

Supporting Information

Synthesis of Functionalized 1,3,2-Benzodiazaborole Cores Using Bench Stable Components

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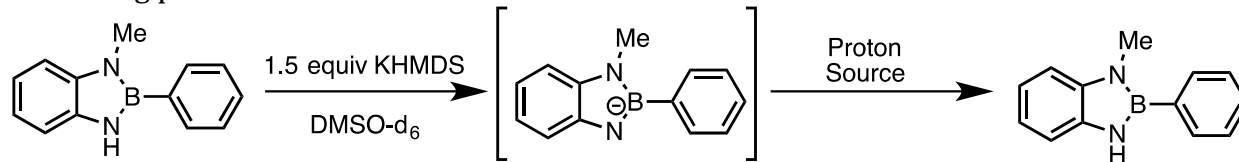
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Bracketing pKa studies:



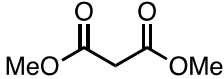
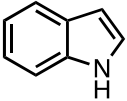
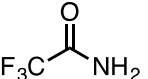
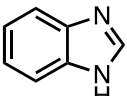
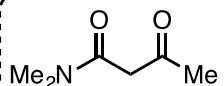
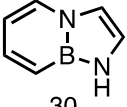

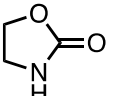
	pKa (DMSO)	Deprotonated?	Reference pKas
	15.7	Yes	 20.95
	17.2	Yes	 16.4
	18.2	50/50	 30
	19.6	No	
	20.9	No	

Table of Bond Lengths

Name	Structure	Bond Lengths (Angstroms)												
		1-2	2-3	3-4	4-5	5-6	6-7	7-8	8-9	4-9	9-1	1-10	2-11	3-12
2a		1.391	1.358	1.398	1.361	1.367	1.425	1.374	1.502	1.460	1.441	-	1.490	-
2b		1.395	1.360	1.395	1.360	1.367	1.425	1.375	1.503	1.459	1.441	1.449	1.491	-
3		-	-	1.390	1.396	1.389	1.389	1.389	1.396	1.412	1.390	-	-	-
5a		1.437	1.437	1.393	1.388	1.395	1.395	1.395	1.388	1.410	1.393	-	1.555	-
6a		1.439	1.438	1.392	1.387	1.395	1.395	1.395	1.388	1.411	1.392	-	1.545	-
6d		1.435	1.435	1.395	1.388	1.394	1.396	1.394	1.388	1.411	1.392	-	1.516	-
7a		1.436	1.437	1.394	1.387	1.395	1.395	1.395	1.387	1.410	1.395	-	1.570	-
7f		1.435	1.439	1.395	1.388	1.397	1.394	1.396	1.386	1.411	1.393	-	1.571	1.447
8a		1.385	1.368	1.435	1.401	1.385	1.405	1.387	1.393	1.418	1.380	-	1.491	-
8b		1.391	1.370	1.432	1.400	1.386	1.404	1.388	1.394	1.418	1.381	1.447	1.492	-
8c		1.389	1.372	1.441	1.401	1.386	1.404	1.387	1.393	1.416	1.377	-	1.492	1.497
9		1.380	1.307	1.389	1.395	1.388	1.404	1.389	1.391	1.410	1.384	-	1.490	-

Computational Compounds:

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 2-methyl "fused" BN-indole (**2a**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.490475
3	7	0	1.178547	0.000000	2.230146
4	5	0	0.860734	-0.000407	3.635206
5	6	0	1.567411	-0.000592	4.961107
6	6	0	0.768291	-0.001067	6.079391
7	6	0	-0.655215	-0.001367	6.010606
8	6	0	-1.311820	-0.001203	4.812170
9	7	0	-0.599500	-0.000740	3.653037
10	6	0	-1.064105	-0.000518	2.334604
11	1	0	-2.114133	-0.000694	2.090567
12	1	0	-2.392921	-0.001426	4.737981
13	1	0	-1.238601	-0.001733	6.921783
14	1	0	1.215785	-0.001229	7.069454
15	1	0	2.643916	-0.000384	5.095247
16	1	0	2.074207	0.000495	1.773503
17	1	0	-1.020462	0.000151	-0.383250
18	1	0	0.509768	-0.882814	-0.398970
19	1	0	0.510065	0.882620	-0.399061

E_{Tot}: -406.713074625 Hartree

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 1,2-dimethyl "fused" BN-indole (**2b**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	-3.138225	-0.847908	0.000167
2	6	0	-1.668843	-0.592351	-0.000067
3	7	0	-1.126480	0.693132	0.000175
4	5	0	0.309979	0.580185	0.000122
5	6	0	1.507881	1.488215	0.000171
6	6	0	2.738917	0.876037	0.000075
7	6	0	2.895337	-0.540490	-0.000091
8	6	0	1.815460	-1.378101	-0.000079
9	7	0	0.558633	-0.857467	-0.000004
10	6	0	-0.670586	-1.516467	-0.000077
11	1	0	-0.753647	-2.591377	-0.000140
12	1	0	1.912733	-2.457423	-0.000193
13	1	0	3.887176	-0.972785	-0.000201
14	1	0	3.645823	1.474384	0.000081
15	1	0	1.473492	2.572725	0.000271
16	6	0	-1.935596	1.895488	-0.000307
17	1	0	-1.276740	2.762270	-0.000456
18	1	0	-2.573790	1.957170	0.886216
19	1	0	-2.573621	1.956518	-0.886874

20	1	0	-3.331418	-1.920638	-0.000928
21	1	0	-3.625174	-0.419926	0.881854
22	1	0	-3.625869	-0.418037	-0.880198

E_{Tot}: -446.028825381 Hartree

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of *o*-phenylenediamine (**3**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.389082
3	6	0	1.209633	0.000000	2.072587
4	6	0	2.432967	0.000000	1.400385
5	6	0	2.432967	0.000000	-0.011303
6	6	0	1.209633	0.000000	-0.683505
7	1	0	1.216069	0.000000	-1.768950
8	7	0	3.622025	0.000000	-0.730961
9	1	0	3.597916	0.000000	-1.733809
10	1	0	4.525158	0.000000	-0.300448
11	7	0	3.622025	0.000000	2.120043
12	1	0	4.525158	0.000000	1.689530
13	1	0	3.597916	0.000000	3.122891
14	1	0	1.216069	0.000000	3.158032
15	1	0	-0.930979	0.000000	1.942111
16	1	0	-0.930979	0.000000	-0.553029
17	0	0	1.214200	0.000000	0.694541
18	0	0	1.214200	1.000000	0.694541
19	0	0	1.214200	-1.000000	0.694540

E_{Tot}: -343.061786471 Hartree

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5a**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	4.305261	0.690310	-0.101690
2	6	0	3.109330	1.400448	-0.204267
3	6	0	1.917291	0.698103	-0.099649
4	6	0	1.917338	-0.698092	0.099884
5	6	0	3.109442	-1.400383	0.204128
6	6	0	4.305310	-0.690220	0.101033
7	1	0	5.246890	-1.219847	0.178860
8	1	0	3.112788	-2.473298	0.359247
9	7	0	0.592388	-1.125573	0.155726
10	5	0	-0.286691	-0.000039	0.000328
11	7	0	0.592328	1.125521	-0.155165
12	1	0	0.364934	2.088169	-0.337085
13	6	0	-1.842093	-0.000064	0.000335
14	6	0	-2.572608	-1.170387	-0.256590
15	6	0	-3.962543	-1.174483	-0.258884

16	6	0	-4.662436	-0.000008	-0.000514
17	6	0	-3.962551	1.174552	0.258471
18	6	0	-2.572710	1.170300	0.257045
19	1	0	-2.047631	2.094775	0.474093
20	1	0	-4.500848	2.092542	0.464417
21	1	0	-5.746151	0.000117	-0.001361
22	1	0	-4.500822	-2.092527	-0.464638
23	1	0	-2.047451	-2.094896	-0.473357
24	1	0	0.365234	-2.088232	0.337905
25	1	0	3.112536	2.473327	-0.359644
26	1	0	5.246796	1.219974	-0.179824

E_{Tot}: -598.536528558 Hartree

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 2-vinyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6a**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.389848
3	6	0	1.195837	0.000000	2.124305
4	5	0	1.190825	-0.000528	3.679699
5	7	0	0.121818	0.391972	4.555430
6	6	0	0.523195	0.245797	5.881637
7	6	0	-0.144301	0.497908	7.071628
8	6	0	0.523585	0.245294	8.269621
9	6	0	1.828723	-0.248222	8.273685
10	6	0	2.504194	-0.500516	7.079890
11	6	0	1.844319	-0.247955	5.885750
12	7	0	2.254188	-0.393541	4.562058
13	1	0	3.156267	-0.777468	4.337662
14	1	0	3.519026	-0.881690	7.086359
15	1	0	2.326394	-0.437935	9.216800
16	1	0	0.019902	0.434659	9.209610
17	1	0	-1.159063	0.879324	7.071712
18	1	0	-0.778848	0.775802	4.325280
19	1	0	1.973428	0.145330	1.809187
20	1	0	-0.951187	-0.014325	1.911874
21	1	0	-0.939065	-0.004498	-0.541313
22	1	0	0.764661	0.157912	-0.400065
23	1	0	0.106870	0.116889	-0.855962

E_{Tot}: -484.170539338 Hartree

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 2-(1-propynyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6d**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	0.000000	0.000000	0.000000
2	6	0	1.523352	-0.225828	0.000000
3	6	0	2.711567	-0.401973	0.000000

4	5	0	4.234919	-0.627801	0.000000
5	7	0	5.120374	0.488071	0.000000
6	6	0	6.455252	-0.009223	0.000000
7	6	0	7.718021	0.650030	0.000000
8	6	0	8.920335	-0.113934	0.000000
9	6	0	8.859880	-1.537151	0.000000
10	6	0	7.597111	-2.196404	0.000000
11	6	0	6.394797	-1.432440	0.000000
12	7	0	5.022556	-1.814742	0.000000
13	1	0	4.750888	-2.870344	0.000000
14	1	0	7.550852	-3.285421	0.000000
15	1	0	9.779868	-2.121721	0.000000
16	1	0	9.886582	0.390513	0.000000
17	1	0	7.764280	1.739048	0.000000
18	1	0	4.942527	1.543187	0.000000
19	1	0	-0.208708	1.069832	0.000000
20	1	0	-0.434754	-0.454997	-0.889981
21	1	0	-0.434754	-0.454997	0.889981

E_{Tot}: -482.932836614 Hartree

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 2-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7a**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	5	0	0.000000	0.000000	1.570050
3	7	0	1.132880	0.000000	2.451855
4	6	0	0.702979	0.007694	3.778662
5	6	0	1.411869	0.010963	4.970647
6	6	0	0.694015	0.018463	6.167164
7	6	0	-0.700640	0.022269	6.166076
8	6	0	-1.417294	0.018622	4.968836
9	6	0	-0.707237	0.011441	3.777358
10	7	0	-1.136160	0.005994	2.450577
11	1	0	-2.115342	0.006976	2.220250
12	1	0	-2.501460	0.021511	4.971694
13	1	0	-1.237177	0.028100	7.107008
14	1	0	1.229335	0.021315	7.108779
15	1	0	2.496030	0.007902	4.974567
16	1	0	2.111719	-0.004322	2.220184
17	1	0	1.007039	-0.082904	-0.415749
18	1	0	-0.588248	-0.829424	-0.404610
19	1	0	-0.439947	0.919343	-0.399934

E_{Tot}: -406.749628439 Hartree

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 1,2-dimethyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7f**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	0.000000	0.000000	0.000000
2	7	0	0.000000	0.000000	1.447194
3	6	0	1.186373	0.000000	2.181121
4	6	0	2.510522	0.000148	1.763908
5	6	0	3.511180	0.000095	2.738108
6	6	0	3.192365	-0.000070	4.094778
7	6	0	1.861896	-0.000177	4.518569
8	6	0	0.865526	-0.000156	3.555443
9	7	0	-0.522603	-0.000152	3.667934
10	5	0	-1.113008	-0.000194	2.359503
11	6	0	-2.642963	-0.000360	2.002118
12	1	0	-3.273383	0.000228	2.894624
13	1	0	-2.922468	-0.878257	1.410722
14	1	0	-2.922440	0.876775	1.409604
15	1	0	-0.975141	-0.000875	4.566126
16	1	0	1.616193	-0.000280	5.574573
17	1	0	3.985748	-0.000106	4.832218
18	1	0	4.550284	0.000192	2.432030
19	1	0	2.767270	0.000293	0.711663

E_{Tot}: -446.067218958 Hartree

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 2-methylindole (**8a**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	-3.265731	-0.995310	0.000000
2	6	0	-1.811961	-0.664456	0.000000
3	7	0	-1.379781	0.651756	0.000000
4	6	0	0.000000	0.690478	0.000000
5	6	0	0.877004	1.772516	0.000000
6	6	0	2.236358	1.496480	0.000000
7	6	0	2.709076	0.173424	0.000000
8	6	0	1.832696	-0.899535	0.000000
9	6	0	0.453772	-0.652869	0.000000
10	6	0	-0.716363	-1.484192	0.000000
11	1	0	-0.745252	-2.562619	0.000000
12	1	0	2.208705	-1.916307	0.000000
13	1	0	3.777583	-0.006086	0.000000
14	1	0	2.945626	2.315428	0.000000
15	1	0	0.515284	2.794568	0.000000
16	1	0	-1.984724	1.455268	0.000000
17	1	0	-3.403294	-2.076129	0.000000
18	1	0	-3.772288	-0.592815	0.883136
19	1	0	-3.772288	-0.592815	-0.883136

E_{Tot}: -403.255153596 Hartree

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 1,2-dimethylindole (**8b**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	0.000000	0.000000	0.000000
2	7	0	0.000000	0.000000	1.446886
3	6	0	1.143486	0.000000	2.221924
4	6	0	2.484512	0.000000	1.840093
5	6	0	3.439585	0.000000	2.847209
6	6	0	3.067843	0.000000	4.201432
7	6	0	1.733626	0.000000	4.576652
8	6	0	0.747057	0.000000	3.583494
9	6	0	-0.684573	0.000000	3.589409
10	6	0	-1.108473	0.000000	2.287135
11	6	0	-2.504481	0.000000	1.760522
12	1	0	-3.205295	0.000000	2.594814
13	1	0	-2.715960	0.882923	1.149127
14	1	0	-2.715960	-0.882923	1.149127
15	1	0	-1.331253	0.000000	4.452860
16	1	0	1.457590	0.000000	5.625061
17	1	0	3.839580	0.000000	4.962008
18	1	0	4.490434	0.000000	2.583395
19	1	0	2.779744	0.000000	0.797678
20	1	0	-1.022819	0.000000	-0.368852
21	1	0	0.505664	0.887466	-0.390757
22	1	0	0.505664	-0.887466	-0.390757

E_{Tot}: -442.573440367 Hartree

Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 2,3-dimethylindole (**8c**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	3.131834	-0.914686	0.000102
2	6	0	1.697530	-0.504982	-0.000124
3	7	0	0.701867	-1.473723	-0.000500
4	6	0	-0.535576	-0.869224	-0.000063
5	6	0	-1.815800	-1.417436	0.000110
6	6	0	-2.890427	-0.539754	0.000197
7	6	0	-2.692101	0.850635	0.000025
8	6	0	-1.415245	1.390731	-0.000174
9	6	0	-0.310913	0.529221	-0.000136
10	6	0	1.114781	0.737625	-0.000237
11	6	0	1.793369	2.071535	0.000255
12	1	0	1.517513	2.661017	0.880465
13	1	0	2.879997	1.975624	-0.000030
14	1	0	1.517080	2.661977	-0.879231
15	1	0	-1.276651	2.465967	-0.000308
16	1	0	-3.553252	1.508199	0.000045
17	1	0	-3.899557	-0.934033	0.000366

18	1	0	-1.971576	-2.490424	0.000145
19	1	0	0.866614	-2.465659	0.001913
20	1	0	3.783282	-0.042213	-0.002685
21	1	0	3.380016	-1.510823	0.884495
22	1	0	3.378751	-1.515558	-0.881407

E_{Tot}: -442.573440367 Hartree

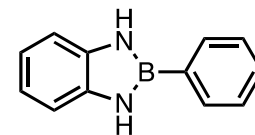
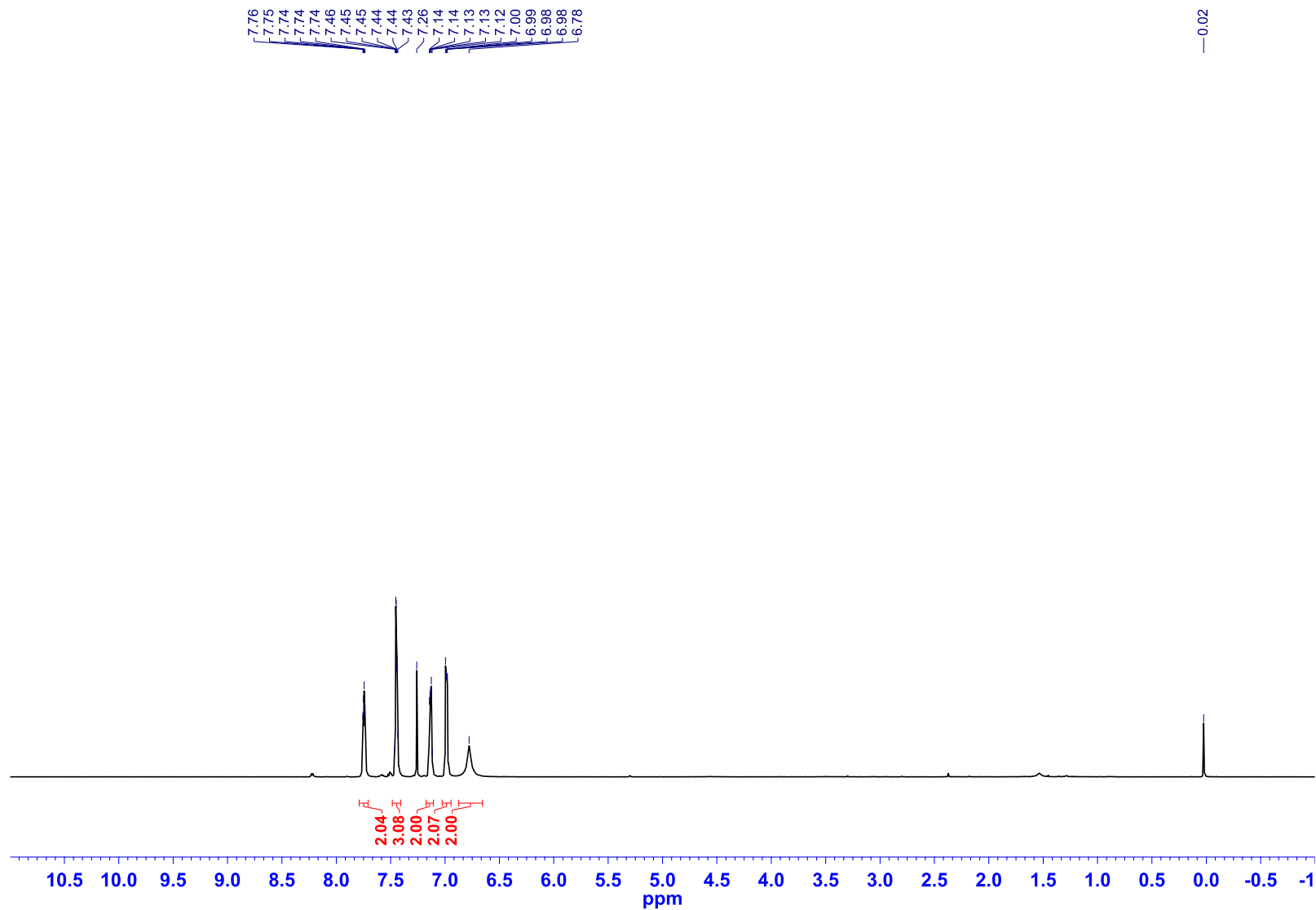
Atomic Coordinates for [B3LYP/6-311+G(2d,p)] optimized geometry value of total energy of 2-methylbenzimidazole (**9**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	X
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.489979
3	7	0	1.169044	0.000000	2.223021
4	6	0	0.817737	-0.000007	3.561390
5	6	0	1.559842	0.000019	4.737512
6	6	0	0.845000	-0.000008	5.928595
7	6	0	-0.559207	-0.000058	5.940137
8	6	0	-1.291790	-0.000074	4.761740
9	6	0	-0.592446	-0.000049	3.554920
10	7	0	-1.064197	-0.000031	2.248840
11	1	0	-2.374704	-0.000087	4.766707
12	1	0	-1.077515	-0.000077	6.891424
13	1	0	1.382881	0.000005	6.868924
14	1	0	2.643472	0.000067	4.734306
15	1	0	2.102780	0.000114	1.847164
16	1	0	0.505834	0.883738	-0.399361
17	1	0	0.505645	-0.883856	-0.399338
18	1	0	-1.029667	0.000111	-0.351102

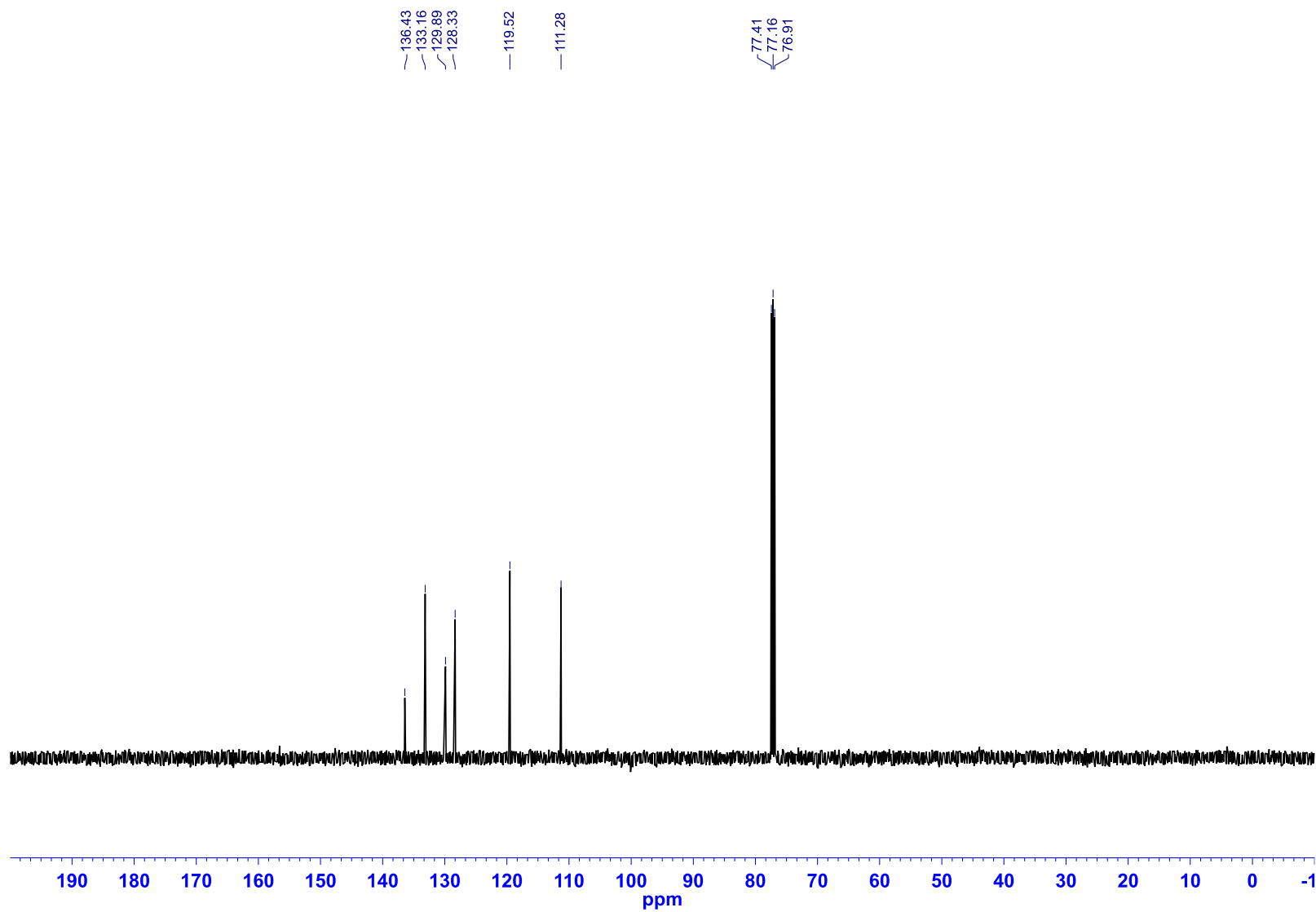
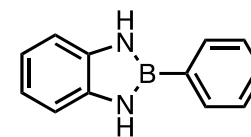
E_{Tot}: -419.31208368 Hartree

NMR Data:

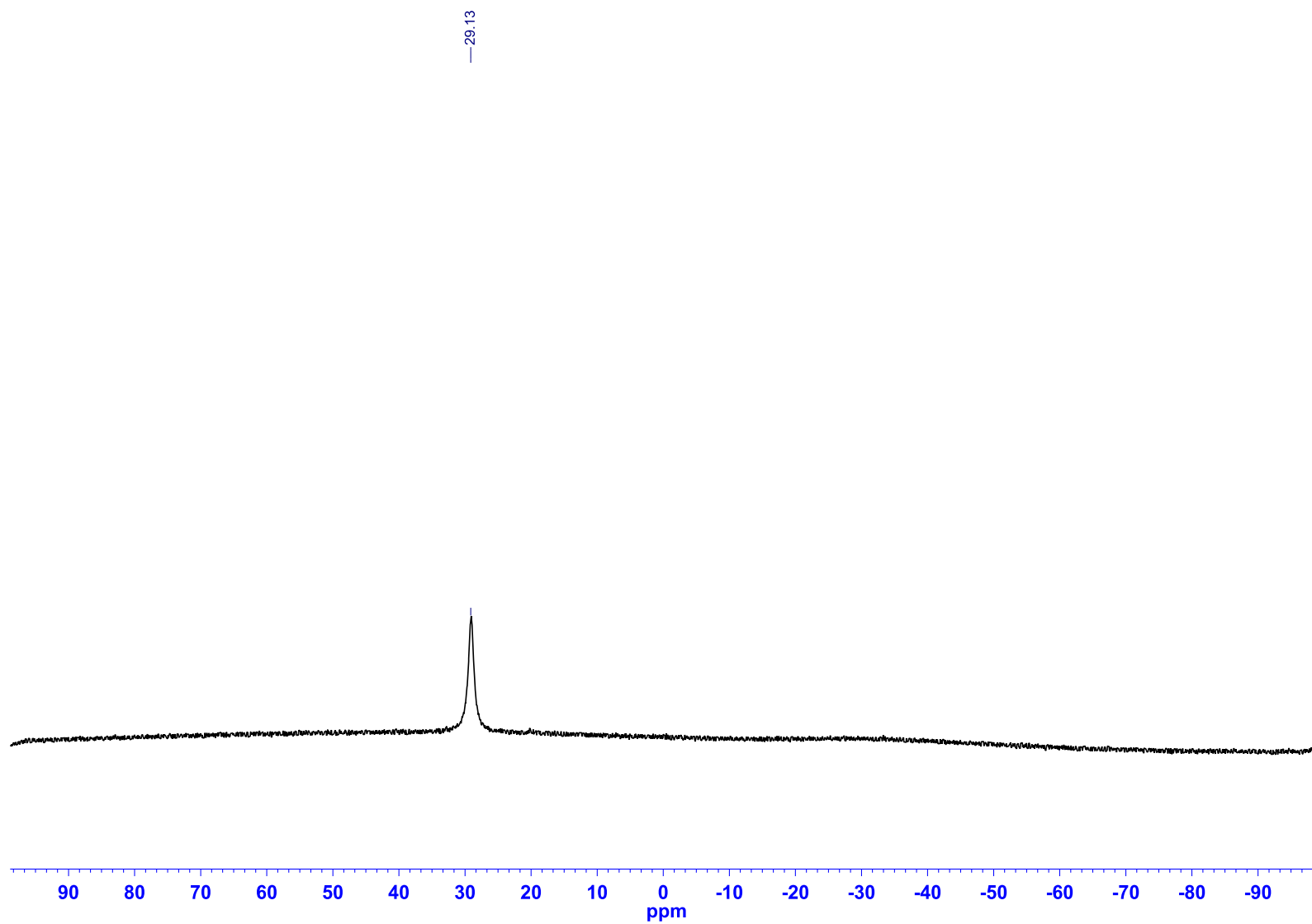
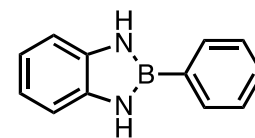
^1H NMR (500.4 MHz, CDCl_3) of 2-Phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5a**)



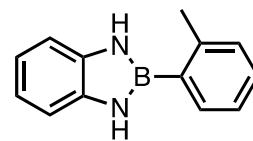
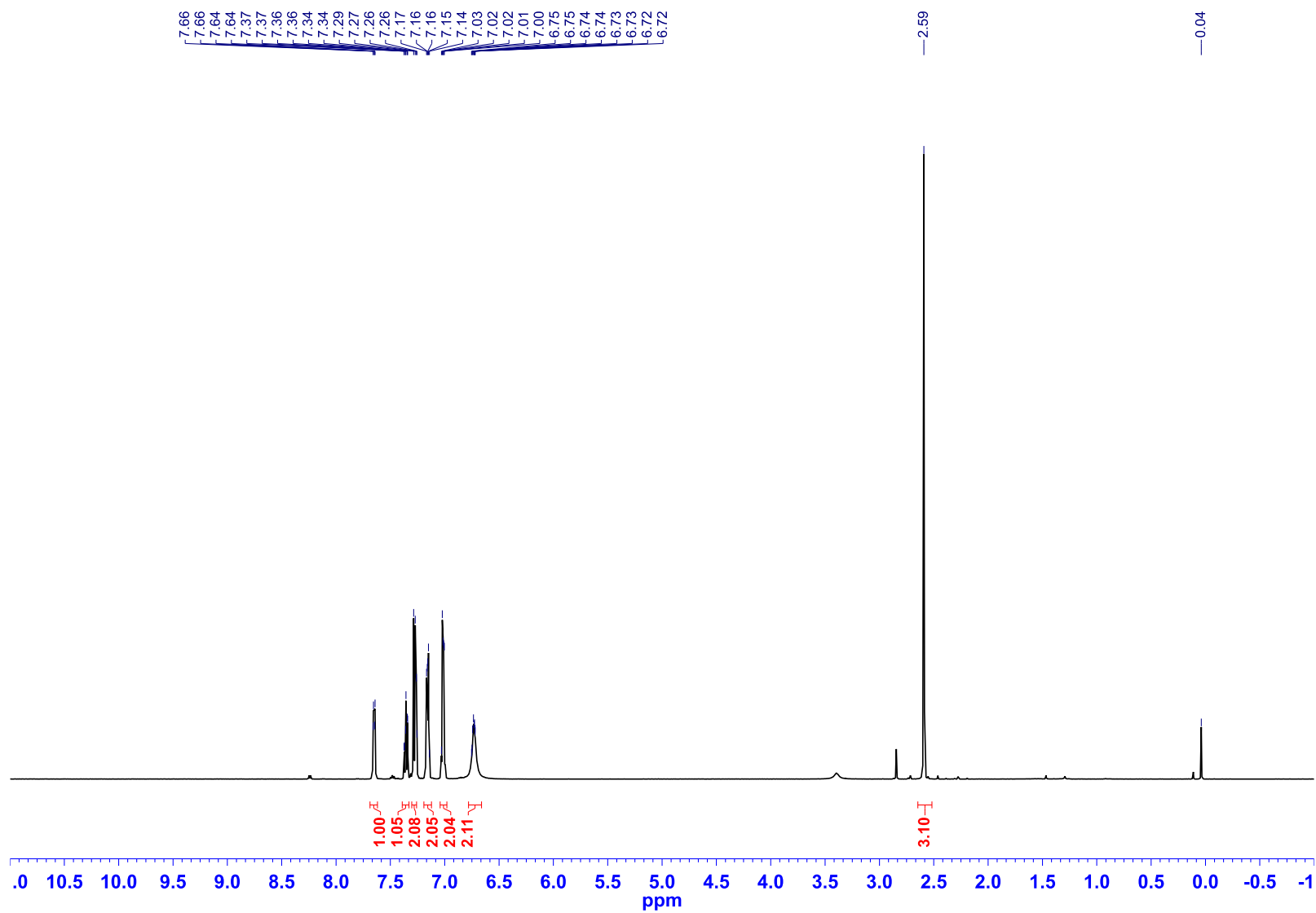
^{13}C NMR (125.8 MHz, CDCl_3) of 2-Phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5a**)



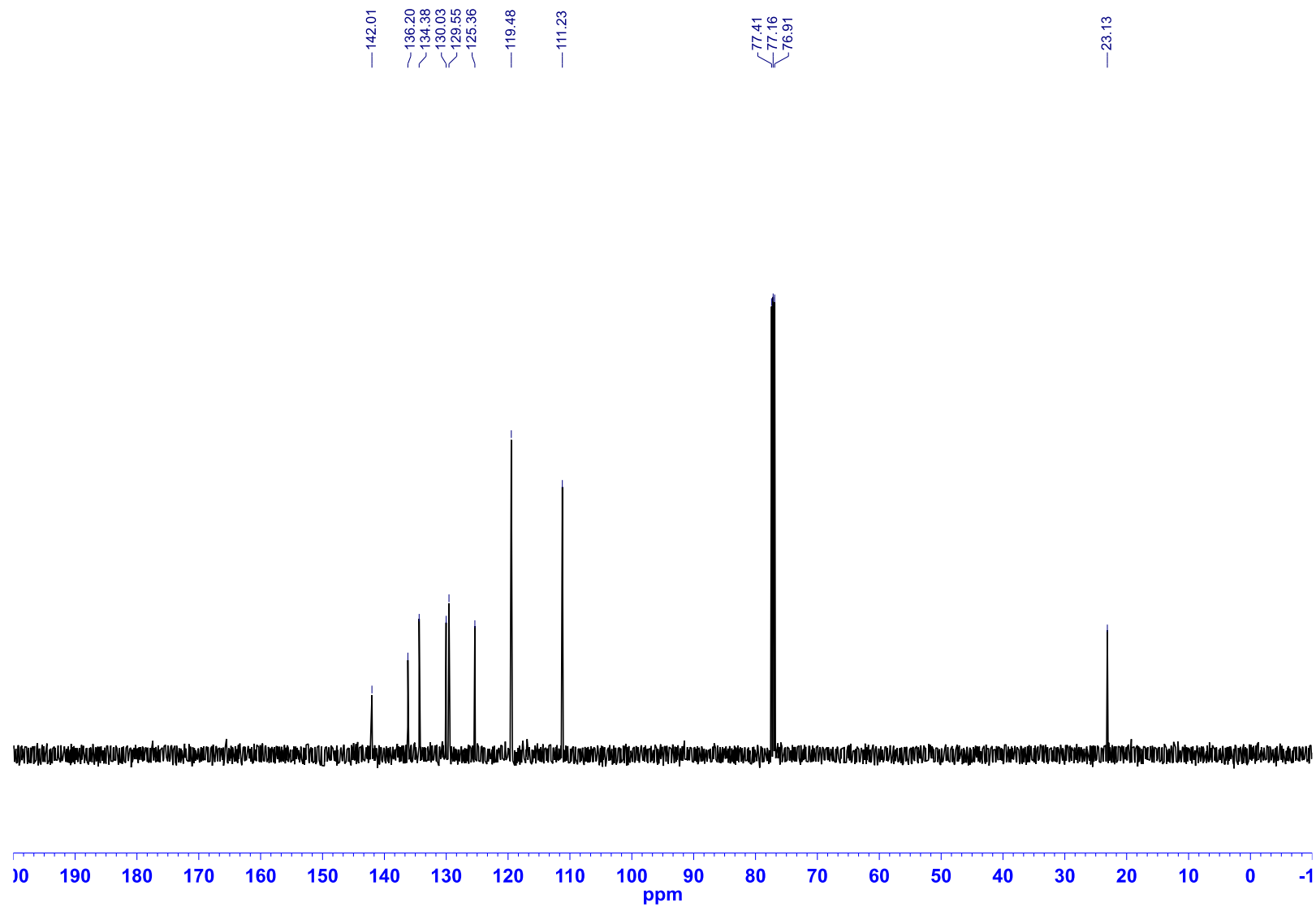
^{11}B NMR (128.4 MHz, MeCN) of 2-Phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5a**)



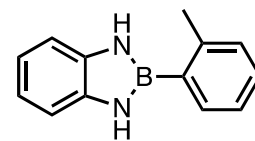
^1H NMR (500.4 MHz, CDCl_3) of 2-(*o*-tolyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5b**)



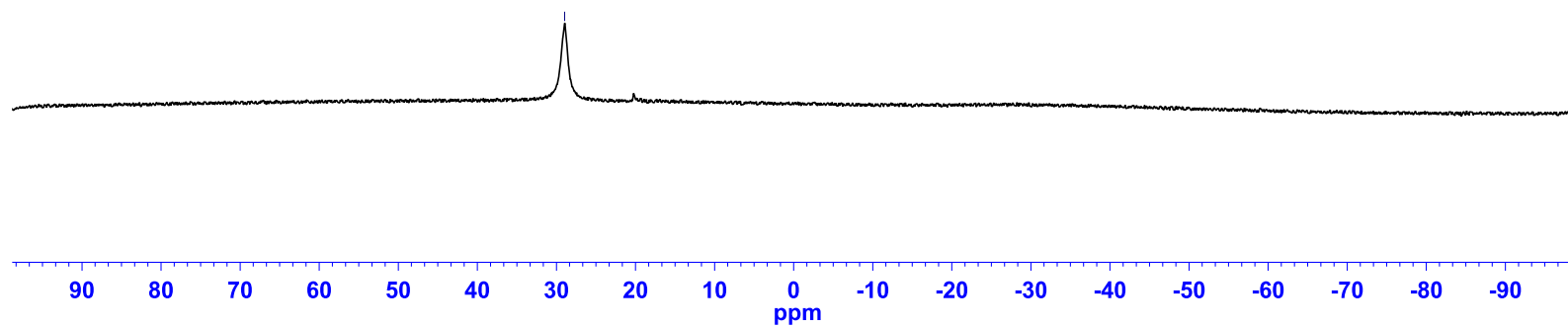
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(*o*-tolyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5b**)



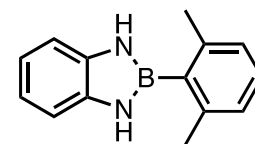
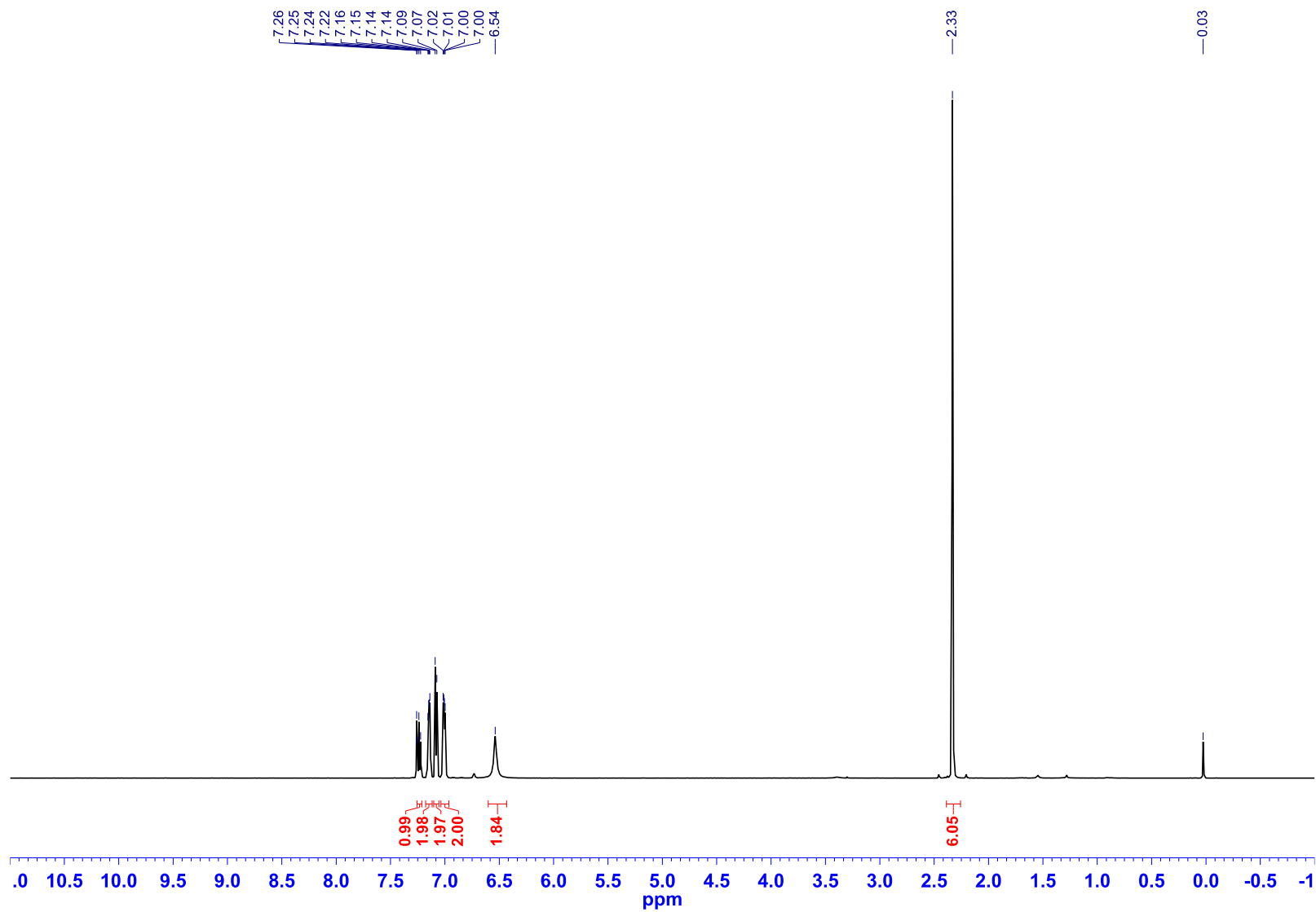
^{11}B NMR (128.4 MHz, MeCN) of 2-(*o*-tolyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5b**)



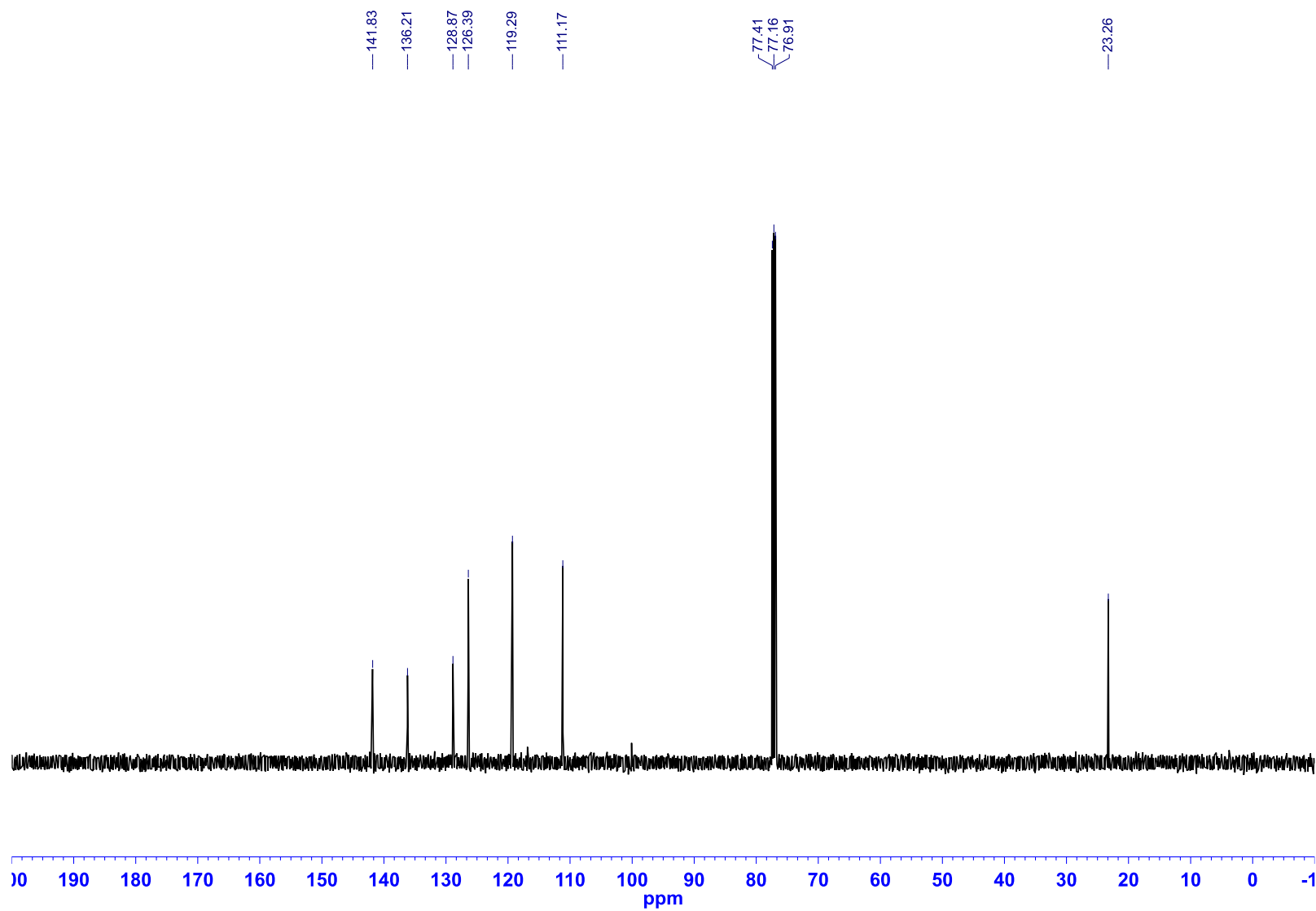
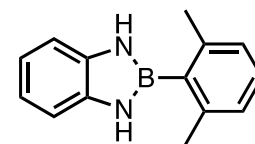
—28.97



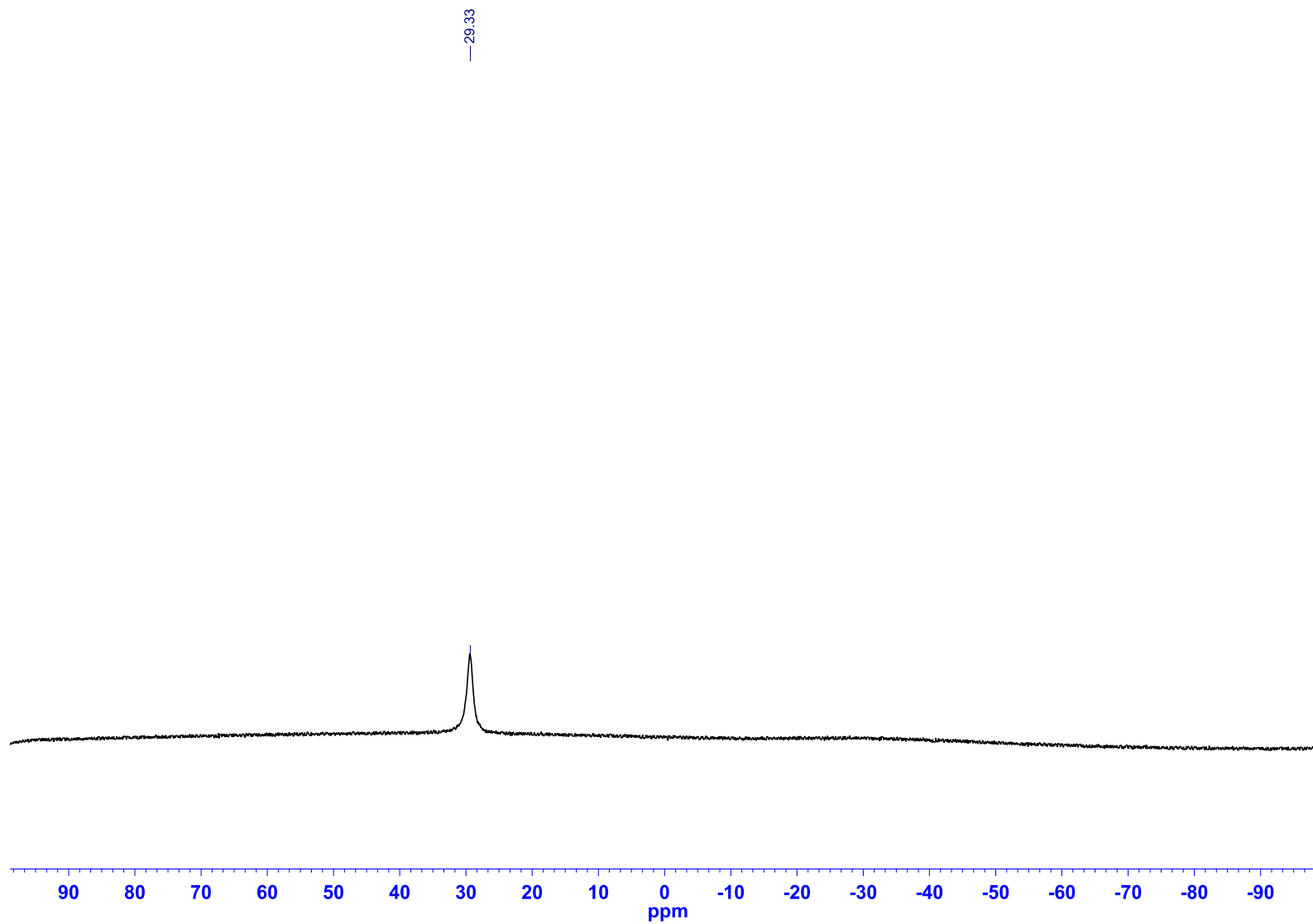
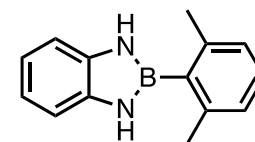
^1H NMR (500.4 MHz, CDCl_3) of 2-(2,6-dimethylphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5c**)



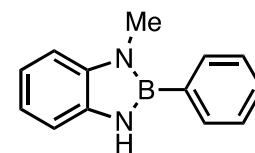
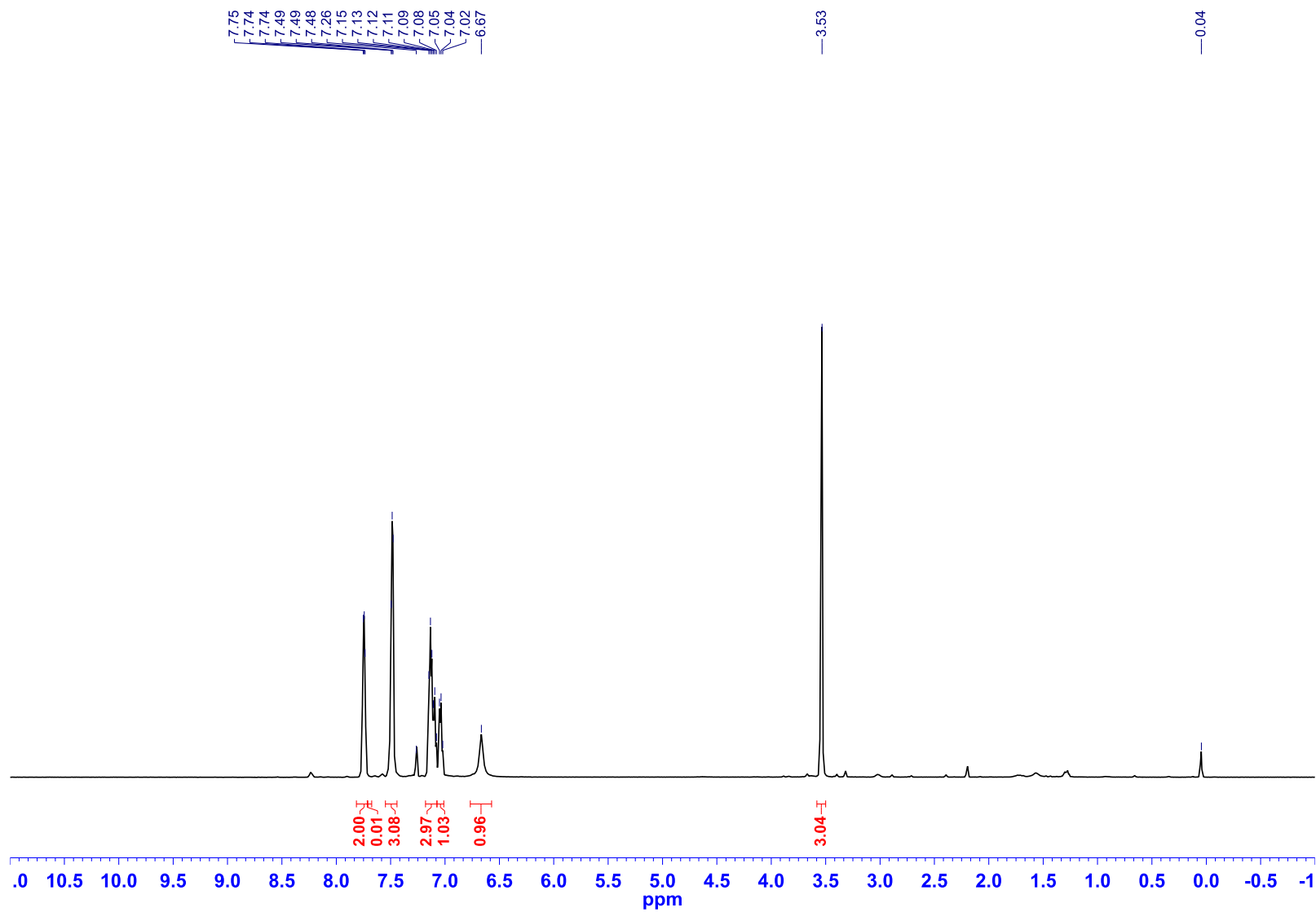
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(2,6-dimethylphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5c**)



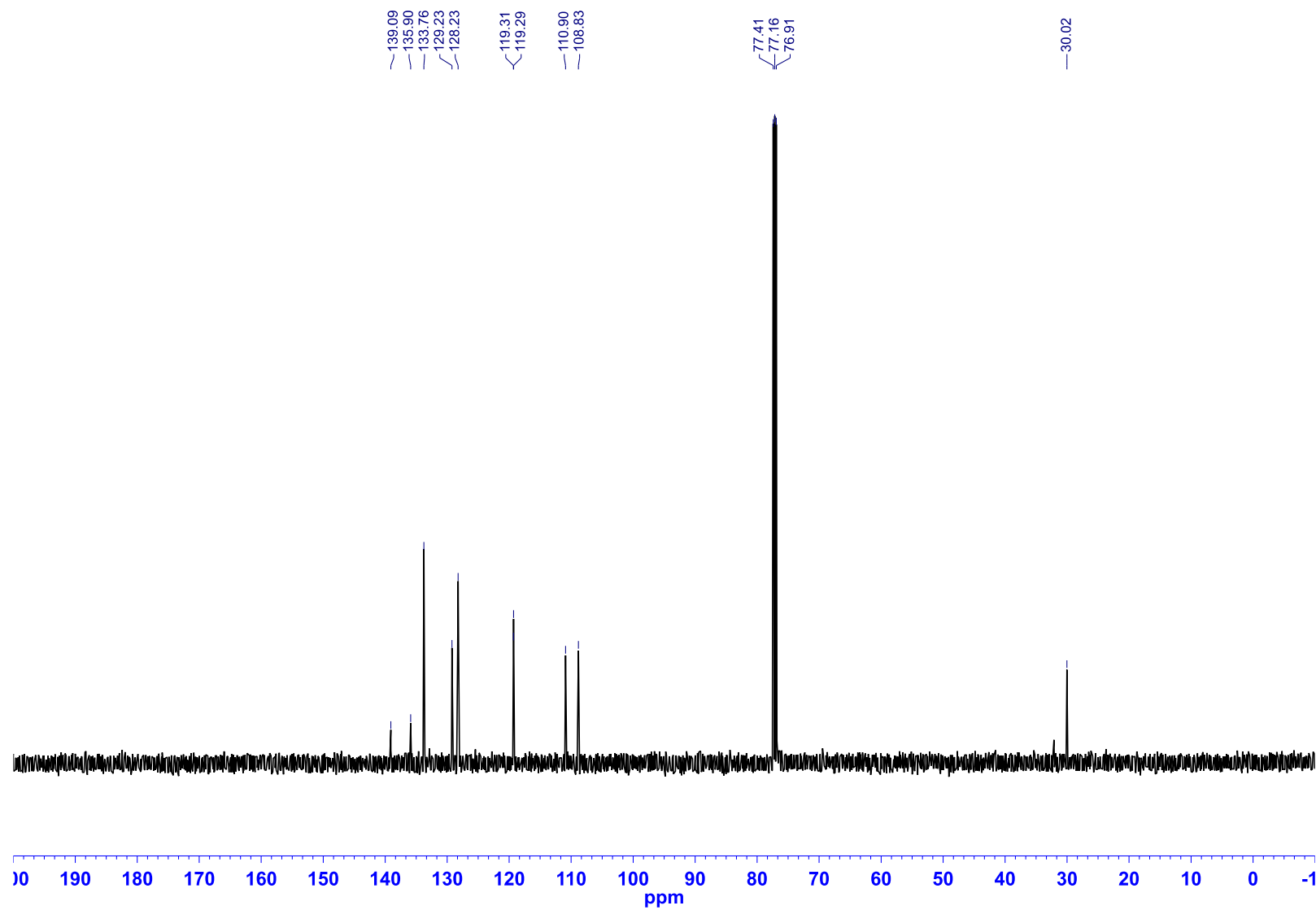
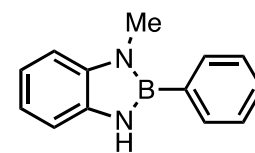
^{11}B NMR (128.4 MHz, MeCN) of 2-(2,6-dimethylphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5c**)



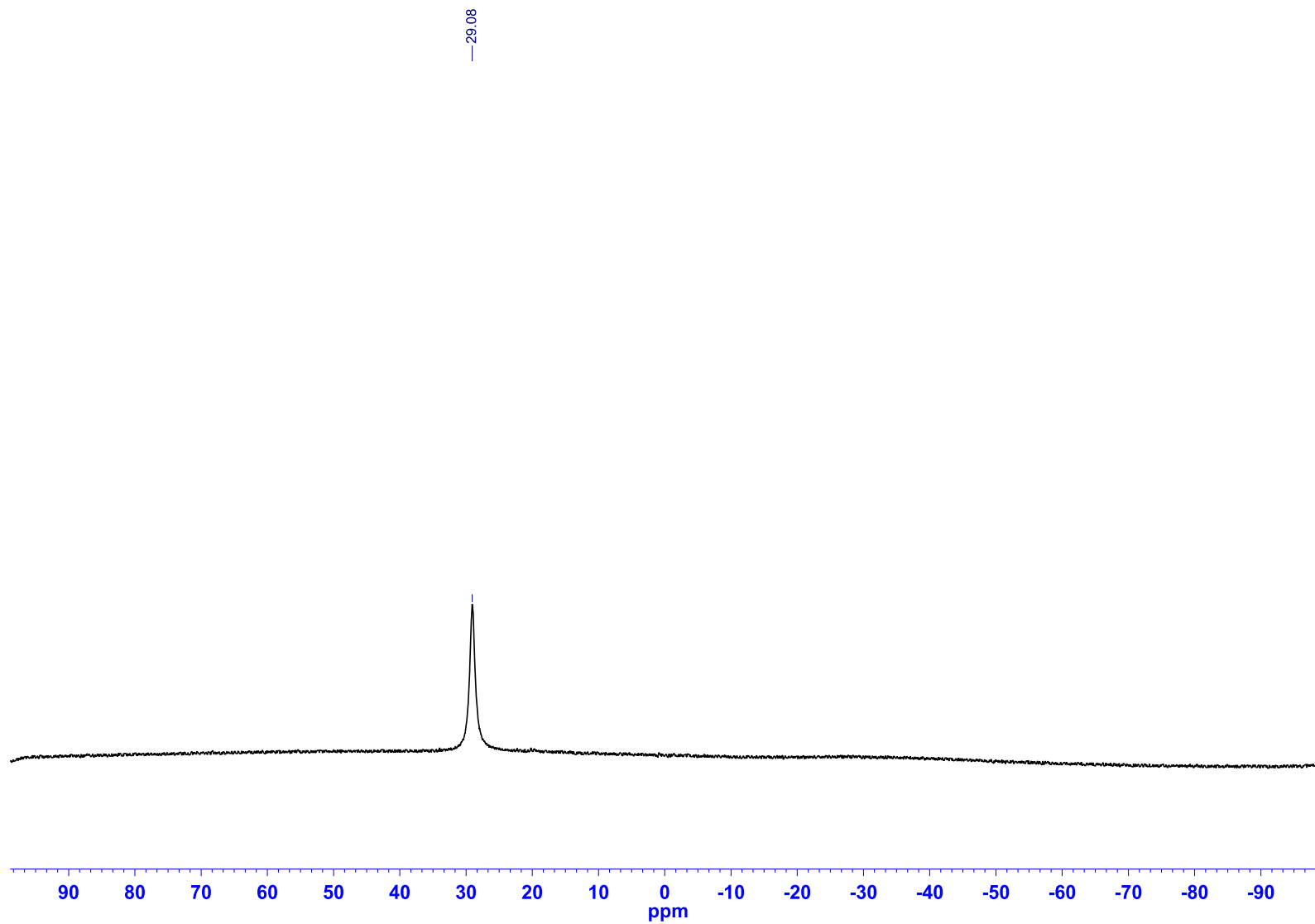
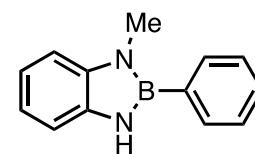
^1H NMR (500.4 MHz, CDCl_3) of 1-methyl-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5d**)



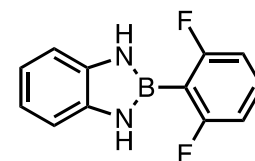
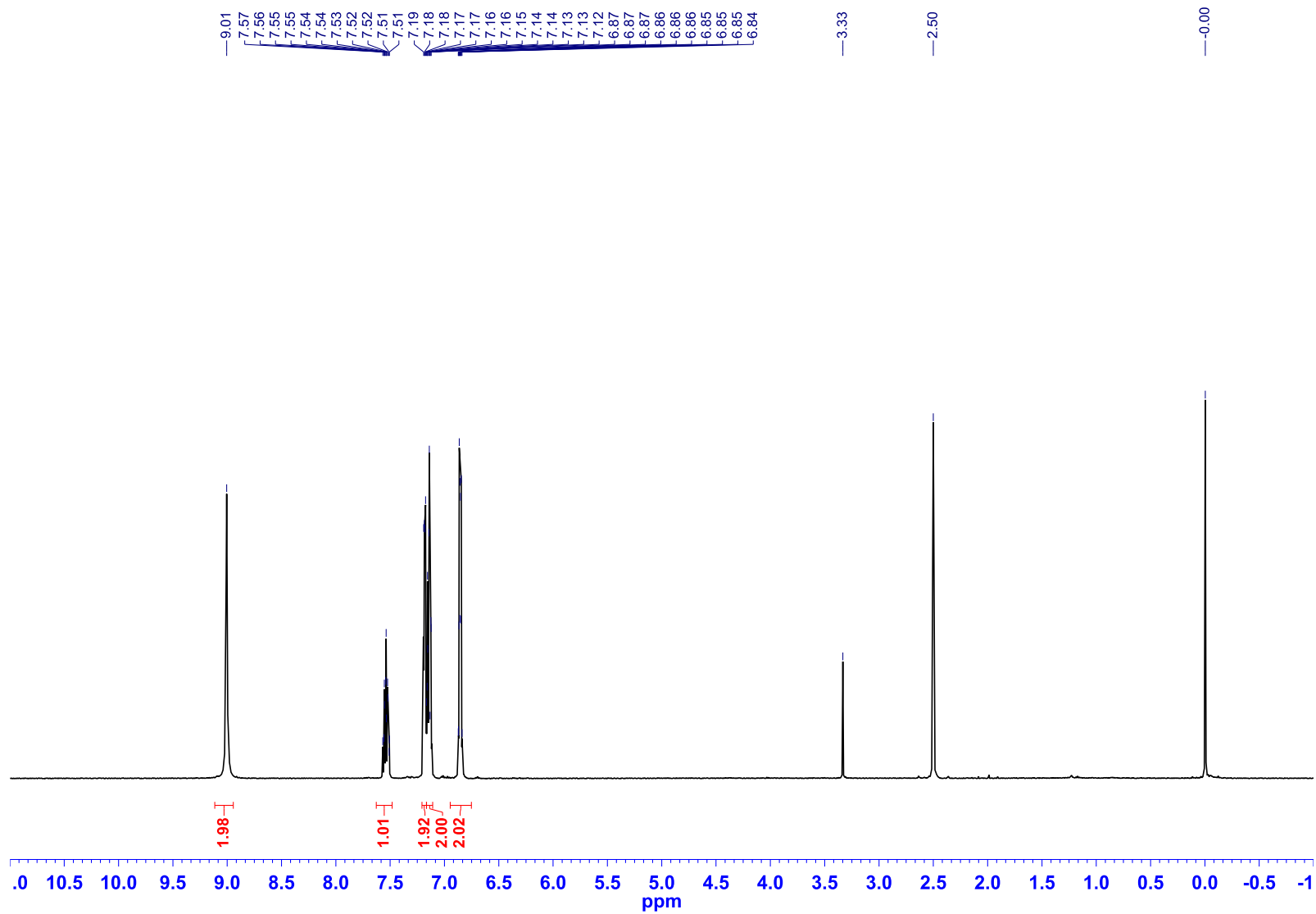
^{13}C NMR (125.8 MHz, CDCl_3) of 1-methyl-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5d**)



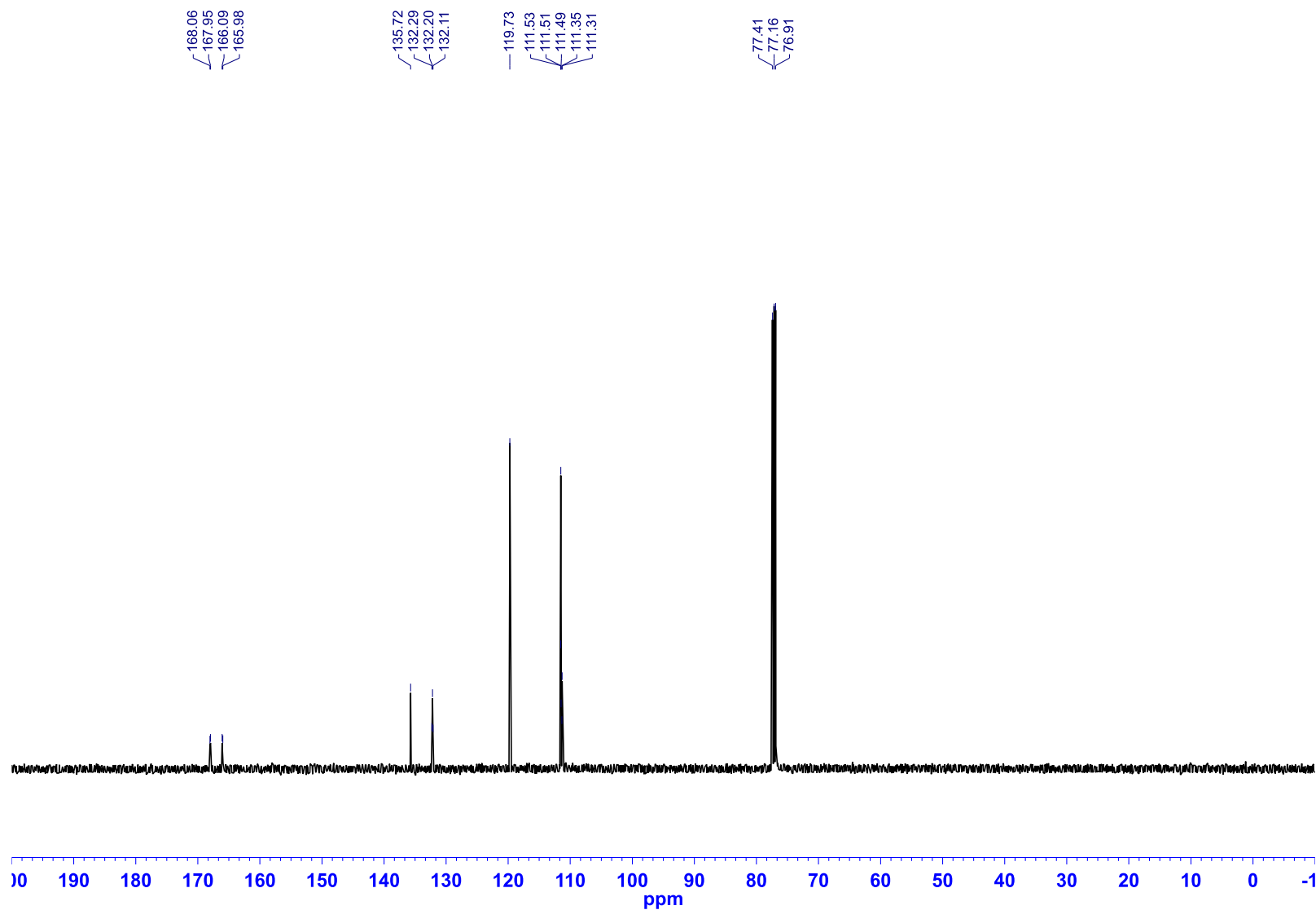
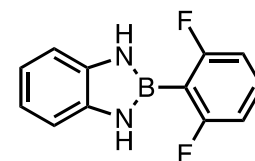
^{11}B NMR (128.4 MHz, MeCN) of 1-methyl-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5d**)



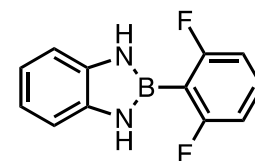
^1H NMR (500.4 MHz, $\text{DMSO-}d_6$) of 2-(2,6-difluorophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5e**)



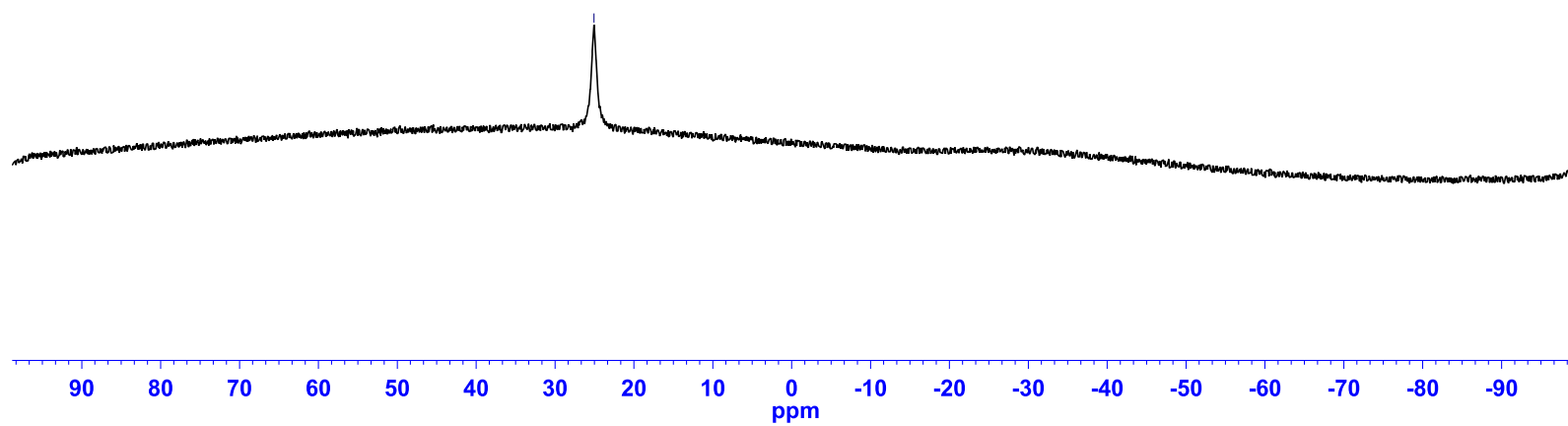
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(2,6-difluorophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5e**)



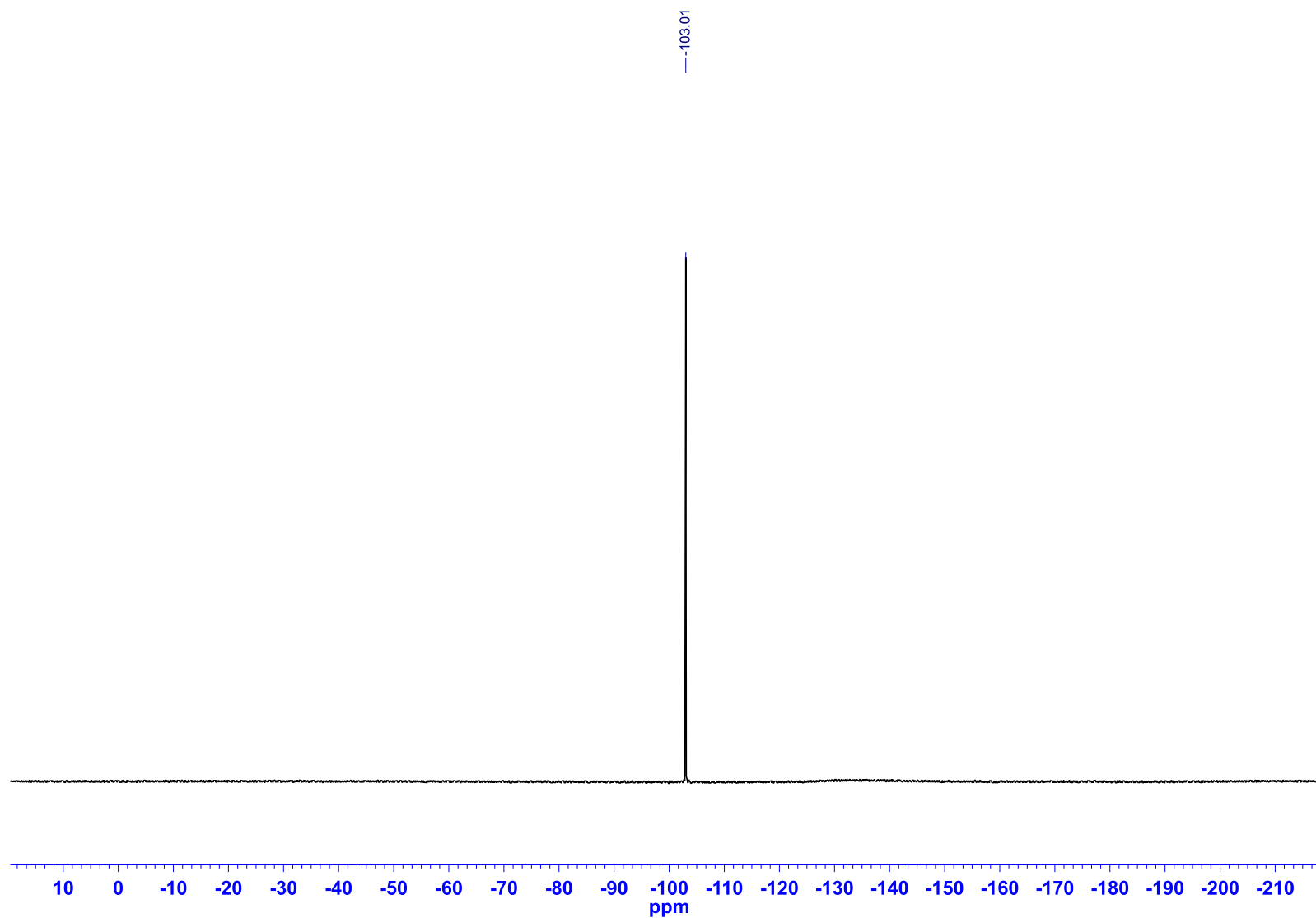
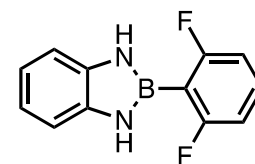
^{11}B NMR (128.4 MHz, MeCN) of 2-(2,6-difluorophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5e**)



— 25.06

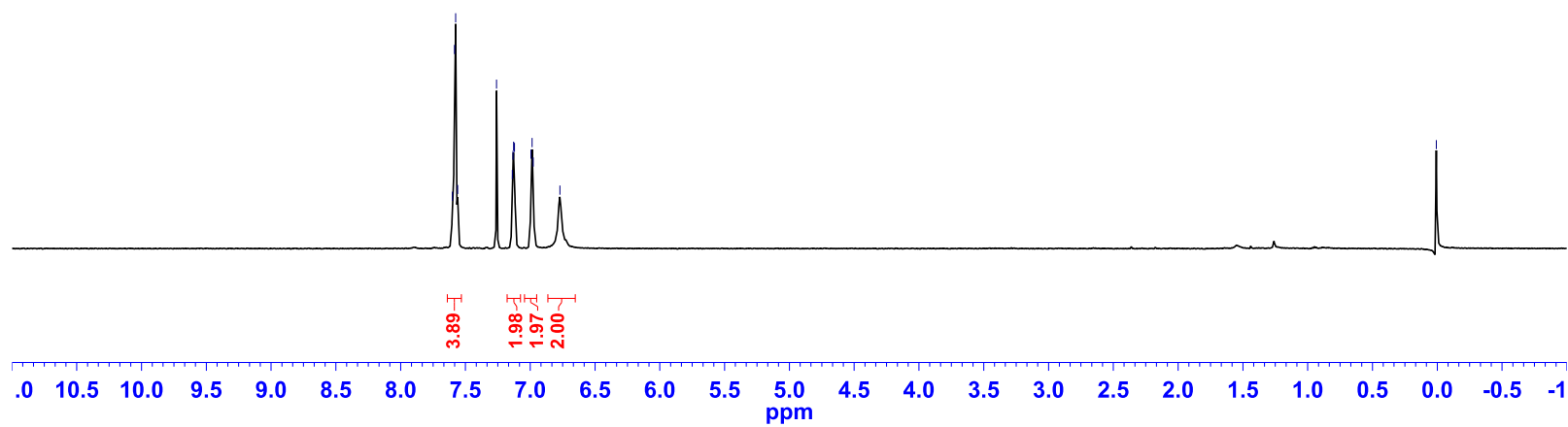
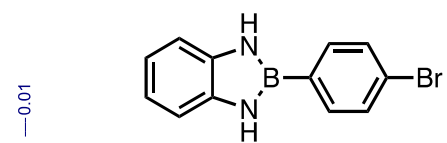


^{19}F NMR (282.4 MHz, CDCl_3) of 2-(2,6-difluorophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5e**)

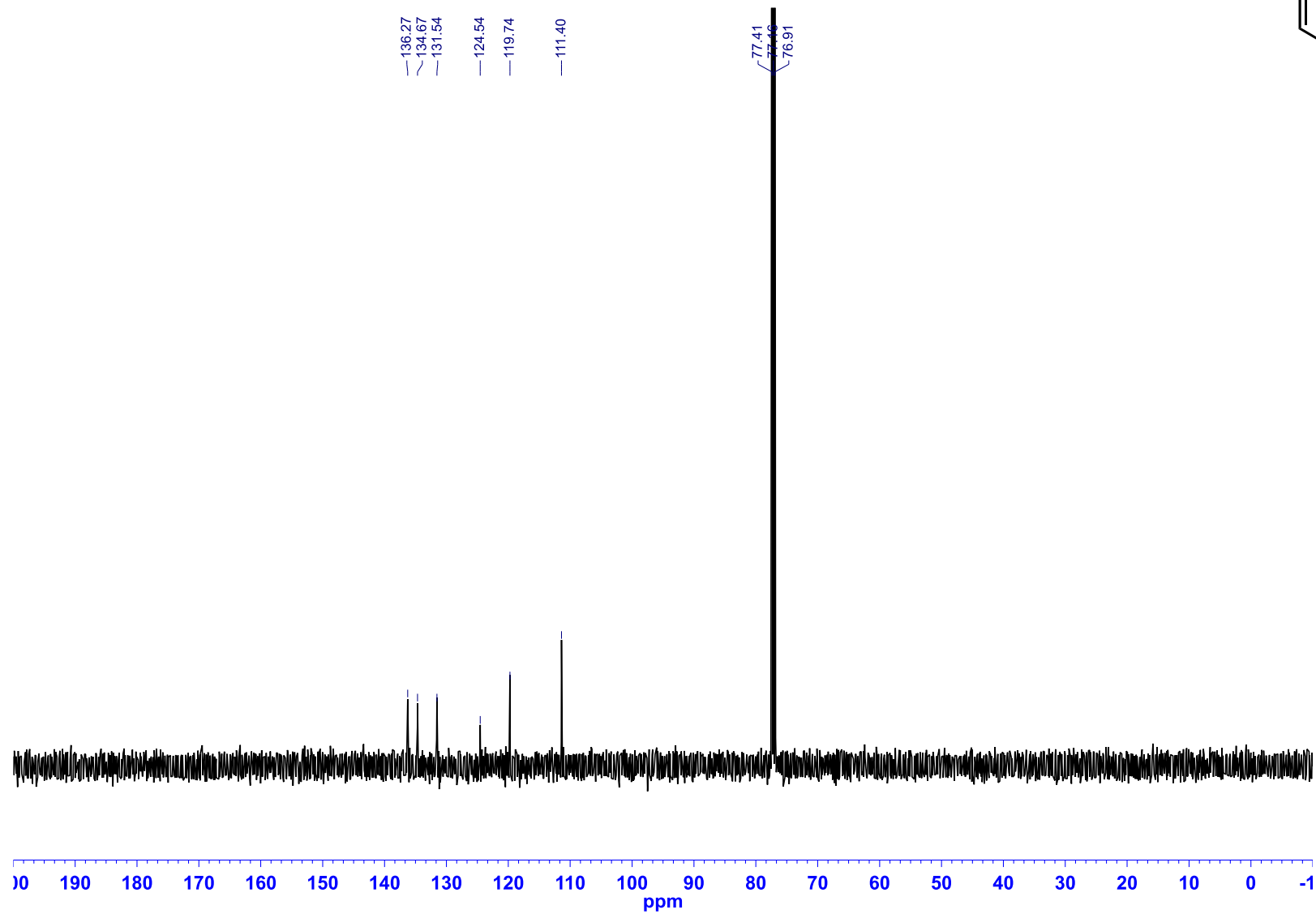
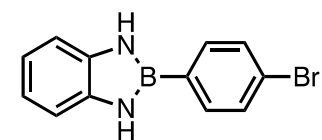


^1H NMR (500.4 MHz, CDCl_3) of 2-(4-bromophenyl)-2,3-dihydro-1H-1,3,2-benzodiazaborole (**5f**)

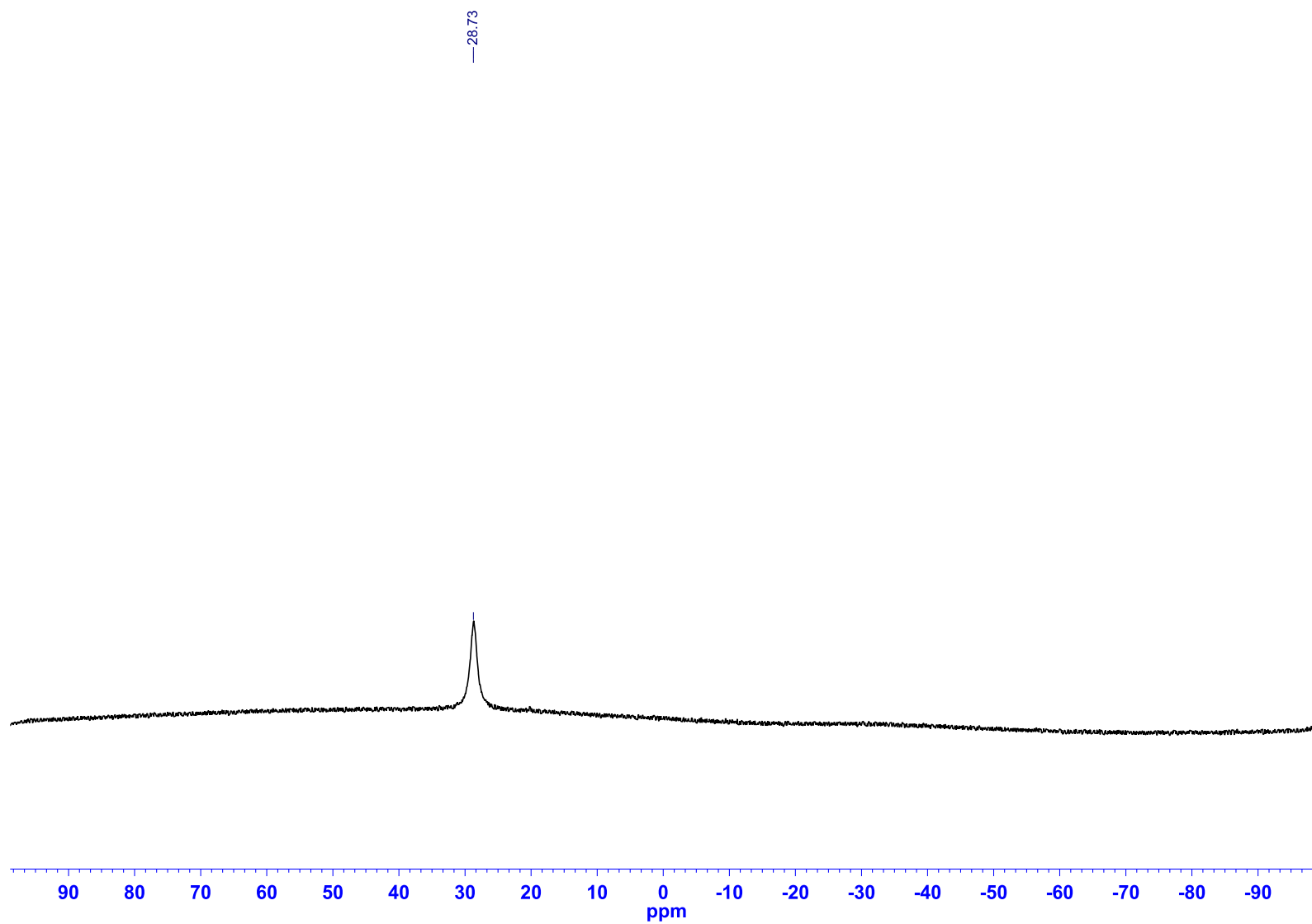
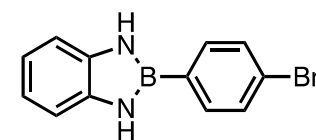
7.60
7.58
7.56
7.26
7.14
7.13
7.13
7.12
6.99
6.98
6.77



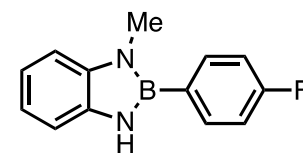
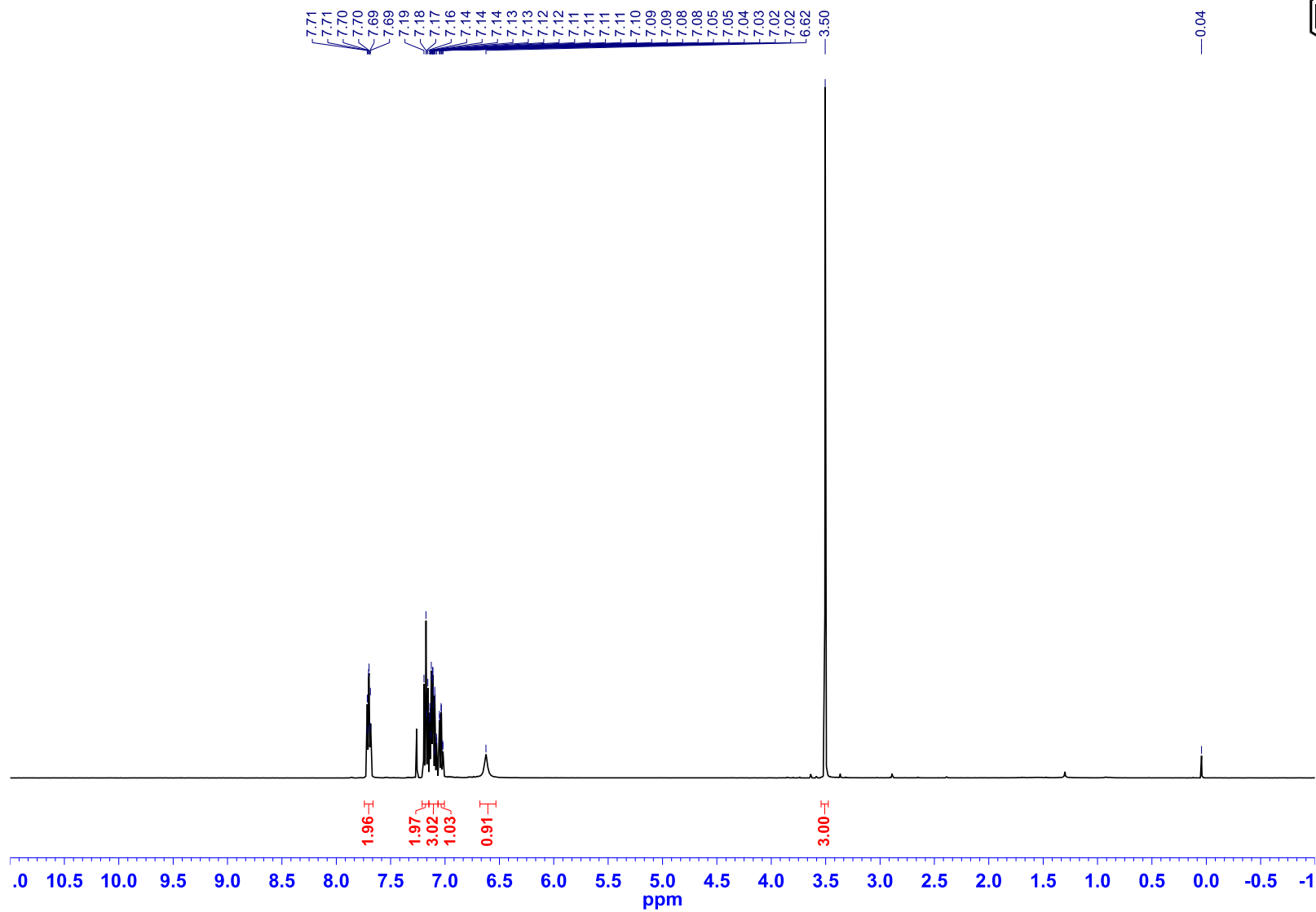
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(4-bromophenyl)-2,3-dihydro-1H-1,3,2-benzodiazaborole (**5f**)



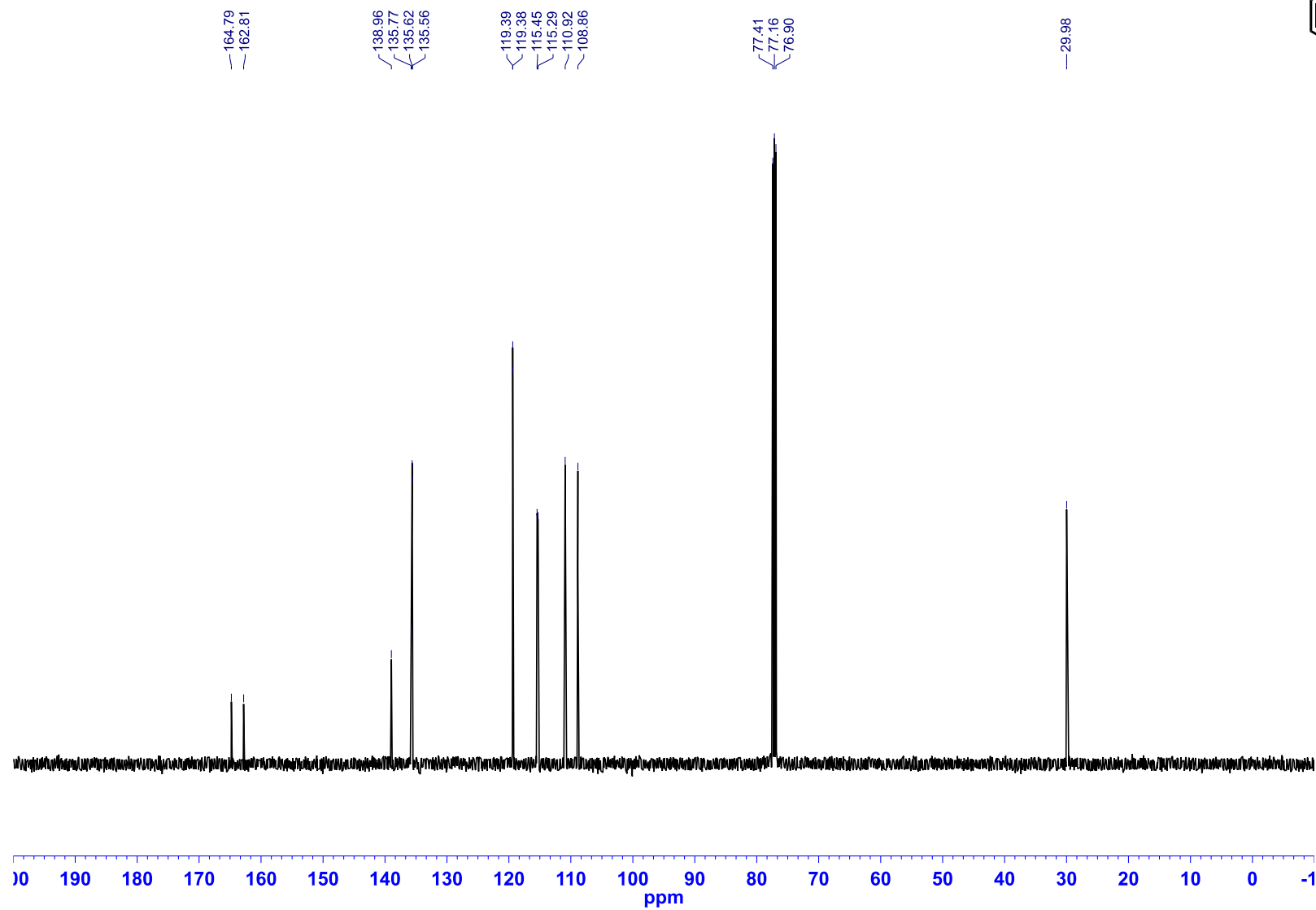
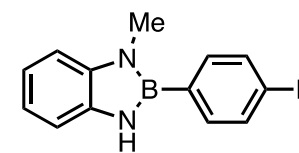
^{11}B NMR (128.4 MHz, MeCN) of 2-(4-bromophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5f**)



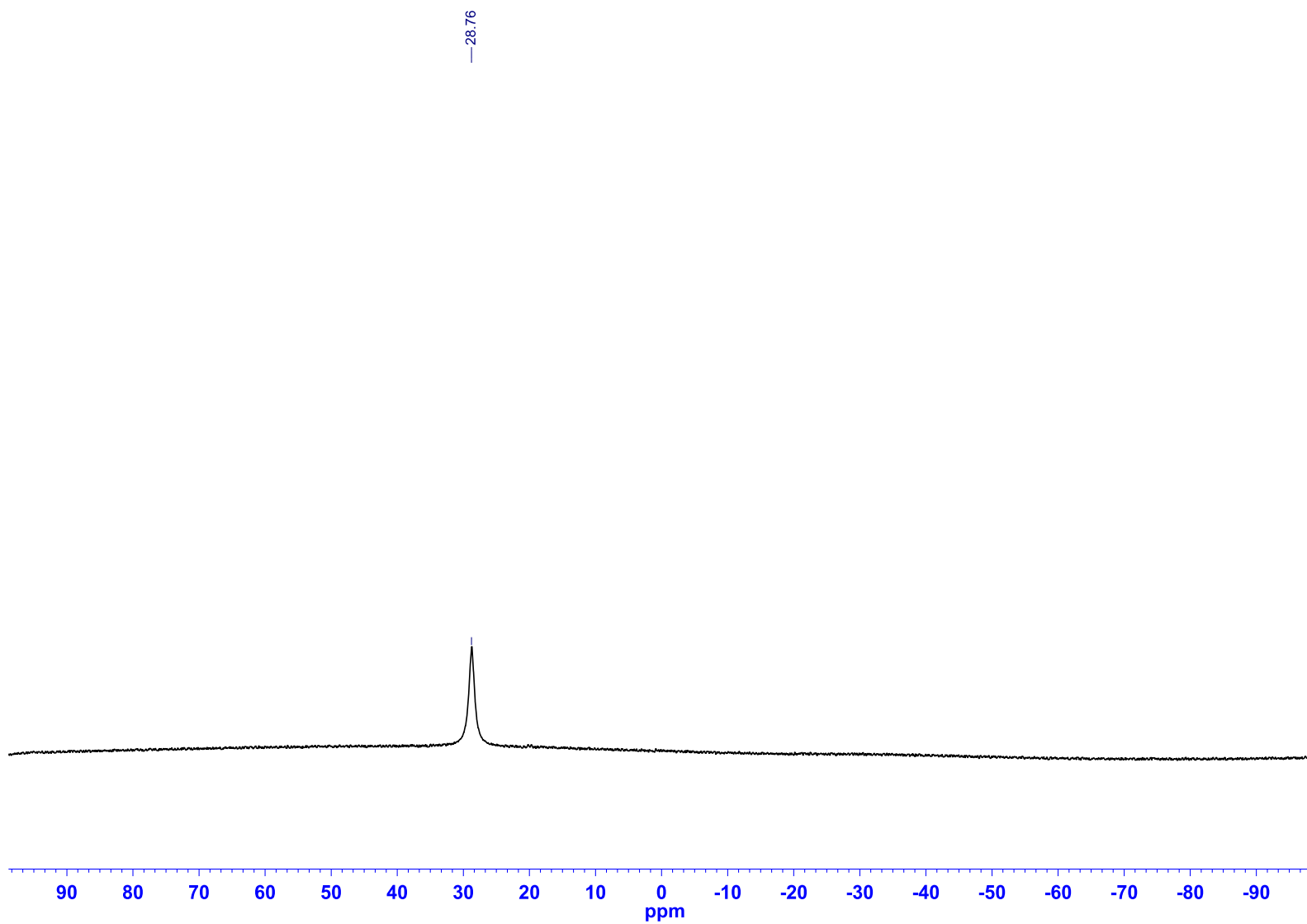
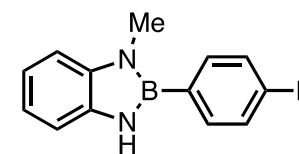
^1H NMR (500.4 MHz, CDCl_3) of 2-(4-fluorophenyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5g**)



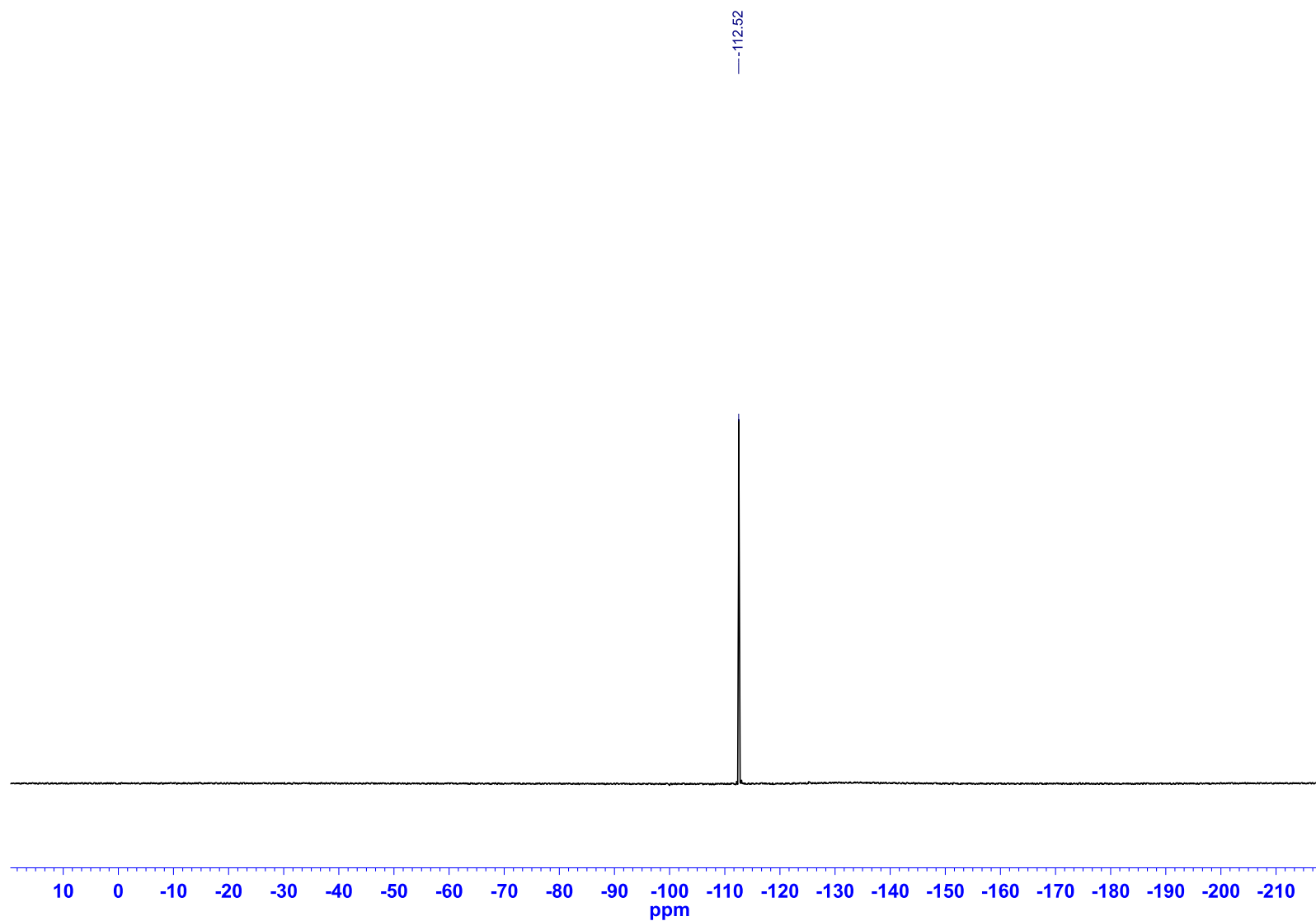
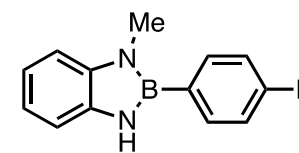
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(4-fluorophenyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5g**)



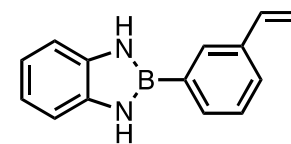
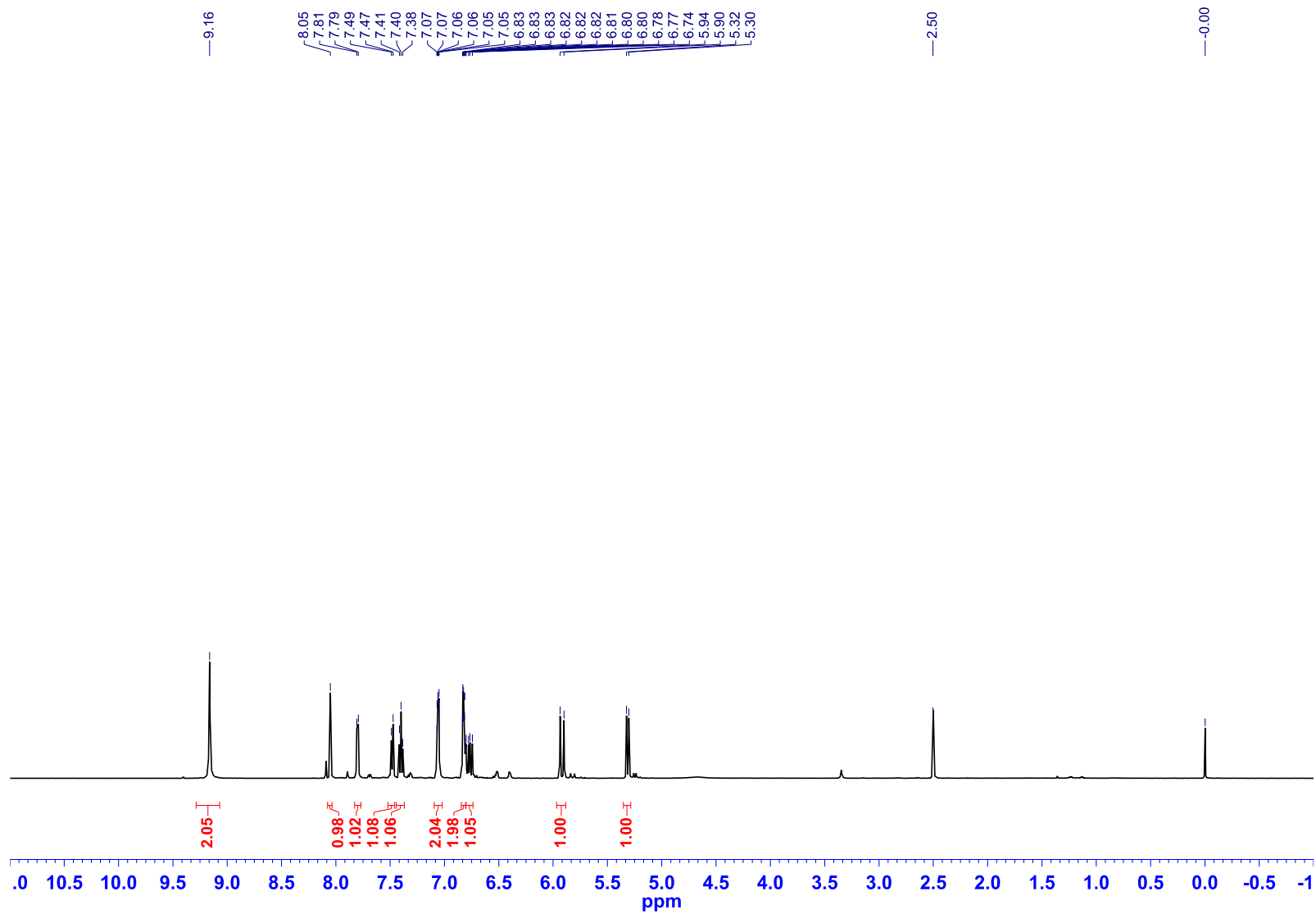
^{11}B NMR (128.4 MHz, MeCN) of 2-(4-fluorophenyl)-1-methy-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5g**)



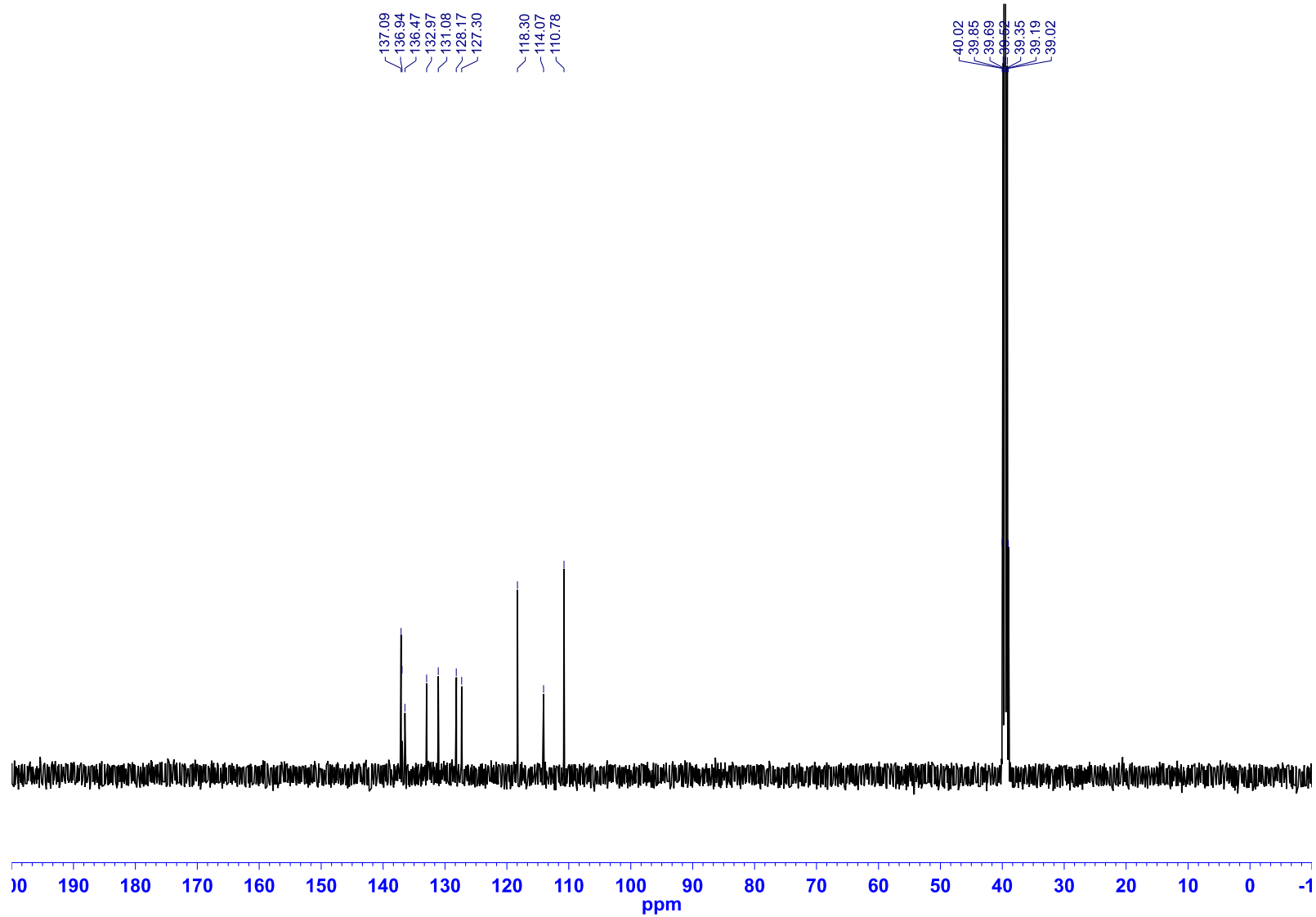
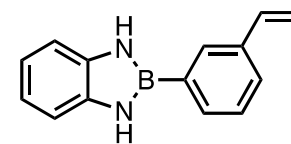
^{19}F NMR (282.4 MHz, CDCl_3) of 2-(4-fluorophenyl)-1-methy-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5g**)



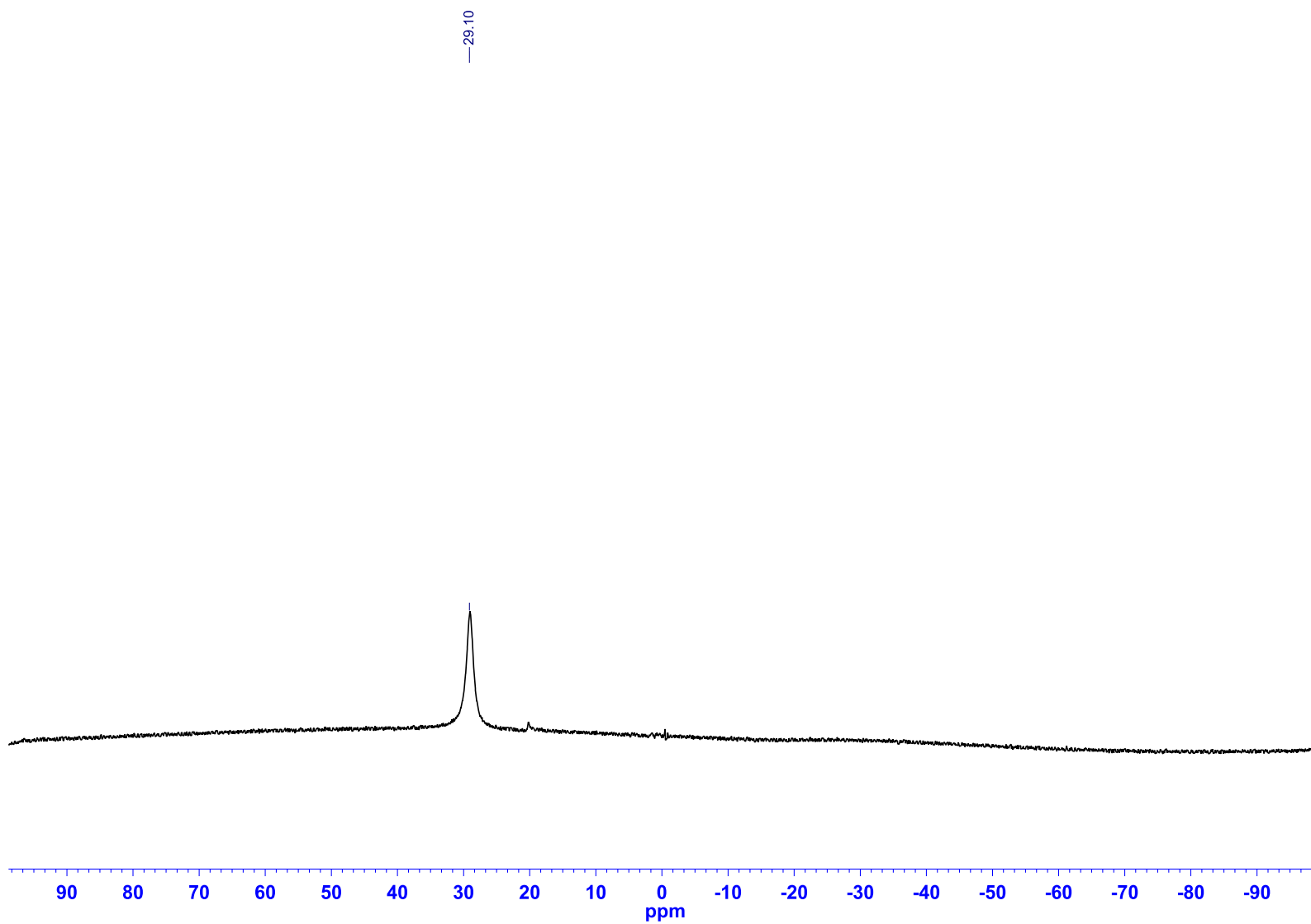
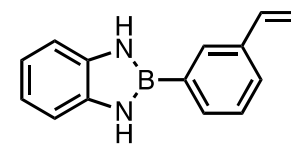
^1H NMR (500.4 MHz, $\text{DMSO-}d_6$) of 2-(3-vinylphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5h**)



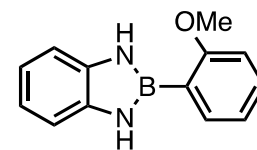
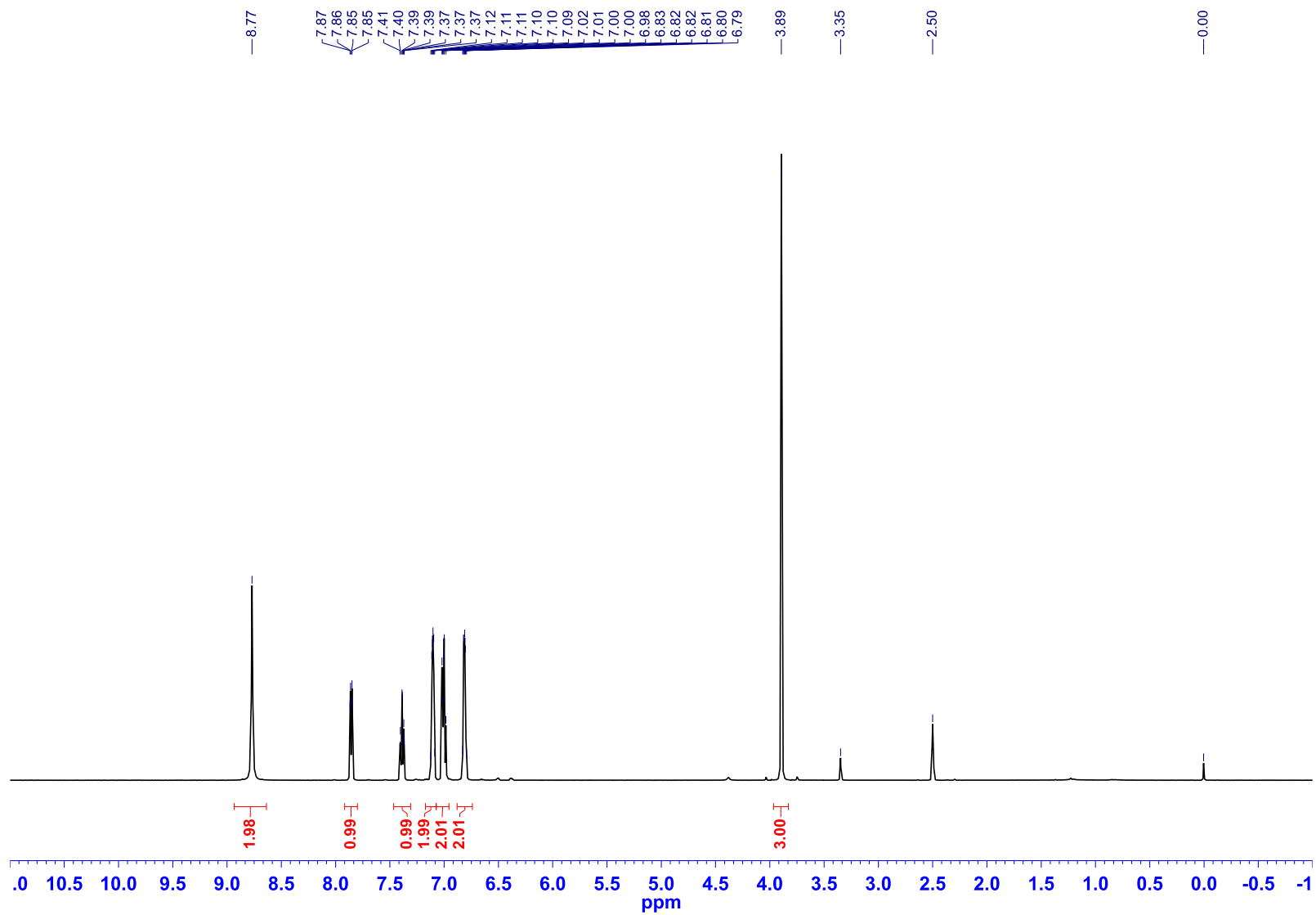
^{13}C NMR (125.8 MHz, $\text{DMSO-}d_6$) of 2-(3-vinylphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5h**)



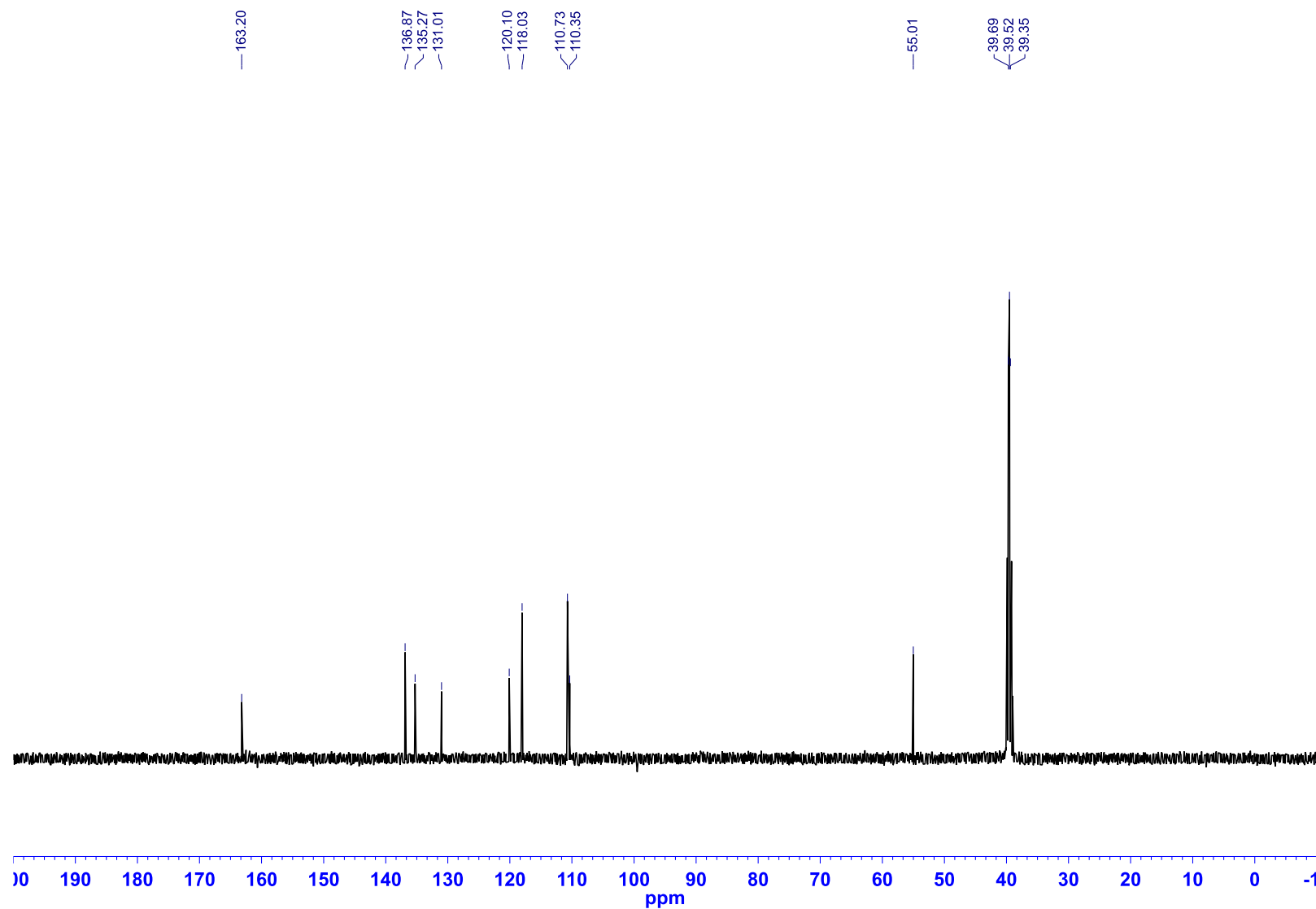
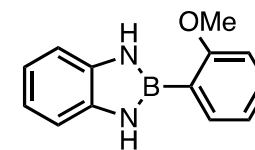
^{11}B NMR (128.4 MHz, MeCN) of 2-(3-vinylphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5h**)



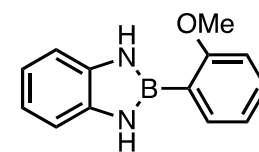
^1H NMR (500.4 MHz, $\text{DMSO-}d_6$) of 2-(2-methoxyphenyl)-2,3-dihydro-1H-1,3,2-benzodiazaborole (**5i**)



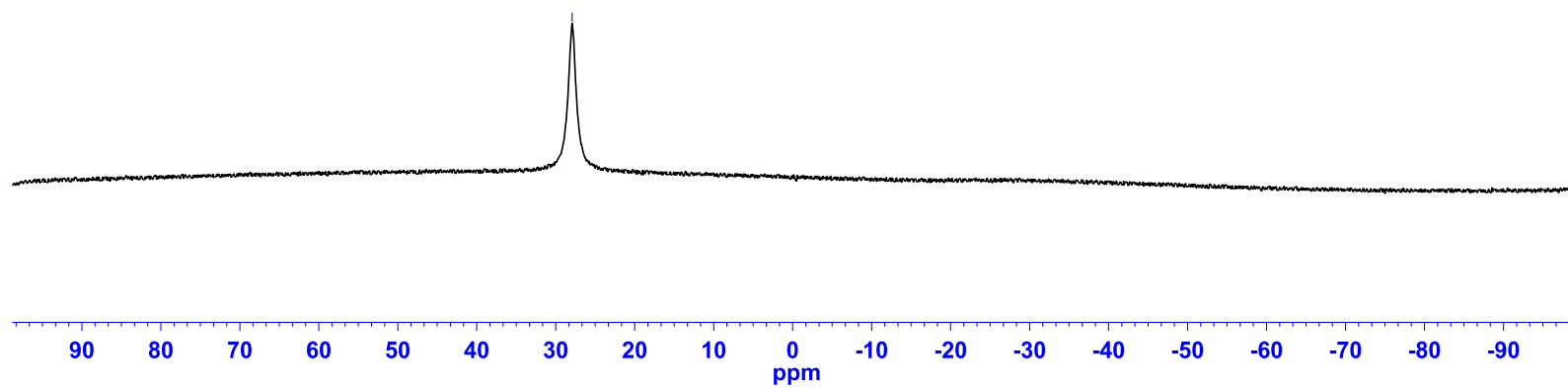
^{13}C NMR (125.8 MHz, $\text{DMSO-}d_6$) of 2-(2-methoxyphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5i**)



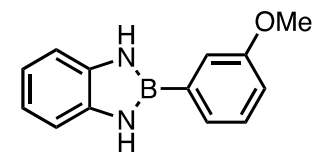
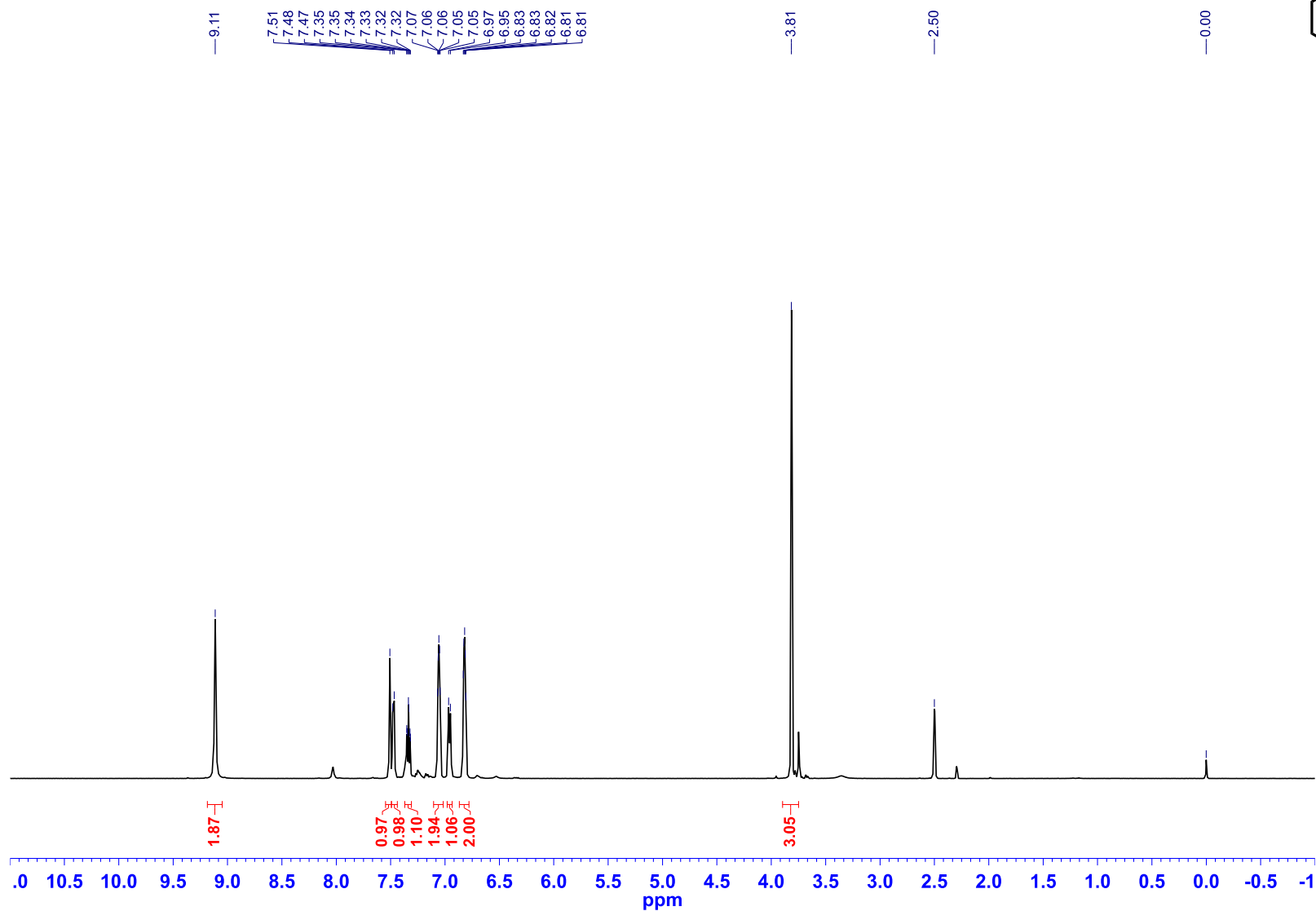
^{11}B NMR (128.4 MHz, MeCN) of 2-(2-methoxyphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5i**)



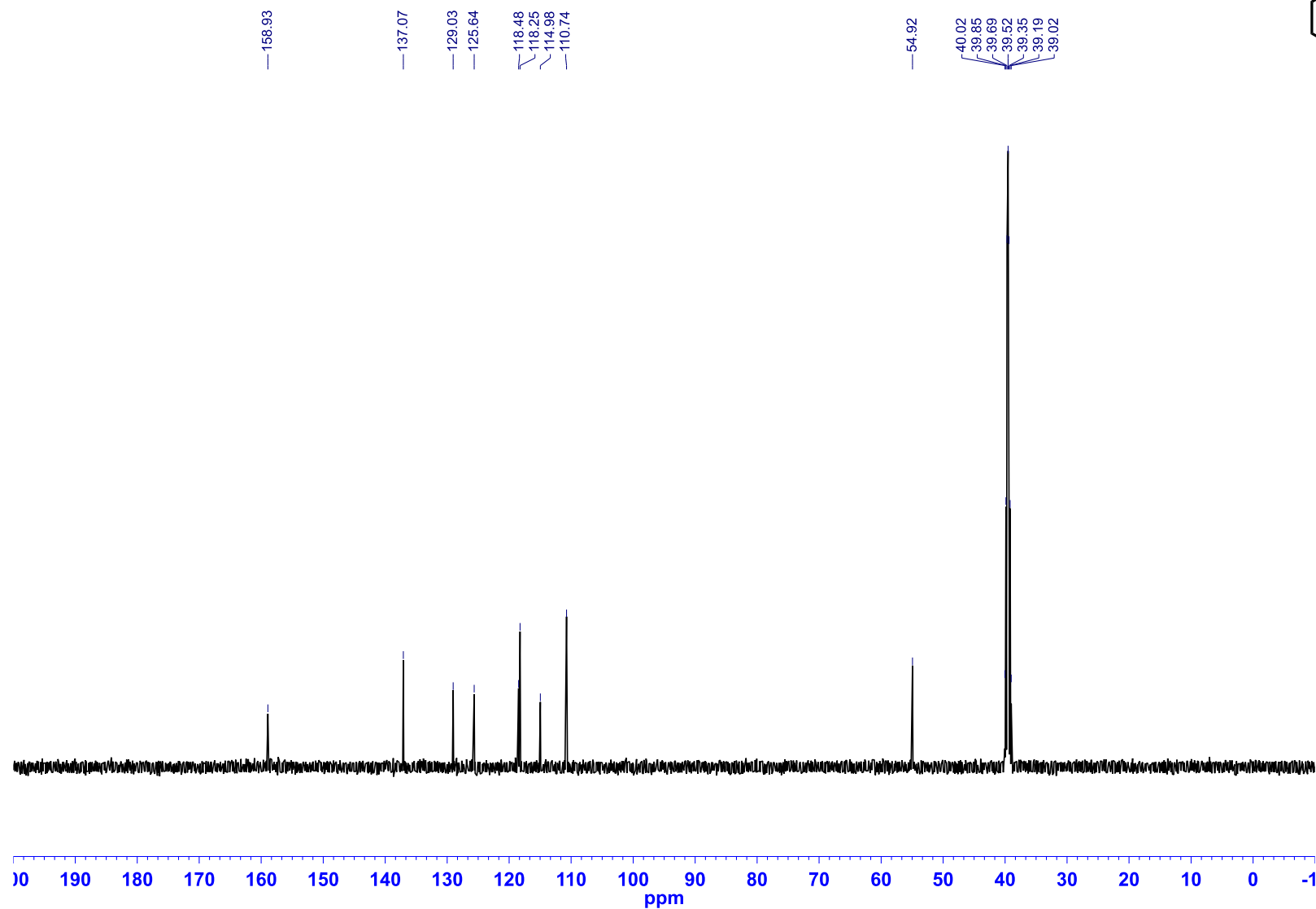
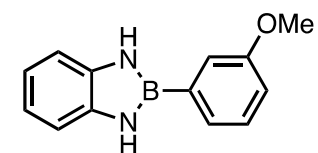
—27.93



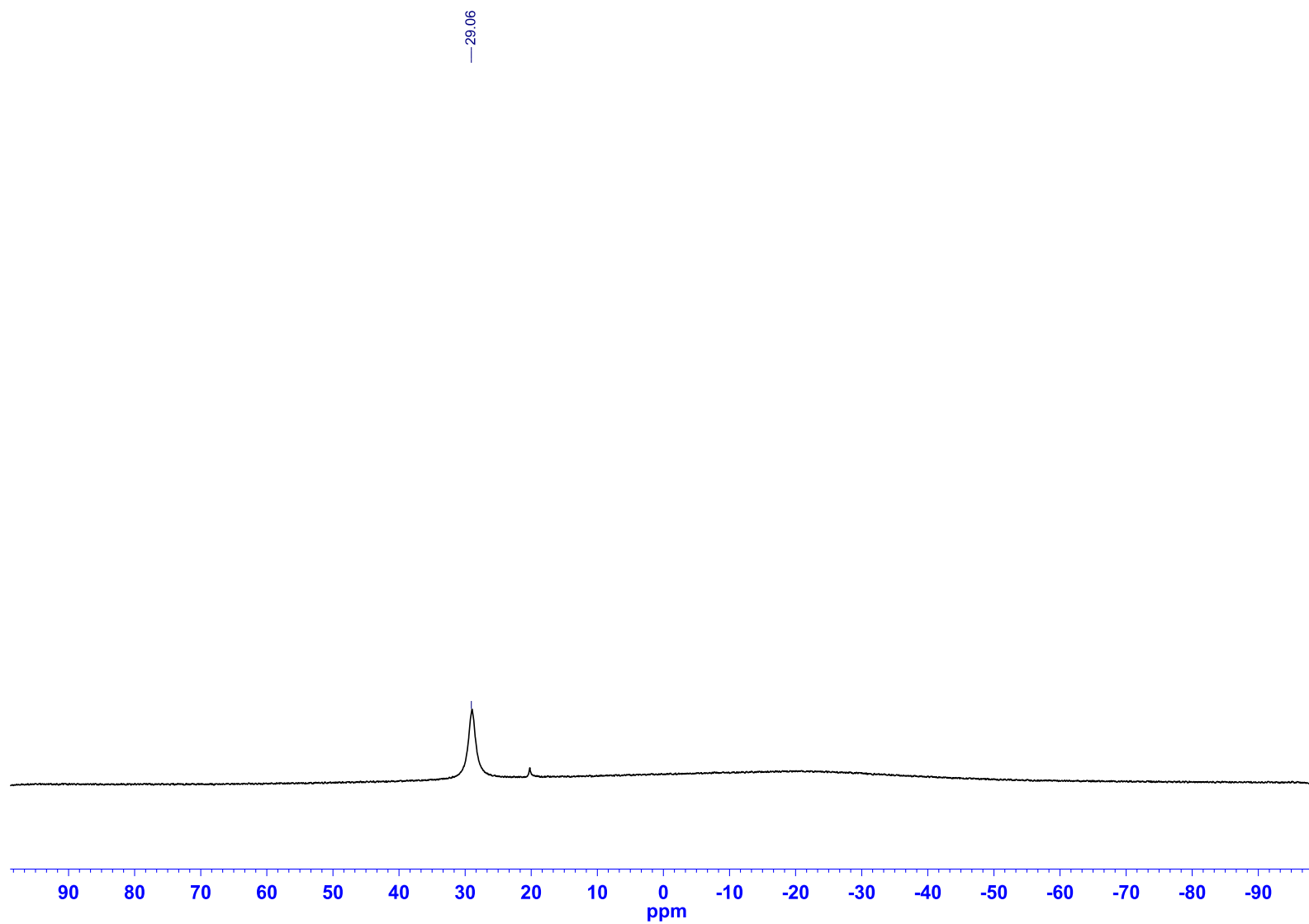
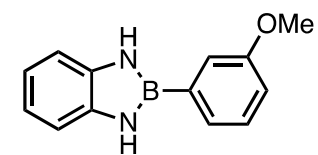
^1H NMR (500.4 MHz, $\text{DMSO-}d_6$) of 2-(3-methoxyphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5j**)



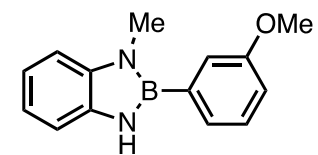
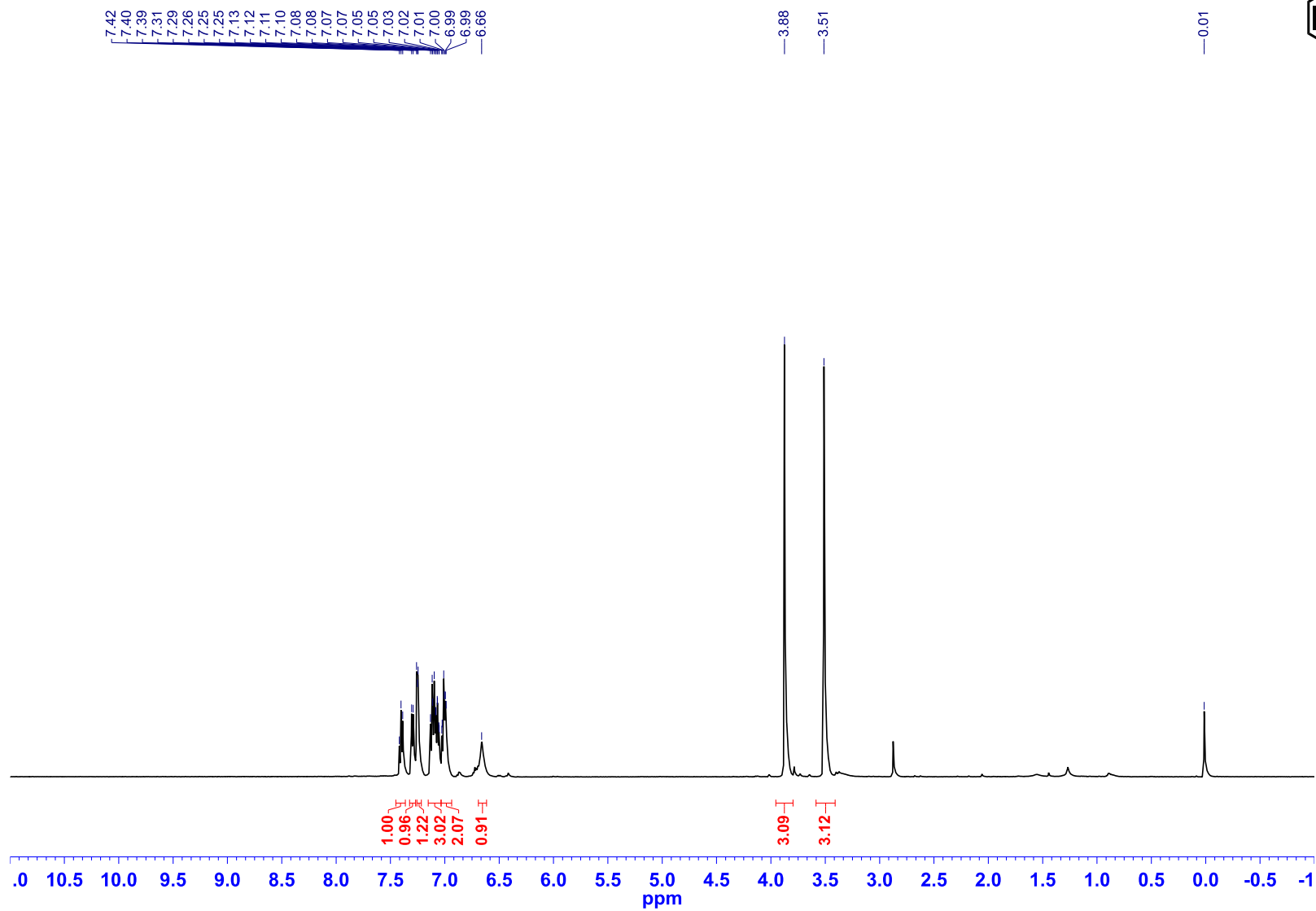
^{13}C NMR (125.8 MHz, $\text{DMSO-}d_6$) of 2-(3-methoxyphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5j**)



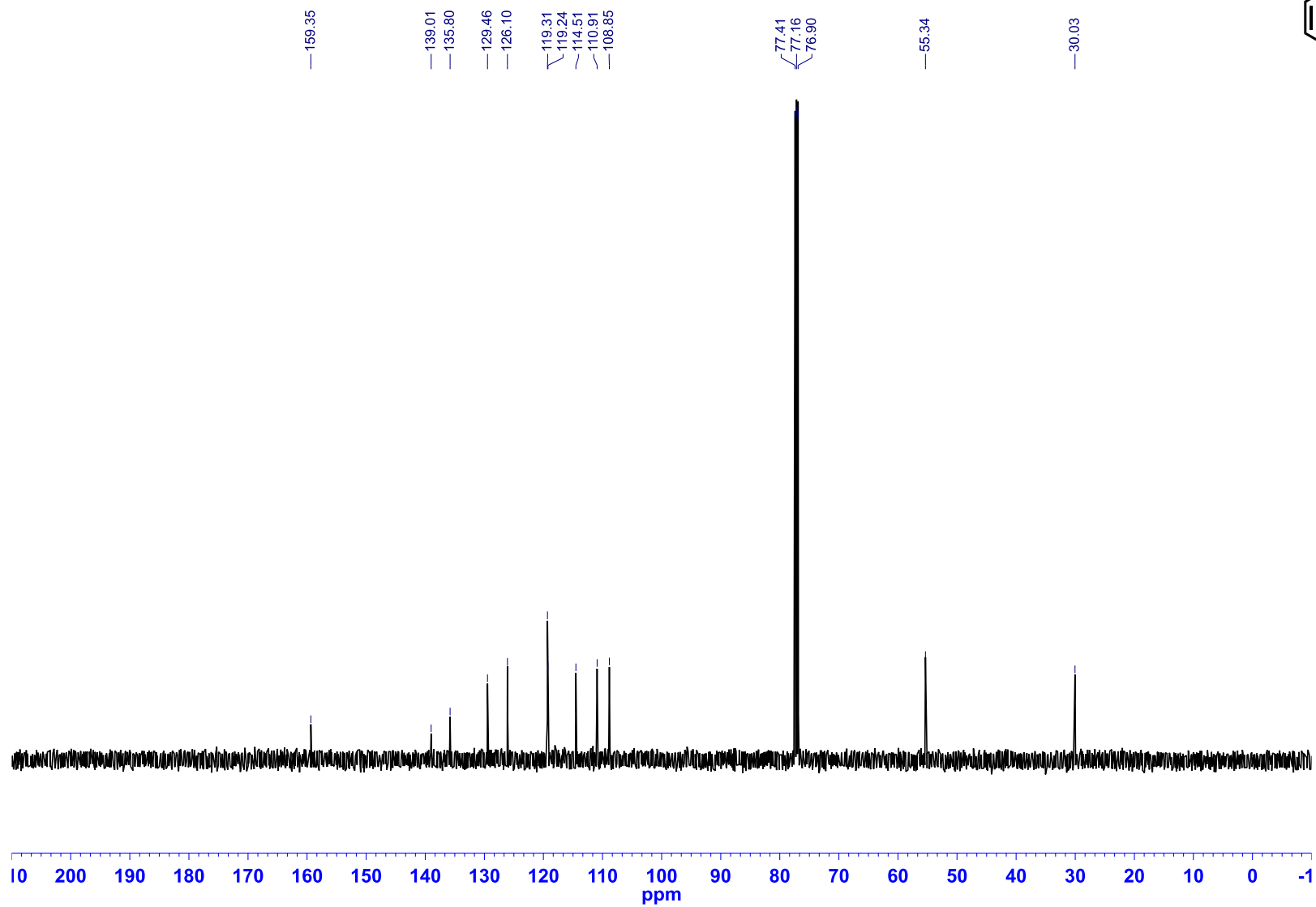
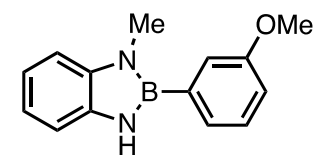
^{11}B NMR (128.4 MHz, MeCN) of 2-(3-methoxyphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5j**)



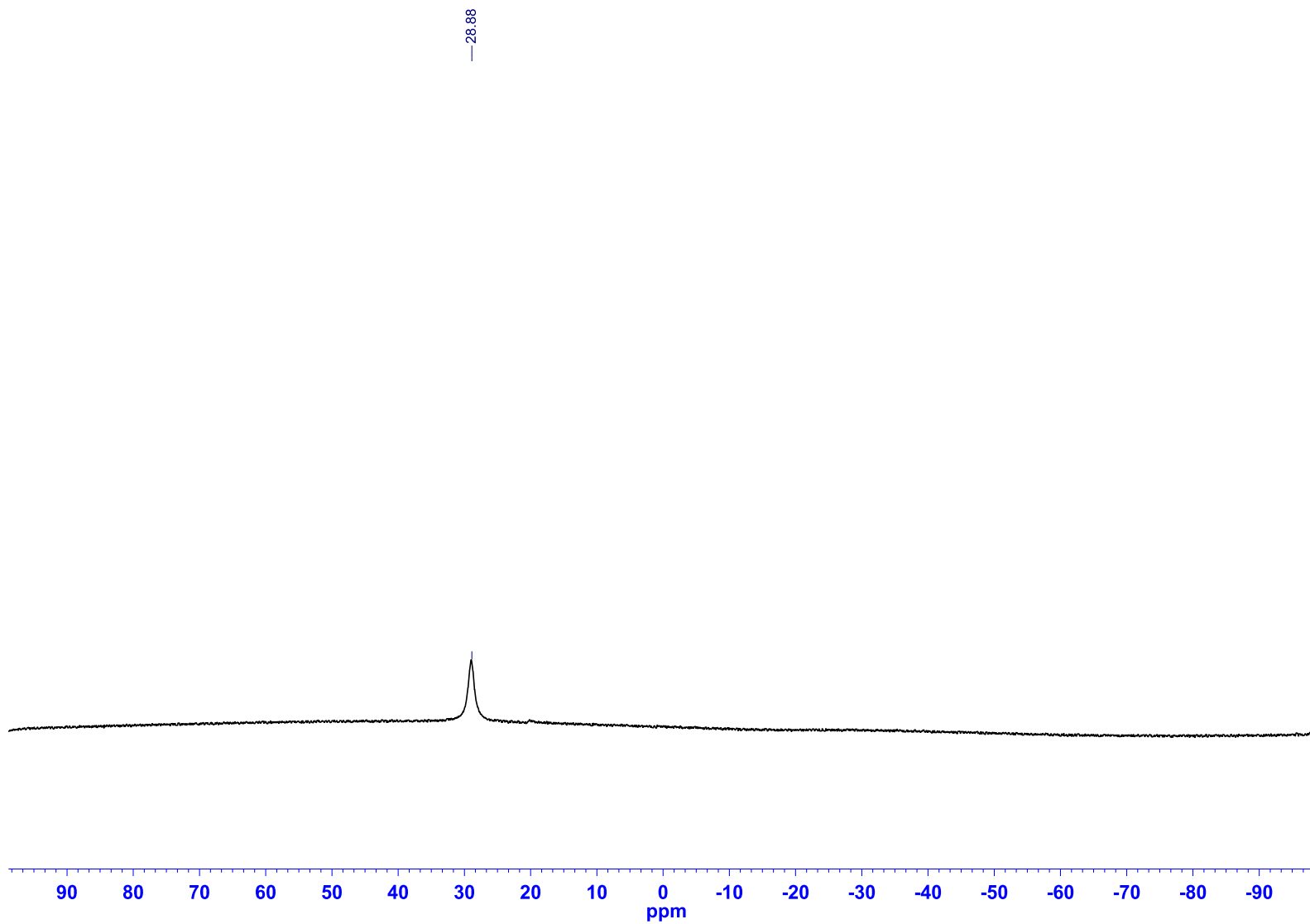
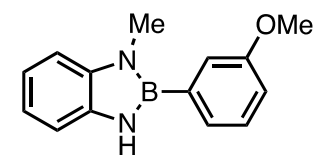
^1H NMR (500.4 MHz, CDCl_3) of 2-(3-methoxyphenyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5k**)



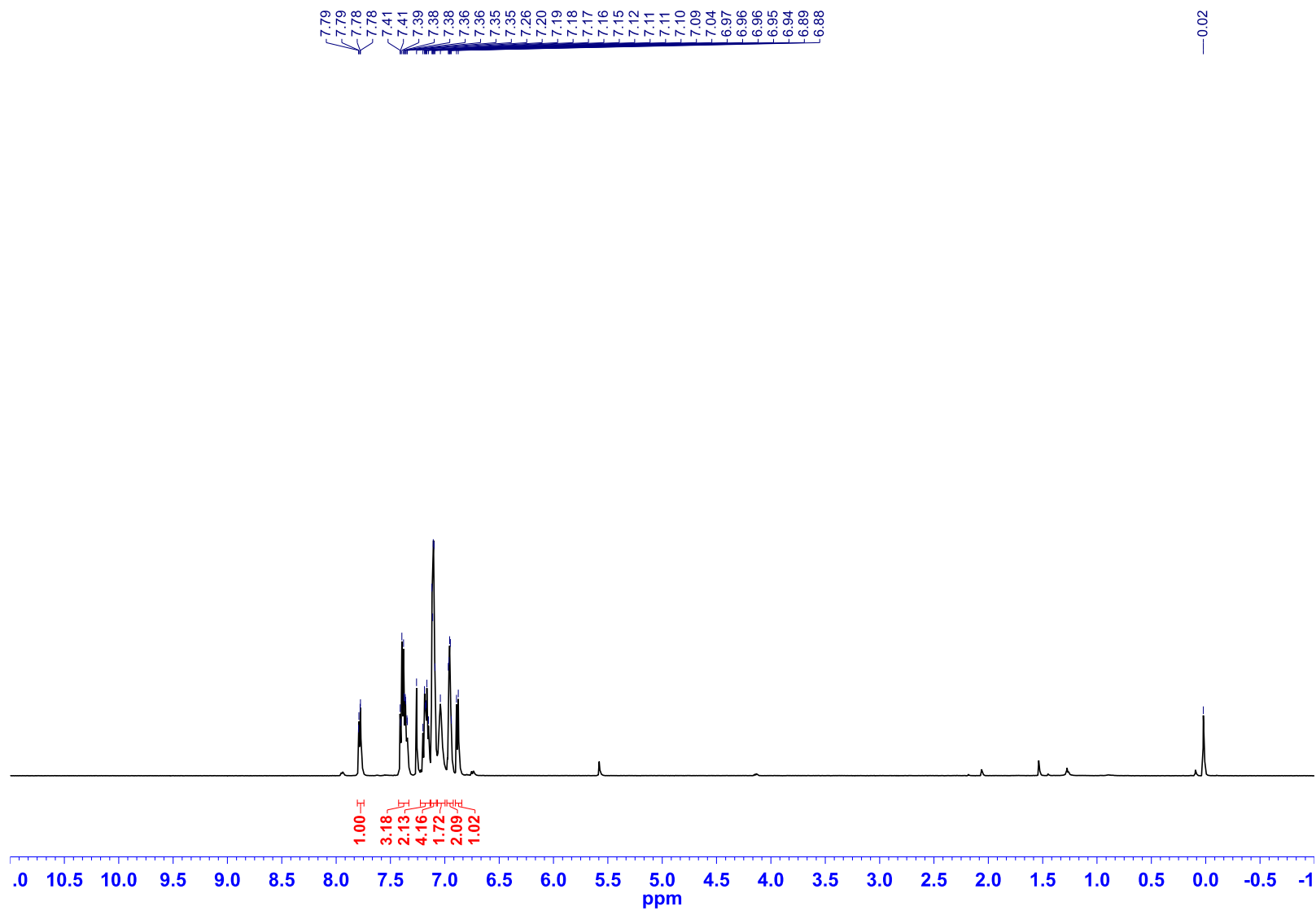
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(3-methoxyphenyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5k**)



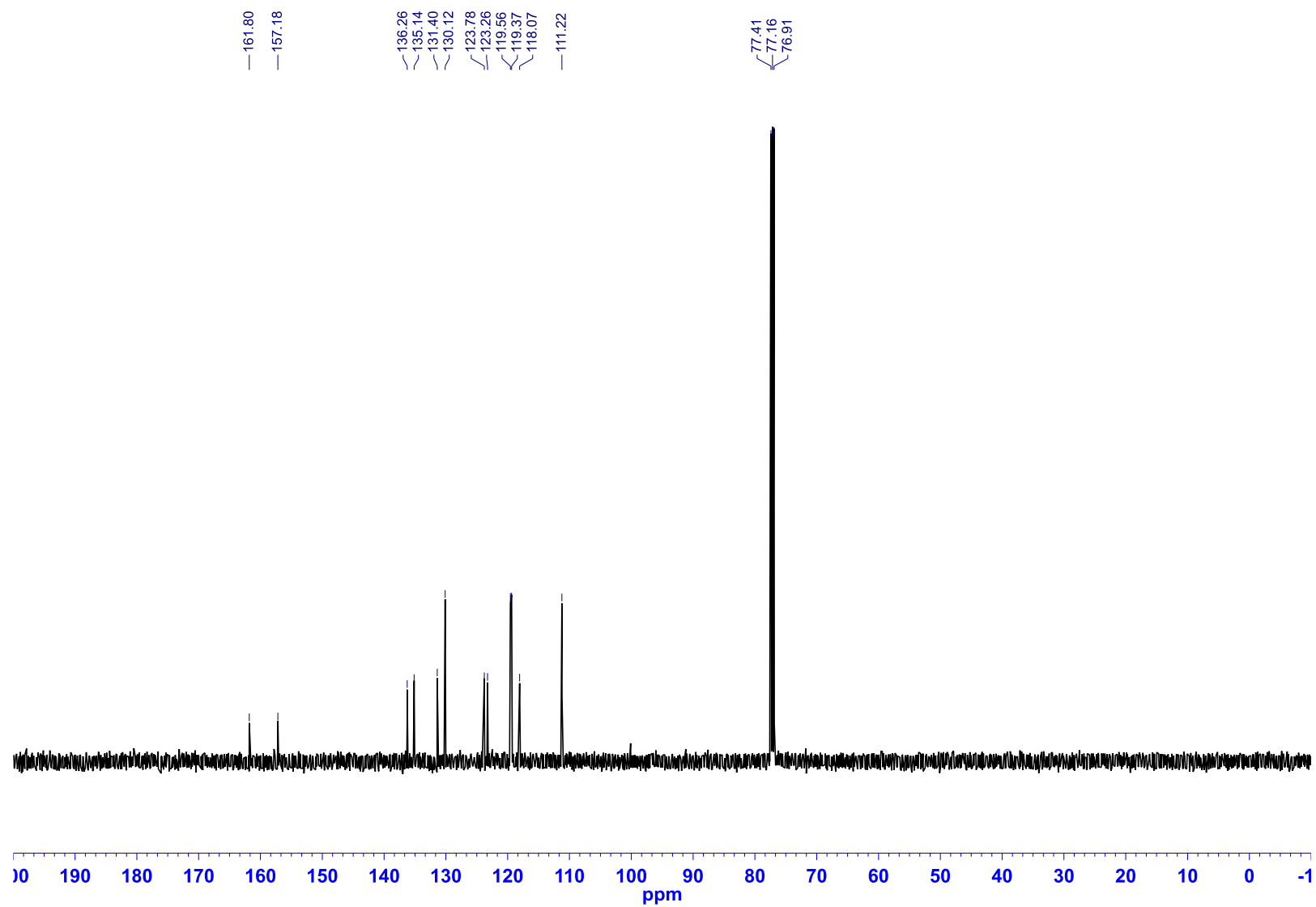
^{11}B NMR (128.4 MHz, MeCN) of 2-(3-methoxyphenyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5k**)



^1H NMR (500.4 MHz, CDCl_3) of 2-(2-phenoxyphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**51**)

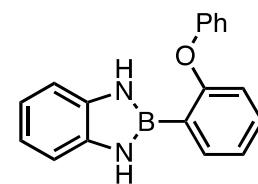
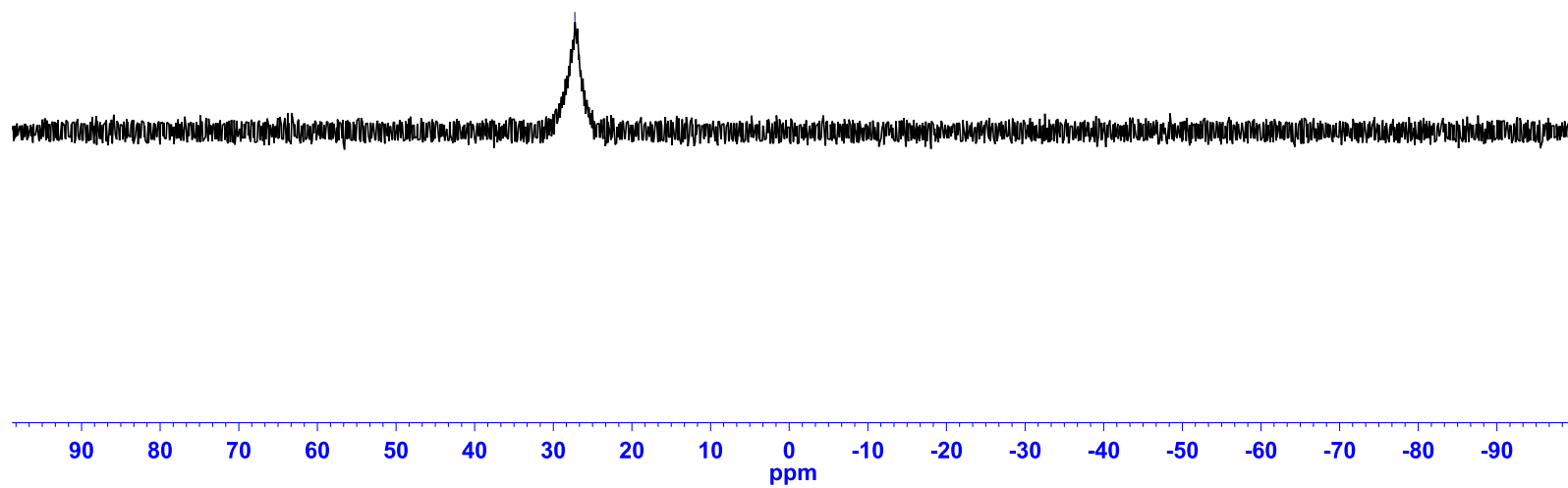


^{13}C NMR (125.8 MHz, CDCl_3) of 2-(2-phenoxyphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5I**)

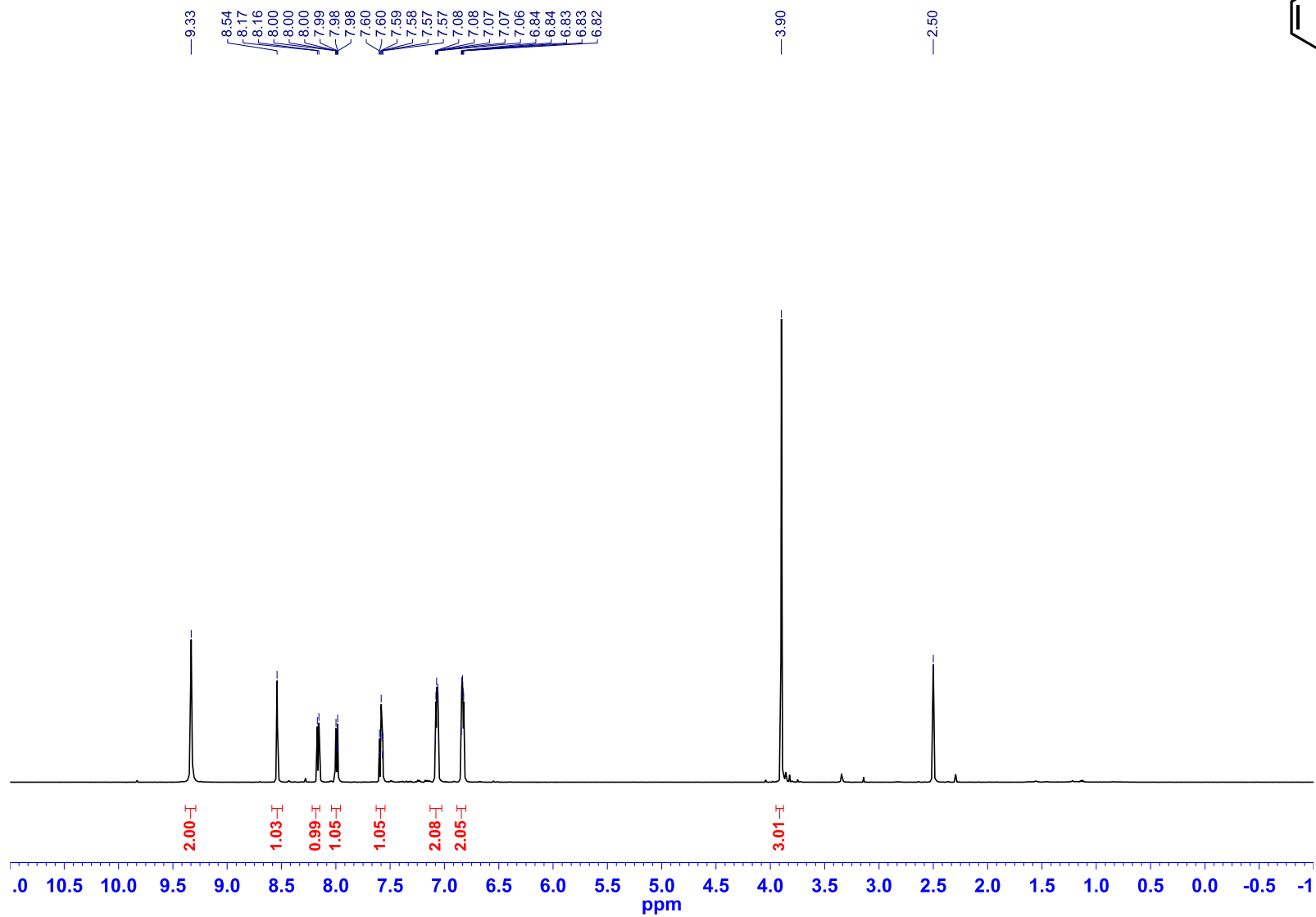
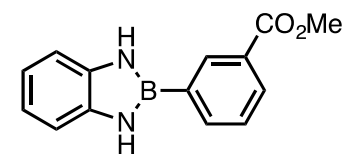


^{11}B NMR (128.4 MHz, CDCl_3) of 2-(2-phenoxyphenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**51**)

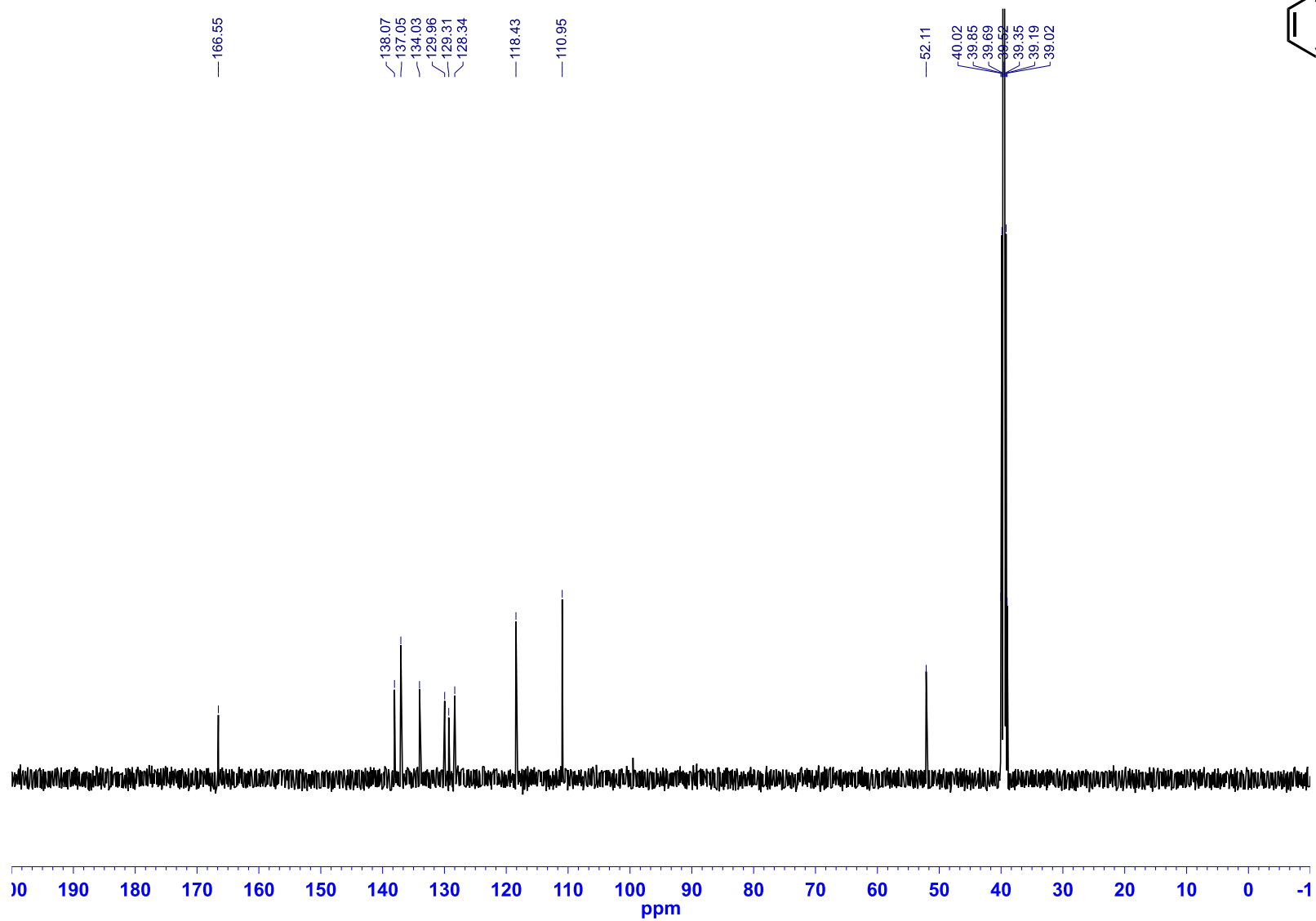
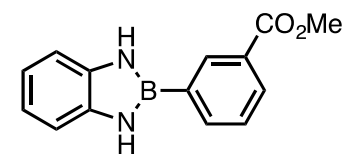
—27.26



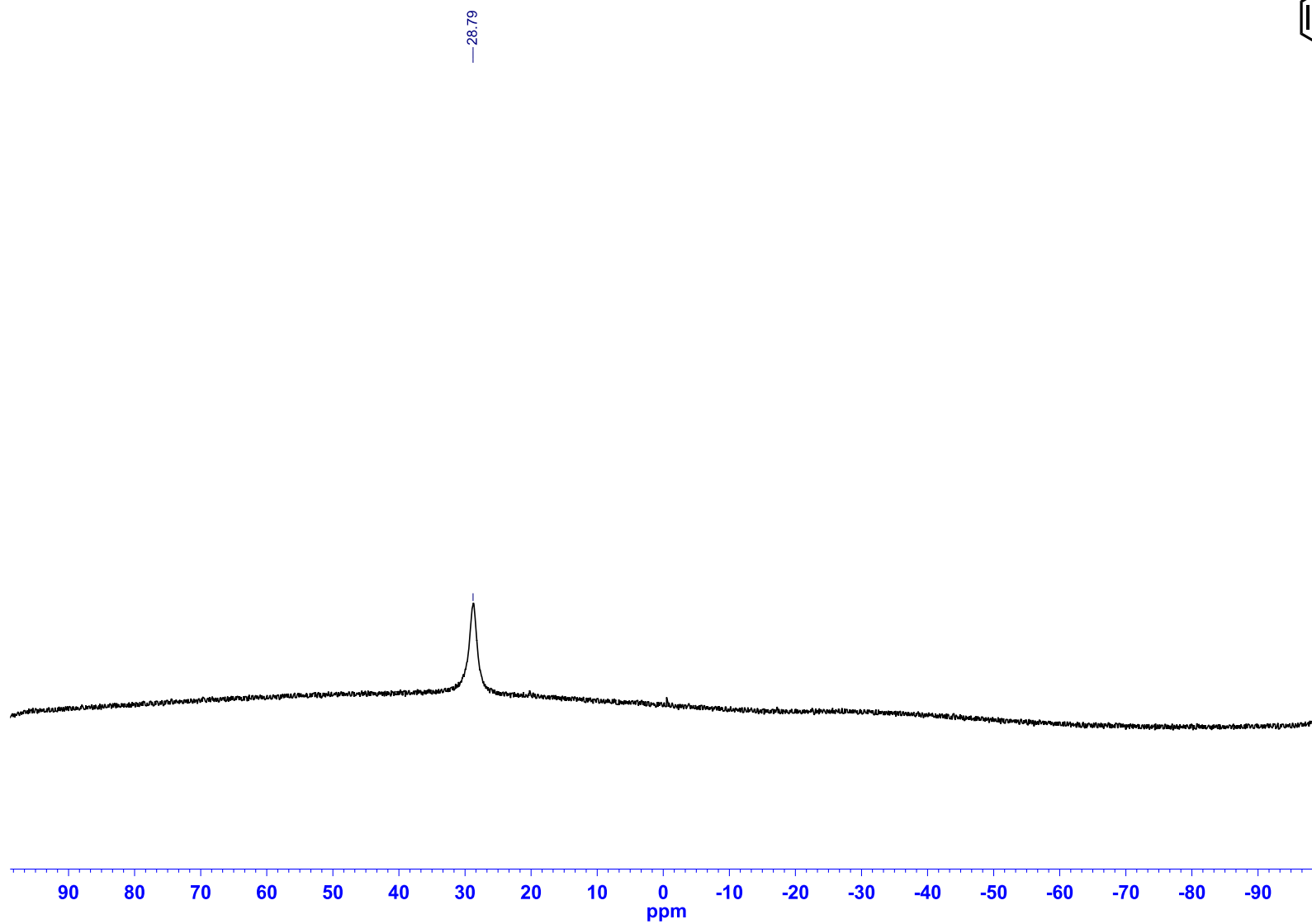
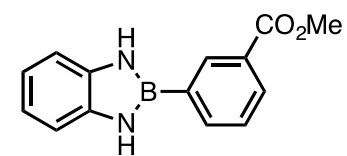
^1H NMR (500.4 MHz, $\text{DMSO-}d_6$) of 2-(4-(methoxycarbonyl)phenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5m**)



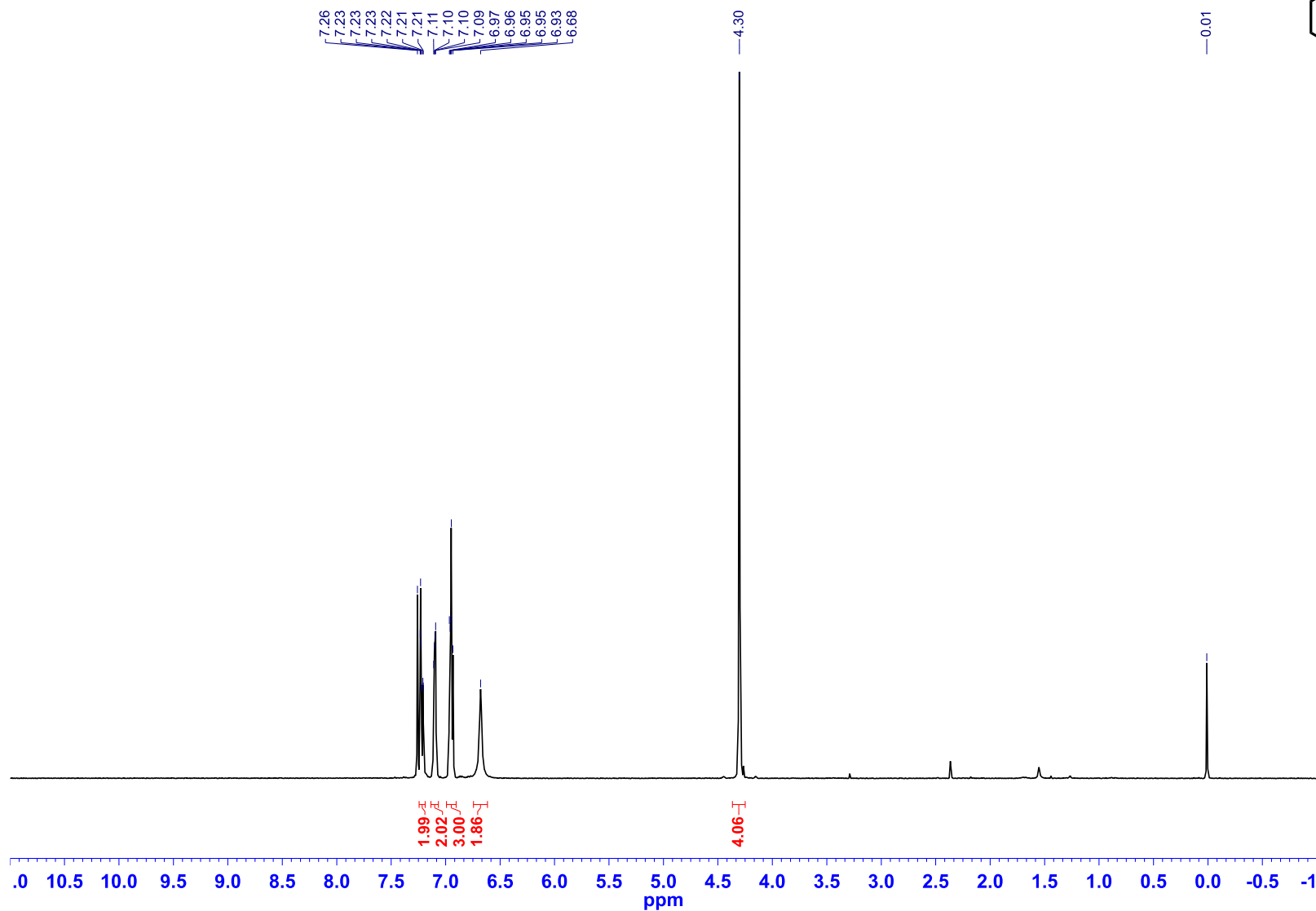
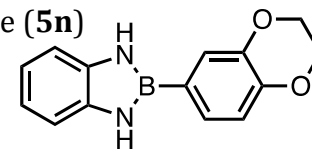
^{13}C NMR (125.8 MHz, $\text{DMSO-}d_6$) of 2-(4-(methoxycarbonyl)phenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5m**)



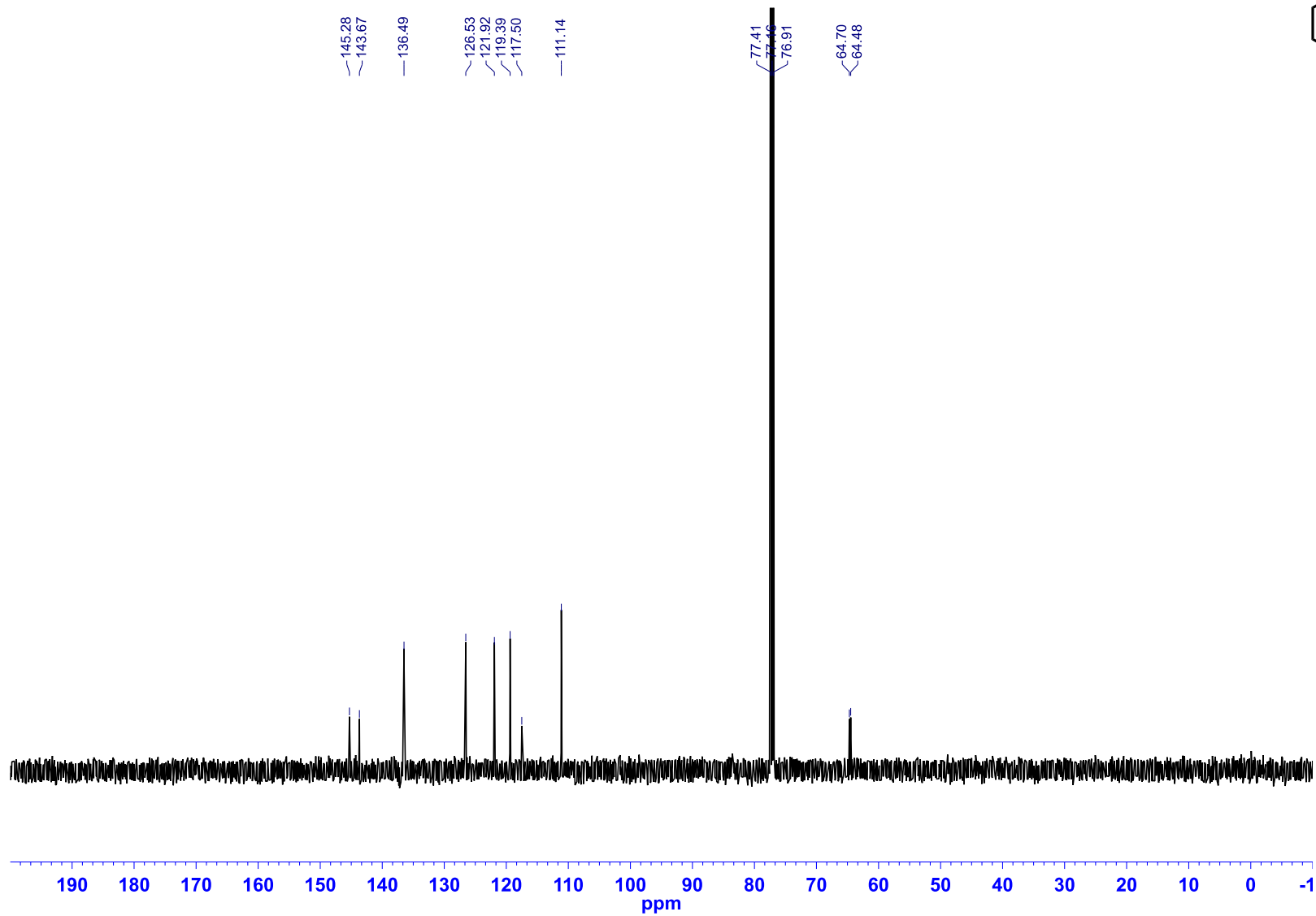
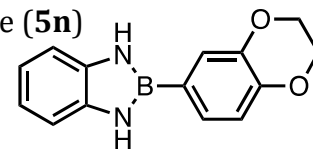
^{11}B NMR (128.4 MHz, MeCN) of 2-(4-(methoxycarbonyl)phenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5m**)



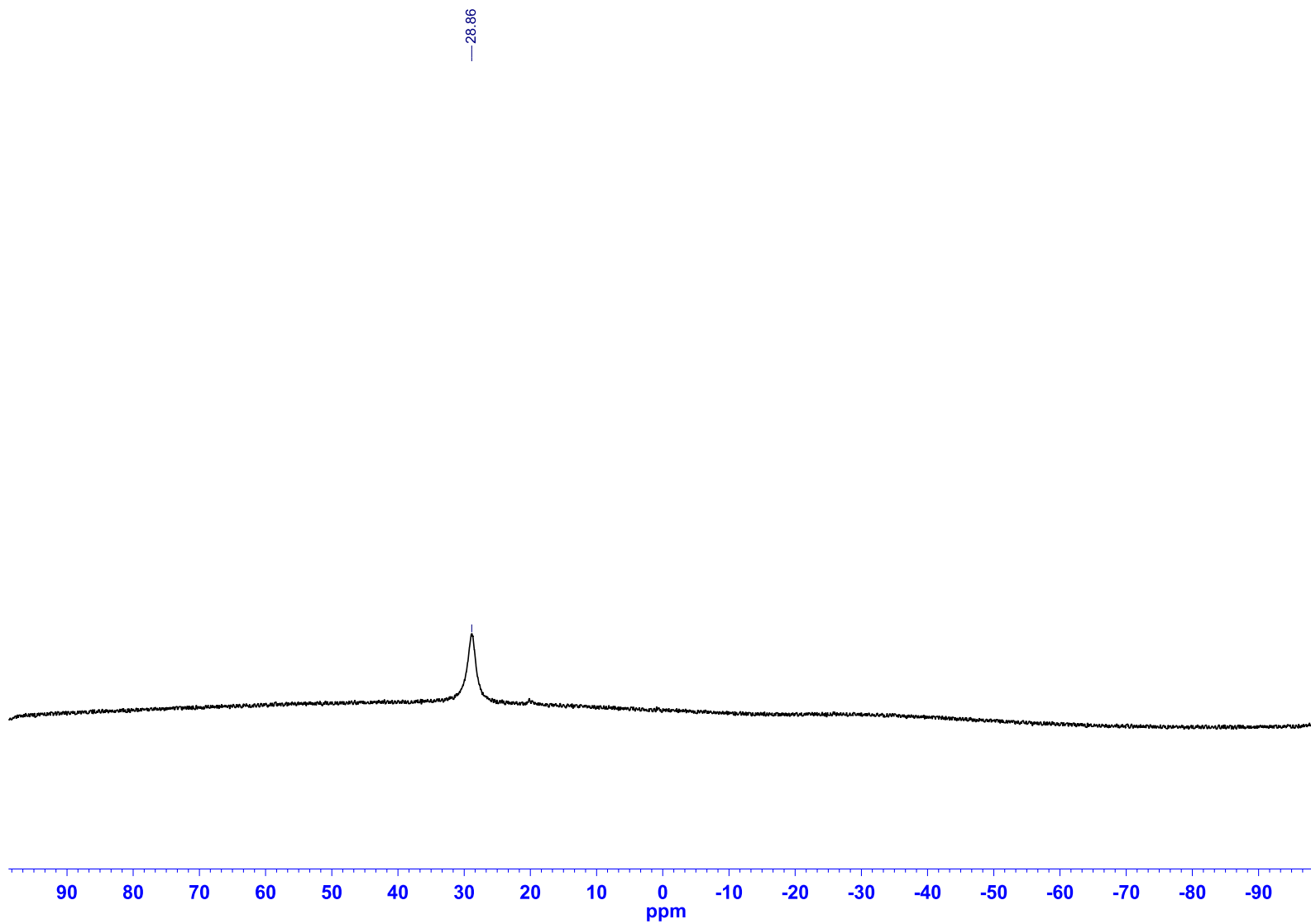
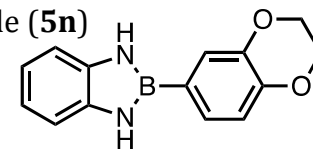
^1H NMR (500.4 MHz, CDCl_3) of 2-(2,3-dihydrobenzo[1,4]dioxin-5-yl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5n**)



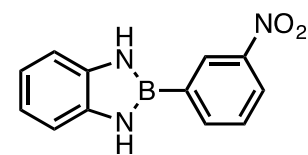
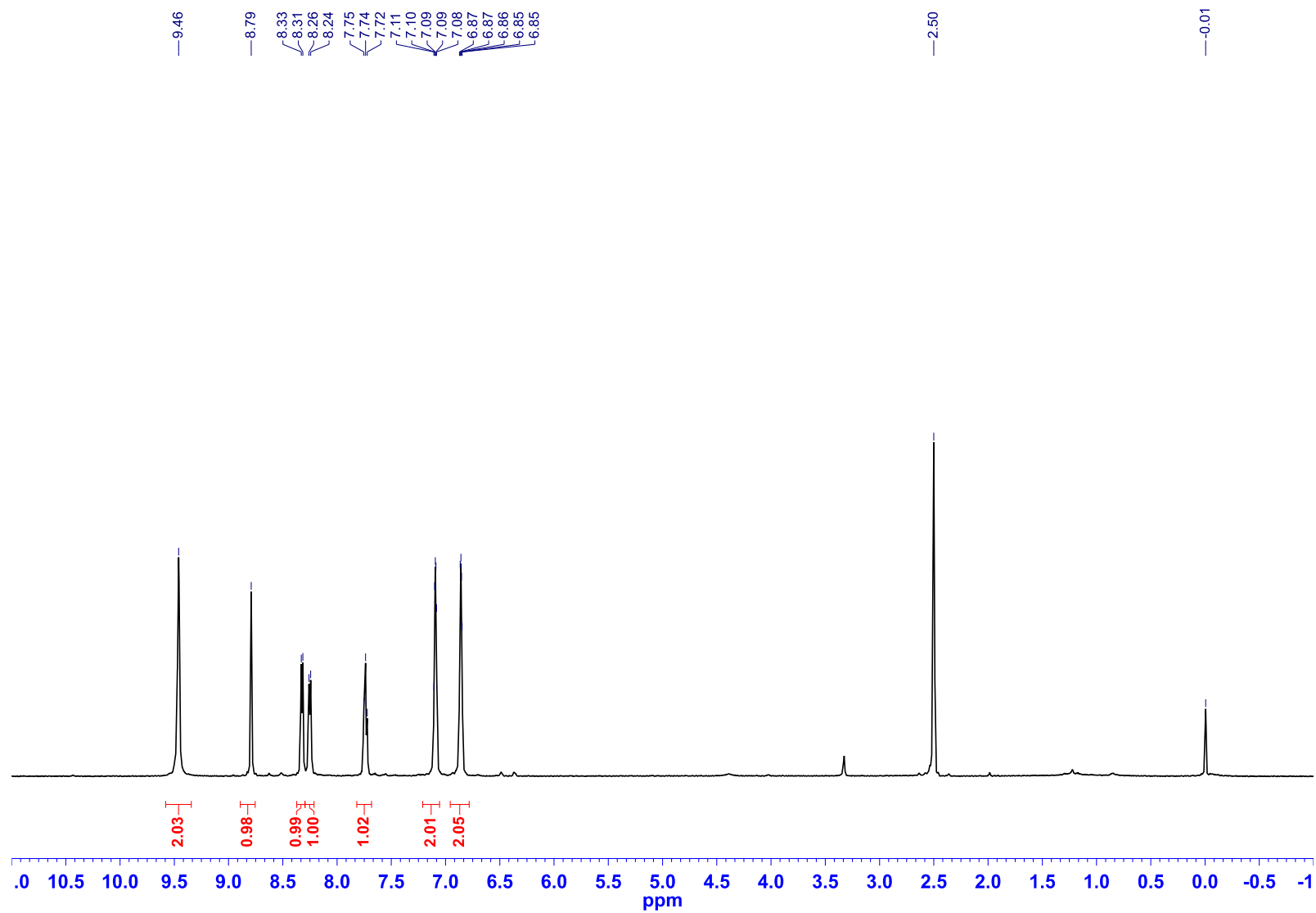
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(2,3-dihydrobenzo[1,4]dioxin-5-yl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5n**)



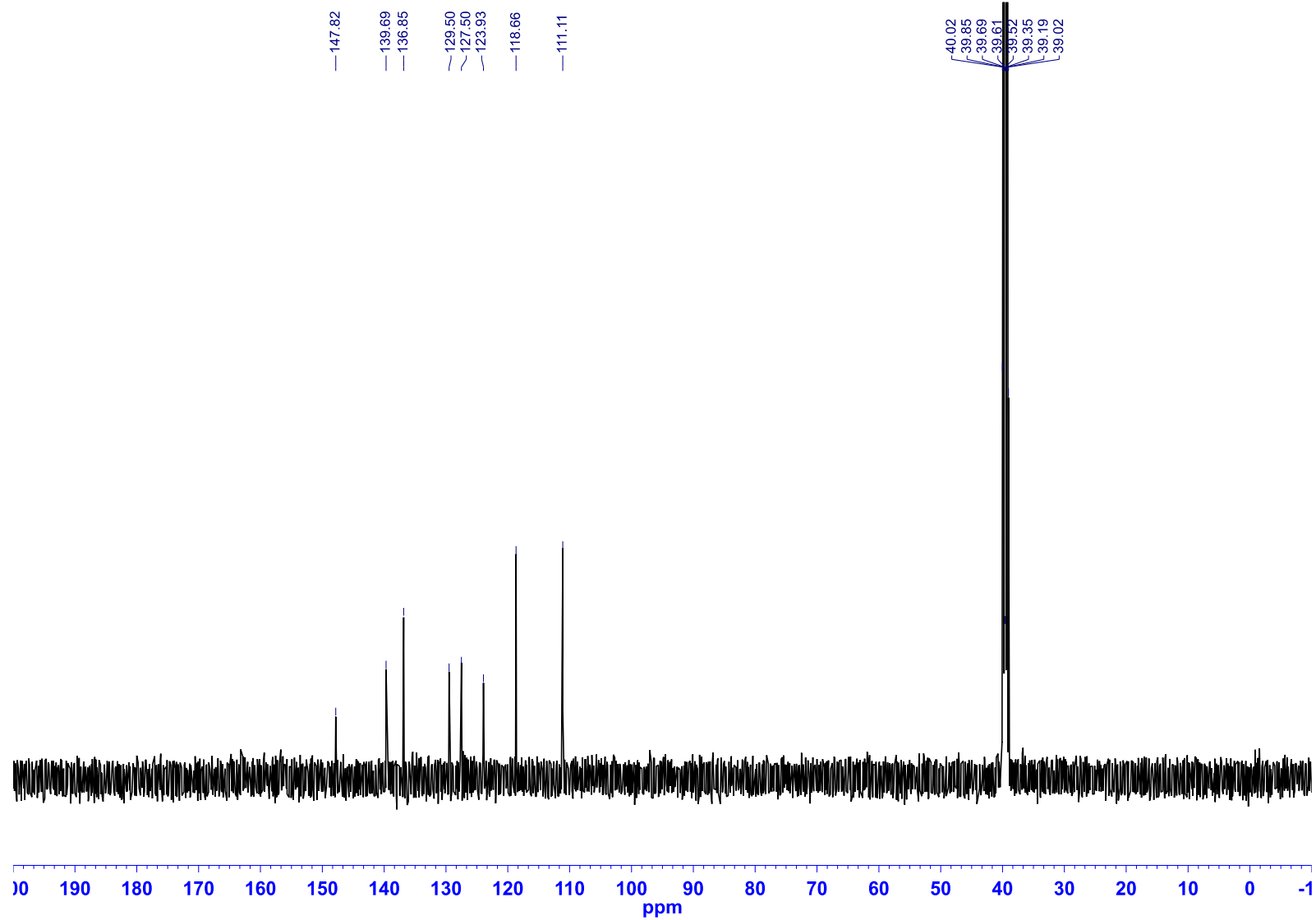
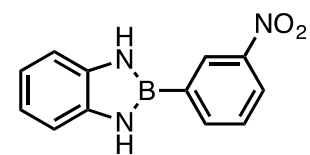
^{11}B NMR (128.4 MHz, MeCN) of 2-(2,3-dihydrobenzo[1,4]dioxin-5-yl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5n**)



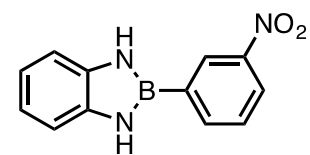
^1H NMR (500.4 MHz, $\text{DMSO-}d_6$) of 2-(3-nitrophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5o**)



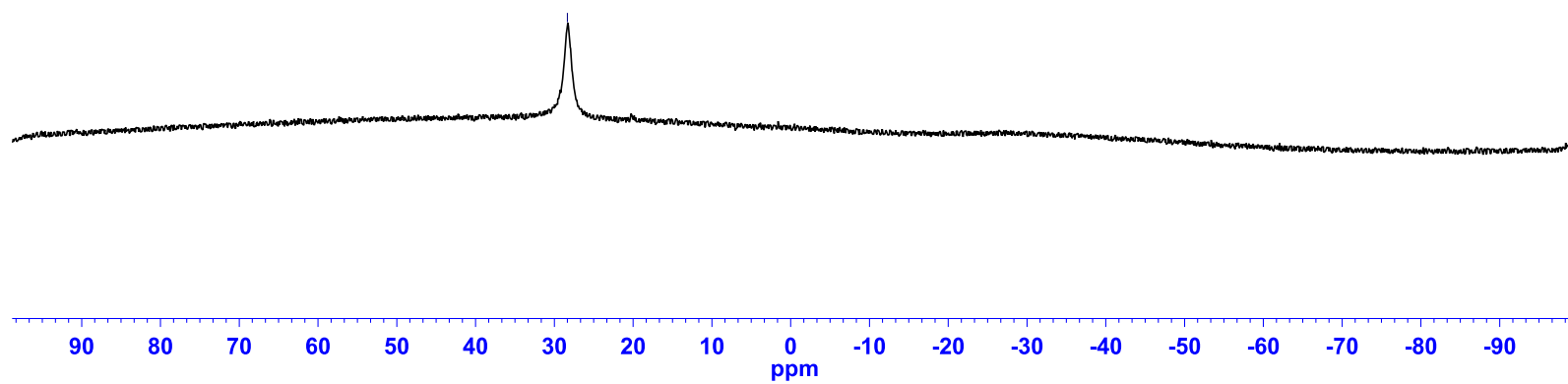
^{13}C NMR (125.8 MHz, $\text{DMSO-}d_6$) of 2-(3-nitrophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5o**)



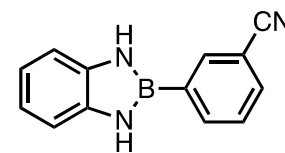
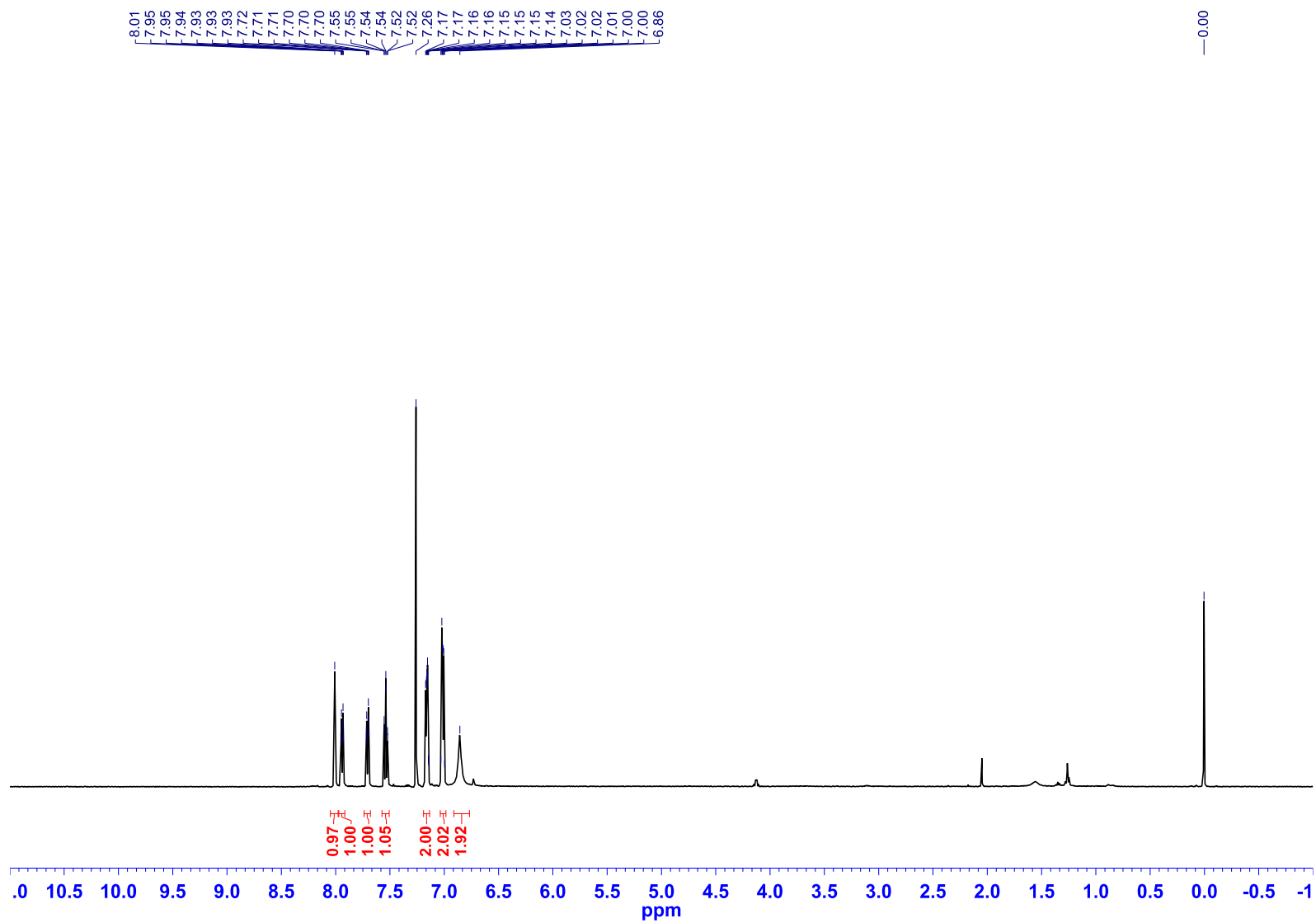
^{11}B NMR (128.4 MHz, MeCN) of 2-(3-nitrophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5o**)



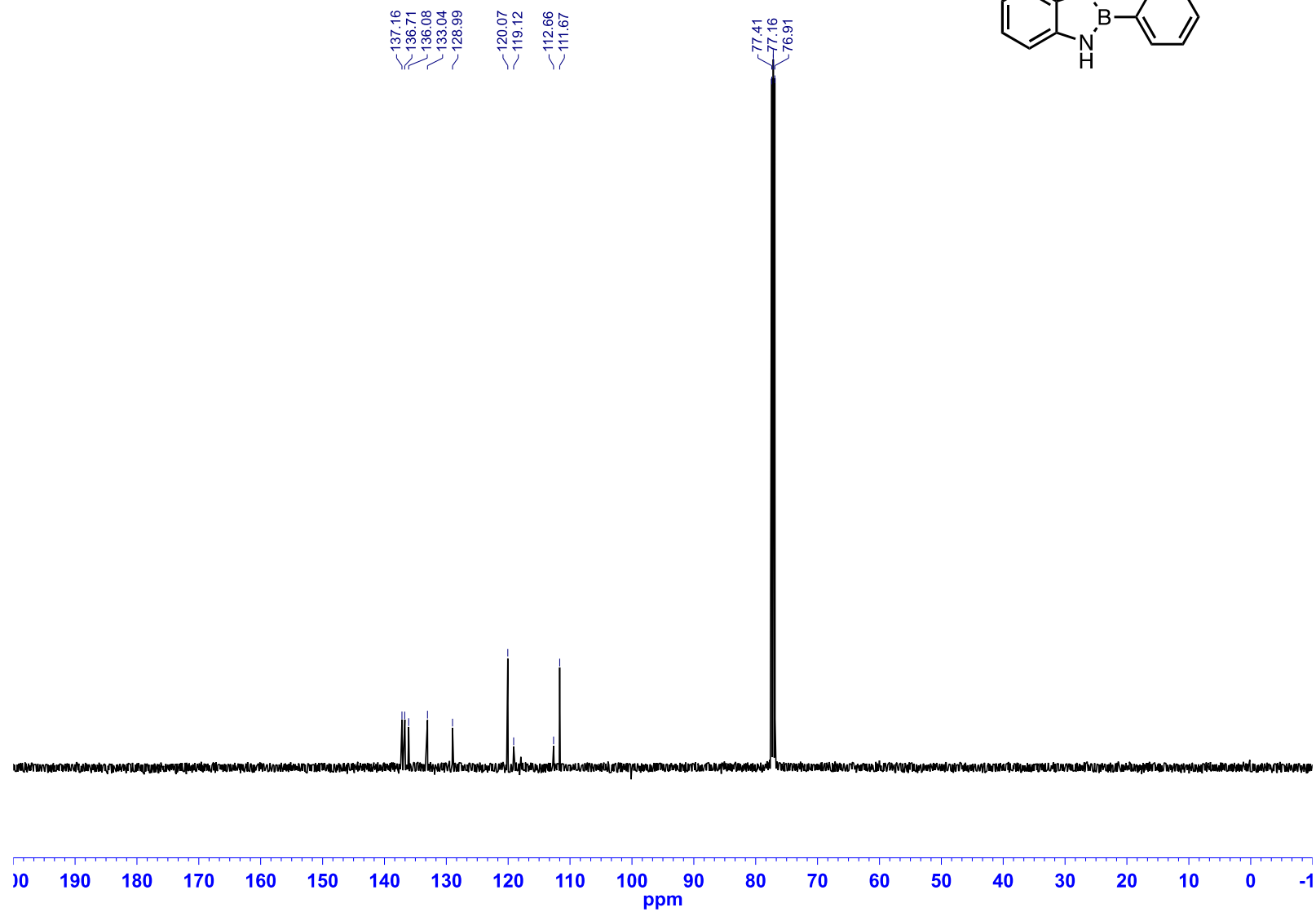
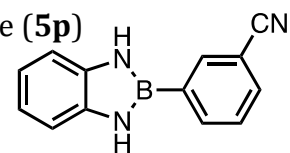
—28.34



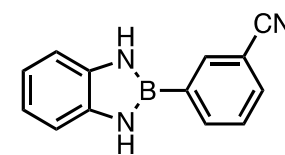
^1H NMR (500.4 MHz, CDCl_3) of 2-(3-cyanophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5p**)



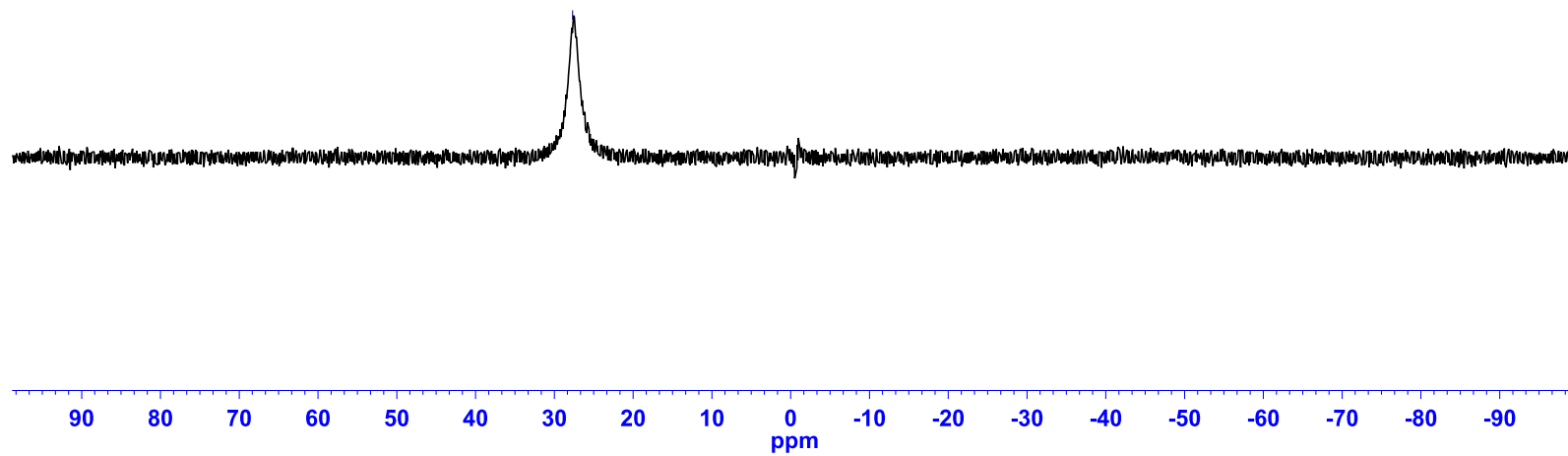
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(3-cyanophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5p**)



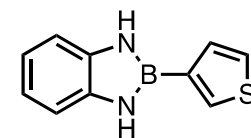
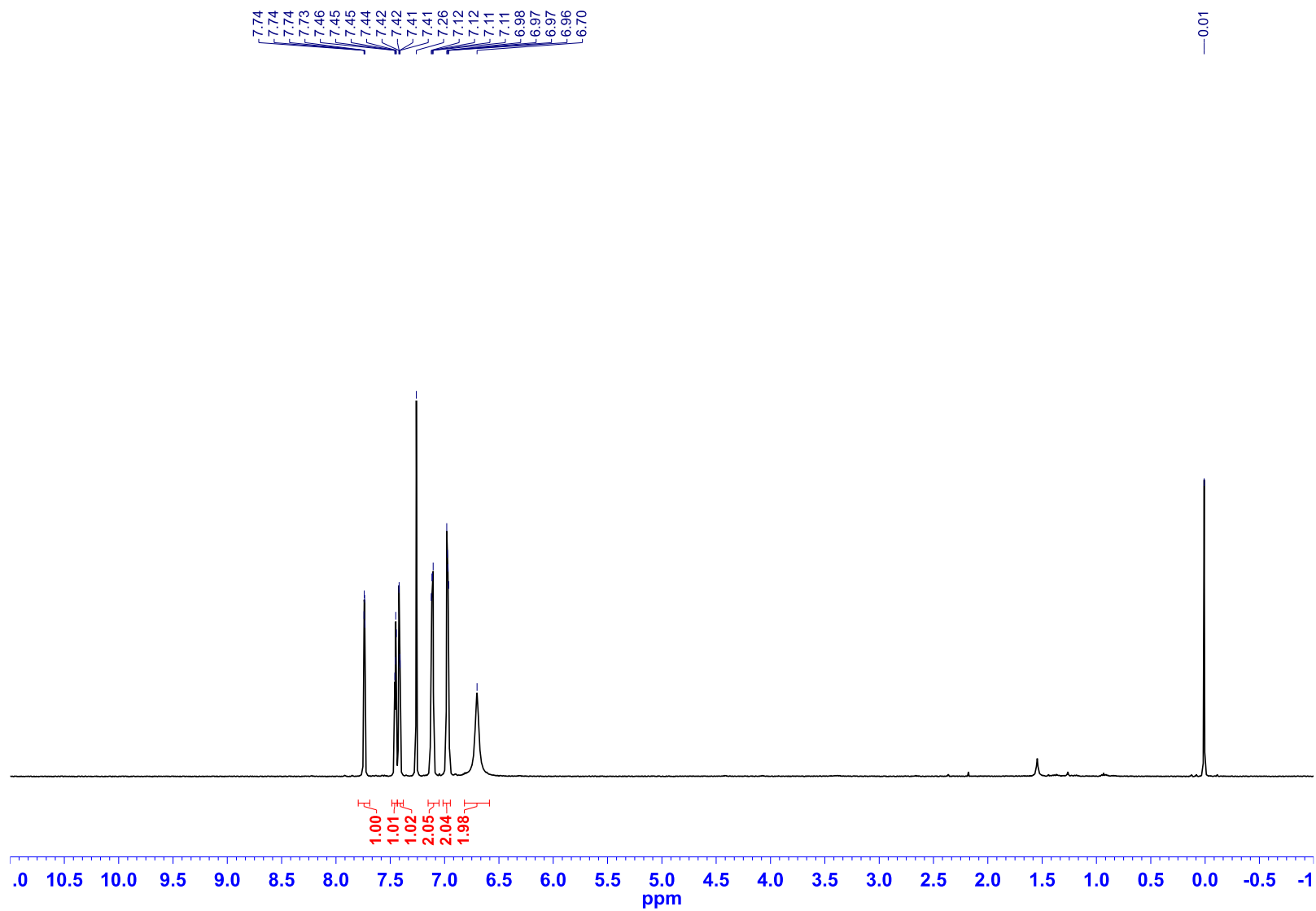
^{11}B NMR (128.4 MHz, CDCl_3) of 2-(3-cyanophenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5p**)



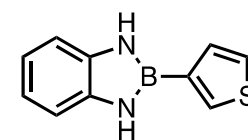
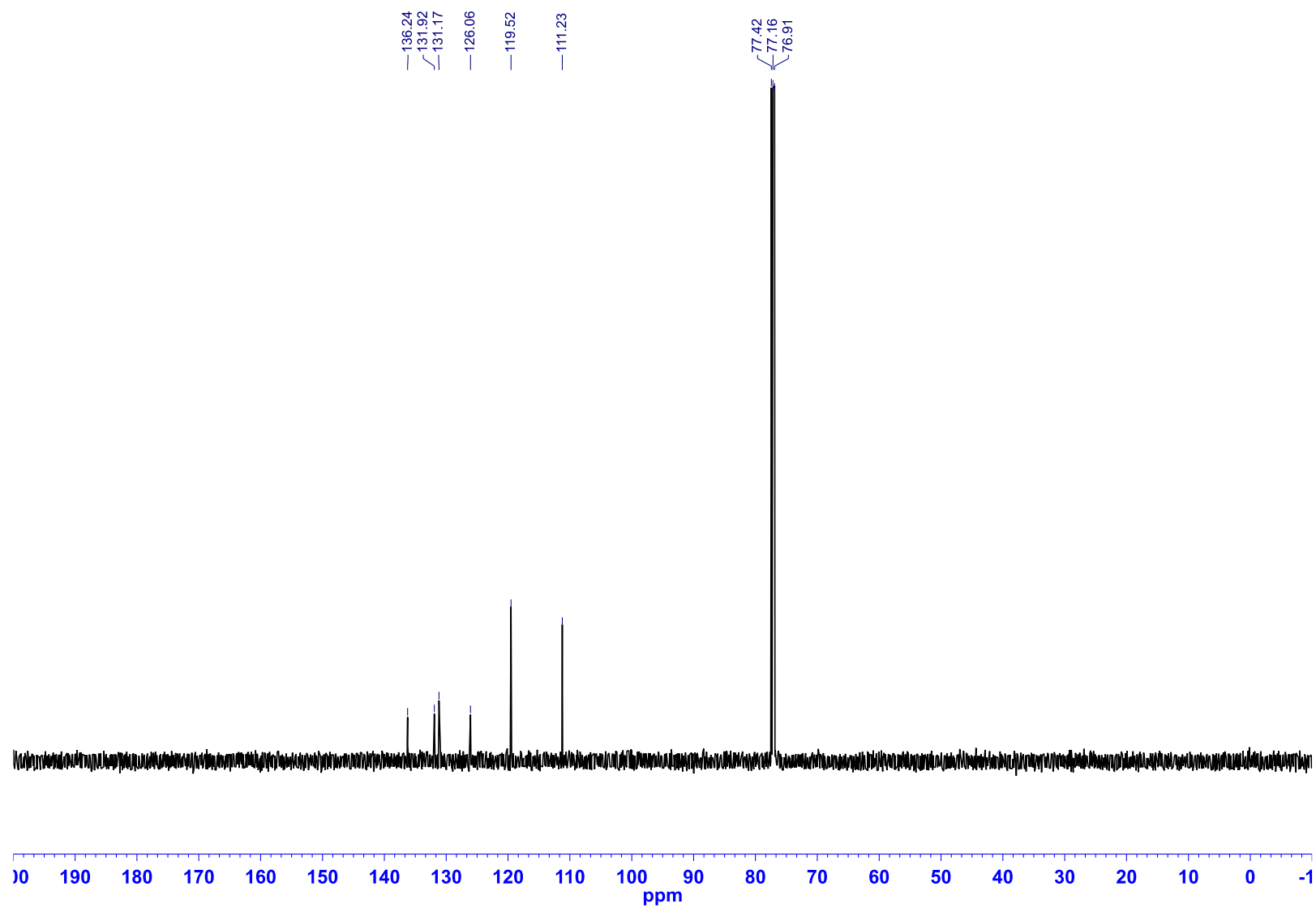
—27.69



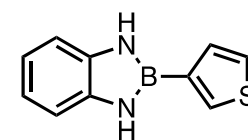
^1H NMR (500.4 MHz, CDCl_3) of 2-(3-thienyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5q**)



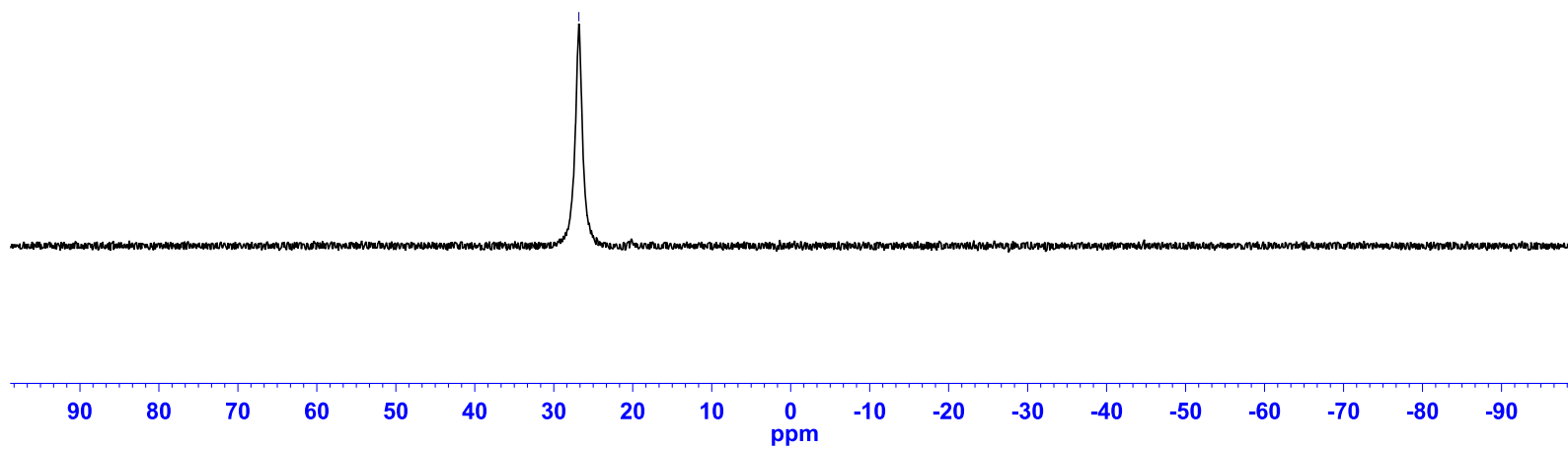
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(3-thienyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5q**)



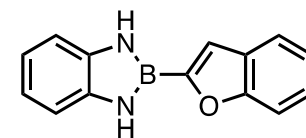
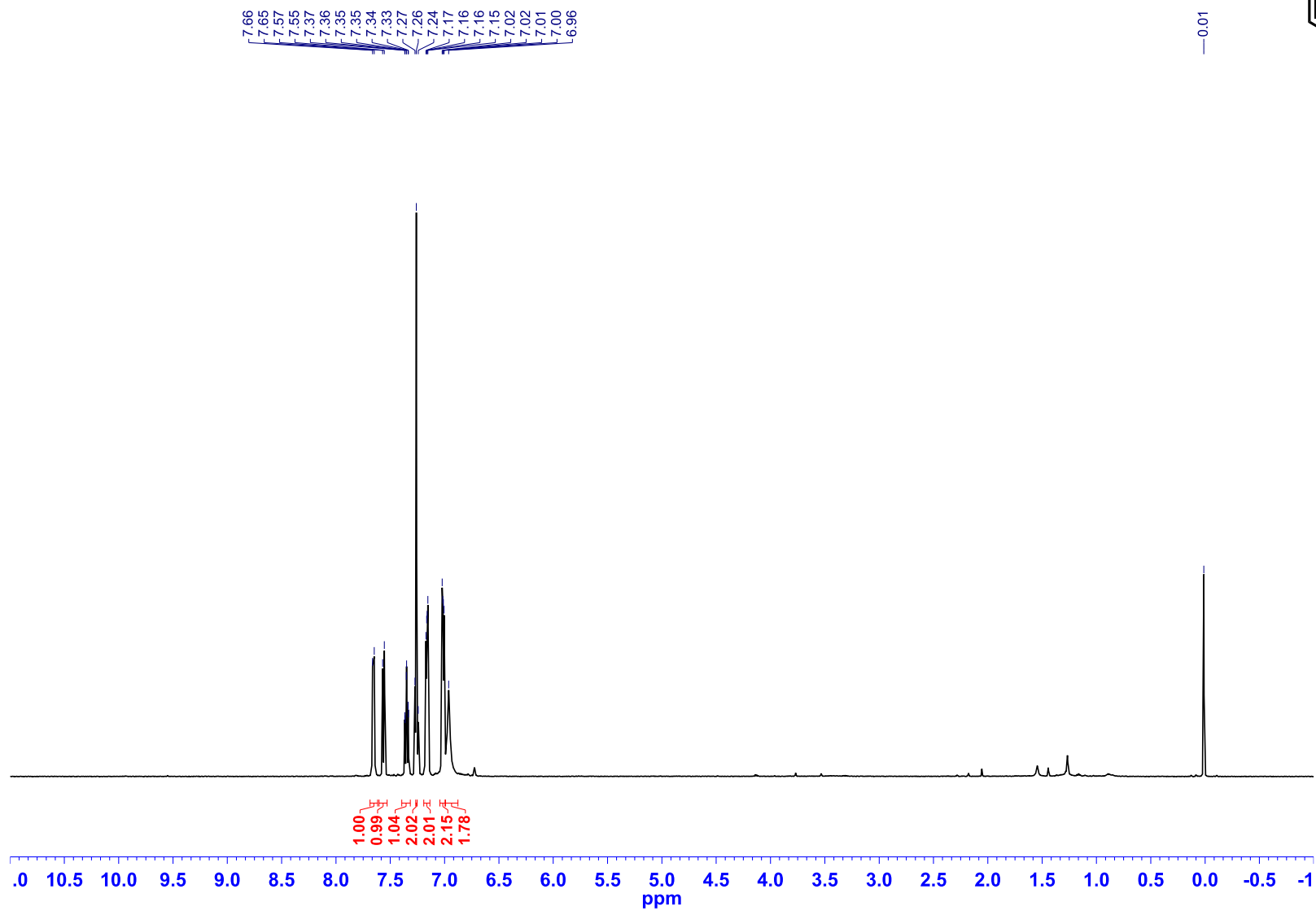
^{11}B NMR (128.4 MHz, MeCN) of 2-(3-thienyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5q**)



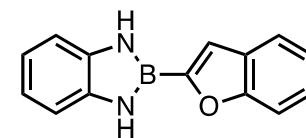
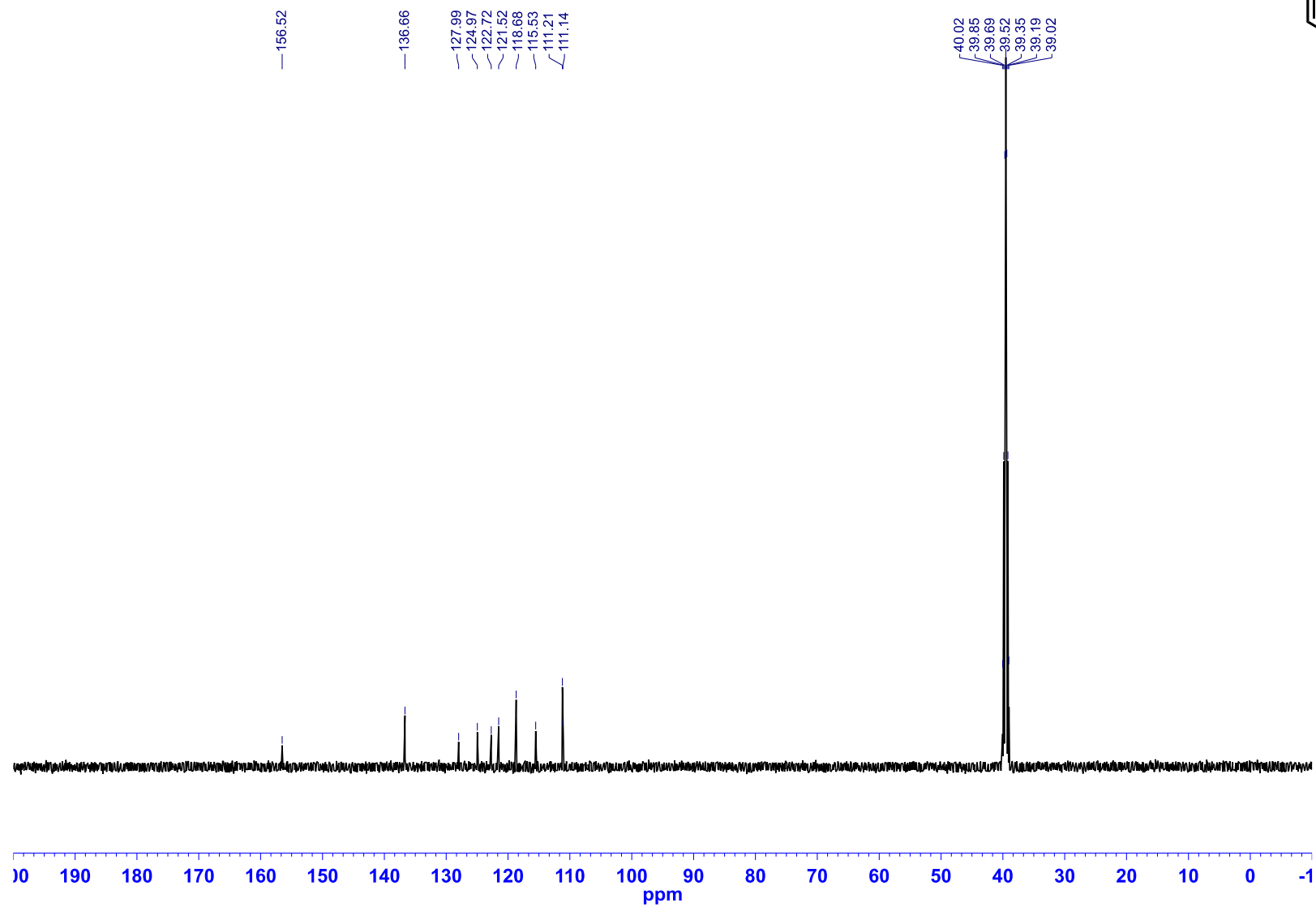
— 26.82



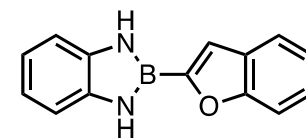
^1H NMR (500.4 MHz, CDCl_3) of 2-(2-benzofuranyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5r**)



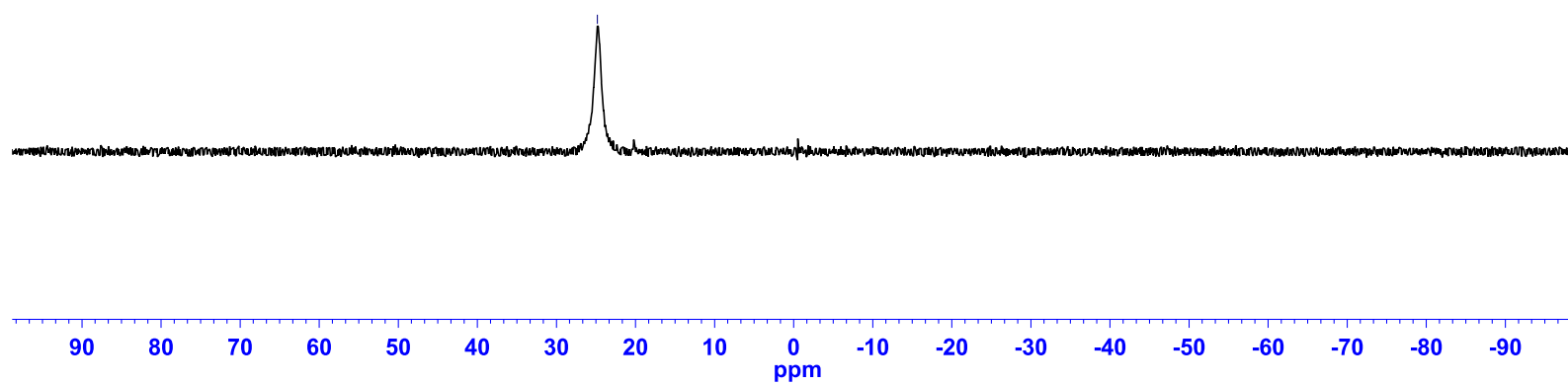
^{13}C NMR (125.8 MHz, $\text{DMSO-}d_6$) of 2-(2-benzofuranyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5r**)



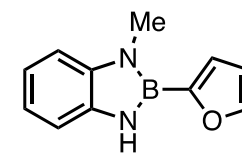
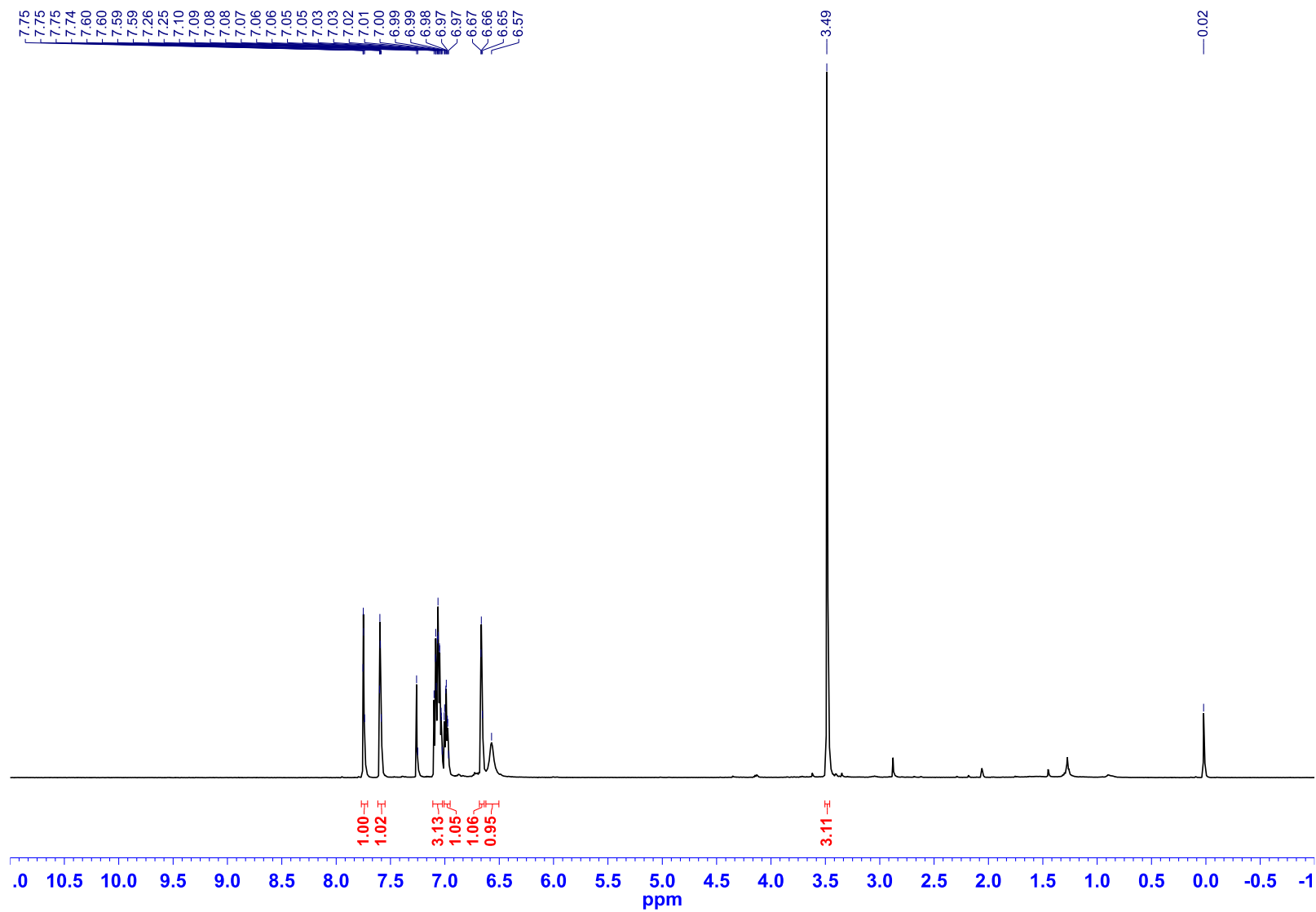
^{11}B NMR (128.4 MHz, MeCN) of 2-(2-benzofuranyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5r**)



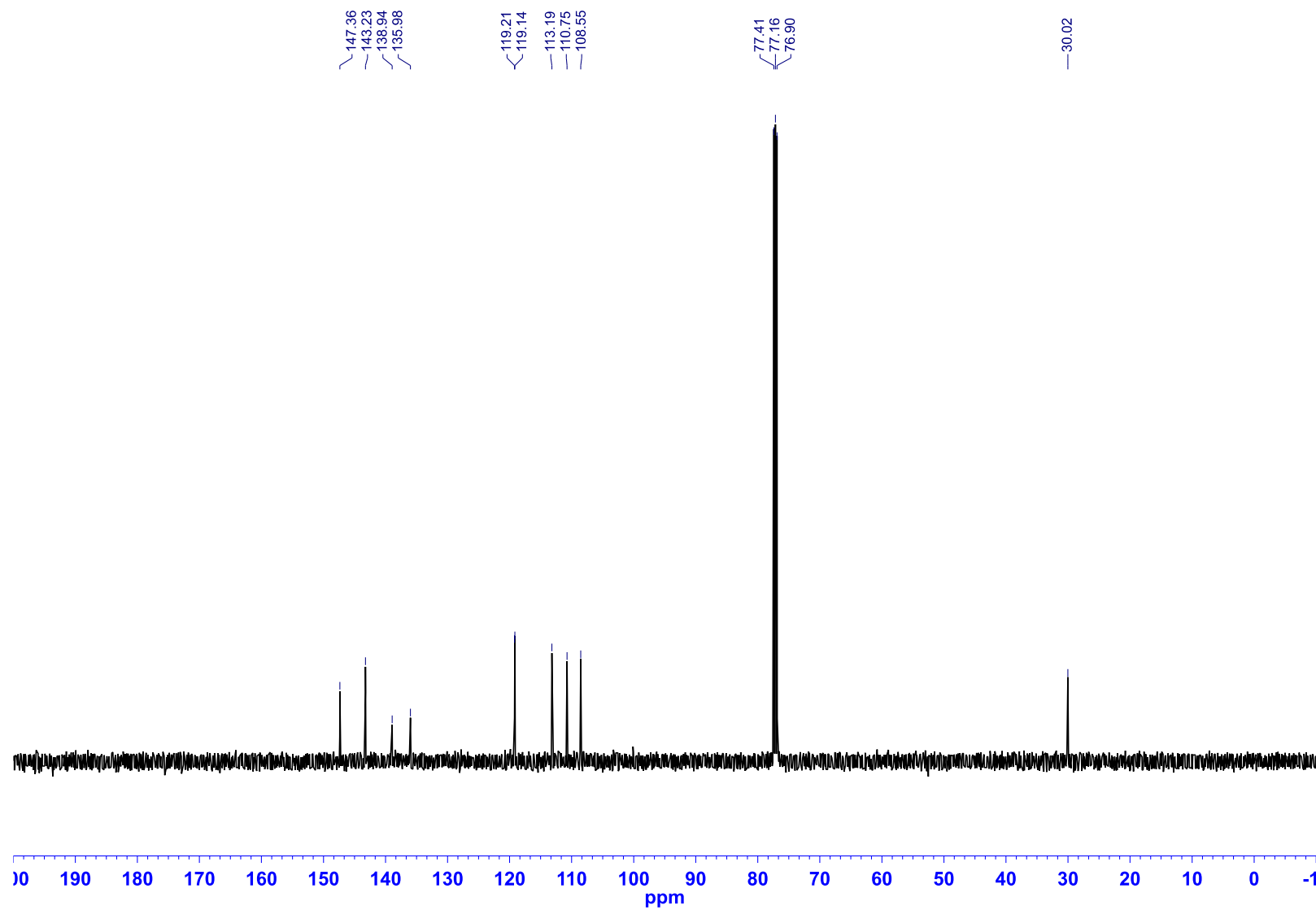
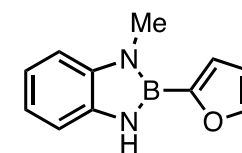
— 24.82



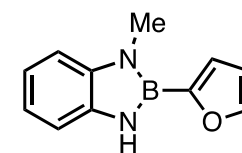
^1H NMR (500.4 MHz, CDCl_3) of 2-(2-furyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5s**)



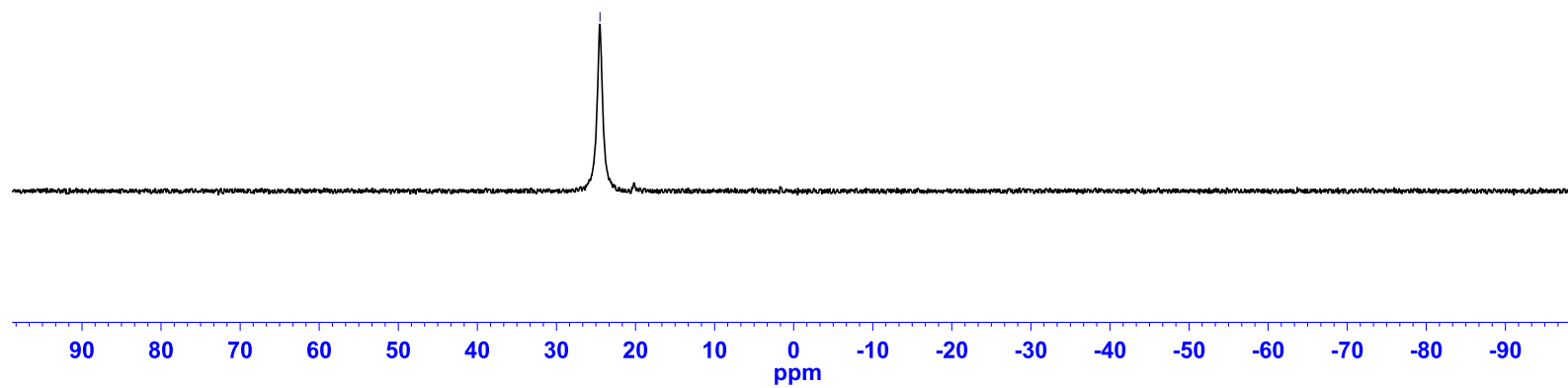
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(2-furyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5s**)



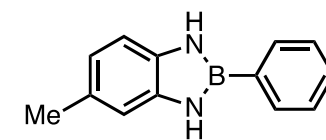
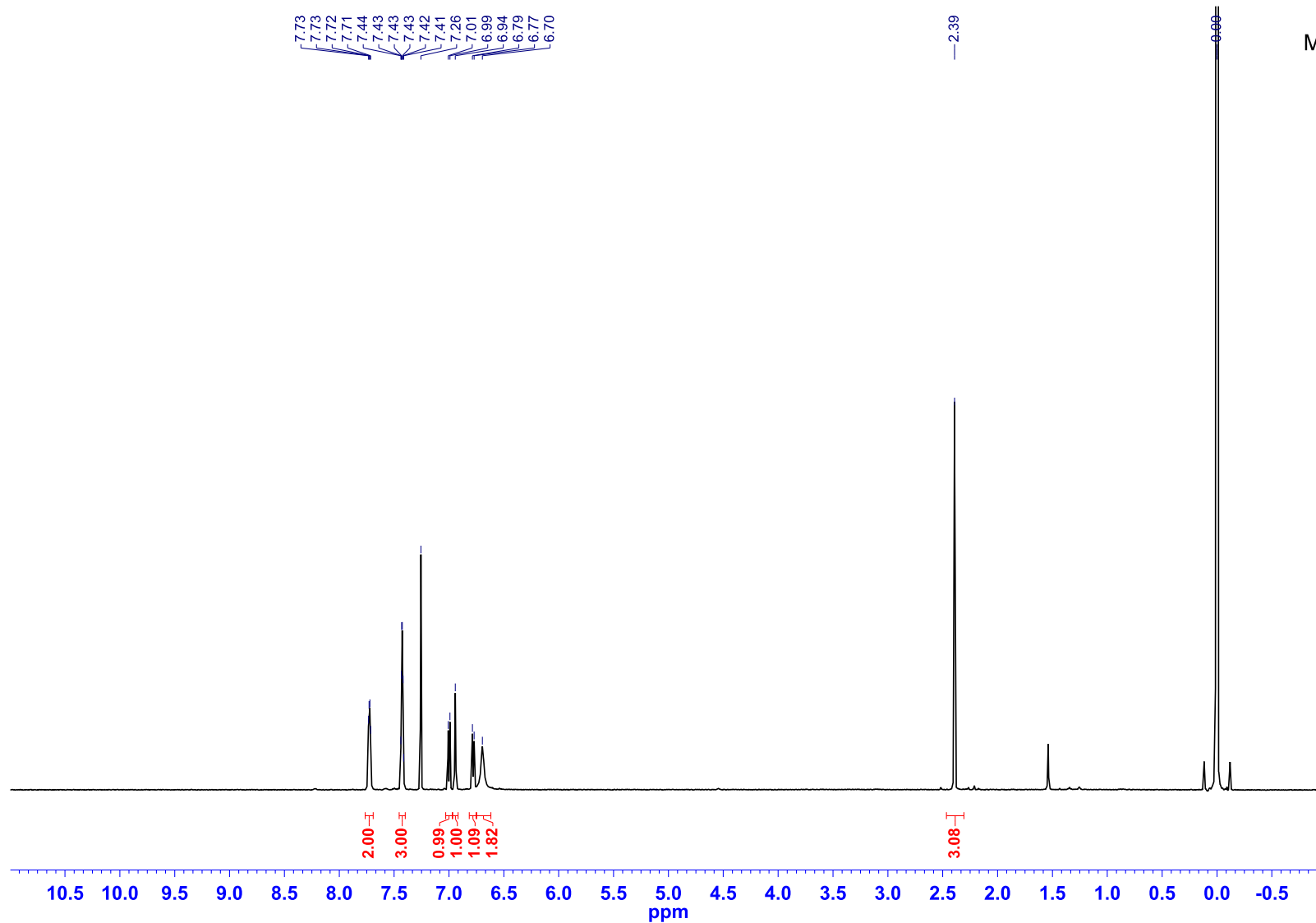
^{11}B NMR (128.4 MHz, MeCN) of 2-(2-furyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5s**)



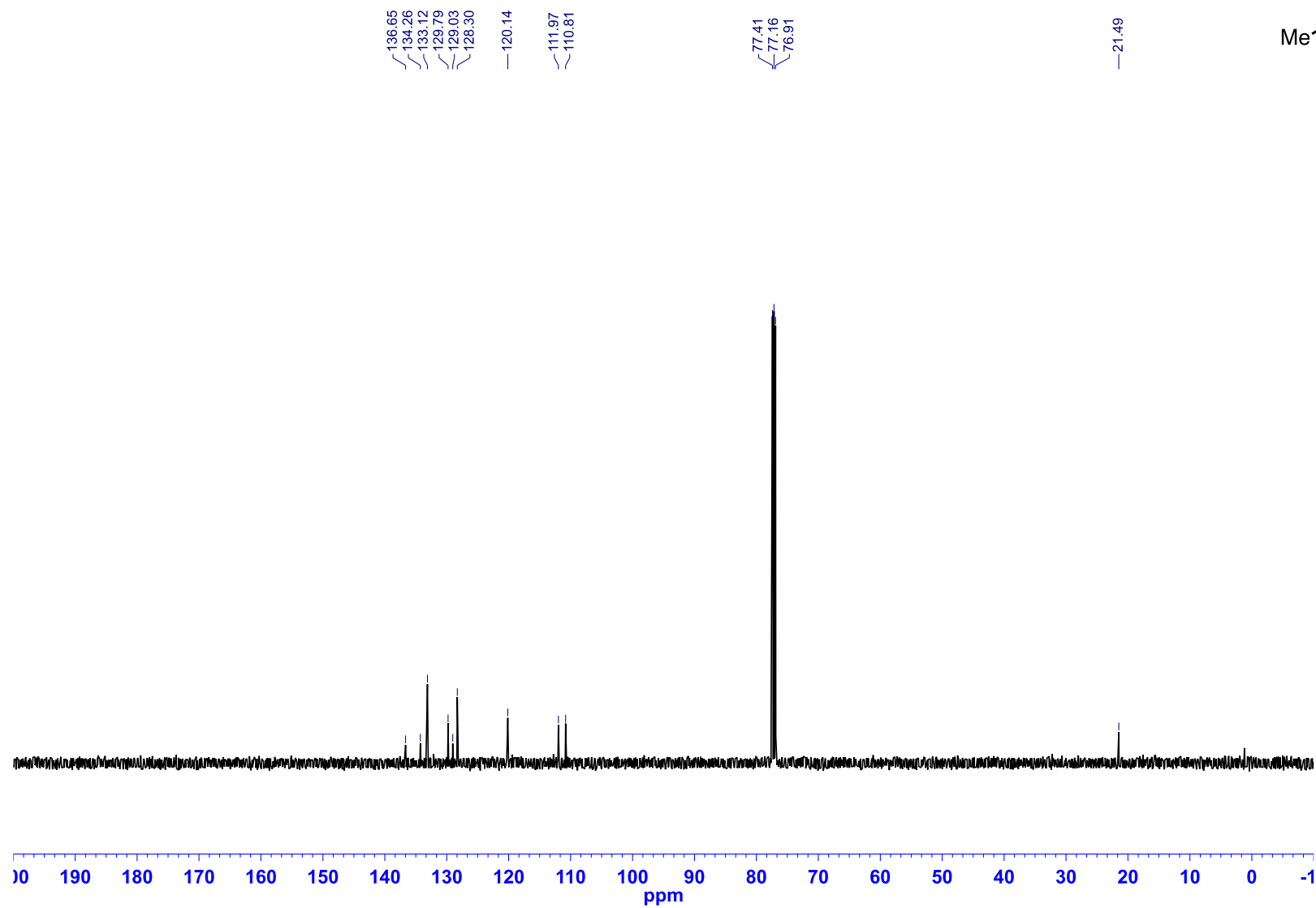
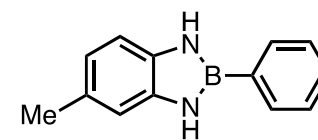
—24.50



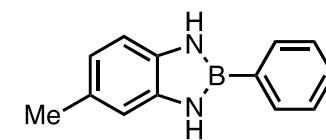
^1H NMR (500.4 MHz, CDCl_3 with 1% TMS) of 5-methyl-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5u**)



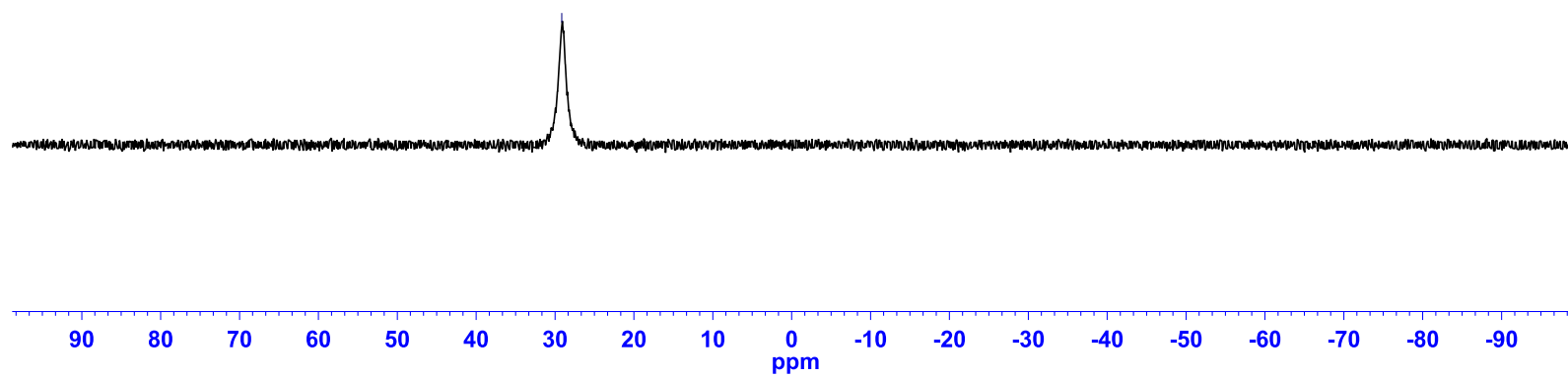
^{13}C NMR (125.8 MHz, CDCl_3) of 5-methyl-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5u**)



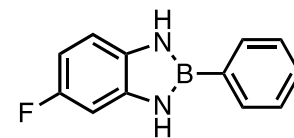
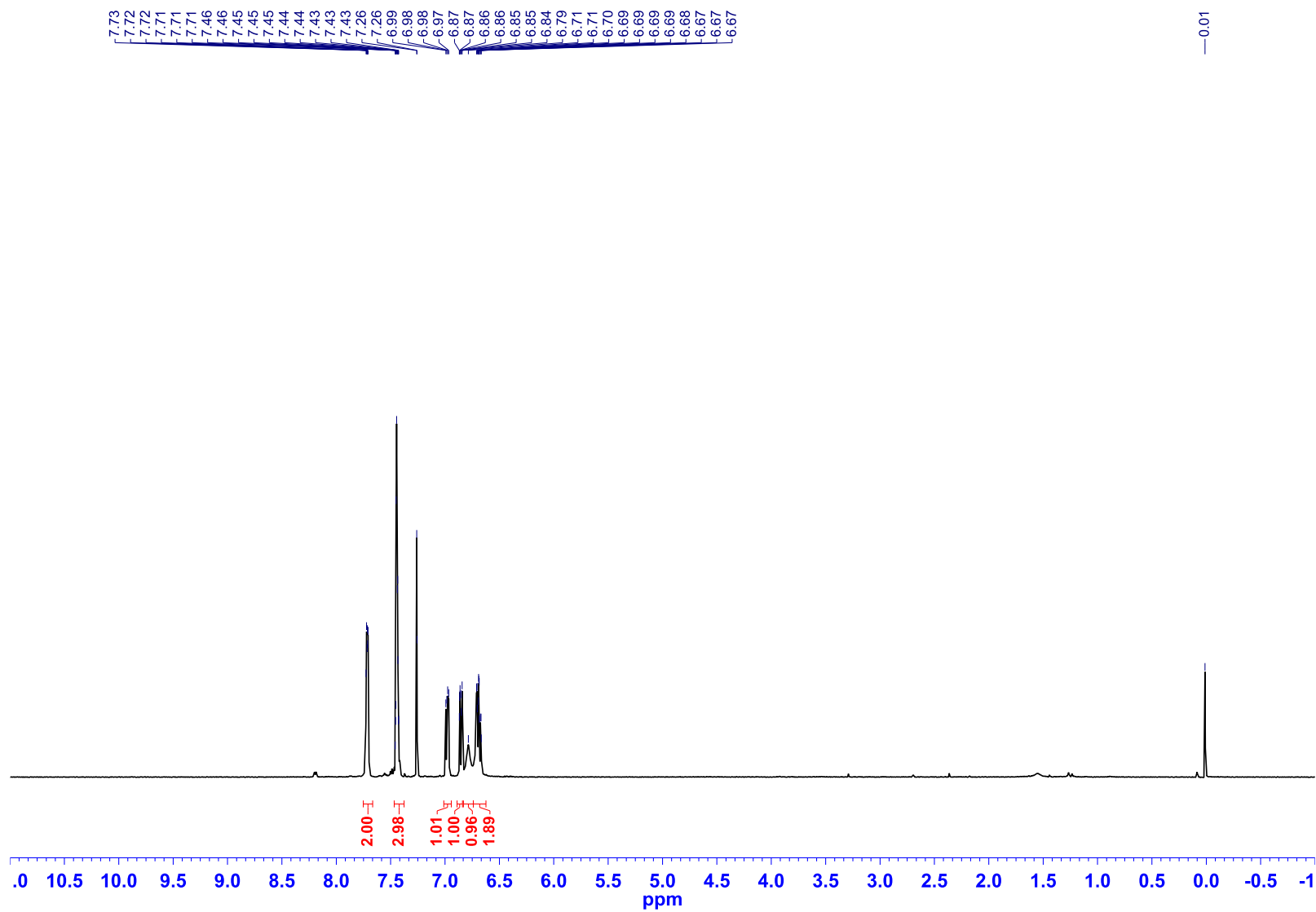
^{11}B NMR (128.4 MHz, MeCN) of 5-methyl-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5u**)



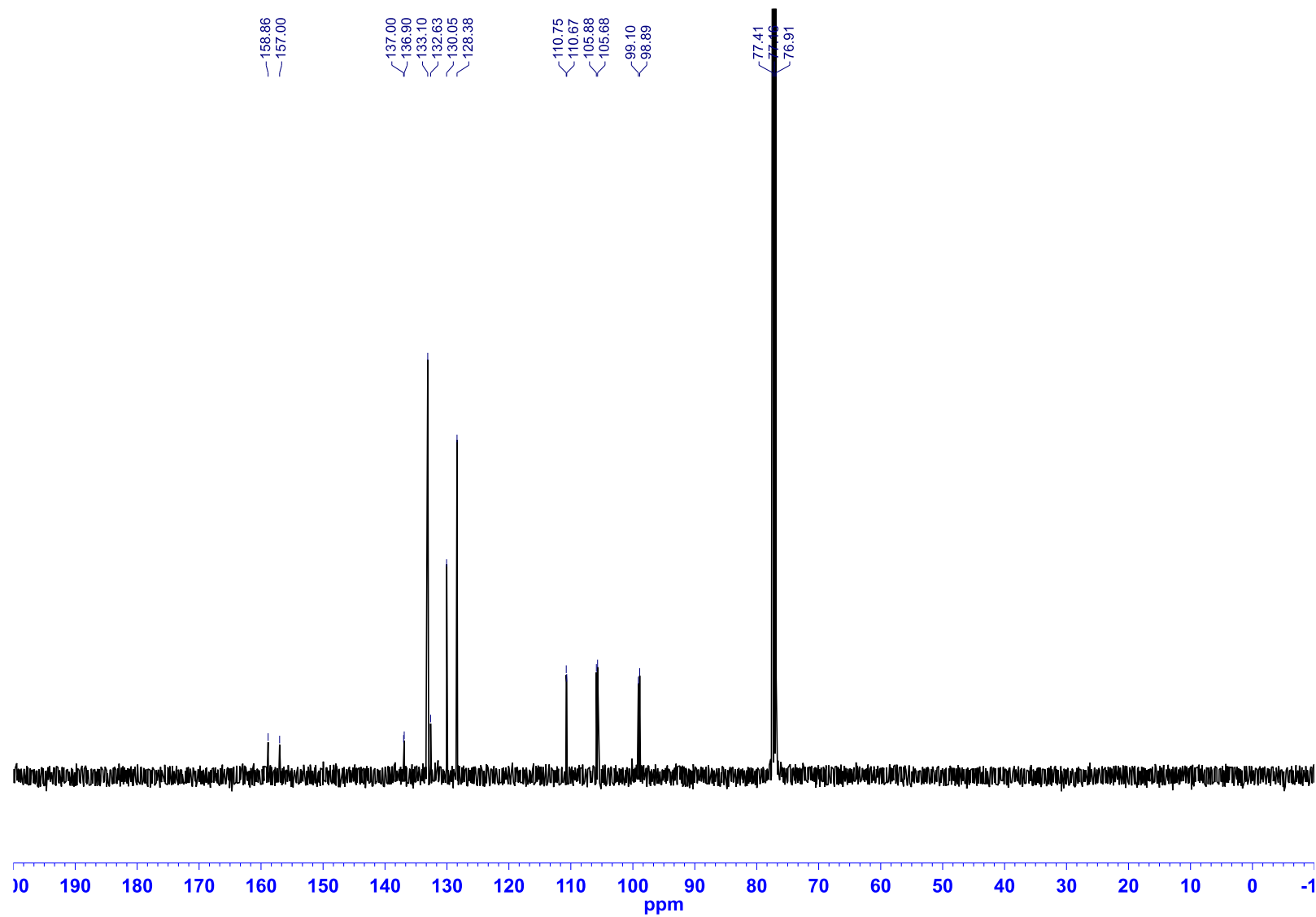
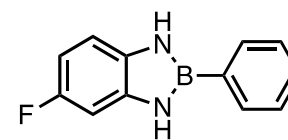
—29.15



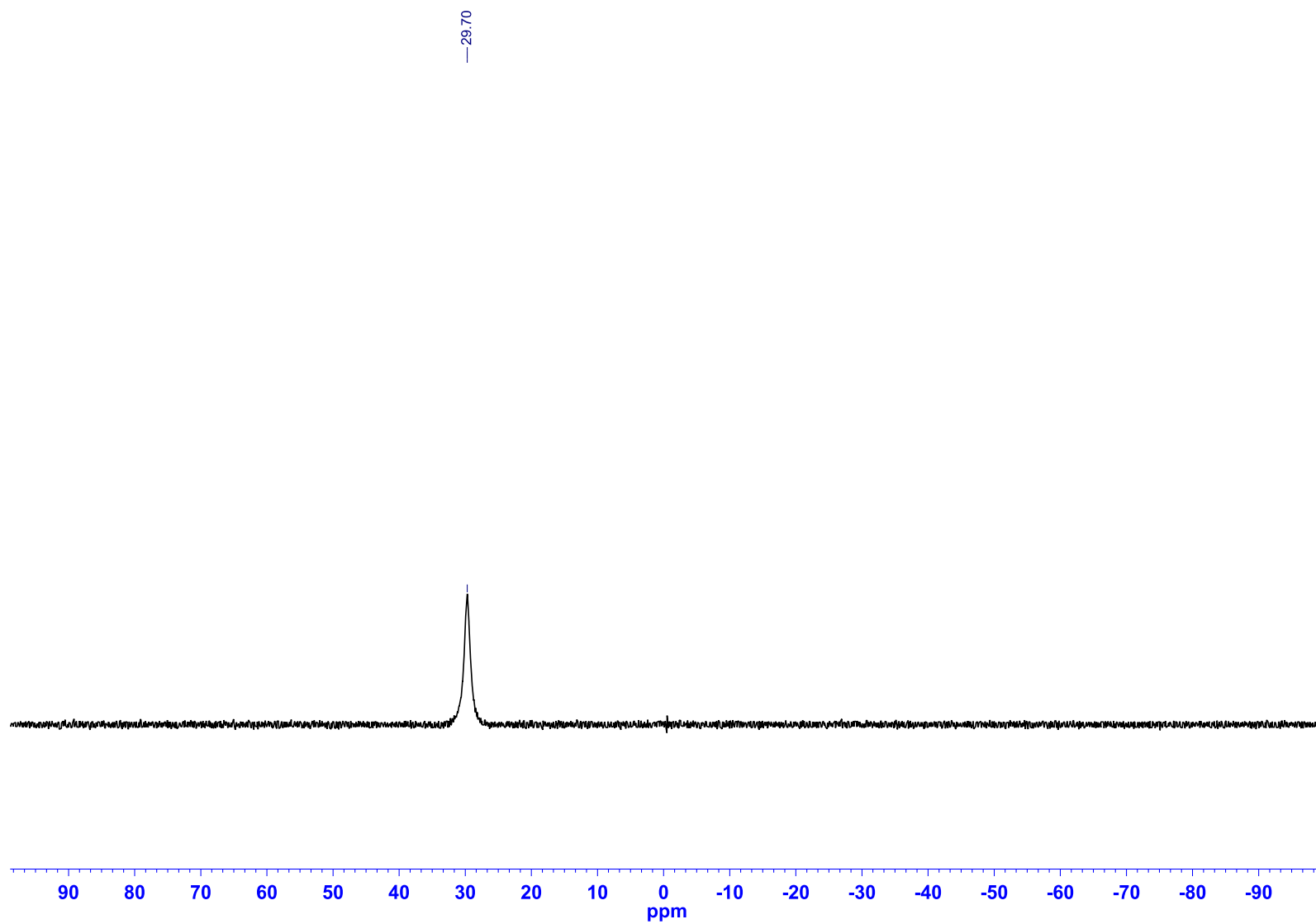
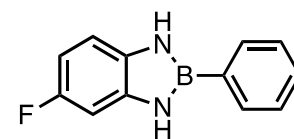
^1H NMR (500.4 MHz, CDCl_3) of 5-fluoro-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5v**)



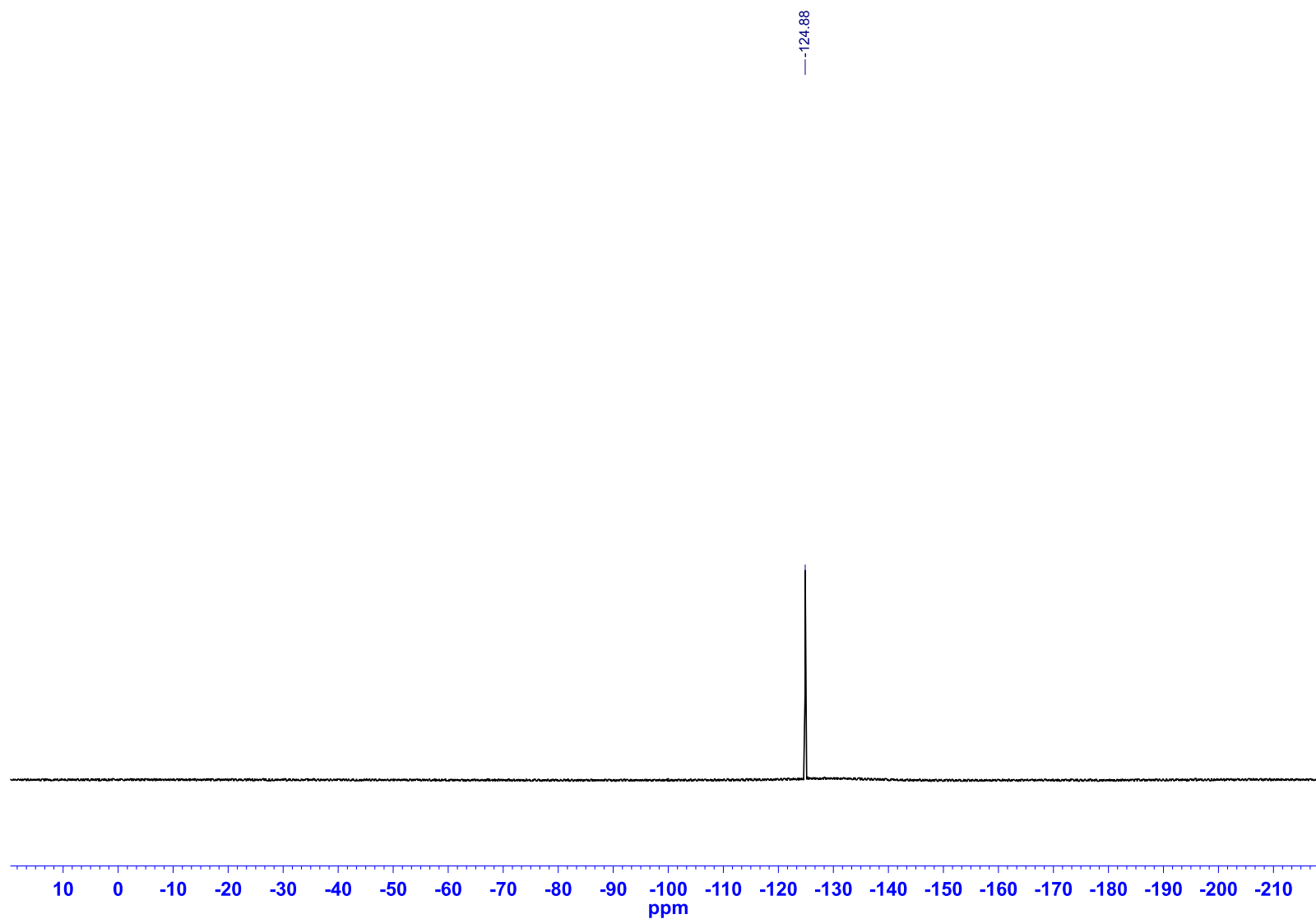
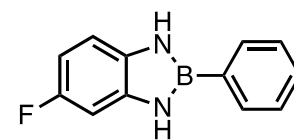
^{13}C NMR (125.8 MHz, CDCl_3) of 5-fluoro-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5v**)



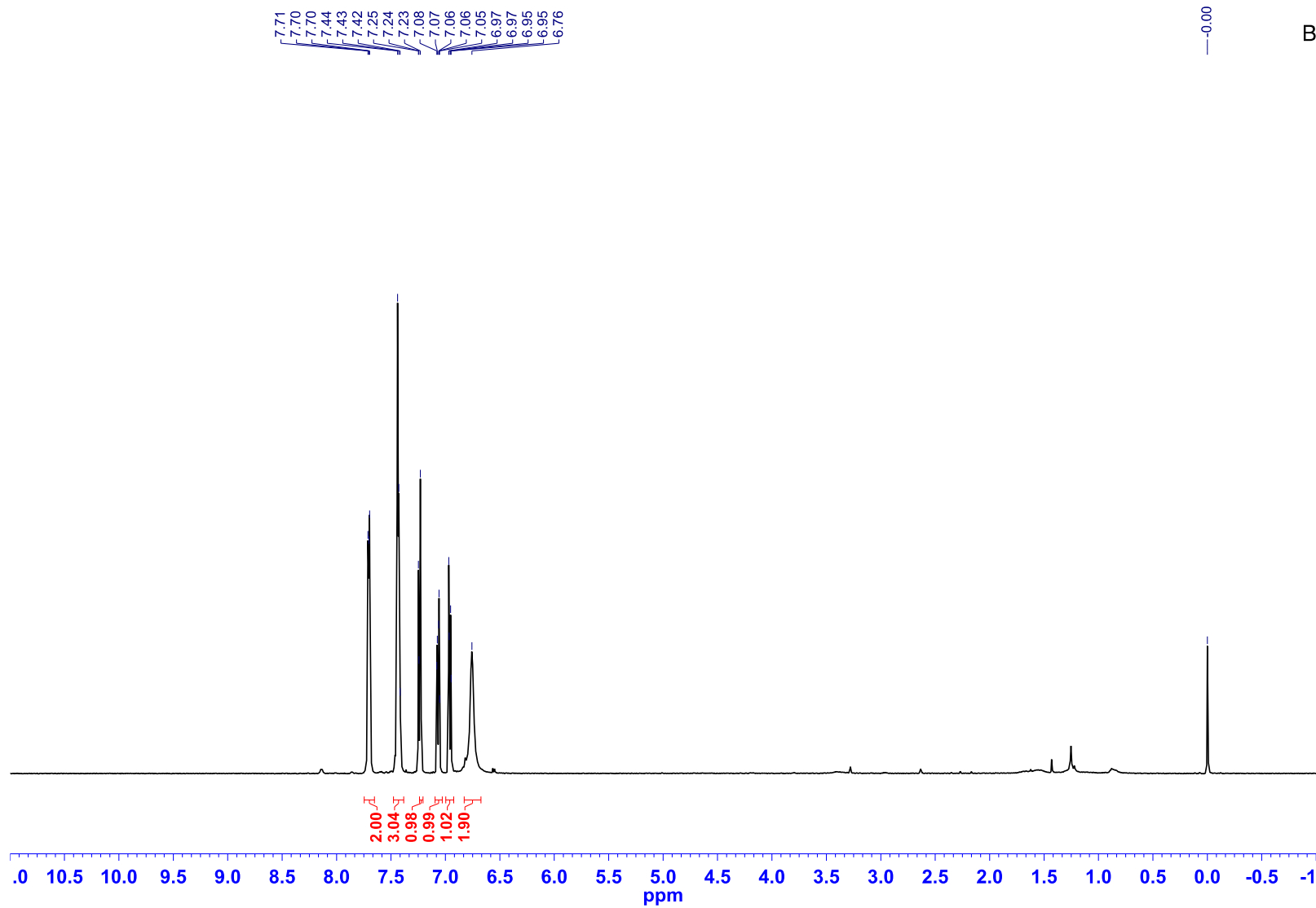
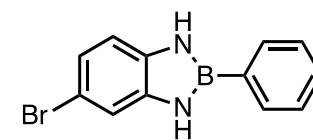
^{11}B NMR (128.4 MHz, MeCN) of 5-fluoro-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5v**)



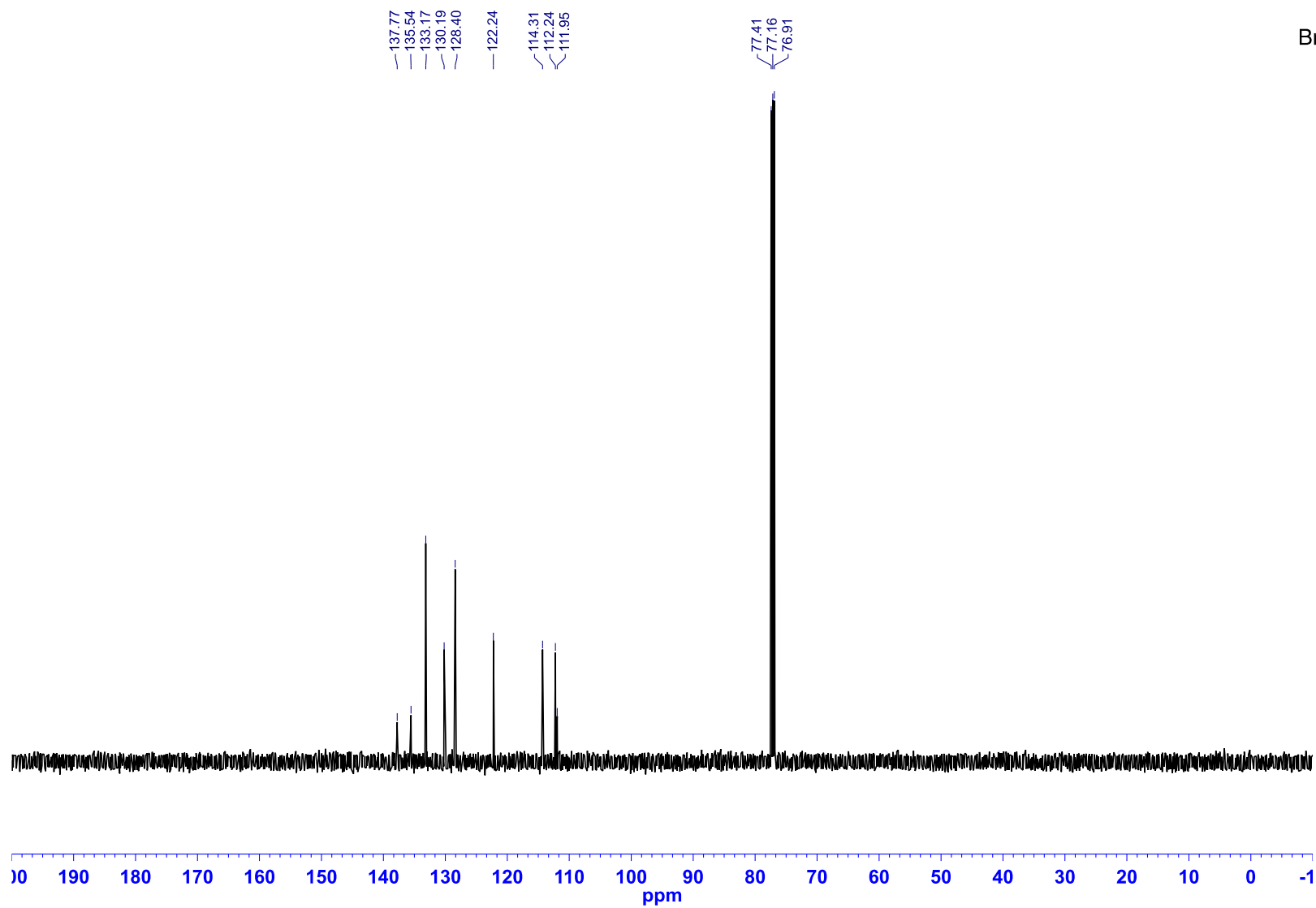
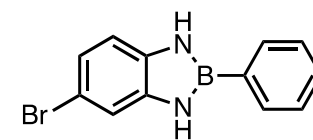
^{19}F NMR (282.4 MHz, CDCl_3) of 5-fluoro-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5v**)



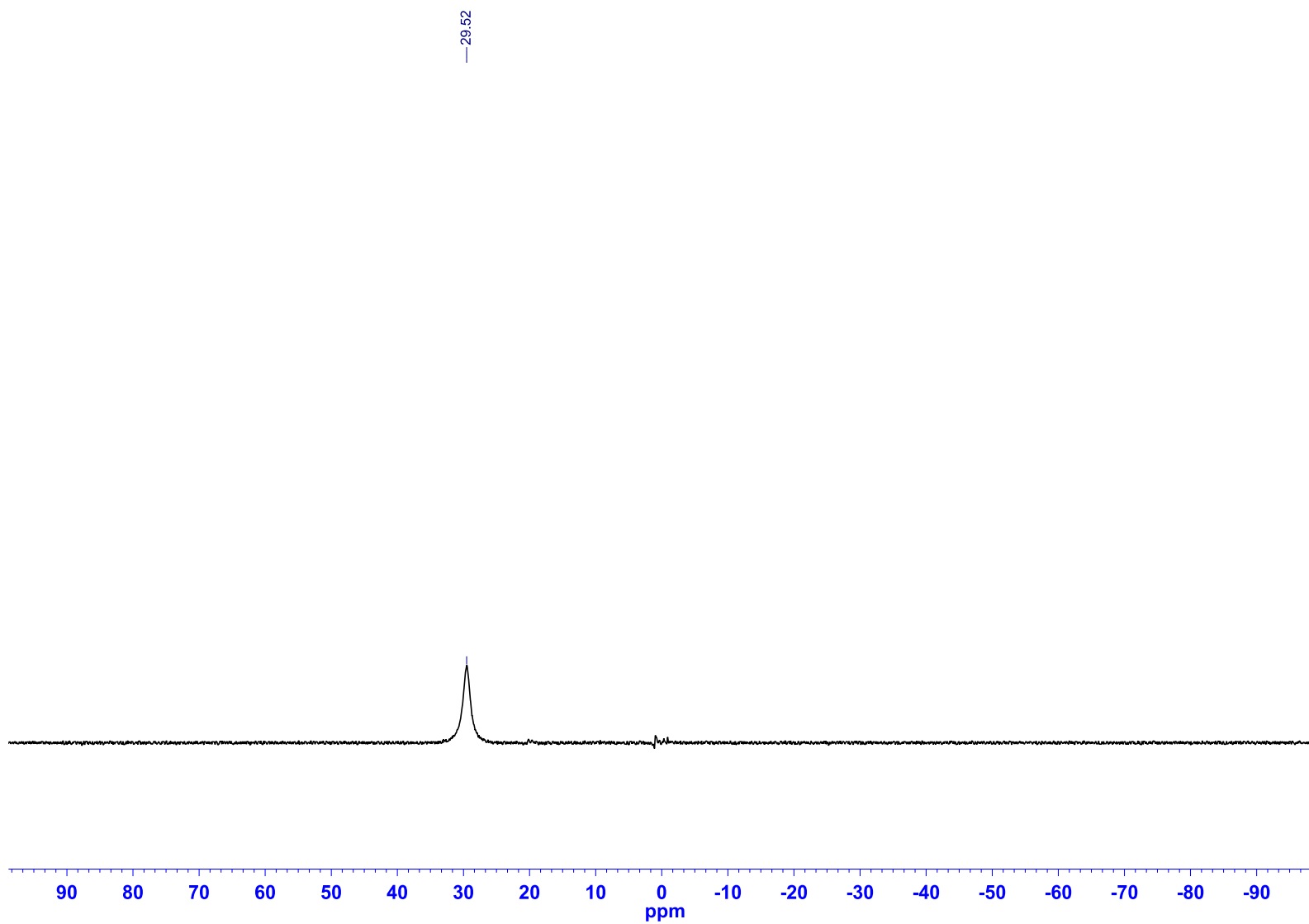
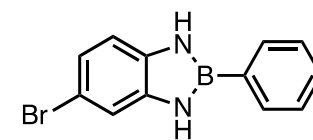
^1H NMR (500.4 MHz, CDCl_3) of 5-bromo-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5w**)



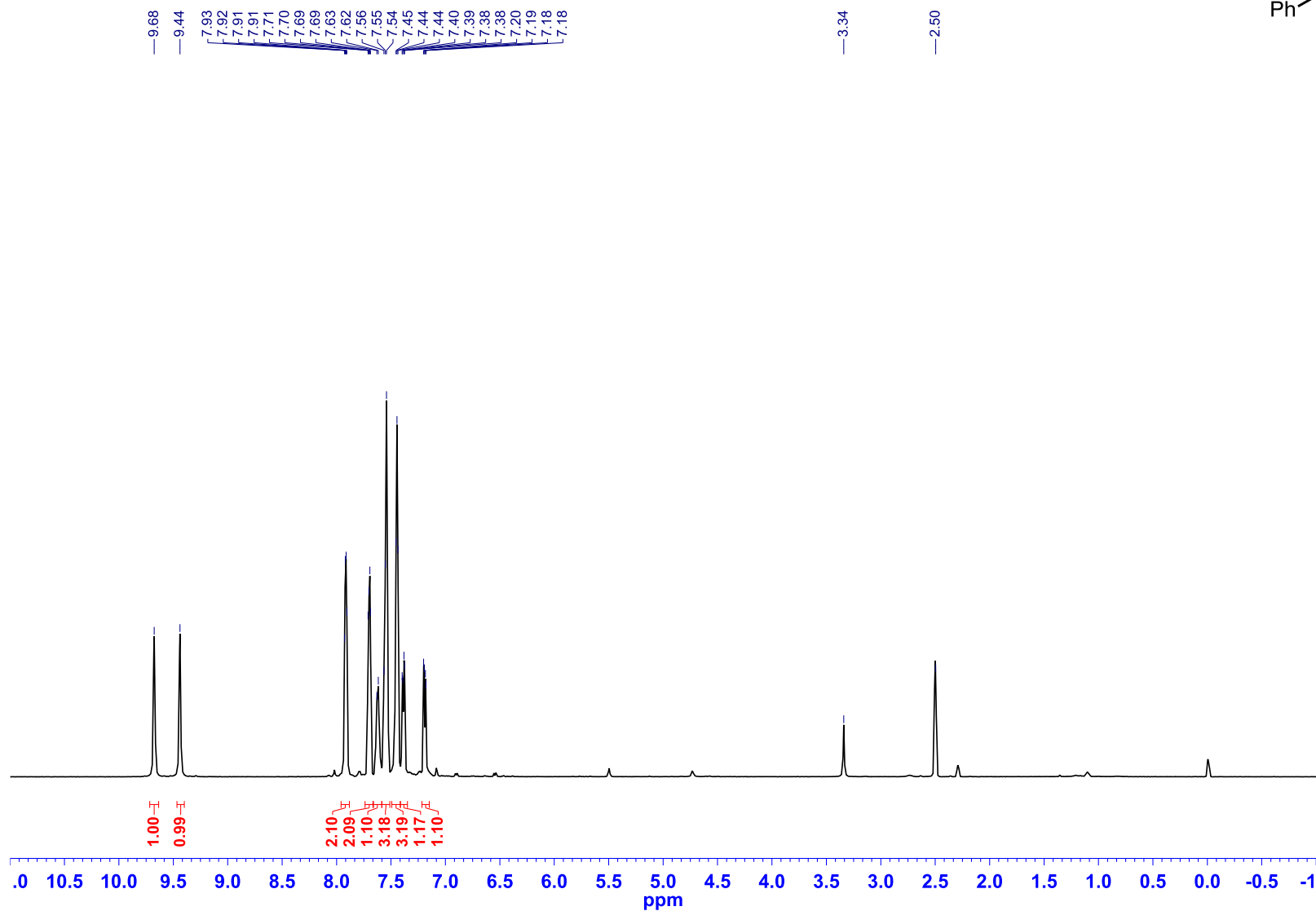
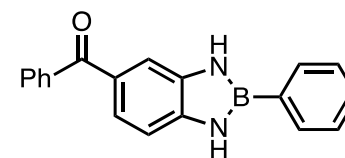
^{13}C NMR (125.8 MHz, CDCl_3) of 5-bromo-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5w**)



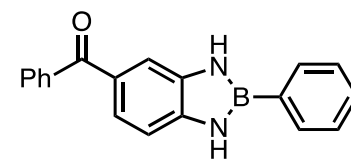
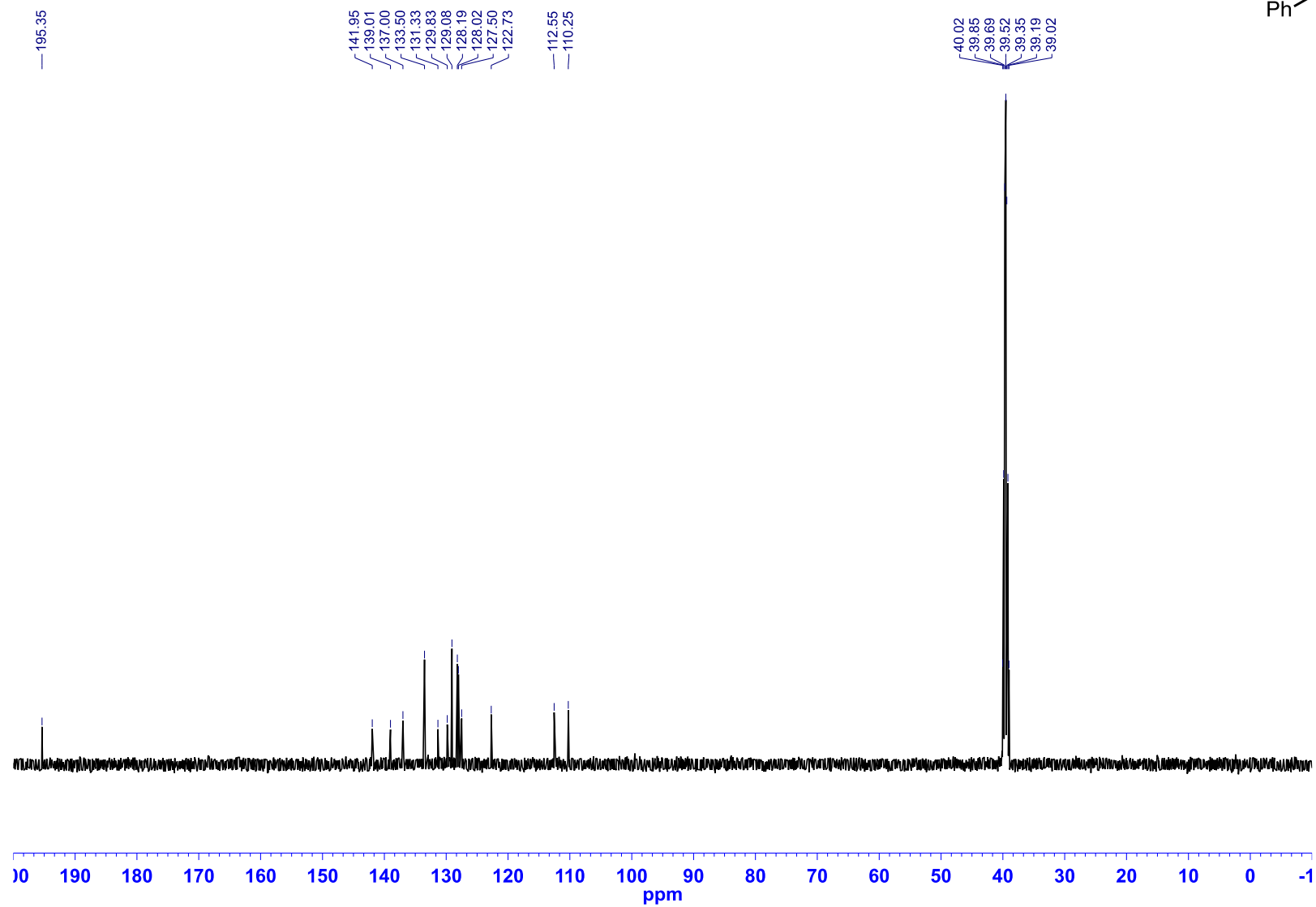
^{11}B NMR (128.4 MHz, MeCN) of 5-bromo-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5w**)



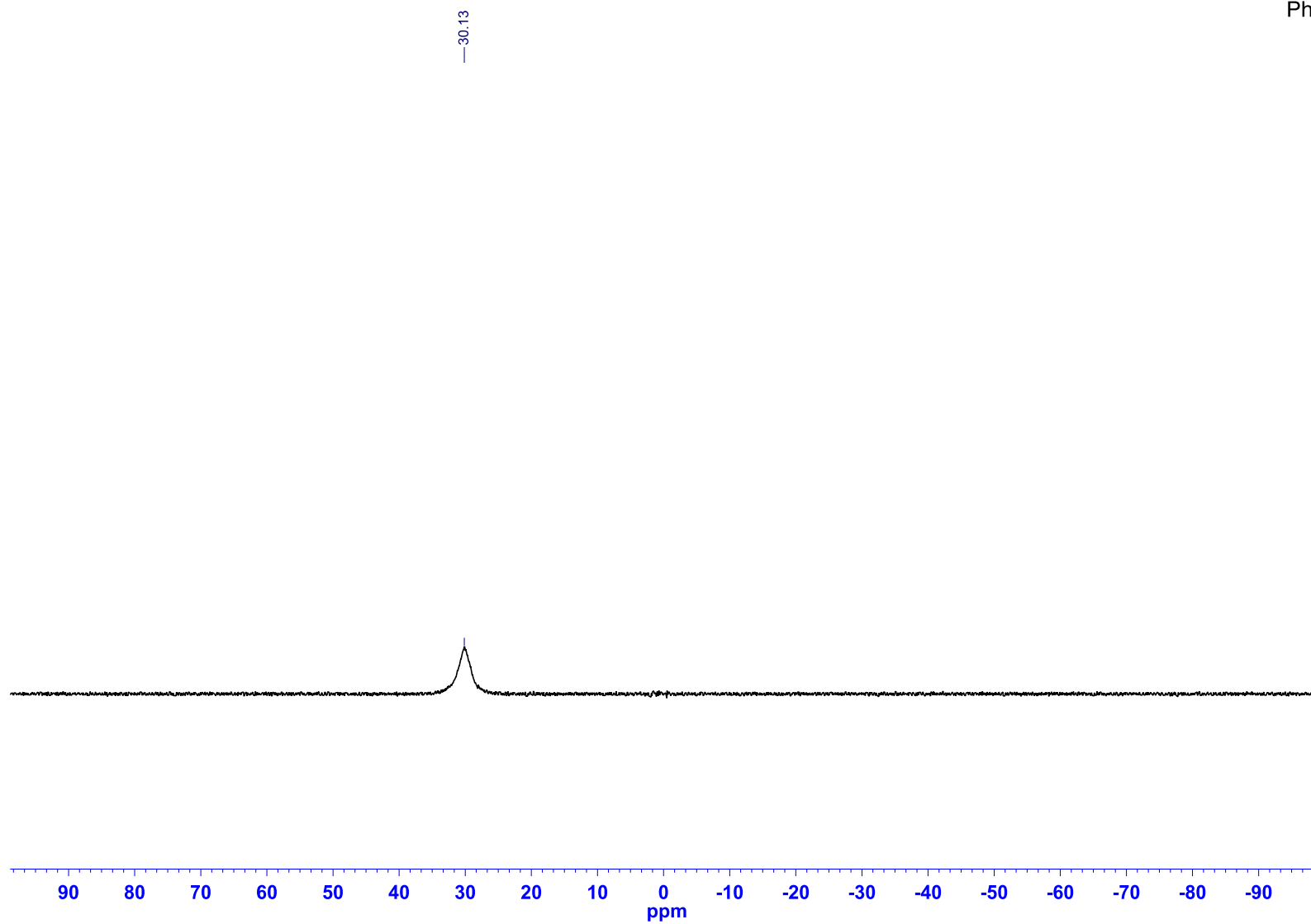
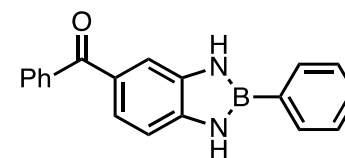
^1H NMR (500.4 MHz, $\text{DMSO-}d_6$) of 5-phenylcarbonyl-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5x**)



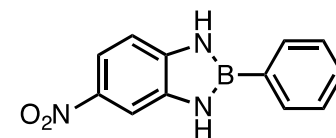
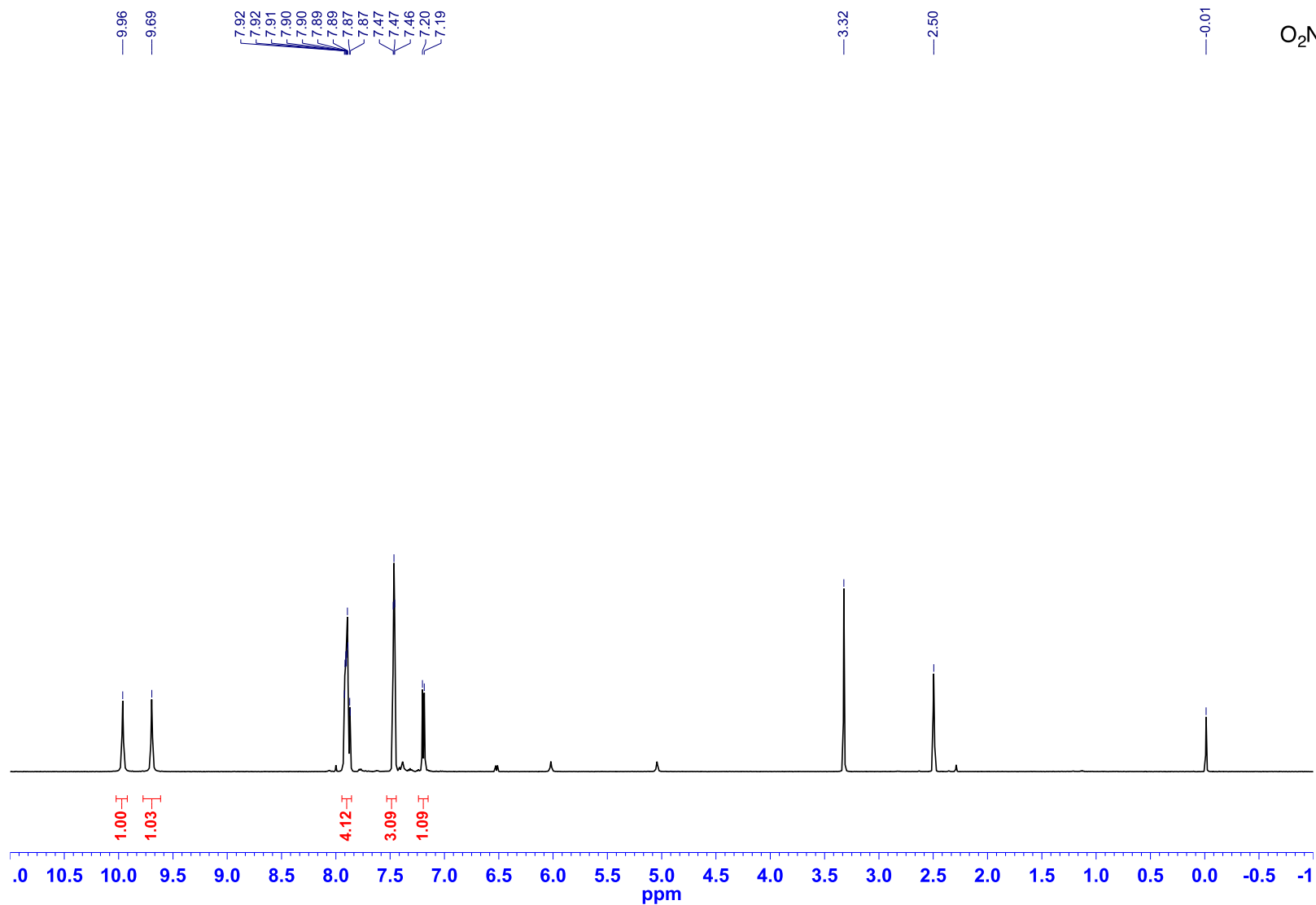
^{13}C NMR (125.8 MHz, $\text{DMSO-}d_6$) of 5-phenylcarbonyl-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5x**)



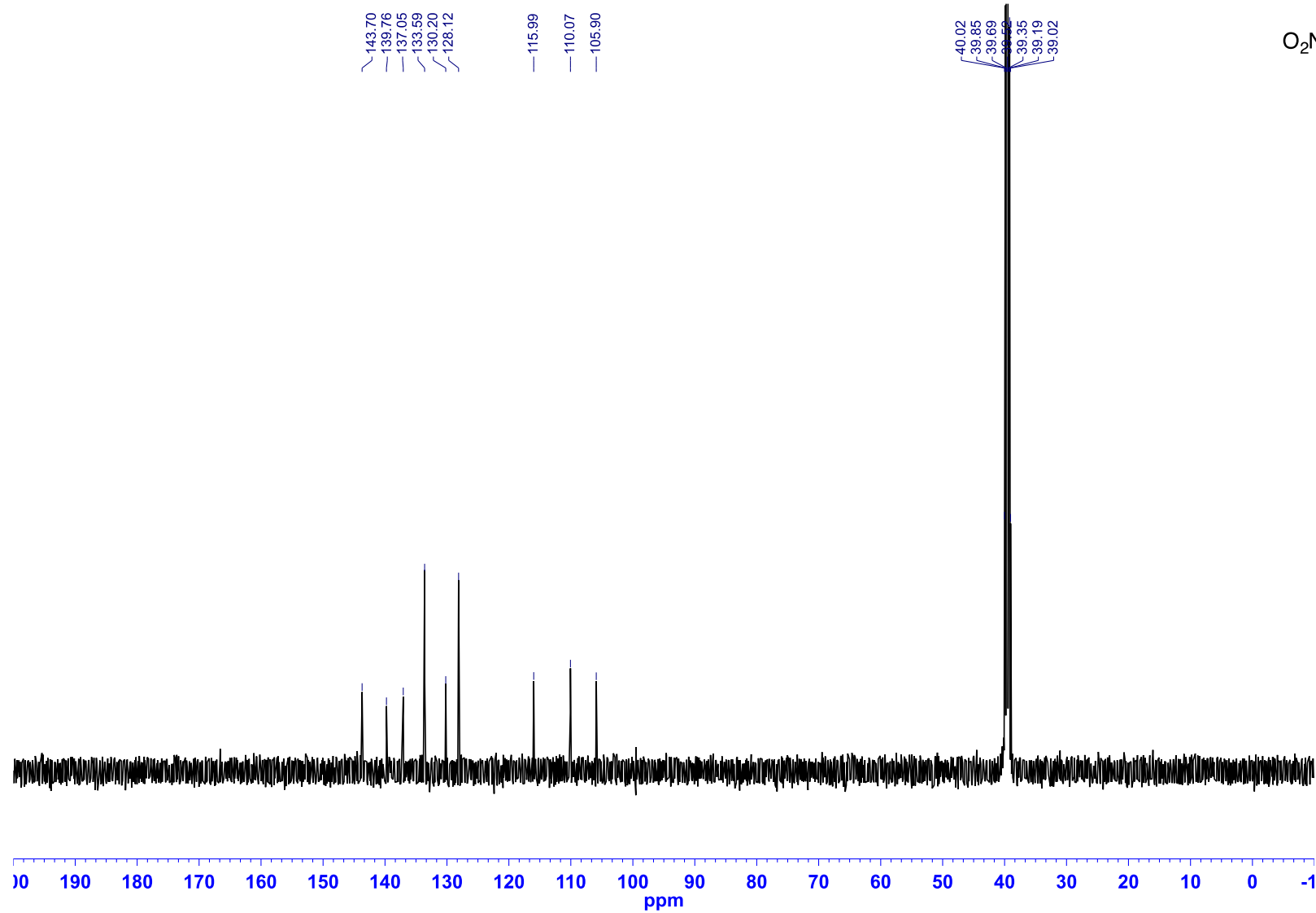
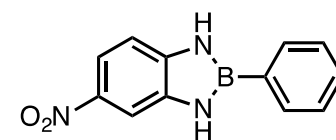
^{11}B NMR (128.4 MHz, MeCN) of 5-phenylcarbonyl-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5x**)



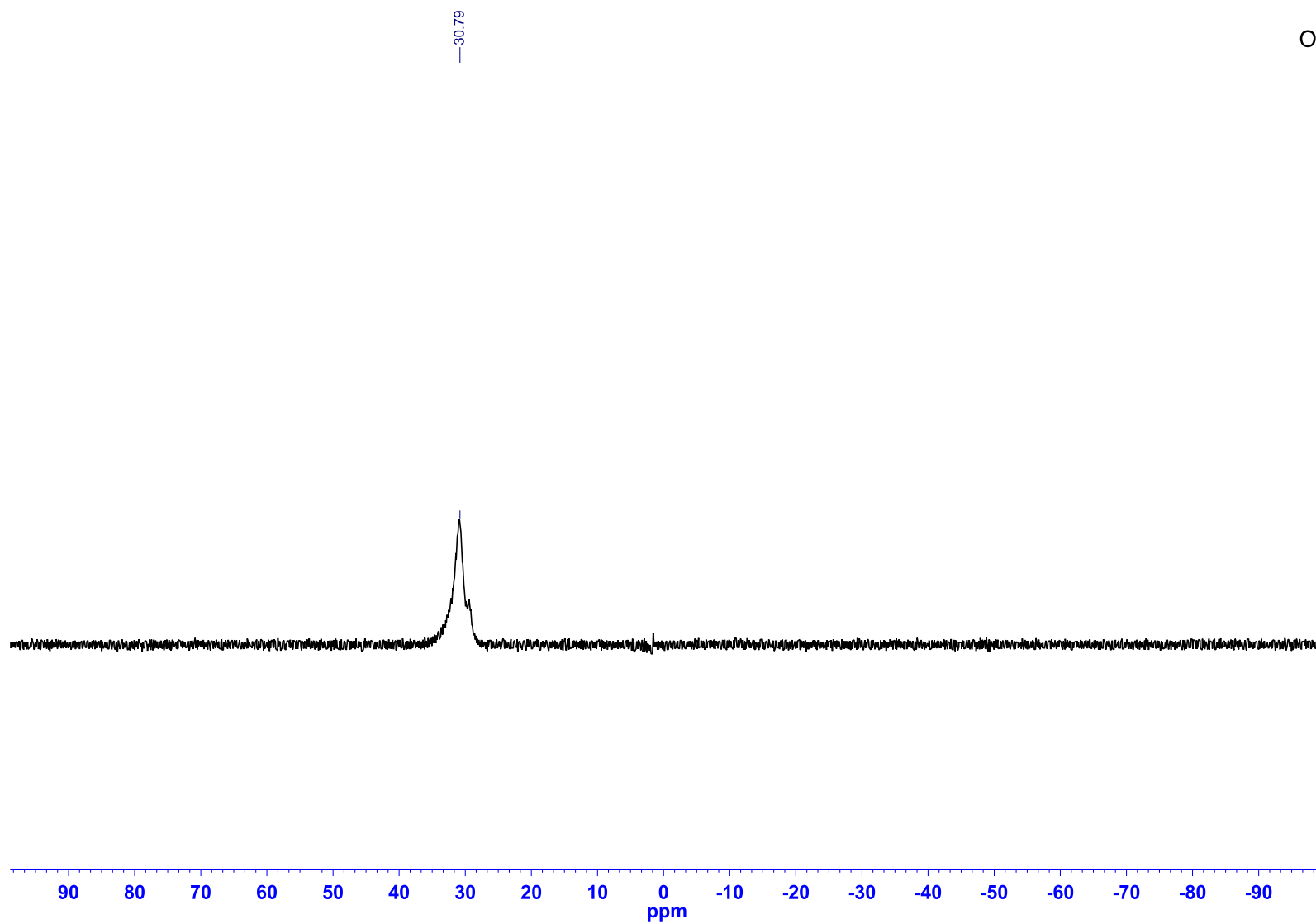
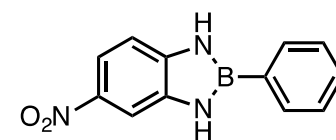
^1H NMR (500.4 MHz, $\text{DMSO-}d_6$) of 5-nitro-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5y**)



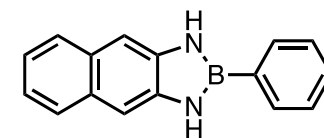
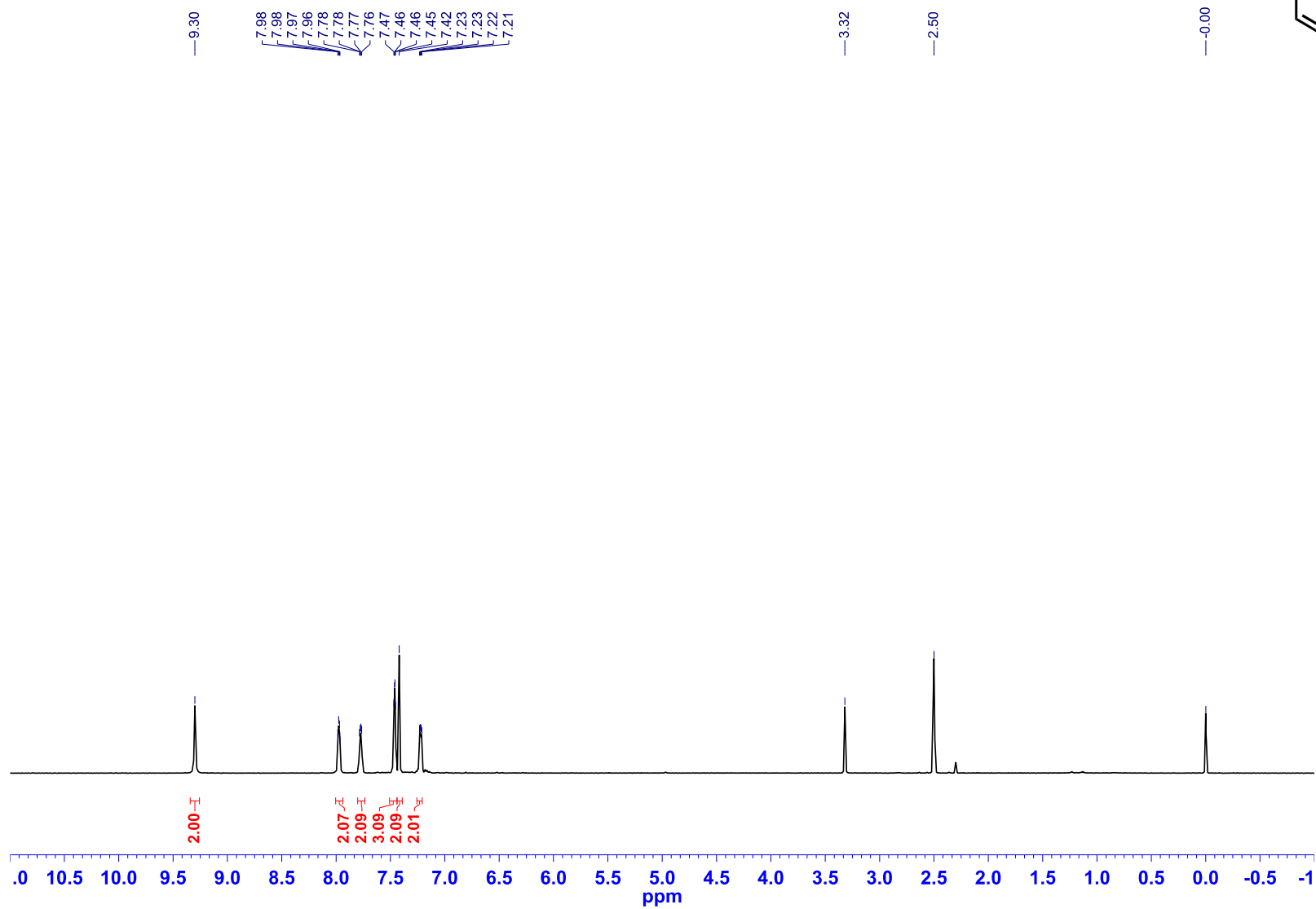
^{13}C NMR (125.8 MHz, $\text{DMSO-}d_6$) of 5-nitro-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5y**)



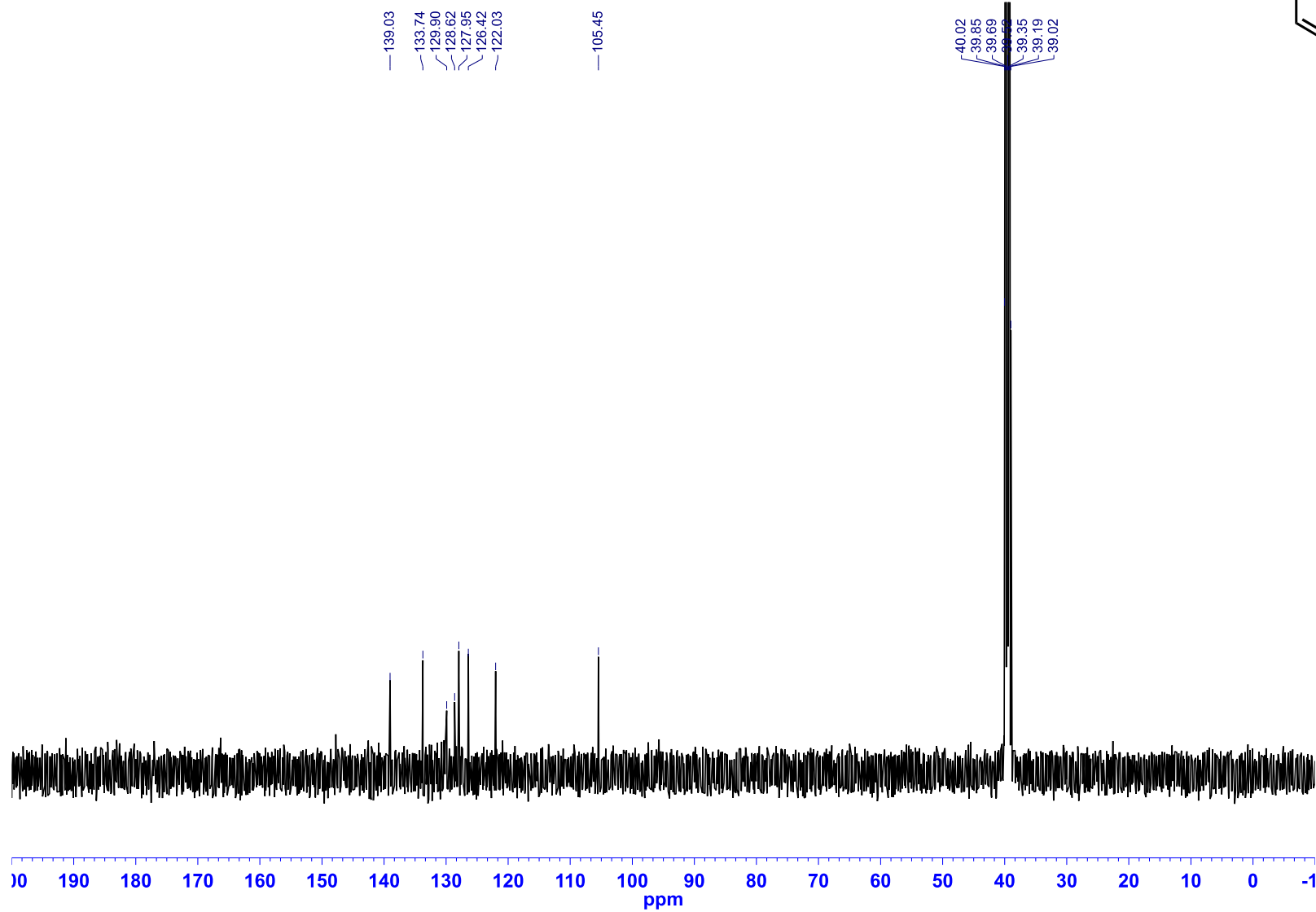
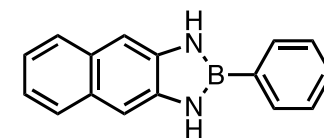
^{11}B NMR (128.4 MHz, MeCN) of 5-nitro-2-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**5y**)



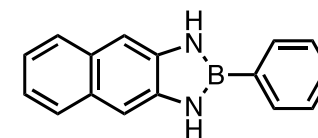
^1H NMR (500.4 MHz, $\text{DMSO-}d_6$) of 2-phenyl-2,3-dihydro-1*H*-1,3,2-naphthodiazaborole (**5z**)



^{13}C NMR (125.8 MHz, $\text{DMSO-}d_6$) of 2-phenyl-2,3-dihydro-1*H*-1,3,2-naphthodiazaborole (**5z**)



^{11}B NMR (128.4 MHz, MeCN) of 2-phenyl-2,3-dihydro-1*H*-1,3,2-naphthodiazaborole (**5z**)

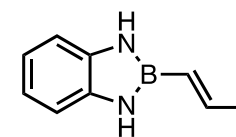
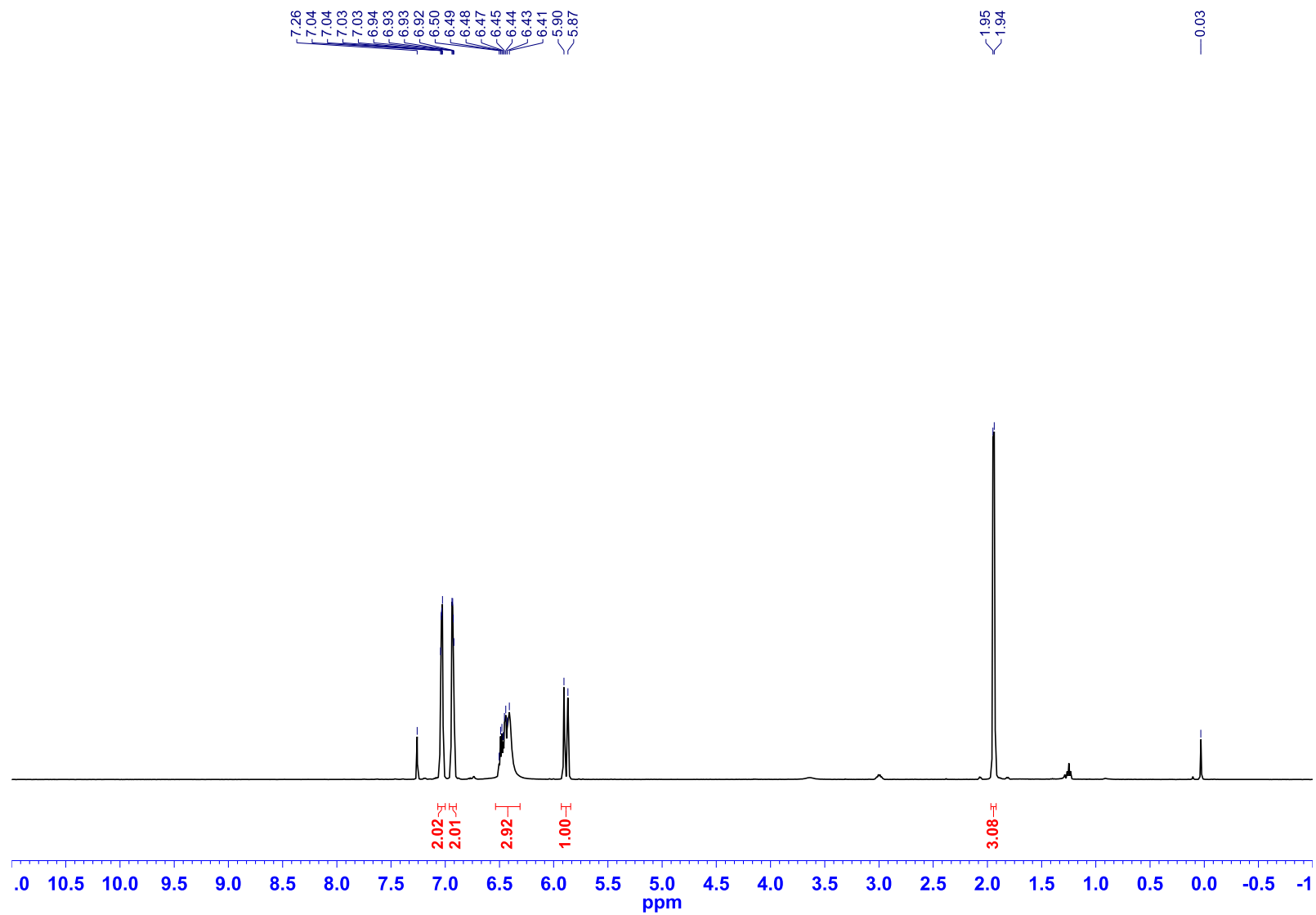


—31.00

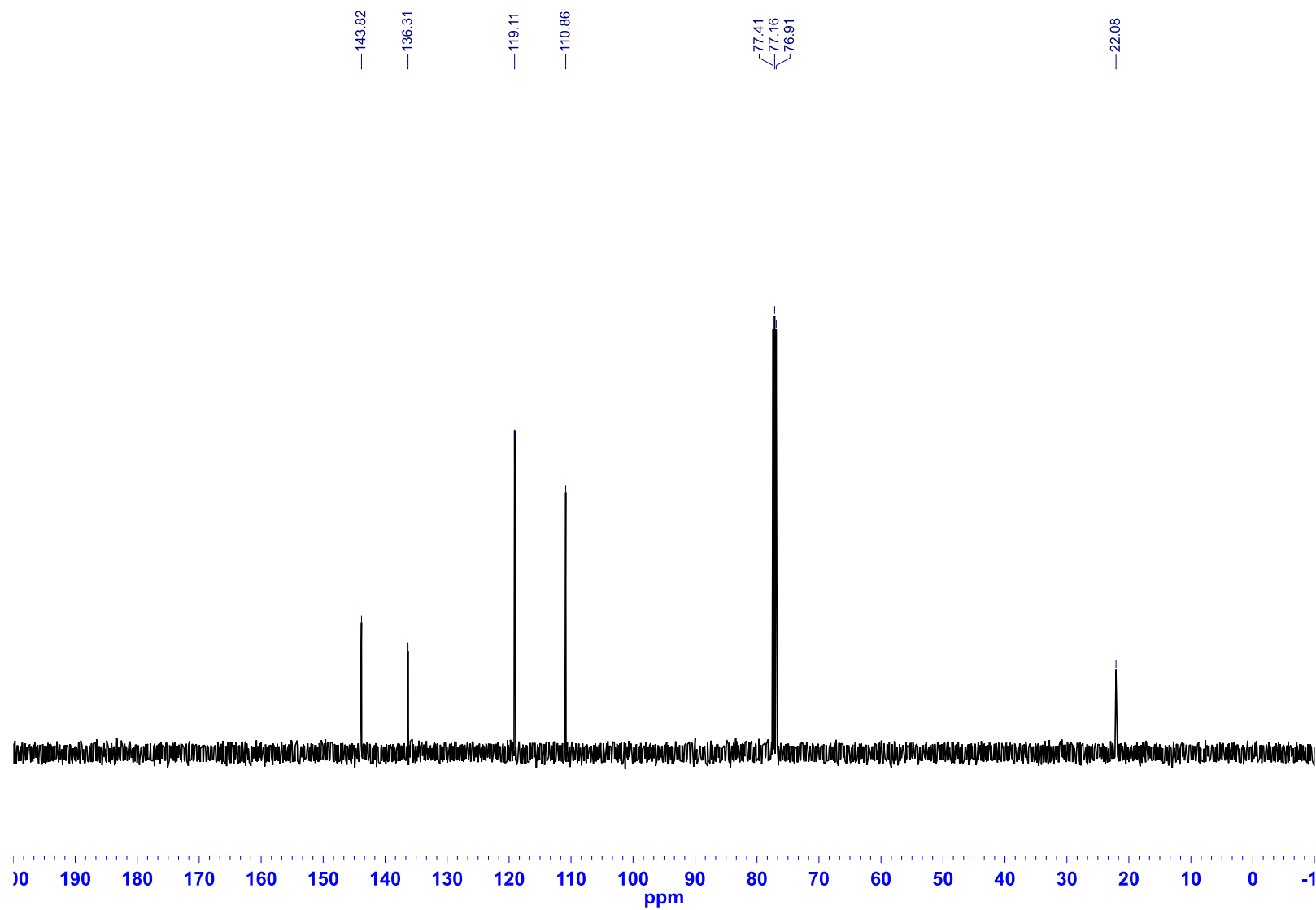
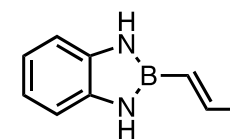


90 80 70 60 50 40 30 20 10 0 ppm -10 -20 -30 -40 -50 -60 -70 -80 -90

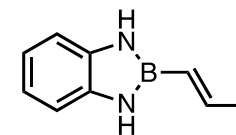
^1H NMR (500.4 MHz, CDCl_3) of (*E*)-2-(1-propenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6a**)



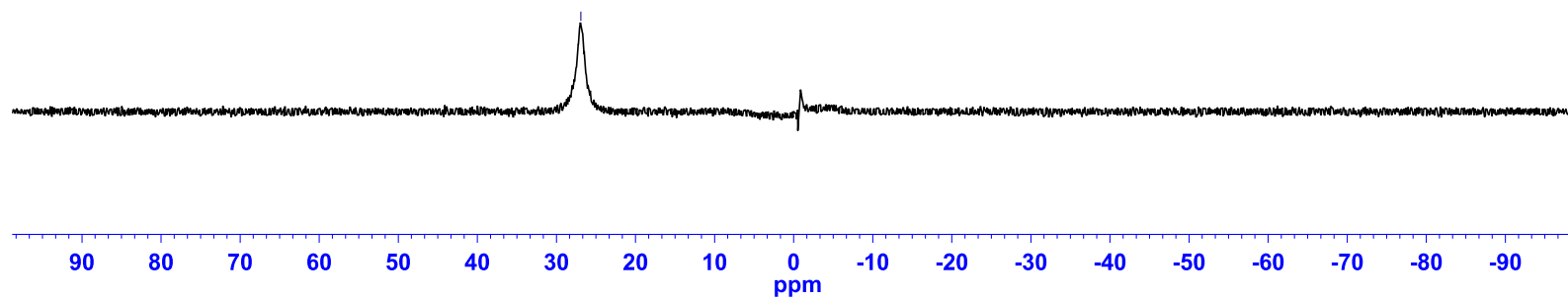
^{13}C NMR (125.8 MHz, CDCl_3) of (*E*)-2-(1-propenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6a**)



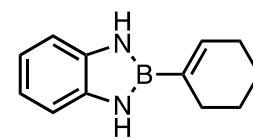
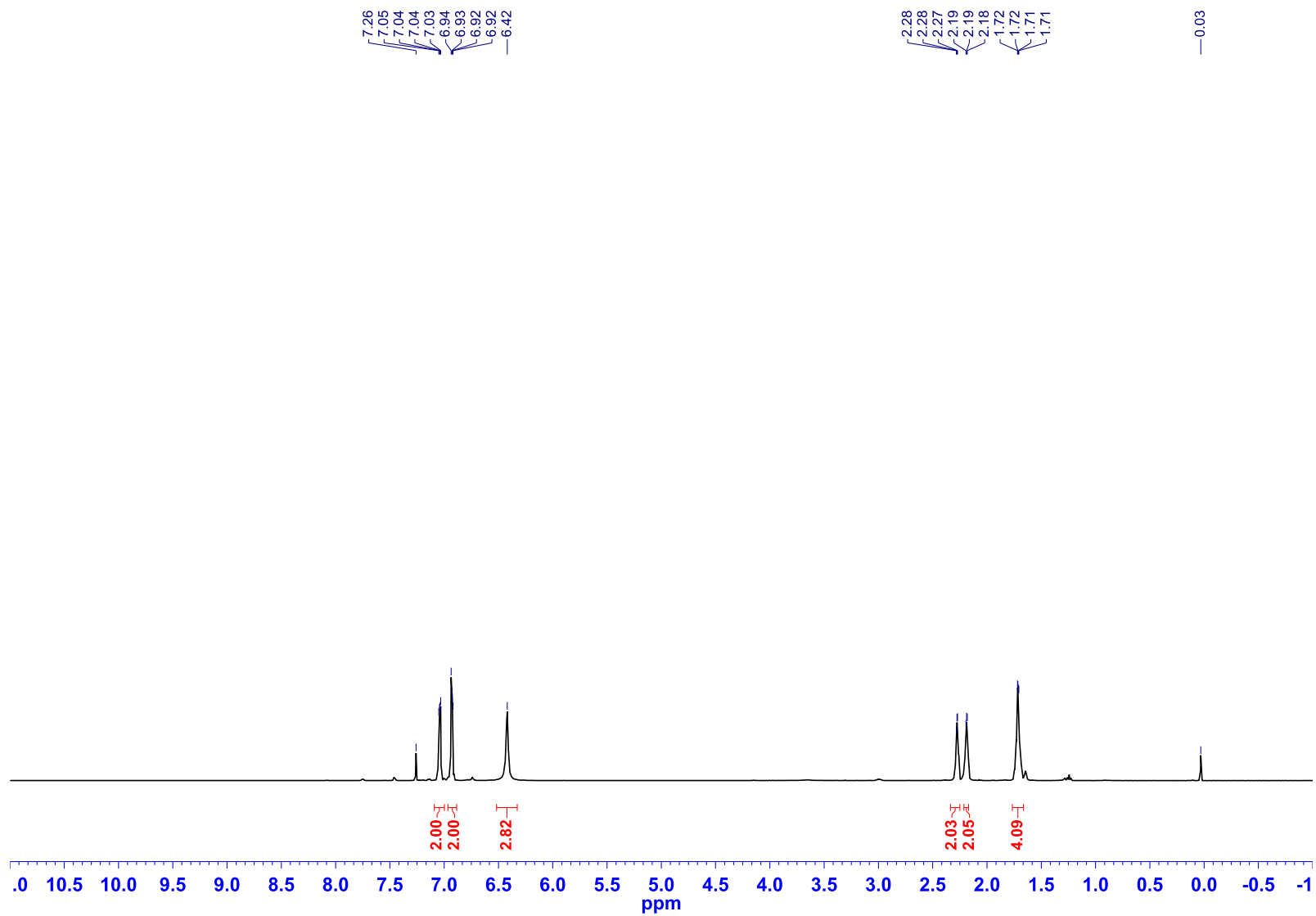
^{11}B NMR (128.4 MHz, CDCl_3) of (*E*)-2-(1-propenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6a**)



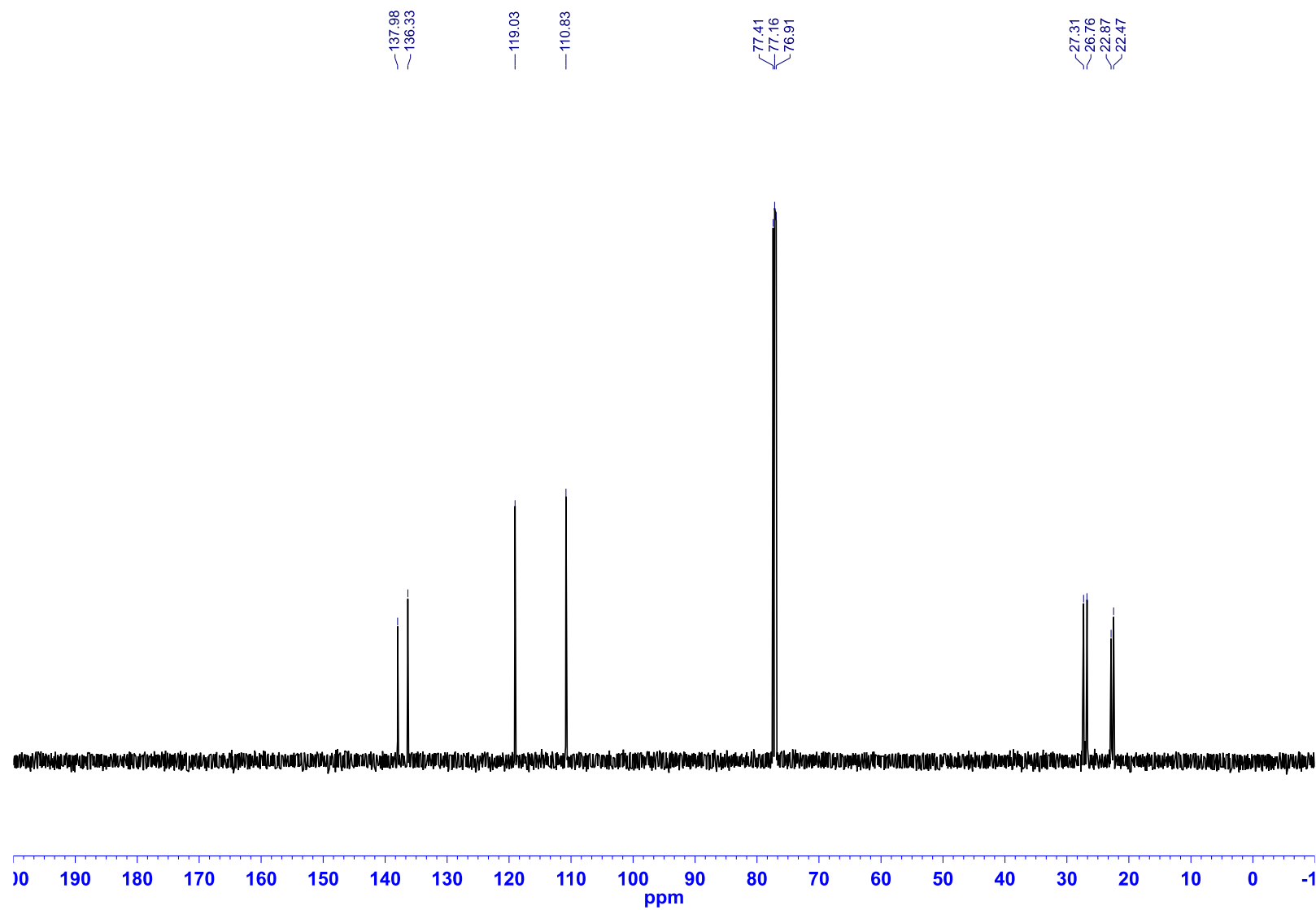
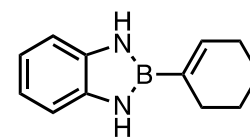
—26.92



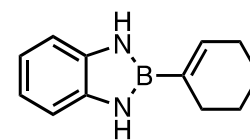
^1H NMR (500.4 MHz, CDCl_3) of 2-(1-cyclohexenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6b**)



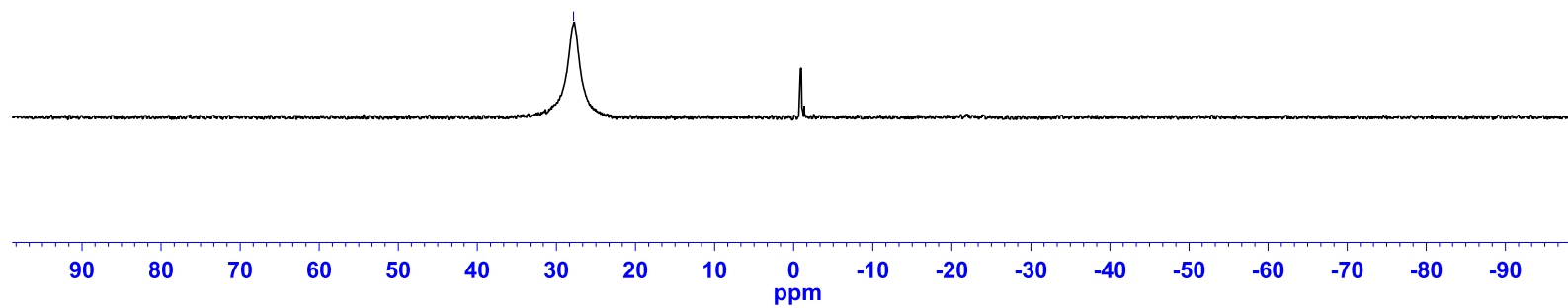
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(1-cyclohexenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6b**)



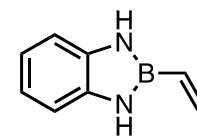
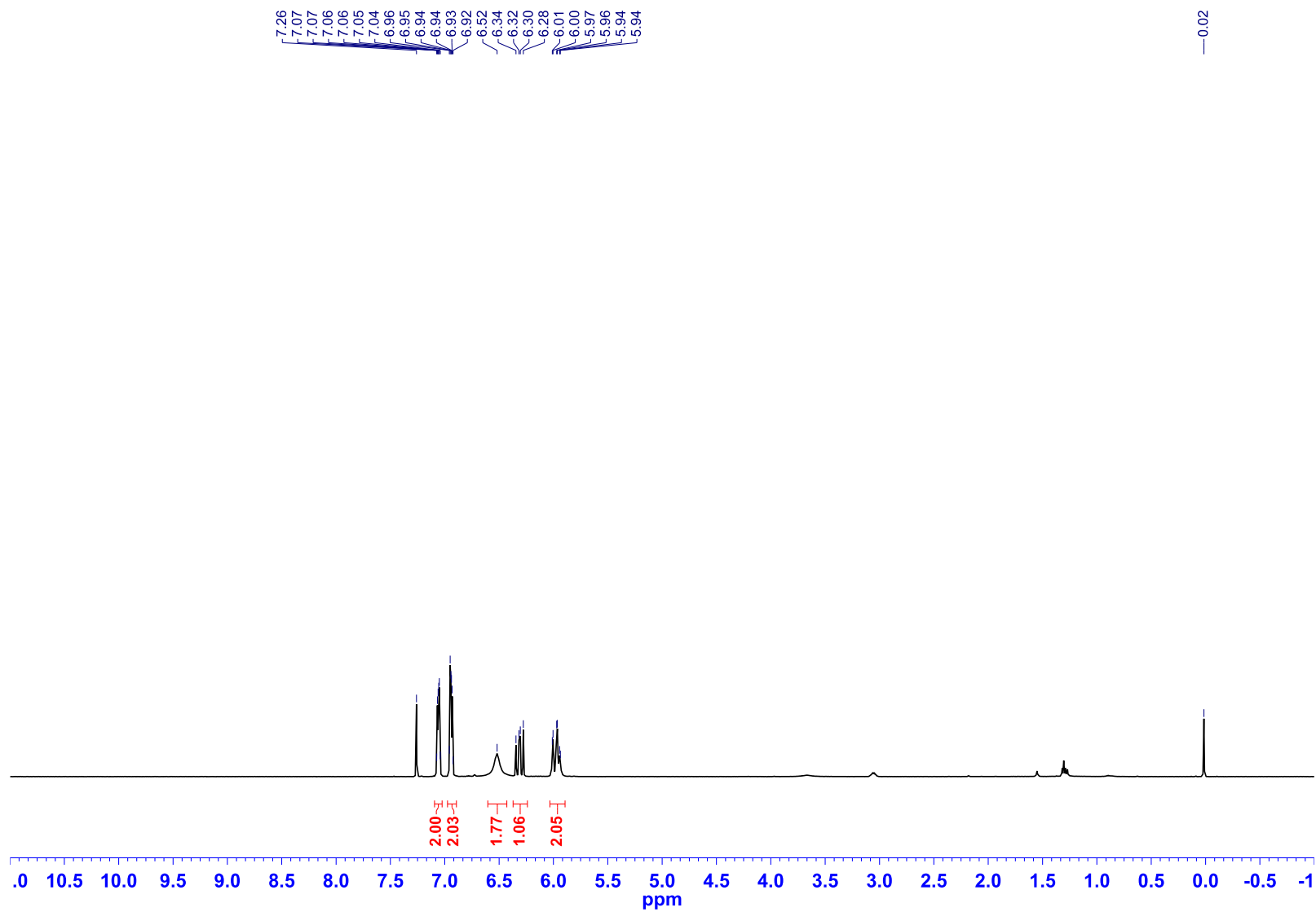
^{11}B NMR (128.4 MHz, CDCl_3) of 2-(1-cyclohexenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6b**)



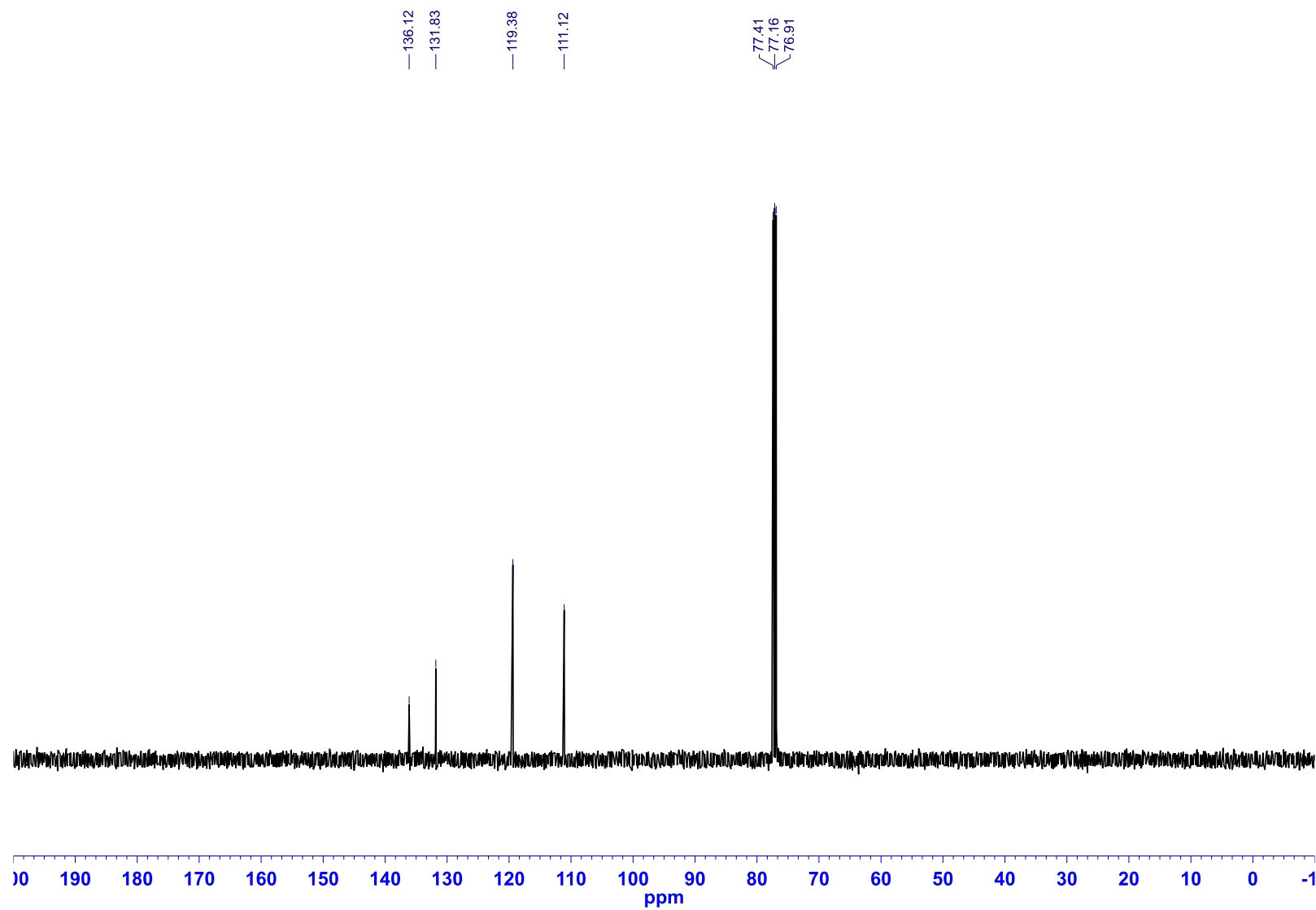
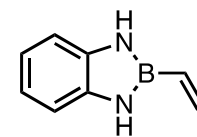
—27.83



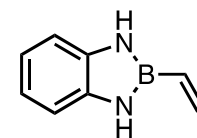
^1H NMR (500.4 MHz, CDCl_3) of 2-vinyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6c**)



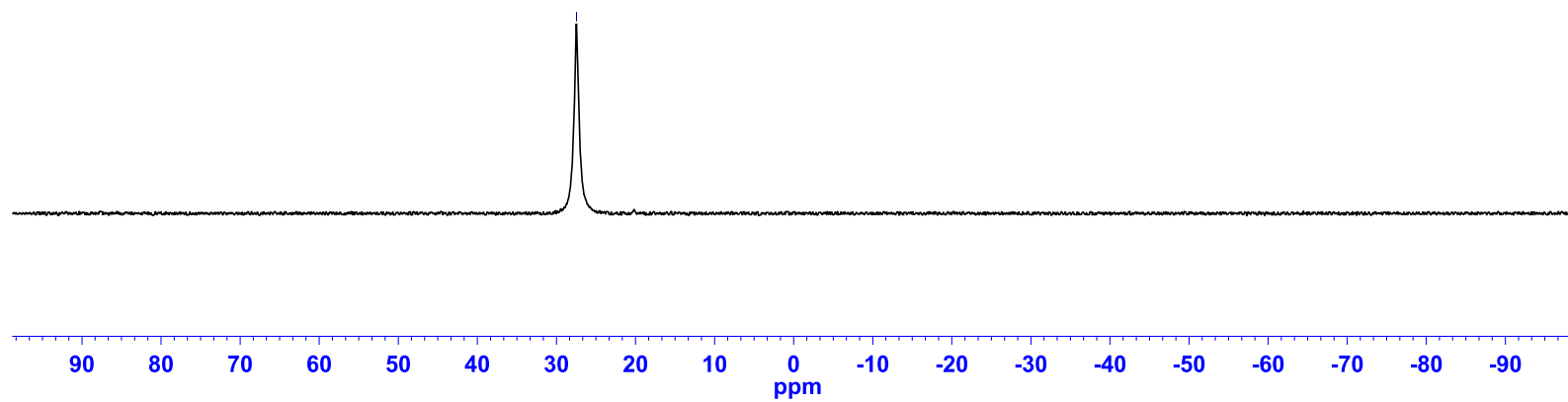
^{13}C NMR (125.8 MHz, CDCl_3) of 2-vinyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6c**)



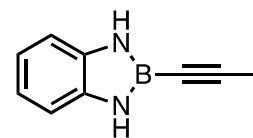
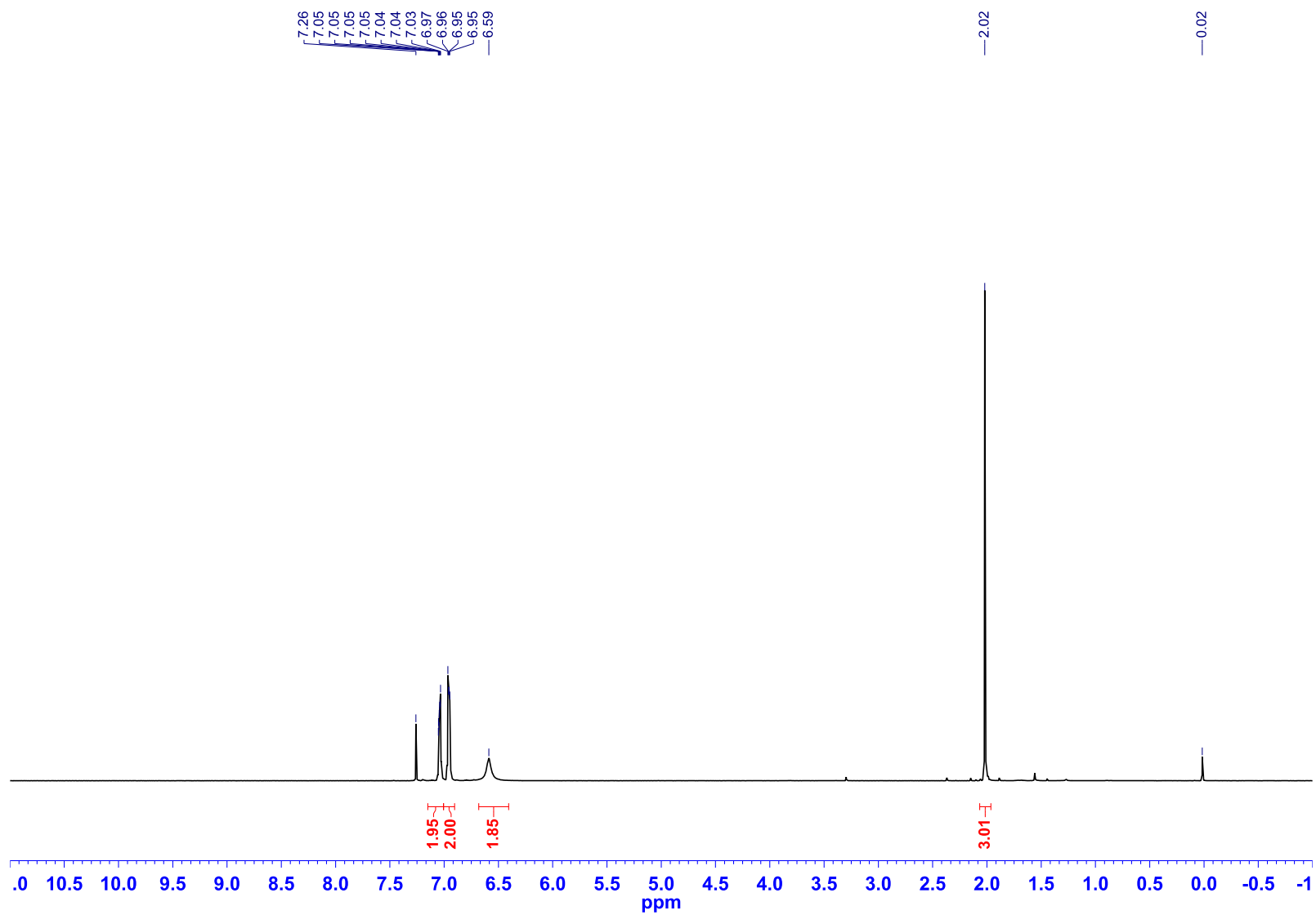
^{11}B NMR (128.4 MHz, MeCN) of 2-vinyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6c**)



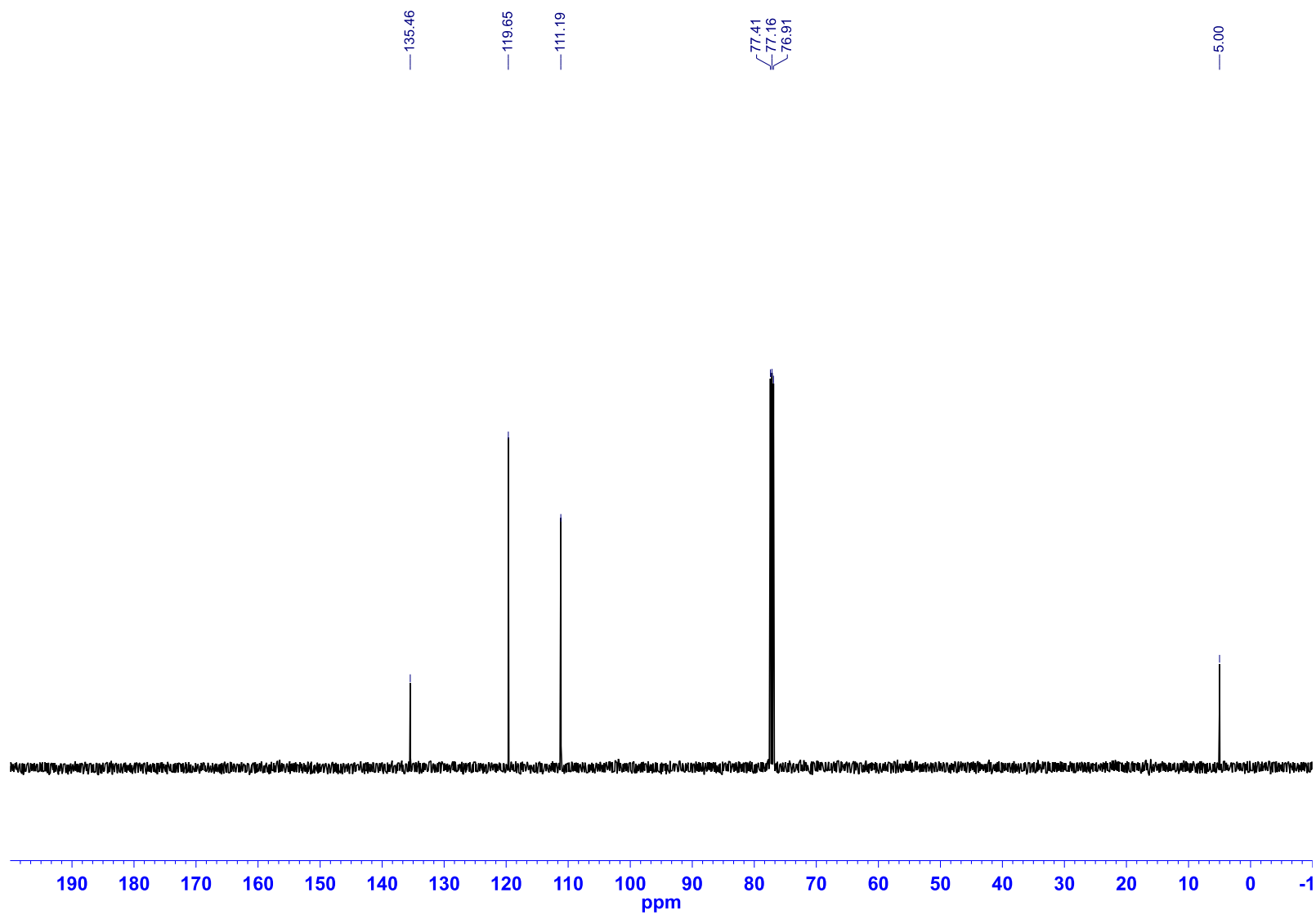
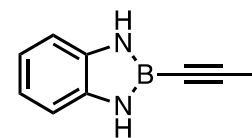
-27.47



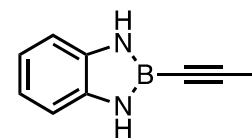
^1H NMR (500.4 MHz, CDCl_3) of 2-(1-propynyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6d**)



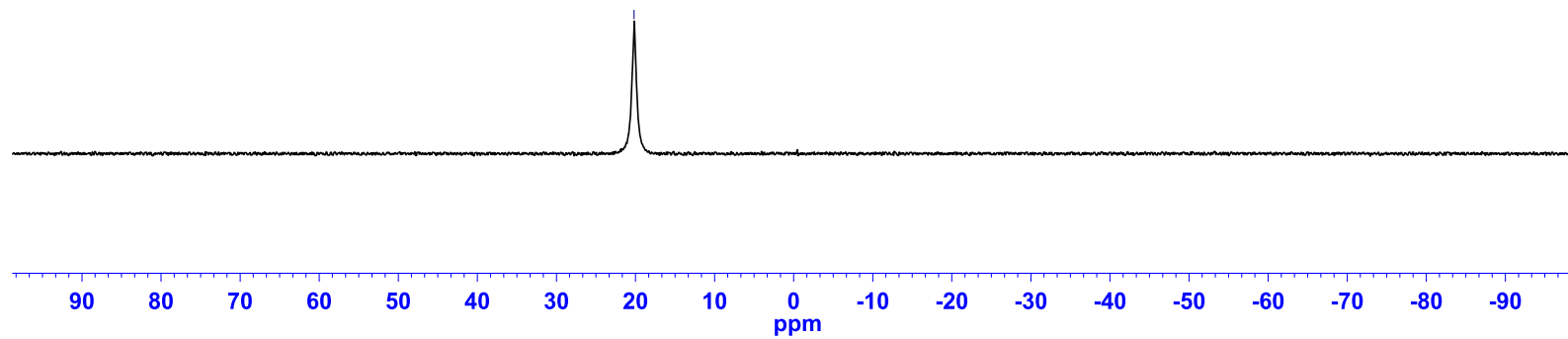
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(1-propynyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6d**)



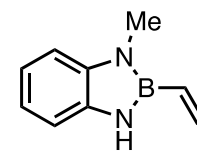
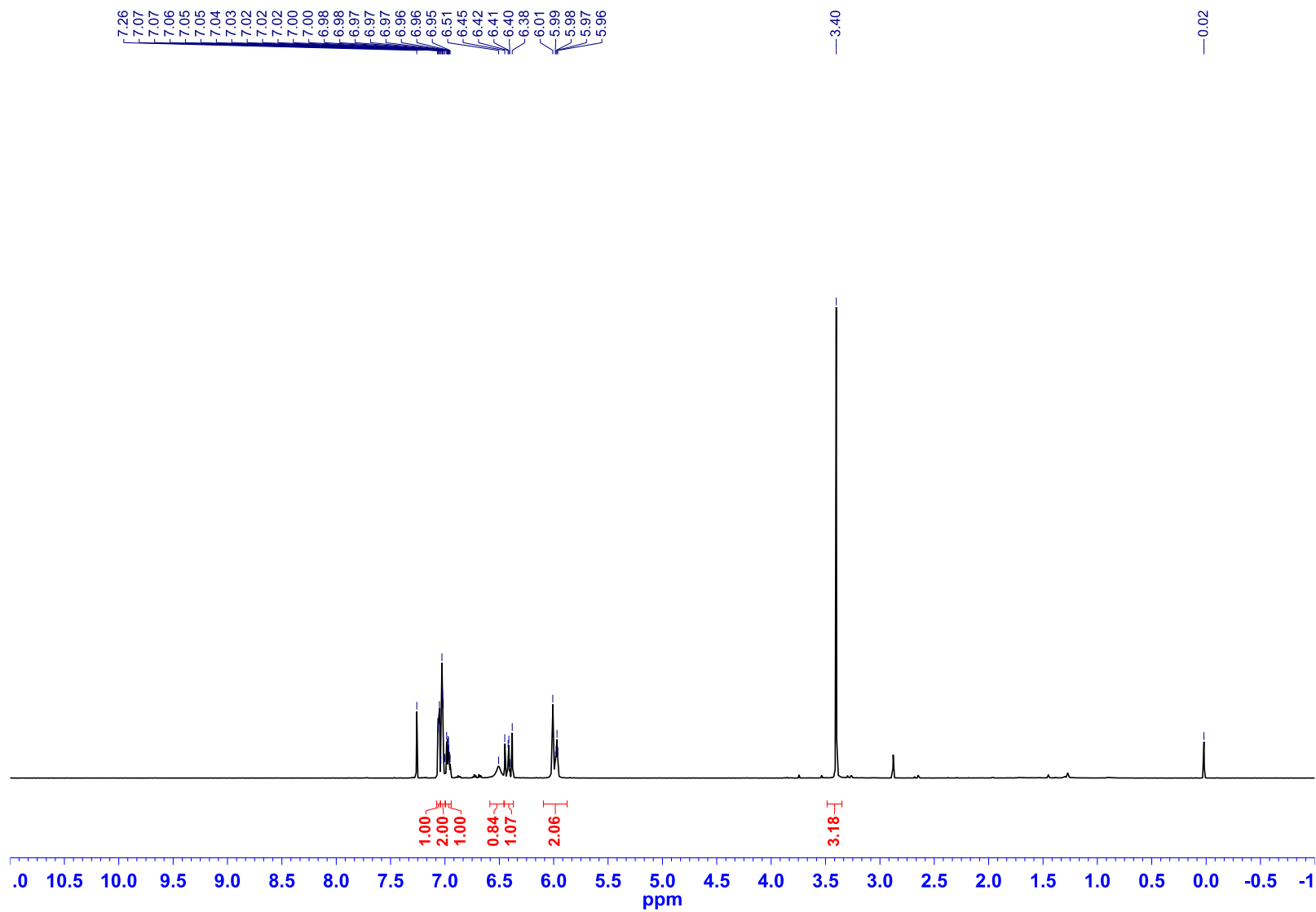
^{11}B NMR (128.4 MHz, MeCN) of 2-(1-propynyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6d**)



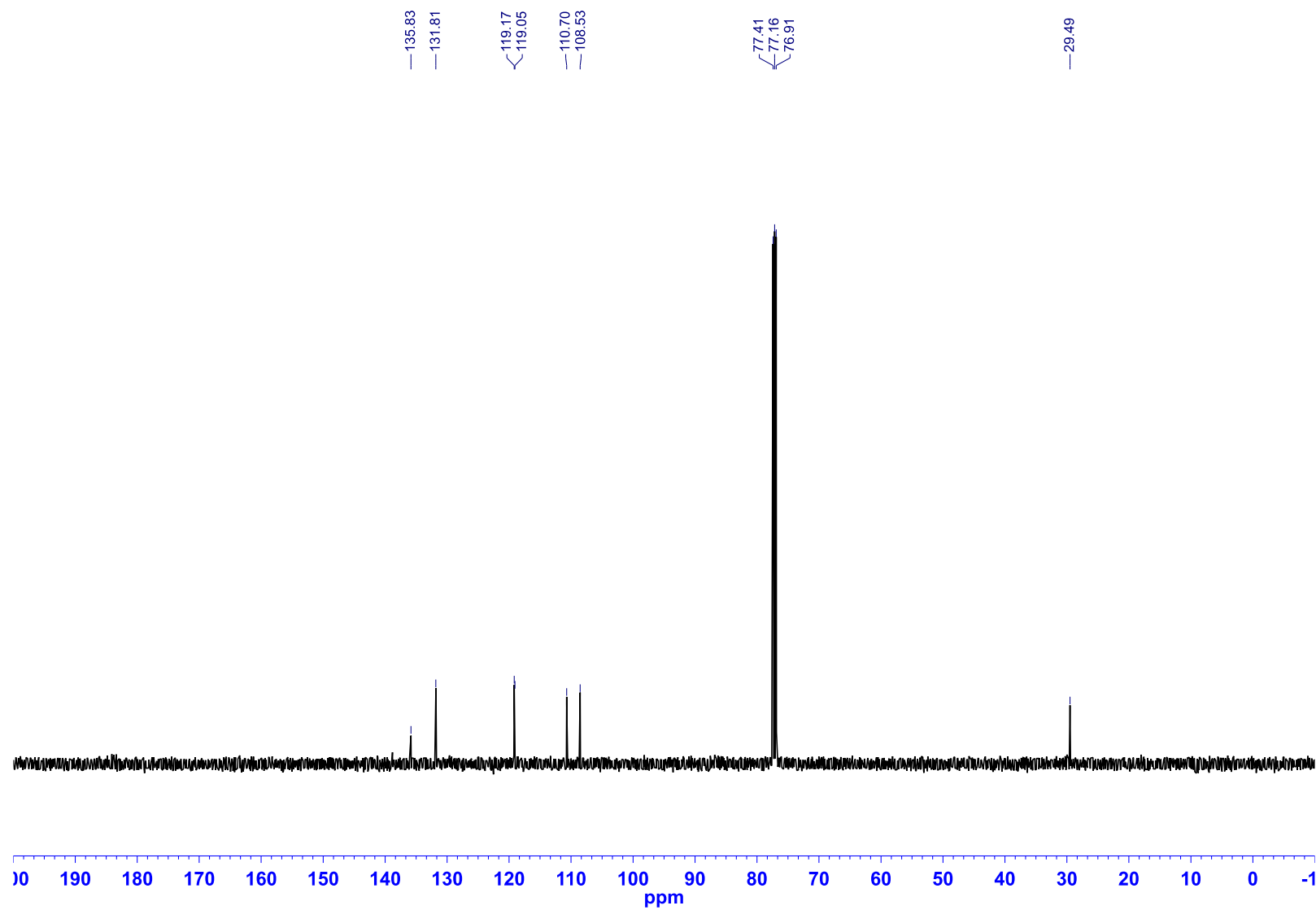
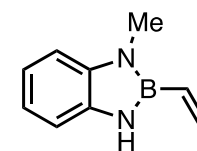
—20.19



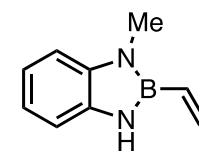
^1H NMR (500.4 MHz, CDCl_3) of 1-methyl-2-vinyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6e**)



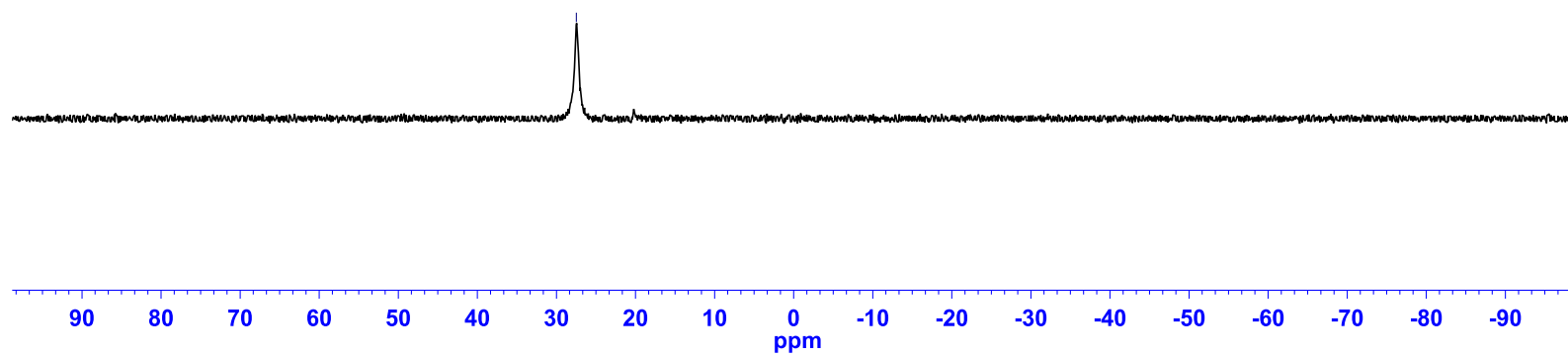
^{13}C NMR (125.8 MHz, CDCl_3) of 1-methyl-2-vinyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6e**)



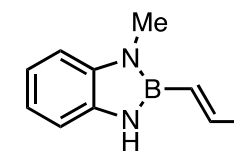
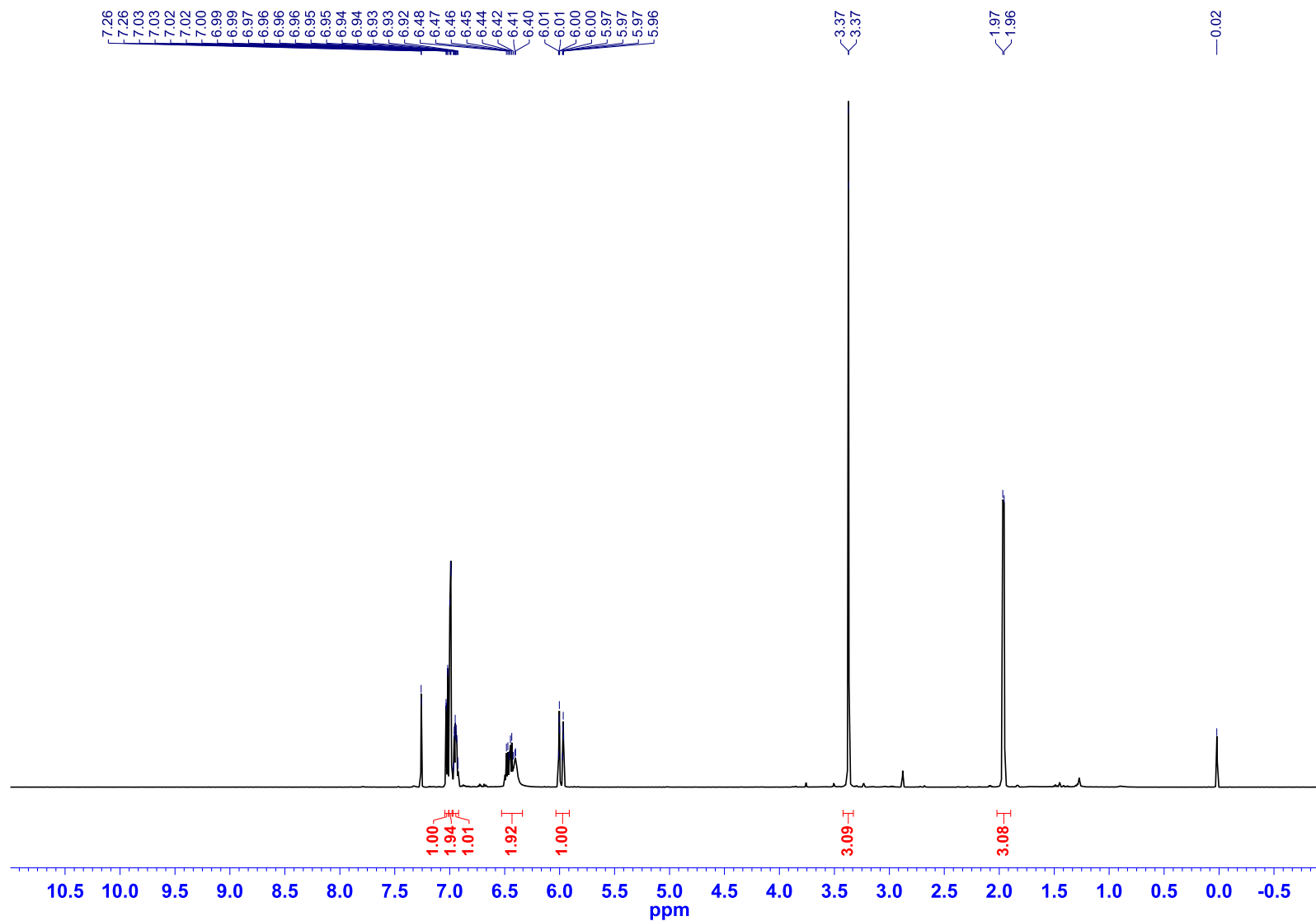
^{11}B NMR (128.4 MHz, MeCN) of 1-methyl-2-vinyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6e**)



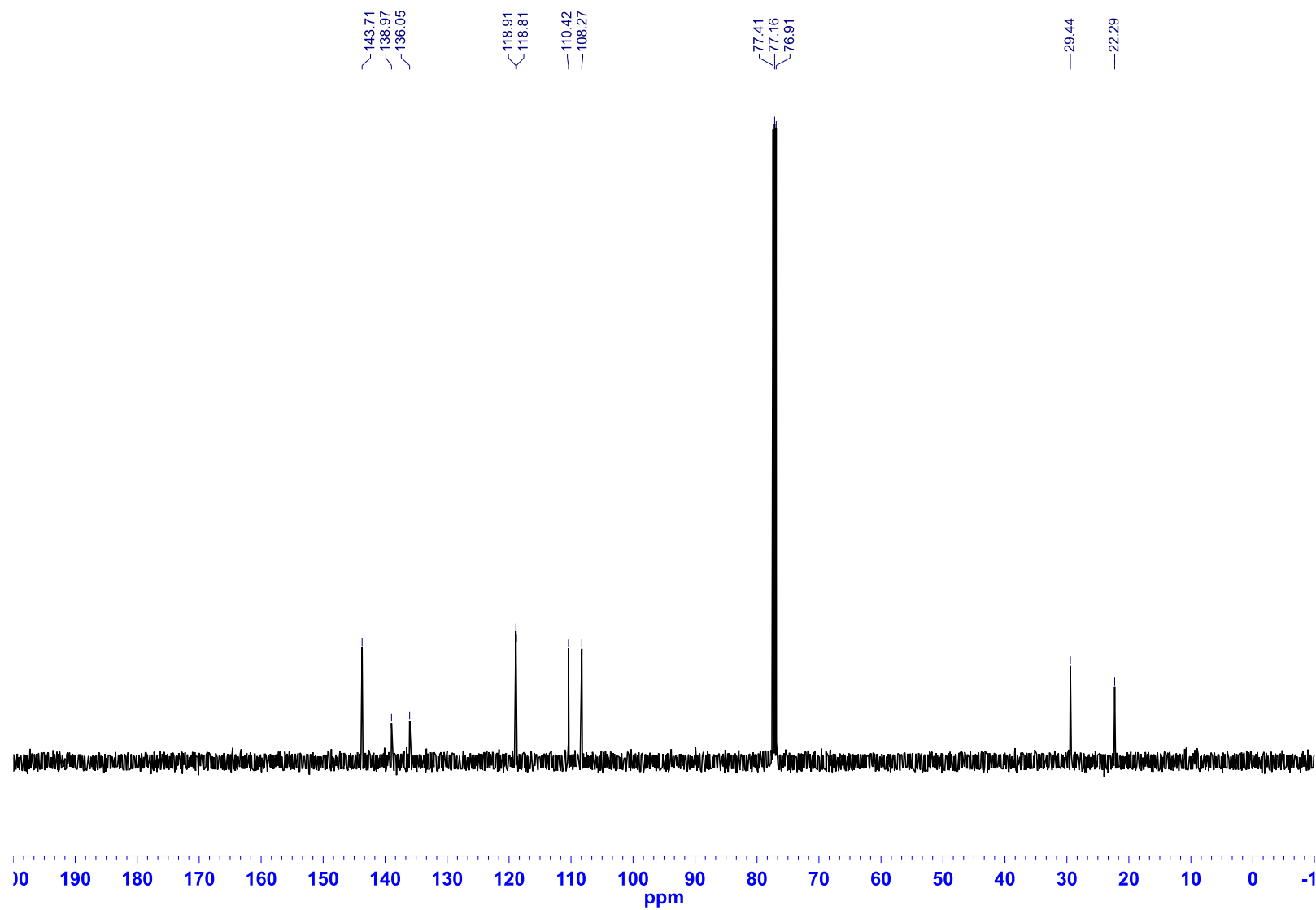
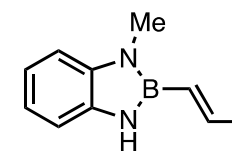
-27.47



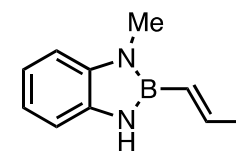
¹H NMR (500.4 MHz, CDCl₃) of (*E*)-1-methyl-2-(1-propenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6f**)



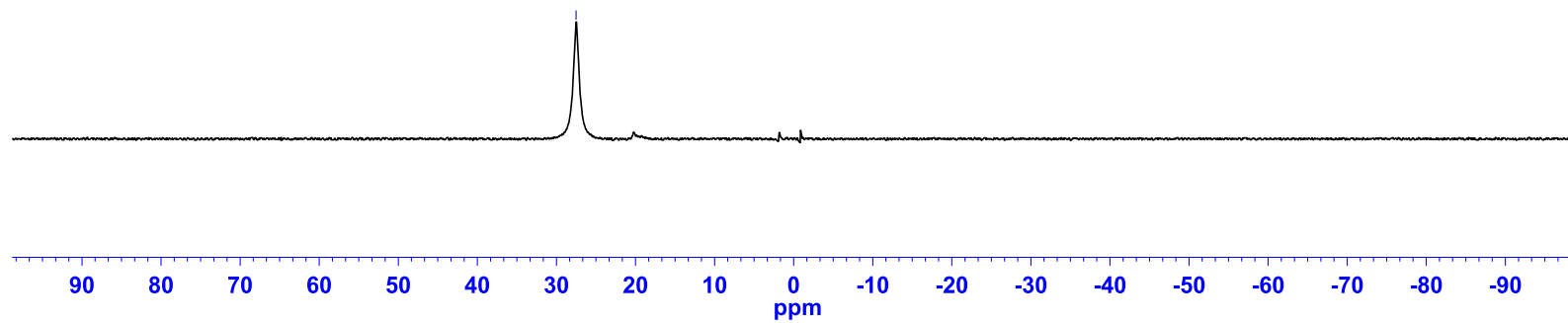
^{13}C NMR (125.8 MHz, CDCl_3) of (*E*)-1-methyl-2-(1-propenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6f**)



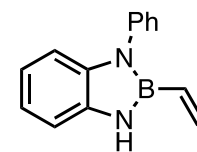
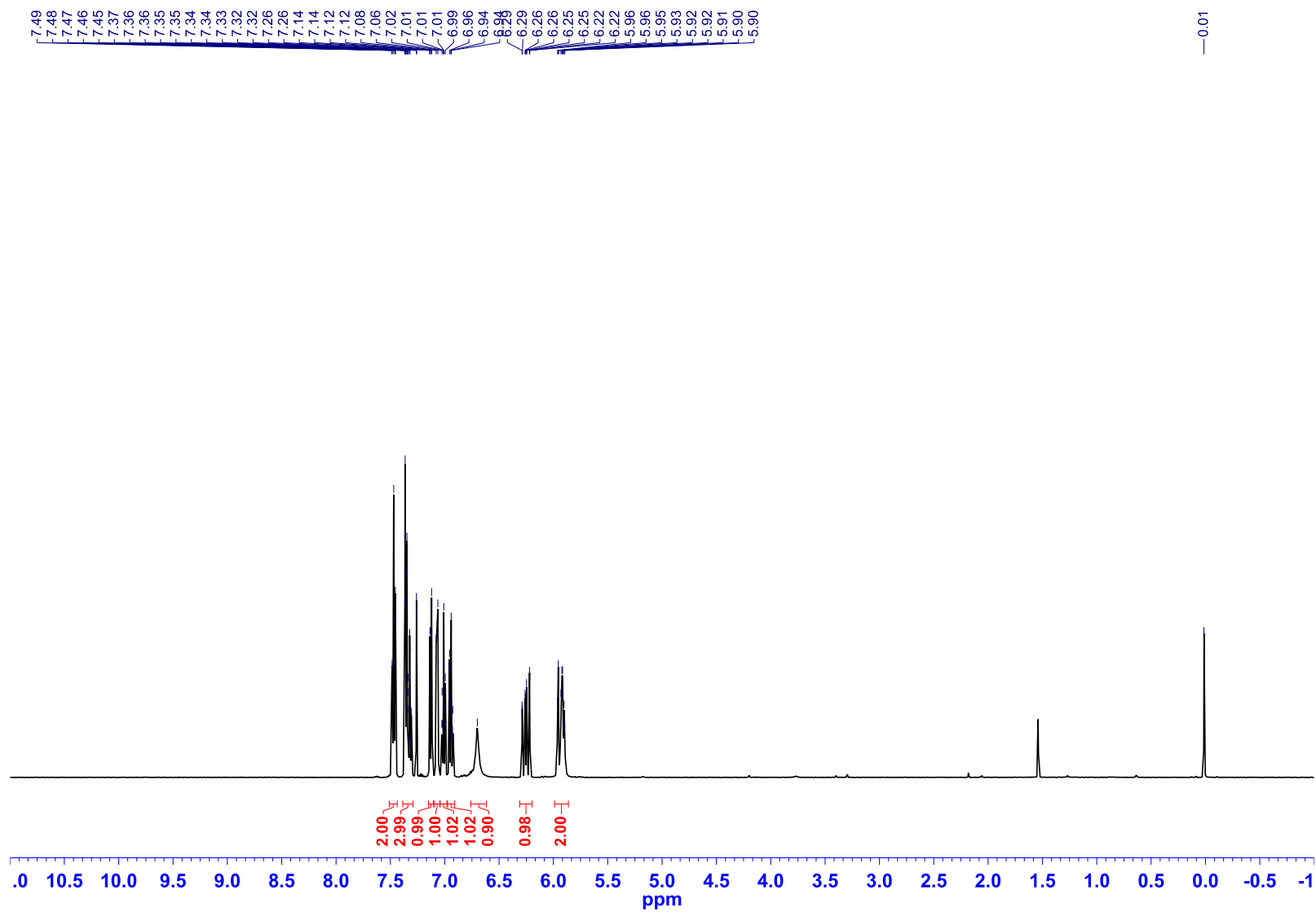
^{11}B NMR (128.4 MHz, MeCN) of (*E*)-1-methyl-2-(1-propenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6f**)



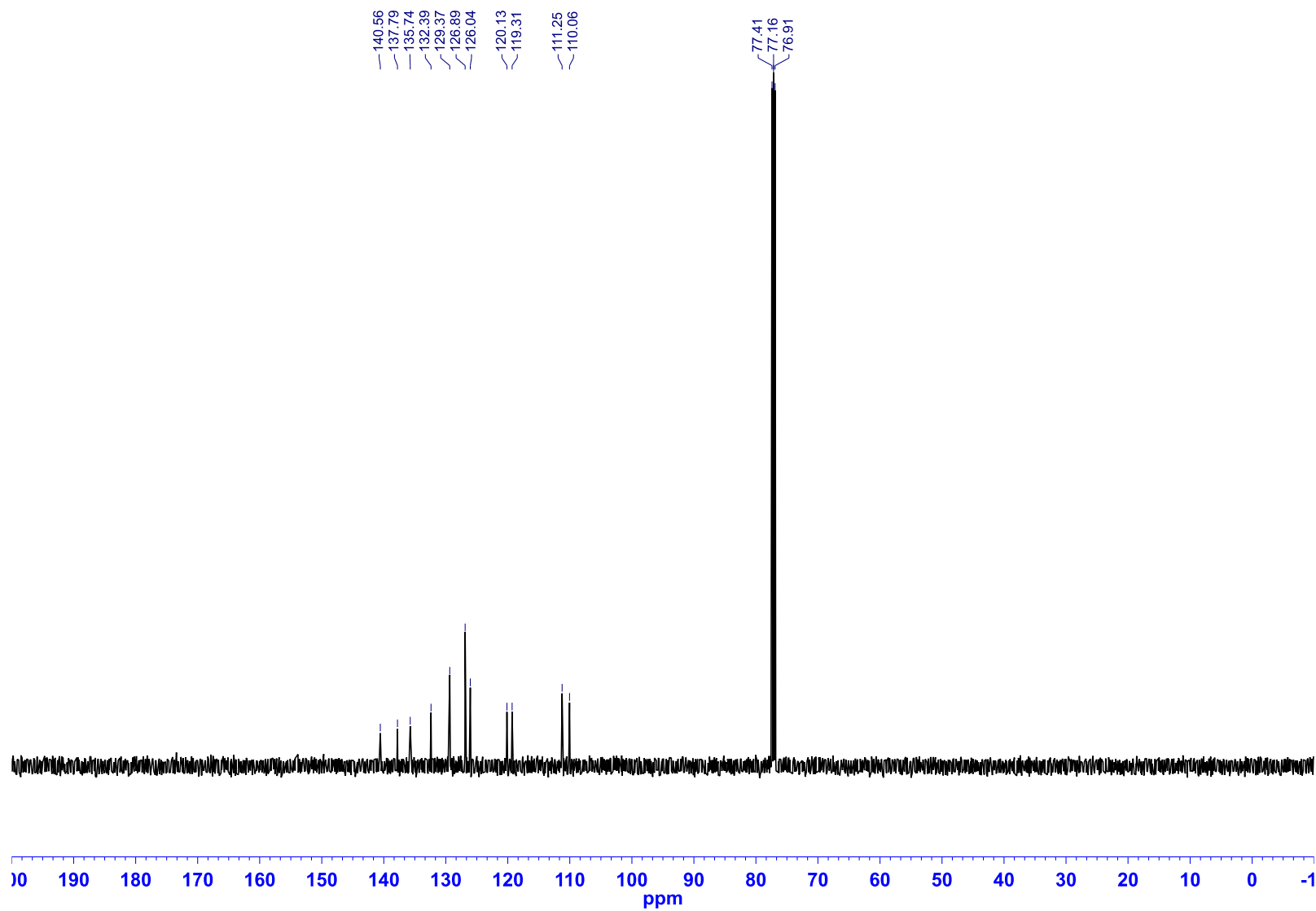
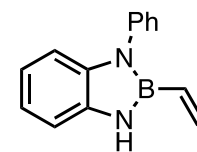
—27.52



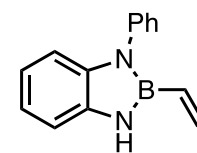
^1H NMR (500.4 MHz, CDCl_3) of 1-phenyl-2-vinyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6g**)



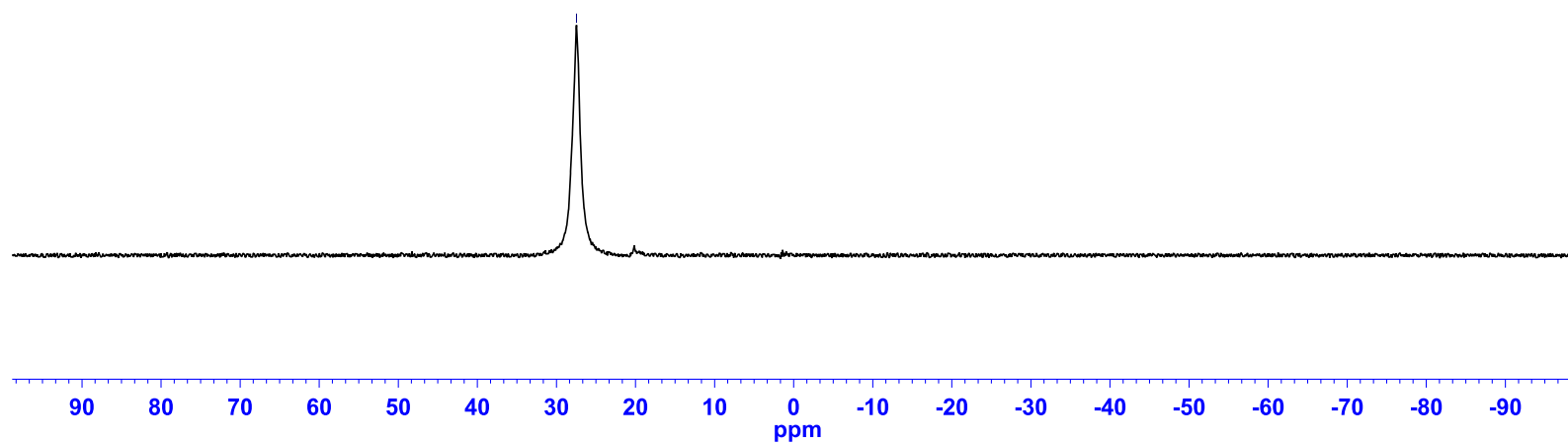
^{13}C NMR (125.8 MHz, CDCl_3) of 1-phenyl-2-vinyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6g**)



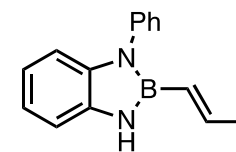
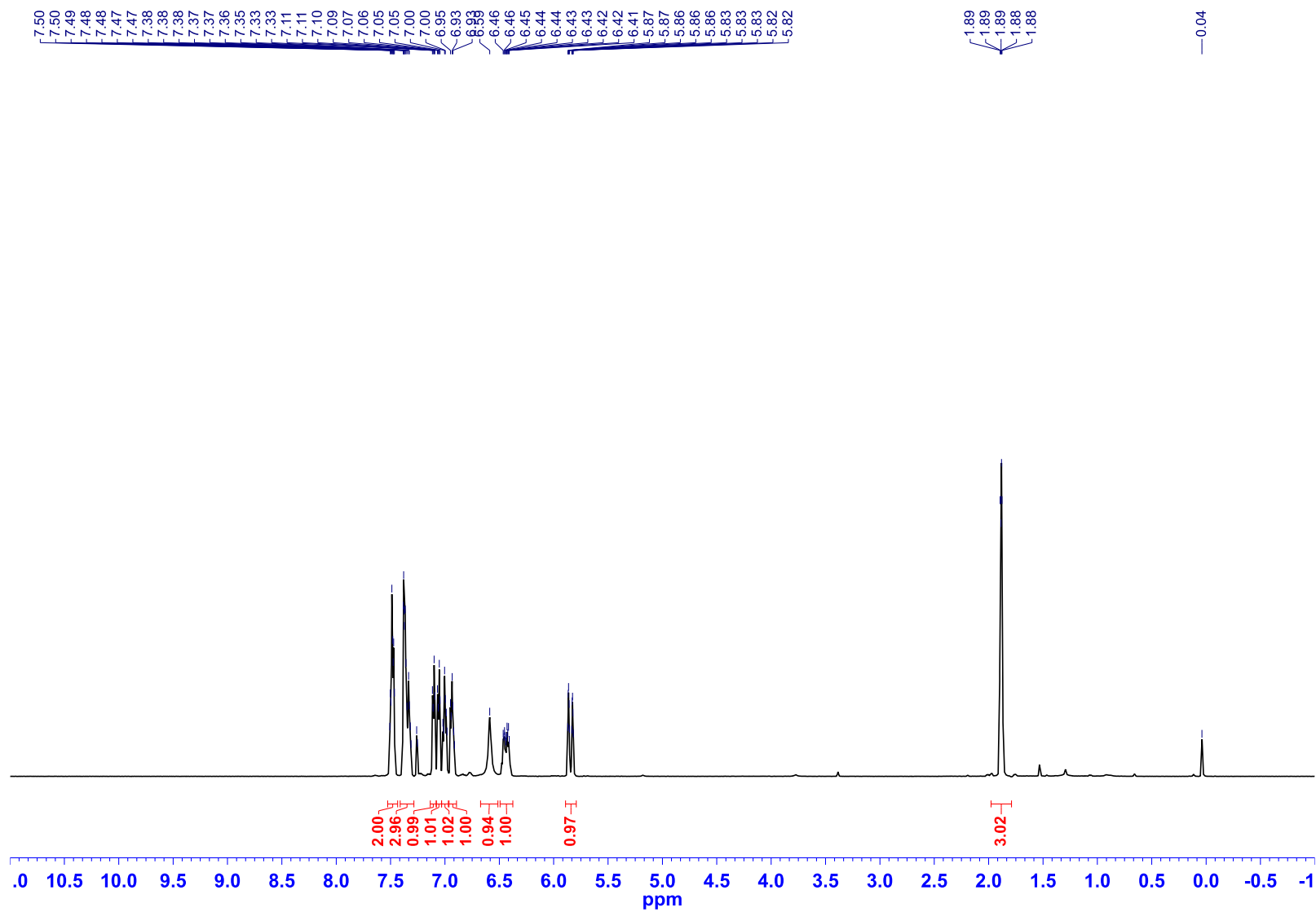
^{11}B NMR (128.4 MHz, MeCN) of 1-phenyl-2-vinyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6g**)



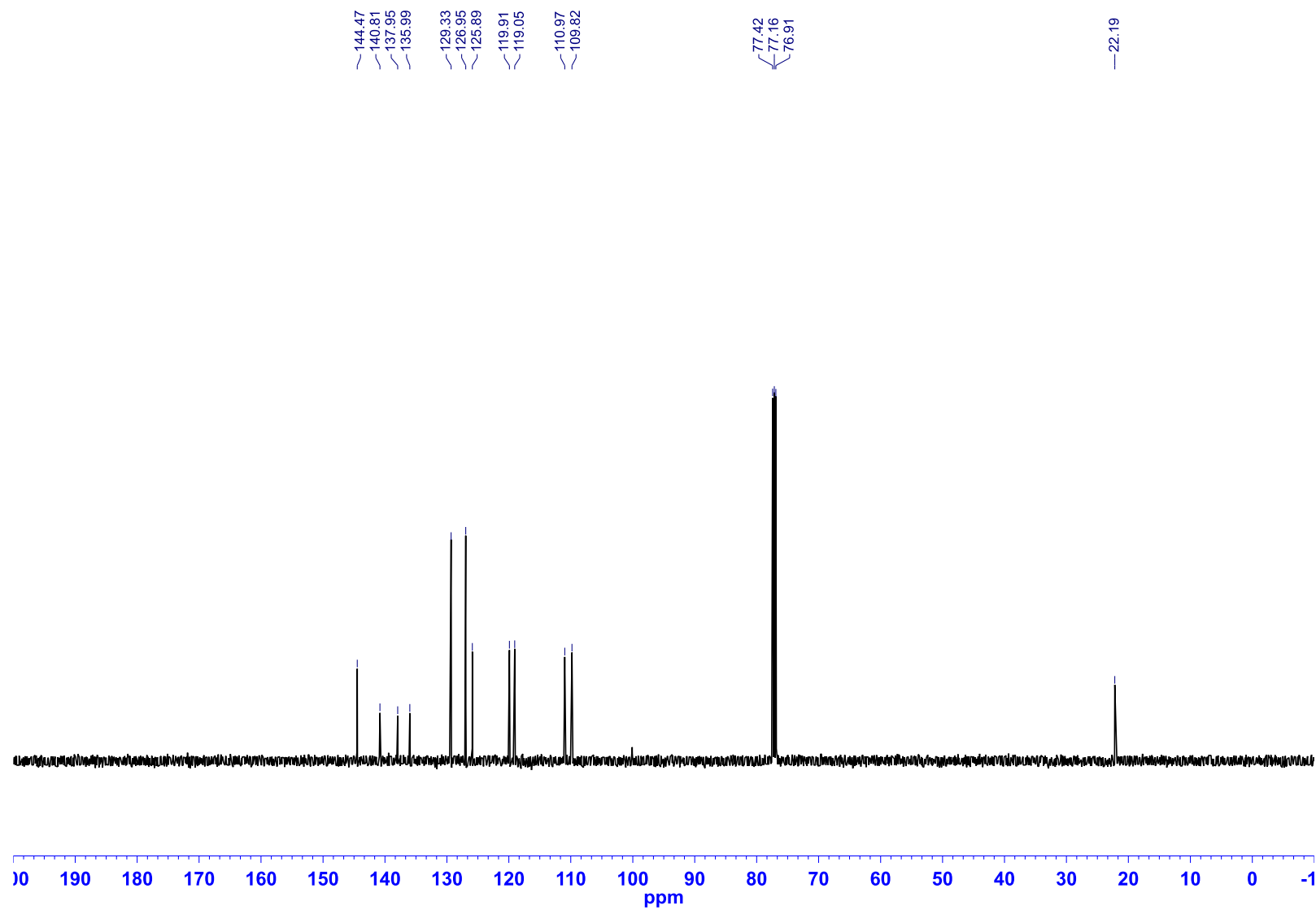
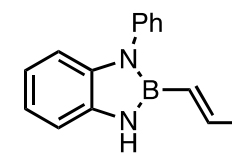
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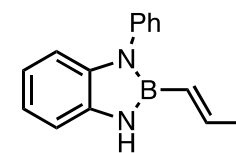
^1H NMR (500.4 MHz, CDCl_3) of (*E*)-1-phenyl-2-(1-propenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6h**)



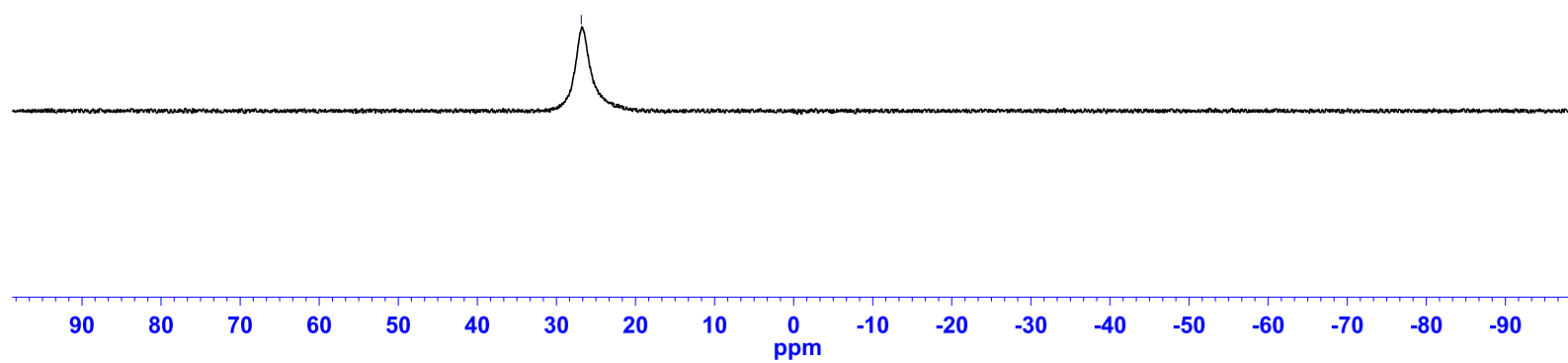
^{13}C NMR (125.8 MHz, CDCl_3) of (*E*)-1-phenyl-2-(1-propenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6h**)



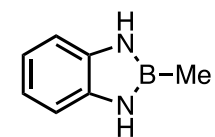
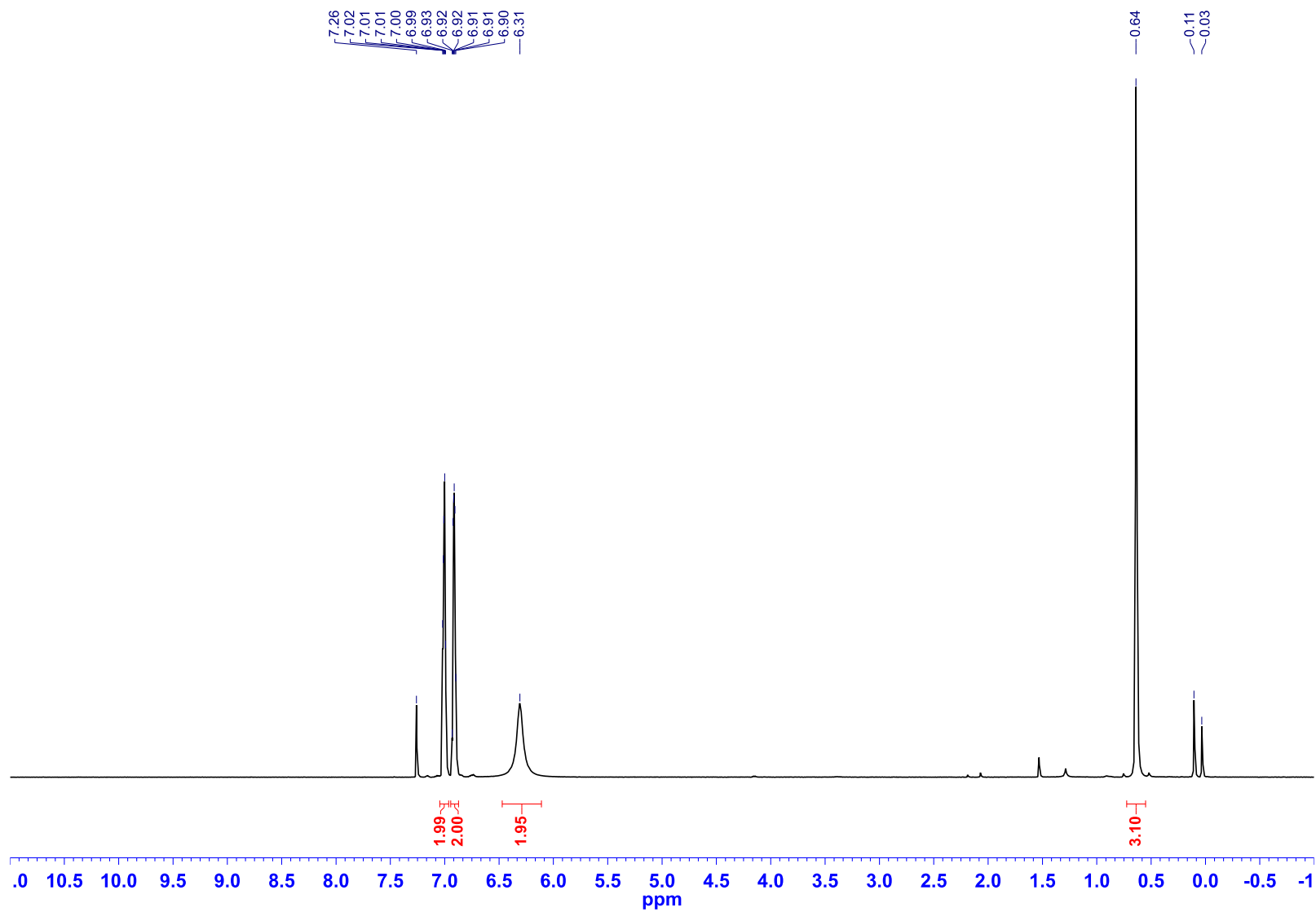
^{11}B NMR (128.4 MHz, CDCl_3) of (*E*)-1-phenyl-2-(1-propenyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**6h**)



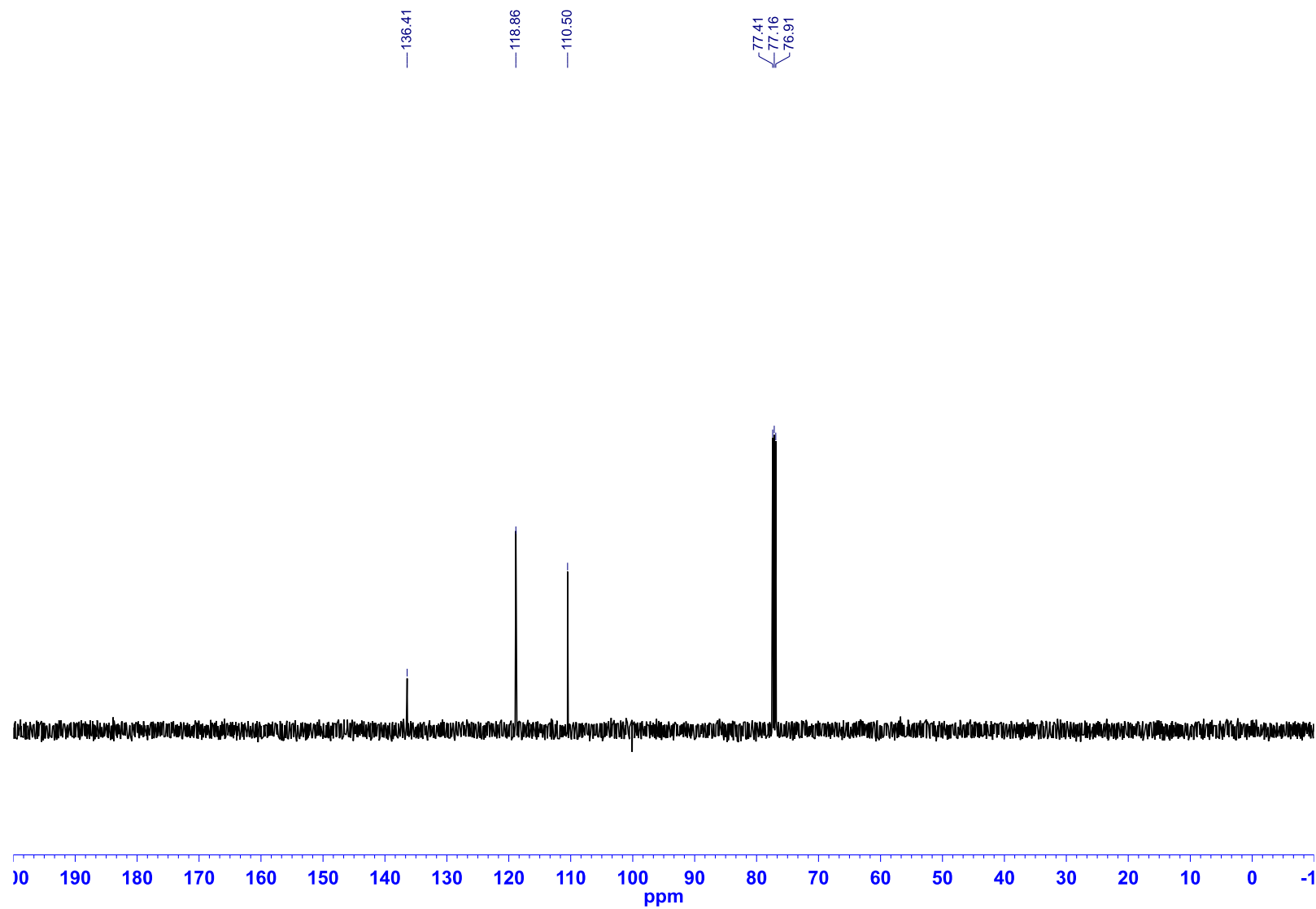
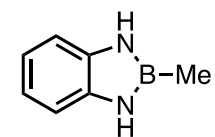
—26.86



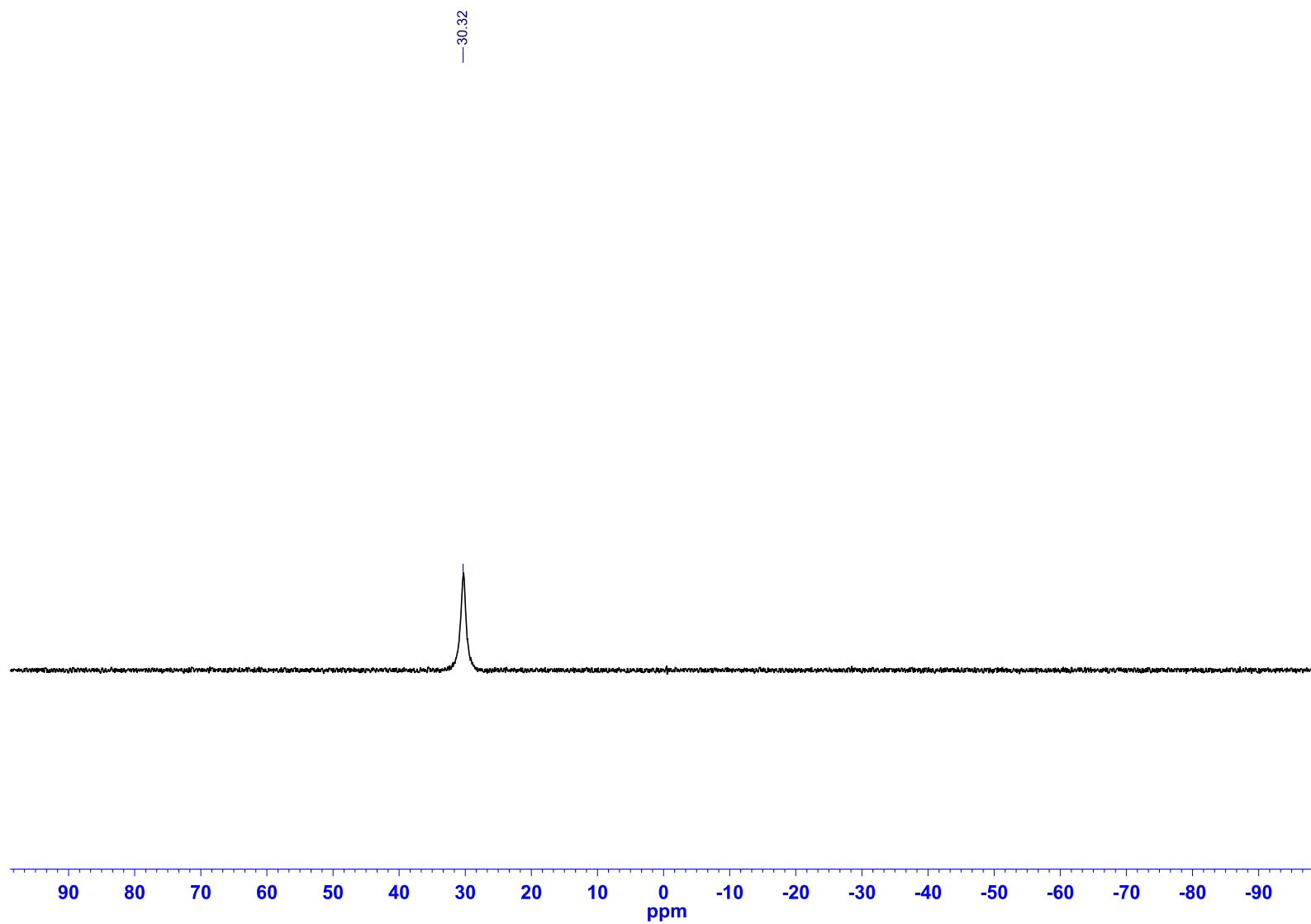
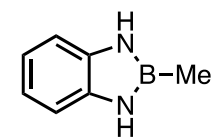
^1H NMR (500.4 MHz, CDCl_3) of 2-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7a**)



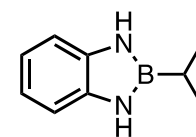
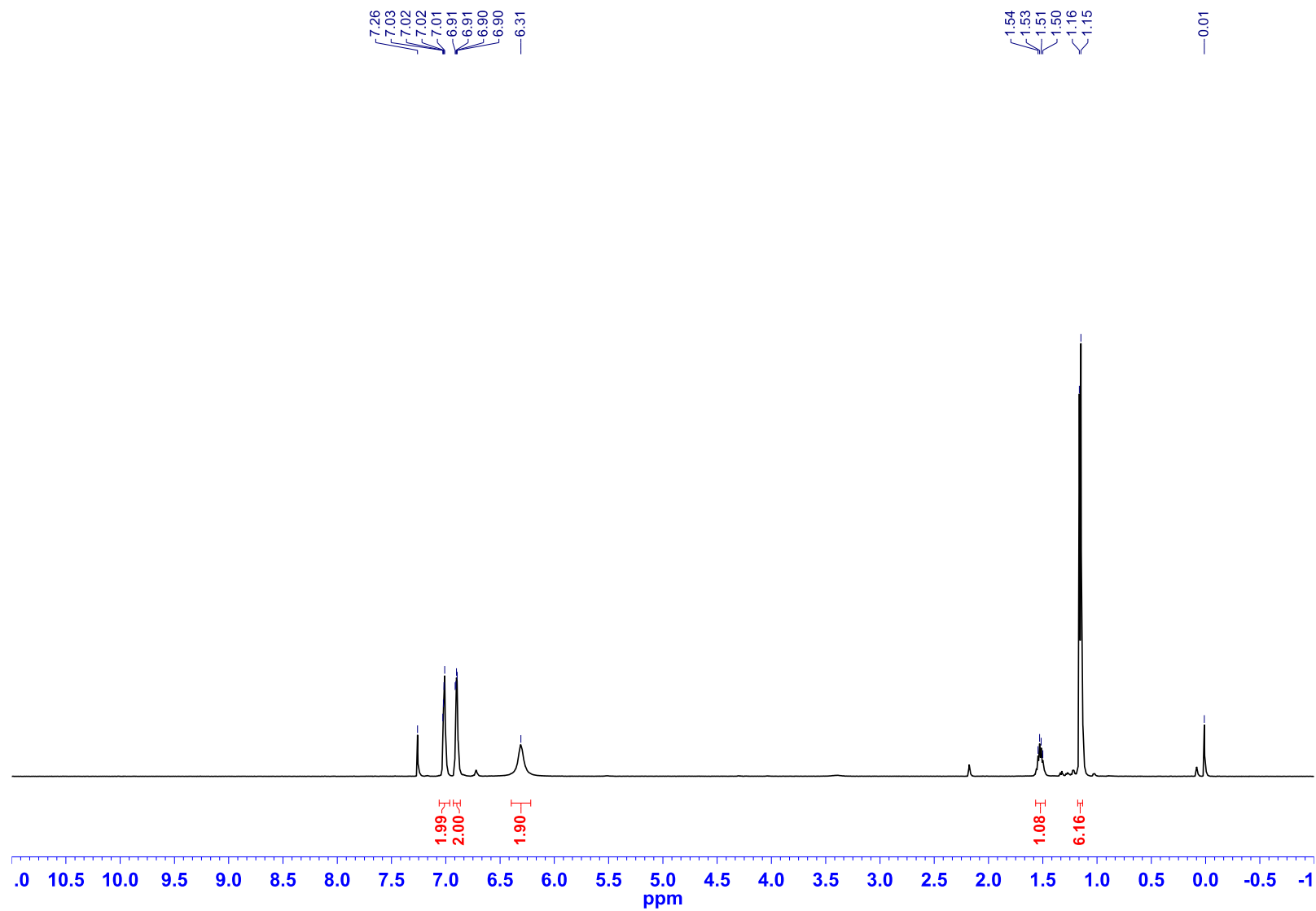
^{13}C NMR (125.8 MHz, CDCl_3) of 2-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7a**)



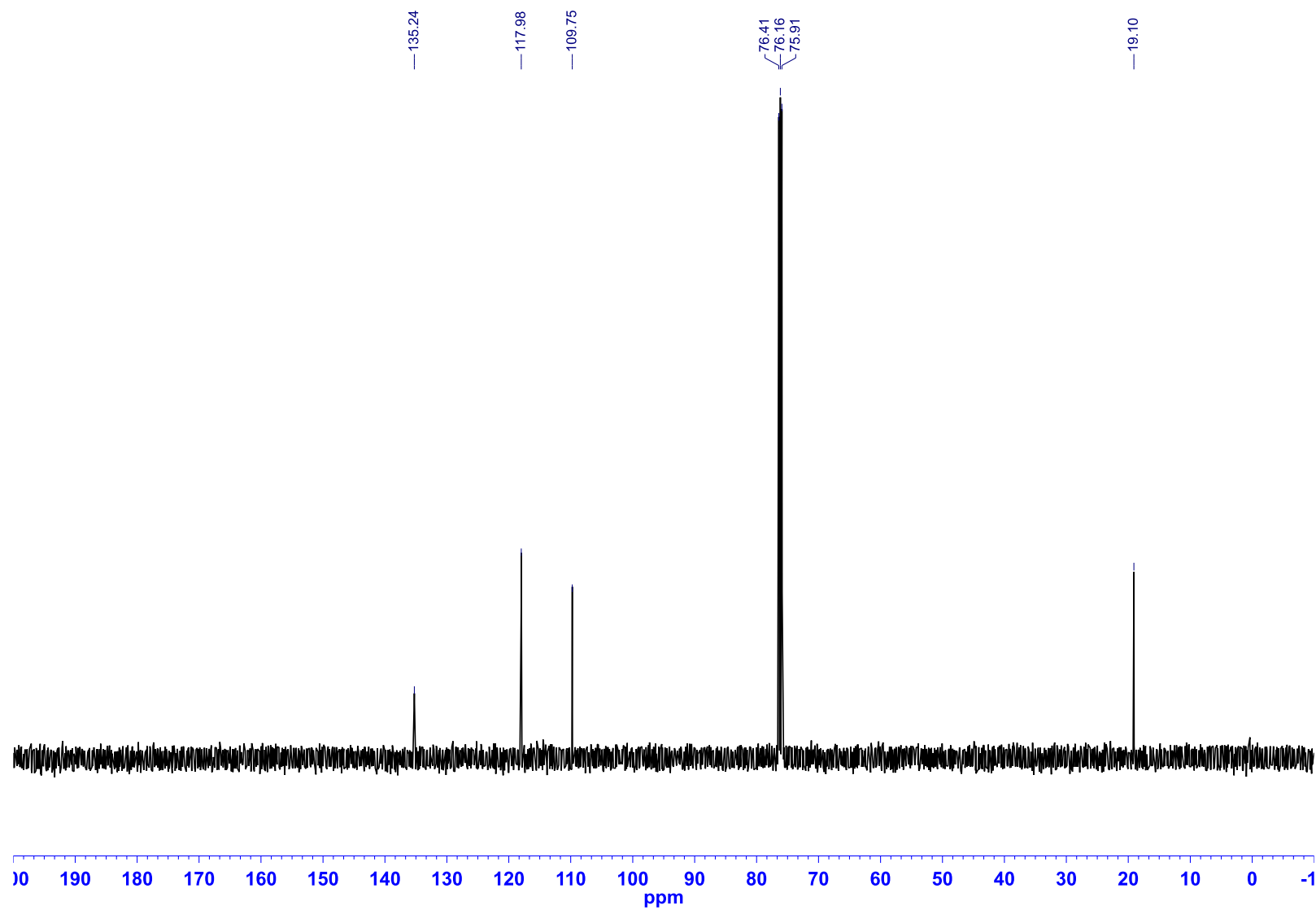
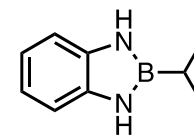
^{11}B NMR (128.4 MHz, CDCl_3) of 2-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7a**)



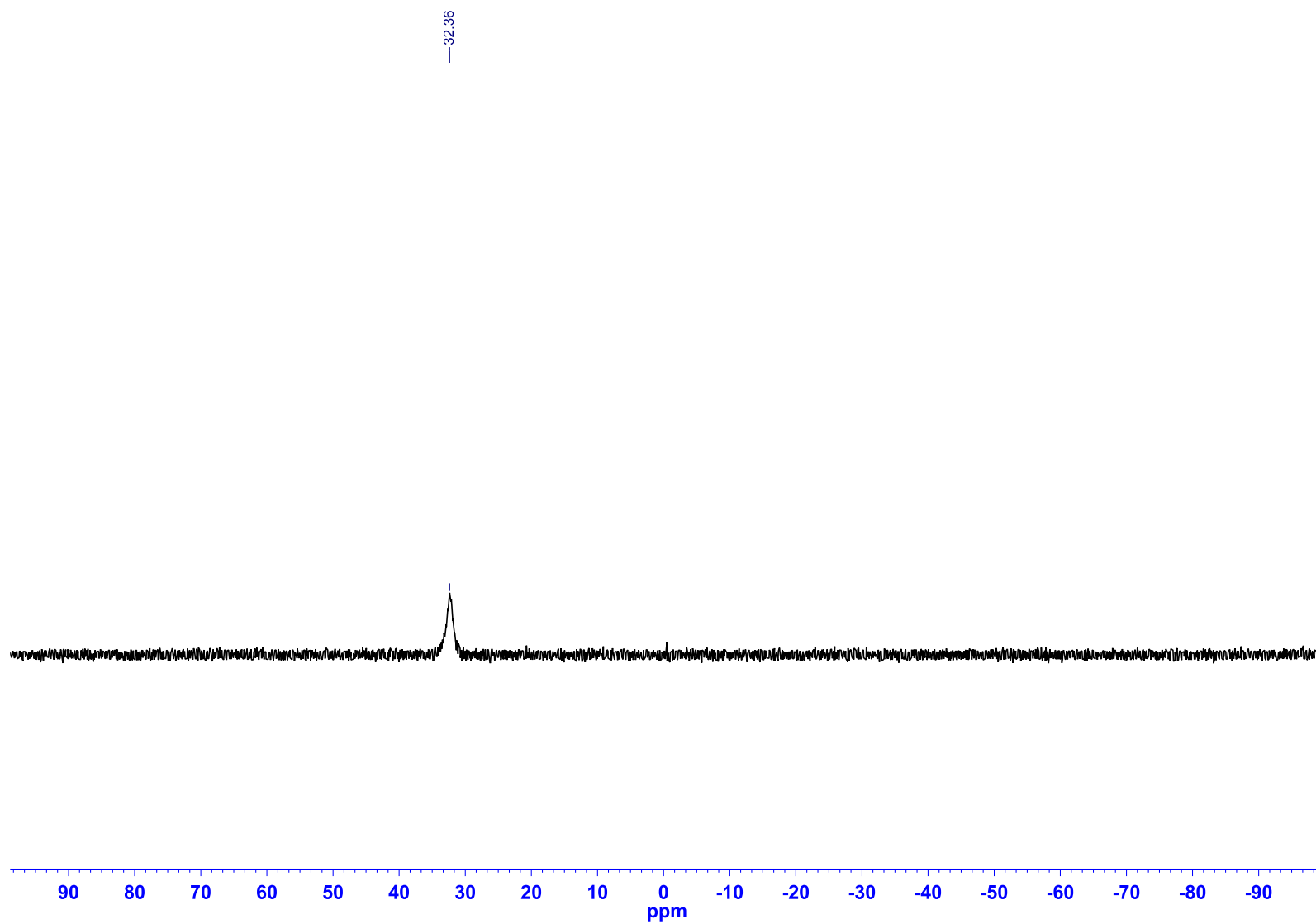
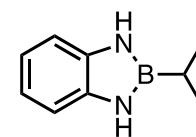
^1H NMR (500.4 MHz, CDCl_3) of 2-isopropyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7b**)



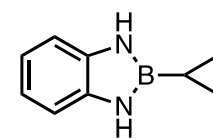
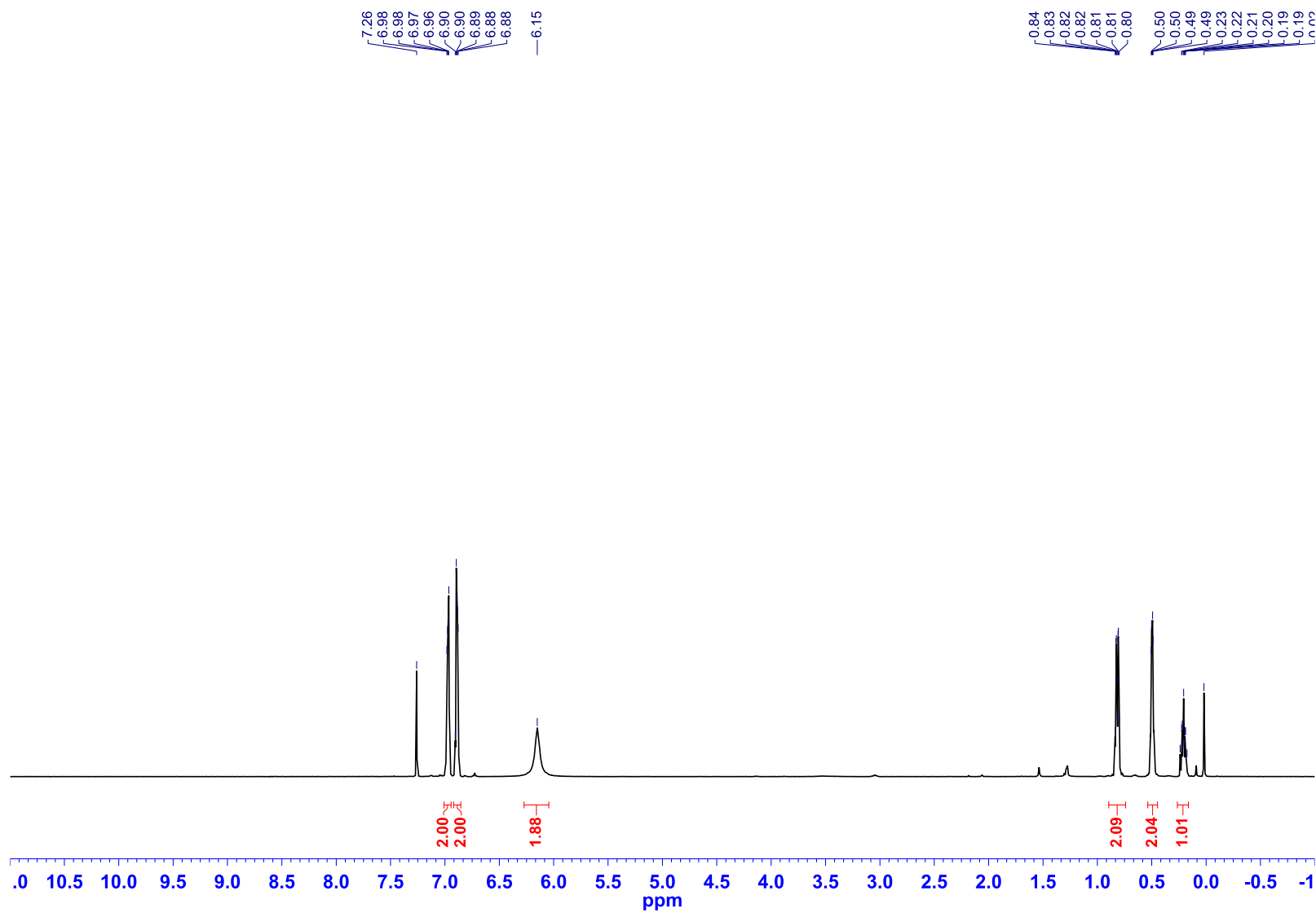
^{13}C NMR (125.8 MHz, CDCl_3) of 2-isopropyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7b**)



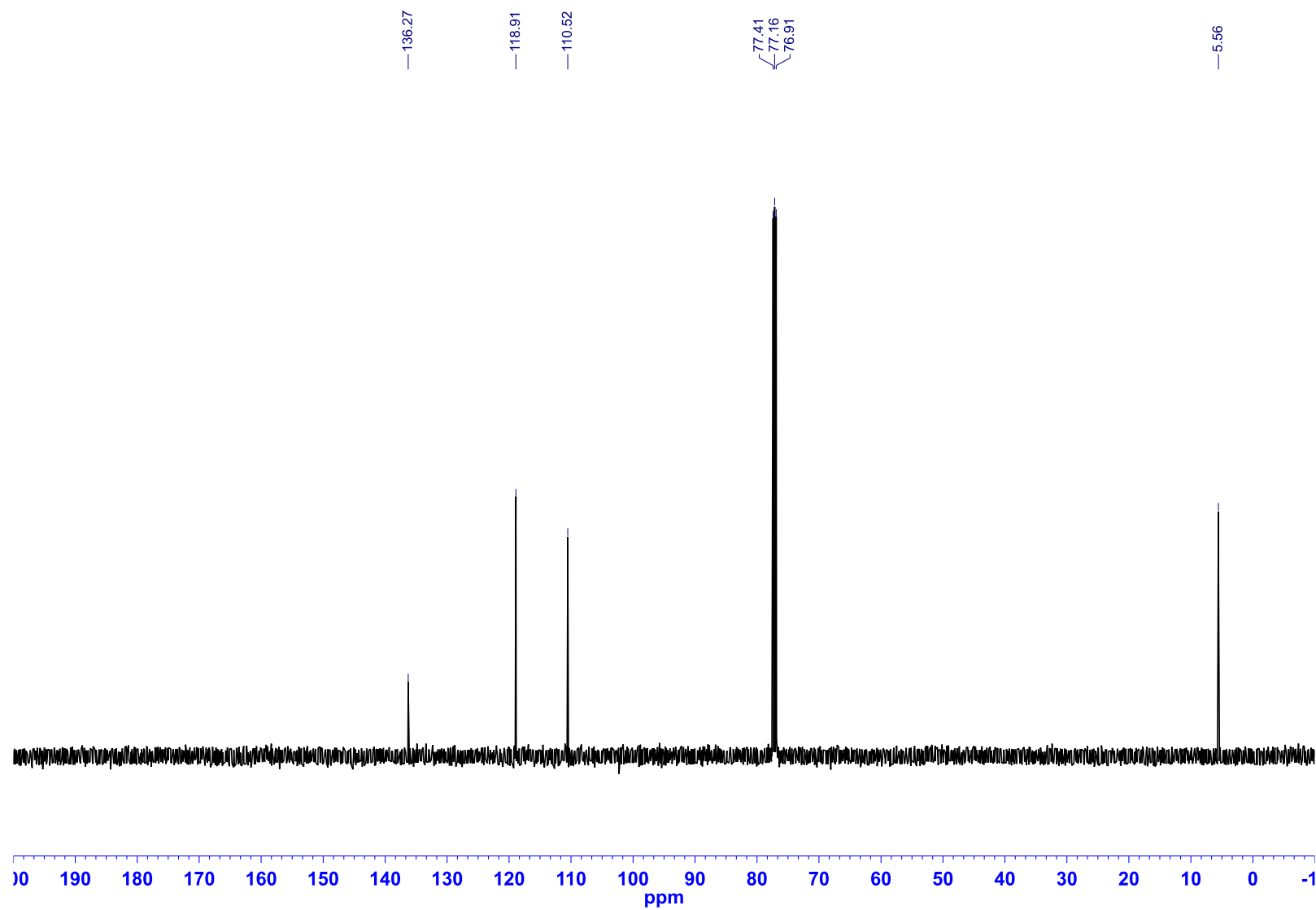
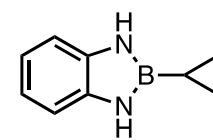
^{11}B NMR (128.4 MHz, CDCl_3) of 2-isopropyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7b**)



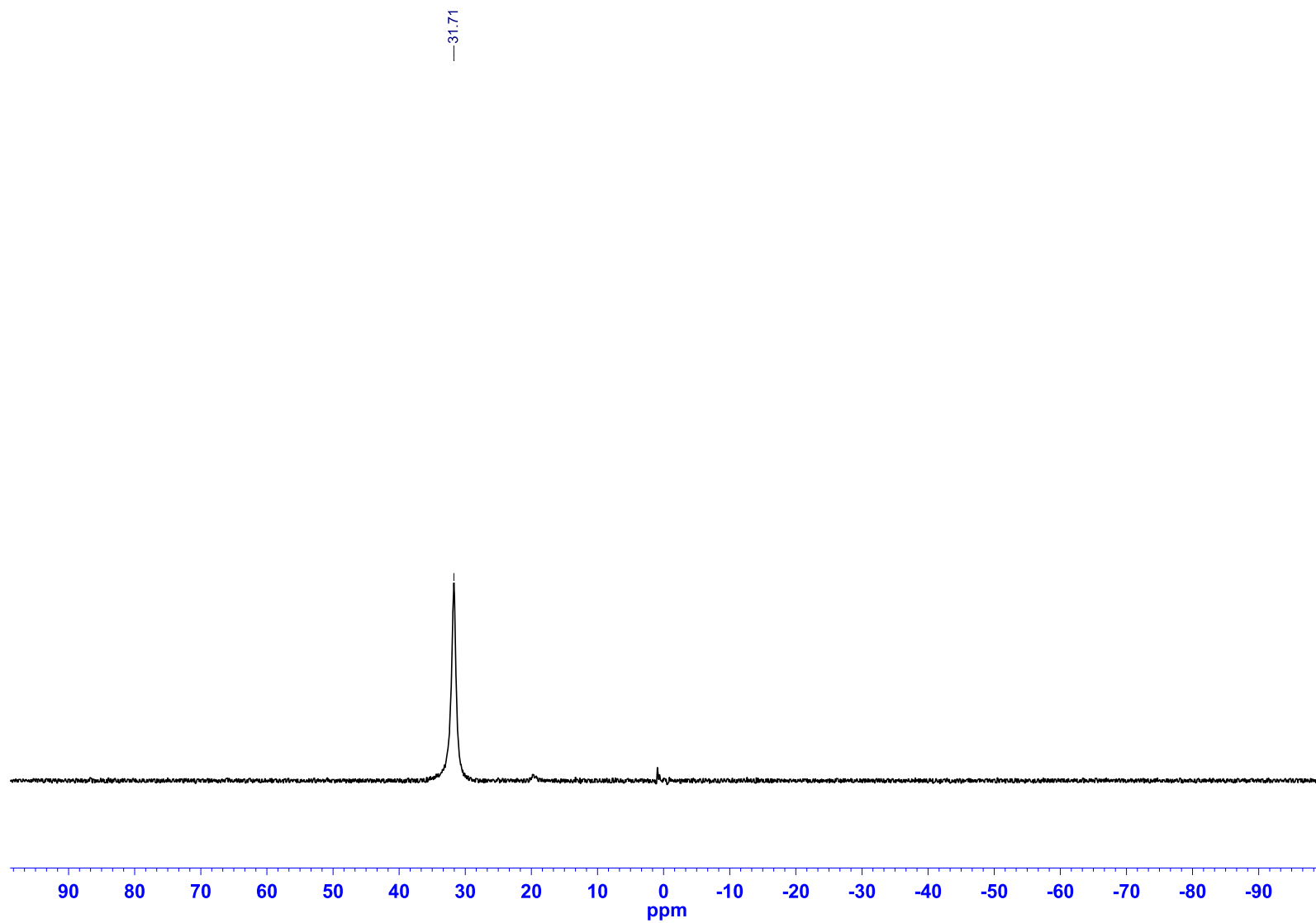
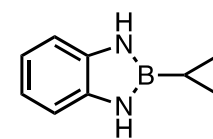
^1H NMR (500.4 MHz, CDCl_3) of 2-cyclopropyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7c**)



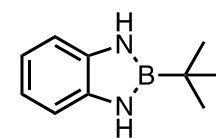
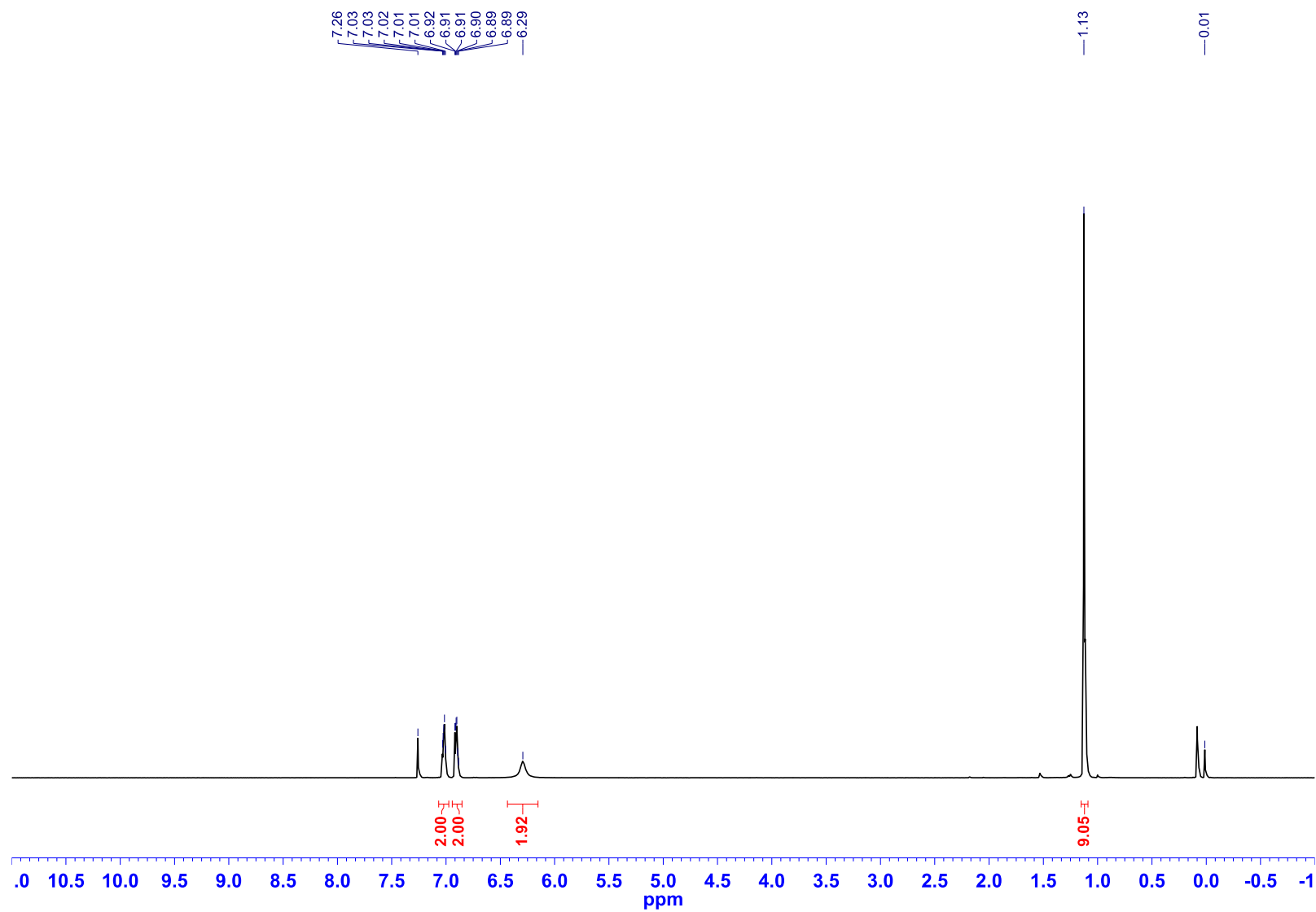
^{13}C NMR (125.8 MHz, CDCl_3) of 2-cyclopropyl-2,3-dihydro-1H-1,3,2-benzodiazaborole (**7c**)



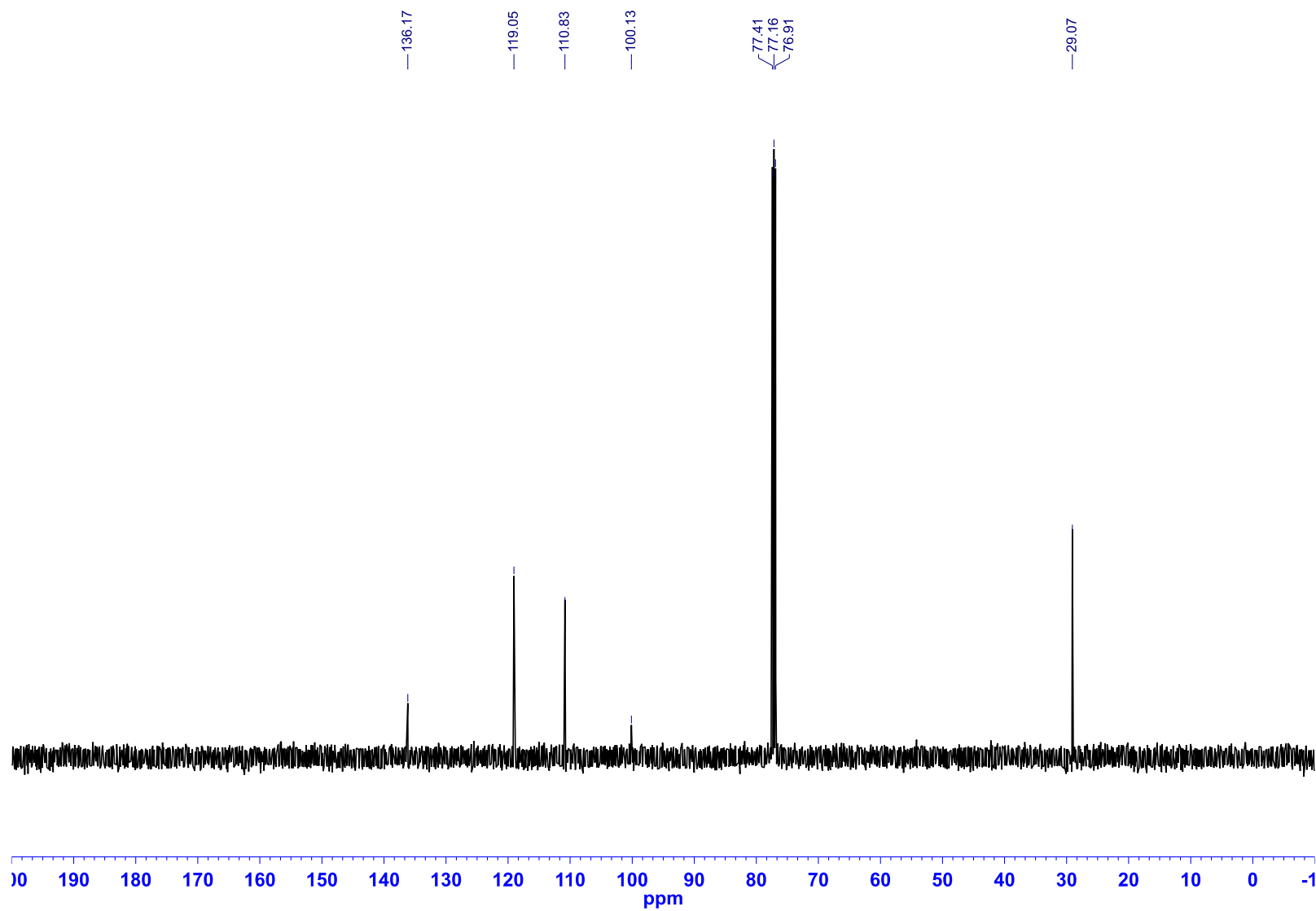
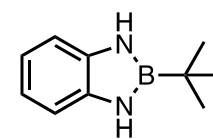
^{11}B NMR (128.4 MHz, MeCN) of 2-cyclopropyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7c**)



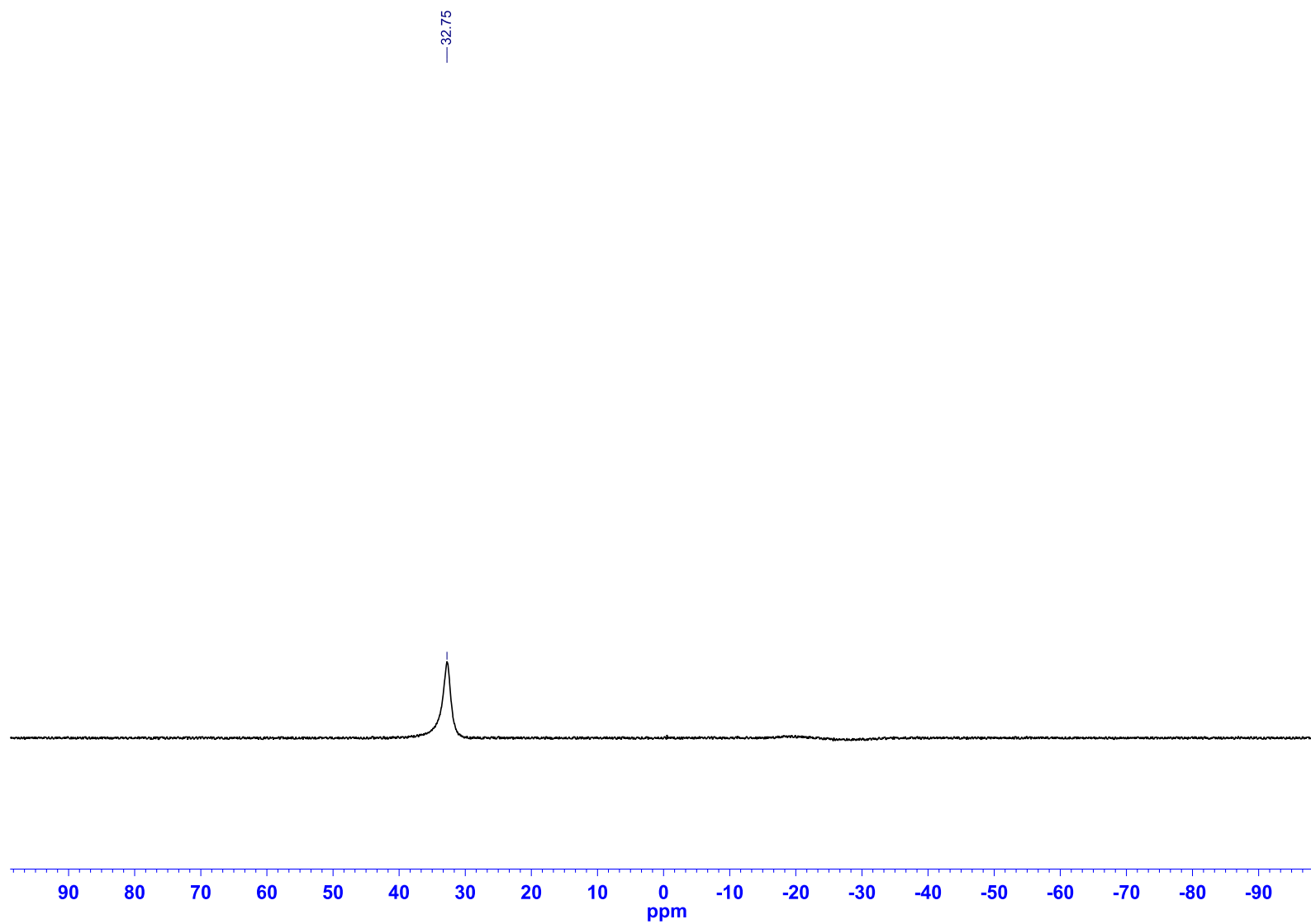
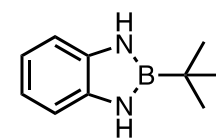
^1H NMR (500.4 MHz, CDCl_3) of 2-(*tert*-butyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7d**)



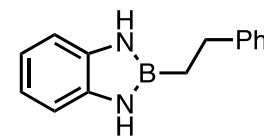
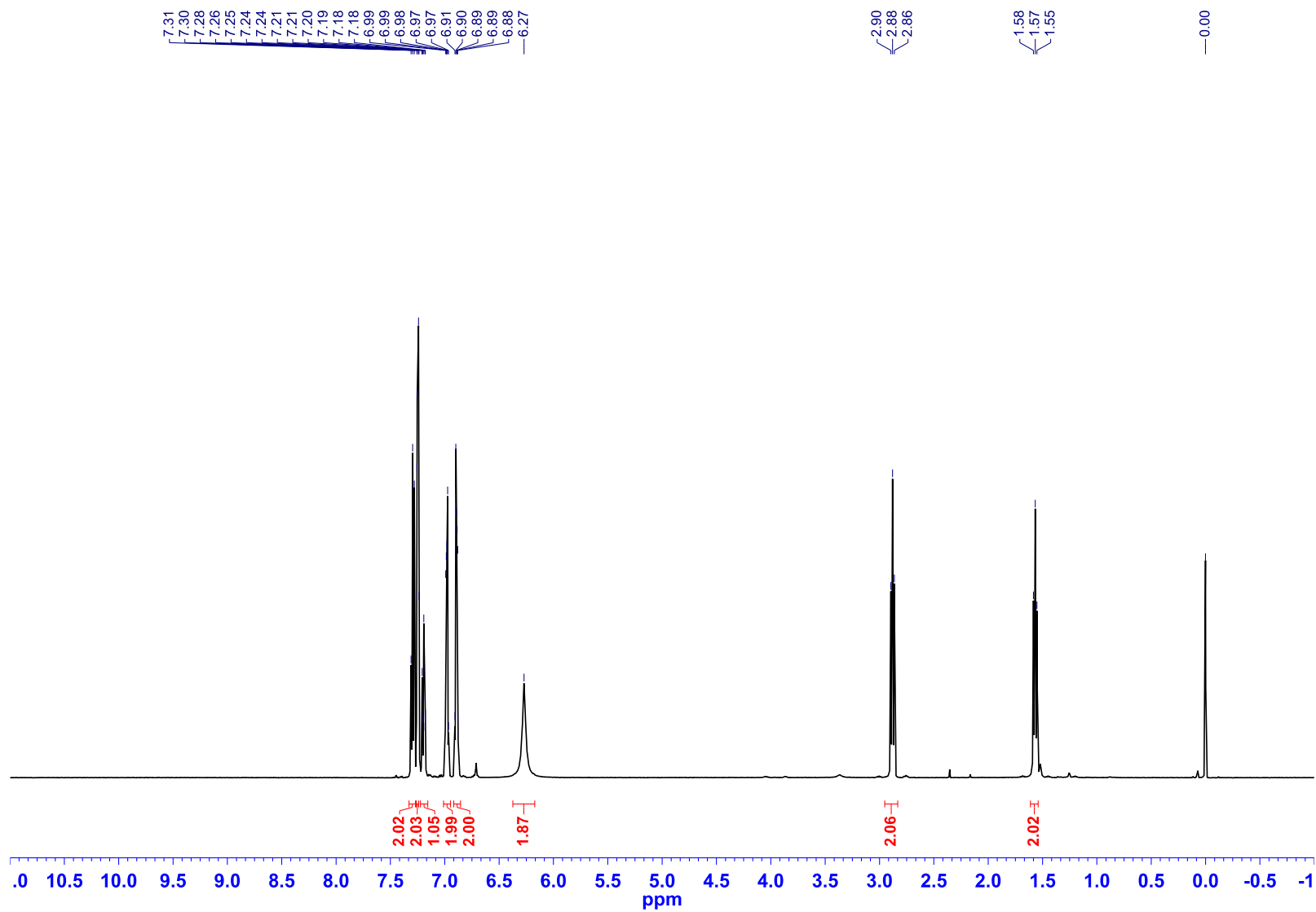
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(*tert*-butyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7d**)



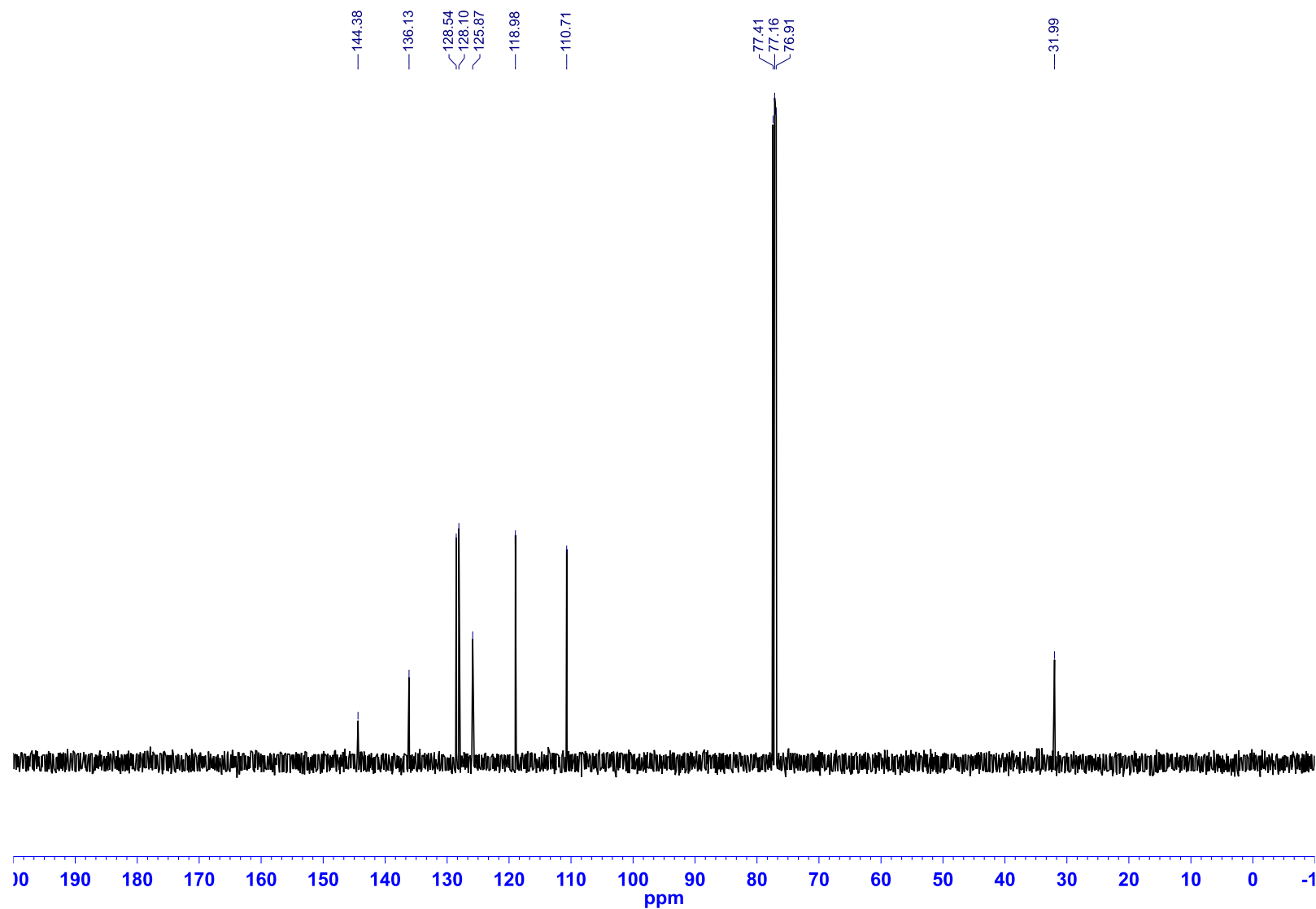
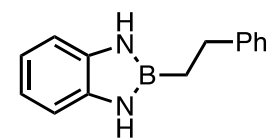
^{11}B NMR (128.4 MHz, CDCl_3) of 2-(*tert*-butyl)-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7d**)



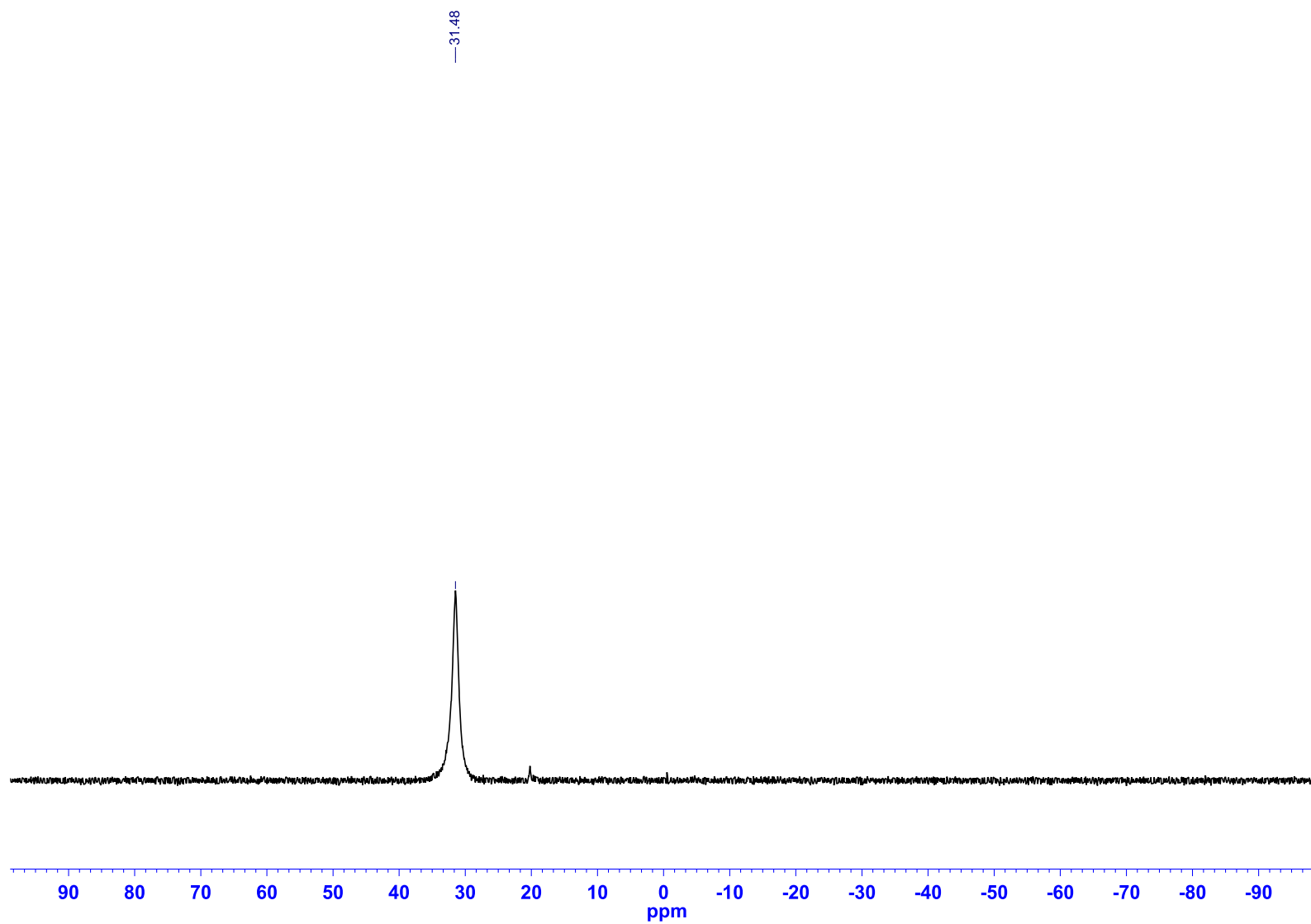
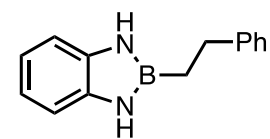
^1H NMR (500.4 MHz, CDCl_3) of 2-phenethyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7e**)



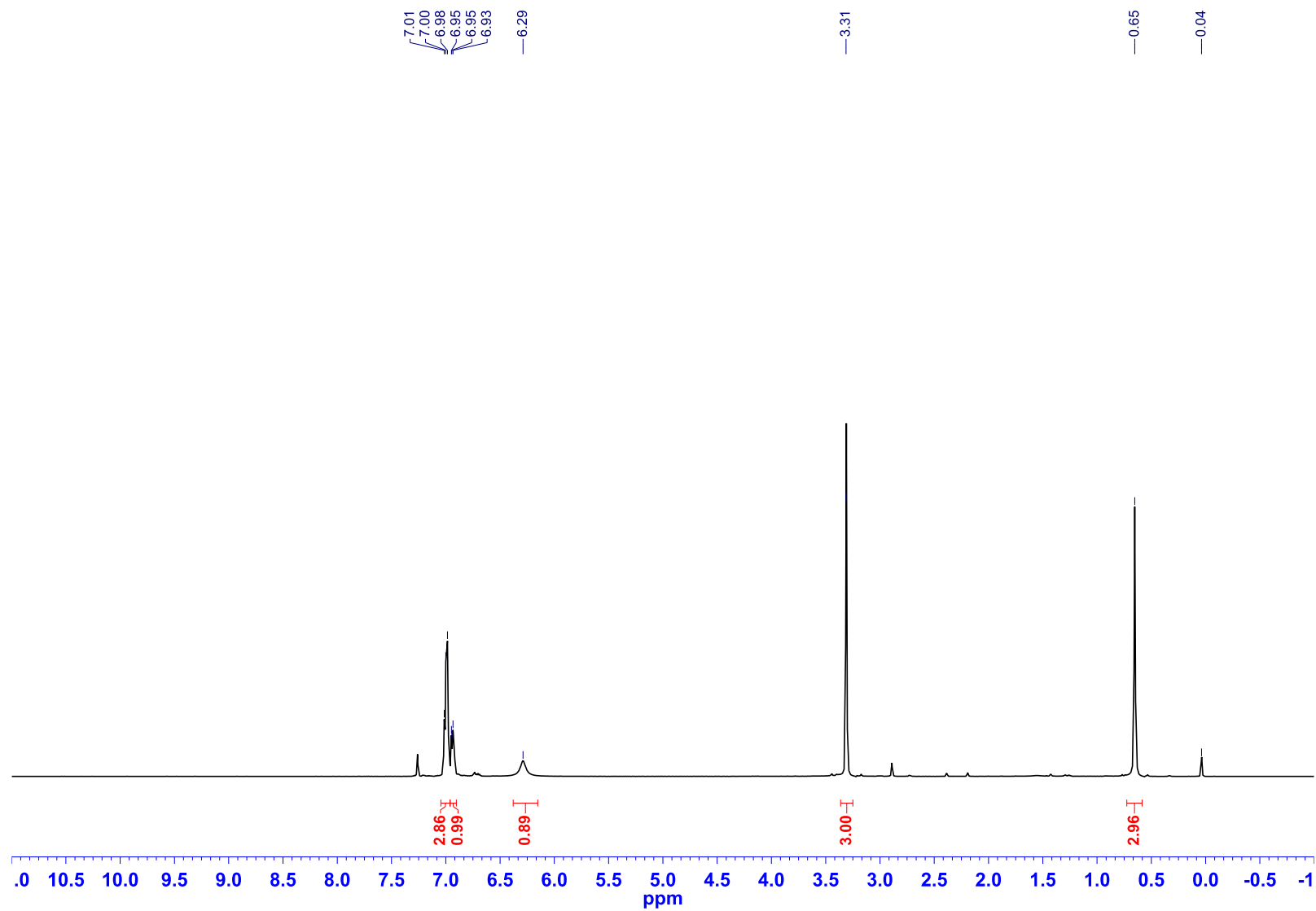
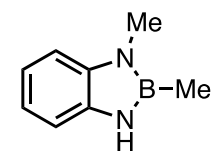
^{13}C NMR (125.8 MHz, CDCl_3) of 2-phenethyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7e**)



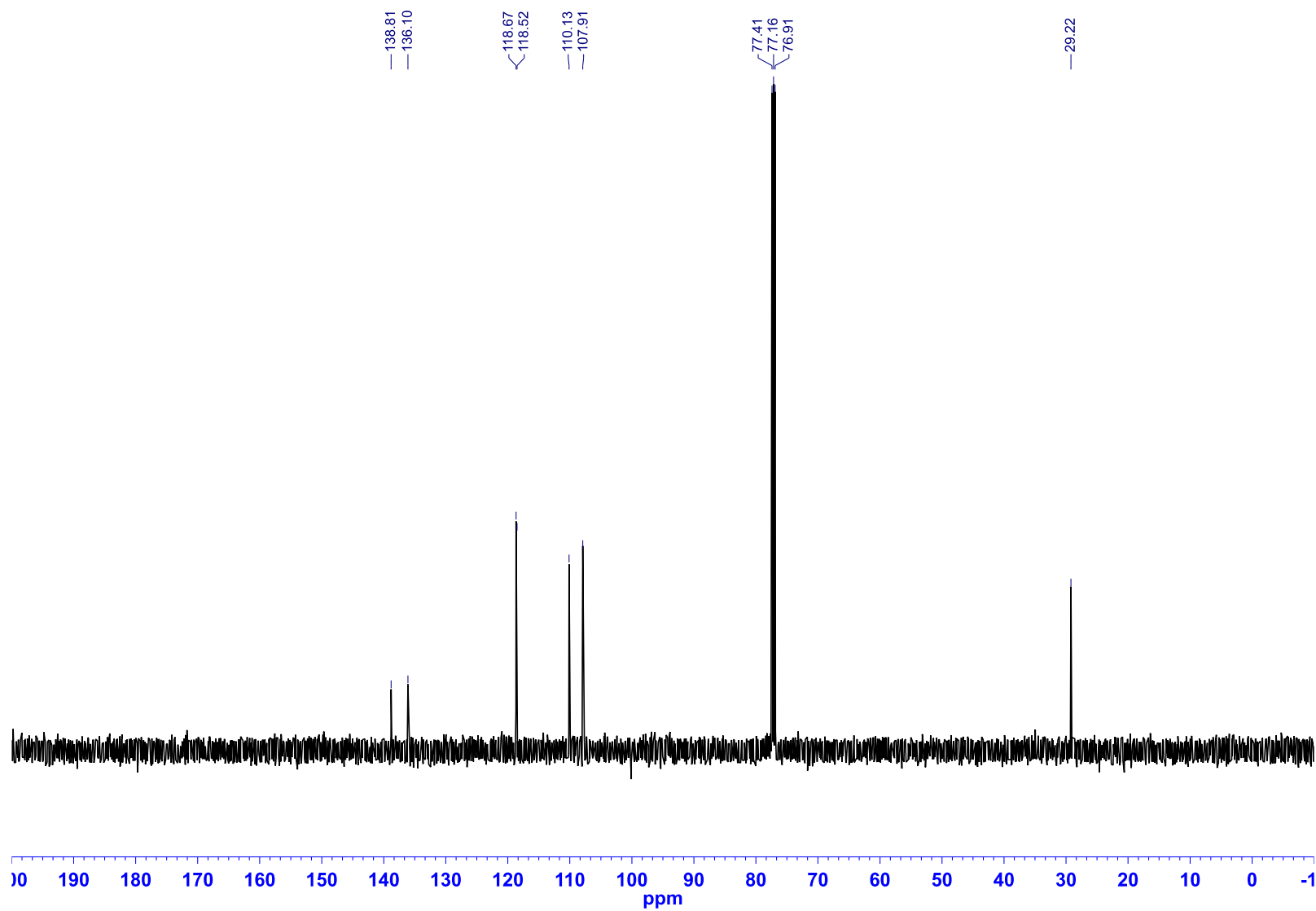
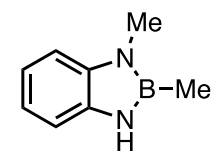
^{11}B NMR (128.4 MHz, MeCN) of 2-phenethyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7e**)



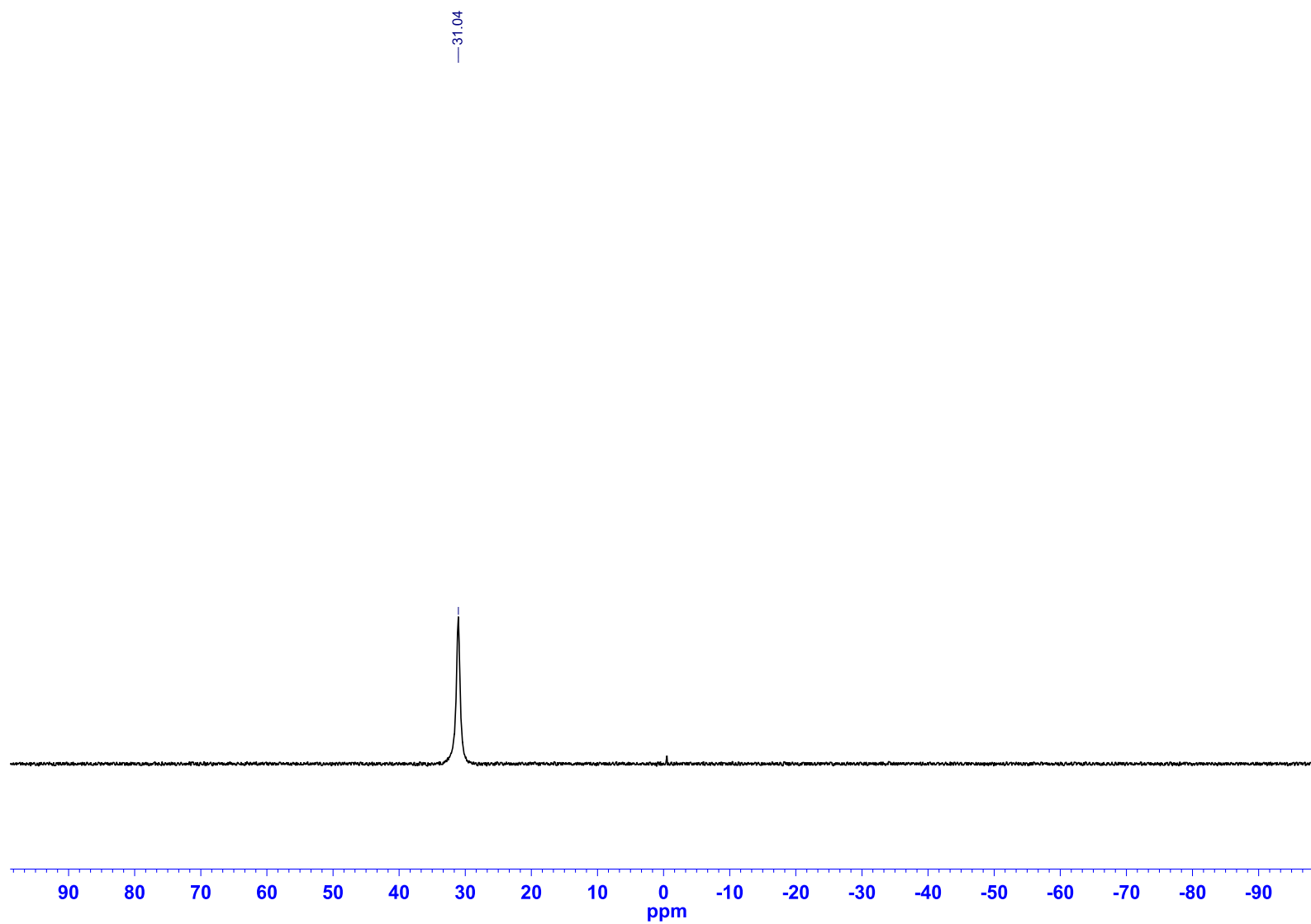
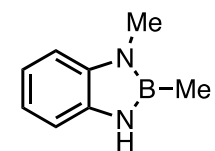
^1H NMR (500.4 MHz, CDCl_3) of 1,2-dimethyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7f**)



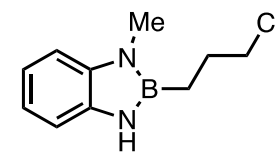
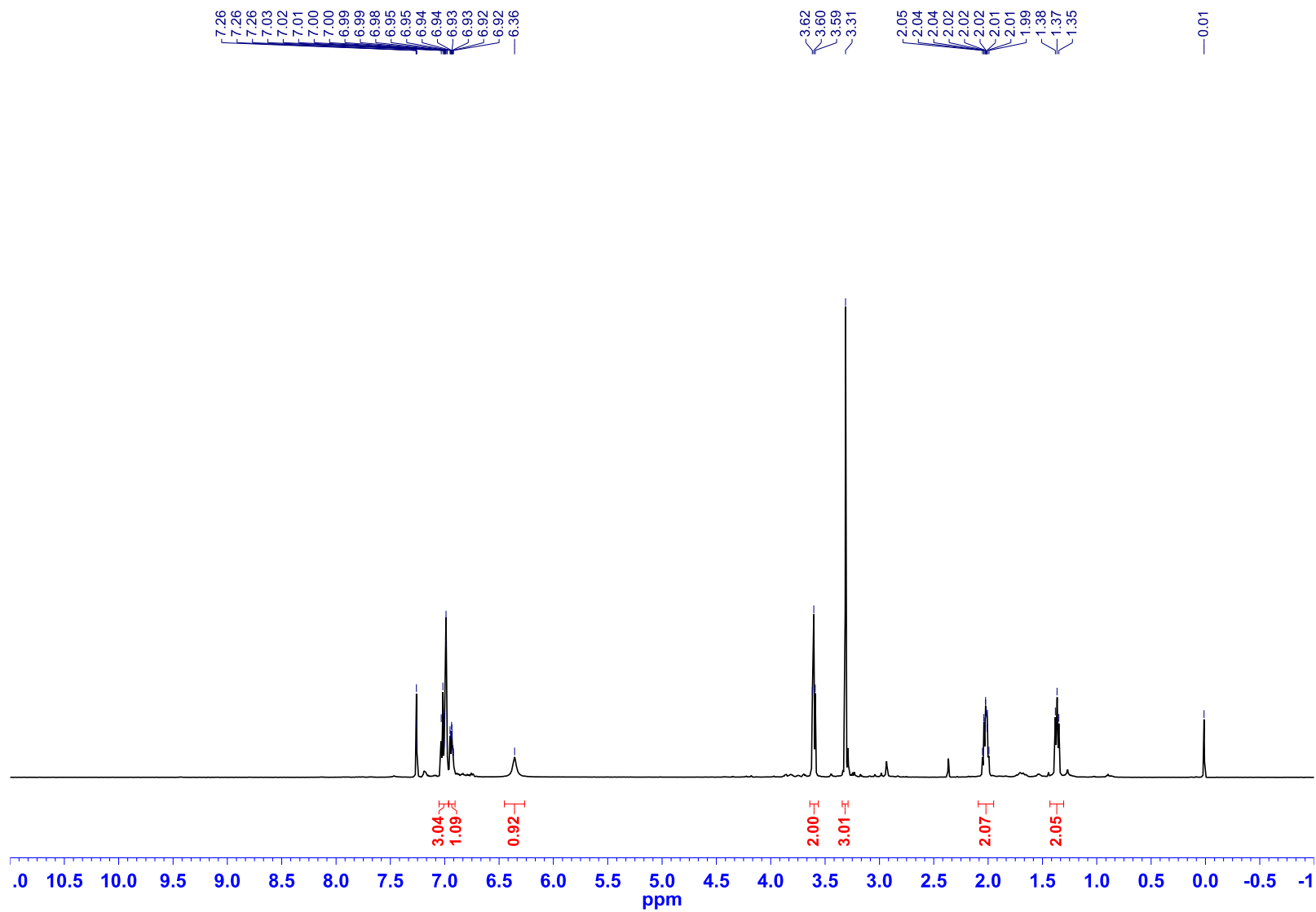
^{13}C NMR (125.8 MHz, CDCl_3) of 1,2-dimethyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7f**)



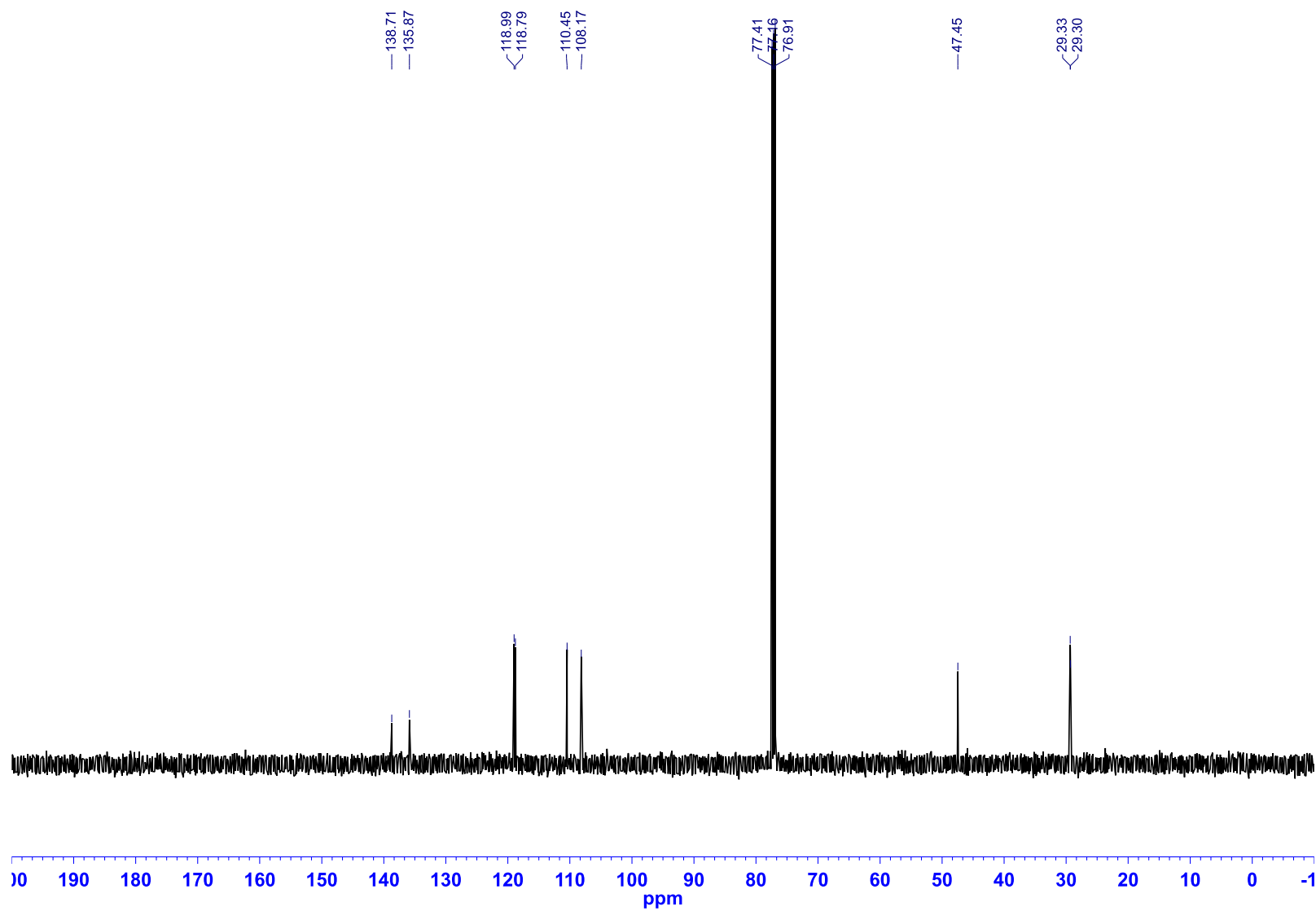
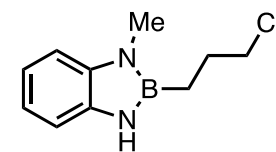
^{11}B NMR (128.4 MHz, MeCN) of 1,2-dimethyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7f**)



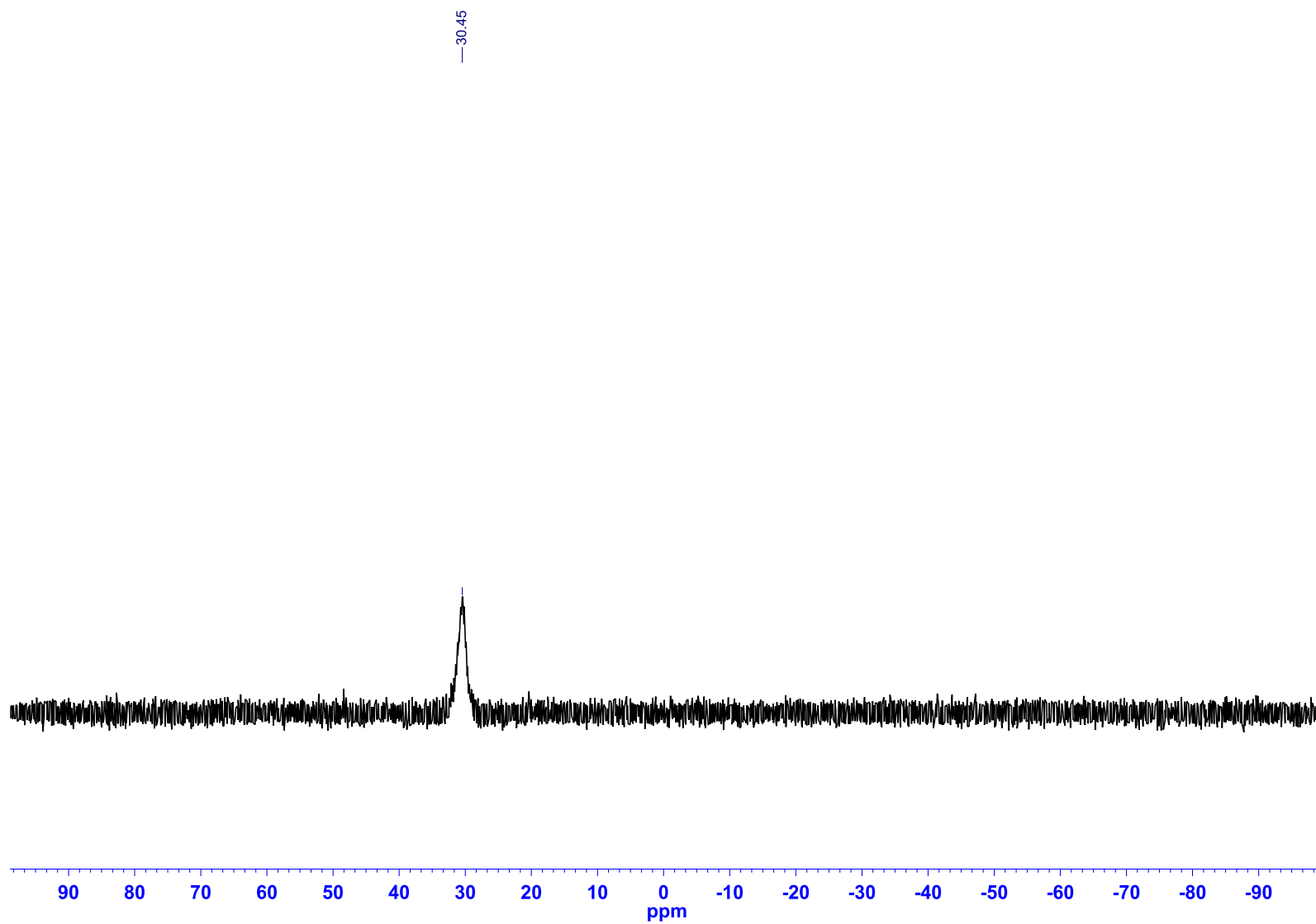
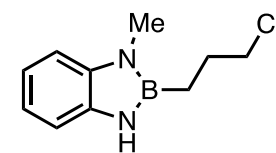
¹H NMR (500.4 MHz, CDCl₃) of 2-(3-chloropropyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7g**)



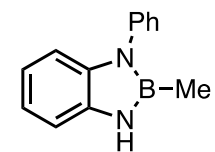
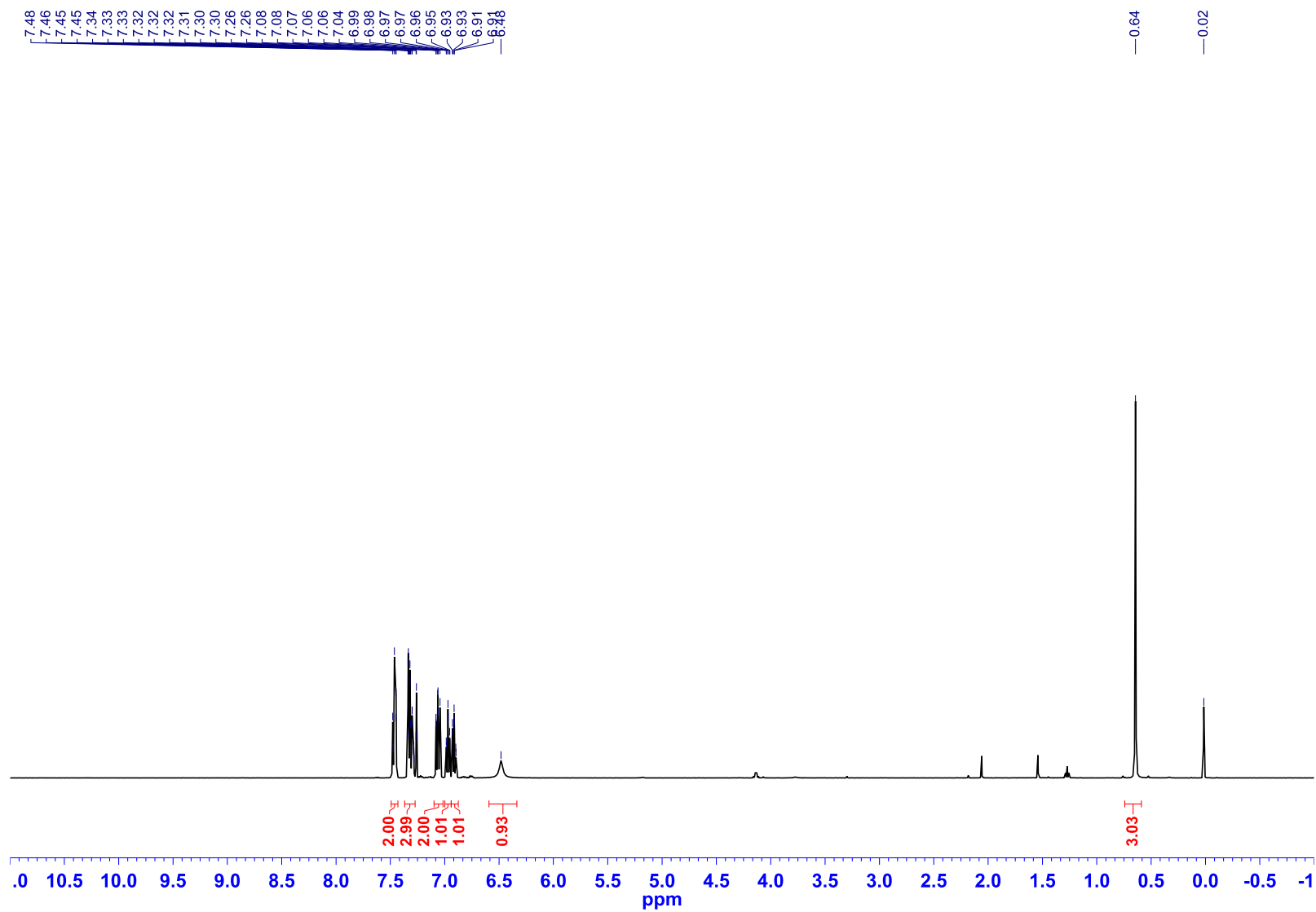
^{13}C NMR (125.8 MHz, CDCl_3) of 2-(3-chloropropyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7g**)



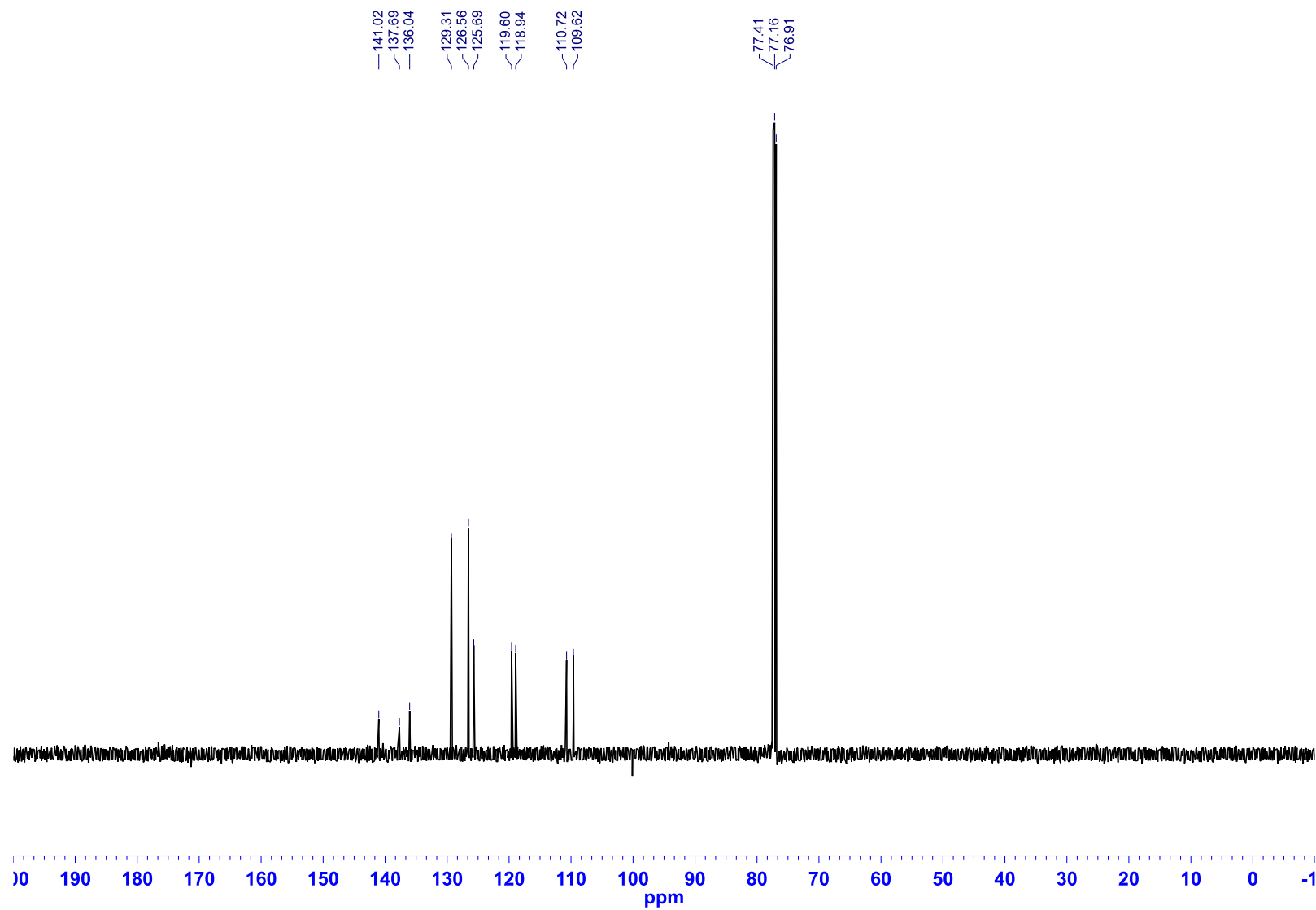
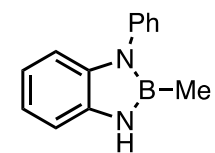
^{11}B NMR (128.4 MHz, CDCl_3) of 2-(3-chloropropyl)-1-methyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7g**)



^1H NMR (500.4 MHz, CDCl_3) of 2-methyl-1-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7h**)



^{13}C NMR (125.8 MHz, CDCl_3) of 2-methyl-1-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7h**)



^{11}B NMR (128.4 MHz, MeCN) of 2-methyl-1-phenyl-2,3-dihydro-1*H*-1,3,2-benzodiazaborole (**7h**)

