281	0.115304
28	1	0	-4.440854	2.785788	0.109594
29	6	0	-8.212464	1.689523	0.082739
30	6	0	-6.497480	-3.429860	0.007078
31	1	0	-4.434124	-2.781515	0.022346
32	6	0	-8.208404	-1.694057	0.028581
33	6	0	-7.877185	3.057182	0.109632
34	1	0	-6.248975	4.483023	0.149538
35	1	0	-9.255122	1.391412	0.040967
36	6	0	-7.869775	-3.061047	0.012447
37	1	0	-6.238169	-4.483548	0.008518
38	1	0	-9.251808	-1.397375	-0.003900
39	6	0	5.875066	1.127709	-0.001618
40	6	0	5.872773	-1.124111	0.024149
41	6	0	5.500106	2.479369	-0.016420
42	6	0	7.250173	0.732347	-0.006052

43	6	0	5.494570	-2.474515	0.043872
44	6	0	7.248470	-0.732271	0.009519
45	6	0	6.508582	3.431000	-0.034885
46	1	0	4.454433	2.757457	-0.012638
47	6	0	8.243242	1.691934	-0.024695
48	6	0	6.500982	-3.428837	0.047744
49	1	0	4.448256	-2.750045	0.054045
50	6	0	8.239493	-1.694422	0.013964
51	6	0	7.888709	3.075834	-0.038697
52	1	0	6.233344	4.478970	-0.043428
53	1	0	9.286925	1.400987	-0.033052
54	6	0	7.881684	-3.077202	0.031900
55	1	0	6.223260	-4.476142	0.058022
56	1	0	9.284001	-1.406258	0.010038
57	7	0	-5.014012	0.001343	0.071327
58	7	0	5.068303	0.003105	0.016874
59	6	0	8.916657	-4.086699	0.034413
60	6	0	10.292486	-3.934523	-0.050037
61	16	0	8.506061	-5.864531	0.160001
62	6	0	11.031459	-5.150207	-0.020492
63	1	0	10.772134	-2.968593	-0.139935
64	6	0	10.247325	-6.269677	0.087567
65	1	0	12.111461	-5.192223	-0.079354
66	1	0	10.546537	-7.305094	0.131769
67	6	0	8.925833	4.082410	-0.057200
68	6	0	10.303418	3.925495	-0.017036
69	16	0	8.517111	5.863150	-0.143716
70	6	0	11.044675	5.139393	-0.051168
71	1	0	10.782722	2.957027	0.041307
72	6	0	10.260872	6.262469	-0.118559
73	1	0	12.126093	5.177807	-0.025374
74	1	0	10.561859	7.297631	-0.156324
75	6	0	-8.927210	-4.073538	0.009111
76	6	0	-10.211229	-3.996825	0.491460
77	16	0	-8.648544	-5.722544	-0.733342
78	6	0	-10.998694	-5.182172	0.307052
79	1	0	-10.584731	-3.116432	1.000289
80	6	0	-10.335292	-6.198244	-0.315767
81	1	0	-12.025044	-5.268675	0.644286
82	1	0	-10.679907	-7.189235	-0.566094
83	6	0	-8.937108	4.066654	0.138417
84	6	0	-10.221319	3.971227	0.616896
85	16	0	-8.662022	5.739459	-0.550139
86	6	0	-11.011695	5.159881	0.470018
87	1	0	-10.593044	3.073960	1.096732
88	6	0	-10.350403	6.197181	-0.119154
89	1	0	-12.038554	5.232831	0.808904
90	1	0	-10.697335	7.194850	-0.337743

Rotational constants (GHZ): 0.0449997 0.0107580 0.0087505
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3702.44940052 A.U. after 7 cycles
Convg = 0.6671D-08 -V/T = 2.0040

Table S8. Cartesian Coordinates (Å) of the Optimized Structure of **P8** at the B3LYP/6-31G Level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.698625	-0.992552	0.323951
2	6	0	0.824439	-0.971160	1.719965
3	6	0	2.096282	-0.974378	2.309498
4	6	0	3.241825	-1.008890	1.502931
5	6	0	3.115645	-1.027214	0.107366
6	6	0	1.844986	-1.014868	-0.482335
7	6	0	-0.698961	-0.992790	-0.323718
8	6	0	-1.845211	-1.018268	0.482400
9	6	0	-3.115938	-1.030350	-0.107324
10	6	0	-3.241934	-1.008736	-1.502866
11	6	0	-2.096311	-0.971730	-2.309543
12	6	0	-0.824572	-0.968234	-1.719731
13	1	0	-0.050289	-0.951593	2.335696
14	1	0	2.192364	-0.952013	3.375020
15	1	0	3.989954	-1.050654	-0.508666
16	1	0	-3.990216	-1.055617	0.508569
17	1	0	-2.192331	-0.947437	-3.375128
18	1	0	0.050089	-0.946504	-2.335184
19	6	0	5.133067	0.352322	2.187206
20	6	0	5.541901	-1.722773	1.225062
21	6	0	4.794351	1.340003	3.040781
22	6	0	6.099652	0.536682	1.219978
23	6	0	5.655204	-3.048249	1.010991
24	6	0	6.365224	-0.817650	0.591494
25	6	0	5.388055	2.606355	2.853501
26	1	0	4.092131	1.170984	3.830543
27	6	0	6.670334	1.727531	0.967882
28	6	0	6.578301	-3.483133	0.037994
29	1	0	5.057888	-3.748324	1.556969
30	6	0	7.235363	-1.165183	-0.374774

31	6	0	6.312010	2.806433	1.797040	
32	1	0	5.138216	3.416365	3.507039	
33	1	0	7.374963	1.849123	0.171856	
34	6	0	7.354651	-2.535913	-0.675942	
35	1	0	6.690207	-4.528074	-0.163525	
36	1	0	7.818809	-0.430189	-0.889231	
37	6	0	-5.133097	0.352728	-2.186999	
38	6	0	-5.542372	-1.722594	-1.225535	
39	6	0	-4.793943	1.340498	-3.040254	
40	6	0	-6.099662	0.537133	-1.220025	
41	6	0	-5.655788	-3.048120	-1.011938	
42	6	0	-6.365512	-0.817344	-0.591735	
43	6	0	-5.387382	2.606960	-2.852792	
44	1	0	-4.091477	1.171668	-3.829793	
45	6	0	-6.669989	1.728101	-0.967451	
46	6	0	-6.579008	-3.483099	-0.039007	
47	1	0	-5.058634	-3.748185	-1.558192	
48	6	0	-7.235484	-1.165019	0.374433	
49	6	0	-6.311699	2.806978	-1.796519	
50	1	0	-5.137436	3.417035	-3.506219	
51	1	0	-7.374677	1.849378	-0.171405	
52	6	0	-7.354937	-2.535862	0.675337	
53	1	0	-6.691093	-4.527995	0.162190	
54	1	0	-7.818608	-0.430091	0.889160	
55	6	0	-6.927547	4.197172	-1.556659	
56	6	0	-7.824683	4.485142	-0.576524	
57	16	0	-6.562781	5.643098	-2.512034	
58	6	0	-8.108261	6.007192	-0.472687	
59	1	0	-8.274080	3.749043	0.057160	
60	6	0	-7.398190	6.723909	-1.384363	
61	1	0	-8.775760	6.442379	0.241174	
62	1	0	-7.347746	7.792437	-1.413706	
63	6	0	-8.328228	-3.005793	1.772693	
64	6	0	-9.121814	-2.183132	2.509146	
65	16	0	-8.573490	-4.694910	2.245679	
66	6	0	-10.123621	-2.973999	3.392431	
67	1	0	-9.070129	-1.115079	2.474804	
68	6	0	-9.990806	-4.318490	3.238966	
69	1	0	-10.843068	-2.514544	4.037880	
70	1	0	-10.653144	-5.047332	3.656693	
71	6	0	8.328077	-3.005981	-1.773080	
72	6	0	9.122100	-2.183527	-2.509391	
73	16	0	8.572671	-4.695074	-2.246381	
74	6	0	10.123778	-2.974610	-3.392551	
75	1	0	9.070825	-1.115420	-2.474708	
76	6	0	9.990533	-4.318973	-3.239150	
77	1	0	10.843615	-2.515281	-4.037643	
78	1	0	10.652644	-5.048105	-3.657096	
79	6	0	6.928075	4.196566	1.557208	S30

80	6	0	7.825022	4.484401	0.576902
81	16	0	6.563633	5.642582	2.512676
82	6	0	8.108903	6.006421	0.473092
83	1	0	8.274254	3.748322	-0.056876
84	6	0	7.399002	6.723330	1.384959
85	1	0	8.776217	6.441573	-0.240879
86	1	0	7.348635	7.791681	1.414254
87	6	0	1.709611	-1.027448	-2.016686
88	1	0	0.801942	-1.523150	-2.290666
89	1	0	1.690919	-0.021763	-2.381336
90	1	0	2.542639	-1.546272	-2.443923
91	6	0	-1.710103	-1.035020	2.016718
92	1	0	-0.801877	-1.530624	2.289339
93	1	0	-1.692392	-0.030388	2.384095
94	1	0	-2.542541	-1.555914	2.442328
95	7	0	-4.576640	-1.026967	-2.118522
96	7	0	4.576479	-1.027208	2.118280

Rotational constants (GHZ): 0.0413703 0.0131930 0.0113712
The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -3782.02533325 A.U. after 37 cycles
Convg = 0.4806D-08 -V/T = 2.0031

Table S9. Cartesian Coordinates (Å) of the Optimized Structure of **P9** at the B3LYP/6-31G Level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.025707	-3.011007	0.433519
2	6	0	3.915776	-3.412965	1.211041
3	6	0	2.991281	-2.460600	1.686675
4	6	0	3.202234	-1.151218	1.369110
5	6	0	4.341953	-0.748691	0.678731
6	6	0	5.240173	-1.642071	0.167726
7	1	0	3.773553	-4.453840	1.440849
8	1	0	2.143151	-2.761713	2.276432
9	1	0	6.085004	-1.313561	-0.410458
10	6	0	3.202862	1.141365	1.373754
11	6	0	2.992446	2.449066	1.696202

12	6	0	3.917653	3.403064	1.224771	
13	6	0	5.027739	3.004085	0.446809	
14	6	0	5.241093	1.636787	0.175267	
15	6	0	4.342283	0.741491	0.682059	
16	1	0	2.143825	2.748219	2.286279	
17	1	0	3.774891	4.443162	1.457689	
18	1	0	6.085489	1.310440	-0.404811	
19	6	0	1.140824	-0.004603	0.811064	
20	6	0	-0.130910	-0.004278	1.390160	
21	6	0	1.270669	-0.004193	-0.582008	
22	6	0	-1.270687	-0.004169	0.582052	
23	1	0	-0.229587	-0.004112	2.461471	
24	6	0	0.130904	-0.004303	-1.390109	
25	1	0	2.246780	-0.003800	-1.032595	
26	6	0	-1.140841	-0.004610	-0.811035	
27	1	0	-2.246791	-0.003752	1.032647	
28	1	0	0.229592	-0.004150	-2.461412	
29	6	0	-3.202882	1.141352	-1.373871	
30	6	0	-3.202257	-1.151222	-1.369215	
31	6	0	-2.992538	2.449053	-1.696384	
32	6	0	-4.342300	0.741499	-0.682187	
33	6	0	-2.991380	-2.460605	-1.686830	
34	6	0	-4.341970	-0.748696	-0.678851	
35	6	0	-3.917773	3.403029	-1.224984	
36	1	0	-2.143952	2.748216	-2.286502	
37	6	0	-5.241121	1.636770	-0.175405	
38	6	0	-3.915907	-3.412931	-1.211213	
39	1	0	-2.143277	-2.761747	-2.276618	
40	6	0	-5.240209	-1.642037	-0.167866	
41	6	0	-5.027793	3.004068	-0.446921	
42	1	0	-3.775082	4.443116	-1.457999	
43	1	0	-6.085528	1.310396	0.404648	
44	6	0	-5.025778	-3.010968	-0.433620	
45	1	0	-3.773761	-4.453801	-1.441098	
46	1	0	-6.085048	-1.313498	0.410287	
47	6	0	5.983605	-4.046099	-0.105203	
48	6	0	7.092737	-3.785613	-0.856679	
49	16	0	5.804563	-5.777813	0.185508	
50	6	0	7.926181	-5.013492	-1.089481	
51	1	0	7.351823	-2.814084	-1.234892	
52	6	0	7.389472	-6.116139	-0.503191	
53	1	0	8.843617	-5.013706	-1.650003	
54	1	0	7.863677	-7.078137	-0.443036	
55	6	0	5.986418	4.041844	-0.088527	
56	6	0	7.087155	3.786063	-0.852620	
57	16	0	5.797514	5.773610	0.194480	
58	6	0	7.732578	5.042917	-1.364048	
59	1	0	7.452368	2.800600	-1.075216	
60	6	0	7.079364	6.159992	-0.949018	

61	1	0	8.606102	5.052024	-1.990752
62	1	0	7.292507	7.160167	-1.277829
63	6	0	-5.983625	-4.046063	0.105229
64	6	0	-7.092614	-3.785606	0.856917
65	16	0	-5.804642	-5.777760	-0.185604
66	6	0	-7.925970	-5.013520	1.089895
67	1	0	-7.351658	-2.814080	1.235187
68	6	0	-7.389374	-6.116137	0.503458
69	1	0	-8.843273	-5.013773	1.650634
70	1	0	-7.863559	-7.078147	0.443398
71	6	0	-5.986414	4.041842	0.088556
72	6	0	-7.087006	3.786079	0.852855
73	16	0	-5.797583	5.773603	-0.194522
74	6	0	-7.732319	5.042947	1.364415
75	1	0	-7.452192	2.800624	1.075522
76	6	0	-7.079195	6.160014	0.949235
77	1	0	-8.605708	5.052063	1.991307
78	1	0	-7.292264	7.160195	1.278080
79	7	0	2.323207	-0.005599	1.684437
80	7	0	-2.323183	-0.005614	-1.684496

Rotational constants (GHZ): 0.0443101 0.0241892 0.0163447
The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -3472.48780067 A.U. after 82 cycles
Convg = 0.3483D-08 -V/T = 2.0032