

Supporting Information

Boron-Dipyrromethene-Functionalized Hemilabile Ligands as “Turn-On” Fluorescent Probes for Coordination Changes in Weak-Link Approach Complexes

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Table of Contents

Absorbance and Emission Spectra	S3
Crystallographic Information	S6
Computational	S7
NMR Spectra	S12
References	S52

Absorbance and Emission Spectra.

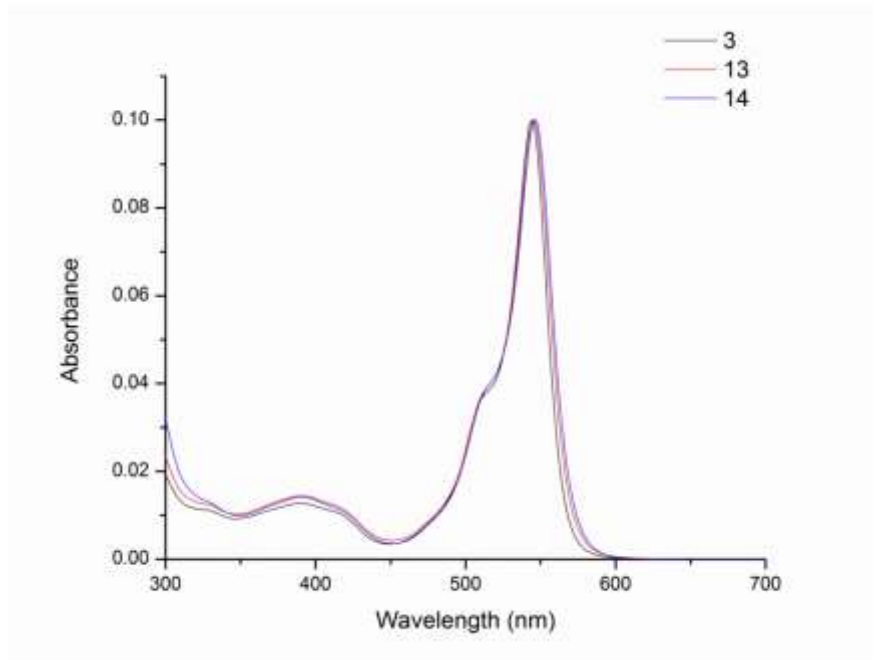


Figure S1. Absorbance spectra of 1.3×10^{-3} mM solutions of compounds **3**, **13** and **14** in CH_2Cl_2 .

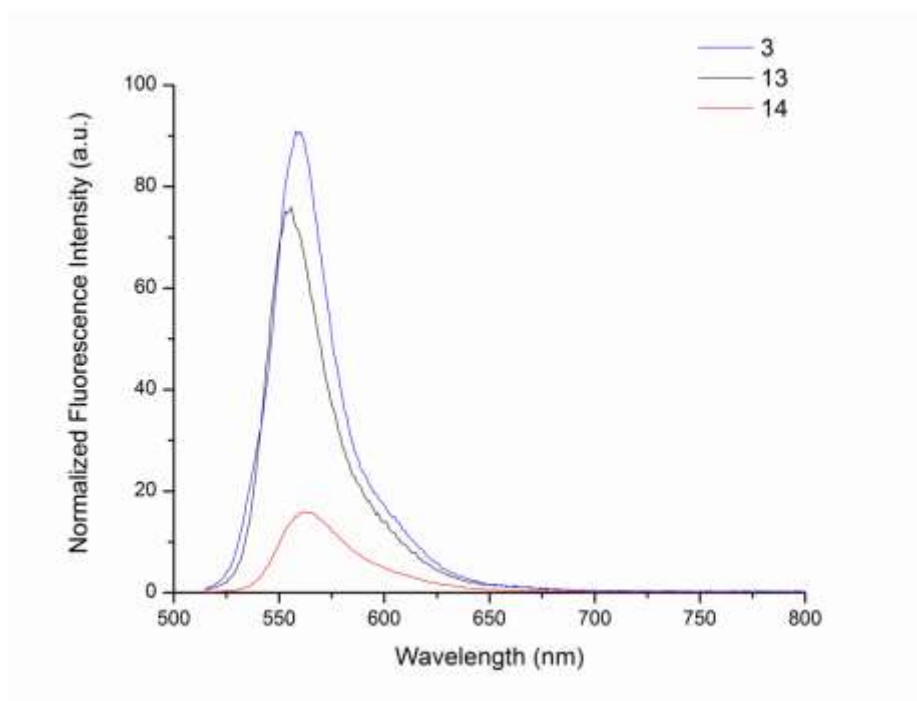


Figure S2. Fluorescence emission spectra of compounds **3**, **13** and **14** normalized relative to their respective quantum yields.

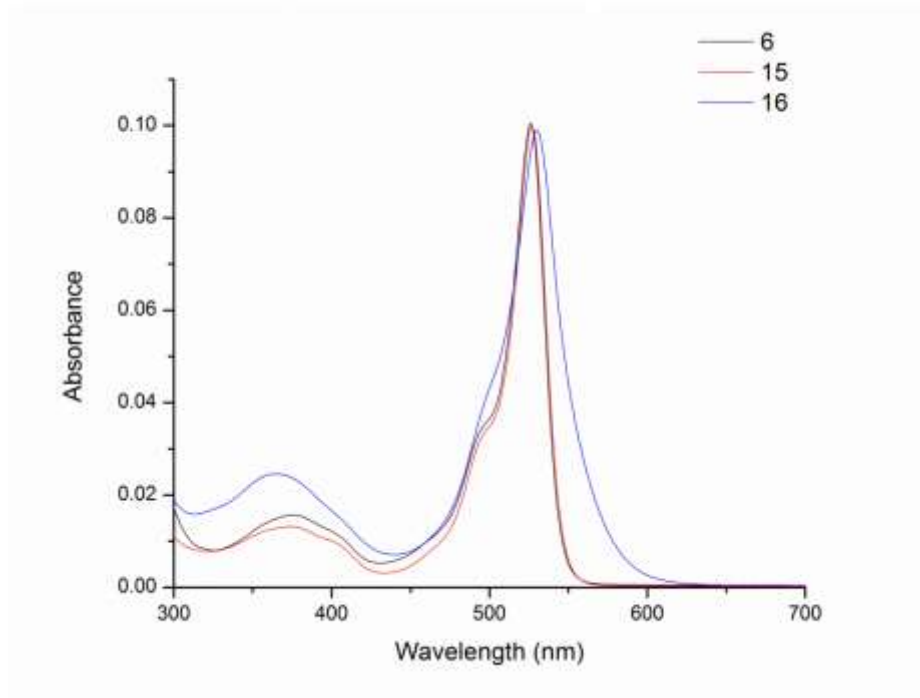


Figure S3. Absorbance spectra of 1.3×10^{-3} mM solutions of compounds **6**, **15** and **16** in CH_2Cl_2 .

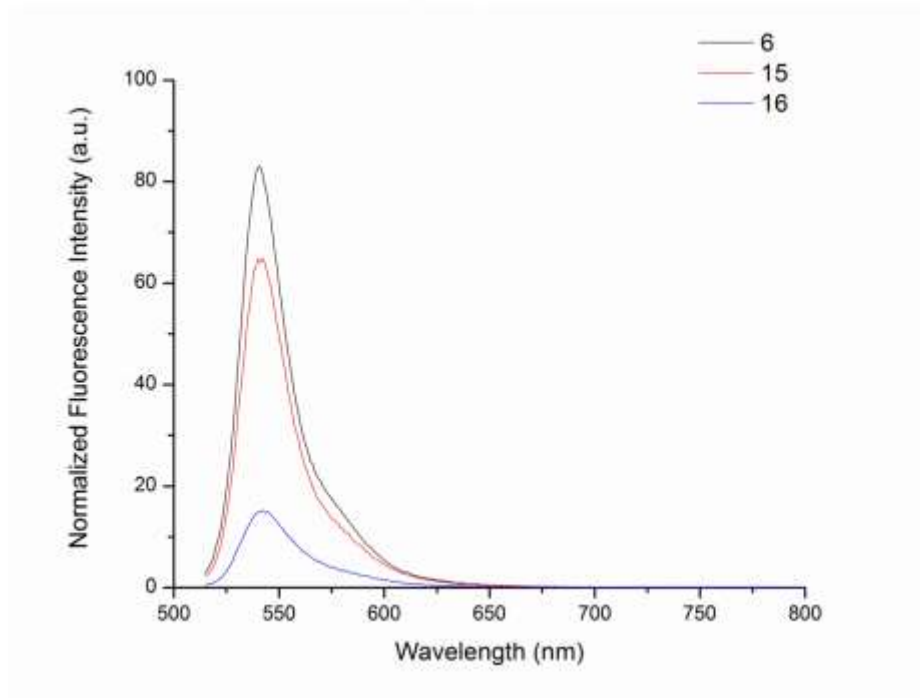


Figure S4. Fluorescence emission spectra of compounds **6**, **15** and **16** normalized relative to their respective quantum yields.

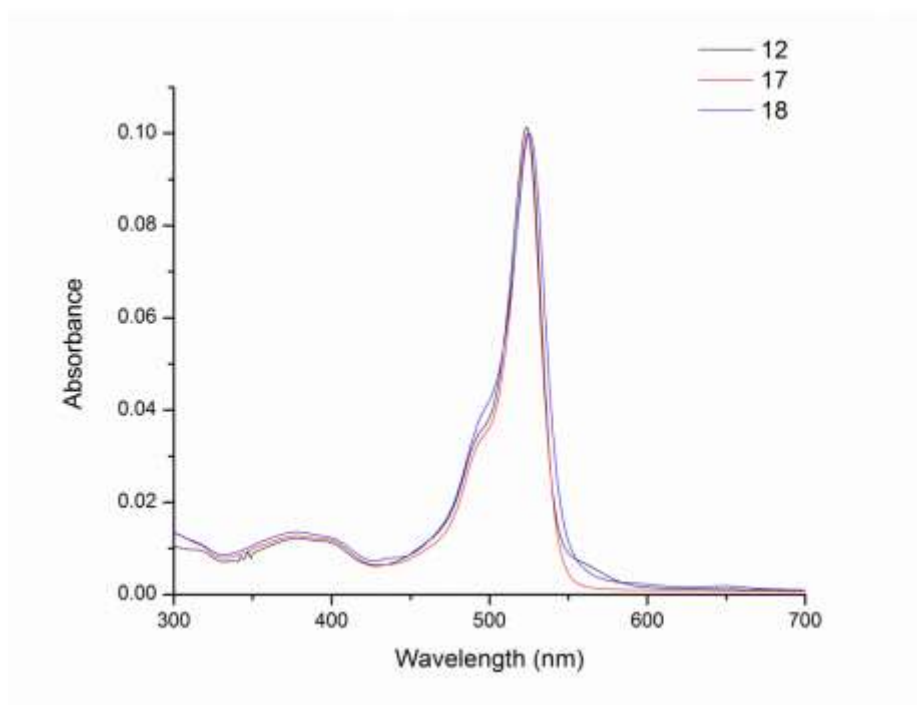


Figure S5. Absorbance spectra of 1.3×10^{-3} mM solutions of compounds **12**, **17** and **18** in CH_2Cl_2 .

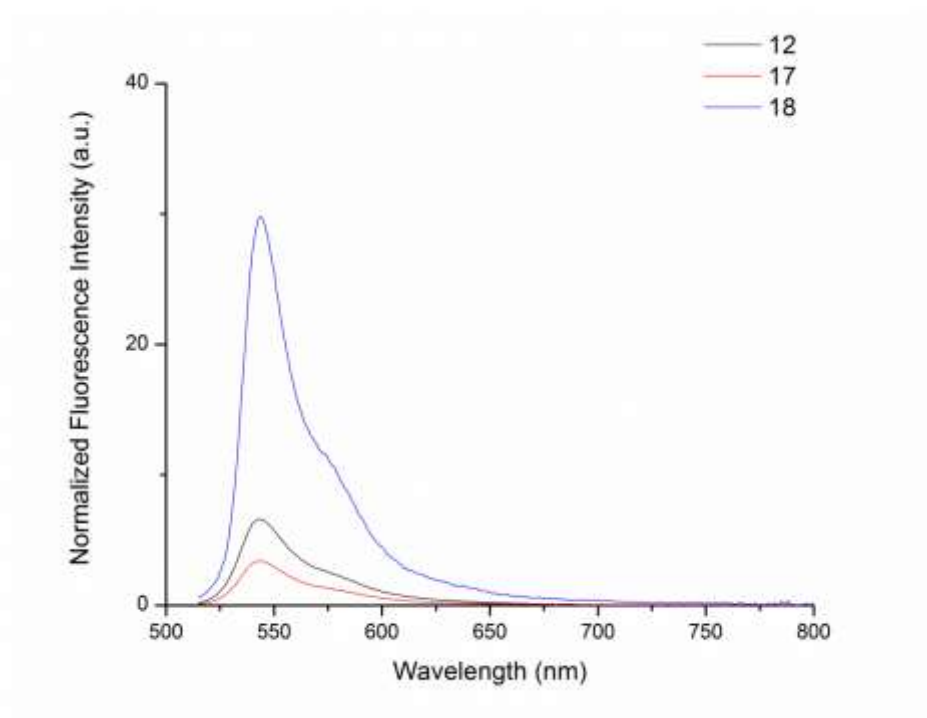


Figure S6. Fluorescence emission spectra of compounds **12**, **17** and **18** normalized relative to their respective quantum yields.

Table S1. Crystallographic Information.

	13	14
Empirical formula	C ₅₂ H ₅₃ BCl ₂ F ₆ N ₂ P ₂ PtS ₂	C ₅₂ H ₅₃ B ₃ F ₁₄ N ₂ P ₂ PtS ₂
Formula weight	1207.02	1325.56
Temperature	100 K	100(2) K
Wavelength	1.54178 Å, CuKα	1.54184 Å, CuKα
Crystal system, space group	Monoclinic, P 1 2 ₁ /n 1	Triclinic, P -1
Unit cell dimensions	a = 17.5965(6) Å b = 10.1996(4) Å β = 95.869(2)° c = 28.7552(9) Å	a = 13.4003(5) Å α = 86.516(2)° b = 17.1690(6) Å β = 88.842(2)° c = 25.3152(11) Å γ = 73.414(2)°
Volume	5133.9(3) Å ³	5571.6(4) Å ³
Z, Calculated density	4, 1.582 Mg/m ³	4, 1.580 Mg/m ³
Absorption coefficient	7.921 mm ⁻¹	6.695 mm ⁻¹
F(000)	2448	2640
Crystal size	0.548 x 0.046 x 0.041 mm	0.275 x 0.12 x 0.02 mm
Theta range for data collection	4.60 to 64.84°	2.690 to 68.056°
Limiting indices	-20 ≤ h ≤ 20, -7 ≤ k ≤ 11, -33 ≤ l ≤ 33	-16 ≤ h ≤ 16, -20 ≤ k ≤ 20, -0 ≤ l ≤ 30
Reflections collected / unique	33501/ 8503 [R(int) = 0.0442]	91587/ 19600 [R(int) = 0.0484]
Completeness to theta	64.84° (97.8%)	67.679° (97.0%)
Absorption correction	Multi-scan	Multi-scan
Max. and min. transmission	0.7526 and 0.5445	1 and 0.543391
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters ^{31b}	8503 / 0 / 620	19600 / 0 / 1384
Goodness-of-fit on F ² ^{31c}	1.424	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0703, wR2 = 0.1776	R1 = 0.0443, wR2 = 0.1124
R indices (all data)	R1 = 0.0798, wR2 = 0.1823	R1 = 0.0525, wR2 = 0.1209
Largest diff. peak and hole	1.687 and -1.477 e-/Å ³	3.099 and -1.406 e-/Å ³

Computational. DFT calculations were made using the Amsterdam Density Functional (ADF2009.01) suite on a 16-core Parallel Quantum Solutions (PQS) computational cluster. The structures prior to geometry optimization were based on coordinates extracted from the X-Ray crystal structure of **13**. Geometry optimizations of model ligand **A** and model ligand **B** were made without restraint in the ADF GUI using basis sets containing triple- ζ functions with one polarization function (TZP), and the local density approximations of Becke¹ and Perdew². This was followed by single point calculations using triple- ζ functions with two polarization functions (TZ2P) and the B3LYP local density approximations of Becke(B3)³, Lee-Yang-Parr (LYP)⁴, Vosko-Wilk-Nusair (VWN)⁵, and the assembly of Stephens et al⁶. Kohn-Sham representations of frontier orbitals were generated by the ADF 2009.01 GUI.

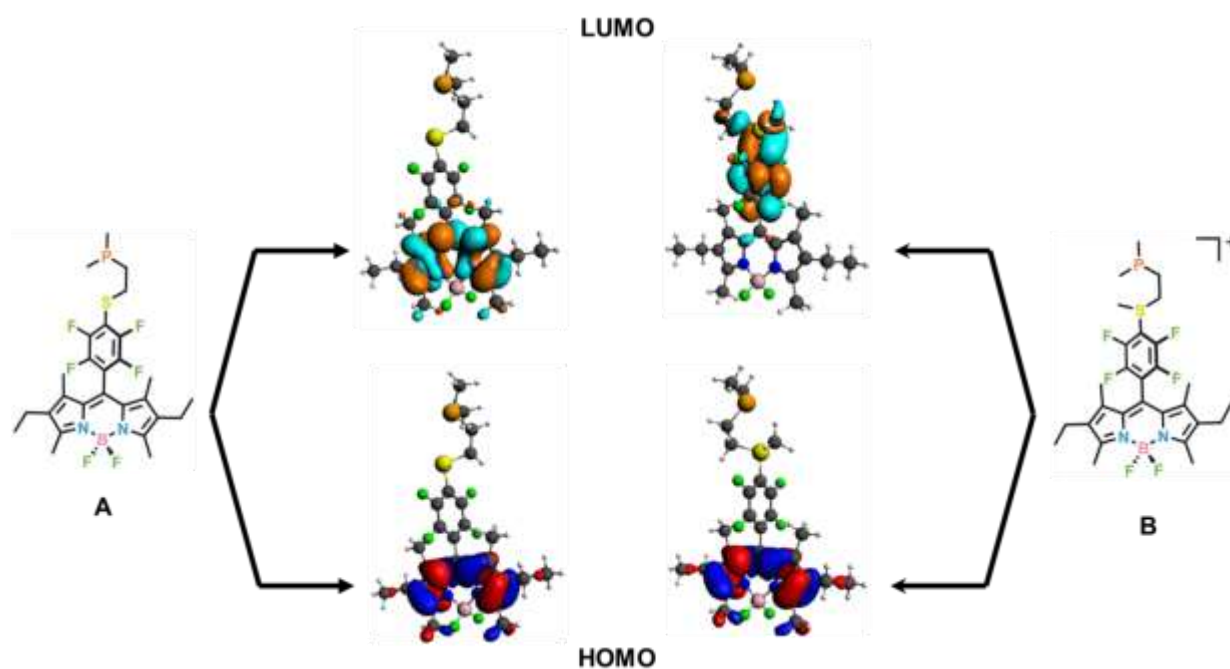


Figure S-X. Kohn-Sham representations of frontier molecular orbitals of model structure **A** and **B**.

We performed theoretical modeling on P,S-Bodipy ligands using DFT-B3LYP theory to confirm the hypothesis that PeT decay pathways are responsible for the decrease in fluorescence observed in closed complexes **14** and **16**, relative to their semi-open analogs **13** and **15**. The model ligands **A** and **B** display a dimethylphosphine moiety, rather than a diphenylphosphine group, given that substitution made the geometry optimization process simpler. Single-point energy calculations show that the meso substituent-centered, frontier orbitals in the model ligand are lowered in energy upon depletion of electron density on the sulfur moiety via methylation. Thus, while the meso substituent-centered LUMO lies too high in energy to interact with the

Bodipy excited state in the neutral ligand, its energy is lowered upon methylation to the extent that PeT can occur.

Table S2. Geometry optimized coordinates for model ligands **A** and **B**.

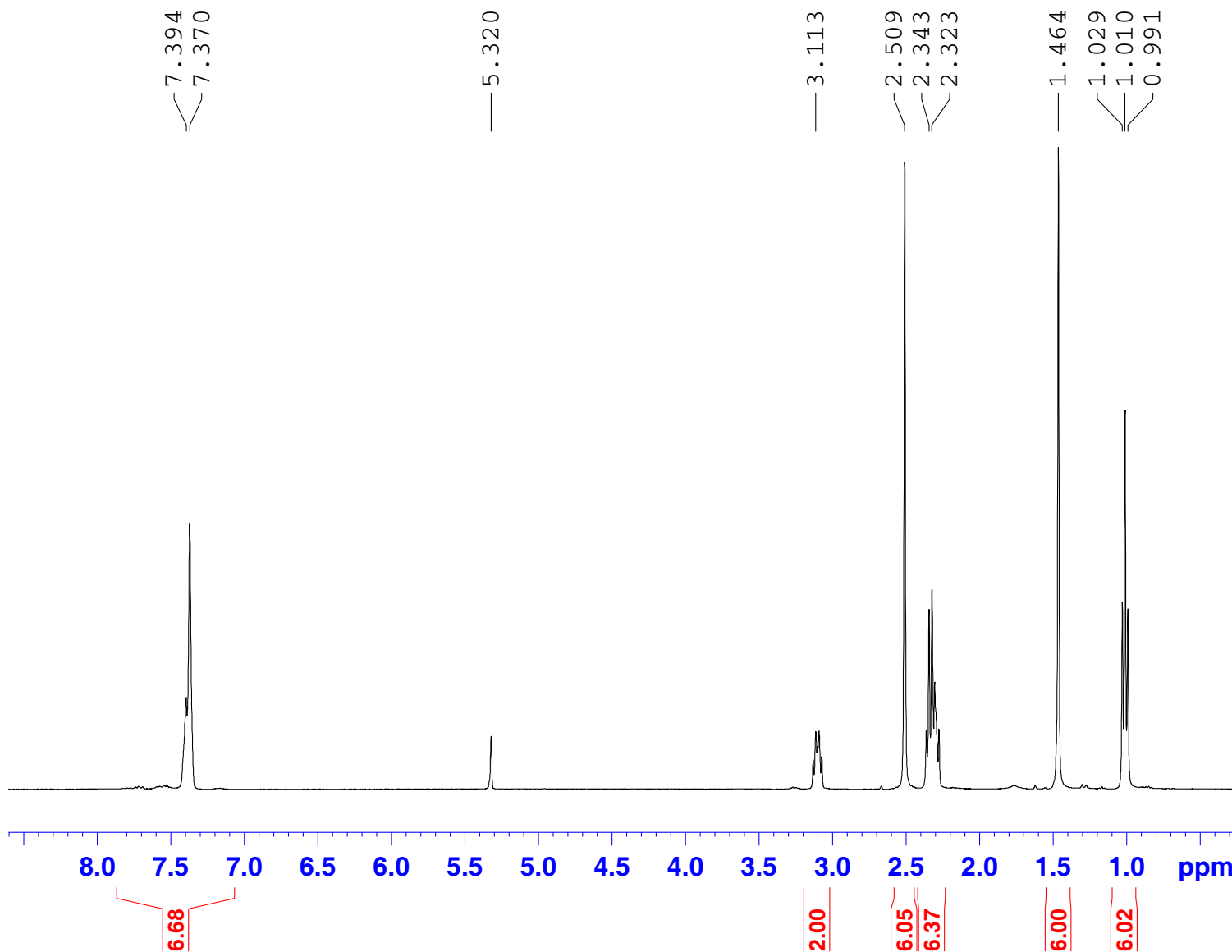
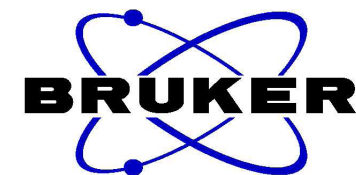
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	Atoms	Coordinates			Charge		Atomic Mass
		x	y	z	Nuclear	Core	
1	H	17.7108	5.9128	11.2593	1	1	1.0078
2	H	20.3081	-3.4662	14.2282	1	1	1.0078
3	H	17.2326	4.553	12.3054	1	1	1.0078
4	C	18.2204	-0.7184	14.94	6	6	12
5	C	18.9904	-5.6425	11.2522	6	6	12
6	C	18.3595	-0.7013	16.3272	6	6	12
7	C	18.8536	1.785	10.0808	6	6	12
8	F	16.9696	-0.7806	14.424	9	9	18.9984
9	C	19.02	2.6652	11.1852	6	6	12
10	H	17.7117	1.7059	8.2728	1	1	1.0078
11	C	19.0842	0.502	11.8999	6	6	12
12	C	19.3504	-3.8077	13.8082	6	6	12
13	H	19.5339	-3.3988	8.1354	1	1	1.0078
14	C	19.3269	-0.6944	14.0827	6	6	12
15	H	19.3606	-4.904	13.8257	1	1	1.0078
16	H	18.556	-3.4744	14.4918	1	1	1.0078
17	C	19.0289	4.1698	11.113	6	6	12
18	N	18.8986	0.5009	10.5129	7	7	14.0031
19	S	19.8836	-0.6306	18.702	16	16	31.9721
20	C	19.1636	-0.7171	12.5973	6	6	12
21	C	20.7279	-0.6095	16.0842	6	6	12
22	H	19.73	4.5658	11.8633	1	1	1.0078
23	H	18.3166	-5.9913	10.4544	1	1	1.0078
24	H	18.5606	-6.0285	12.1887	1	1	1.0078
25	H	21.0725	-5.966	11.8481	1	1	1.0078
26	H	19.4329	4.4858	10.1392	1	1	1.0078
27	C	17.6463	4.8163	11.3214	6	6	12
28	C	19.3598	2.4076	13.7188	6	6	12
29	H	20.3252	2.0994	14.1471	1	1	1.0078
30	H	18.5728	2.0725	14.4104	1	1	1.0078
31	H	19.3408	3.504	13.7084	1	1	1.0078
32	C	20.3852	-6.2618	11.0425	6	6	12
33	H	20.8278	-5.9278	10.0931	1	1	1.0078

34	F	21.9795	-0.5494	16.601	9	9	18.9984
35	F	21.7037	-0.6196	13.936	9	9	18.9984
36	F	17.2318	-0.7809	17.0832	9	9	18.9984
37	B	18.7465	-0.758	9.6142	5	5	11.0093
38	H	20.3296	-7.3603	11.0257	1	1	1.0078
39	F	19.7527	-0.7802	8.6288	9	9	18.9984
40	F	17.4829	-0.7586	8.9886	9	9	18.9984
41	C	19.0742	-1.9545	11.9363	6	6	12
42	C	19.1425	-3.3131	12.4078	6	6	12
43	C	18.9858	-4.1369	11.2856	6	6	12
44	C	18.6555	2.1295	8.643	6	6	12
45	H	18.6378	3.2153	8.5016	1	1	1.0078
46	H	17.7961	-3.1378	8.287	1	1	1.0078
47	H	18.4848	-4.752	8.6334	1	1	1.0078
48	C	18.5911	0.5646	19.292	6	6	12
49	C	19.6175	-0.6236	16.9463	6	6	12
50	H	19.4574	1.6996	8.0274	1	1	1.0078
51	C	18.8335	-3.2867	10.155	6	6	12
52	N	18.8858	-1.9916	10.5501	7	7	14.0031
53	C	18.6479	-3.6728	8.7262	6	6	12
54	H	16.9303	4.4723	10.5614	1	1	1.0078
55	C	20.5838	-0.6484	14.6971	6	6	12
56	C	19.1594	1.8724	12.3322	6	6	12
57	C	19.0285	1.1781	20.6229	6	6	12
58	P	19.3933	-0.0767	21.9737	15	15	30.9738
59	C	17.6567	-0.5425	22.4629	6	6	12
60	C	19.7944	1.1185	23.3452	6	6	12
61	H	19.9015	0.5613	24.2867	1	1	1.0078
62	H	19.019	1.8902	23.4734	1	1	1.0078
63	H	20.7566	1.6063	23.1349	1	1	1.0078
64	H	17.6985	-1.1604	23.3713	1	1	1.0078
65	H	17.1985	-1.1541	21.673	1	1	1.0078
66	H	17.0213	0.336	22.6574	1	1	1.0078
67	H	18.2413	1.8739	20.9616	1	1	1.0078
68	H	19.9497	1.7625	20.4755	1	1	1.0078
69	H	17.6347	0.0397	19.3862	1	1	1.0078
70	H	18.49	1.3396	18.5229	1	1	1.0078

Model Complex B							
	Atoms	Coordinates			Charge		Atomic Mass
		x	y	z	Nuclear	Core	
1	H	17.7629	5.9144	11.3548	1	1	1.0078
2	H	20.2409	-3.4607	14.2856	1	1	1.0078
3	H	17.2227	4.5469	12.3587	1	1	1.0078
4	C	18.1316	-0.9251	14.9312	6	6	12
5	C	19.065	-5.6519	11.1852	6	6	12
6	C	18.2099	-0.9146	16.3216	6	6	12
7	C	18.9281	1.8047	10.1775	6	6	12
8	F	16.9257	-1.0969	14.3682	9	9	18.9984
9	C	19.064	2.6662	11.3058	6	6	12
10	H	17.8724	1.7187	8.3207	1	1	1.0078
11	C	19.1086	0.4884	11.9761	6	6	12
12	C	19.3513	-3.8801	13.792	6	6	12
13	H	19.6809	-3.3578	8.1479	1	1	1.0078
14	C	19.2728	-0.7577	14.1283	6	6	12
15	H	19.4839	-4.9678	13.7659	1	1	1.0078
16	H	18.4788	-3.6785	14.4338	1	1	1.0078
17	C	19.0806	4.1714	11.2579	6	6	12
18	N	18.9603	0.514	10.5869	7	7	14.0031
19	S	19.6425	-0.6859	18.7478	16	16	31.9721
20	C	19.1669	-0.7515	12.6389	6	6	12
21	C	20.5899	-0.5631	16.1799	6	6	12
22	H	19.7436	4.5544	12.0483	1	1	1.0078
23	H	18.3821	-5.9825	10.3879	1	1	1.0078
24	H	18.6497	-6.0676	12.1154	1	1	1.0078
25	H	21.16	-5.9788	11.7405	1	1	1.0078
26	H	19.5369	4.4983	10.3117	1	1	1.0078
27	C	17.6899	4.8185	11.401	6	6	12
28	C	19.3259	2.3707	13.8383	6	6	12
29	H	20.322	2.1509	14.2541	1	1	1.0078
30	H	18.5709	1.9597	14.5256	1	1	1.0078
31	H	19.2093	3.4604	13.8499	1	1	1.0078
32	C	20.4615	-6.2533	10.9369	6	6	12
33	H	20.8881	-5.8904	9.9913	1	1	1.0078
34	F	21.7925	-0.3854	16.7641	9	9	18.9984
35	F	21.6287	-0.4243	14.08	9	9	18.9984

36	F	17.0805	-1.0818	17.0571	9	9	18.9984
37	B	18.8179	-0.7285	9.6538	5	5	11.0093
38	H	20.4102	-7.3502	10.8878	1	1	1.0078
39	F	19.8369	-0.7284	8.6913	9	9	18.9984
40	F	17.5612	-0.7155	9.0279	9	9	18.9984
41	C	19.0991	-1.9797	11.9578	6	6	12
42	C	19.1701	-3.3502	12.3994	6	6	12
43	C	19.0479	-4.1482	11.2582	6	6	12
44	C	18.7756	2.179	8.7437	6	6	12
45	H	18.7114	3.2656	8.6283	1	1	1.0078
46	H	17.9448	-3.0631	8.245	1	1	1.0078
47	H	18.5884	-4.6981	8.5816	1	1	1.0078
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49	C	19.4405	-0.7268	16.9714	6	6	12
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51	C	18.9157	-3.27	10.1413	6	6	12
52	N	18.9477	-1.9854	10.5686	7	7	14.0031
53	C	18.7692	-3.6249	8.7021	6	6	12
54	H	17.0136	4.4879	10.6002	1	1	1.0078
55	C	20.4983	-0.5836	14.7849	6	6	12
56	C	19.1677	1.8527	12.4381	6	6	12
57	C	18.8395	1.3238	20.4987	6	6	12
58	P	19.5136	0.2056	21.8543	15	15	30.9738
59	C	18.0313	0.0178	22.9563	6	6	12
60	C	20.5488	1.4017	22.8162	6	6	12
61	H	20.9072	0.9005	23.7259	1	1	1.0078
62	H	19.9878	2.3027	23.1041	1	1	1.0078
63	H	21.4279	1.6899	22.2243	1	1	1.0078
64	H	18.3238	-0.5651	23.841	1	1	1.0078
65	H	17.2378	-0.5426	22.4416	1	1	1.0078
66	H	17.6327	0.9888	23.2851	1	1	1.0078
67	H	18.0224	1.9679	20.8613	1	1	1.0078
68	H	19.6552	1.985	20.1703	1	1	1.0078
69	H	17.4302	-0.0826	19.5404	1	1	1.0078
70	H	18.1122	1.1337	18.4263	1	1	1.0078
71	C	19.0383	-2.3368	19.2464	6	6	12
72	H	19.7119	-3.0611	18.7725	1	1	1.0078
73	H	18.0045	-2.4782	18.9188	1	1	1.0078
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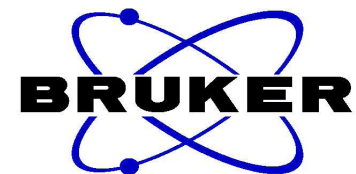
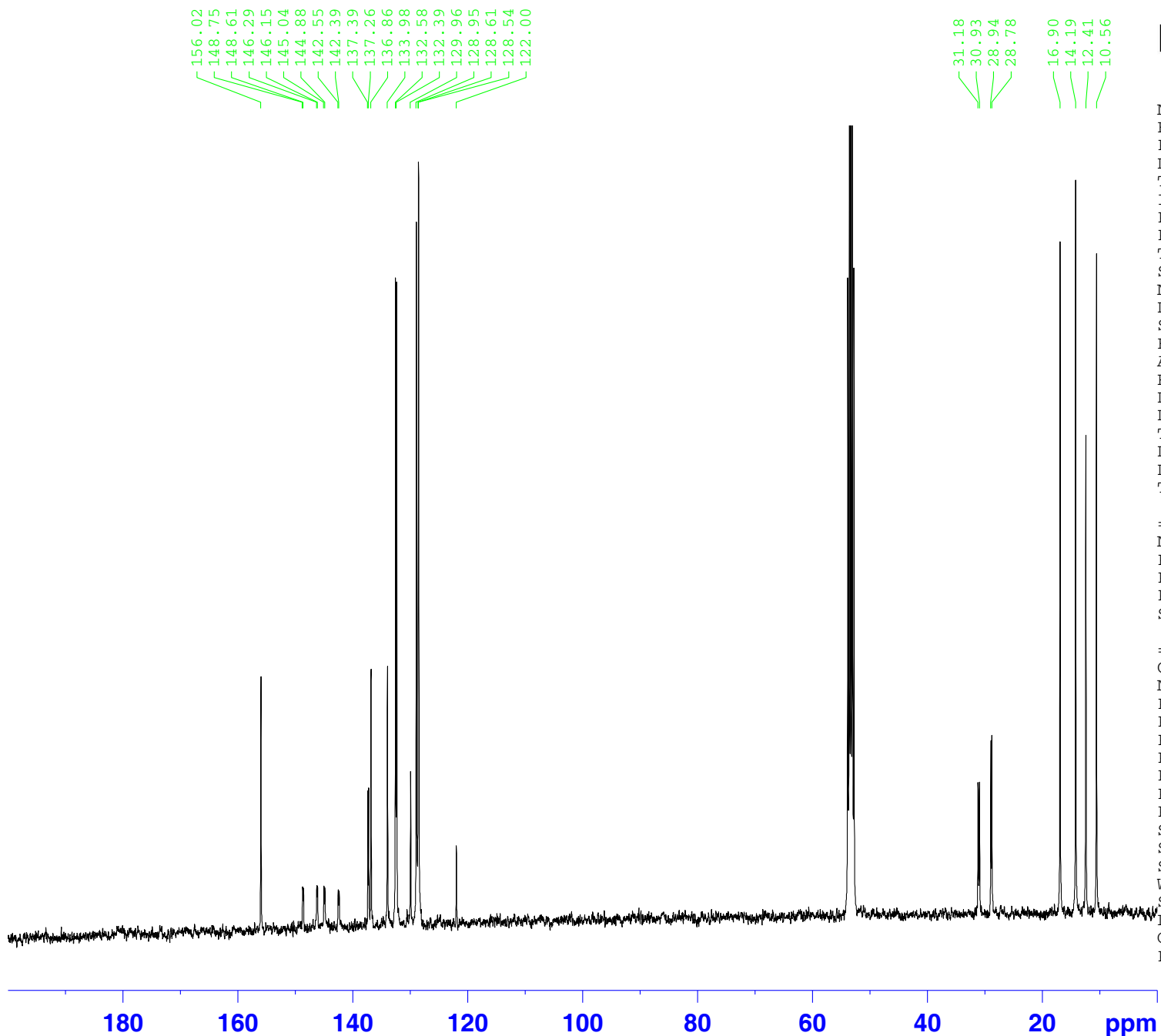
¹H P,S-Bodipy (3)



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$^{13}\text{C}\{^1\text{H}\}$ P,S-Bodipy (3)



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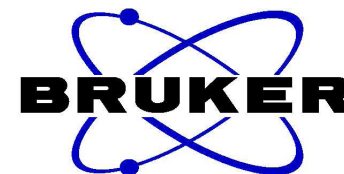
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PL12W     0.48524728 W
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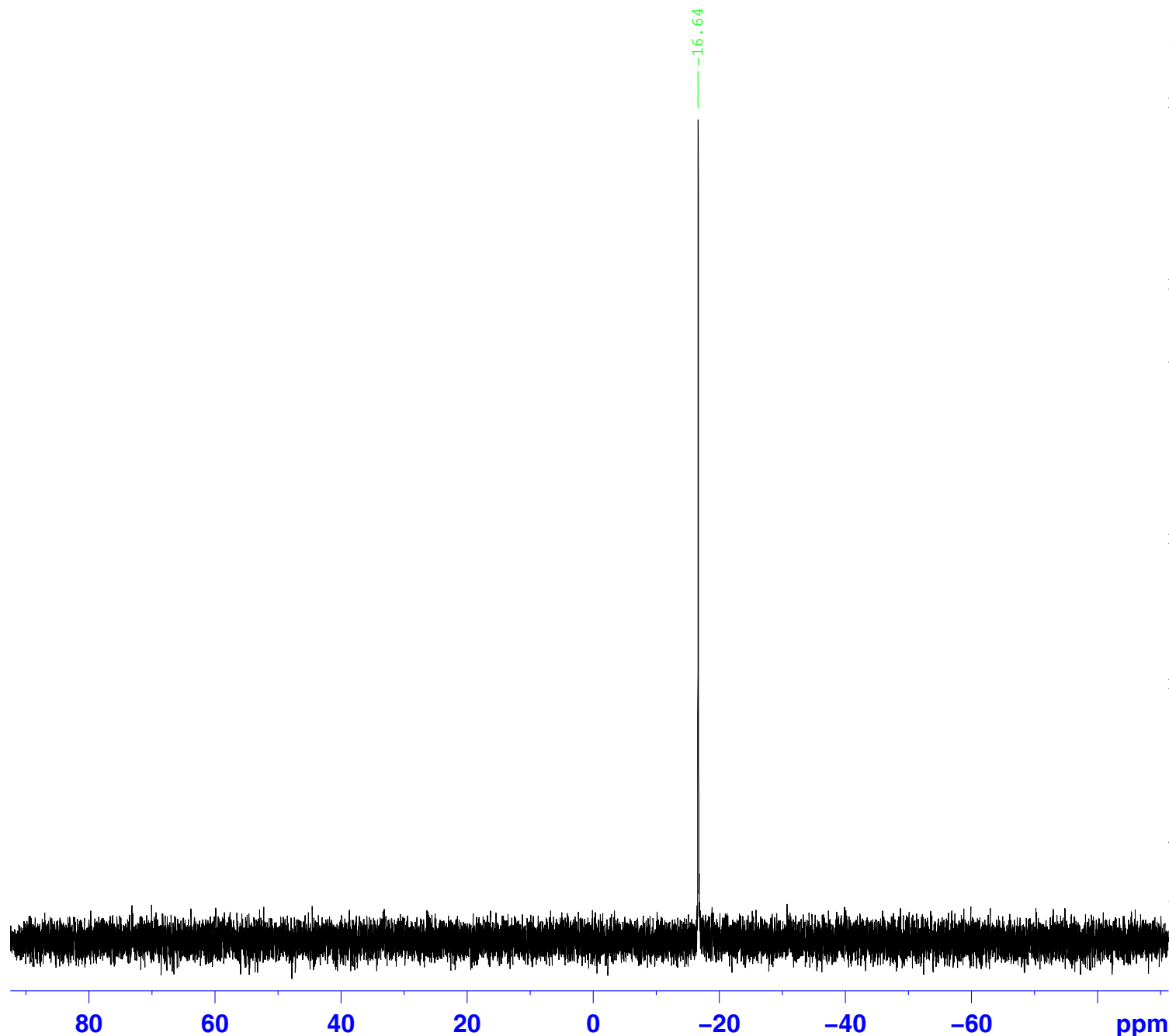
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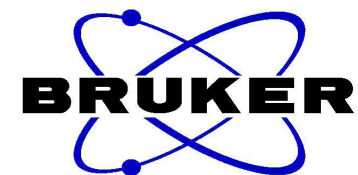
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TE 303.4 K
D1 0.60000002 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
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PL1 3.00 dB
PL1W 12.96693134 W
SFO1 161.9755930 MHz

===== CHANNEL f2 =====
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PL2 -0.50 dB
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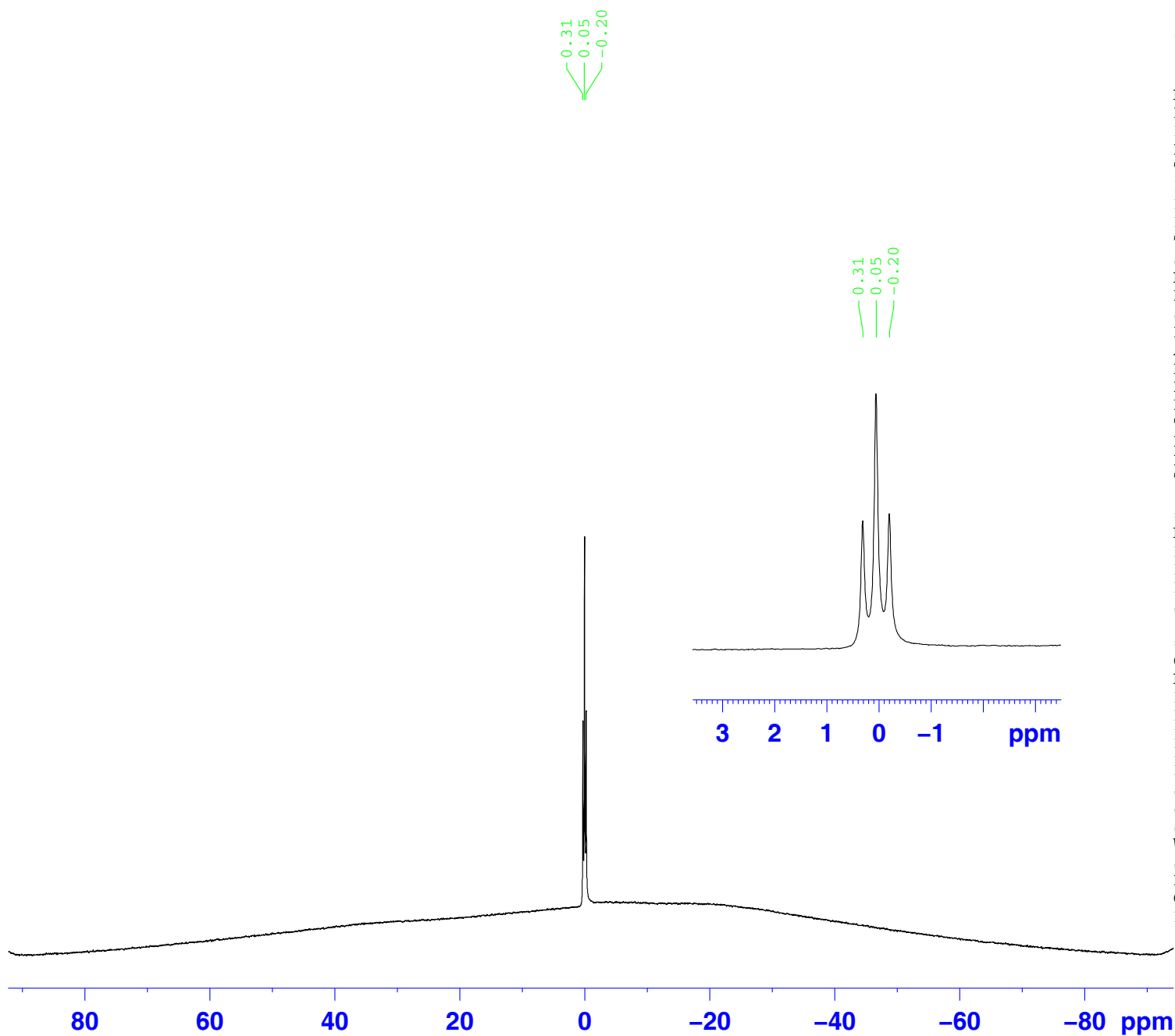
11B{1H} PS-Bodipy (3)



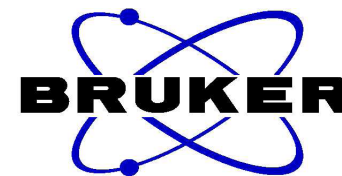
NAME Paper
EXPNO 5
PROCNO 1
Date_ 20120611
Time 15.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 65536
SOLVENT CD2Cl2
NS 72
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 575
DW 20.800 usec
DE 6.50 usec
TE 303.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 12.80 usec
PL1 1.00 dB
PL1W 17.63811874 W
SFO1 128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.20 dB
PL2W 14.48648834 W
PL12W 0.49086621 W
SFO2 400.1316005 MHz
SI 32768
SF 128.3776824 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

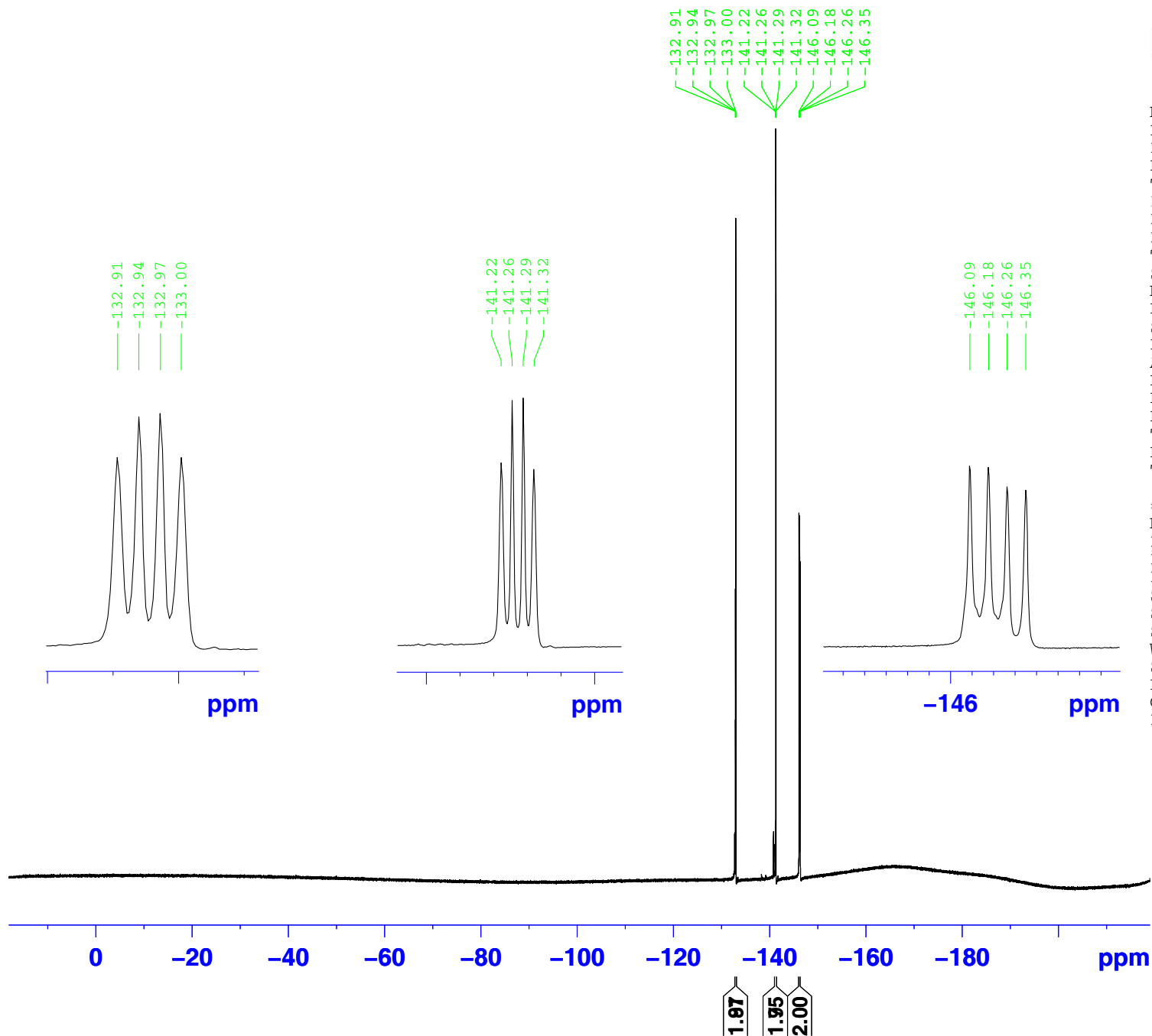


¹⁹F P,S-Bodipy (3)



NAME Paper
 EXPNO 3
 PROCNO 1
 Date_ 20120611
 Time 15.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg
 TD 131072
 SOLVENT CD2C12
 NS 84
 DS 0
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340532 sec
 RG 724
 DW 5.600 usec
 DE 6.50 usec
 TE 303.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 14.75 usec
 PL1 -3.20 dB
 PL1W 18.89306831 W
 SFO1 376.4607164 MHz
 SI 65536
 SF 376.4985425 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

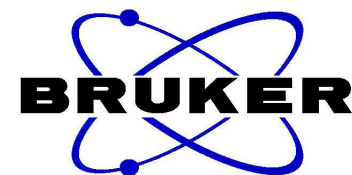


¹H P,S-Bodipy (6)

7.428
7.422
7.410
7.404
7.364
7.359
7.339
7.197
7.177

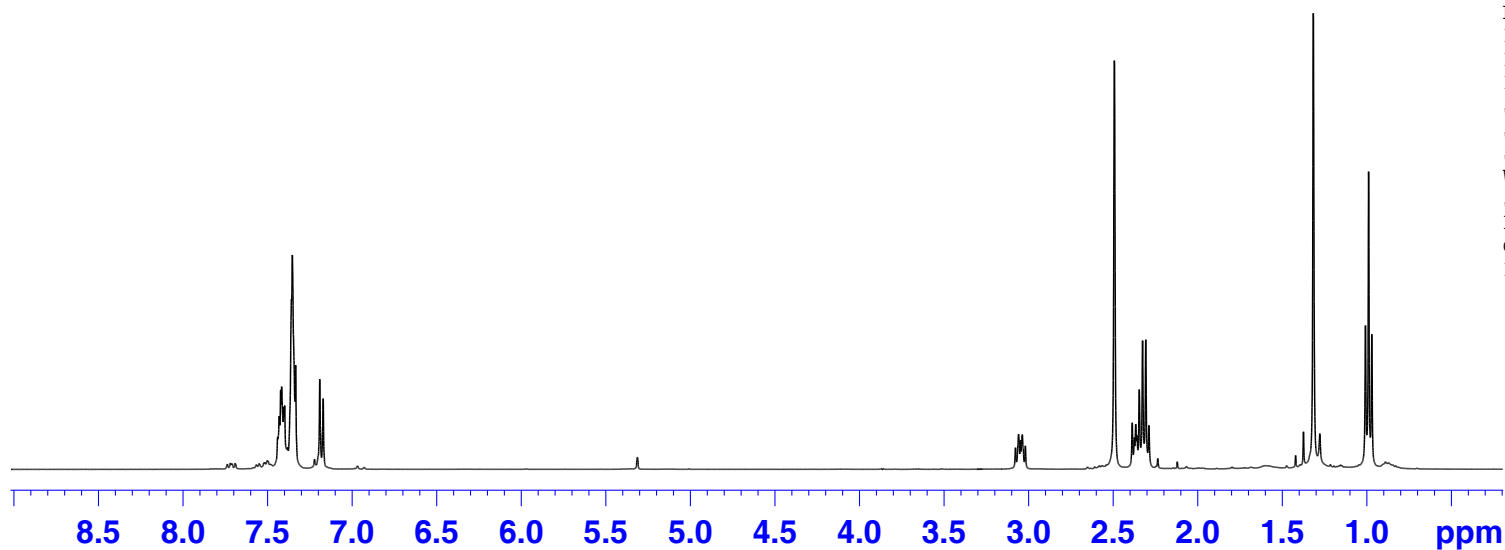
— 5.320

3.066
3.044
2.499
2.394
2.373
2.352
2.333
2.314
2.295
1.323
1.015
0.996
0.978



NAME Paper
EXPNO 40
PROCNO 1
Date_ 20121203
Time 22.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -0.65 dB
PL1W 14.99557495 W
SFO1 400.1624712 MHz
SI 32768
SF 400.1600143 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



12.83

2.09

2.00

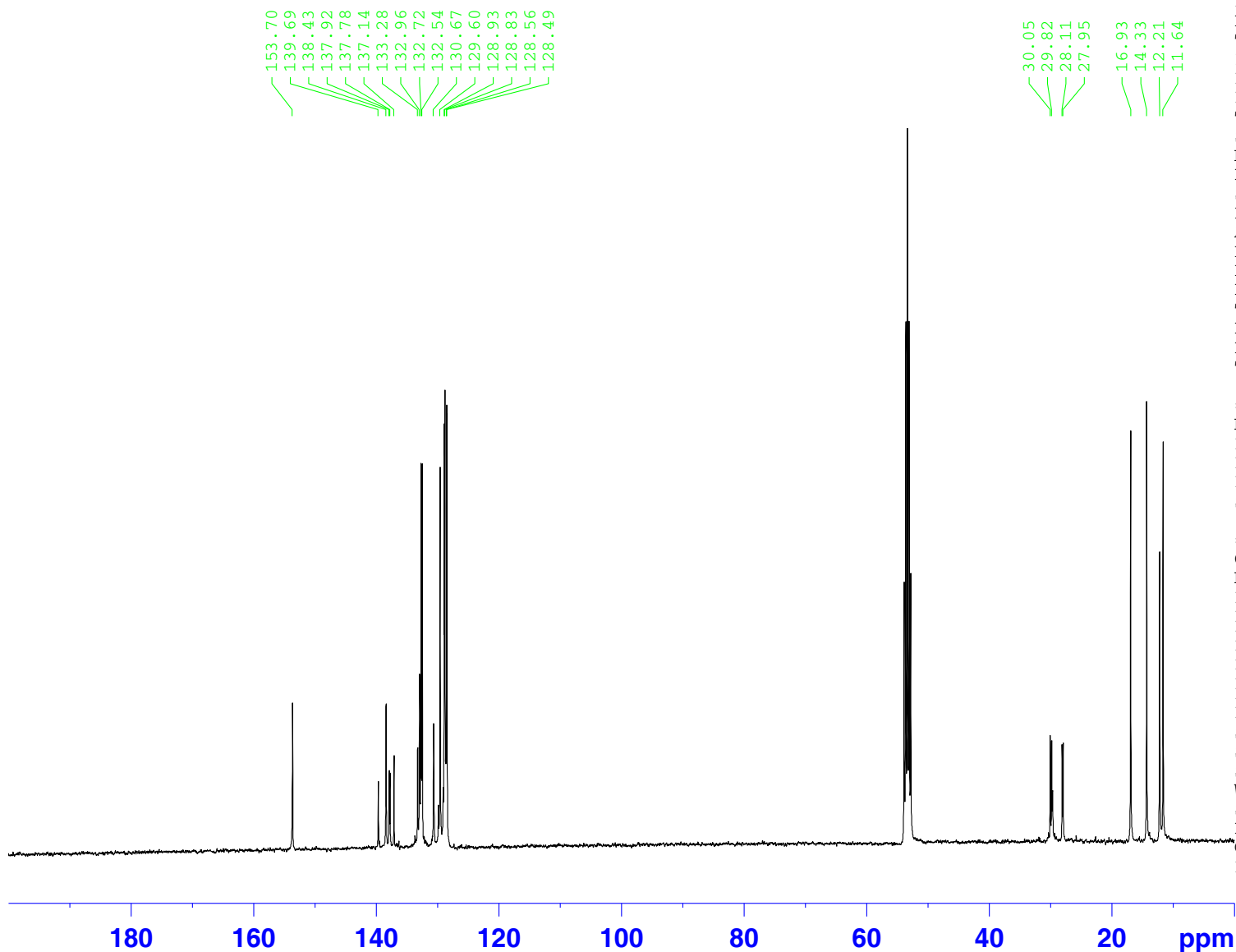
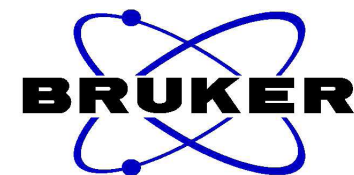
6.06

6.52

6.14

6.49

$^{13}\text{C}\{^1\text{H}\}$ P,S-Bodipy (6)



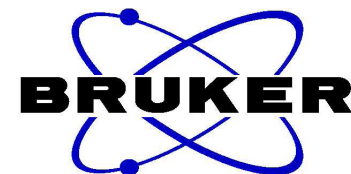
NAME Paper
EXPNO 44
PROCNO 1
Date_ 20121204
Time 3.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 6000
DS 0
SWH 40760.871 Hz
FIDRES 0.621962 Hz
AQ 0.8039582 sec
RG 406
DW 12.267 usec
DE 6.50 usec
TE 303.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^{13}C
P1 9.98 usec
PL1 -3.35 dB
PL1W 83.66055298 W
SFO1 100.6303741 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ^1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.25 dB
PL13 16.25 dB
PL2W 14.48648834 W
PL12W 0.48524728 W
PL13W 0.30617034 W
SFO2 400.1616006 MHz
SI 32768
SF 100.6203145 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

$^{31}\text{P}\{^1\text{H}\}$ P,S-Bodipy (6)

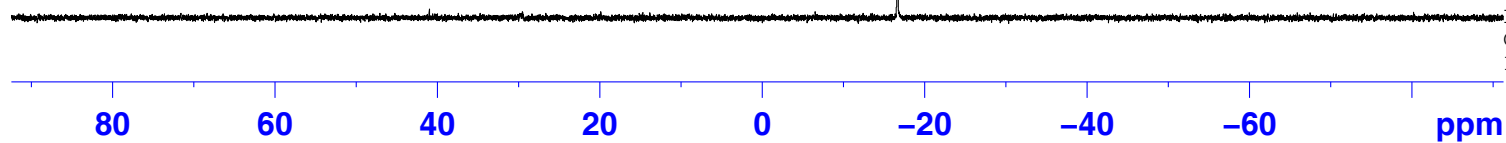
-16.66



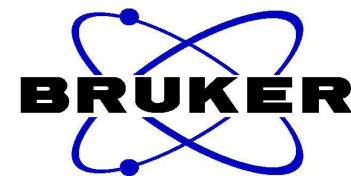
NAME Paper
EXPNO 43
PROCNO 1
Date_ 20121203
Time 23.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2C12
NS 7
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 2050
DW 7.800 usec
DE 6.50 usec
TE 303.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 14.90 usec
PL1 1.95 dB
PL1W 16.51342773 W
SFO1 161.9796378 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.25 dB
PL13 16.25 dB
PL2W 14.48648834 W
PL12W 0.48524728 W
PL13W 0.30617034 W
SFO2 400.1616006 MHz
SI 32768
SF 161.9876419 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



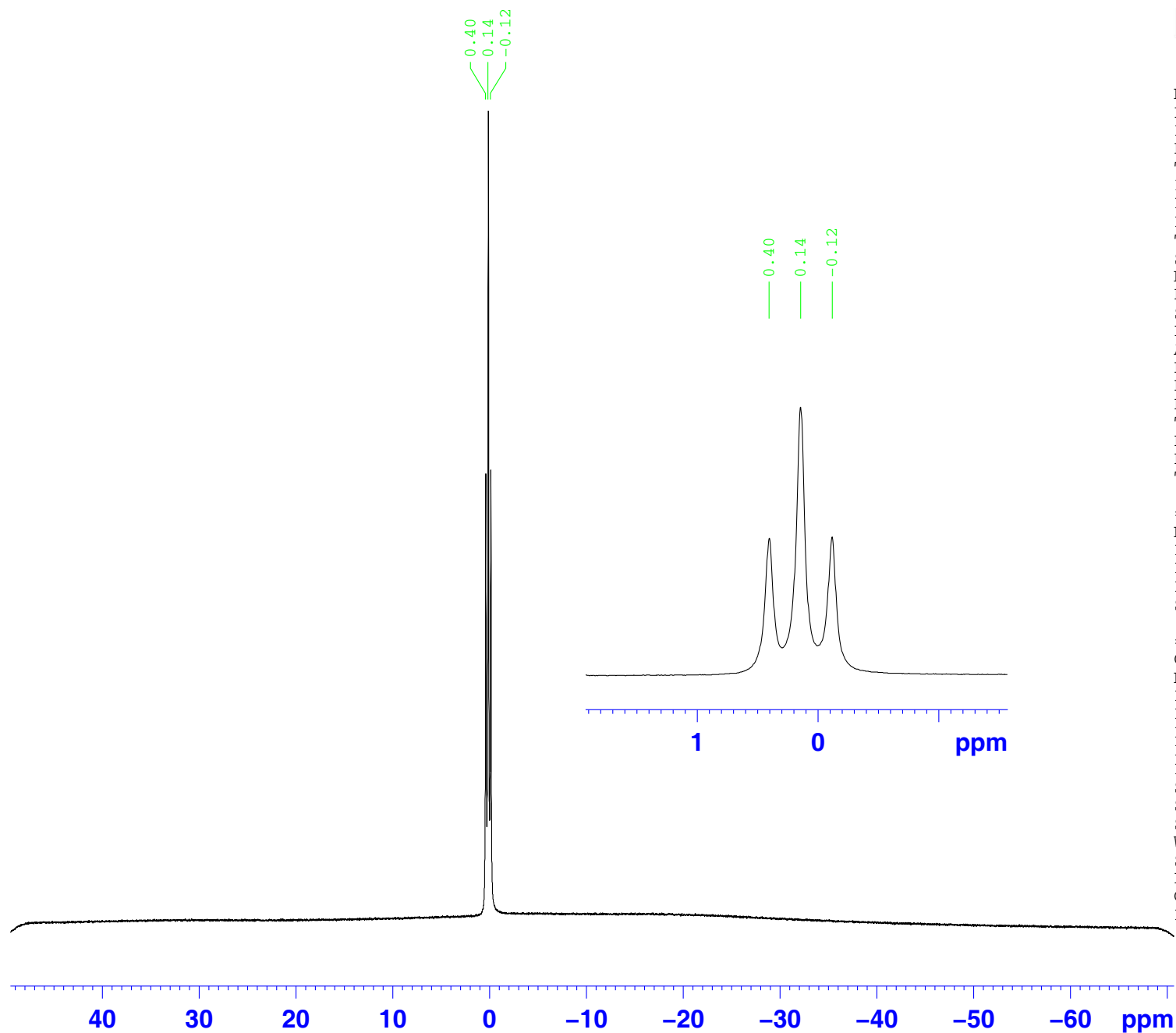
11B{1H} P,S-Bodipy (6)



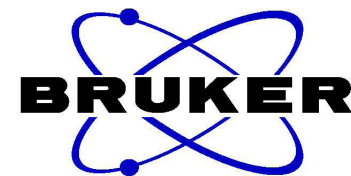
NAME Paper
EXPNO 41
PROCNO 1
Date_ 20121203
Time 22.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 16384
SOLVENT CD2C12
NS 73
DS 0
SWH 15432.099 Hz
FIDRES 0.941901 Hz
AQ 0.5308916 sec
RG 512
DW 32.400 usec
DE 6.50 usec
TE 303.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 12.80 usec
PL1 1.00 dB
PL1W 17.63811874 W
SFO1 128.3859468 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.25 dB
PL2W 14.48648834 W
PL12W 0.48524728 W
SFO2 400.1616006 MHz
SI 32768
SF 128.3873079 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹⁹F P,S-Bodipy (6)



NAME Paper
EXPNO 42
PROCNO 1
Date_ 20121203
Time 23.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CD2C12
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 2050
DW 5.600 usec
DE 6.50 usec
TE 303.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 19.50 usec
PL1 -4.00 dB
PL1W 22.71446419 W
SFO1 376.4889418 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 112.00 usec
PL2 -4.00 dB
PL12 18.00 dB
PL2W 32.43120575 W
PL12W 0.20462708 W
SFO2 400.1616006 MHz
SI 65536
SF 376.5267818 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

-146.06
-146.15
-146.23
-146.32

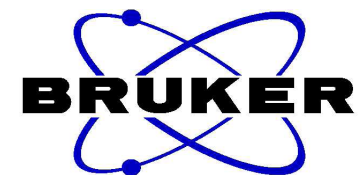
-146.06
-146.15
-146.23
-146.32

-146

ppm

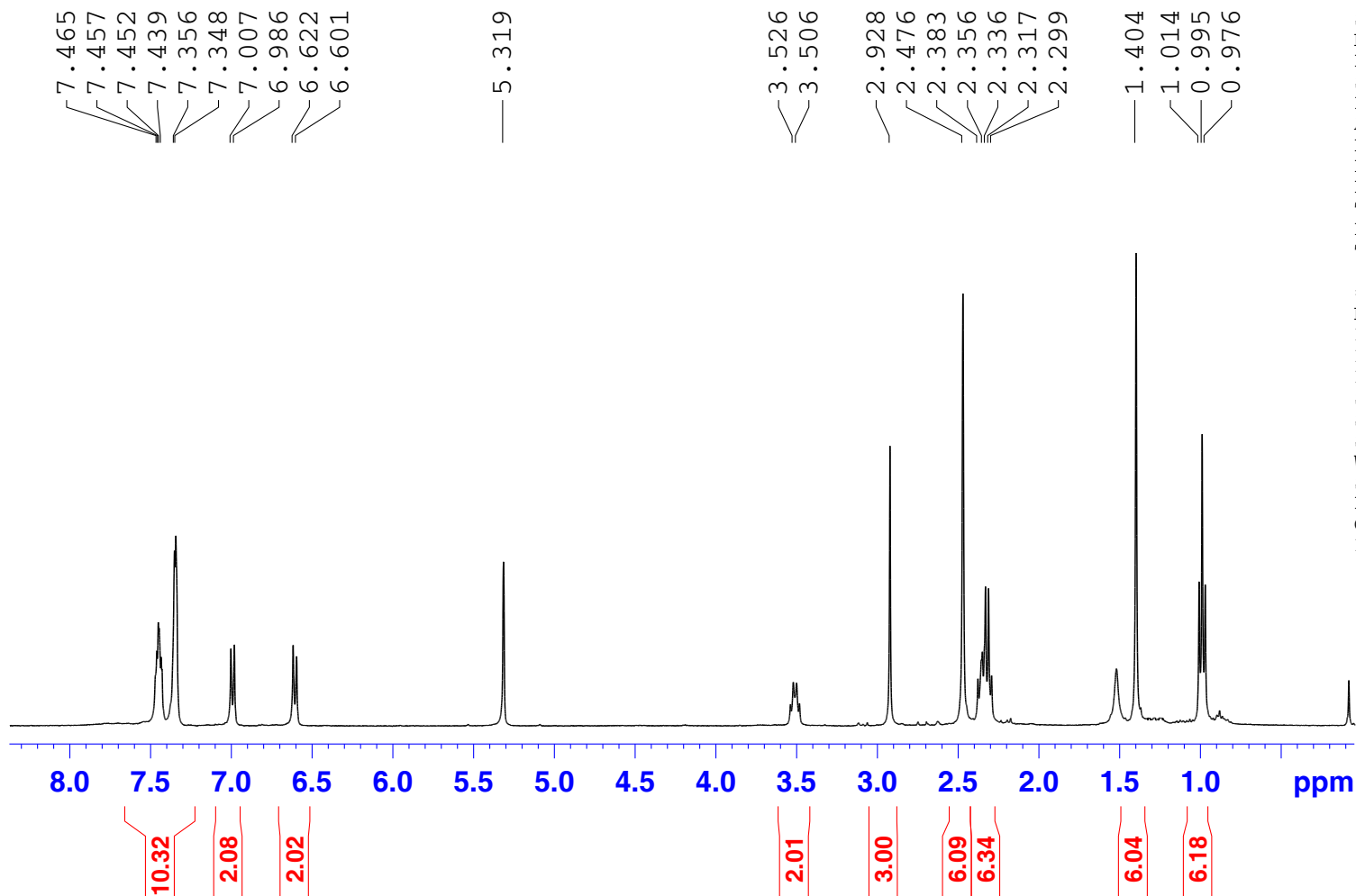
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

¹H P,N-Bodipy (12)



NAME Paper
EXPNO 30
PROCNO 1
Date_ 20121203
Time 12.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 256
DW 60.800 usec
DE 6.50 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -0.65 dB
PL1W 14.99557495 W
SFO1 400.1624712 MHz
SI 32768
SF 400.1600143 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C{¹H} P,N-Bodipy (12)

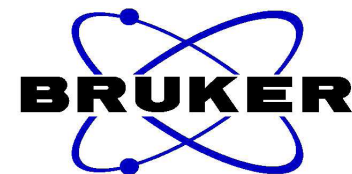
152.79
148.92
141.77
138.65
138.20
138.07
132.70
132.51
131.34
129.04
128.73
128.46
128.41
122.66
112.36

49.55
49.31

37.75

24.96
24.81

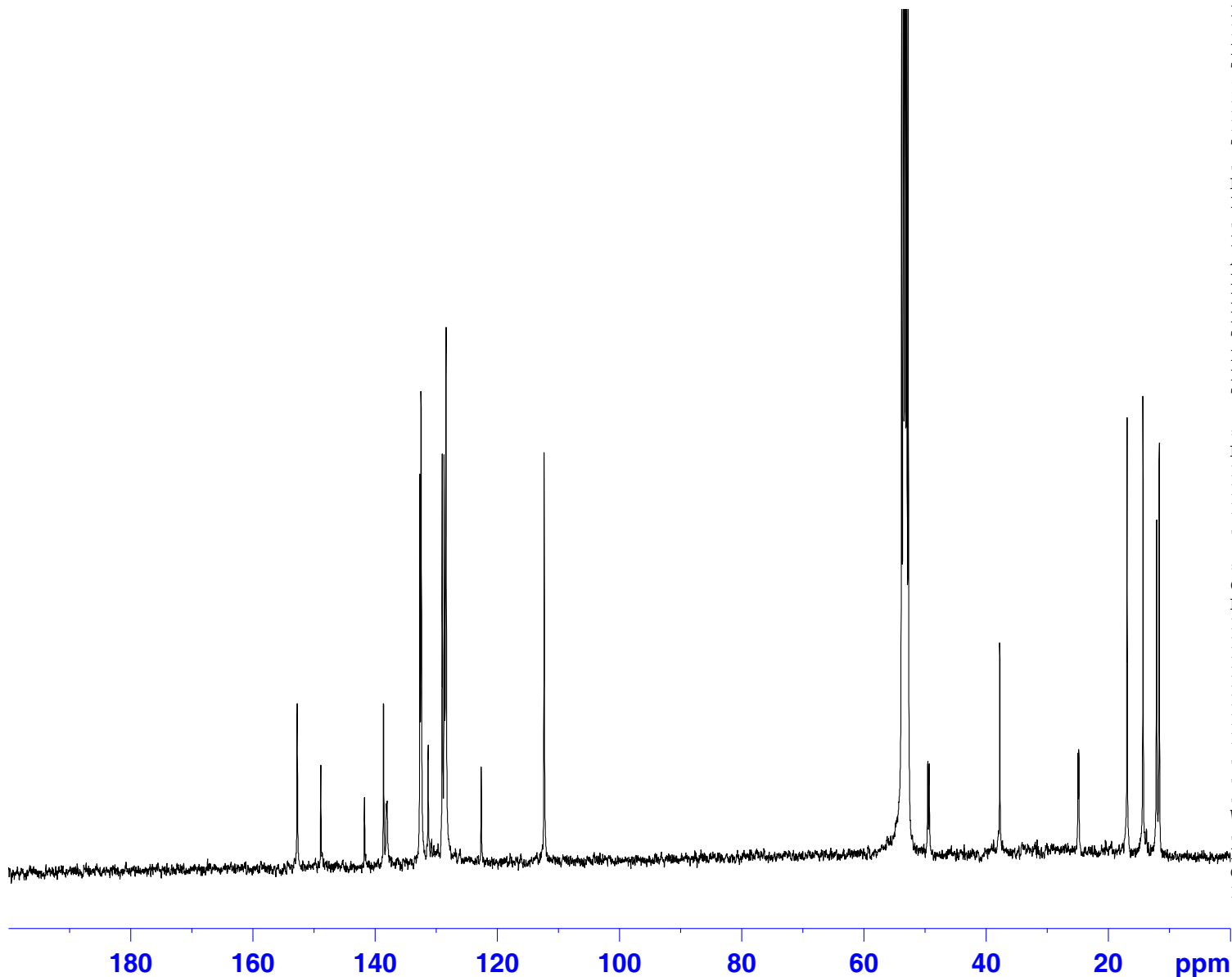
16.91
14.31
12.08
11.65



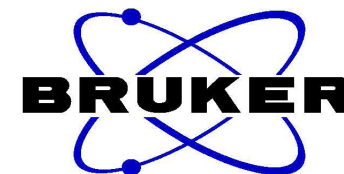
NAME Paper
EXPNO 48
PROCNO 1
Date_ 20121205
Time 8.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 12000
DS 0
SWH 40760.871 Hz
FIDRES 0.621962 Hz
AQ 0.8039582 sec
RG 406
DW 12.267 usec
DE 6.50 usec
TE 306.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 9.98 usec
PL1 -3.35 dB
PL1W 83.66055298 W
SFO1 100.6303741 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.25 dB
PL13 16.25 dB
PL2W 14.48648834 W
PL12W 0.48524728 W
PL13W 0.30617034 W
SFO2 400.1616006 MHz
SI 32768
SF 100.6203176 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40



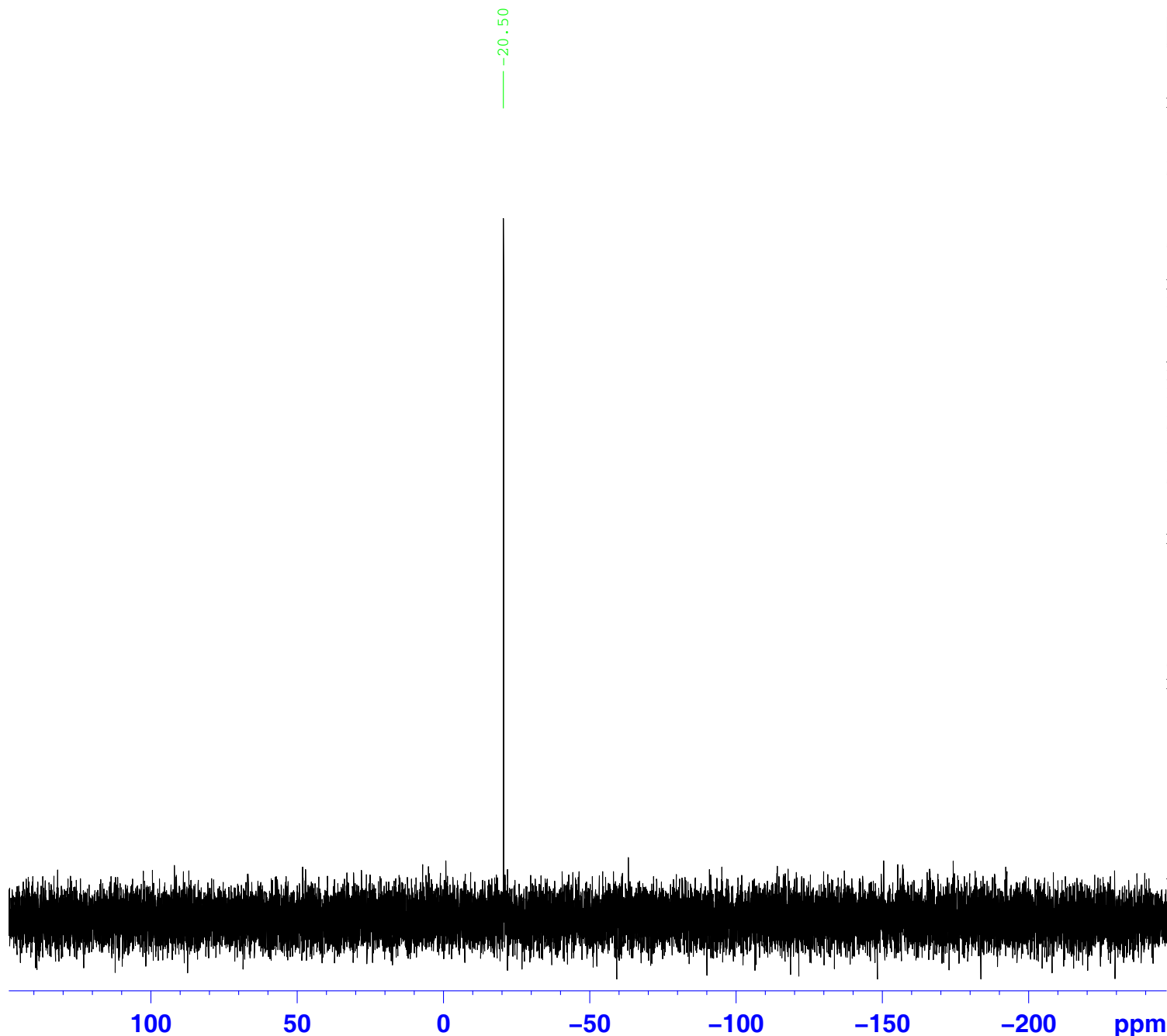
31P{1H} P,N-Bodipy (12)



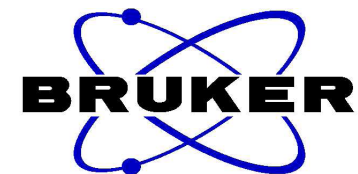
NAME Paper
EXPNO 33
PROCNO 1
Date_ 20121203
Time 14.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2C12
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 2050
DW 7.800 usec
DE 6.50 usec
TE 303.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 14.90 usec
PL1 1.95 dB
PL1W 16.51342773 W
SFO1 161.9796378 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.25 dB
PL13 16.25 dB
PL2W 14.48648834 W
PL12W 0.48524728 W
PL13W 0.30617034 W
SFO2 400.1616006 MHz
SI 32768
SF 161.9876242 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



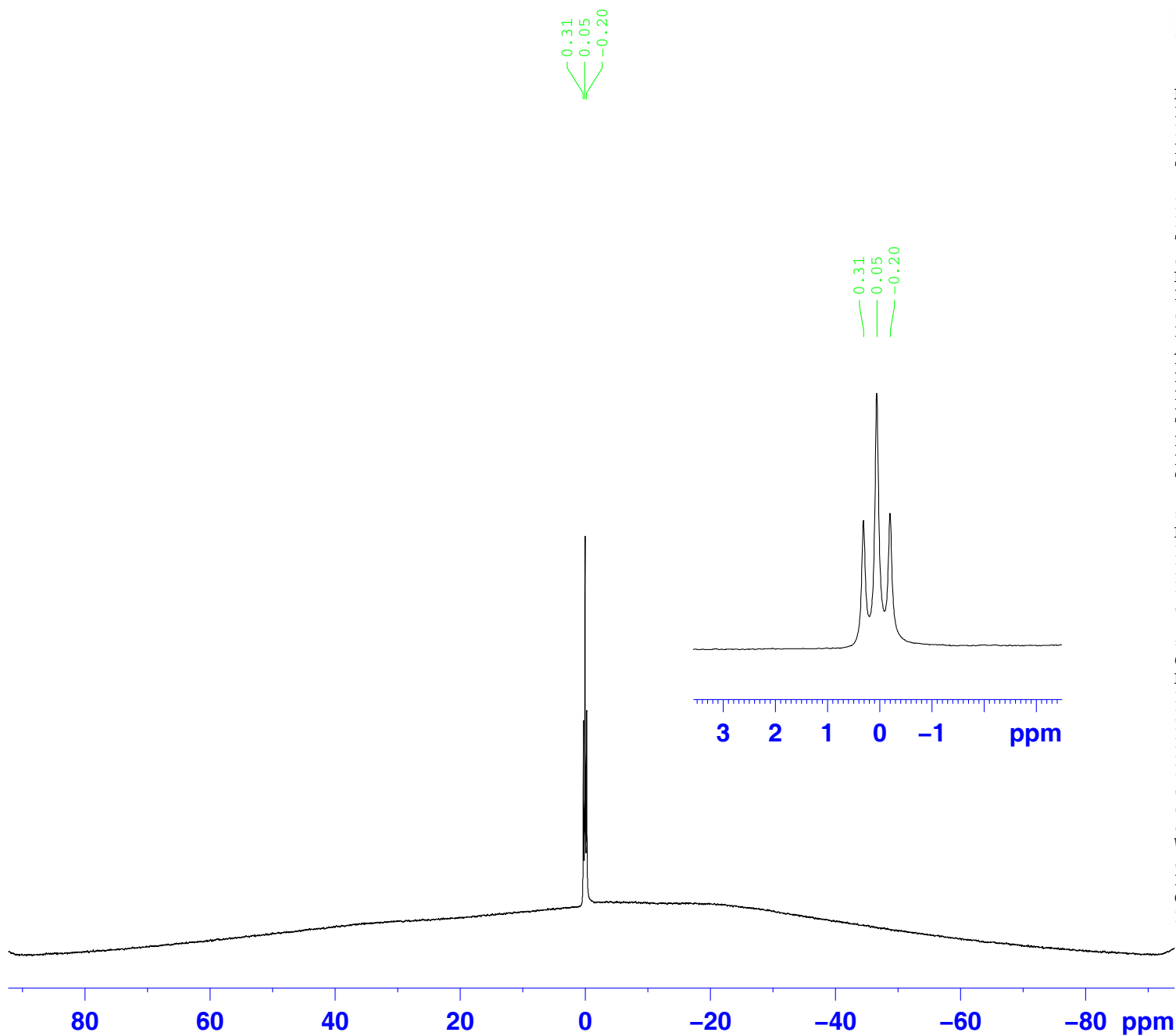
11B{1H} P,N-Bodipy (12)



NAME Paper
EXPNO 5
PROCNO 1
Date_ 20120611
Time 15.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 65536
SOLVENT CD2Cl2
NS 72
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 575
DW 20.800 usec
DE 6.50 usec
TE 303.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

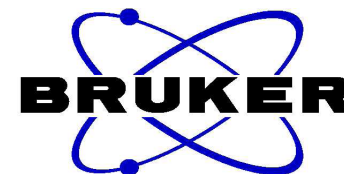
===== CHANNEL f1 =====
NUC1 11B
P1 12.80 usec
PL1 1.00 dB
PL1W 17.63811874 W
SFO1 128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.20 dB
PL2W 14.48648834 W
PL12W 0.49086621 W
SFO2 400.1316005 MHz
SI 32768
SF 128.3776824 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40



¹⁹F P,N-Bodipy (12)

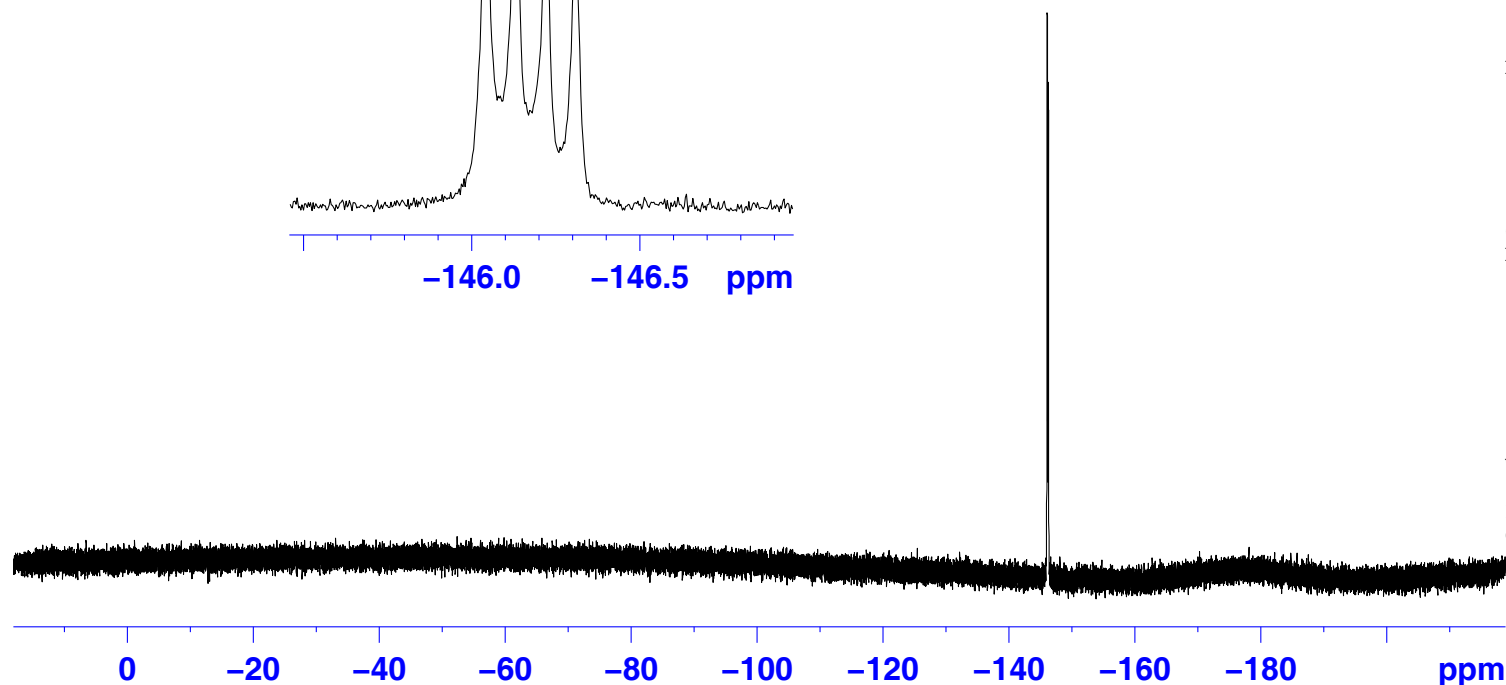
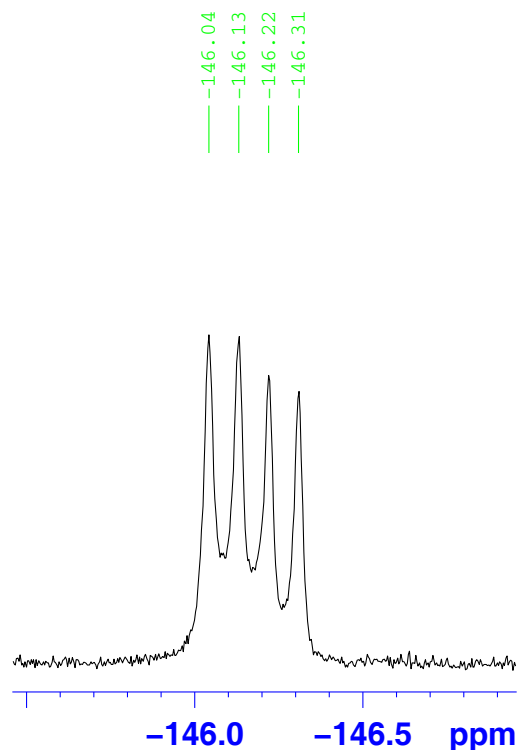
-146.04
-146.13
-146.22
-146.31



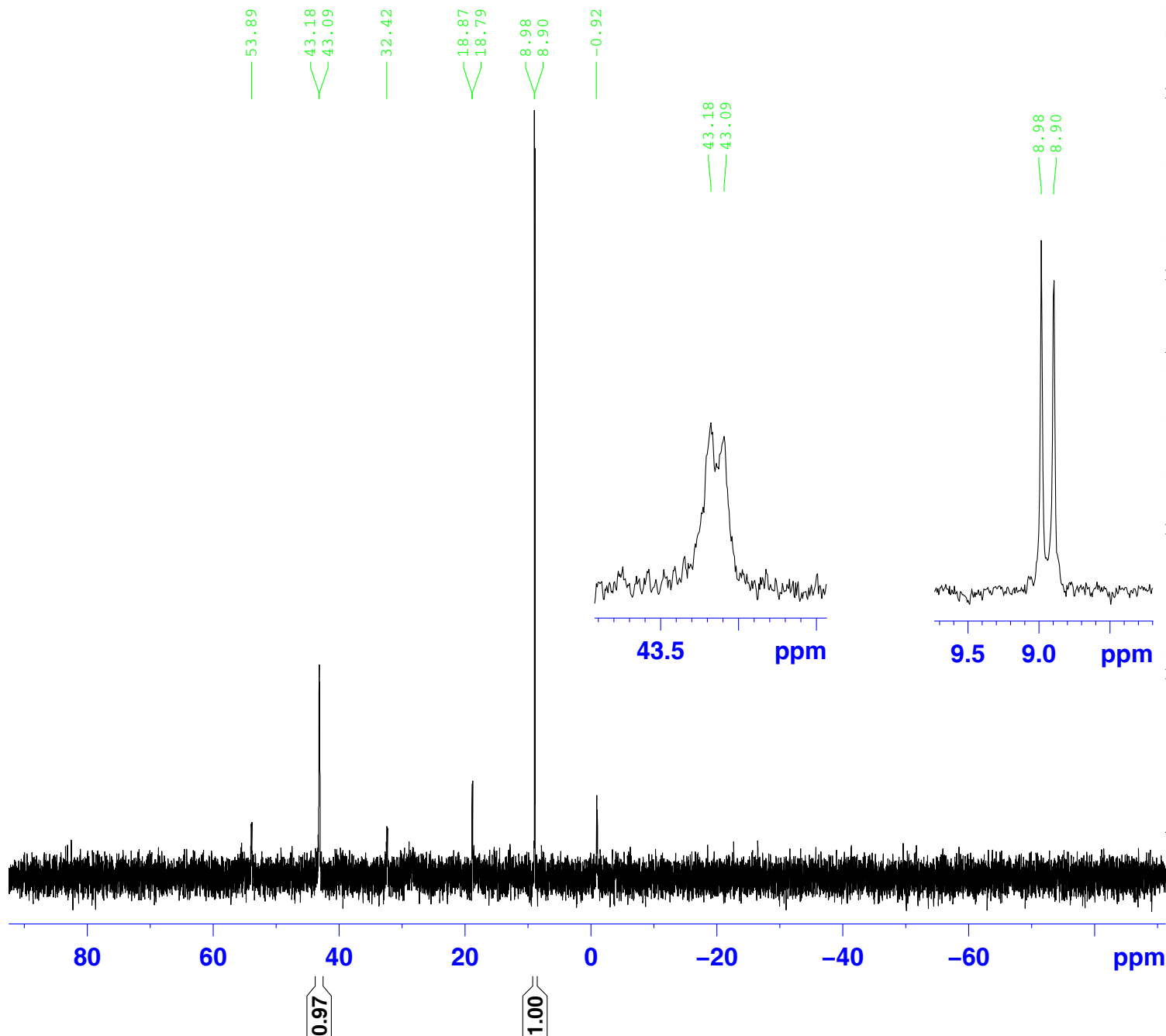
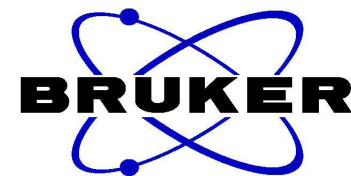
NAME Paper
EXPNO 34
PROCNO 1
Date_ 20121203
Time 13.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CD2Cl2
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 2050
DW 5.600 usec
DE 6.50 usec
TE 303.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 19.50 usec
PL1 -4.00 dB
PL1W 22.71446419 W
SFO1 376.4889418 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 112.00 usec
PL2 -4.00 dB
PL12 18.00 dB
PL2W 32.43120575 W
PL12W 0.20462708 W
SFO2 400.1616006 MHz
SI 65536
SF 376.5267681 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



PS-phF4-pBDP PS-Me Pt Semiopen recryst

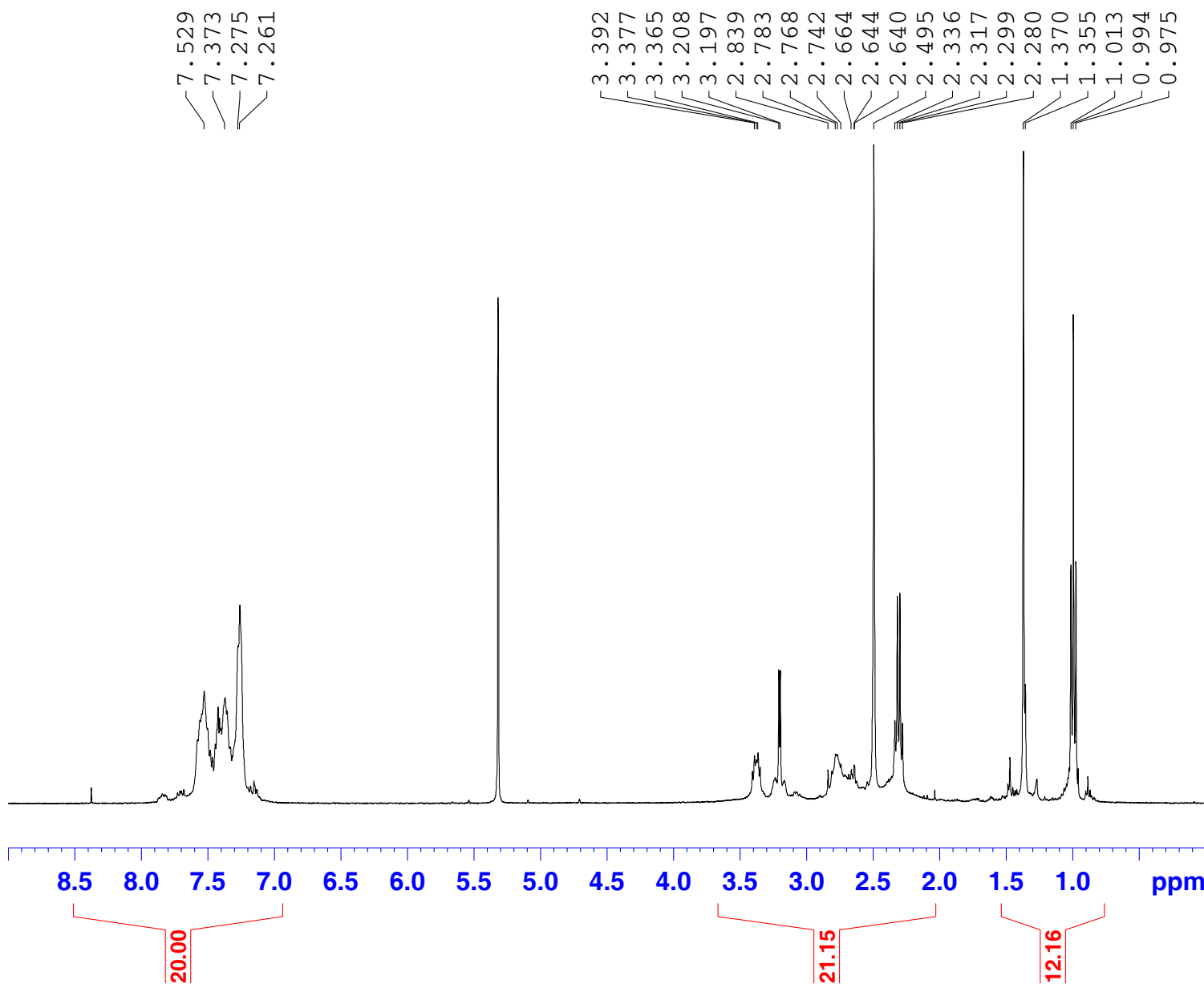
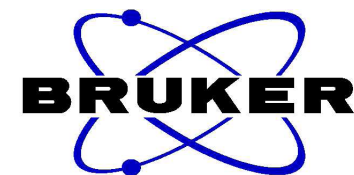


NAME Paper
 EXPNO 6
 PROCNO 2
 Date_ 20120814
 Time 12.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgig
 TD 52080
 SOLVENT CD2C12
 NS 232
 DS 0
 SWH 29761.904 Hz
 FIDRES 0.571465 Hz
 AQ 0.8749940 sec
 RG 1820
 DW 16.800 usec
 DE 6.50 usec
 TE 303.0 K
 D1 0.60000002 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 31P
 P1 15.66 usec
 PL1 3.00 dB
 PL1W 12.96693134 W
 SFO1 161.9755930 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -0.50 dB
 PL12 14.25 dB
 PL2W 14.48648834 W
 PL12W 0.48524728 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 161.9754972 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H [PtCl(κ²-P,S-Me)(P,S-Bodipy)]Cl (13)



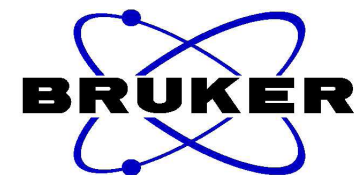
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NAME          Paper
EXPNO          46
PROCNO         1
Date_          20121204
Time           14.11
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zg30
TD             65536
SOLVENT        CD2Cl2
NS             16
DS             2
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ            3.9846387 sec
RG            181
DW            60.800 usec
DE            6.50 usec
TE            303.0 K
D1            1.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1           1H
P1            15.00 usec
PL1           -0.65 dB
PL1W          14.99557495 W
SFO1          400.1624712 MHz
SI            32768
SF            400.1600143 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB           0
PC            1.00
  
```

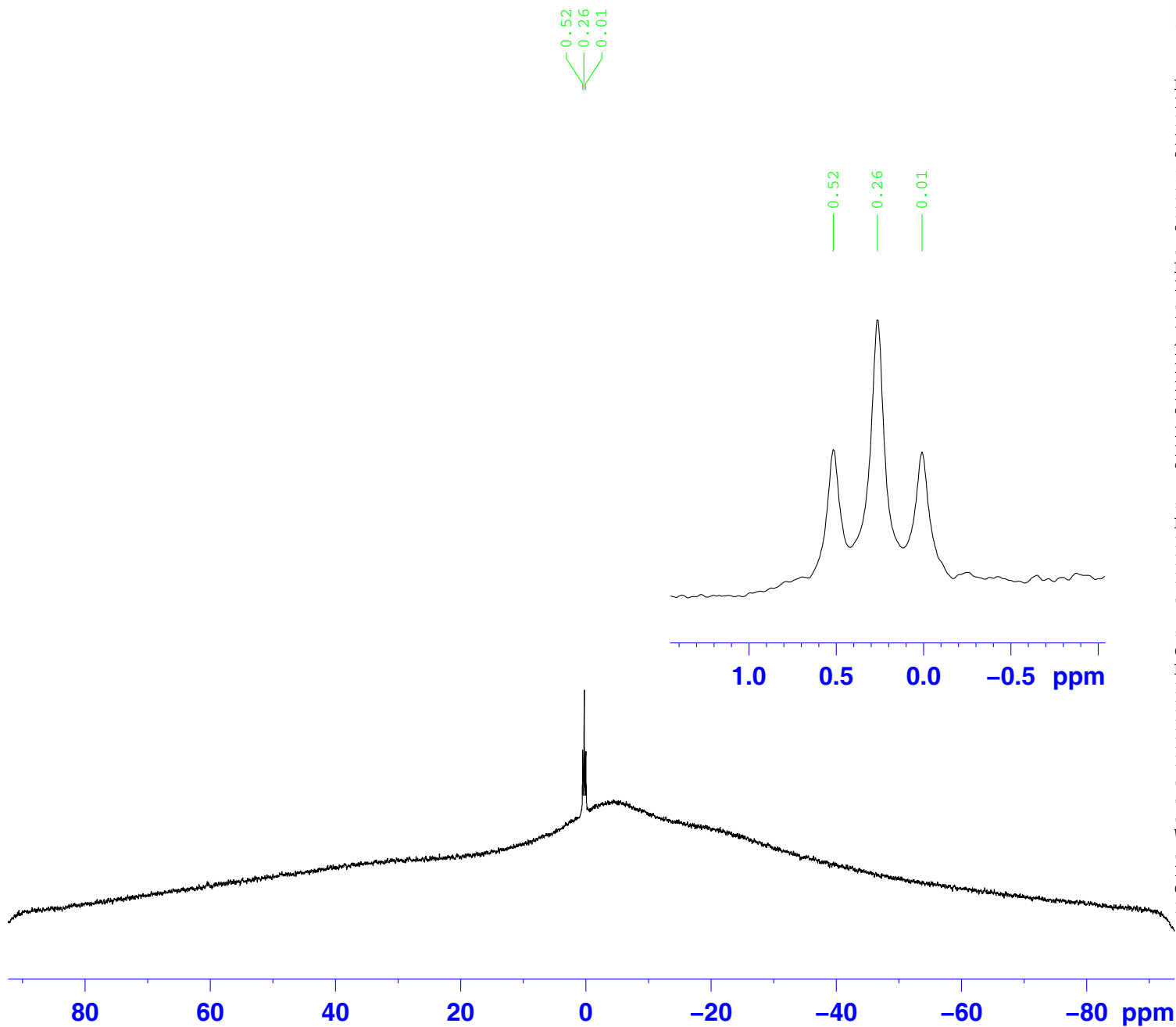
11B{1H} [PtCl(κ^2 -P,S-Me)(P,S-Bodipy)]Cl (13)



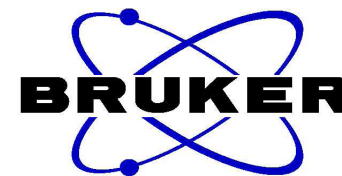
NAME Paper
EXPNO 7
PROCNO 1
Date_ 20120814
Time 12.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 65536
SOLVENT CD2Cl2
NS 38
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 575
DW 20.800 usec
DE 6.50 usec
TE 303.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 12.80 usec
PL1 1.00 dB
PL1W 17.63811874 W
SFO1 128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.20 dB
PL2W 14.48648834 W
PL12W 0.49086621 W
SFO2 400.1316005 MHz
SI 32768
SF 128.3776587 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40



^{19}F [PtCl(κ^2 -P,S-Me)(P,S-Bodipy)]Cl (13)

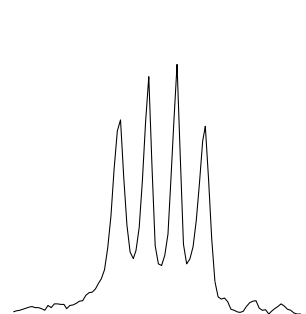


-131.74
-131.77
-131.80
-131.83
-140.43
-140.46
-140.50
-140.53
-146.00
-146.08
-146.17
-146.26

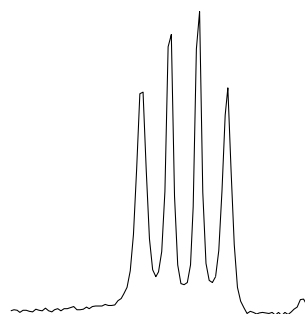
-131.74
-131.77
-131.80
-131.83

-140.43
-140.46
-140.50
-140.53

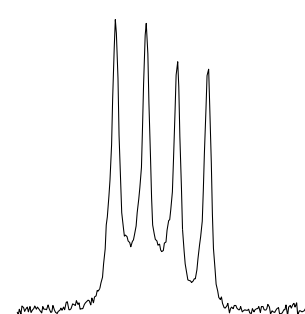
-146.00
-146.08
-146.17
-146.26



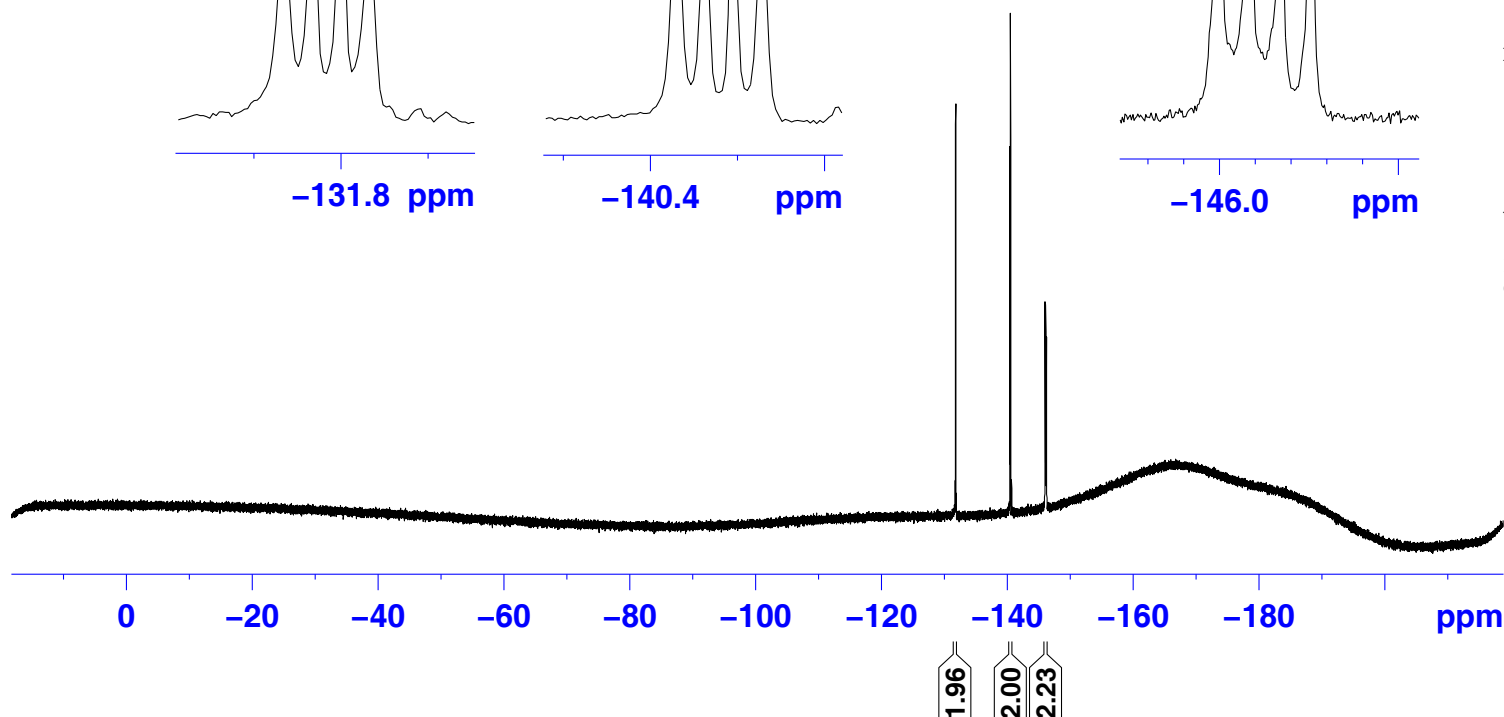
-131.8 ppm



-140.4 ppm



-146.0 ppm

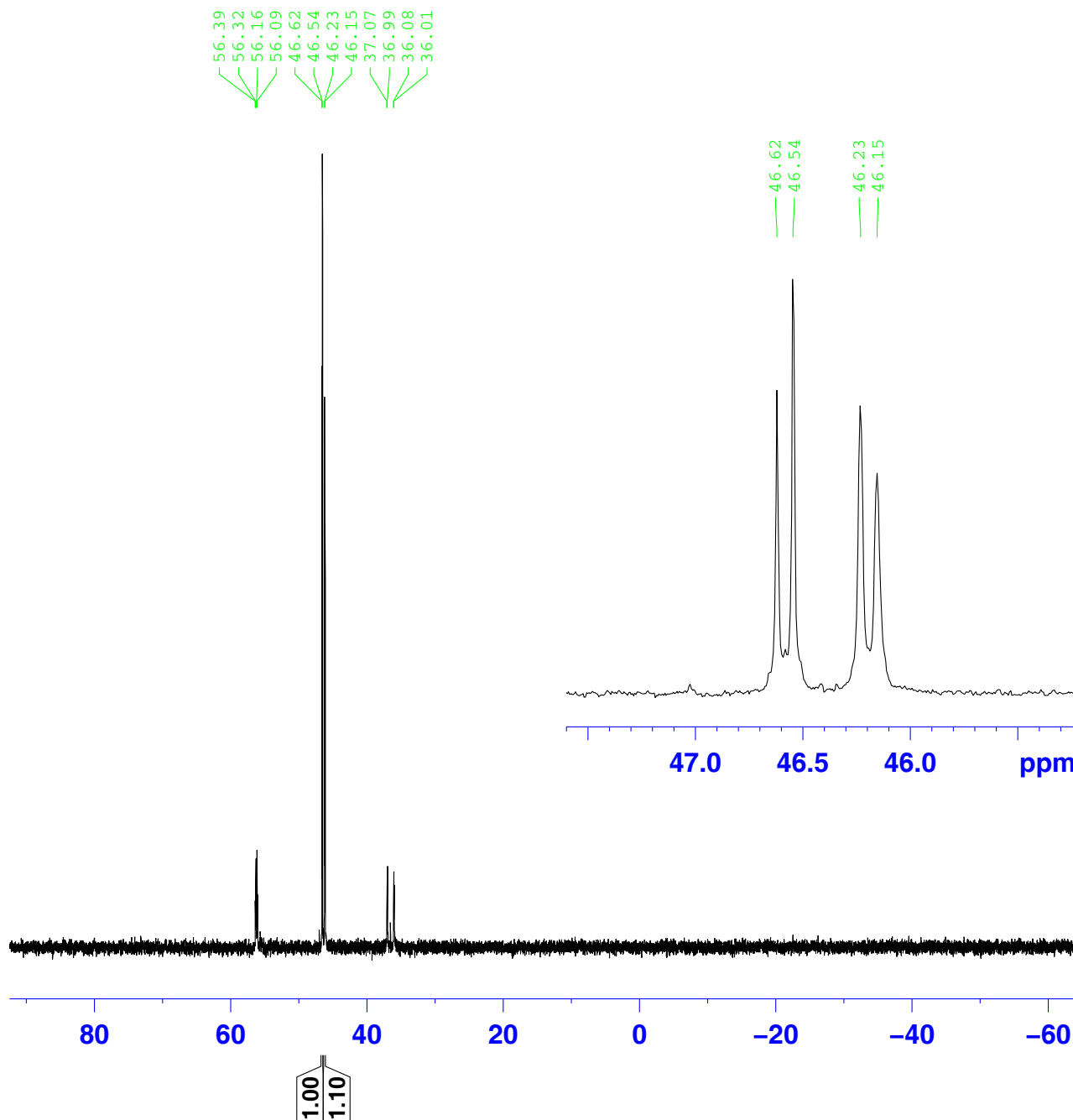
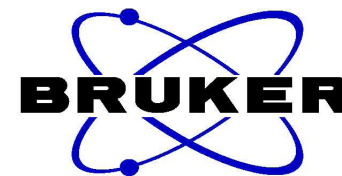


```

NAME      Paper
EXPNO      8
PROCNO     1
Date_      20120814
Time       12.32
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zg
TD         131072
SOLVENT    CD2C12
NS         105
DS         0
SWH        89285.711 Hz
FIDRES     0.681196 Hz
AQ         0.7340532 sec
RG         724
DW         5.600 usec
DE         6.50 usec
TE         303.1 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       19F
P1         14.75 usec
PL1        -3.20 dB
PL1W       18.89306831 W
SFO1       376.4607164 MHz
SI         65536
SF         376.4984751 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

$^{31}\text{P}\{^1\text{H}\} \text{ [Pt}(\kappa^2\text{-P,S-Me})(\kappa^2\text{-P,S-Bodipy})]2\text{BF}_4 \text{ (14)}$



```

NAME          Paper
EXPNO         18
PROCNO        3
Date_         20120814
Time          17.38
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgig
TD            52080
SOLVENT       CD2C12
NS            72
DS            0
SWH           29761.904 Hz
FIDRES        0.571465 Hz
AQ            0.8749940 sec
RG            1820
DW            16.800 usec
DE            6.50 usec
TE            303.1 K
D1            0.60000002 sec
D11           0.03000000 sec
TD0           1
  
```

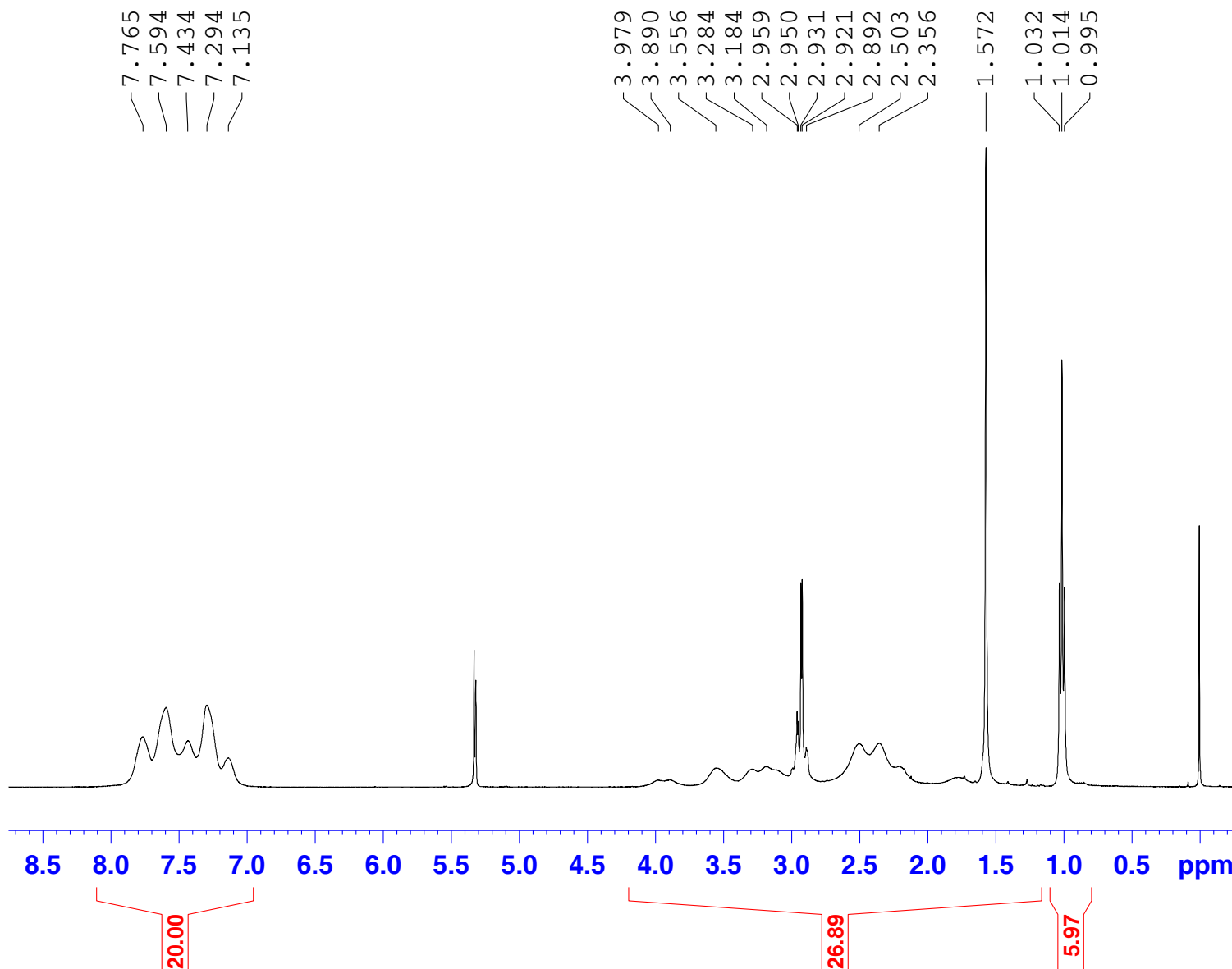
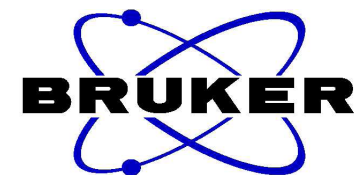
```

===== CHANNEL f1 =====
NUC1          31P
P1            15.66 usec
PL1           3.00 dB
PL1W          12.96693134 W
SFO1          161.9755930 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -0.50 dB
PL12          14.25 dB
PL2W          14.48648834 W
PL12W         0.48524728 W
SFO2          400.1316005 MHz
SI            32768
SF            161.9754972 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

^1H [Pt($\kappa^2\text{-P,S-Me}$)($\kappa^2\text{-P,S-Bodipy}$)] 2BF_4 (14)



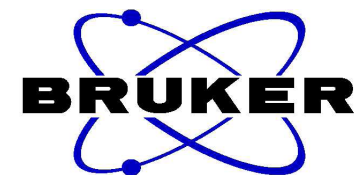
```

NAME          Paper
EXPNO          21
PROCNO         1
Date_          20120814
Time           18.17
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zg
TD             44116
SOLVENT        CD2Cl2
NS             16
DS             0
SWH            11029.412 Hz
FIDRES         0.250009 Hz
AQ            1.9999753 sec
RG             101
DW            45.333 usec
DE             6.50 usec
TE            303.0 K
D1            1.00000000 sec
TD0            1
  
```

```

===== CHANNEL f1 =====
NUC1           1H
P1            14.65 usec
PL1           -0.50 dB
PL1W          14.48648834 W
SFO1          400.1323986 MHz
SI            32768
SF            400.1300153 MHz
WDW            EM
SSB            0
LB            0.30 Hz
GB            0
PC            1.00
  
```

$^{11}\text{B}\{^1\text{H}\} [\text{Pt}(\kappa^2\text{-P}, \text{S-Me})(\kappa^2\text{-P}, \text{S-Bodipy})]_2\text{BF}_4$ (14)



```

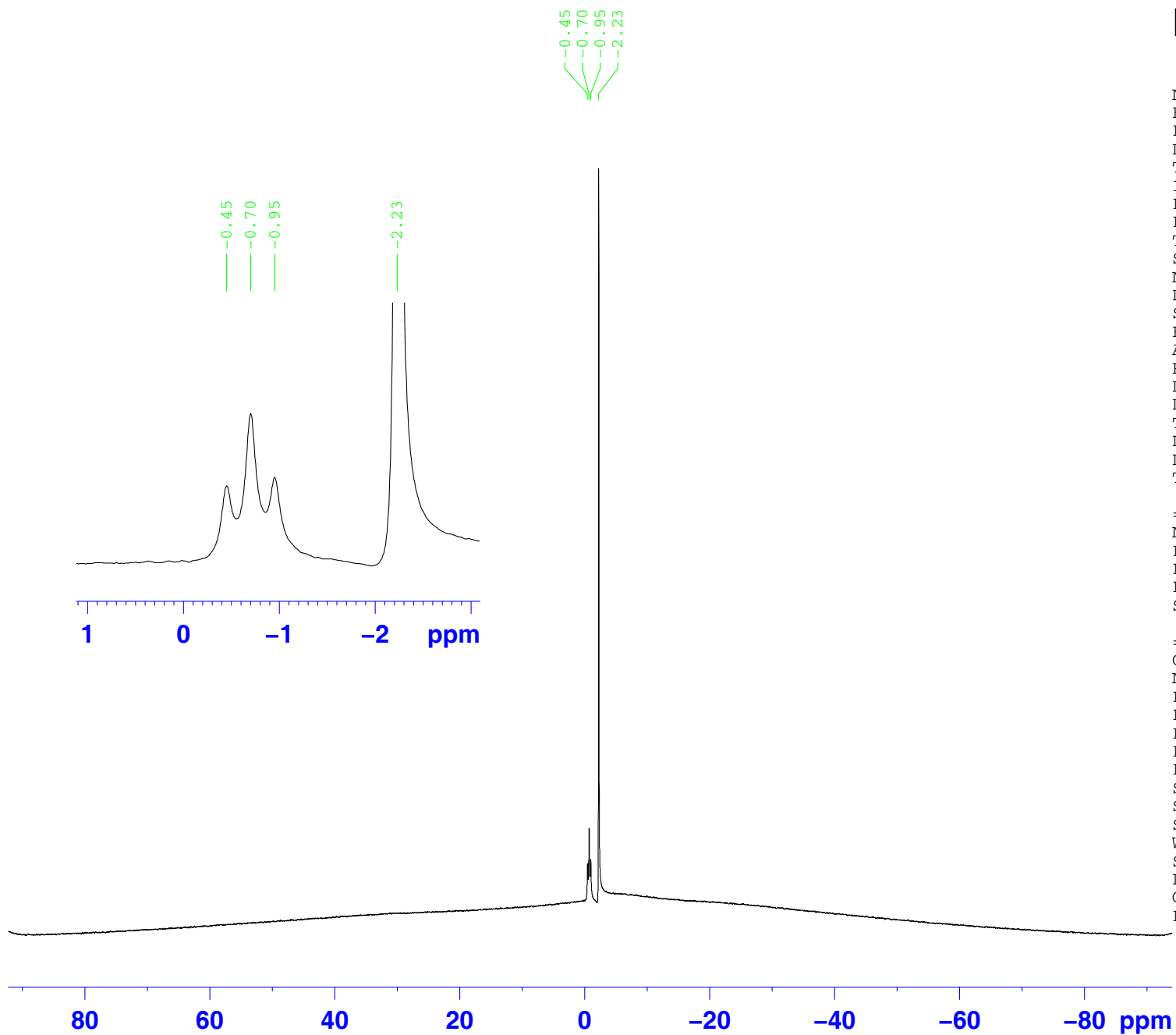
NAME      Paper
EXPNO     20
PROCNO    1
Date_     20120814
Time      18.13
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgig
TD        65536
SOLVENT   CD2Cl2
NS        44
DS        0
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        575
DW        20.800 usec
DE        6.50 usec
TE        303.0 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

```

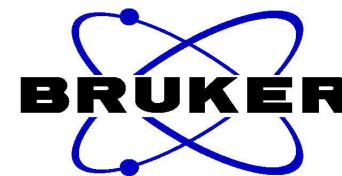
===== CHANNEL f1 =====
NUC1      11B
P1        12.80 usec
PL1       1.00 dB
PL1W      17.63811874 W
SFO1      128.3776050 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -0.50 dB
PL12      14.20 dB
PL2W      14.48648834 W
PL12W     0.49086621 W
SFO2      400.1316005 MHz
SI        32768
SF        128.3777762 MHz
WDW       EM
SSB       0
LB        5.00 Hz
GB        0
PC        1.40
  
```



^{19}F [Pt($\kappa^2\text{-P,S-Me}$)($\kappa^2\text{-P,S-Bodipy}$)] 2BF_4 (14)

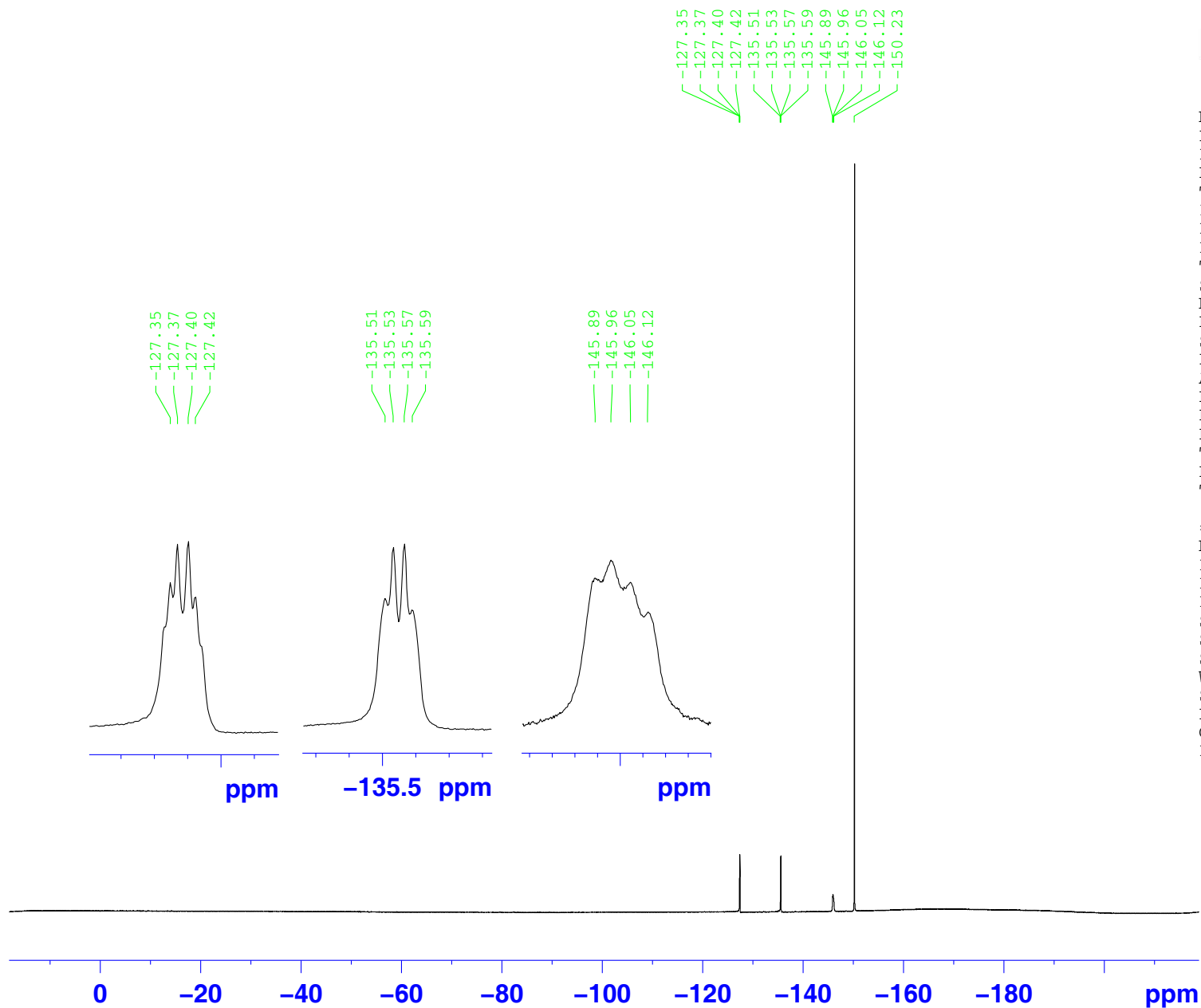


```

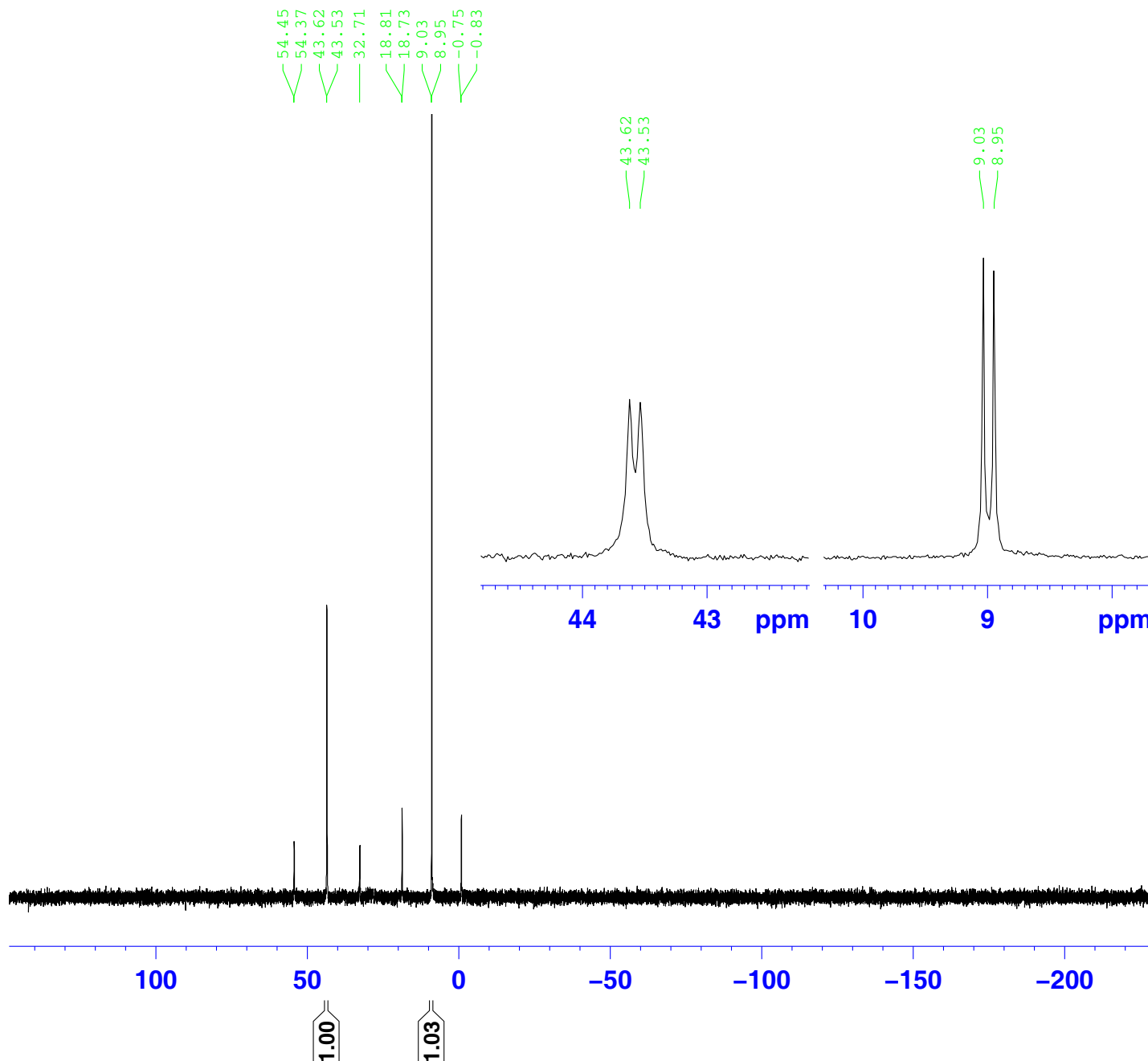
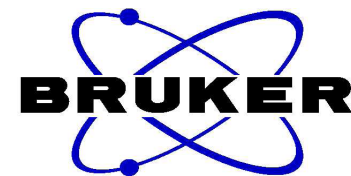
NAME          Paper
EXPNO         19
PROCNO        1
Date_         20120814
Time          17.51
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg
TD            131072
SOLVENT       CD2C12
NS            177
DS            0
SWH           89285.711 Hz
FIDRES        0.681196 Hz
AQ            0.7340532 sec
RG            724
DW            5.600 usec
DE            6.50 usec
TE            303.0 K
D1            1.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          19F
P1            14.75 usec
PL1           -3.20 dB
PL1W          18.89306831 W
SFO1          376.4607164 MHz
SI            65536
SF            376.4985194 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



$^{31}\text{P}\{^1\text{H}\}$ [PtCl(κ^2 -P,S-Me)(P,S-Bodipy)]Cl (15)

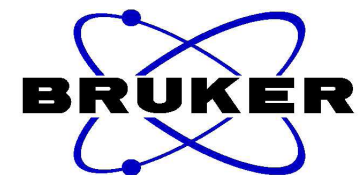


NAME Paper
EXPNO 55
PROCNO 1
Date_ 20121206
Time 11.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2C12
NS 123
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 2050
DW 7.800 usec
DE 6.50 usec
TE 303.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^{31}P
P1 14.90 usec
PL1 1.95 dB
PL1W 16.51342773 W
SFO1 161.9796378 MHz

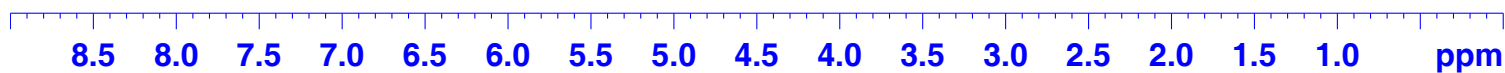
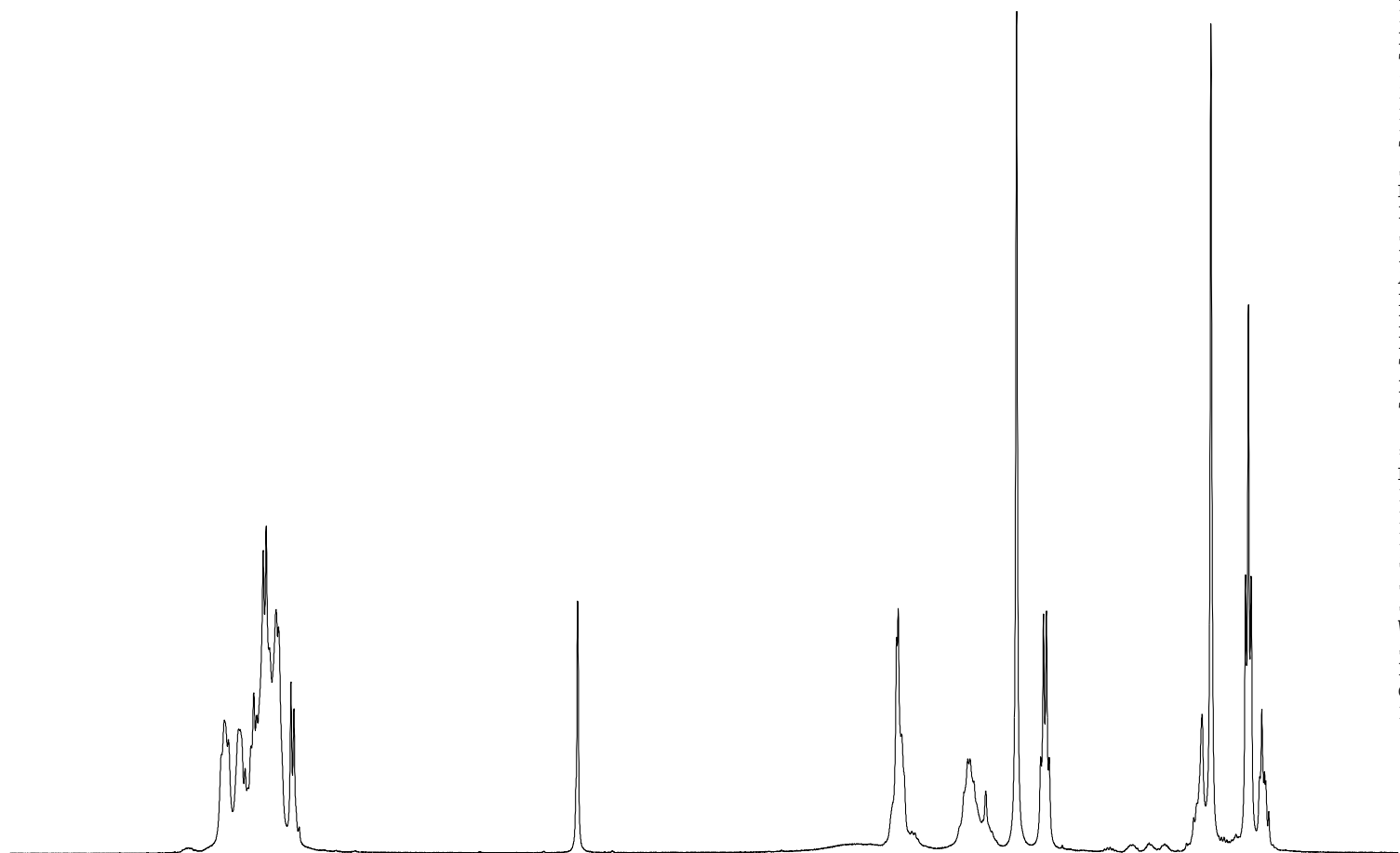
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ^1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.25 dB
PL13 16.25 dB
PL2W 14.48648834 W
PL12W 0.48524728 W
PL13W 0.30617034 W
SFO2 400.1616006 MHz
SI 32768
SF 161.9876419 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

$^{31}\text{P}\{^1\text{H}\}$ [PtCl(κ^2 -P,S-Me)(P,S-Bodipy)]Cl (15)



NAME Paper
EXPNO 54
PROCNO 1
Date_ 20121206
Time 11.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.50 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

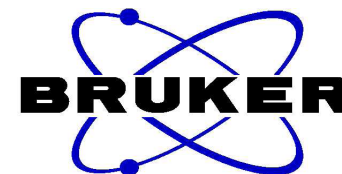
===== CHANNEL f1 =====
NUC1 ^1H
P1 15.00 usec
PL1 -0.65 dB
PL1W 14.99557495 W
SFO1 400.1624712 MHz
SI 32768
SF 400.1600143 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



24.00

32.74

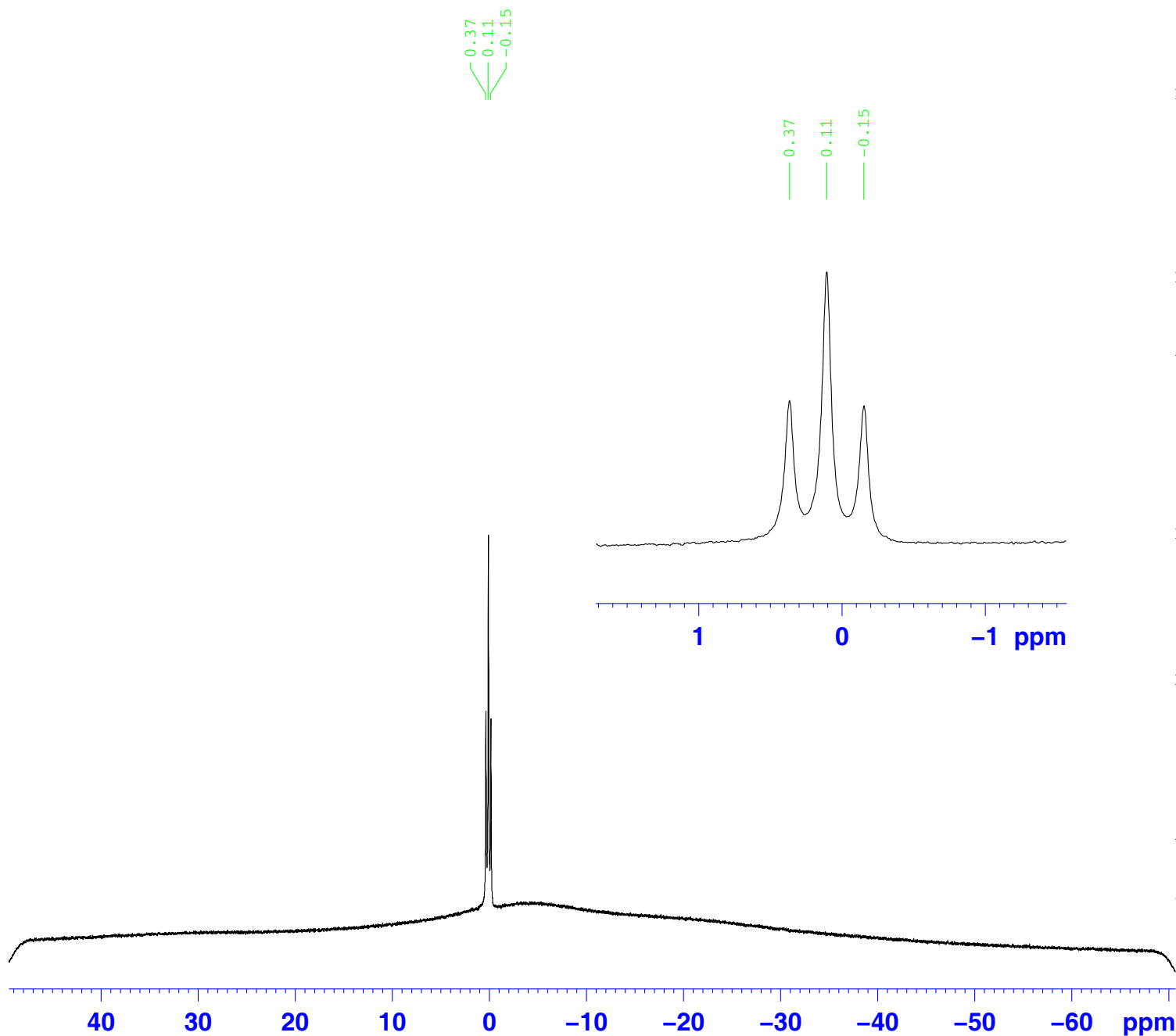
$^{19}\text{F}\{^1\text{H}\} \text{ [PtCl}(\kappa^2\text{-P,S-Me) (P,S-Bodipy)]Cl (15)}$



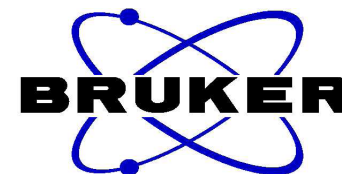
NAME Paper
EXPNO 53
PROCNO 1
Date_ 20121205
Time 20.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 16384
SOLVENT CD2Cl2
NS 166
DS 0
SWH 15432.099 Hz
FIDRES 0.941901 Hz
AQ 0.5308916 sec
RG 812
DW 32.400 usec
DE 6.50 usec
TE 303.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 12.80 usec
PL1 1.00 dB
PL1W 17.63811874 W
SFO1 128.3859468 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.25 dB
PL2W 14.48648834 W
PL12W 0.48524728 W
SFO2 400.1616006 MHz
SI 32768
SF 128.3873074 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



^{19}F [PtCl(κ^2 -P,S-Me)(P,S-Bodipy)]Cl (15)



```

NAME          Paper
EXPNO         52
PROCNO        1
Date_         20121205
Time          19.58
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgfhigqn
TD            131072
SOLVENT       CD2Cl2
NS            16
DS            4
SWH           89285.711 Hz
FIDRES        0.681196 Hz
AQ            0.7340532 sec
RG            2050
DW            5.600 usec
DE            6.50 usec
TE            302.9 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0           1
  
```

```

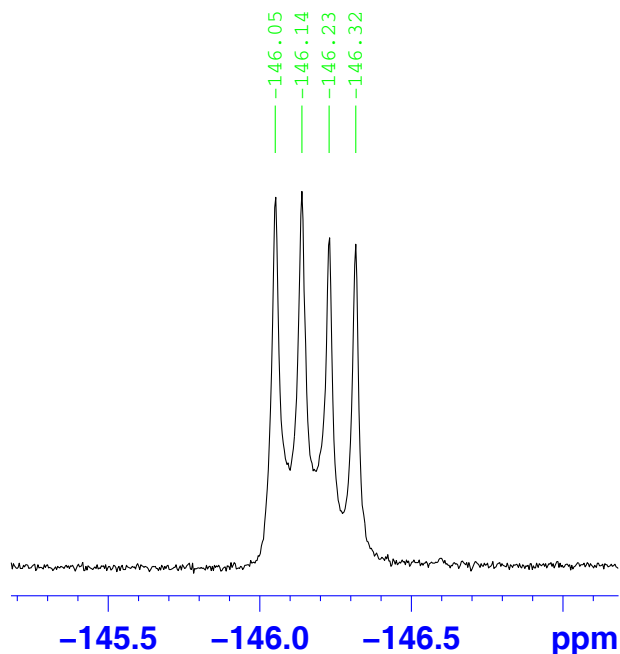
===== CHANNEL f1 =====
NUC1          19F
P1            19.50 usec
PL1           -4.00 dB
PL1W          22.71446419 W
SFO1          376.4889418 MHz
  
```

```

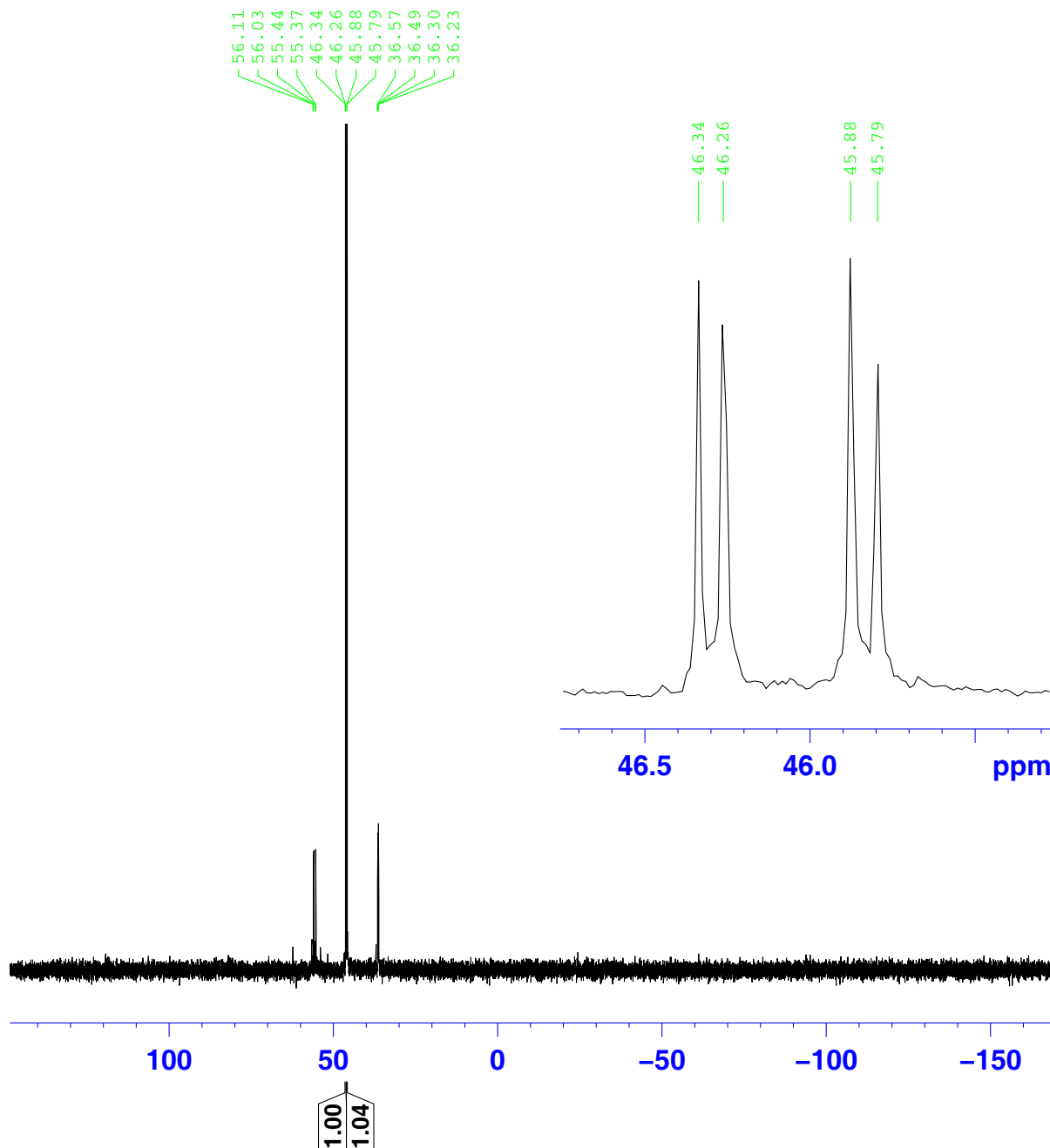
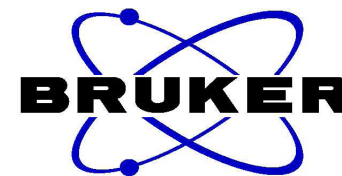
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         112.00 usec
PL2           -4.00 dB
PL12          18.00 dB
PL2W          32.43120575 W
PL12W         0.20462708 W
SFO2          400.1616006 MHz
SI            65536
SF            376.5267652 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

-146.05
-146.14
-146.23
-146.32

-146.05
-146.14
-146.23
-146.32



$^{31}\text{P}\{^1\text{H}\} \text{ [Pt}(\kappa^2\text{-P,S-Me})(\kappa^2\text{-P,S-Bodipy)]2BF}_4 \text{ (16)}$



```

NAME          Paper
EXPNO         56
PROCNO        2
Date_         20121206
Time          16.10
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CD2C12
NS            161
DS            4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            2050
DW            7.800 usec
DE            6.50 usec
TE            303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
```

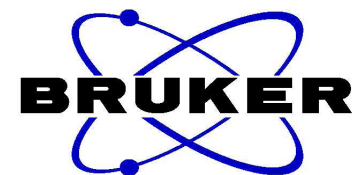
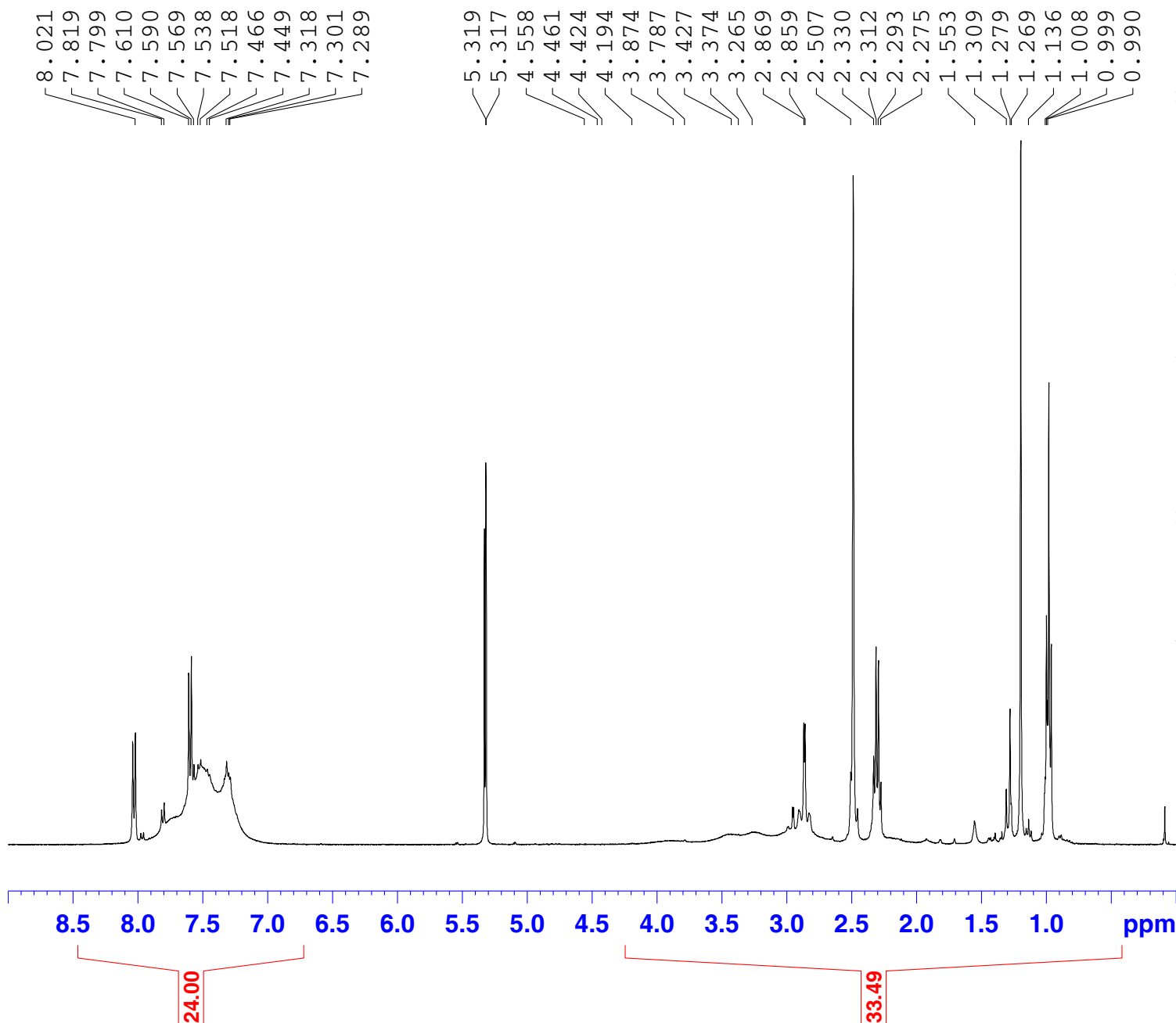
```

===== CHANNEL f1 =====
NUC1          31P
P1            14.90 usec
PL1           1.95 dB
PL1W          16.51342773 W
SFO1          161.9796378 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -0.50 dB
PL12          14.25 dB
PL13          16.25 dB
PL2W          14.48648834 W
PL12W         0.48524728 W
PL13W         0.30617034 W
SFO2          400.1616006 MHz
SI            32768
SF            161.9876419 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

^1H [Pt($\kappa^2\text{-P,S-Me}$)($\kappa^2\text{-P,S-Bodipy}$)] 2BF_4 (16)



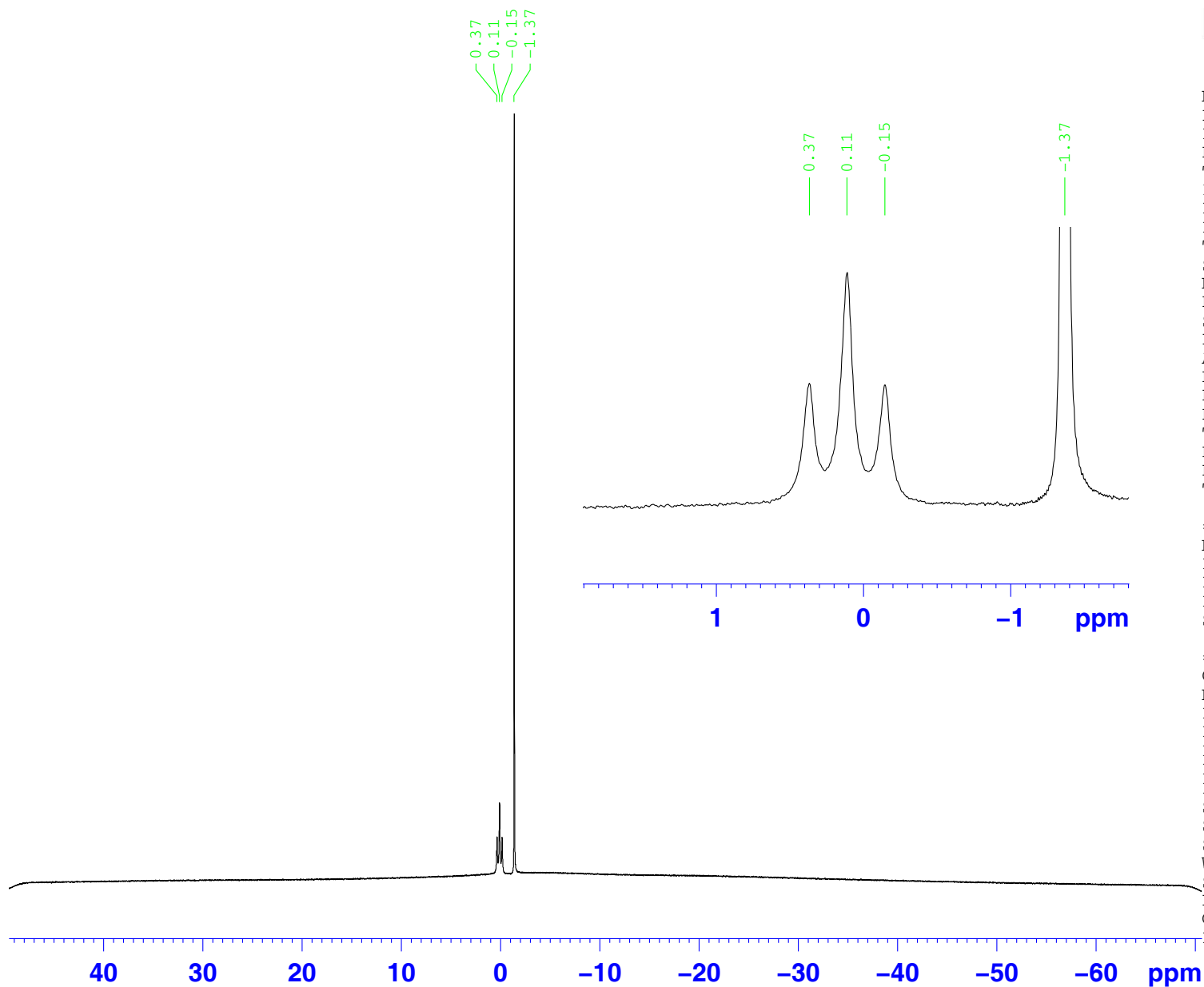
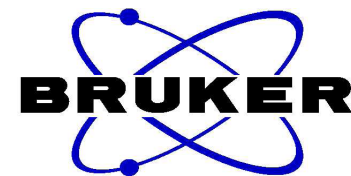
```

NAME      Paper
EXPNO      59
PROCNO     1
Date_      20121206
Time       16.29
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zg30
TD         65536
SOLVENT    CD2Cl2
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         181
DW         60.800 usec
DE         6.50 usec
TE         303.0 K
D1         1.00000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1       1H
P1         15.00 usec
PL1        -0.65 dB
PL1W       14.99557495 W
SFO1       400.1624712 MHz
SI         32768
SF         400.1600143 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

$^{11}\text{B}\{^1\text{H}\} [\text{Pt}(\kappa^2\text{-P}, \text{S-Me})(\kappa^2\text{-P}, \text{S-Bodipy})]_2\text{BF}_4$ (16)

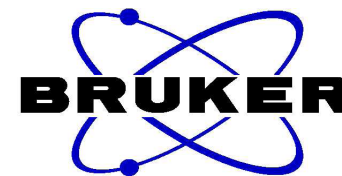


NAME Paper
 EXPNO 57
 PROCNO 1
 Date_ 20121206
 Time 16.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgig
 TD 16384
 SOLVENT CD2Cl2
 NS 96
 DS 0
 SWH 15432.099 Hz
 FIDRES 0.941901 Hz
 AQ 0.5308916 sec
 RG 812
 DW 32.400 usec
 DE 6.50 usec
 TE 303.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ^{11}B
 P1 12.80 usec
 PL1 1.00 dB
 PL1W 17.63811874 W
 SFO1 128.3859468 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ^1H
 PCPD2 80.00 usec
 PL2 -0.50 dB
 PL12 14.25 dB
 PL2W 14.48648834 W
 PL12W 0.48524728 W
 SFO2 400.1616006 MHz
 SI 32768
 SF 128.3873045 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

^{19}F [Pt($\kappa^2\text{-P,S-Me}$)($\kappa^2\text{-P,S-Bodipy}$)] 2BF_4 (16)



```

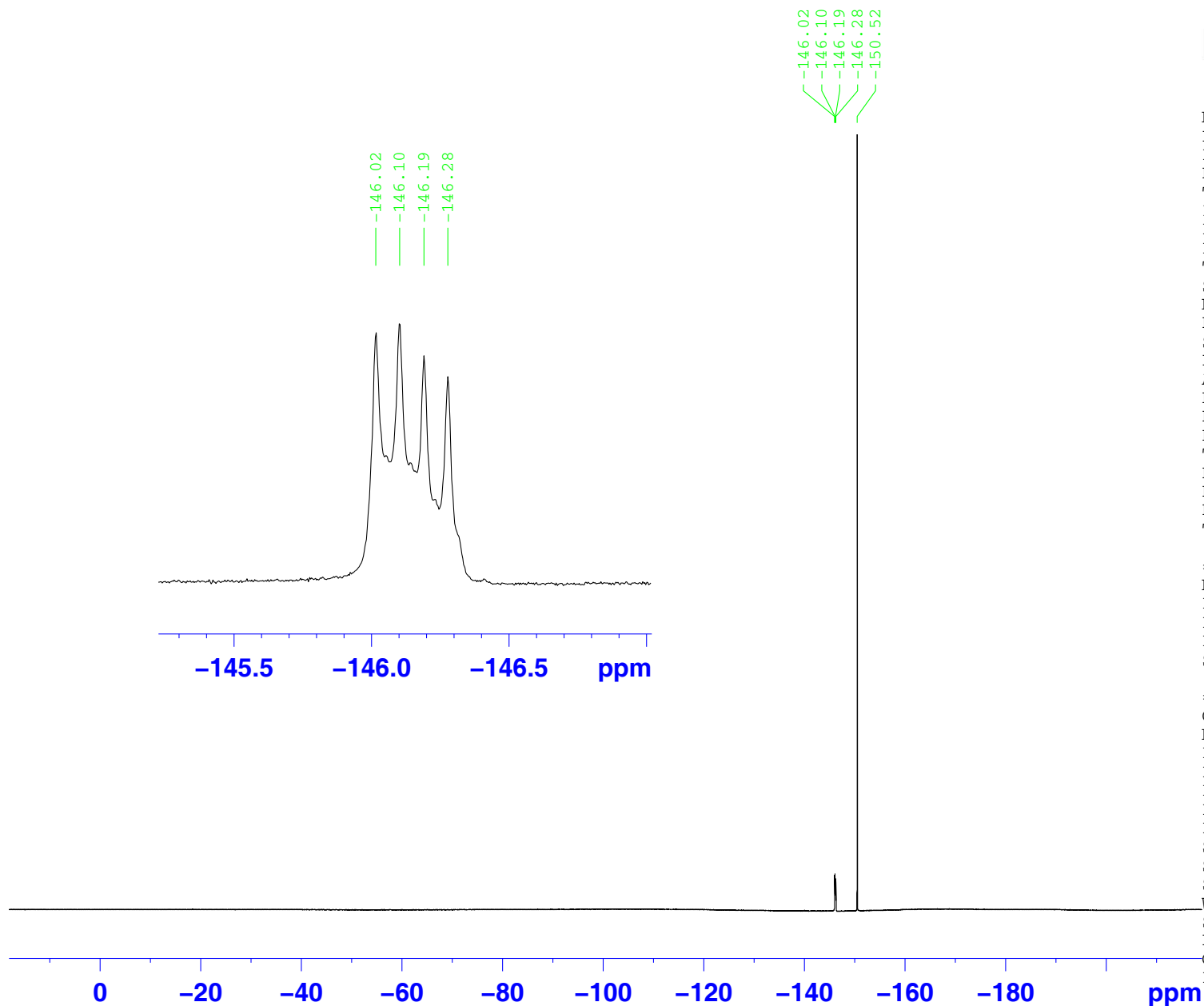
NAME          Paper
EXPNO          58
PROCNO         1
Date_          20121206
Time           16.25
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zgfhigqn
TD             131072
SOLVENT        CD2C12
NS             121
DS             4
SWH            89285.711 Hz
FIDRES         0.681196 Hz
AQ             0.7340532 sec
RG             2050
DW             5.600 usec
DE             6.50 usec
TE             303.0 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0            1
  
```

```

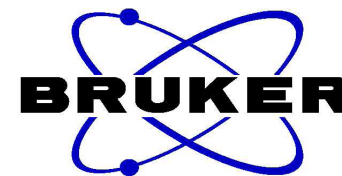
===== CHANNEL f1 =====
NUC1           19F
P1             19.50 usec
PL1            -4.00 dB
PL1W           22.71446419 W
SFO1           376.4889418 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2           1H
PCPD2          112.00 usec
PL2            -4.00 dB
PL12           18.00 dB
PL2W           32.43120575 W
PL12W          0.20462708 W
SFO2           400.1616006 MHz
SI             65536
SF             376.5267722 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB             0
PC             1.00
  
```



$^{31}\text{P}\{^1\text{H}\} \text{ [PtCl}(\kappa^2\text{-P,S-Me) (P,S-Bodipy)]Cl}$ (17)



```

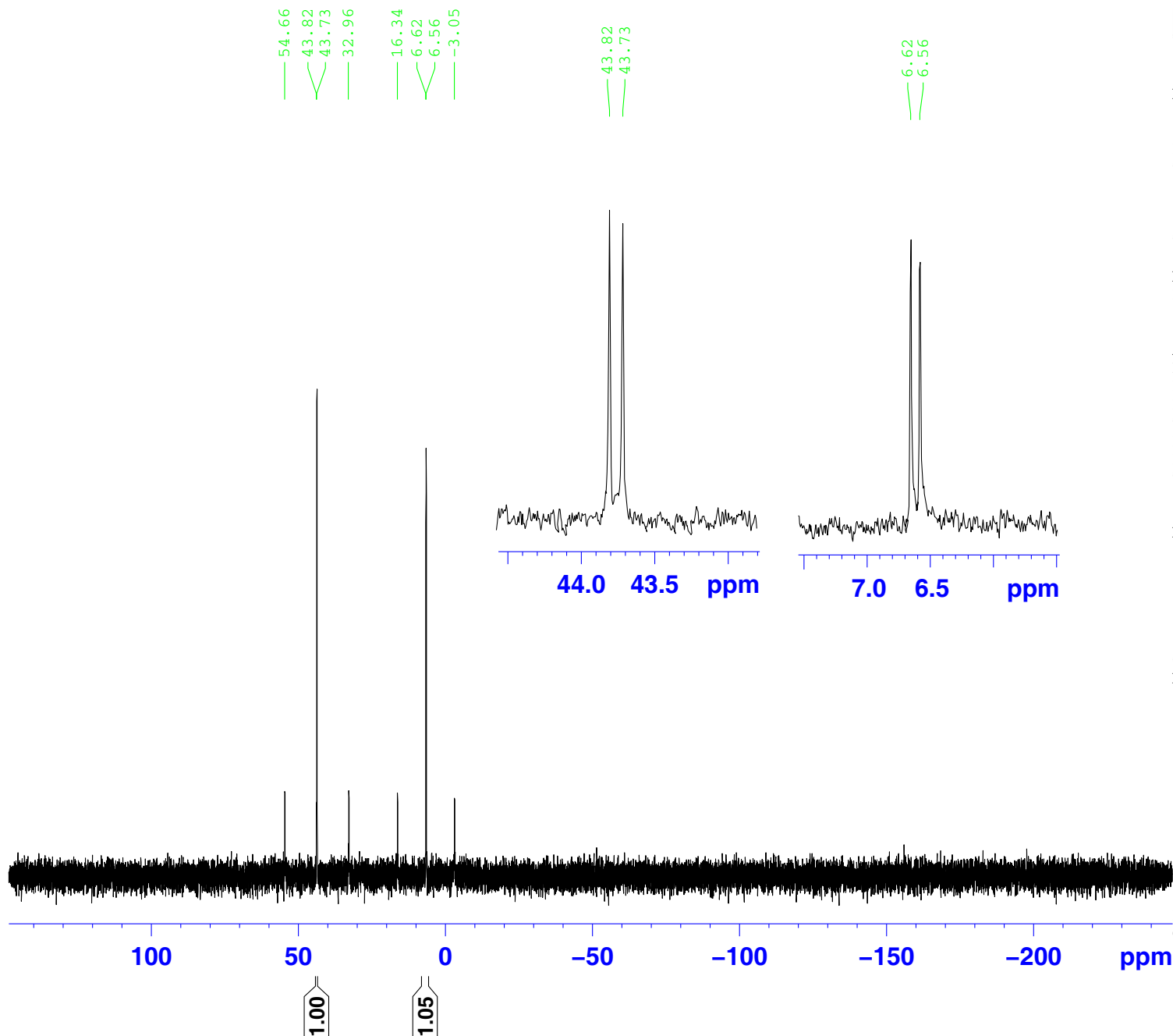
NAME          Paper
EXPNO          60
PROCNO         1
Date_          20121208
Time           14.30
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zgpg30
TD             65536
SOLVENT        CD2C12
NS             220
DS             4
SWH            64102.563 Hz
FIDRES         0.978127 Hz
AQ            0.5112308 sec
RG            2050
DW            7.800 usec
DE            6.50 usec
TE            303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
```

```

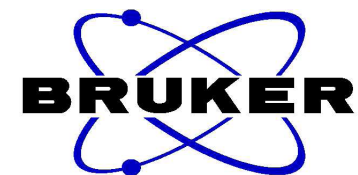
===== CHANNEL f1 =====
NUC1           31P
P1            14.90 usec
PL1           1.95 dB
PL1W          16.51342773 W
SFO1          161.9796378 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2           1H
PCPD2          80.00 usec
PL2           -0.50 dB
PL12          14.25 dB
PL13          16.25 dB
PL2W          14.48648834 W
PL12W         0.48524728 W
PL13W         0.30617034 W
SFO2          400.1616006 MHz
SI            32768
SF            161.9876419 MHz
WDW            EM
SSB            0
LB            1.00 Hz
GB            0
PC            1.40
  
```

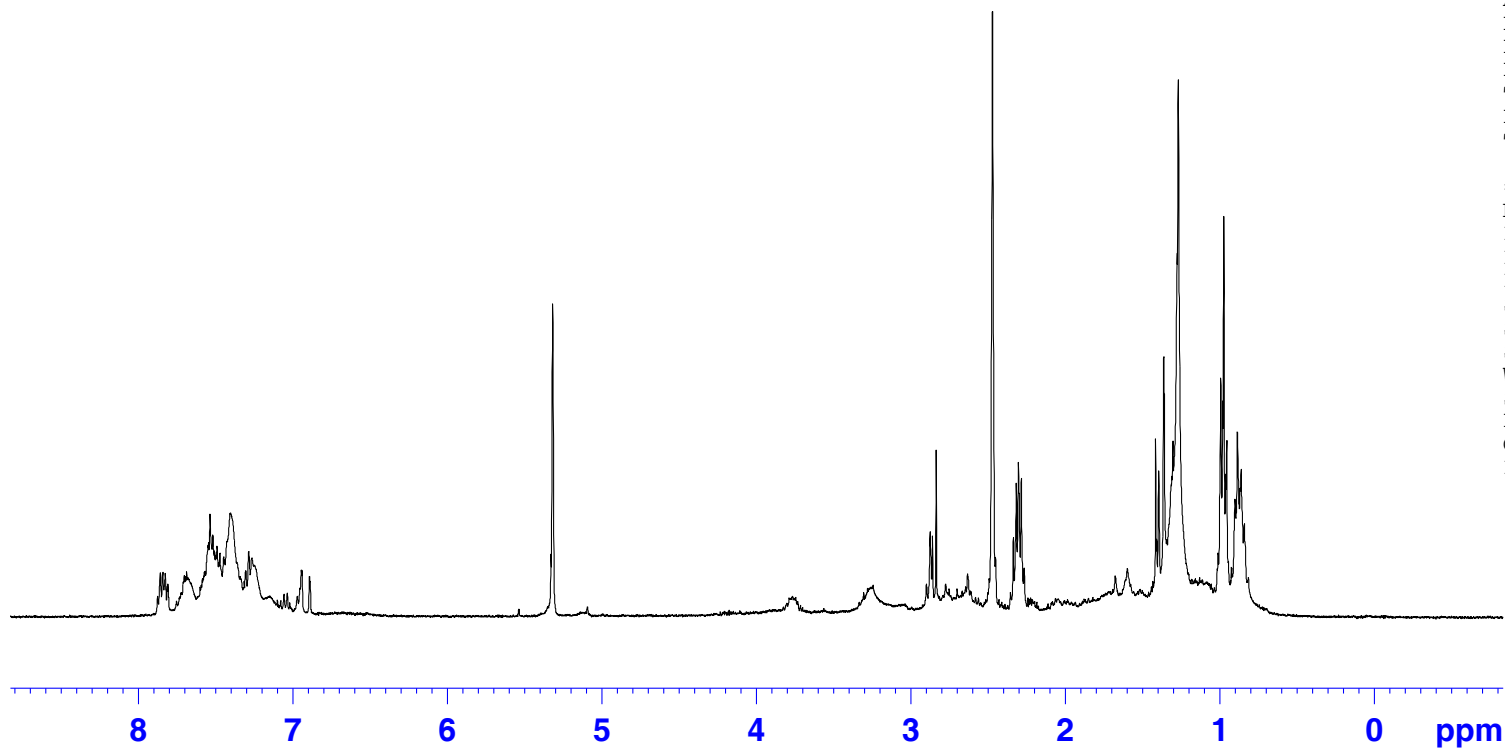


^1H [PtCl(κ^2 -P,S-Me)(P,S-Bodipy)]Cl (17)

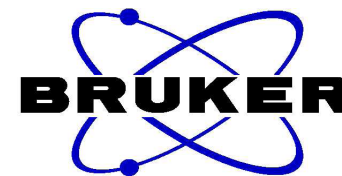


```
NAME          Paper
EXPNO          63
PROCNO         1
Date_          20121208
Time           14.40
INSTRUM        spect
PROBHD 5 mm PABBO BB-
PULPROG        zg30
TD             65536
SOLVENT        CD2Cl2
NS             16
DS             2
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ             3.9846387 sec
RG             181
DW             60.800 usec
DE             6.50 usec
TE             303.0 K
D1             1.00000000 sec
TD0            1
```

```
===== CHANNEL f1 =====
NUC1           1H
P1             15.00 usec
PL1            -0.65 dB
PL1W           14.99557495 W
SFO1           400.1624712 MHz
SI             32768
SF             400.1600143 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB             0
PC             1.00
```



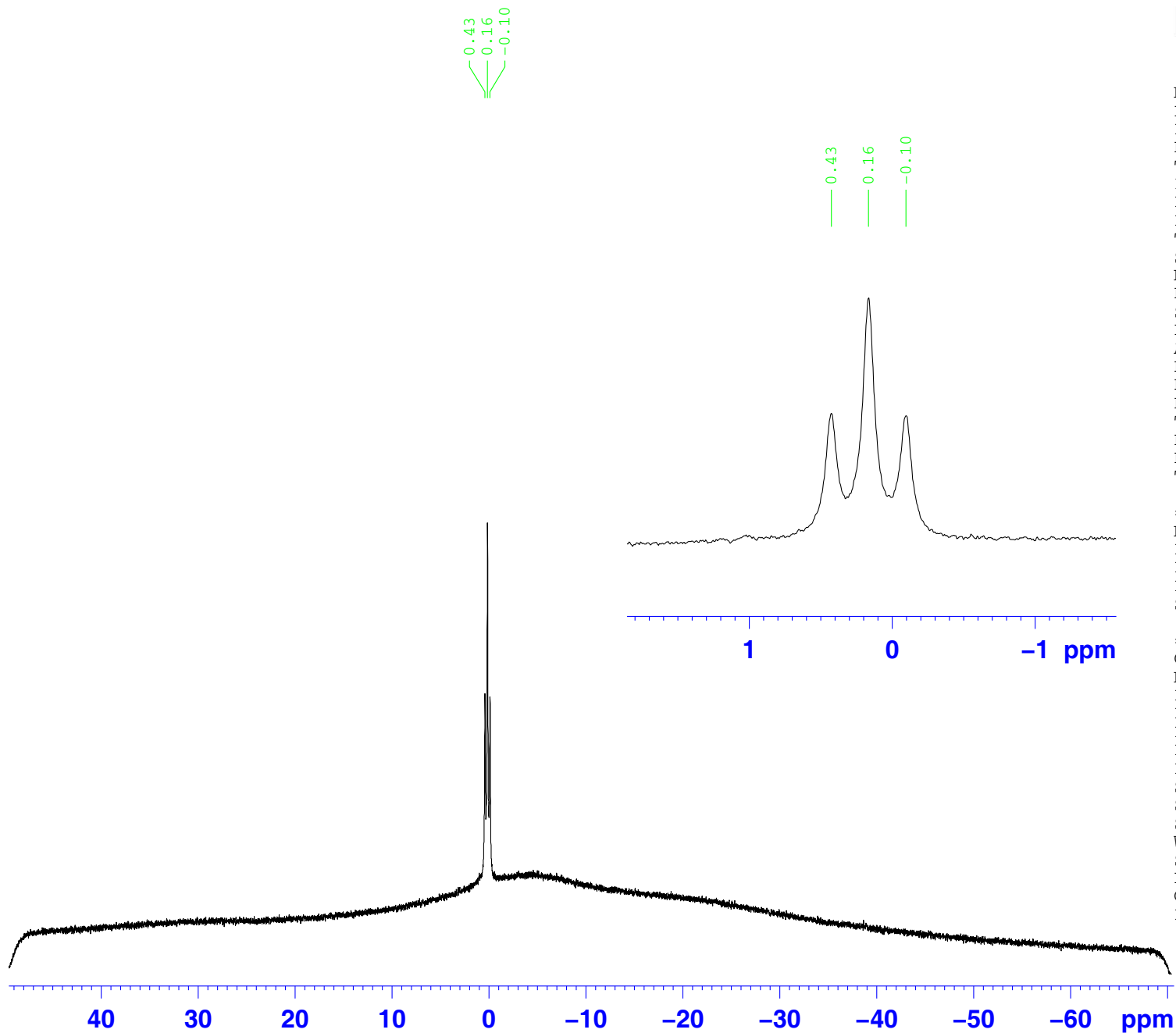
$^{11}\text{B}\{^1\text{H}\} [\text{PtCl}(\kappa^2\text{-P,S-Me})(\text{P,S-Bodipy})]\text{Cl}$ (17)



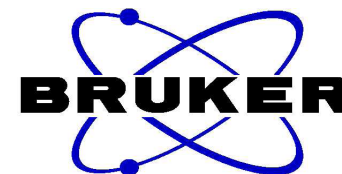
NAME Paper
EXPNO 61
PROCNO 1
Date_ 20121207
Time 14.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgig
TD 16384
SOLVENT CD2Cl2
NS 96
DS 0
SWH 15432.099 Hz
FIDRES 0.941901 Hz
AQ 0.5308916 sec
RG 812
DW 32.400 usec
DE 6.50 usec
TE 303.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^{11}B
P1 12.80 usec
PL1 1.00 dB
PL1W 17.63811874 W
SFO1 128.3859468 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ^1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.25 dB
PL2W 14.48648834 W
PL12W 0.48524728 W
SFO2 400.1616006 MHz
SI 32768
SF 128.3873041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



^{19}F [PtCl(κ^2 -P,S-Me)(P,S-Bodipy)]Cl (17)



```

NAME          Paper
EXPNO          62
PROCNO         1
Date_          20121207
Time           14.09
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zgfhigqn
TD             131072
SOLVENT        CD2Cl2
NS              41
DS              4
SWH            89285.711 Hz
FIDRES         0.681196 Hz
AQ             0.7340532 sec
RG             2050
DW             5.600 usec
DE             6.50 usec
TE             303.0 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0            1
  
```

```

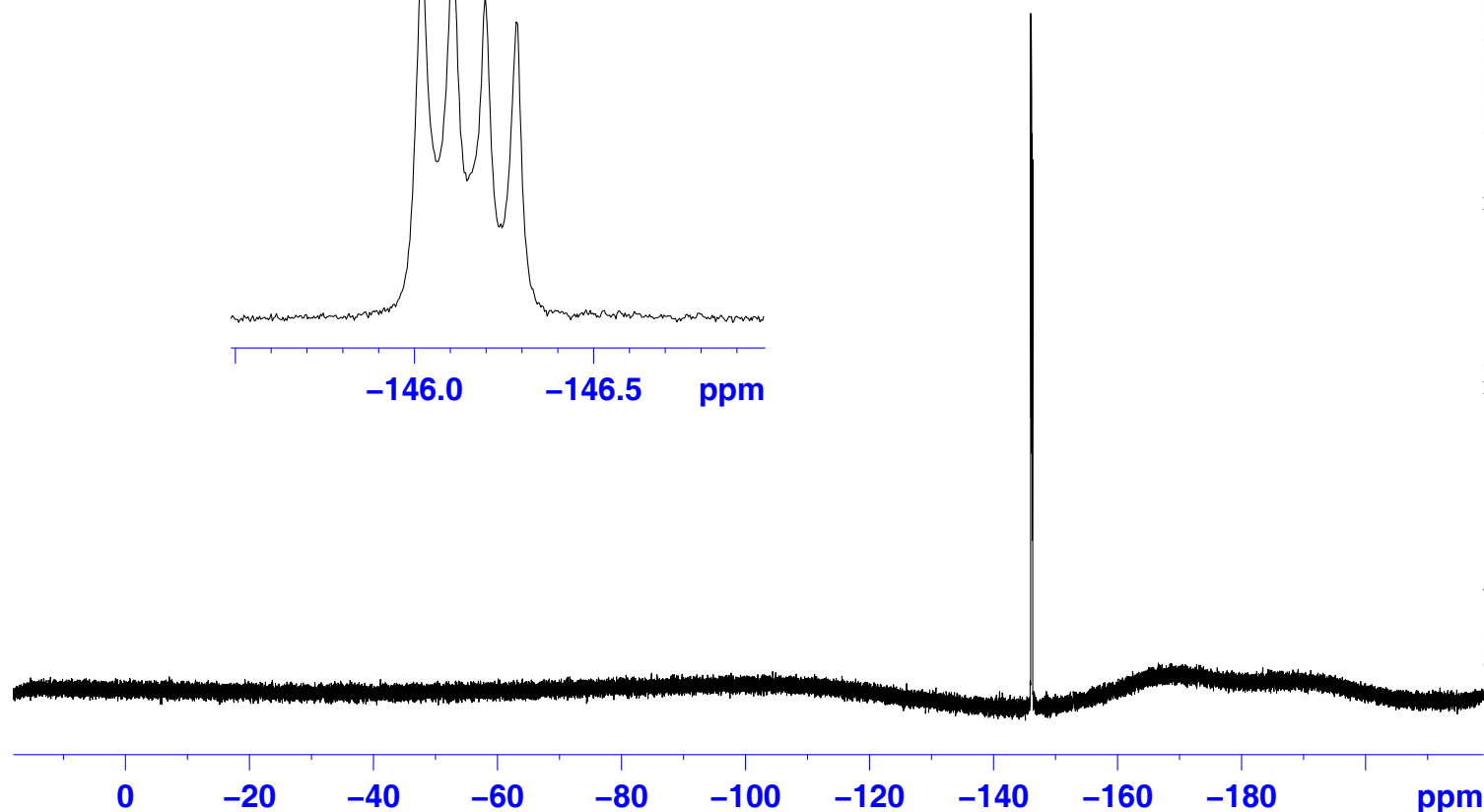
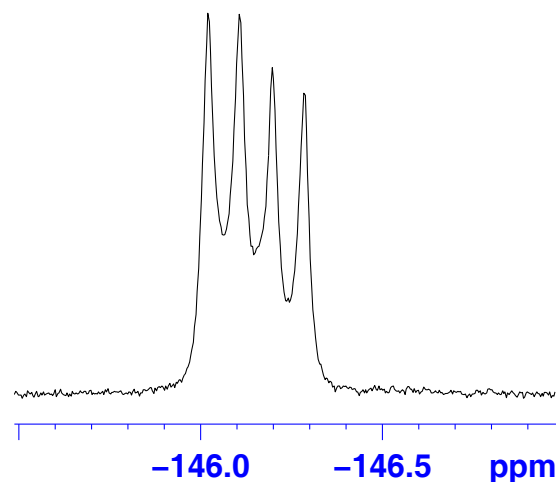
===== CHANNEL f1 =====
NUC1           19F
P1             19.50 usec
PL1            -4.00 dB
PL1W           22.71446419 W
SFO1           376.4889418 MHz
  
```

```

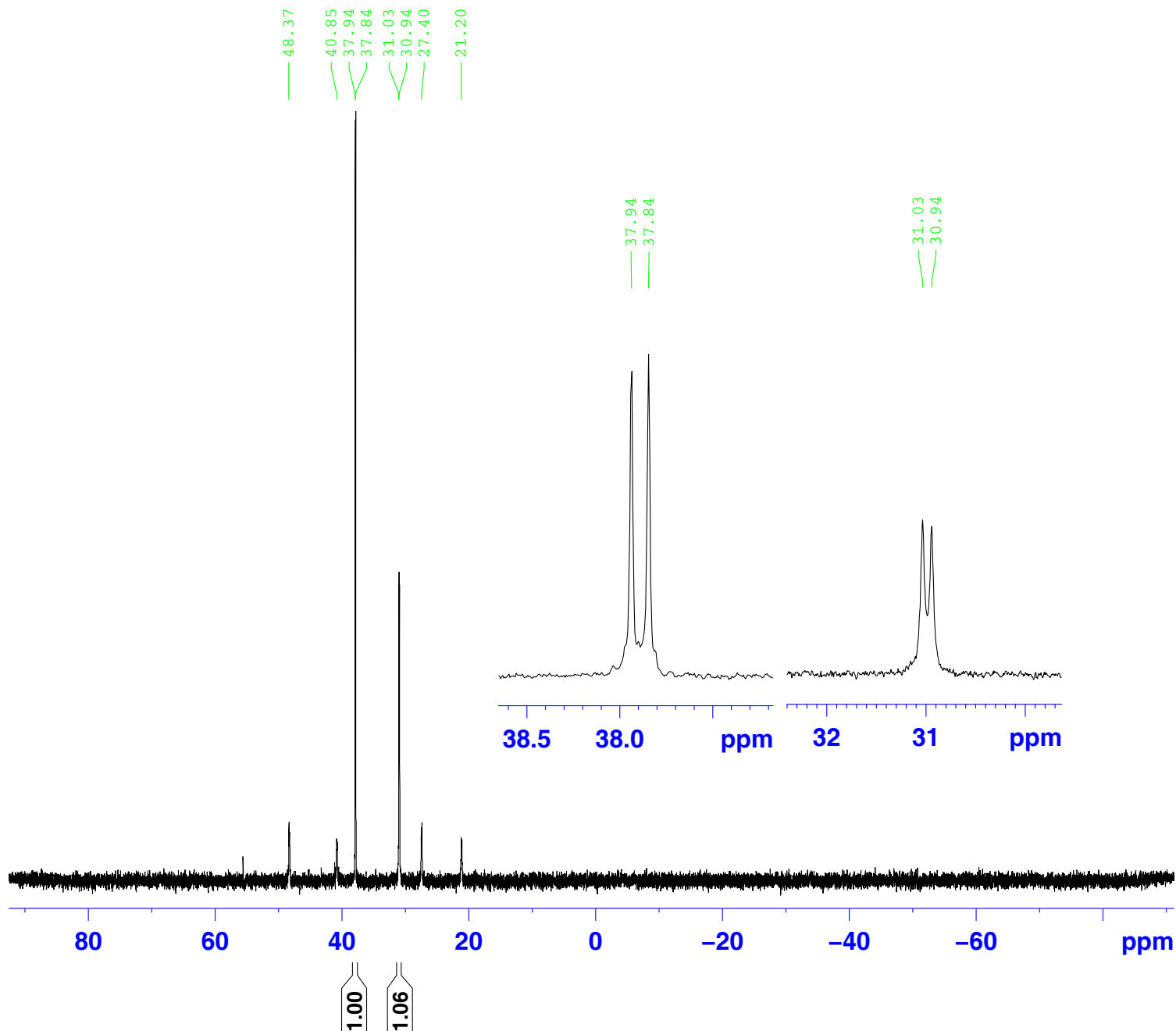
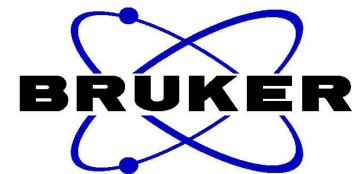
===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2            1H
PCPD2          112.00 usec
PL2            -4.00 dB
PL12           18.00 dB
PL2W           32.43120575 W
PL12W          0.20462708 W
SFO2           400.1616006 MHz
SI             65536
SF             376.5267678 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB             0
PC             1.00
  
```

-146.02
-146.11
-146.20
-146.29

-146.02
-146.11
-146.20
-146.29



^{31}P { ^1H } [Pt($\kappa^2\text{-P,S-Me}$)($\kappa^2\text{-P,S-Bodipy}$)] 2BF_4 (18)

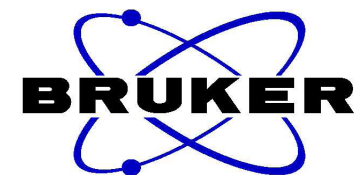


NAME Paper
EXPNO 68
PROCNO 1
Date_ 20121210
Time 12.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD 2Cl_2
NS 220
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 2050
DW 7.800 usec
DE 6.50 usec
TE 303.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^{31}P
P1 14.90 usec
PL1 1.95 dB
PL1W 16.51342773 W
SFO1 161.9796378 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ^1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 14.25 dB
PL13 16.25 dB
PL2W 14.48648834 W
PL12W 0.48524728 W
PL13W 0.30617034 W
SFO2 400.1616006 MHz
SI 32768
SF 161.9876419 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

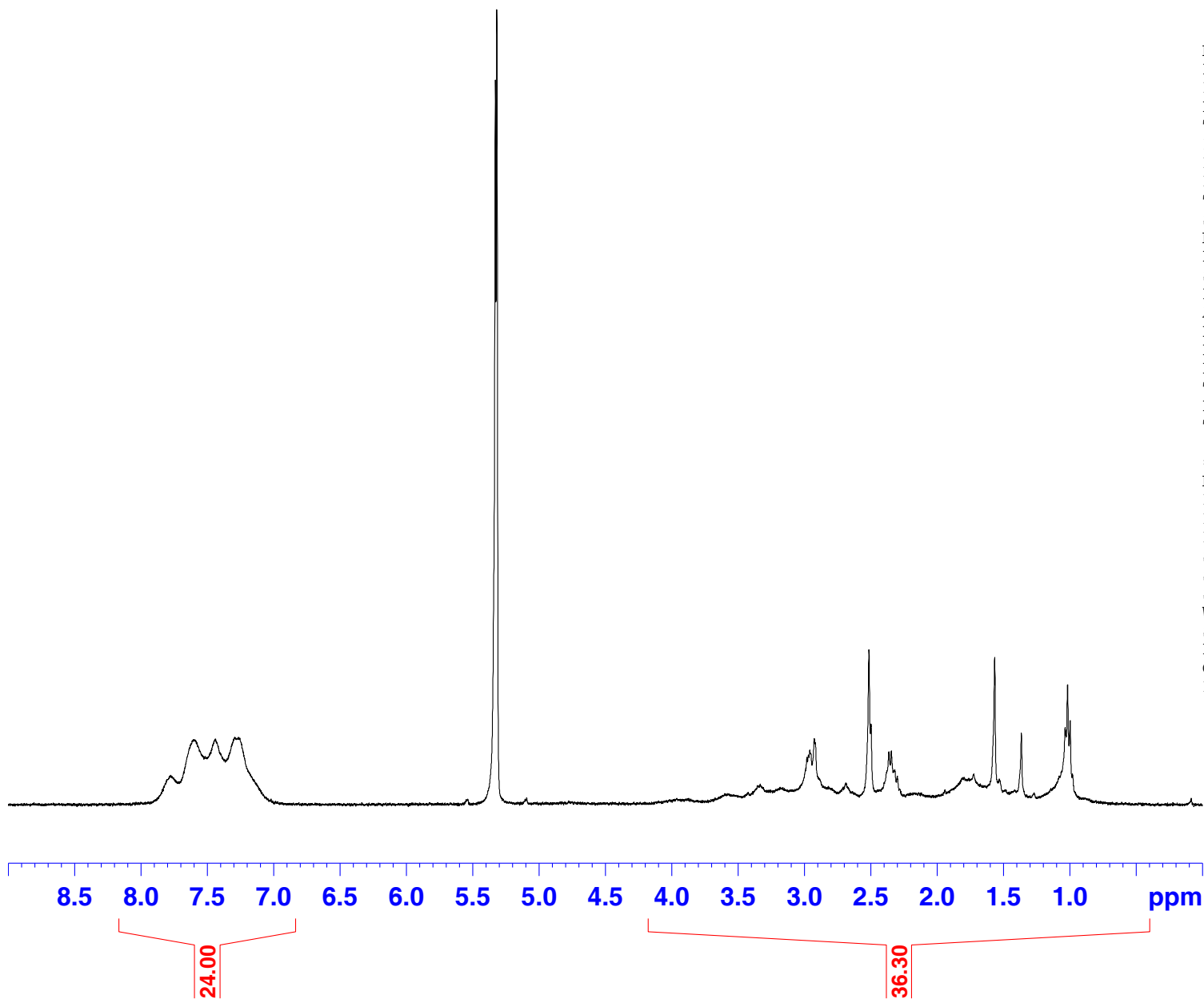
^1H [Pt(κ^2 -P,S-Me)(κ^2 -P,S-Bodipy)] 2BF_4 (18)



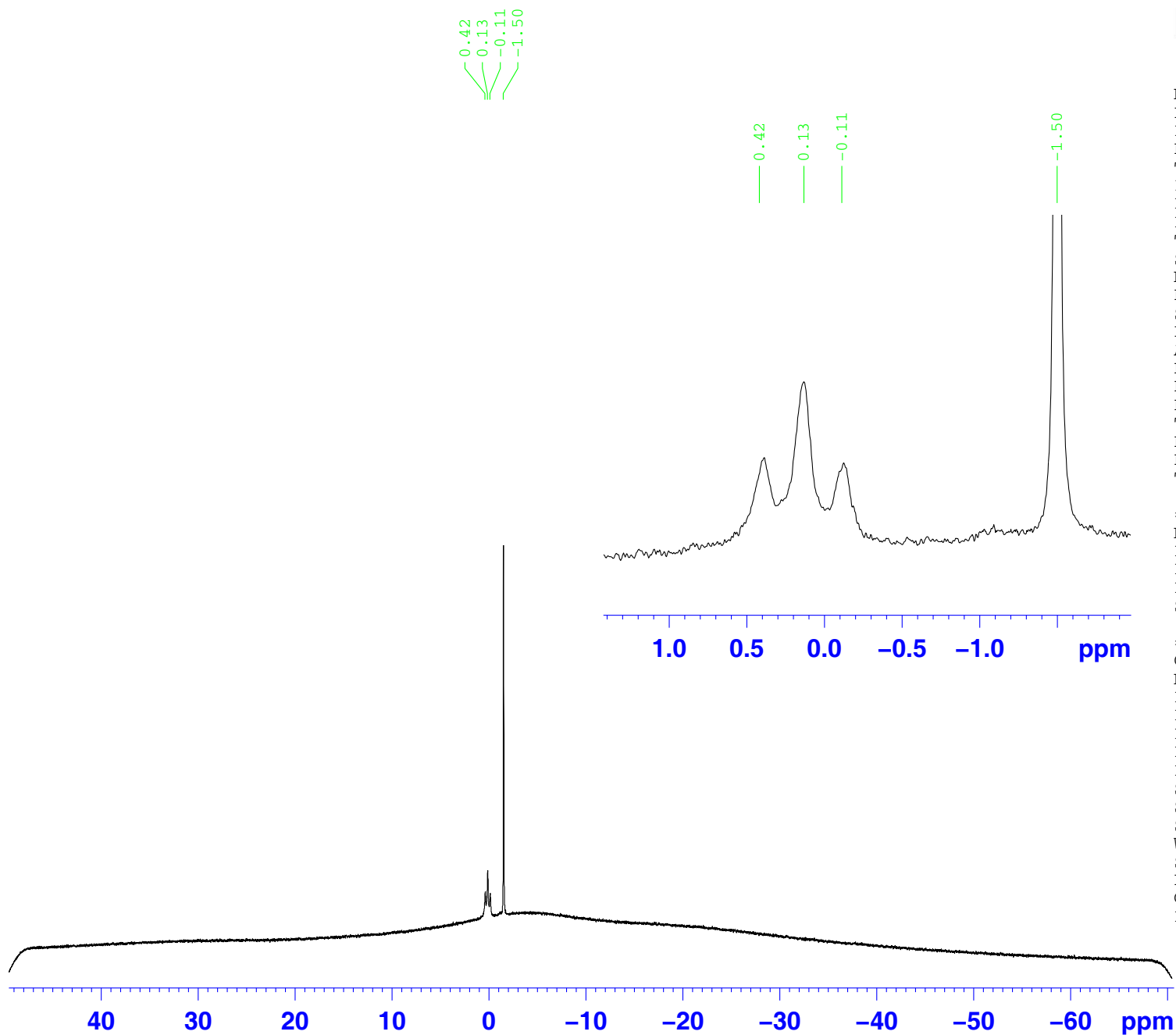
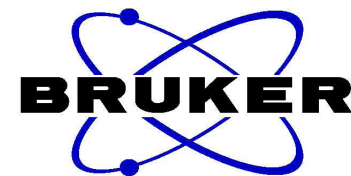
NAME	Paper
EXPNO	70
PROCNO	1
Date_	20121210
Time	14.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CD 2Cl_2
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	322
DW	60.800 usec
DE	6.50 usec
TE	303.1 K
D1	1.00000000 sec
TD0	1

===== CHANNEL f1 =====

NUC1	^1H
P1	15.00 usec
PL1	-0.65 dB
PL1W	14.99557495 W
SFO1	400.1624712 MHz
SI	32768
SF	400.1600143 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



$^{11}\text{B}\{^1\text{H}\} [\text{Pt}(\kappa^2\text{-P}, \text{S-Me})(\kappa^2\text{-P}, \text{S-Bodipy})]_2\text{BF}_4$ (18)

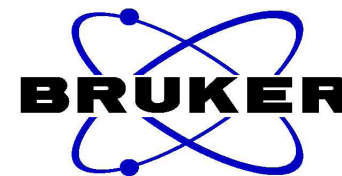


NAME Paper
 EXPNO 66
 PROCNO 1
 Date_ 20121210
 Time 15.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgig
 TD 16384
 SOLVENT CD2C12
 NS 252
 DS 0
 SWH 15432.099 Hz
 FIDRES 0.941901 Hz
 AQ 0.5308916 sec
 RG 812
 DW 32.400 usec
 DE 6.50 usec
 TE 303.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ^{11}B
 P1 12.80 usec
 PL1 1.00 dB
 PL1W 17.63811874 W
 SFO1 128.3859468 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ^1H
 PCPD2 80.00 usec
 PL2 -0.50 dB
 PL12 14.25 dB
 PL2W 14.48648834 W
 PL12W 0.48524728 W
 SFO2 400.1616006 MHz
 SI 32768
 SF 128.3873041 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

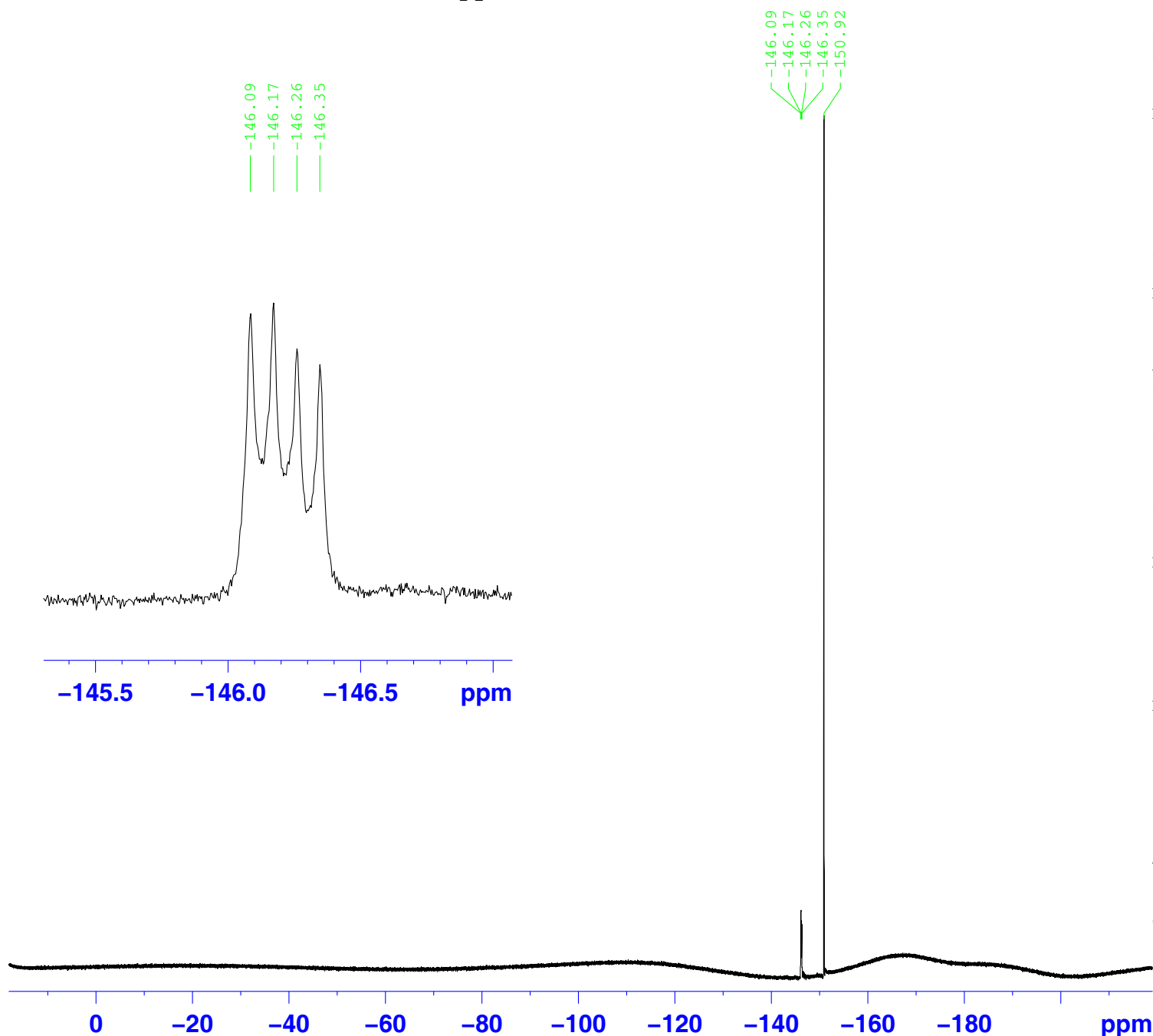
^{19}F [Pt($\kappa^2\text{-P,S-Me}$)($\kappa^2\text{-P,S-Bodipy}$)] 2BF_4 (18)



NAME Paper
EXPNO 67
PROCNO 1
Date_ 20121210
Time 15.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CD2Cl2
NS 245
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 2050
DW 5.600 usec
DE 6.50 usec
TE 303.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^{19}F
P1 19.50 usec
PL1 -4.00 dB
PL1W 22.71446419 W
SFO1 376.4889418 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ^1H
PCPD2 112.00 usec
PL2 -4.00 dB
PL12 18.00 dB
PL2W 32.43120575 W
PL12W 0.20462708 W
SFO2 400.1616006 MHz
SI 65536
SF 376.5267722 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



References

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- (2) Perdew, J. P.; Yue, W. *Phys. Rev. B* **1986**, *33*, 8800–8802.
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- (4) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785–789.
- (5) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200–1211.
- (6) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623–11627.