

# Supporting Information

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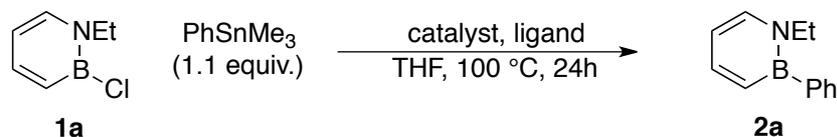
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## ***General***

All oxygen- and moisture-sensitive manipulations were carried out under an inert atmosphere using either standard Schlenk techniques or a glove box. Tetrahydrofuran, diethyl ether, dichloromethane, and pentane were purified by passing through a neutral alumina column under argon. Toluene was refluxed with sodium/benzophenone overnight and distilled. All other chemicals and solvents were purchased and used as received.  $^1\text{H}$  NMR spectra were recorded on a Varian Unity/Inova 300, Varian Inova 500 or Unity/Inova 600 spectrometer at ambient temperature.  $^{11}\text{B}$  NMR spectra were recorded on a Varian Unity/Inova 300 spectrometer at ambient temperature.  $^{13}\text{C}$  NMR spectra were recorded on a Unity/Inova 600 or Varian Inova 500 spectrometer at ambient temperature.  $^{31}\text{P}$  NMR spectra were recorded on a Varian Inova 500 spectrometer at ambient temperature.  $^{11}\text{B}$  NMR chemical shifts were externally referenced to  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  ( $\delta$  0).  $^{19}\text{F}$  NMR chemical shifts were not referenced.  $^{31}\text{P}$  NMR chemical shifts were externally referenced to 1%  $\text{H}_3\text{PO}_4$  in  $\text{D}_2\text{O}$  ( $\delta$  0).

### Catalyst Survey (Table 1)



**General Procedure.** To a 4 mL pressure vessel was added *N*-ethyl-2-chloro-1,2-azaborine **1a**<sup>1</sup> (52 mg, 0.368 mmol), trimethyl(phenyl)tin (98 mg, 0.405 mmol), the catalyst, ligand and 2.0 mL THF. The vessel was sealed and heated to 100 °C for 24h. The reaction was then cooled to room temperature, diluted with Et<sub>2</sub>O to 10 mL, and *n*-hexadecane (100 μL) as the GC internal standard was added. The yield was determined by GC analysis, and reported as the average of two trials.

**Entry 1:** The general procedure was followed, no catalyst was added. GC analysis indicated no product formation.

**Entry 2:** The general procedure was followed, using Pd(PPh<sub>3</sub>)<sub>4</sub> (21 mg, 0.018 mmol). GC analysis indicated no product formation.

**Entry 3:** The general procedure was followed, using Pd<sub>2</sub>(dba)<sub>3</sub> (8.0 mg, 0.009 mmol) and PCy<sub>3</sub> (10 mg, 0.037 mmol). GC analysis indicated no product formation.

**Entry 4:** The general procedure was followed, using Pd<sub>2</sub>(dba)<sub>3</sub> (8.0 mg, 0.009 mmol) and *rac*-BINAP (11 mg, 0.018 mmol). GC analysis indicated no product formation.

**Entry 5:** The general procedure was followed, using [Ir(cod)Cl]<sub>2</sub> (6.0 mg, 0.009 mmol). GC analysis indicated the formation of **2a** in <5% yield.

**Entry 6:** The general procedure was followed, using Rh(PPh<sub>3</sub>)<sub>3</sub>Cl (17 mg, 0.018 mmol). GC analysis indicated the formation of **2a** in 18% yield.

**Entry 7:** The general procedure was followed, using [Rh(cod)Cl]<sub>2</sub> (4.5 mg, 0.009 mmol). GC analysis indicated the formation of **2a** in 43% yield.

**Entry 8:** The general procedure was followed, using [Rh(cod)<sub>2</sub>]BF<sub>4</sub> (7.5 mg, 0.018 mmol). GC analysis indicated the formation of **2a** in 42% yield.

**Entry 9:** The general procedure was followed, using [Rh(nbd)Cl]<sub>2</sub> (4.2 mg, 0.009 mmol). GC

analysis indicated the formation of **2a** in 71% yield.

**Entry 10:** The general procedure was followed, using [Rh(nbd)<sub>2</sub>]<sub>2</sub>BF<sub>4</sub> (7 mg, 0.018 mmol). GC analysis indicated the formation of **2a** in 67% yield.

**Entry 11:** The general procedure was followed, using Rh(cod)(dppb)BF<sub>4</sub> (15 mg, 0.018 mmol). GC analysis indicated the formation of **2a** in 22% yield.

**Entry 12:** To a 20 mL vial was added chlorobis(ethylene)rhodium dimer (3.5 mg, 0.009 mmol) and *rac*-BINAP (11 mg, 0.018 mmol) followed by 2.0 mL THF. The solution was stirred for 15 min then transferred to a 4 mL pressure vessel containing **1a** (52 mg, 0.368 mmol) and trimethyl(phenyl)tin (98 mg, 0.405 mmol). The reaction was heated to 100 °C for 24h then cooled to room temperature, diluted with 10 mL of Et<sub>2</sub>O, and *n*-hexadecane (100 μL) as the internal standard was added. GC analysis indicated the formation of **2a** in 83% yield.

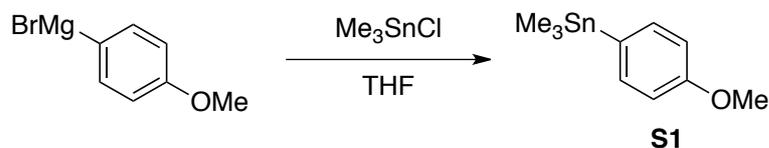
**Entry 13:** The procedure for entry 12 was followed using *p*-tolBINAP (12 mg, 0.018 mmol). GC analysis indicated the formation of **2a** in 91% yield.

**Entry 14:** The procedure for entry 12 was followed using BIPHEP (9.6 mg, 0.018 mmol). GC analysis indicated the formation of **2a** in 95% yield.

**Entry 15:** The procedure for entry 12 was followed using chlorobis(ethylene)rhodium dimer (1.4 mg, 0.0036 mmol) and BIPHEP (3.8 mg, 0.0072 mmol). GC analysis indicated the formation of **2a** in 89% yield.

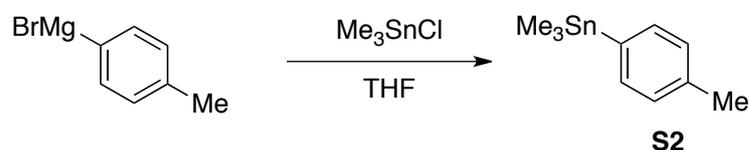
### Preparation of Arylstannanes

#### (4-Methoxyphenyl)trimethylstannane (S1) [CAS 940-00-1]:



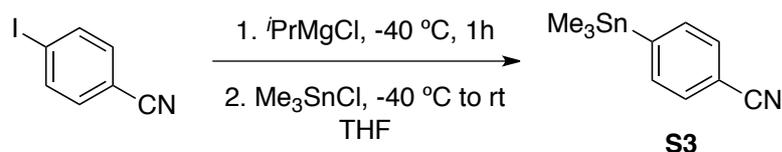
To a solution of trimethyltin chloride (1.71 g, 8.58 mmol) in THF (50 mL) was added 4-methoxyphenylmagnesium bromide (17.0 mmol, 0.5M in THF) at rt. The solution was stirred at 60 °C for 1h then cooled to rt. The reaction was quenched with saturated  $\text{NH}_4\text{Cl}$  and extracted with  $\text{Et}_2\text{O}$  (3 x 20 mL). The combined organic extracts were shaken with brine (50 mL) and dried over  $\text{Na}_2\text{SO}_4$ . After removal of volatiles under reduced pressure the crude material was purified by fractional distillation (1.47 g, 63% yield).  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45 (d,  $J = 8.4$  Hz, 2H), 6.97 (d,  $J = 8.4$  Hz, 2H), 3.85 (s, 3H), 0.31 (s, 9H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  159.92, 136.91, 132.43, 114.03, 55.03, -9.48; HRMS (EI+) calcd for  $\text{C}_{10}\text{H}_{16}\text{OSn}$  ( $\text{M}^+$ ) 272.02231, found 272.02265.

#### (4-Methylphenyl)trimethylstannane (S2) [CAS 937-12-2]:



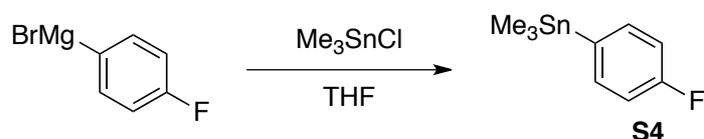
To a solution of trimethyltin chloride (2.0 g, 10.0 mmol) in THF (10 mL) was added *p*-tolylmagnesium bromide (11.0 mmol, 1.0M in THF). The solution was stirred at rt for 3h then quenched with saturated  $\text{NH}_4\text{Cl}$  and extracted with  $\text{Et}_2\text{O}$  (3 x 20 mL). The combined extracts were shaken with brine (50 mL) and dried over  $\text{Na}_2\text{SO}_4$ . After removal of volatiles under reduced pressure the crude material was purified by distillation (30 °C, 150 mTorr) (1.34 g, 48% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.43 (d,  $J = 7.7$  Hz, 2H), 7.22 (d,  $J = 7.7$  Hz, 2H), 2.38 (s, 3H), 0.31 (s, 9H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  138.27, 137.98, 135.81, 128.94, 21.40, -9.58; HRMS (EI+) calcd for  $\text{C}_{10}\text{H}_{16}\text{Sn}$  ( $\text{M}^+$ ) 256.02740, found 256.02639.

**(4-Cyanophenyl)trimethylstannane (S3) [CAS 58666-77-6]:**



To 4-iodobenzonitrile (2.00 g, 8.7 mmol) in THF (30 mL) at  $-40\text{ }^\circ\text{C}$  was added isopropylmagnesium chloride (9.6 mmol, 2M in  $\text{Et}_2\text{O}$ ). After 1h at  $-40\text{ }^\circ\text{C}$  trimethyltin chloride was added (2.09 g, 9.6 mmol) and the reaction was allowed to warm to rt. The reaction was quenched with saturated  $\text{NH}_4\text{Cl}$  and extracted with  $\text{Et}_2\text{O}$  (3 x 20 mL). The combined extracts were shaken with brine (50 mL) and dried over  $\text{Na}_2\text{SO}_4$ . The volatiles were removed under reduced pressure. (2.20 g, 95% yield)  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64-7.59 (m, 4H), 0.36 (s, 9H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  150.26, 136.30, 130.85, 119.13, 111.84, -9.49; HRMS (EI+) calcd for  $\text{C}_{10}\text{H}_{13}\text{NSn}$  ( $\text{M}^+$ ) 267.00700, found 267.00648.

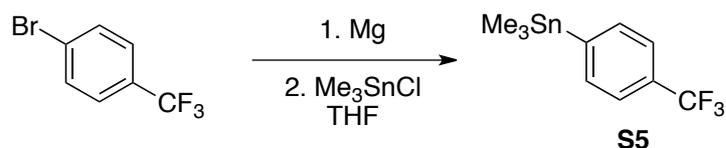
**(4-Fluorophenyl)trimethylstannane (S4) [CAS 14101-14-5]:**



To a solution of trimethyltin chloride (2.0 g, 10.0 mmol) in THF was added (4-fluorophenyl)magnesium bromide (11.0 mmol, 2.0M in  $\text{Et}_2\text{O}$ ). The solution was stirred at rt for 3h then quenched with saturated  $\text{NH}_4\text{Cl}$  and extracted with  $\text{Et}_2\text{O}$  (3 x 20mL). The combined extracts were shaken with brine (50 mL) and dried over  $\text{Na}_2\text{SO}_4$ . After removal of volatiles under reduced pressure crude material was purified by silica gel chromatography (1%  $\text{EtOAc}$ /hexanes) (v/v). (0.98 g, 38% yield)

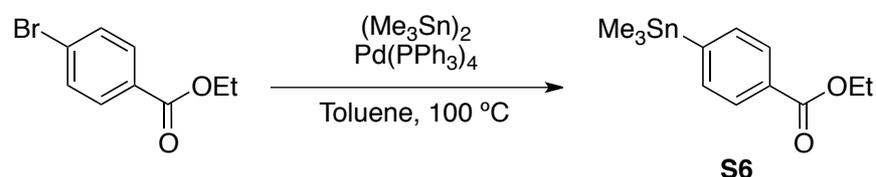
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.47 (dd,  $J = 8.3, 6.5$  Hz, 2H), 7.08 (dd,  $J = 9.5$  Hz, 8.3 Hz, 2H), 0.32 (s, 9H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  163.33 (d,  $J = 246.6$  Hz), 137.27 (d,  $J = 6.7$  Hz), 137.08, 115.18 (d,  $J = 19.1$  Hz), -9.46;  $^{19}\text{F}$  NMR (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -113.32; HRMS (EI+) calcd for  $\text{C}_9\text{H}_9\text{FSn}$  ( $\text{M}^+$ ) 260.00233, found 260.00192.

**(4-Trifluoromethylphenyl)trimethylstannane (S5) [CAS 17315-40-1]:**



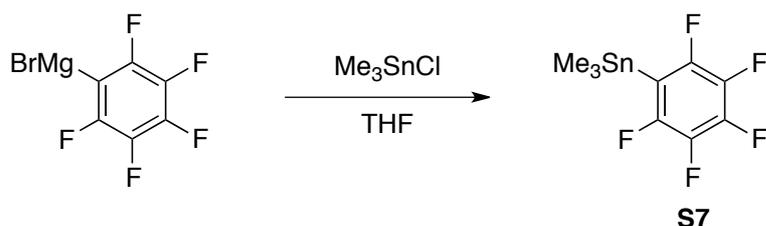
To a vigorously stirring suspension of magnesium turnings (0.55 g, 23.0 mmol) in THF (40 mL) was added 4-bromobenzotrifluoride (4.0 g, 17.8 mmol) and 4 drops of 1,2-dibromoethane. The reaction was brought to reflux for 16h. After cooling to rt, trimethyltin chloride (1.77 g, 8.88 mmol) was added and the solution was refluxed for 2h. The reaction was cooled to rt and quenched with saturated NH<sub>4</sub>Cl and extracted with Et<sub>2</sub>O (3 x 20 mL). The combined extracts were shaken with brine (50 mL) and dried over Na<sub>2</sub>SO<sub>4</sub>. Volatiles were removed under reduced pressure and crude material was purified by silica gel chromatography (hexanes) (0.80 g, 15%). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.74-7.48 (m, 4H), 0.36 (s, 9H); <sup>19</sup>F NMR (282 MHz, CDCl<sub>3</sub>) δ -62.85. These spectroscopic data correspond to previously reported data.<sup>2</sup>

**Ethyl 4-(trimethylstannyl)benzoate (S6) [CAS 69849-40-7]:**



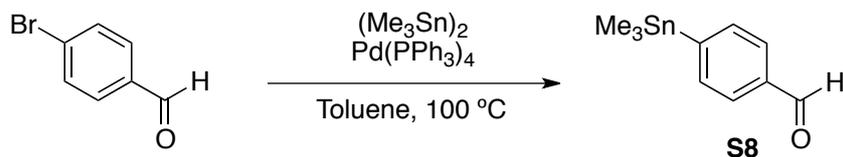
To ethyl 4-bromobenzoate (1.0 g, 5.4 mmol) in 15 mL toluene was added tetrakis(triphenylphosphine)palladium (0.31 g, 0.27 mmol), and hexamethylditin (2.29 g, 7.0 mmol). The solution was brought to 100 °C for 24h then cooled to rt. After removal of volatiles under reduced pressure the crude material was purified by silica gel chromatography (5% EtOAc/hexanes) (v/v) (0.64 g, 47% yield). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.00 (d, *J* = 8.1 Hz, 2H), 7.60 (d, *J* = 8.1 Hz, 2H), 4.40 (q, *J* = 7.2 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H), 0.35 (s, 9H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 166.94, 149.44, 135.73, 130.19, 128.48, 60.85, 14.35, -9.53; HRMS (EI+) calcd for C<sub>12</sub>H<sub>18</sub>O<sub>2</sub>Sn (M<sup>+</sup>) 314.03288, found 314.03348.

**(Pentafluorophenyl)trimethyltin (S7) [CAS 1015-53-8]:**



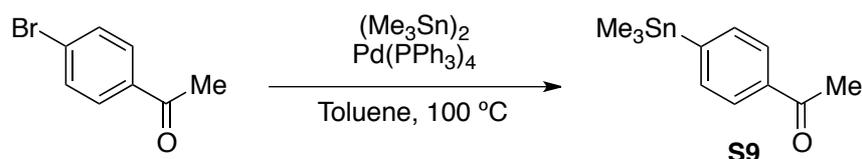
To a solution of trimethyltin chloride (2.0 g, 10.0 mmol) in THF (10 mL) was added pentafluorophenylmagnesium bromide (11.0 mmol, 0.5M in THF). The solution was stirred at rt for 1h then quenched with saturated  $\text{NH}_4\text{Cl}$  and extracted with  $\text{Et}_2\text{O}$  (3 x 20 mL). The combined extracts were shaken with brine (50 mL) and dried over  $\text{Na}_2\text{SO}_4$ . After removal of volatiles under reduced pressure the crude material was purified by distillation (35-45 °C, 150 mTorr) (2.16 g, 30% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  0.50 (s, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  150.48-147.07 (m), 143.26-139.85 (m), 138.55-135.08 (m), 112.05-109.70 (m), -7.57 (t,  $J = 2.4$  Hz);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -121.64 (m, 2F), -152.82 (tt,  $J = 19.4$ , 2.1 Hz, 1F), -160.70 (m, 2F); HRMS (EI+) calcd for  $\text{C}_9\text{H}_9\text{F}_5\text{Sn}$  ( $\text{M}^+$ ) 331.96464, found 331.96403.

**(4-Formylphenyl)trimethylstannane (S8) [CAS 65488-26-8]:**



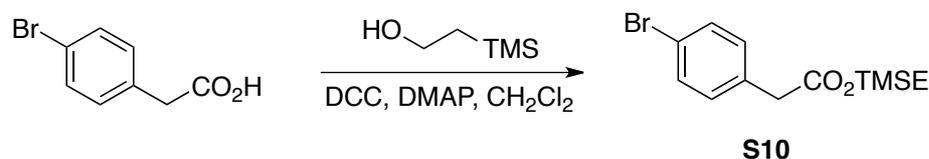
To a solution of 4-bromobenzaldehyde (1.0 g, 5.4 mmol) in toluene (20 mL) was added tetrakis(triphenylphosphine)palladium (0.31 g, 0.27 mmol), and hexamethylditin (2.29 g, 7.0 mmol). The solution was brought to 100 °C for 24h then cooled to rt. Volatiles were removed under reduced pressure and the crude material was passed through a plug of silica gel (10% EtOAc/hexanes) (v/v). Distillation provided **S7** (0.60 g, 41% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.03 (s, 1H), 7.84 (d,  $J = 7.9$  Hz, 2H), 7.71 (d,  $J = 7.9$  Hz, 2H), 0.37 (s, 9H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  192.76, 152.43, 136.36, 136.11, 128.59, -9.49; HRMS (EI+) calcd for  $\text{C}_{10}\text{H}_{14}\text{OSn}$  ( $\text{M}^+$ ) 270.00667, found 270.00533.

**(4-Acetylphenyl)trimethylstannane (S9) [CAS 58666-79-8]:**



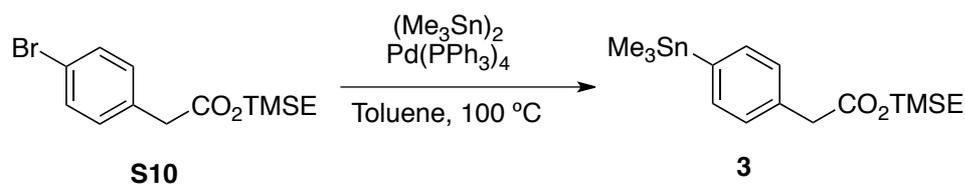
To a solution of 4-bromoacetophenone (1.0 g, 5.4 mmol) in toluene (15 mL) was added tetrakis(triphenylphosphine)palladium (0.31 g, 0.27 mmol), and hexamethylditin (2.29 g, 7.0 mmol). The solution was brought to  $100\text{ }^\circ\text{C}$  for 24h then cooled to rt. After removal of volatiles under reduced pressure the crude material was purified by silica gel chromatography (10% EtOAc/hexanes) (v/v) (1.22 g, 66% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (d,  $J = 8.1$  Hz, 2H), 7.64 (d,  $J = 8.0$  Hz, 2H), 2.62 (s, 3H), 0.35 (s, 9H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  198.49, 150.18, 136.80, 136.01, 127.22, 26.57, -9.53; HRMS (EI+) calcd for  $\text{C}_{11}\text{H}_{16}\text{OSn}$  ( $\text{M}^+$ ) 284.02231, found 284.02317.

**(2-Trimethylsilyl)ethyl 4-bromophenylacetate (S10) [CAS 483334-56-1]:**



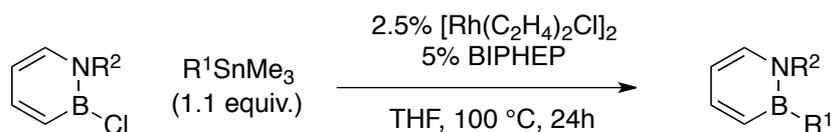
To a solution of 4-bromophenylacetic acid (2.00 g, 9.32 mmol) in  $\text{CH}_2\text{Cl}_2$  (40 mL) was added 4-dimethylaminopyridine (56 mg, 0.48 mmol),  $N,N'$ -dicyclohexylcarbodiimide (2.12 g, 10.2 mmol) and 2-(trimethylsilyl)ethanol (2.20 g, 18.6 mmol). The reaction was stirred at rt for 14h. The crude material was filtered through a medium porosity frit and volatiles were removed under reduced pressure. Purification by silica gel chromatography (5% EtOAc/hexanes) (v/v) provided **S10** (2.50 g, 85% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.50 (d,  $J = 8.3$  Hz, 2H), 7.21 (d,  $J = 8.4$  Hz, 2H), 4.31-4.13 (m, 2H), 3.59 (s, 2H), 1.13-0.93 (m, 2H), 0.07 (s, 9H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  170.93, 133.60, 131.46, 131.12, 120.77, 63.15, 40.75, 17.16, -1.89; HRMS (EI+) calcd for  $\text{C}_{13}\text{H}_{19}\text{BrO}_2\text{Si}$  ( $\text{M}^+$ ) 314.03377, found 314.03434.

**(2-Trimethylsilyl)ethyl (4-trimethylstannyl)phenylacetate (3):**



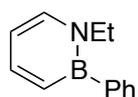
To **S10** (1.00 g, 3.17 mmol) in 15 mL toluene was added tetrakis(triphenylphosphine)palladium (0.37 g, 0.32 mmol), and hexamethylditin (2.08 g, 6.34 mmol). The solution was brought to 100 °C for 24h then cooled to rt. After removal of volatiles under reduced pressure the crude material was purified by silica gel chromatography (1% EtOAc/hexanes) (v/v) (0.49 g, 39% yield). <sup>1</sup>H NMR (500 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 7.50 (d, *J* = 7.7 Hz, 2H), 7.28 (d, *J* = 7.4 Hz, 2H), 4.24-4.18 (m, 2H), 3.61 (s, 2H), 1.08-0.99 (m, 2H), 0.32 (s, 9H), 0.08 (s, 9H); <sup>13</sup>C NMR (126 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 178.57, 147.69, 142.95, 141.43, 135.94, 69.98, 48.37, 24.22, 5.15, -2.97; HRMS (EI+) calcd for C<sub>16</sub>H<sub>28</sub>O<sub>2</sub>SiSn (M<sup>+</sup>) 400.08806, found 400.08763.

### Substrate scope (Table 2)



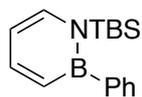
**General procedure.** To a 20 mL vial was added chlorobis(ethylene)rhodium dimer (7.0 mg, 0.018 mmol) and BIPHEP (19 mg, 0.037 mmol) followed by 2.0 mL THF. The solution was stirred for 15 min, then transferred to a 15 mL pressure vessel containing **1a** (104 mg, 0.736 mmol) and the arylstannane (0.810 mmol) in 2.0 mL THF. The vessel was sealed and heated at 100 °C for 24 h. The reaction was allowed to cool to room temperature, and volatiles were removed under reduced pressure. Purification of crude material by silica gel chromatography (ether/pentane) provides the product.

### Compound 2a:



The general procedure was followed using trimethyl(phenyl)tin (196 mg, 0.810 mmol) (107 mg, 79% yield). A duplicate reaction gave 74% yield. <sup>1</sup>H NMR (300 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 7.80 (m, 1H), 7.70 (m, 2H), 7.58-7.24 (m, 4H), 6.98 (dd, *J* = 10.8, 1.7 Hz, 1H), 6.57 (td, *J* = 6.6, 1.6 Hz, 1H), 4.01 (q, *J* = 7.2 Hz, 2H), 1.44 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 142.64, 142 (br), 138.23, 132.82, 131 (br), 127.69, 127.36, 111.55, 48.35, 18.35; <sup>11</sup>B NMR (96 MHz) δ 35.32. These spectroscopic data correspond to previously reported data.<sup>1</sup>

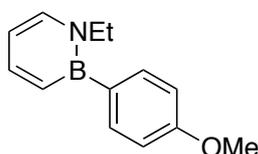
### Compound 2b:



To a 20 mL vial was added chlorobis(ethylene)rhodium dimer (4.3 mg, 0.011 mmol) and BIPHEP (11 mg, 0.021 mmol) followed by 1.0 mL THF. The solution was stirred for 15 min then transferred to a 15 mL pressure vessel containing *N*-TBS-2-chloro-1,2-azaborine **1b**<sup>3</sup> (100 mg, 0.44 mmol) and trimethyl(phenyl)tin (116 mg, 0.48 mmol) in 1.0 mL THF. The pressure vessel was sealed and heated at 100 °C for 24 h. The reaction was allowed to cool to

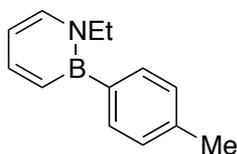
room temperature, and volatiles were removed under reduced pressure. Purification of crude material by silica gel chromatography (ether/pentane) provides **2b** (90 mg, 76% yield). A duplicate reaction gave 74% yield.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.66 (dd,  $J = 10.8$  Hz, 6.3 Hz, 1H), 7.51 (d,  $J = 6.8$  Hz, 1H), 7.45 (m, 2H), 7.34 (m, 3H), 6.73 (d,  $J = 10.9$  Hz, 1H), 6.51 (m, 1H), 0.98 (s, 9H), 0.13 (s, 6H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  146 (br), 142.84, 138.26, 133 (br), 132.00, 126.67, 126.55, 111.84, 26.74, 18.86, -2.26;  $^{11}\text{B}$  NMR (96 MHz)  $\delta$  38.04; HRMS (EI+) calcd for  $\text{C}_{16}\text{H}_{24}\text{BNSi}$  ( $\text{M}^+$ ) 269.17711, found 269.17646.

### Compound 2c:



The general procedure was followed using (4-methoxyphenyl)trimethylstannane (**S1**) (219 mg, 0.810 mmol) (125 mg, 80%) A duplicate reaction gave 75% yield.  $^1\text{H}$  NMR (300 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.69 (m, 1H), 7.56 (m, 2H), 7.37 (d,  $J = 6.6$  Hz, 1H), 7.03 (m, 2H), 6.87 (m 1H), 6.46 (td,  $J = 6.6$  Hz, 1.6Hz, 1H), 3.96 (q,  $J = 7.2$  Hz, 2H), 3.90 (s, 3H), 1.40 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  158.68, 141.67, 137.58, 133.63, 133 (br), 131 (br), 112.62, 110.51, 54.30, 47.50, 17.59;  $^{11}\text{B}$  NMR (96 MHz)  $\delta$  35.71; HRMS (EI+) calcd for  $\text{C}_{13}\text{H}_{16}\text{BNO}$  ( $\text{M}^+$ ) 213.13250, found 213.13230.

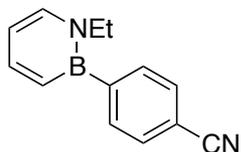
### Compound 2d:



The general procedure was followed using (4-methylphenyl)trimethylstannane (**S2**) (206 mg, 0.810 mmol) (102 mg, 70% yield). A duplicate reaction gave 77% yield.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.67 (dd,  $J = 10.7$  Hz, 6.5 Hz, 1H), 7.49 (d,  $J = 7.7$  Hz, 2H), 7.35 (d, 1H,  $J = 6.8$  Hz, 1H), 7.27 (d,  $J = 7.5$  Hz, 2H), 6.84 (d,  $J = 10.9$  Hz, 1H), 6.45 (t,  $J = 6.6$  Hz, 1H), 3.92 (q,  $J = 7.2$  Hz, 2H), 2.43 (s, 3H), 1.36 (t,  $J = 7.2\text{Hz}$ , 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  141.72, 138 (br), 137.51, 136.31, 132.16, 131 (br), 127.71, 110.59, 47.55, 20.47, 17.60;  $^{11}\text{B}$

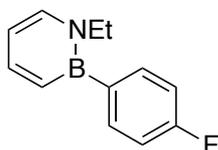
NMR (96 MHz)  $\delta$  35.76; HRMS (EI+) calcd for  $C_{13}H_{16}BN$  ( $M^+$ ) 197.13758, found 197.13710.

**Compound 2e:**



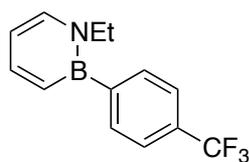
The general procedure was followed using (4-cyanophenyl)trimethylstannane (**S3**) (215 mg, 0.810 mmol) (81% yield). A duplicate reaction gave 80% yield.  $^1H$  NMR (600 MHz,  $CD_2Cl_2$ )  $\delta$  7.69 (m, 5H), 7.41 (d,  $J = 4.4$  Hz, 1H), 6.84 (dd,  $J = 10.8$  Hz, 0.9 Hz, 1H), 6.54 (dt,  $J = 1.5$  Hz  $J = 6.7$  Hz, 1H), 3.89 (q,  $J = 7.0$  Hz, 2H), 1.35 (t,  $J = 7.0$  Hz, 3H);  $^{13}C$  NMR (150 MHz,  $CD_2Cl_2$ )  $\delta$  148 (br), 143.20, 138.32, 133.15, 130.98, 131 (br), 119.32, 112.21, 110.89, 48.46, 18.25;  $^{11}B$  NMR (96 MHz)  $\delta$  35.10; HRMS (EI+) calcd for  $C_{13}H_{13}BN_2$  ( $M^+$ ) 208.11719, found 208.11641.

**Compound 2f:**



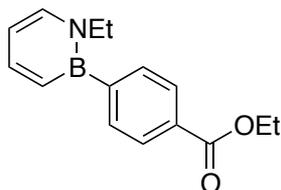
The general procedure was followed using (4-fluorophenyl)trimethylstannane (**S4**) (210 mg, 0.810 mmol) (122 mg, 78% yield). A duplicate reaction gave 77% yield.  $^1H$  NMR (300 MHz,  $CD_2Cl_2$ )  $\delta$  7.71 (m, 1H), 7.59 (dd,  $J = 8.3$  Hz, 6.3 Hz, 2H), 7.39 (d,  $J = 6.7$  Hz, 1H), 7.17 (m, 2H), 6.85 (m, 1H), 6.50 (m, 1H), 3.92 (q,  $J = 7.2$  Hz, 2H), 1.37 (t,  $J = 7.2$  Hz, 3H);  $^{13}C$  NMR (150 MHz,  $CD_2Cl_2$ )  $\delta$  162.8 (d,  $J = 245$  Hz), 142.64, 138.21, 134.5 (d,  $J = 7.3$  Hz), 131 (br), 114.4 (d,  $J = 19.6$  Hz) 111.53, 48.22, 18.17 (one C bonded to B was not observed);  $^{11}B$  NMR (96 MHz)  $\delta$  35.45;  $^{19}F$  NMR (282 MHz)  $\delta$  -115.6 (m); HRMS (EI+) calcd for  $C_{12}H_{13}BFN$  ( $M^+$ ) 201.11251, found 201.11244.

### Compound 2g:



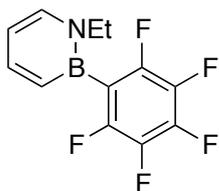
The general procedure was followed using (4-trifluoromethylphenyl)-trimethylstannane (**S5**) (250 mg, 0.810 mmol) (95 mg, 51% yield). A duplicate reaction gave 61% yield.  $^1\text{H}$  NMR (300 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.73 (m, 5H), 7.42 (d,  $J = 6.7$  Hz, 1H), 6.87 (dd,  $J = 10.8$  Hz, 1.7 Hz, 1H), 6.56 (dt,  $J = 6.6$  Hz, 1.6 Hz, 1H), 3.91 (q,  $J = 7.0$  Hz, 2H), 1.37 (t,  $J = 7.0$  Hz, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  147 (br), 142.95, 138.19, 132.86, 131 (br), 128.97 (q,  $J = 32$  Hz), 124.70 (q,  $J = 272$  Hz), 124.04 (q,  $J = 4.0$  Hz), 111.91, 48.37, 18.15;  $^{11}\text{B}$  NMR (96 MHz)  $\delta$  35.45;  $^{19}\text{F}$  NMR (282 MHz)  $\delta$  -62.75 (s); HRMS (EI+) calcd for  $\text{C}_{13}\text{H}_{13}\text{BF}_3\text{N}$  ( $\text{M}^+$ ) 251.10932, found 251.10905.

### Compound 2h:



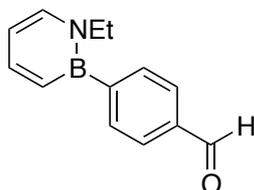
The general procedure was followed using ethyl 4-(trimethylstannyl)benzoate (**S6**) (254 mg, 0.810 mmol) (132 mg, 70% yield). A duplicate reaction gave 80% yield.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  8.06 (d,  $J = 8.3$  Hz, 2H), 7.68 (dd,  $J = 10.8$  Hz, 6.5 Hz, 1H), 7.63 (d,  $J = 8.1$  Hz, 2H), 7.35 (d,  $J = 6.8$  Hz, 1H), 6.81 (d,  $J = 10.8$  Hz, 1H), 6.48 (td,  $J = 6.6$  Hz, 1.4 Hz, 1H), 4.39 (q,  $J = 7.1$  Hz, 2H), 3.85 (q,  $J = 7.2$  Hz, 2H), 1.42 (t,  $J = 7.1$  Hz, 3H), 1.30 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  166.70, 147 (br), 142.81, 138.20, 132.55, 131 (br), 129.32, 128.30, 111.78, 60.72, 48.40, 18.17, 14.14;  $^{11}\text{B}$  NMR (96 MHz)  $\delta$  35.30; HRMS (EI+) calcd for  $\text{C}_{15}\text{H}_{18}\text{BNO}_2$  ( $\text{M}^+$ ) 255.14306, found 255.14276.

### Compound 2i:



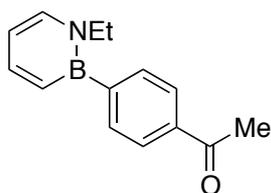
The general procedure was followed using (pentafluorophenyl)trimethyltin (**S7**) (300 mg, 0.810 mmol) and a reaction time of 48h (77 mg, 38% yield). A duplicate reaction gave 41% yield.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.73 (dd,  $J = 10.5$  Hz, 6.7 Hz, 1H), 7.47 (d,  $J = 6.7$  Hz, 1H), 6.82 (d,  $J = 10.8$  Hz, 1H), 6.59 (td,  $J = 6.7$  Hz, 1.4 Hz, 1H), 3.74 (q,  $J = 7.3$  Hz, 2H), 1.28 (t,  $J = 7.3$  Hz, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  146.1 (m,  $J = 242$  Hz), 143.42; 140.8 (m,  $J = 252$  Hz), 138.65, 137.3 (m,  $J = 250$  Hz), 130 (br), 113.17, 49.53, 17.62 (one C bonded to B was not observed);  $^{11}\text{B}$  NMR (96 MHz)  $\delta$  31.45;  $^{19}\text{F}$  NMR (282 MHz)  $\delta$  -131.8 (m, 2F), -156.0 (m, 1F), -163.2 (m, 2F); HRMS (EI+) calcd for  $\text{C}_{12}\text{H}_9\text{BF}_5\text{N}$  ( $\text{M}^+$ ) 273.07483, found 273.07504.

### Compound 2j:



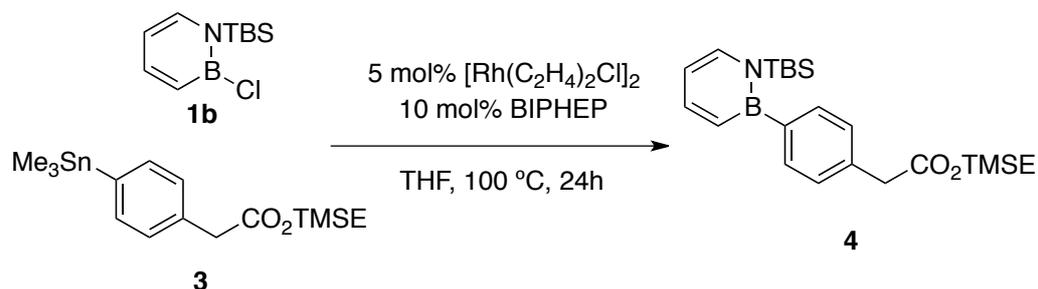
The general procedure was followed using (4-formylphenyl)trimethylstannane (**S8**) (218 mg, 0.810 mmol) (65 mg, 41% yield). A duplicate reaction gave 38% yield.  $^1\text{H}$  NMR (300 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  10.09 (s, 1H), 7.94 (d,  $J = 8.2$  Hz, 2H), 7.74 (m, 3H), 7.41 (d,  $J = 4.4$  Hz, 1H), 6.84 (dd,  $J = 10.8$  Hz, 0.9 Hz, 1H), 6.54 (t,  $J = 6.4$  Hz, 1H), 3.89 (q,  $J = 7.2$  Hz, 2H), 1.35 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  191.82, 149 (br), 142.31, 137.60, 134.75, 132.46, 130 (br), 127.88, 111.31, 47.81, 17.53;  $^{11}\text{B}$  NMR (96 MHz)  $\delta$  35.45; HRMS (EI+) calcd for  $\text{C}_{13}\text{H}_{14}\text{BNO}$  ( $\text{M}^+$ ) 211.11685, found 211.11616.

### Compound 2k:



The general procedure was followed using (4-acetylphenyl)trimethylstannane (**S9**) (229 mg, 0.810 mmol) (109 mg, 66% yield). A duplicate reaction gave 66% yield.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.99 (d,  $J = 7.9$  Hz, 2H), 7.68 (m, 3H), 7.37 (d,  $J = 6.7$  Hz, 1H), 6.82 (d,  $J = 10.8$  Hz, 1H), 6.49 (t,  $J = 6.5$  Hz, 1H), 3.86 (q,  $J = 7.2$  Hz, 2H), 2.63 (s, 3H), 1.32 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  197.99, 148 (br), 142.88, 138.26, 136.00, 132.79, 131 (br), 127.18, 111.87, 48.43, 26.42, 18.22;  $^{11}\text{B}$  NMR (96 MHz)  $\delta$  35.45; HRMS (EI+) calcd for  $\text{C}_{14}\text{H}_{16}\text{BNO}$  ( $\text{M}^+$ ) 225.13250, found 225.13320.

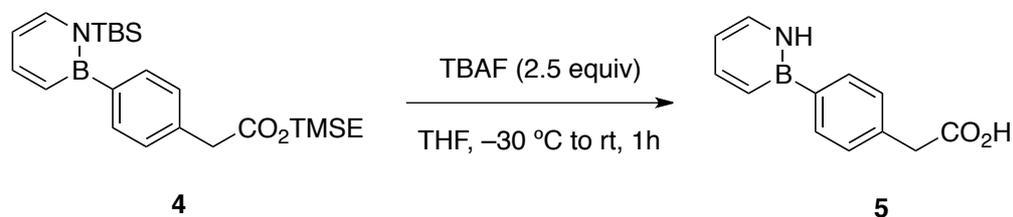
### Compound 4:



To a 20 mL vial was added chlorobis(ethylene)rhodium dimer (8.0 mg, 0.02 mmol) and BIPHEP (21 mg, 0.04 mmol), followed by 2.0 mL THF. The solution was stirred for 15 min, then transferred to a 15 mL pressure vessel containing **1b** (100 mg, 0.44 mmol) and **3** (160 mg, 0.40 mmol) in 2.0 mL THF. The pressure vessel was sealed and heated at 100 °C for 24h. The reaction was allowed to cool to room temperature, and volatiles were removed under reduced pressure. Purification of crude material by silica gel chromatography (ether/pentane) provides the product. (77% yield based on **3**).  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.65 (dd,  $J = 11.0, 6.3$  Hz, 1H), 7.49 (d,  $J = 6.7$  Hz, 1H), 7.38 (d,  $J = 7.3$  Hz, 2H), 7.25 (d,  $J = 7.5$  Hz, 2H), 6.70 (d,  $J = 10.9$  Hz, 1H), 6.49 (t,  $J = 6.6$  Hz, 1H), 4.25 (t,  $J = 8.7$  Hz, 2H), 3.66 (s, 2H), 1.05 (t,  $J = 8.8$  Hz, 2H), 0.94 (s, 9H), 0.10 (s, 15H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  171.72, 144 (br), 142.83, 138.32z, 132.75, 132.18, 127.59, 111.82, 62.83, 41.47, 26.69, 18.82, 17.23,

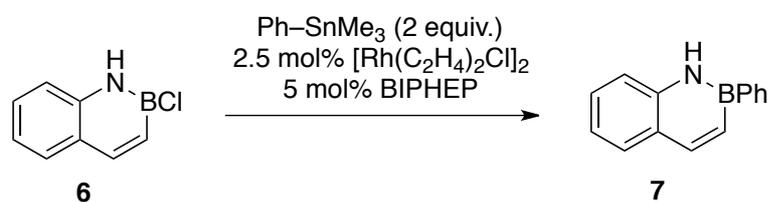
-1.79, -2.23 (one C bonded to B was not observed);  $^{11}\text{B}$  NMR (96 MHz)  $\delta$  38.88; HRMS (EI+) calcd for  $\text{C}_{23}\text{H}_{39}\text{BNO}_2\text{Si}_2$  (M+H) $^+$  428.2612, found 428.2608.

### BN Felbinac (5):



To a 20 mL vial was added **4** (43 mg, 0.10 mmol), TBAF (1.0 mL, 0.25M in THF) and 2.0 mL THF at  $-30\text{ }^\circ\text{C}$ . The solution was stirred and brought to room temperature over 1h. Volatiles were removed under reduced pressure. Purification of crude material by silica gel chromatography using  $\text{CH}_2\text{Cl}_2/\text{MeOH}/\text{AcOH}$  95:4:1 (v/v) as the eluent affords the title compound as a white solid (88% yield).  $^1\text{H}$  NMR (300 MHz,  $(\text{CD}_3)_2\text{CO}$ )  $\delta$  9.96 (br s, 1H), 7.88 (d,  $J = 7.4$  Hz, 2H), 7.76 (dd,  $J = 11.2, 6.5$  Hz, 1H), 7.55 (t,  $J = 7.2$  Hz, 1H), 7.38 (d,  $J = 7.5$  Hz, 2H), 7.18 (d,  $J = 11.2$  Hz, 1H), 6.40 (dt,  $J = 7.1, 3.7$  Hz, 1H), 3.67 (s, 2H); the COOH is not observed;  $^{13}\text{C}$  NMR (126 MHz,  $(\text{CD}_3)_2\text{CO}$ )  $\delta$  171.93, 144.32, 135.45, 134.93, 132.46, 128.98, 127.6 (br) 110.44, 40.50 (one C bonded to B was not observed);  $^{11}\text{B}$  NMR (96 MHz)  $\delta$  34.17; HRMS (EI+) calcd for  $\text{C}_{12}\text{H}_{13}\text{BNO}_2$  (M+H) $^+$  214.1039, found 214.1031.

### Compound 7 (Equation 1) [CAS 24341-84-2]:



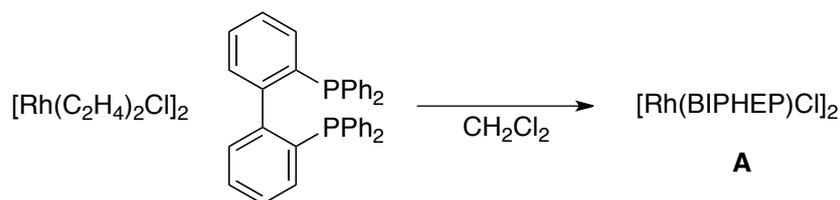
To a 10 mL vial was added chlorobis(ethylene)rhodium dimer (3.0 mg, 0.0077 mmol) and BIPHEP (8.0 mg, 0.015 mmol) then 1.0 mL THF. The solution was stirred for 15 min then transferred to a 8 mL pressure vessel containing 2-chloro-1,2-benzazaborine **6**<sup>4</sup> (50 mg, 0.31 mmol) and trimethyl(phenyl)stannane (147 mg, 0.61 mmol) in 1.0 mL THF. The vessel was sealed and heated at  $100\text{ }^\circ\text{C}$  for 24h. The reaction was allowed to cool to room temperature, and volatiles were removed under reduced pressure. Purification of crude material by silica

gel chromatography (ether/pentane) provides the product (43 mg, 69% yield). A duplicate reaction gave 72% yield.

$^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  8.32 (br s, 1H), 8.21 (d,  $J = 11.5$  Hz, 1H), 7.99 (dd,  $J = 7.3$ , 2.0 Hz, 2H), 7.73 (d,  $J = 7.8$  Hz, 1H), 7.52 (m, 4H), 7.44 (d,  $J = 8.1$  Hz, 1H), 7.34 (dd,  $J = 11.5$ , 2.0 Hz, 1H), 7.26 (t,  $J = 7.4$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  145.51, 140.22, 132.68, 129.67, 129.38, 128.45, 128.19, 125.70, 121.09, 118.26; the signals for the carbon atoms connected to boron are not observed;  $^{11}\text{B}$  NMR (96 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  33.55. These spectroscopic data correspond to previously reported data.<sup>5</sup>

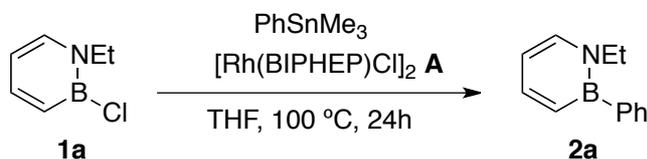
## Mechanistic Studies

### [Rh(BIPHEP)Cl]<sub>2</sub> (A):



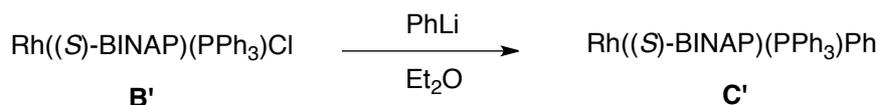
To a vial containing BIPHEP (549 mg, 1.05 mmol) suspended in 7.0 mL CH<sub>2</sub>Cl<sub>2</sub> was added [Rh(C<sub>2</sub>H<sub>4</sub>)<sub>2</sub>Cl]<sub>2</sub> (200 mg, 0.525 mmol) in 5.0 mL CH<sub>2</sub>Cl<sub>2</sub>. The solution was stirred for 18h then volatiles were removed under reduced pressure to give the title compound as a red powder (694 mg, 99% yield). <sup>1</sup>H NMR (500 MHz, C<sub>6</sub>D<sub>6</sub>) δ 8.16 (br, 8H), 8.07 (br s, 8H), 7.12 (br, 4H), 7.04 (t, *J* = 7.5 Hz, 8H), 6.96 (dt, *J* = 16.9 Hz, 7.4 Hz, 8H), 6.90 (t, *J* = 7.5 Hz, 8H), 6.69 (t, *J* = 7.5 Hz, 4H), 6.59 (t, *J* = 7.7 Hz, 4H), 6.38 (d, *J* = 7.6 Hz, 4H); <sup>31</sup>P NMR (202 MHz, C<sub>6</sub>D<sub>6</sub>) δ 46.46 (d, *J*<sub>Rh-P</sub> = 193.3 Hz).

### Complex A as a Catalyst in Arylstannane Addition Reaction (Equation 2):

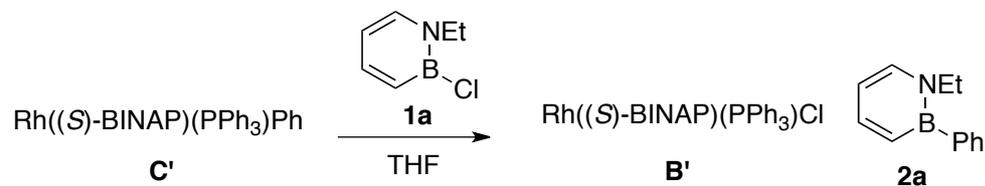


To a 15 mL pressure vessel was added [Rh(BIPHEP)Cl]<sub>2</sub> (A) (12 mg, 0.009 mmol), **1a** (52 mg, 0.368 mmol) and trimethyl(phenyl)tin (98 mg, 0.405 mmol) and 2.0 mL THF. The reaction was heated to 100 °C for 24h. At the conclusion of the reaction, the mixture was cooled to room temperature, diluted with Et<sub>2</sub>O to 10 mL, and then *n*-hexadecane (100 μL) as the GC internal standard was added. GC analysis indicated the formation of **2a** in 85% yield.



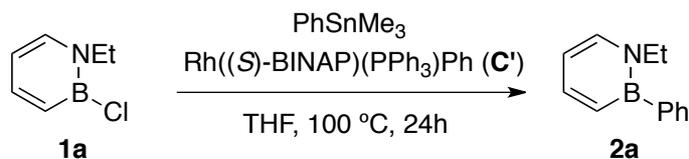
**Rh((S)-BINAP)(PPh<sub>3</sub>)Ph (C') [CAS 434314-09-7]:**

Complex **C'** was prepared according to a published procedure.<sup>6</sup> To a suspension of **B'** (250 mg, 0.244 mmol) in Et<sub>2</sub>O (40 mL) at 0 °C was added phenyllithium (0.230 mL, 0.415 mmol, 1.8 M in Bu<sub>2</sub>O). The solution was slowly warmed to room temperature over 18h. The red solution was filtered through an acrodisc and passed through a plug of neutral alumina with Et<sub>2</sub>O. Volatiles were removed under reduced pressure to provide **C'** as a red powder (184 mg, 71%). <sup>1</sup>H NMR (500 MHz, C<sub>6</sub>D<sub>6</sub>) δ 8.41 (dd, *J* = 8.7 Hz, 6.6 Hz, 1H), 8.21 (t, *J* = 8.0 Hz, 2H), 7.83 (m, 3H), 7.53- 7.39 (m, 10H), 7.47-7.35 (m, 3H), 7.31 (d, *J* = 8.2 Hz, 1H), 7.26 (d, *J* = 8.1 Hz, 1H), 7.21-7.16 (m, 2H), 7.16-7.05 (m, 6H), 6.91-6.83 (m, 10H), 6.57-6.48 (m, 4H), 6.42-6.27 (m, 9H); <sup>31</sup>P NMR (202 MHz, C<sub>6</sub>D<sub>6</sub>) δ 32.14 (ddd, *J*<sub>Rh-P</sub> = 121 Hz, *J*<sub>PP-cis</sub> = 39 Hz, *J*<sub>PP-trans</sub> = 30 Hz), 29.55 (ddd, *J*<sub>PP-trans</sub> = 325 Hz, *J*<sub>Rh-P</sub> = 170 Hz, *J*<sub>PP-cis</sub> = 29 Hz), 26.27 (ddd, *J*<sub>PP-trans</sub> = 325 Hz, *J*<sub>Rh-P</sub> = 178 Hz, *J*<sub>PP-cis</sub> = 39 Hz). These spectroscopic data correspond to previously reported data.<sup>6</sup>

**Reaction of C' and 1a (Figure 2)**

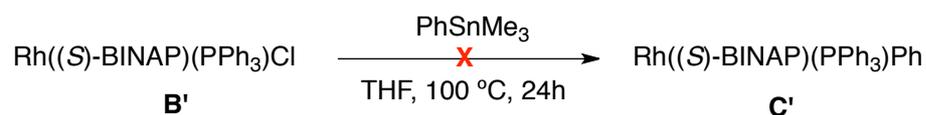
To a J-Young tube was added **C'** (48 mg, 0.045 mmol), **1a** (32 mg, 0.225 mmol) and THF-*d*8 (1.1 mL). The reaction was followed by <sup>31</sup>P NMR (202 MHz, 25 °C). Conversion to **B'** was complete at 1h at room temperature. Unreacted **1a** and formation of **2a** was observed by <sup>1</sup>H and <sup>11</sup>B NMR.

### Complex C' as a Catalyst in Arylstannane Addition Reaction (Equation 3)



To a 15 mL pressure vessel was added **C'** (31 mg, 0.029 mmol), **1a** (82 mg, 0.58 mmol), trimethyl(phenyl)tin (154 mg, 0.64 mmol) and 2.0 mL THF. The reaction was sealed and heated at 100 °C for 24h. At the conclusion of the reaction, the mixture was cooled to room temperature, diluted to 10 mL with Et<sub>2</sub>O, and *n*-hexadecane (100 μL) as the GC internal standard was added. GC analysis indicated the formation of **2a** in 62% yield.

### Attempted Regeneration of C' by Trimethyl(phenyl)tin



To a 15 mL pressure vessel was added **B'** (30 mg, 0.029 mmol), trimethyl(phenyl)tin (154 mg, 0.64 mmol) and 2.0 mL THF. The reaction was heated at 100 °C for 24h, then cooled to room temperature. The solution was concentrated *in vacuo* to 0.5 mL. <sup>31</sup>P NMR analysis indicated no formation of **C'**.

## *Kinetic Studies by Reaction Calorimetry*

### **General Experimental Procedure for Reaction Calorimetry**

Reactions were performed in a Setaram C80 Calvet calorimeter with Setsoft 2000 software. In a glove box, a stainless steel mixing cell (approx. volume 4.6 mL) was charged with **1b** (82 mg, 0.36 mmol) and trimethyl(phenyl)tin (181 mg, 0.750 mmol) and toluene to give a 1.0 mL solution. To the upper chamber was added 1.0 mL [Rh(BIPHEP)Cl]<sub>2</sub> (**A**) solution (18 mM in toluene). The reference cell was left empty under air. Both cells were loaded into the calorimeter at 100 °C and the heat flow was allowed to equilibrate (approx. 2h). Data collection was initiated, and both plungers were depressed. Heat flow measurements were recorded every 6s. Data collection was halted when heat flow reached equilibrium.

The thermodynamic heat of reaction was obtained through integration of the complete heat flow versus time curve and moles of limiting substrate by equation (1).

$$\Delta H_{\text{rxn}} = \frac{\int_0^{\infty} q \, dt}{\text{mol}} \quad (1)$$

Heat flow is directly related to rate through equation (2).

$$\text{heat flow} = q = (\Delta H_{\text{rxn}})(\text{volume})(\text{rate}) \quad (2)$$

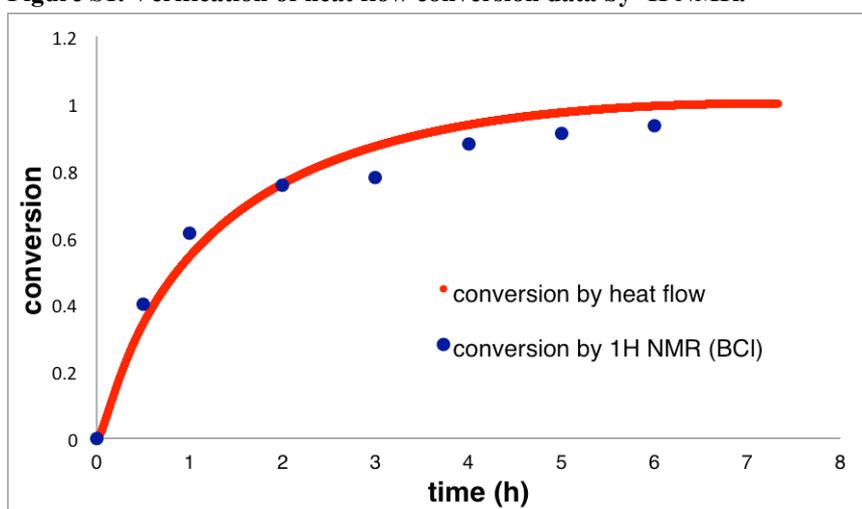
Integration of the heat flow curve from t=0 to t=t divided by the complete area under the curve provides conversion (equation (3)).

$$(\text{Conv})_t = \frac{\text{area to time } t}{\text{total area}} = \frac{\int_0^t q \, dt}{\int_0^{\infty} q \, dt} \quad (3)$$

### Conversion by $^1\text{H}$ NMR Experiment

In a glovebox, a 20 mL scintillation vial flask was charged with **1b** ([BCl]) (164 mg, 0.720 mmol), trimethyl(phenyl)tin (361 mg, 1.50 mmol), Rh catalyst **A** ([Rh(BIPHEP)Cl]<sub>2</sub>) (24 mg, 0.018 mmol) and 4,4'-di-*tert*-butylbiphenyl (96 mg, 0.36 mmol) as an internal standard. Toluene was added to give 4.0 mL of solution ([BCl]=0.18M, [PhSn]=0.38M, [Rh]<sub>total</sub> = 9mM). Six 0.5 mL aliquots were transferred to J-Young NMR tubes. The tubes were sealed and brought to 100 °C. Results are shown in Figure S1.

Figure S1. Verification of heat flow conversion data by  $^1\text{H}$  NMR.



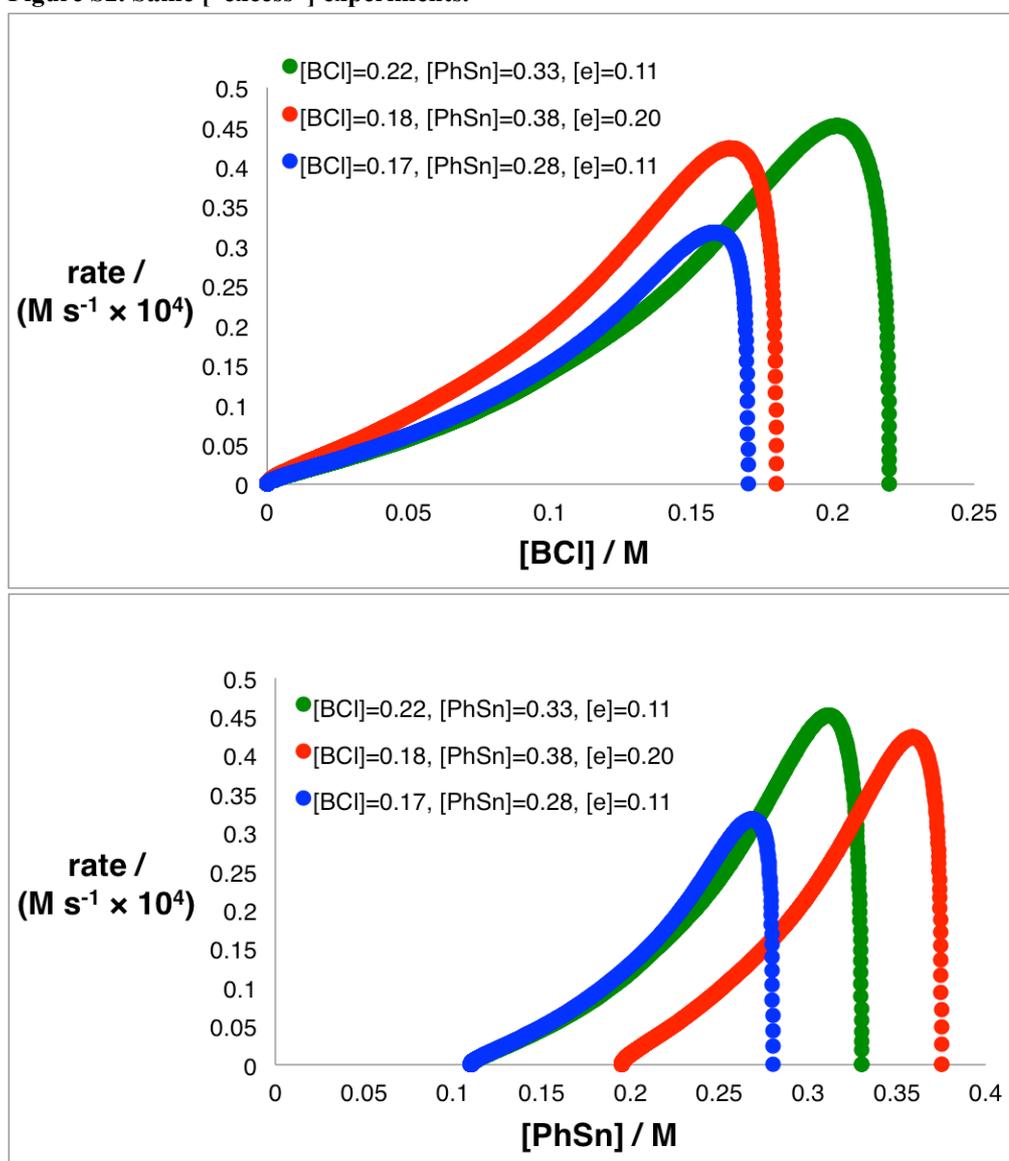
## Reaction Progress Kinetic Analysis

The method of reaction progress kinetic analysis developed by D.G. Blackmond and coworkers was followed.<sup>7</sup>

### Same [“excess”] Experiments

Reactions ran at the same [“excess”] showed overlay in rate vs. [BCl] rate vs. [PhSn] (Figure S2) indicating negligible catalyst degradation or product inhibition.

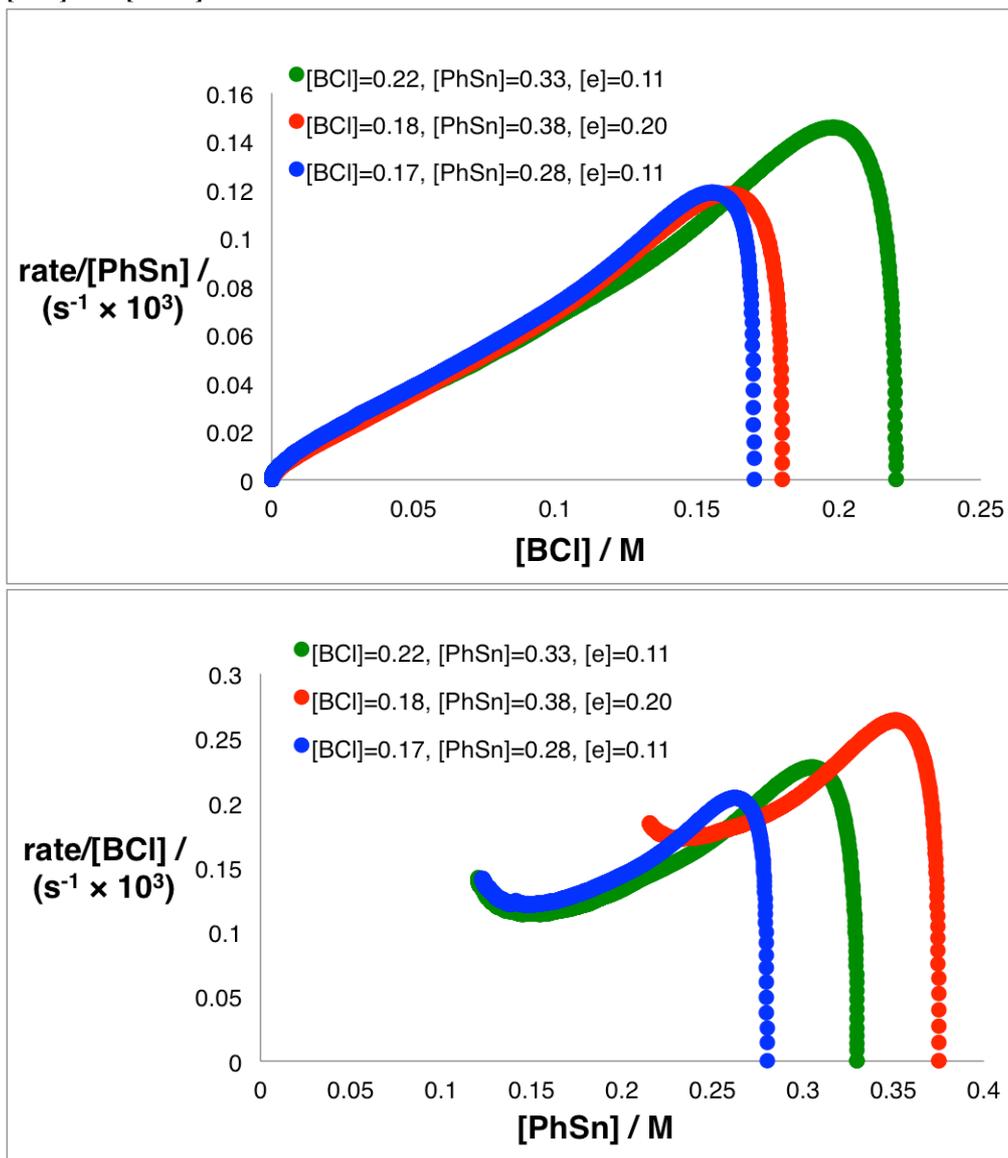
Figure S2. Same [“excess”] experiments.



### Different ["excess"] Experiments (Figure S3)

Reactions ran at different ["excess"] showed overlay when rate/[PhSn] versus [BCl] and rate/[BCl] versus [PhSn] (Figure S3) were plotted. This confirms first order behavior in both reactants.

Figure S3. Different ["excess"] plots. Determination of the reaction order with respect to [BCl] and [PhSn].



## Reaction Order In $[\text{Rh}]_{\text{total}}$

Plots of rate versus  $[\text{BCl}]$  and rate/ $[\text{Rh}]_{\text{total}}$  versus  $[\text{BCl}]$  (Figure S4) showed no overlay. A plot of rate/ $[\text{Rh}]_{\text{total}}^{1/2}$  vs.  $[\text{BCl}]$  showed overlay (Figure S5) evident of half order kinetics in  $[\text{Rh}]_{\text{total}}$ .

Figure S4. Plots to determine reaction order with respect to  $[\text{Rh}]_{\text{total}}$ .

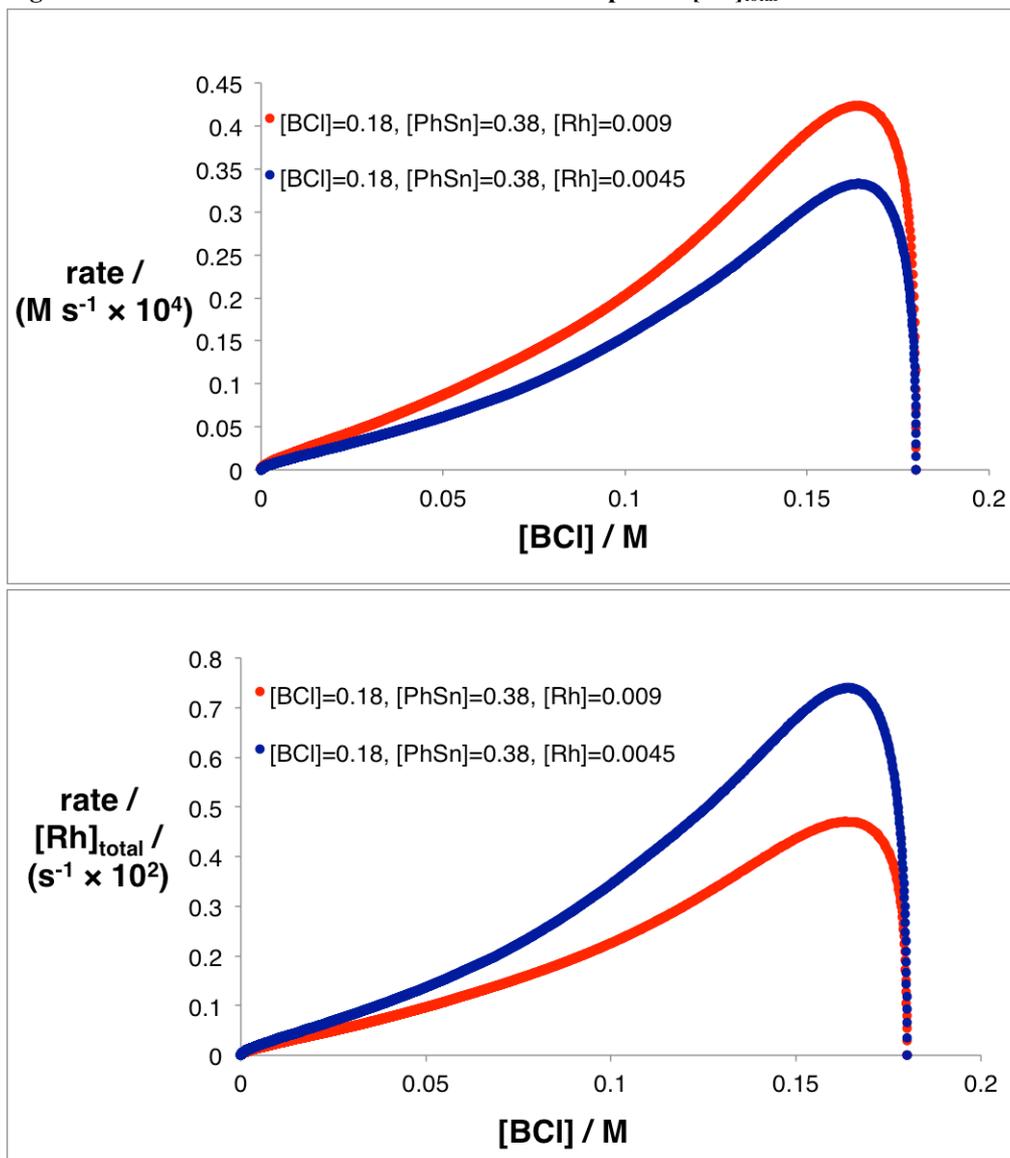
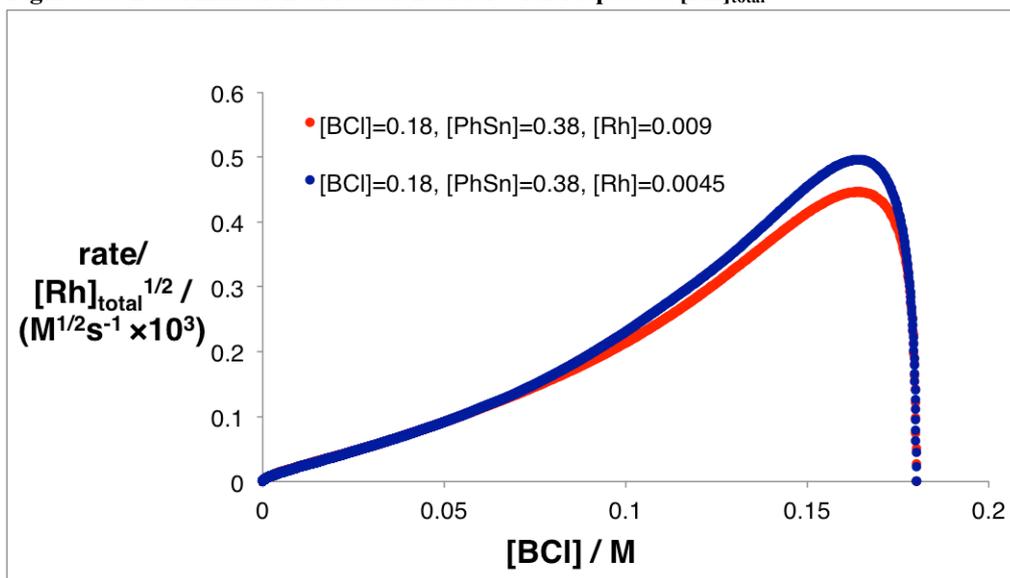


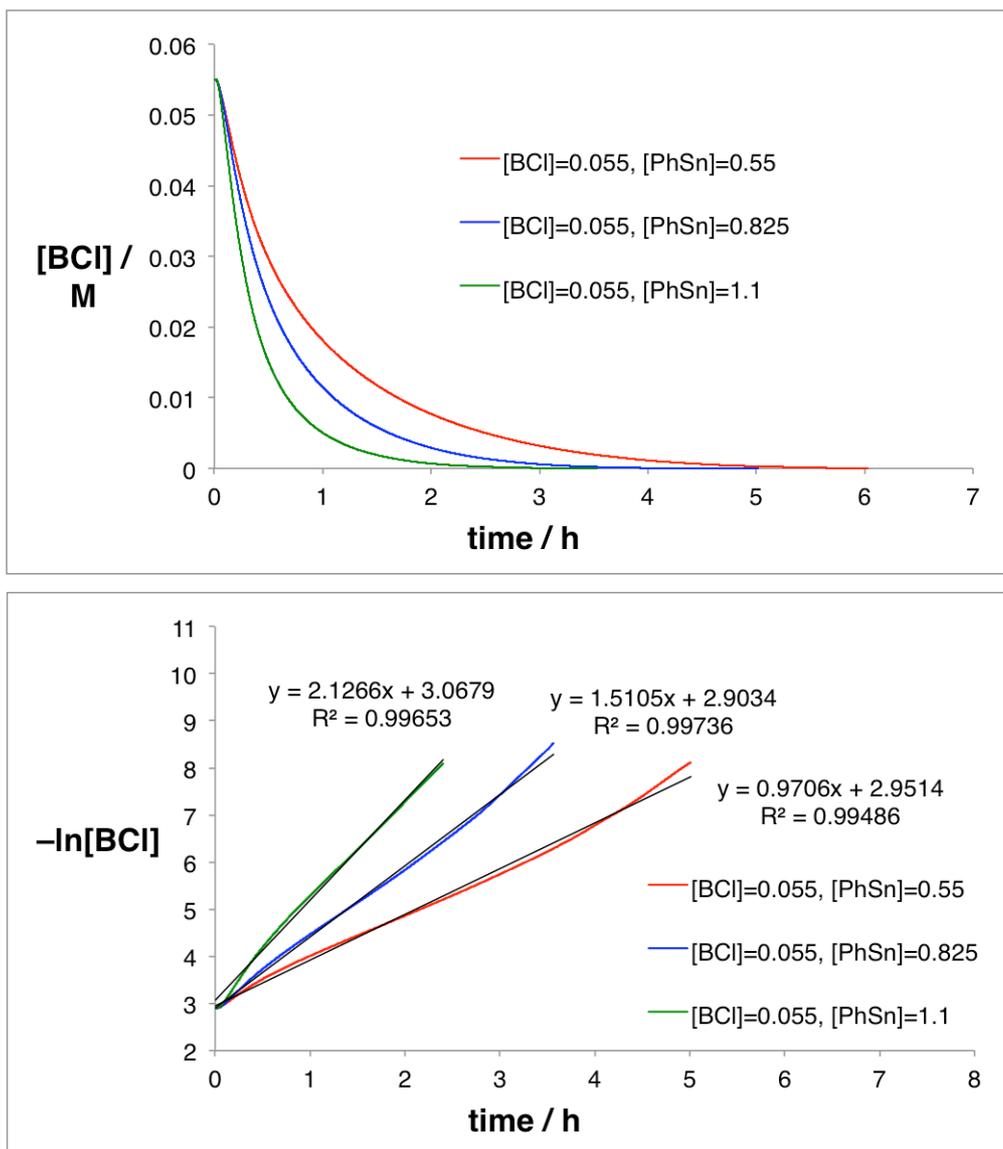
Figure S5. Determination of reaction order with respect to  $[\text{Rh}]_{\text{total}}$ .



## Pseudo-First Order Experiments

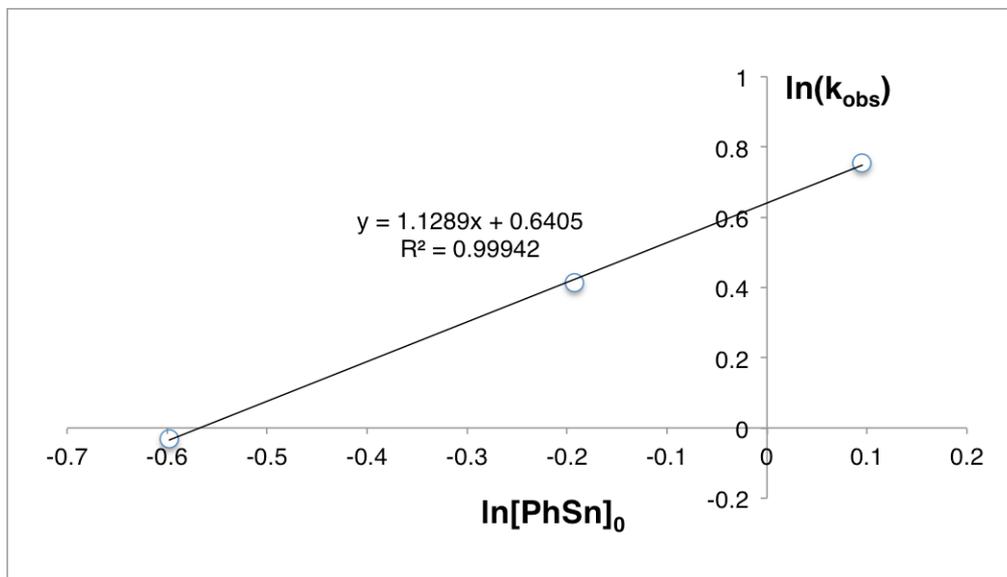
The general procedure for reaction calorimetry was followed. Plots of  $[BCl]$  versus time and  $-\ln[BCl]$  versus time are shown in Figure S6. Under pseudo-first order conditions, the slope of the  $-\ln[BCl]$  versus time plot is  $k_{obs}$ . Further, the linear nature of the pseudo-first order plot indicates first order behavior in  $[BCl]$ .

Figure S6. Plots under pseudo-first order conditions.



First order kinetics in [PhSn] is supported by a plot of  $\ln(k_{\text{obs}})$  versus  $\ln[\text{PhSn}]_0$  (slope = 1.1289) (See Figure S7).

**Figure S7. Determination of the reaction order in [PhSn] under pseudo-first order reaction conditions.**



### Modeling to Experimental Data

The empirical rate equation is shown in equation (4). Good fits between experimental rate data and calculated rate were found when  $k'=7.39\times 10^{-3}$ . The fitted data is plotted in Figure S8. Goodness of fit is shown in Table S1.

$$\text{rate} = k'[\text{BCl}][\text{PhSn}][\text{Rh}]_{\text{total}}^{1/2} \quad (4)$$

Figure S8. Fitted rate data.

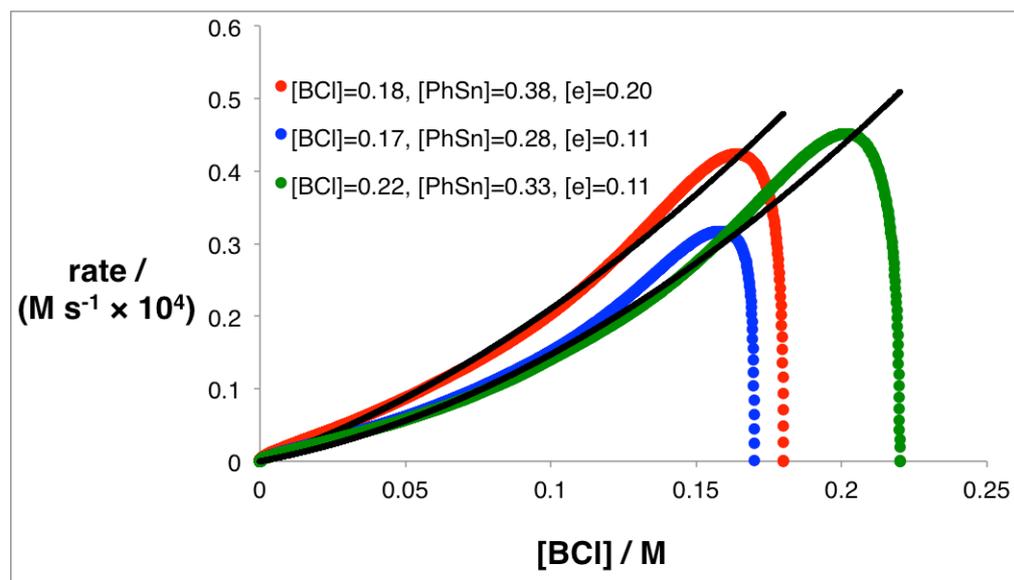
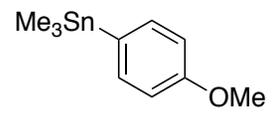


Table S1. Goodness of fit for calculated rates in Figure S8.

experiment	$R^2$ (0 to 85% conv.)
[BCl]=0.17, [PhSn]=0.28, [e]=0.11	0.984
[BCl]=0.18, [PhSn]=0.38, [e]=0.20	0.994
[BCl]=0.22, [PhSn]=0.33, [e]=0.11	0.945

## References

- (1) Marwitz, A. J. V.; Abbey, E. R.; Jenkins, J. T.; Zakharov, L. N.; Liu, S.-Y. *Org. Lett.* **2007**, *9*, 4905–4908.
- (2) Hayashi, T.; Ishigedani, M. *Tetrahedron* **2001**, *57*, 2589–2595.
- (3) Marwitz, A. J. V.; Matus, M. H.; Zakharov, L. N.; Dixon, D. A.; Liu, S.-Y. *Angew. Chem. Int. Ed.* **2009**, *48*, 973–977.
- (4) Dewar, M.; Dietz, R. *J. Chem. Soc.* **1959**, 2728–2730.
- (5) Pan, J.; Kampf, J. W.; Ashe, A. J. *Organometallics* **2009**, *28*, 506–511.
- (6) Hayashi, T.; Takahashi, M.; Takaya, Y.; Ogasawara, M. *J. Am. Chem. Soc.* **2002**, *124*, 5052–5058.
- (7) Blackmond, D. G. *Angew. Chem. Int. Ed.* **2005**, *44*, 4302–4320.



S1

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: H

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 8001.6 Hz

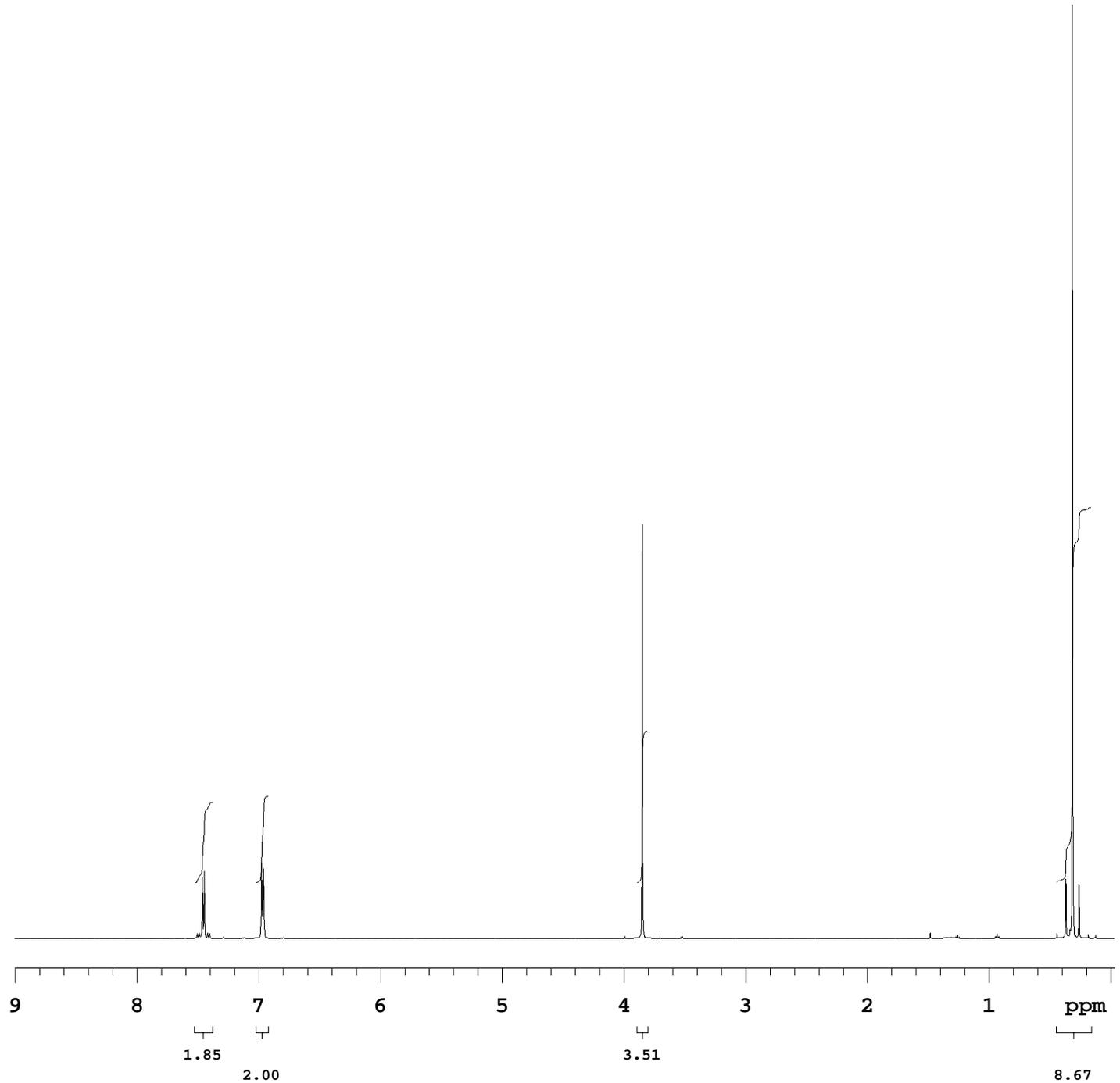
8 repetitions

OBSERVE H1, 500.1042443

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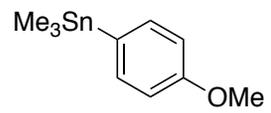
FT size 32768

Total time 1 minute



Archive dir:

File: H



S1

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

168 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

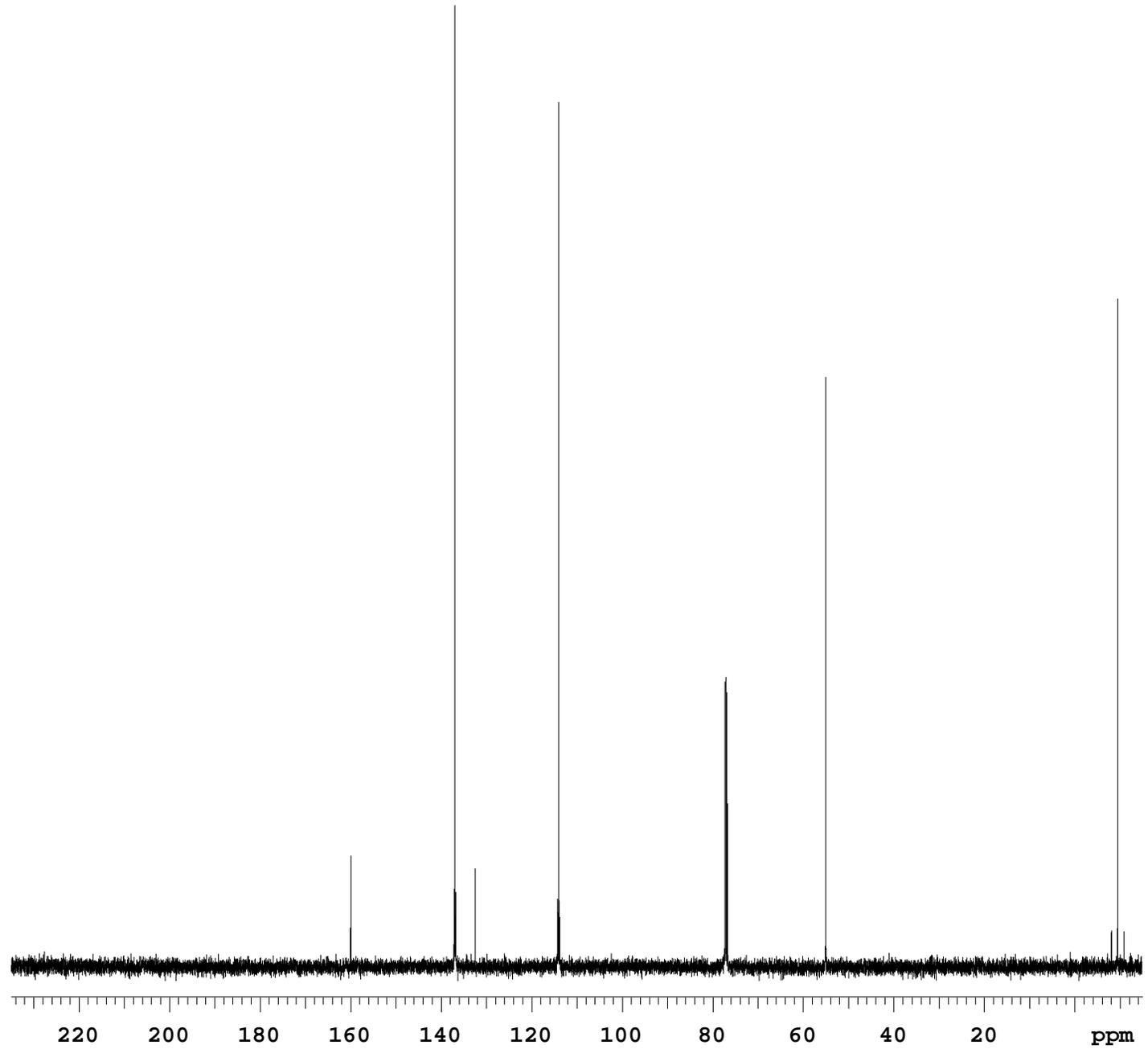
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DATA PROCESSING

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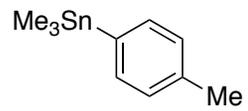
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Total time 5 minutes



Archive dir:

File: C



S2

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: H

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 8001.6 Hz

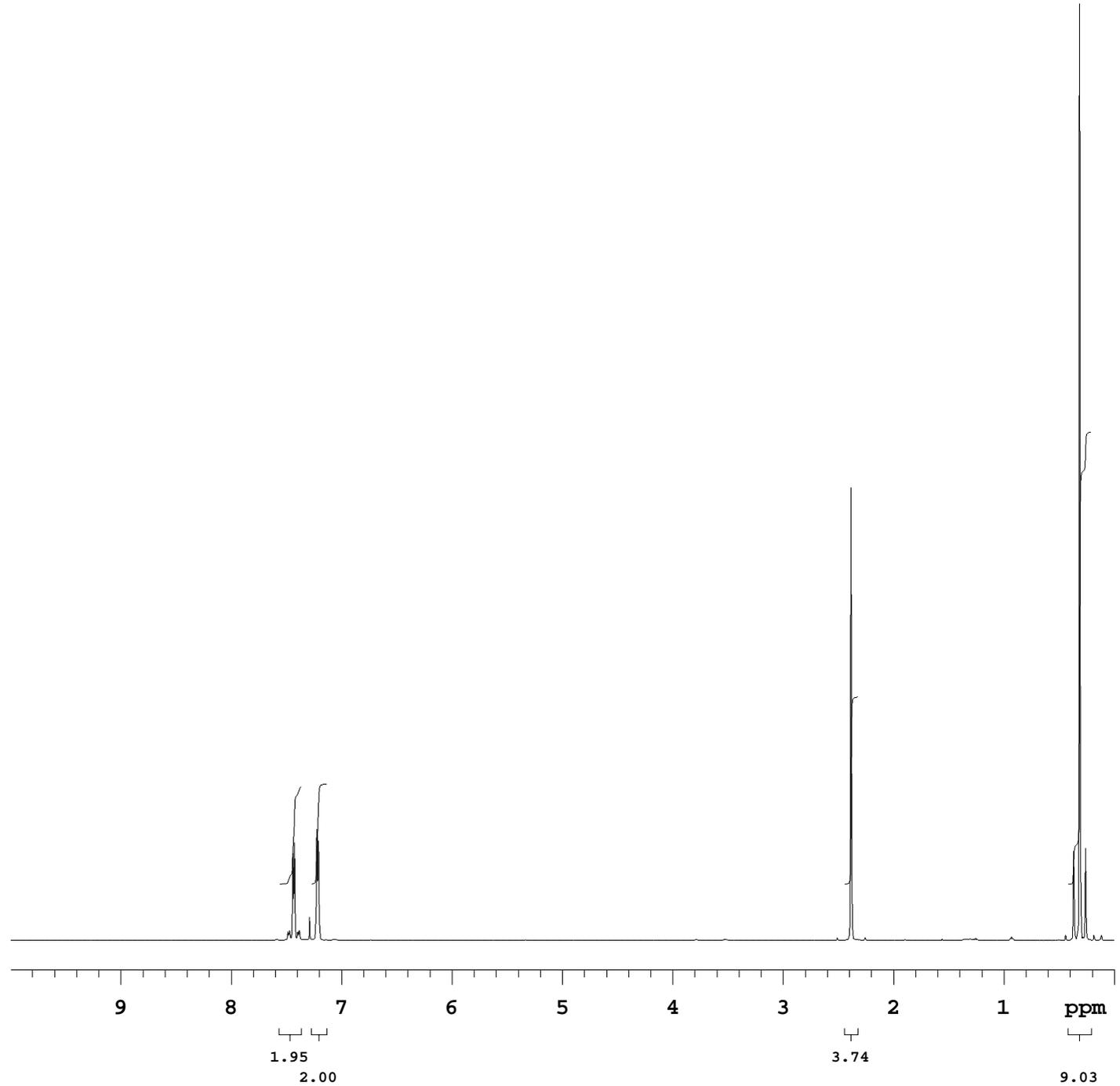
8 repetitions

OBSERVE H1, 500.1042443

DATA PROCESSING

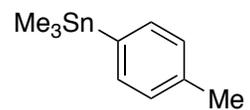
FT size 32768

Total time 1 minute



Archive dir:

File: H



S2

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

156 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

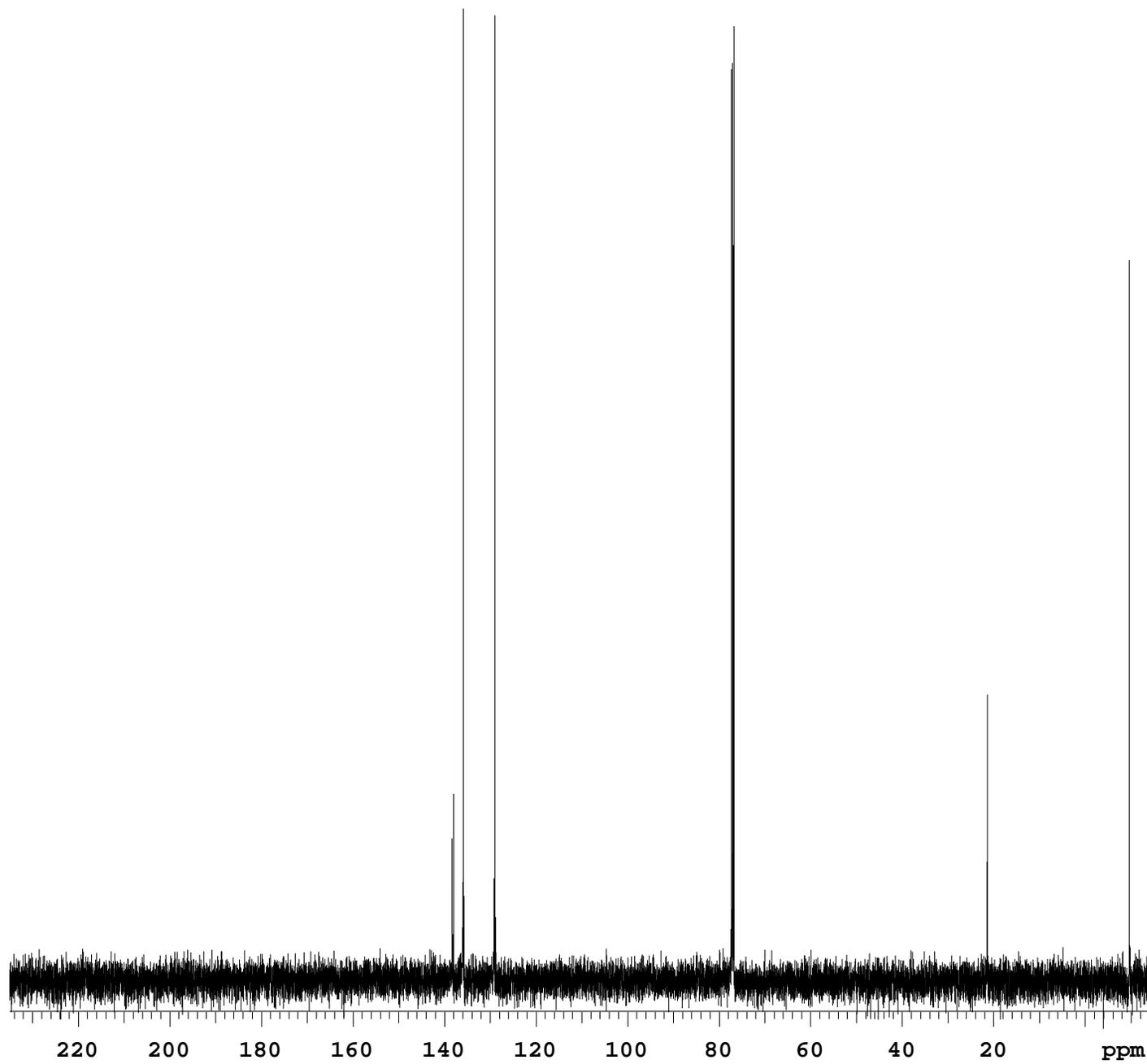
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DATA PROCESSING

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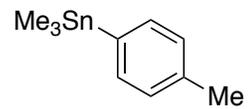
FT size 65536

Total time 5 minutes



Archive dir:

File: C



S2

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

156 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

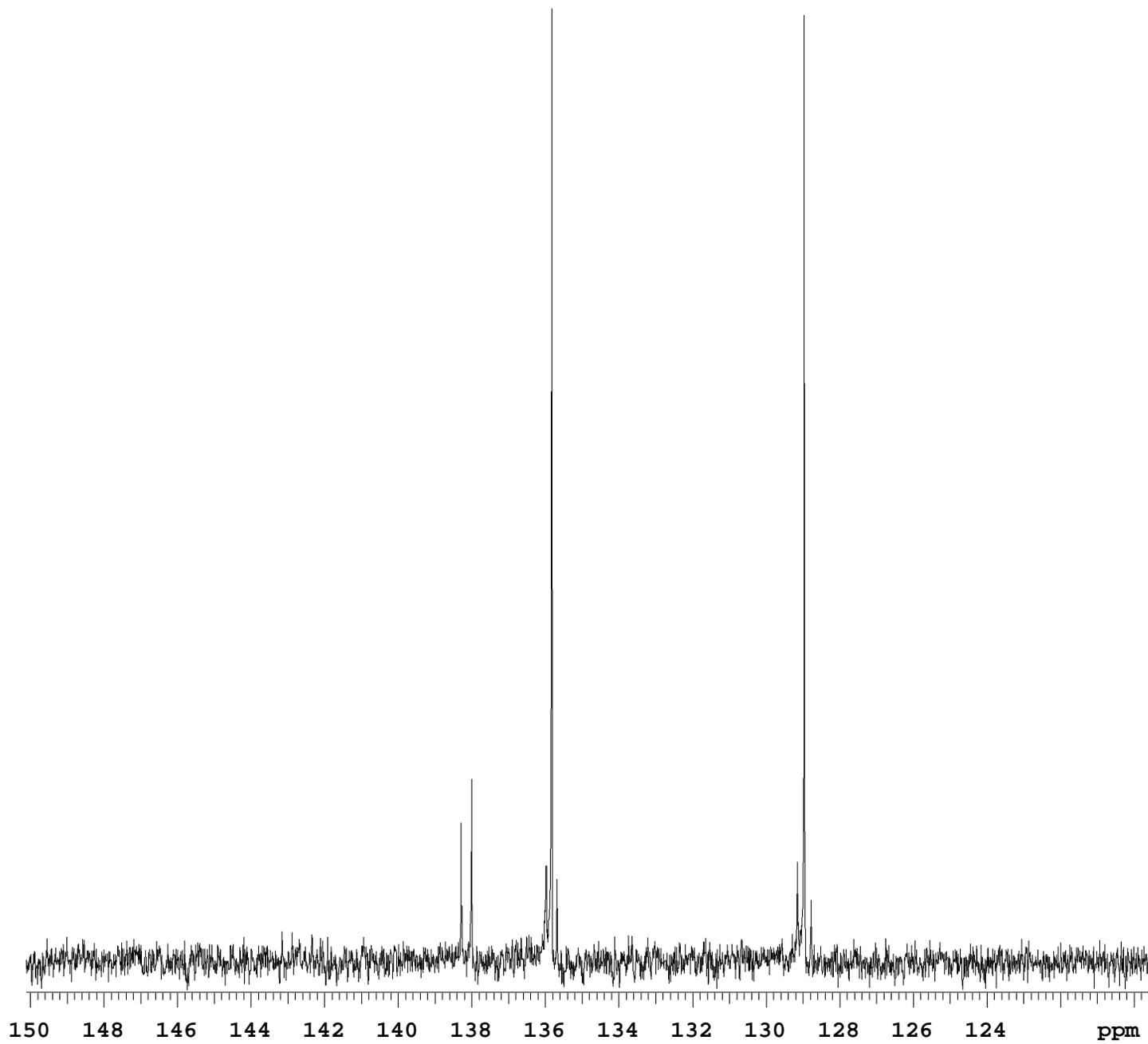
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DATA PROCESSING

Line broadening 1.0 Hz

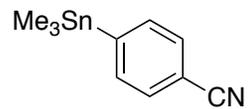
FT size 65536

Total time 5 minutes



Archive dir:

File: C



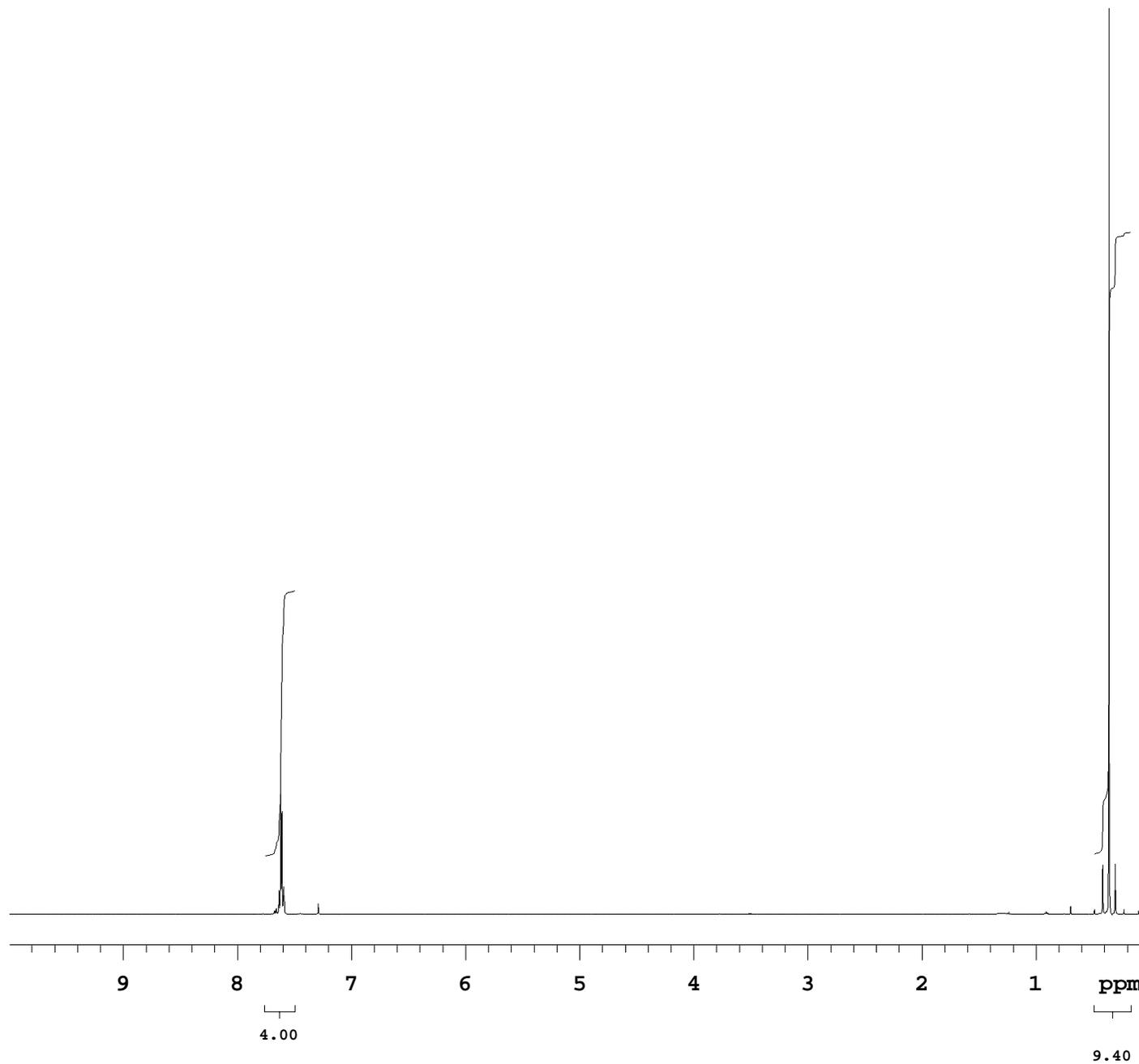
S3

UO Inova-500 standard 1H  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: H  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8001.6 Hz  
8 repetitions

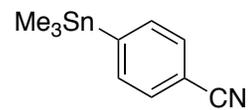
OBSERVE H1, 500.1042443

DATA PROCESSING  
FT size 32768  
Total time 1 minute



Archive dir:

File: H



S3

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

184 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

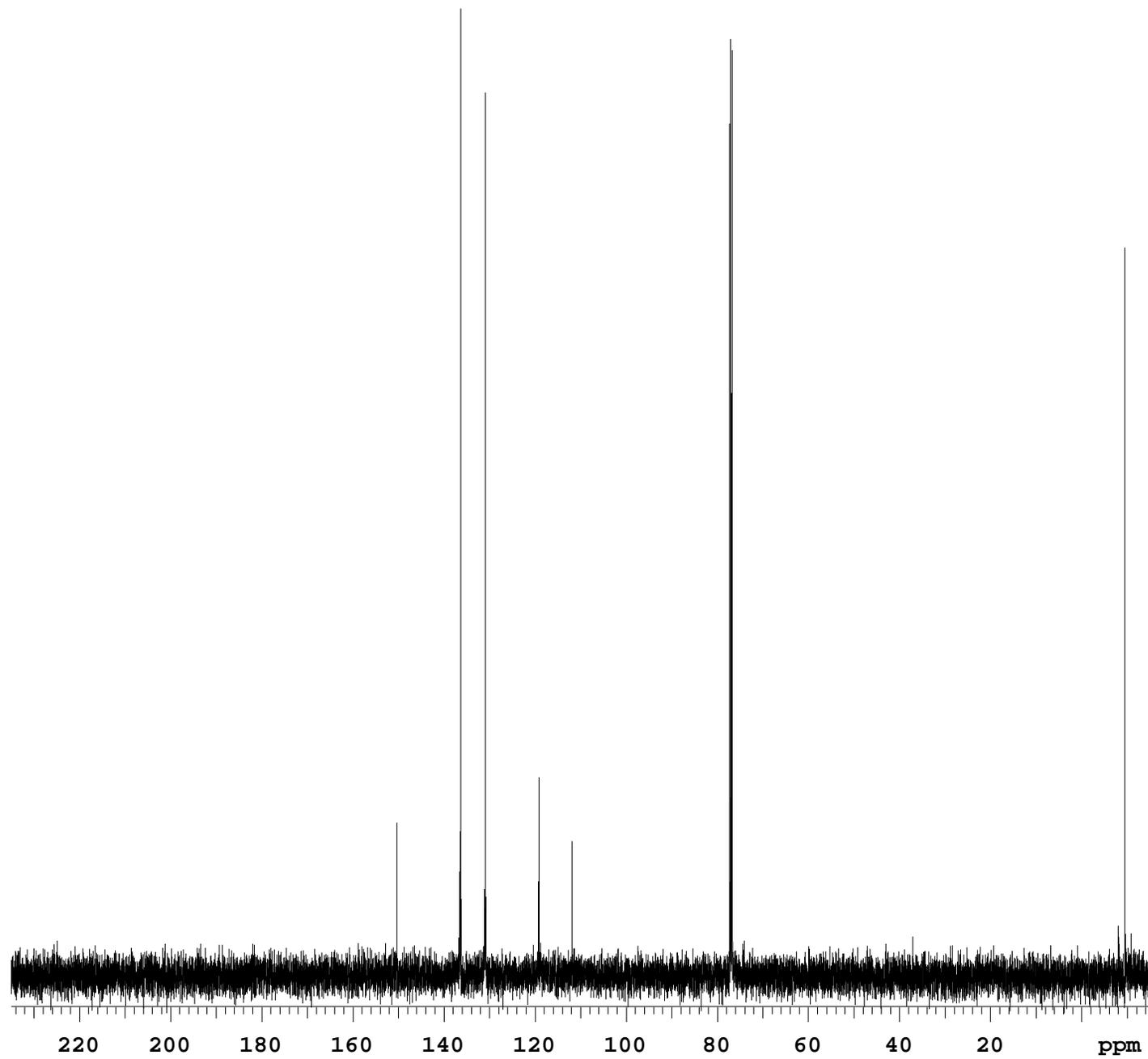
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DATA PROCESSING

Line broadening 1.0 Hz

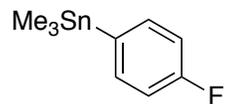
FT size 65536

Total time 6 minutes



Archive dir:

File: C



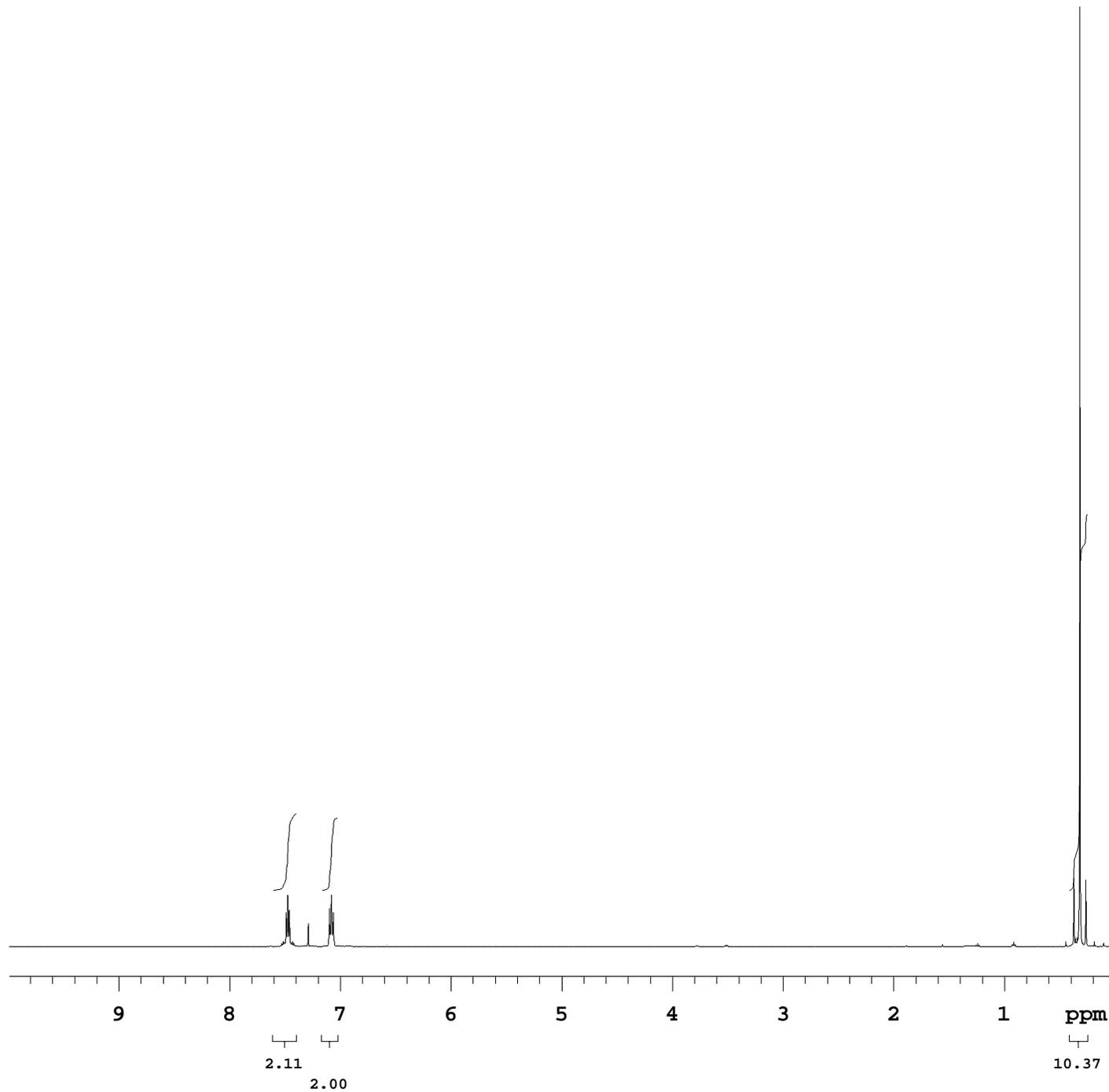
S4

UO Inova-500 standard 1H  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: H  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8001.6 Hz  
8 repetitions

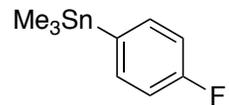
OBSERVE H1, 500.1042443

DATA PROCESSING  
FT size 32768  
Total time 1 minute



Archive dir:

File: H



S4

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

524 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

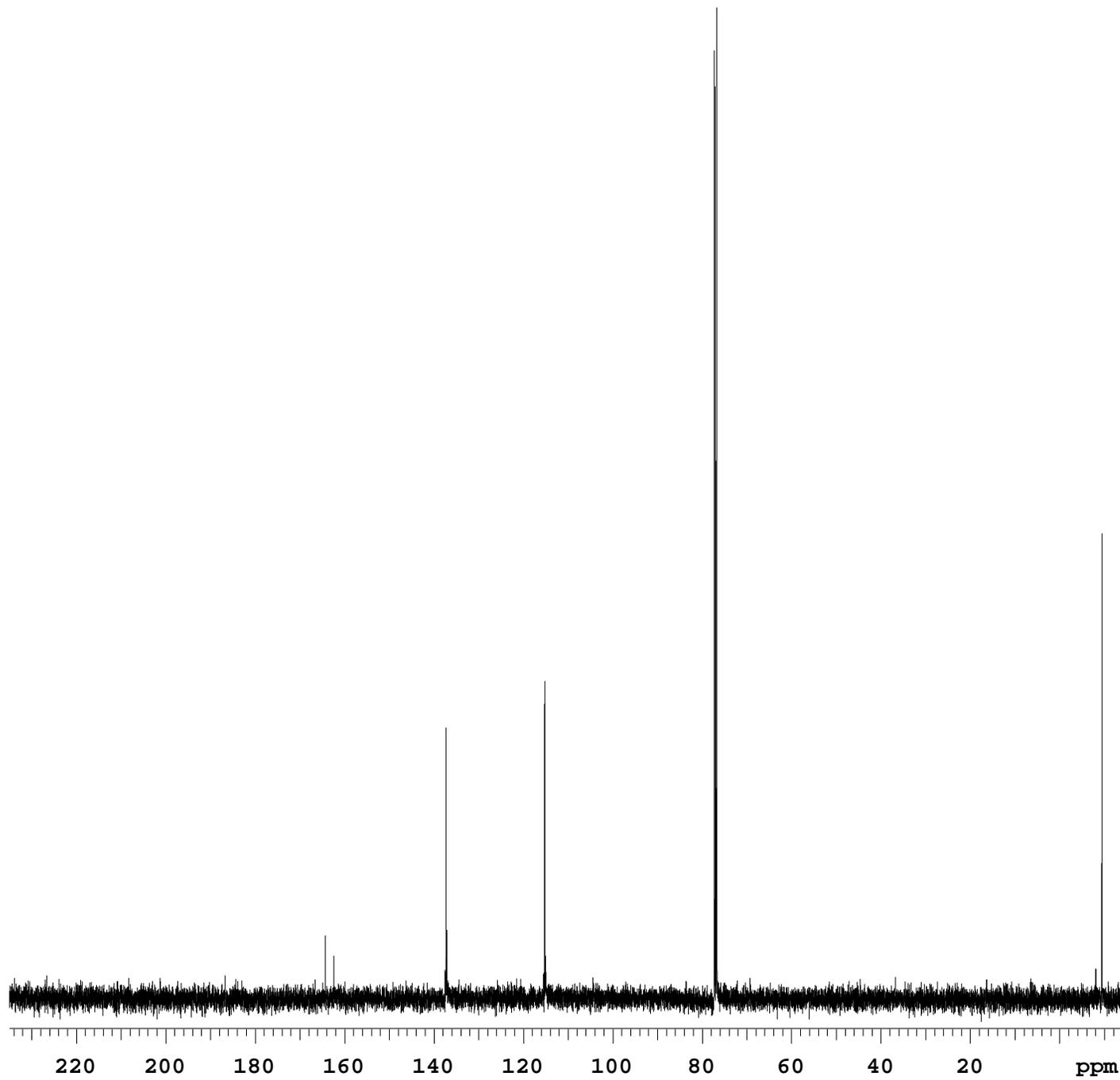
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DATA PROCESSING

Line broadening 1.0 Hz

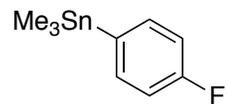
FT size 65536

Total time 17 minutes



Archive dir:

File: C



S4

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

524 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

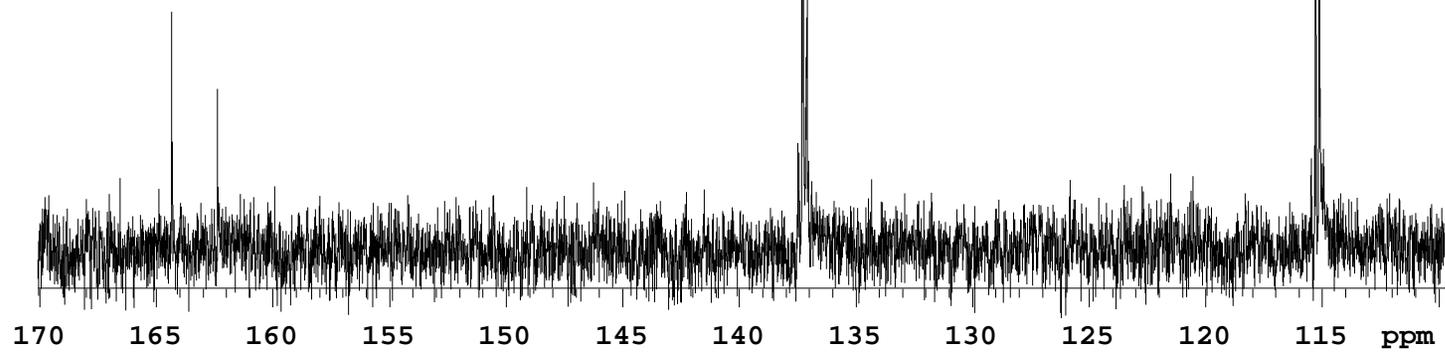
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

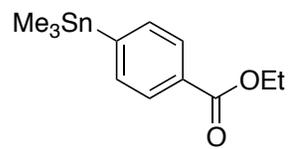
FT size 65536

Total time 17 minutes



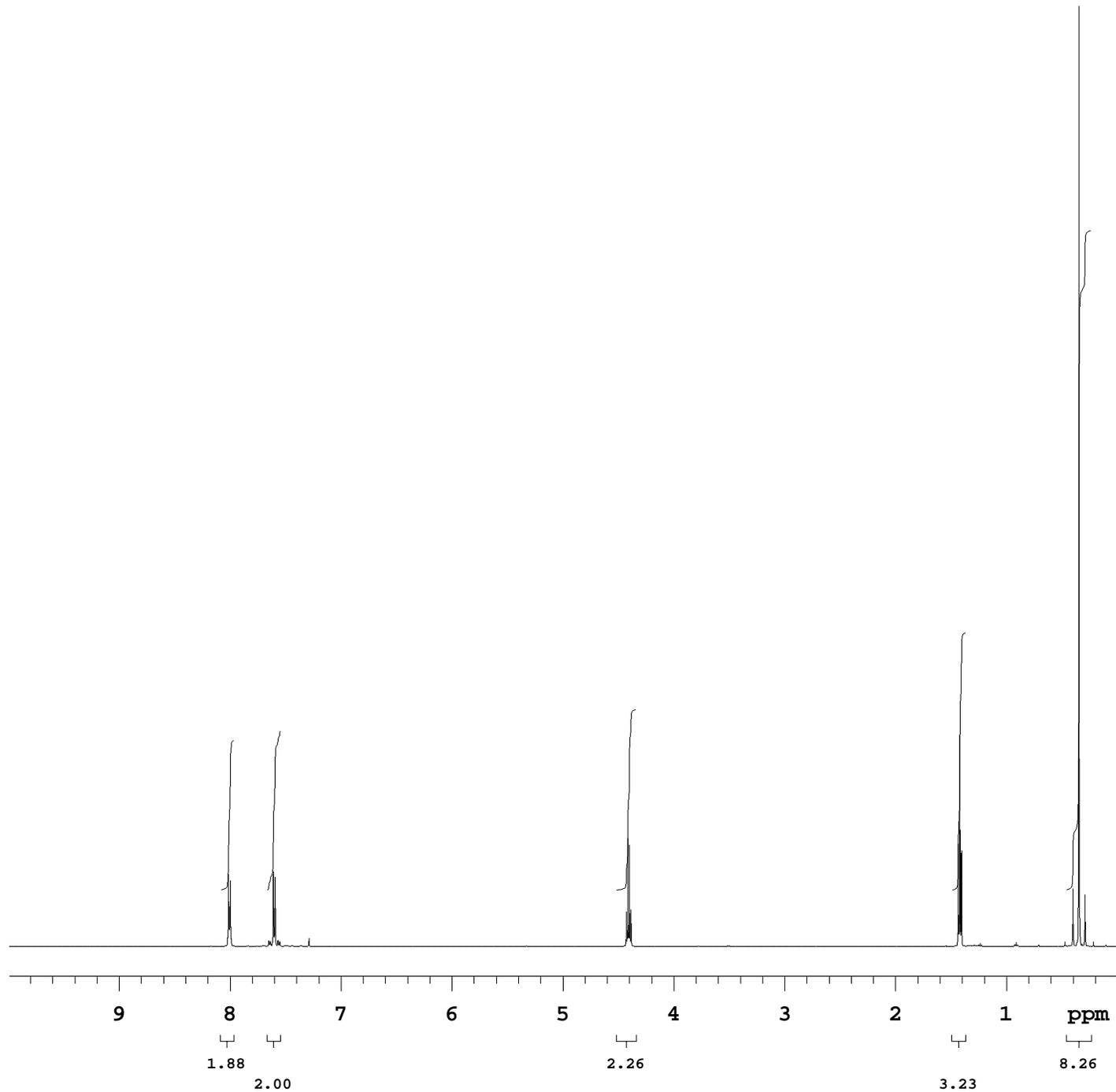
Archive dir:

File: C



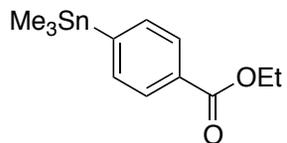
S6

UO Inova-500 standard 1H  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: H  
INOVA-500 "sunofnmr.uoregon.edu"  
PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8001.6 Hz  
8 repetitions  
OBSERVE H1, 500.1042443  
DATA PROCESSING  
FT size 32768  
Total time 1 minute



Archive dir:

File: H



S6

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

212 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

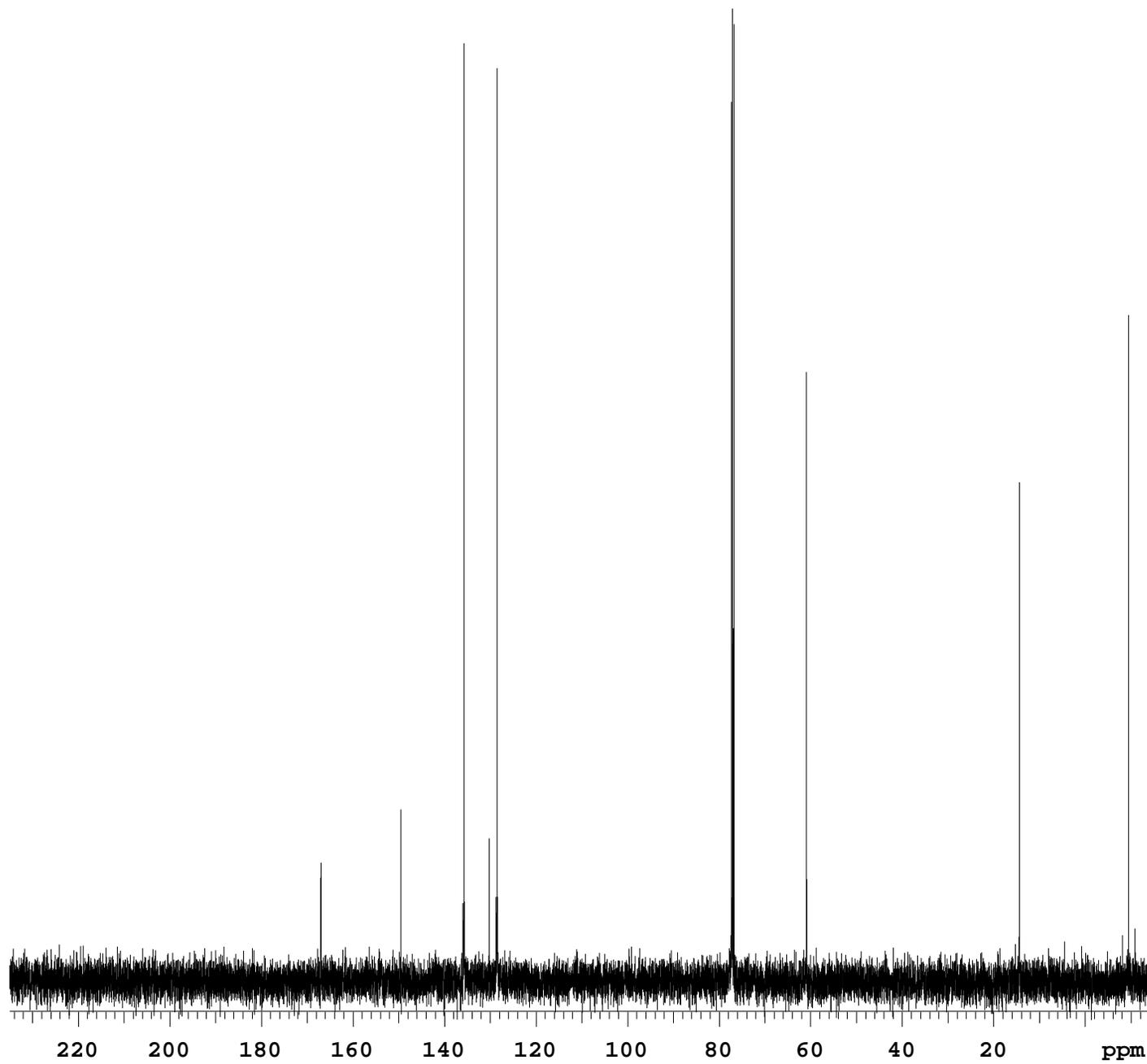
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

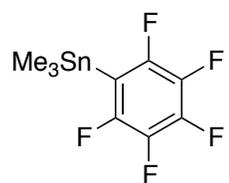
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Total time 7 minutes



Archive dir:

File: C



S7

UO Inova-500 standard 1H

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: H

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 8001.6 Hz

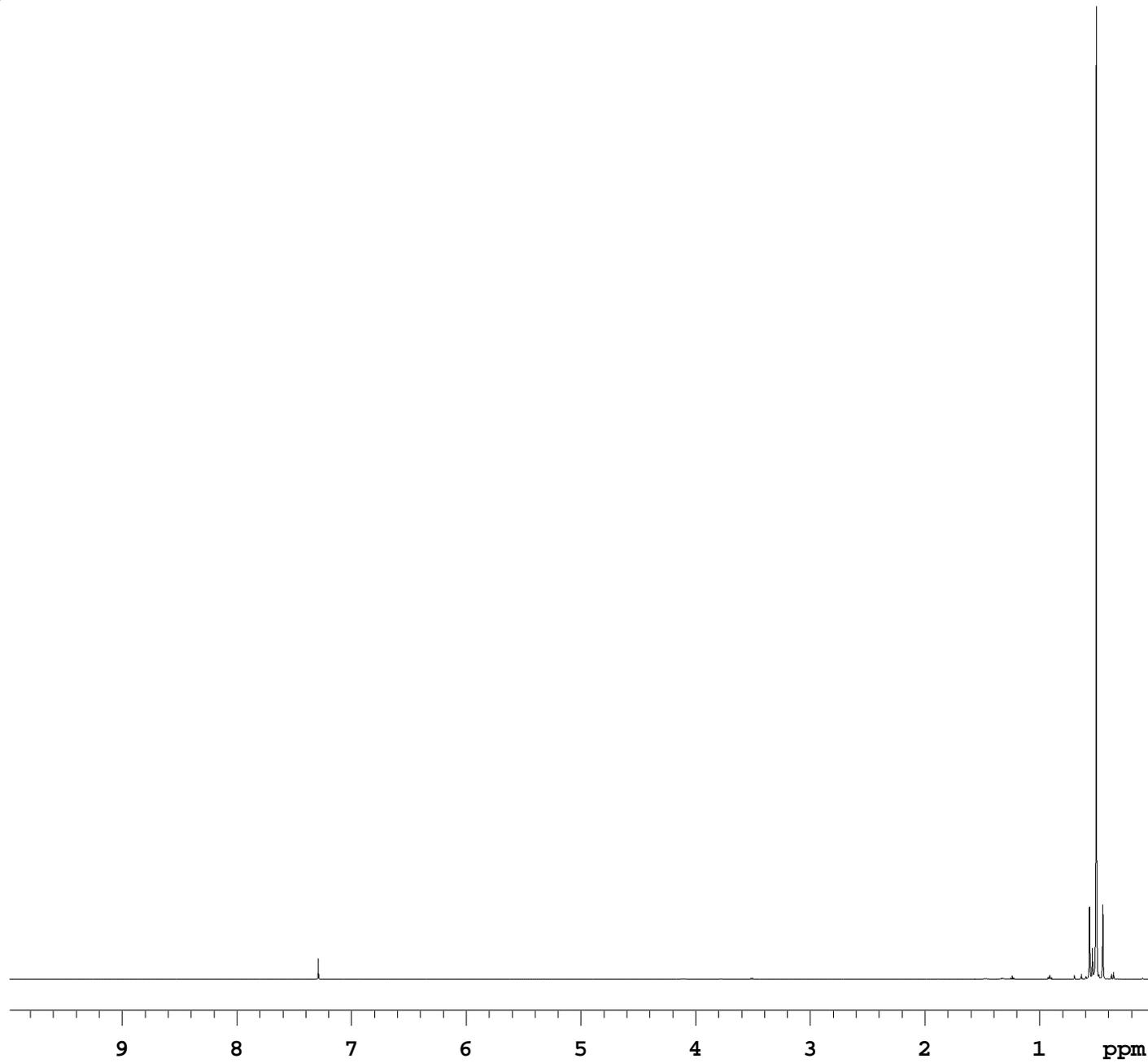
8 repetitions

OBSERVE H1, 500.1042443

DATA PROCESSING

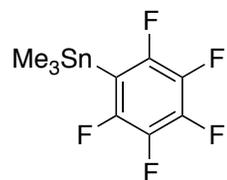
FT size 32768

Total time 1 minute



Archive dir:

File: H



S7

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

1316 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

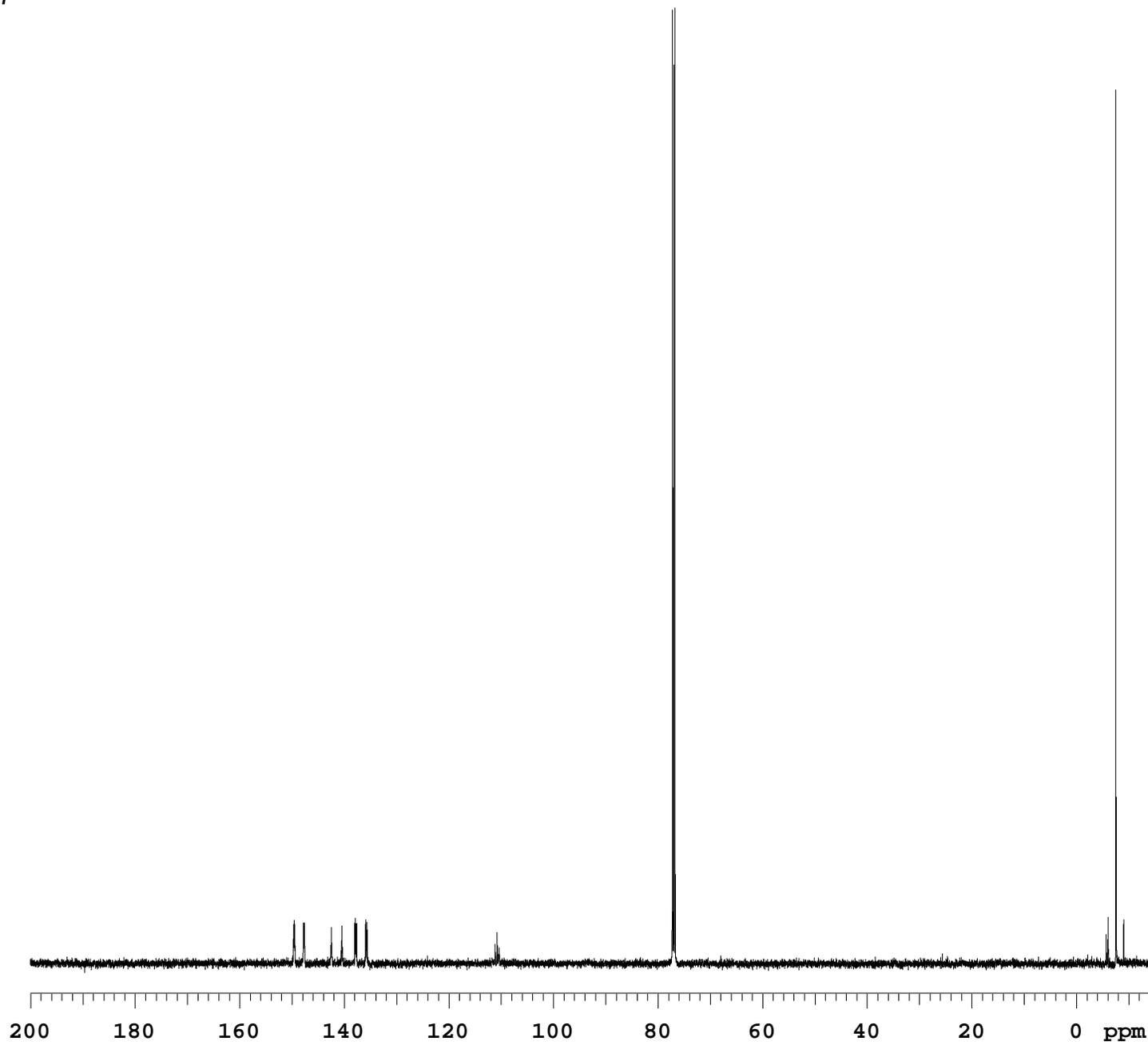
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

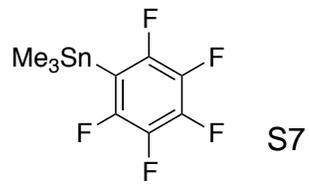
FT size 65536

Total time 65 minutes



Archive dir:

File: C



UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

1316 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

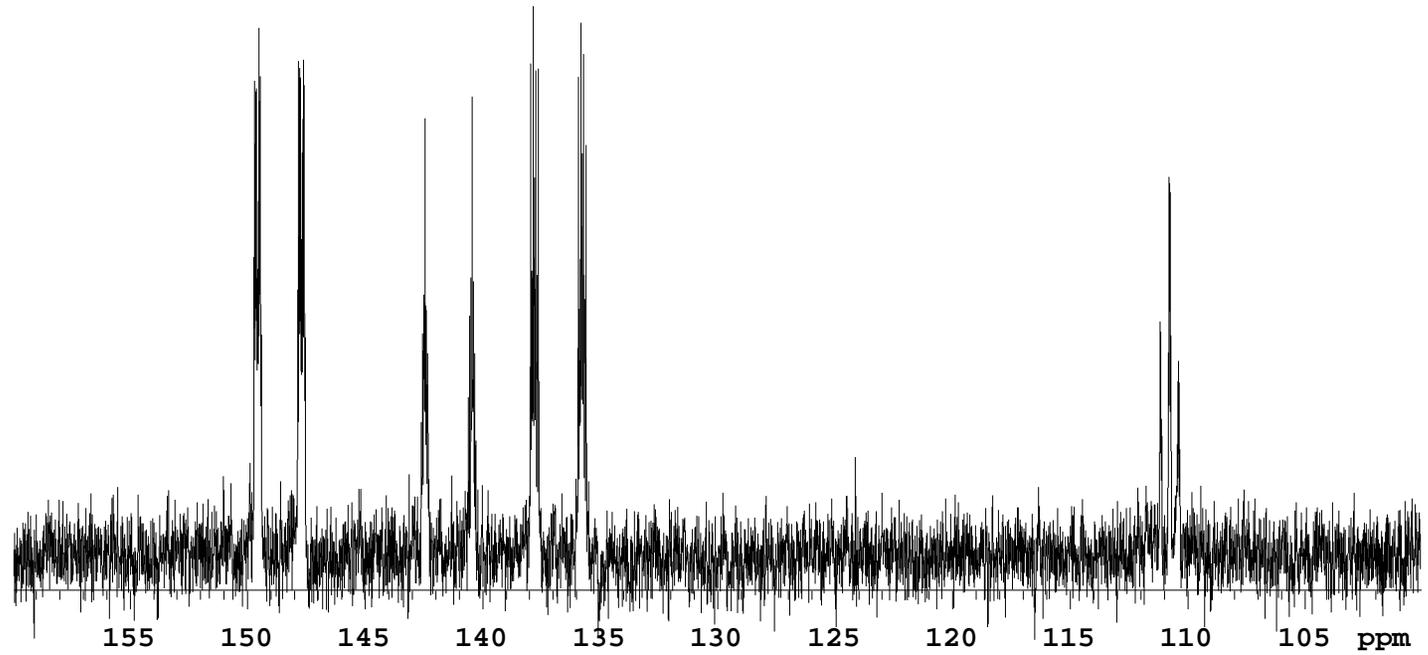
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

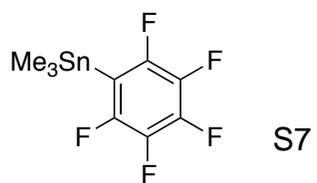
FT size 65536

Total time 65 minutes



Archive dir:

File: C



UO Inova-500 standard 19F

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: F

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 30.0 degrees

Acq. time 1.000 sec

Width 100.0 kHz

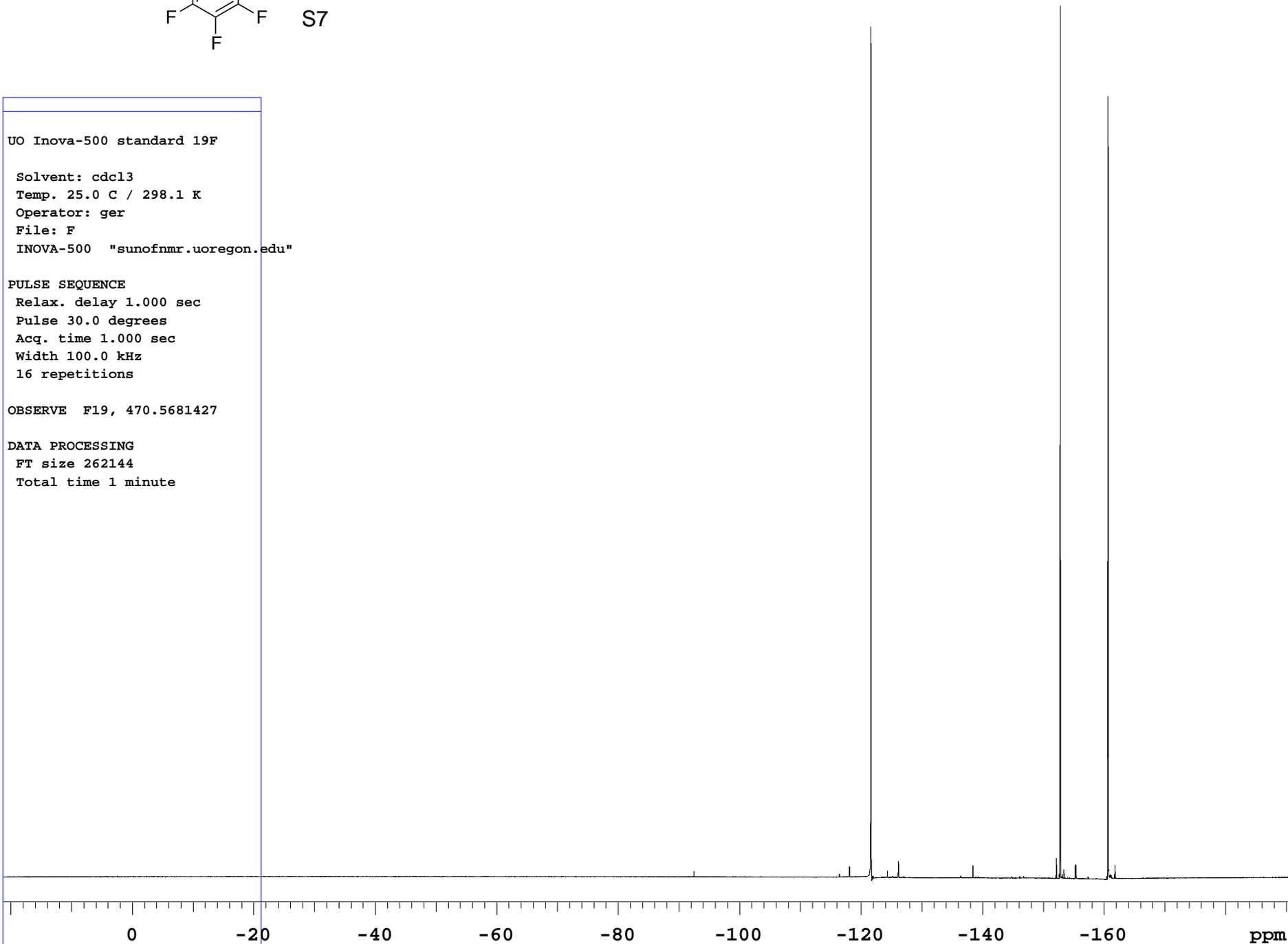
16 repetitions

OBSERVE F19, 470.5681427

DATA PROCESSING

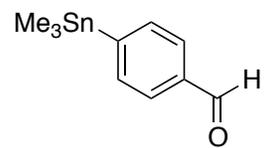
FT size 262144

Total time 1 minute



Archive dir:

File: F



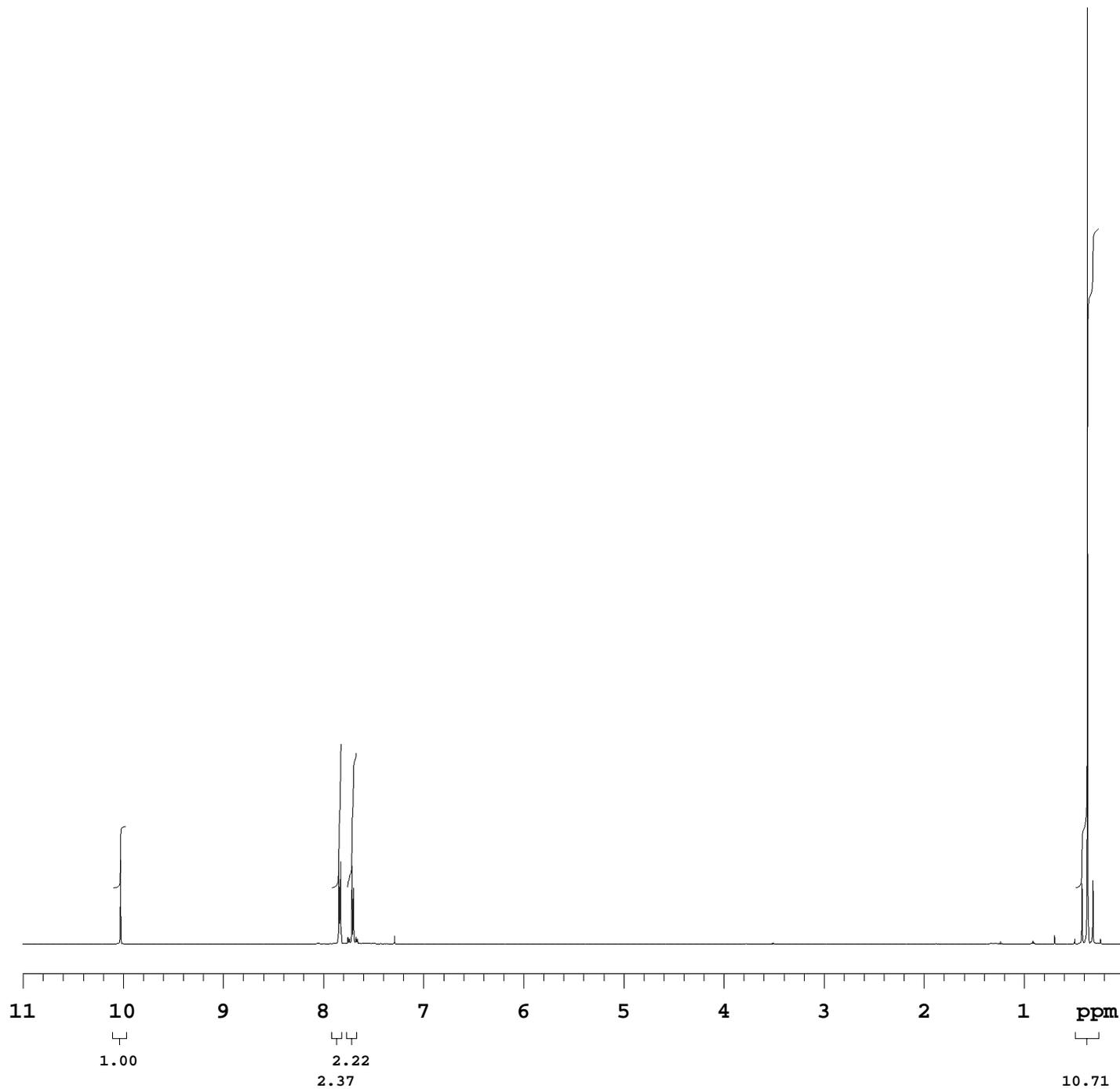
S8

UO Inova-500 standard 1H  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: H  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8001.6 Hz  
8 repetitions

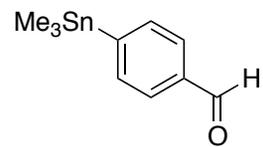
OBSERVE H1, 500.1042443

DATA PROCESSING  
FT size 32768  
Total time 1 minute



Archive dir:

File: H



S8

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

208 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

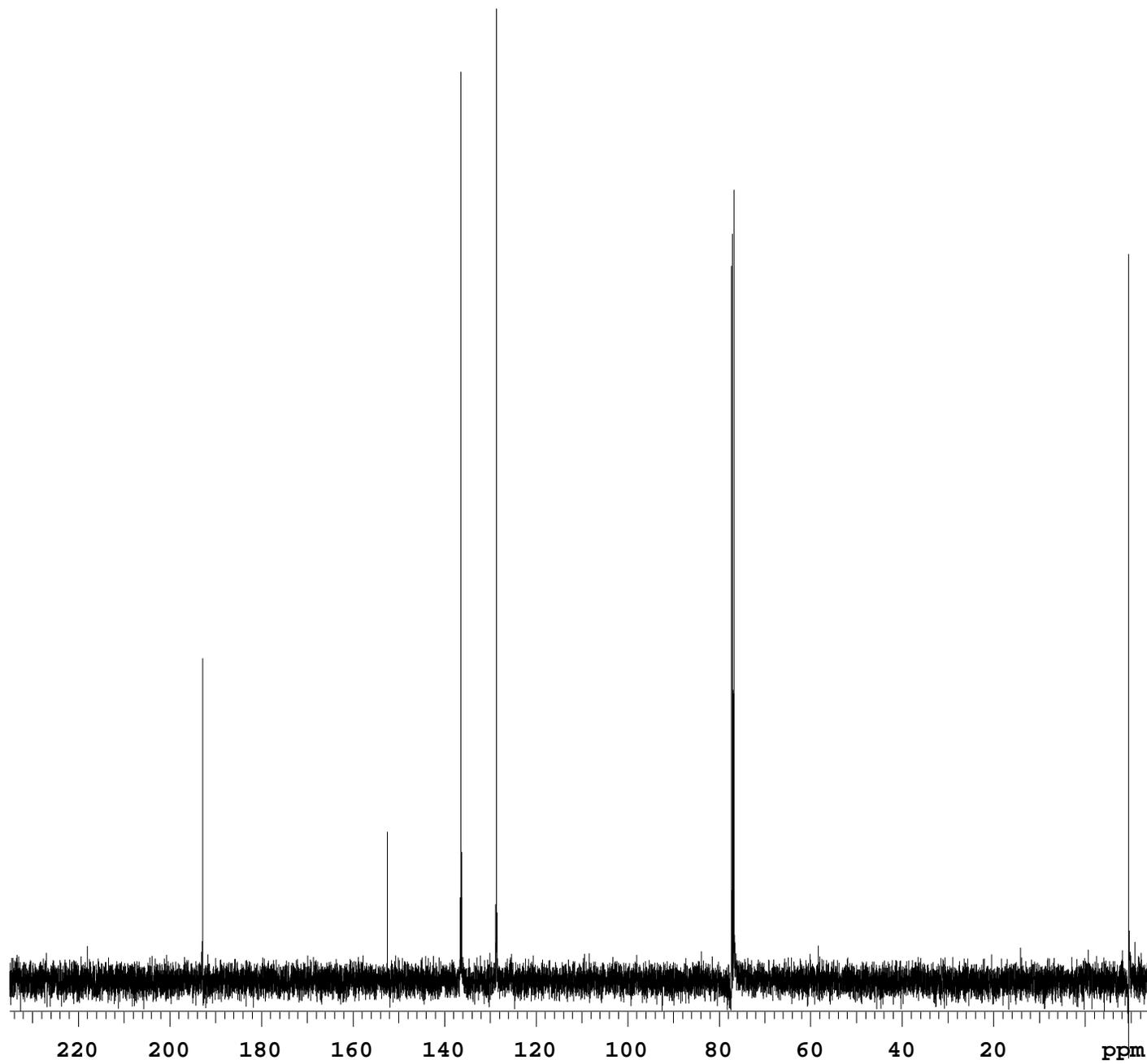
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

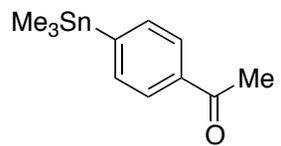
FT size 65536

Total time 6 minutes



Archive dir:

File: C



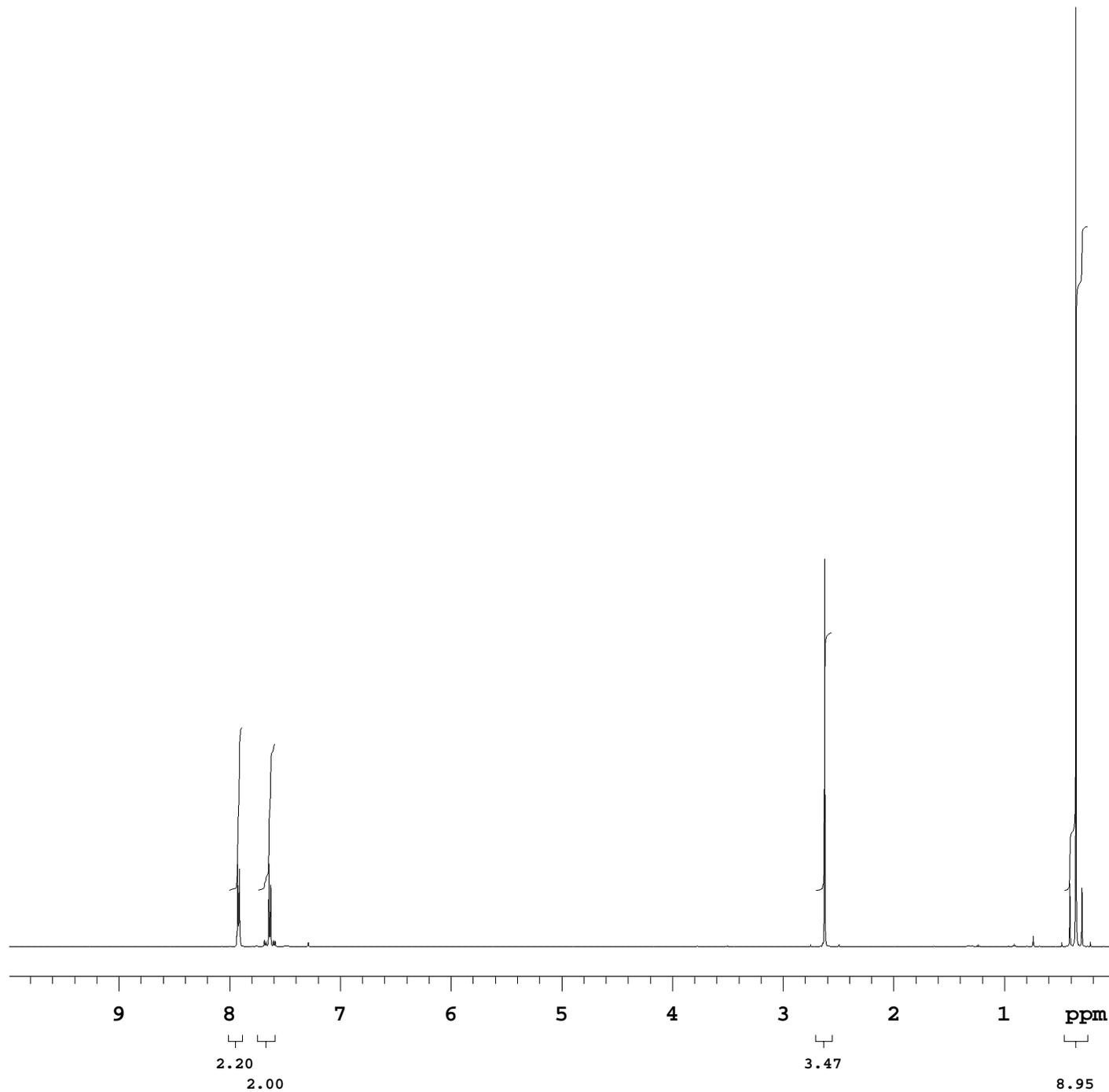
S9

UO Inova-500 standard 1H  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: H  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8001.6 Hz  
8 repetitions

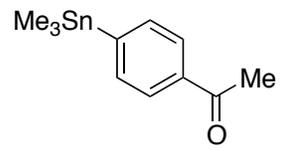
OBSERVE H1, 500.1042443

DATA PROCESSING  
FT size 32768  
Total time 1 minute



Archive dir:

File: H



S9

UO Inova-500 Carbon-13

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

284 repetitions

OBSERVE C13, 125.7513123

DECOUPLE H1, 500.1067449

Power 39 dB

continuously on

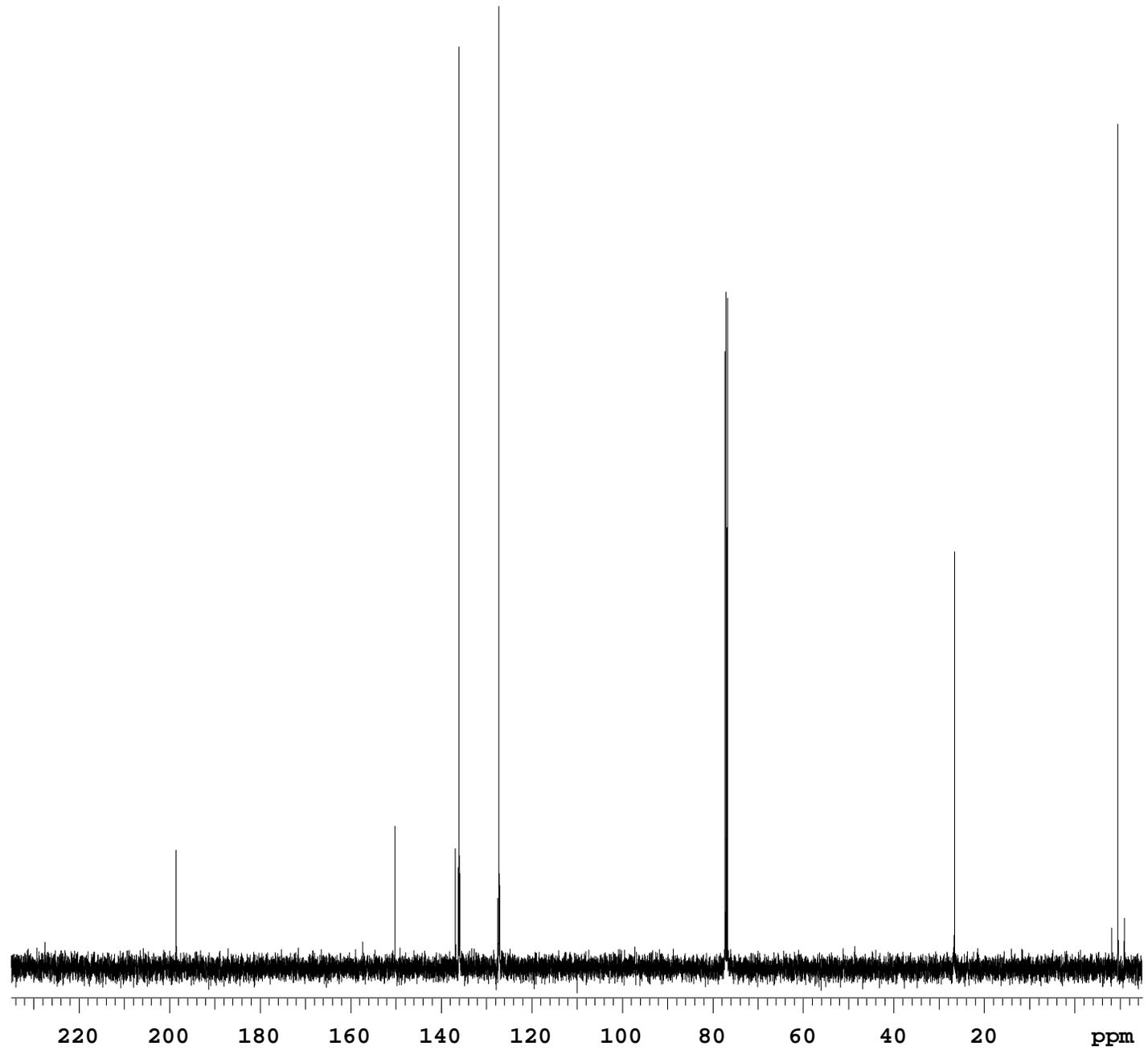
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

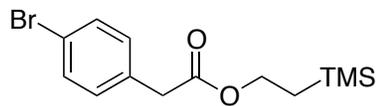
FT size 65536

Total time 9 minutes



Archive dir:

File: C



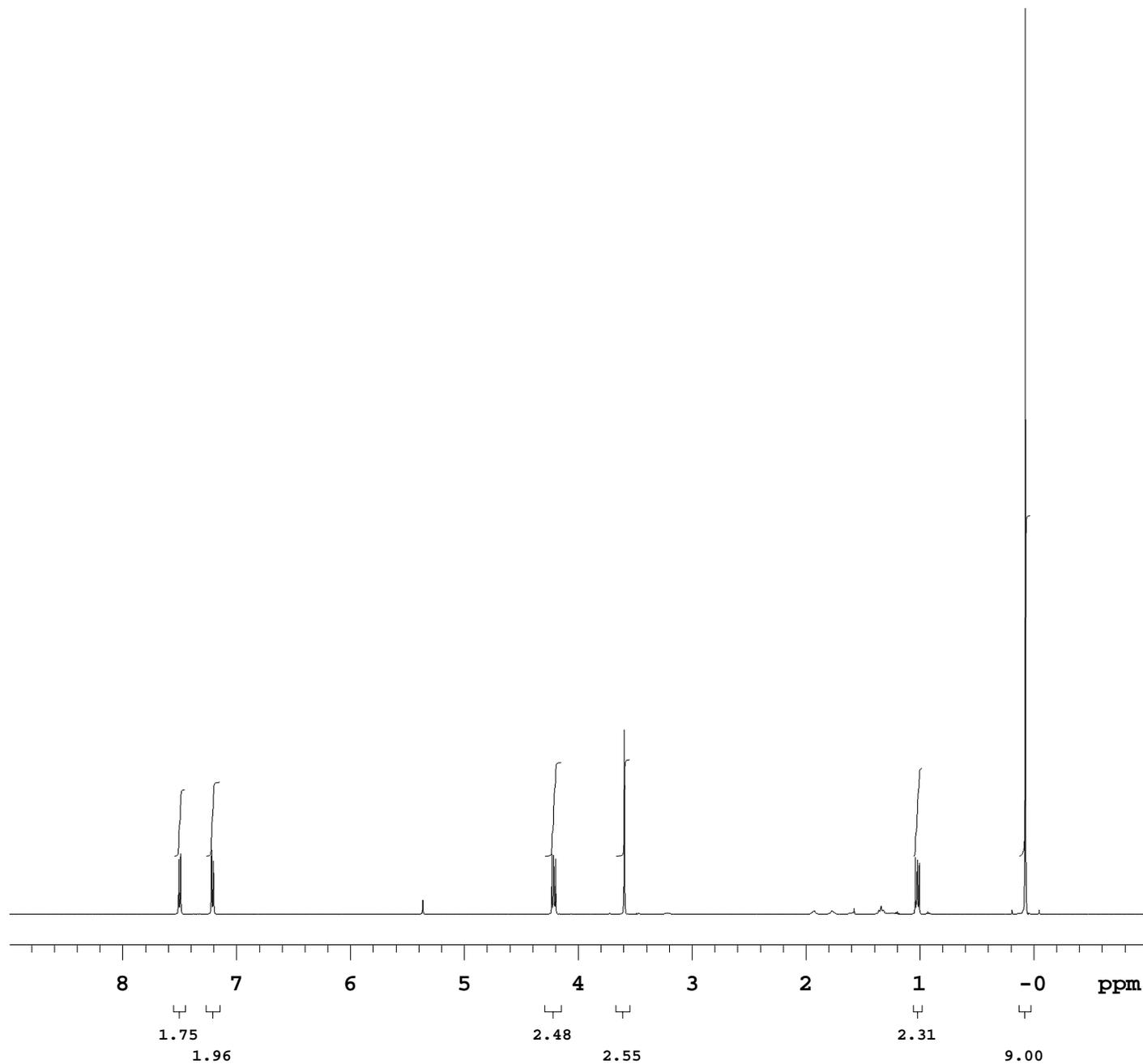
S10

UO Inova-500 standard 1H  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: H  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8001.6 Hz  
8 repetitions

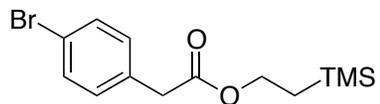
OBSERVE H1, 500.1052045

DATA PROCESSING  
FT size 32768  
Total time 1 minute



Archive dir:

File: H



S10

UO Inova-500 Carbon-13

Solvent: cd2cl2

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

264 repetitions

OBSERVE C13, 125.7515537

DECOUPLE H1, 500.1077051

Power 39 dB

continuously on

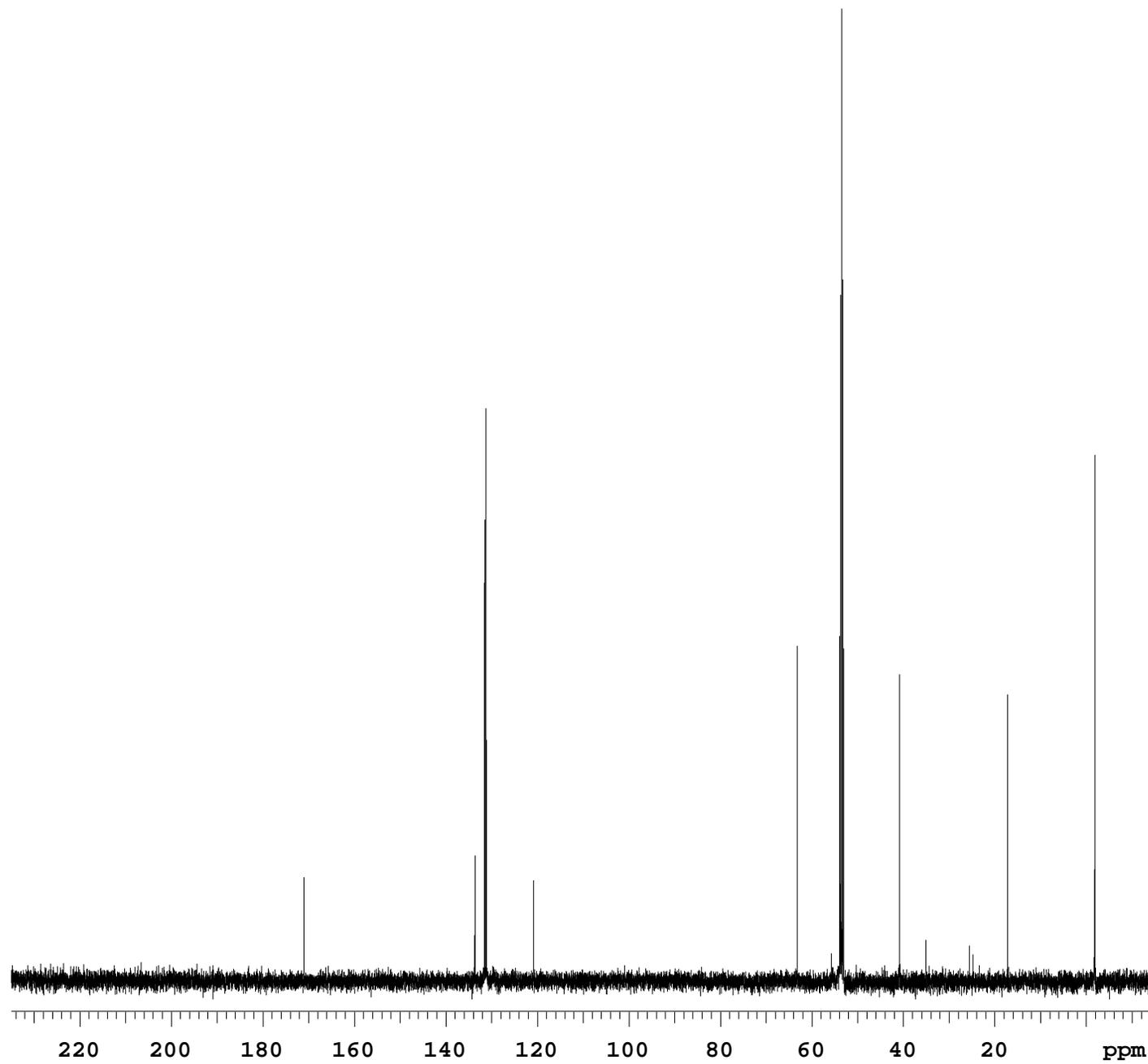
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

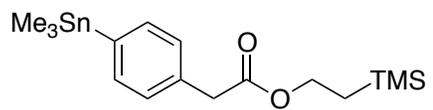
FT size 65536

Total time 8 minutes



Archive dir:

File: C



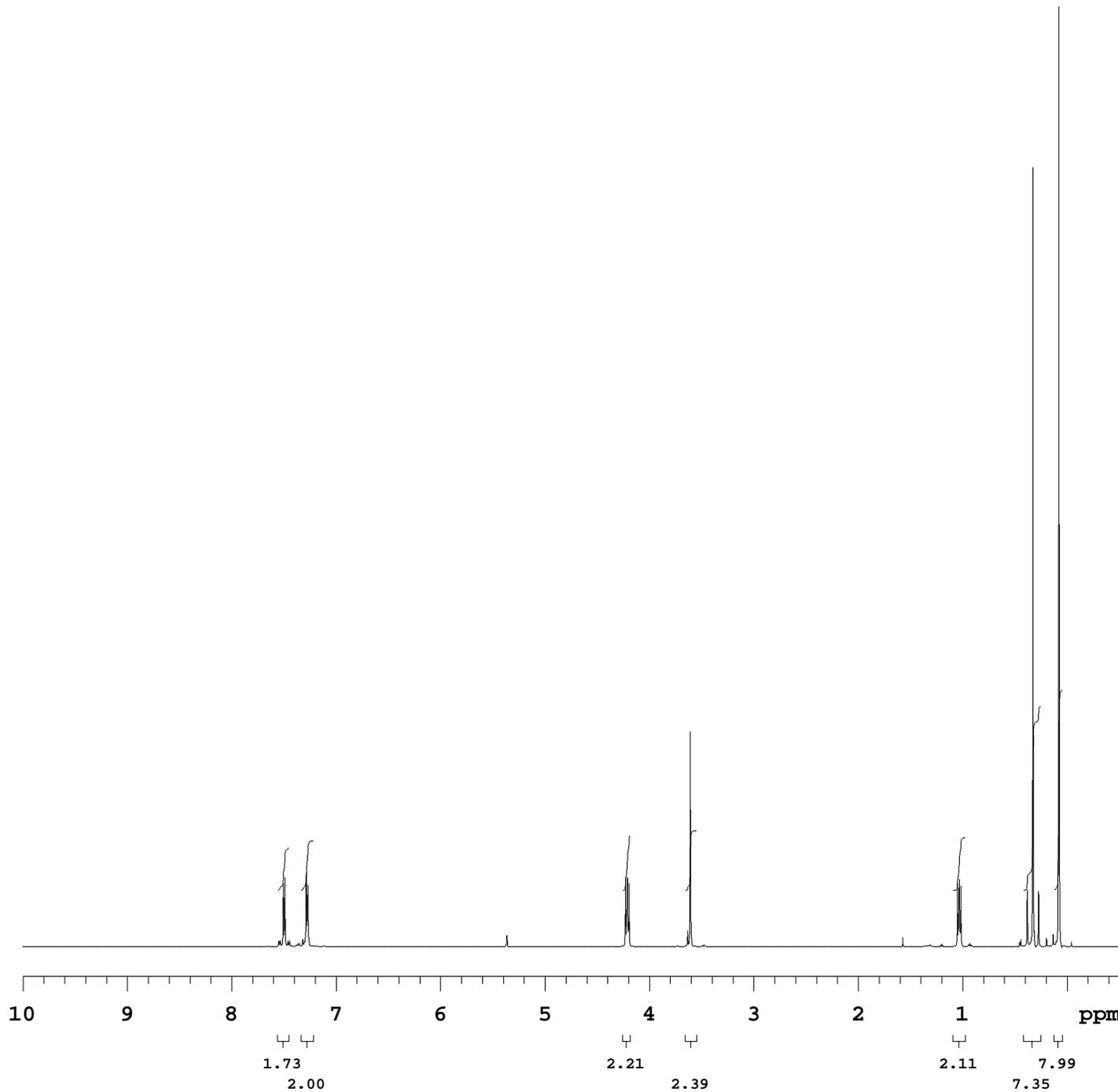
3

UO Inova-500 standard 1H  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: H  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8001.6 Hz  
8 repetitions

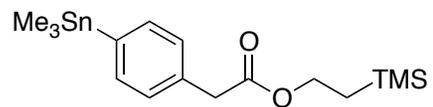
OBSERVE H1, 500.1052045

DATA PROCESSING  
FT size 32768  
Total time 1 minute



Archive dir:

File: H



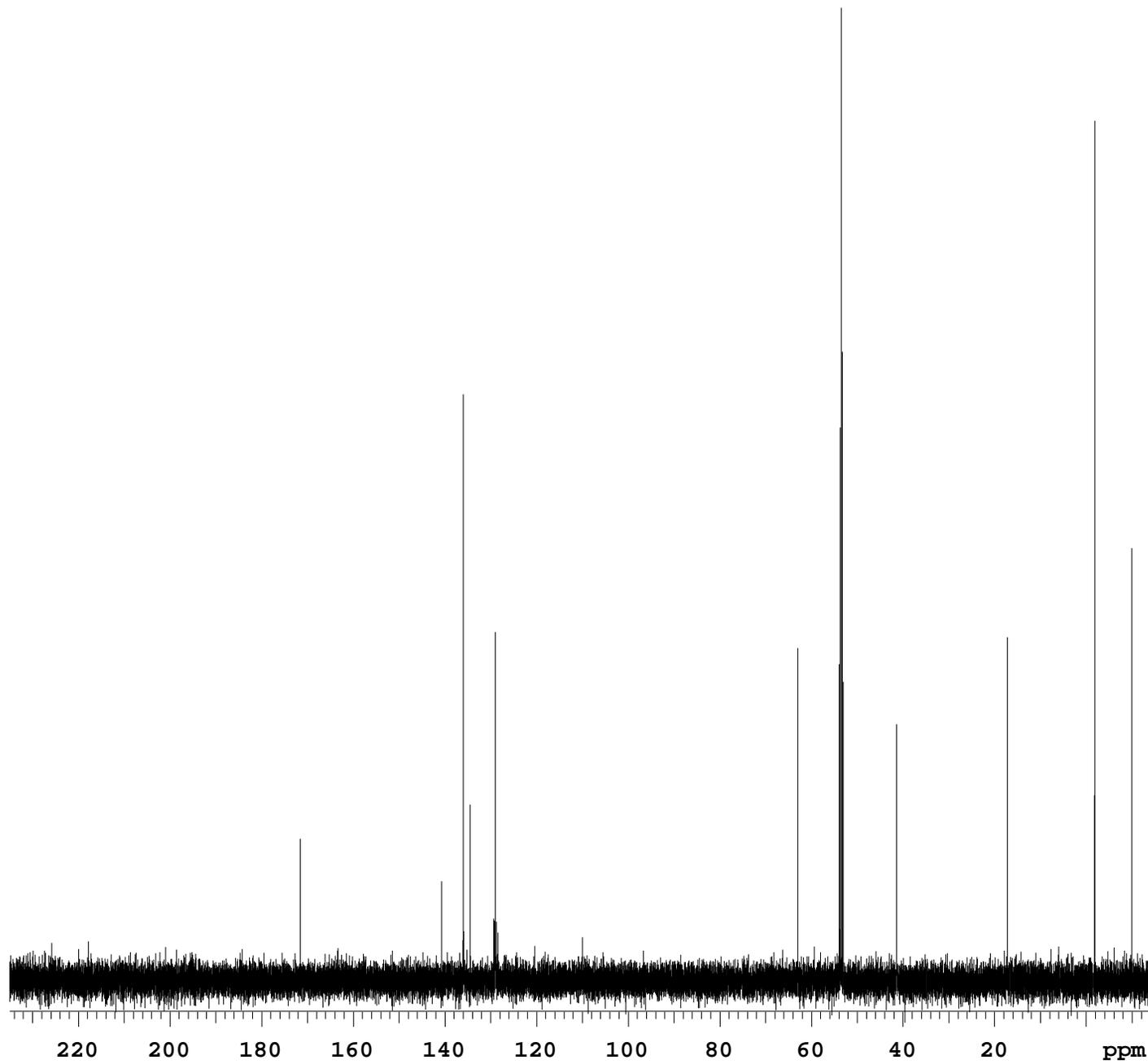
3

UO Inova-500 standard 1H  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: C  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.000 sec  
Width 31434.2 Hz  
380 repetitions

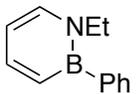
OBSERVE C13, 125.7515537  
DECOUPLE H1, 500.1077051  
Power 39 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
FT size 65536  
Total time 12 minutes



Archive dir:

File: C



2a

UO Inova-300-North  
Boron-11

Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: H  
INOVA-500 "sunofnmr.uoregon.edu"

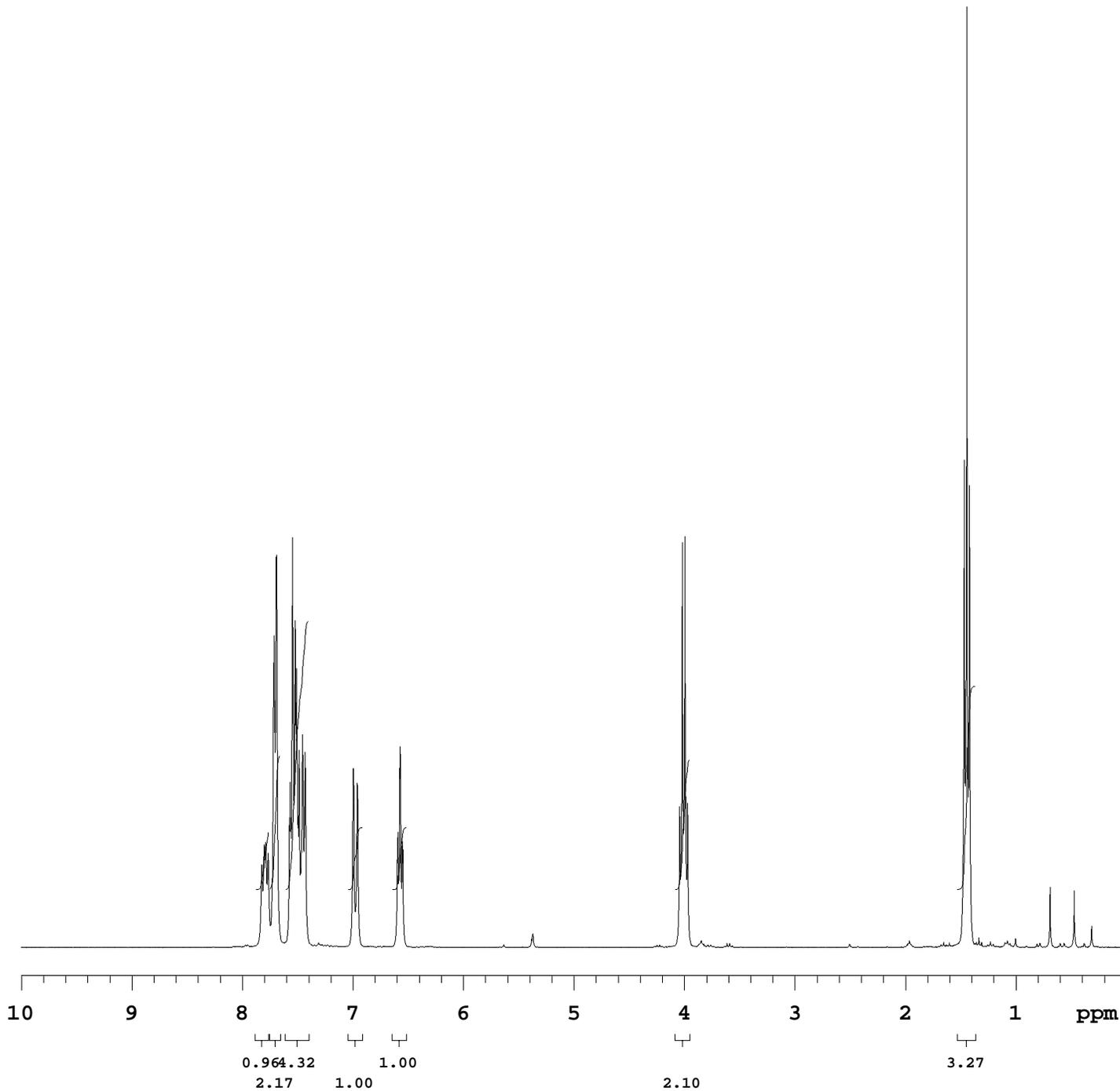
PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 4800.8 Hz  
8 repetitions

OBSERVE H1, 300.0510060

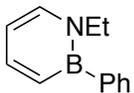
DATA PROCESSING

FT size 32768  
Total time 1 minute



Archive dir:

File: H



2a

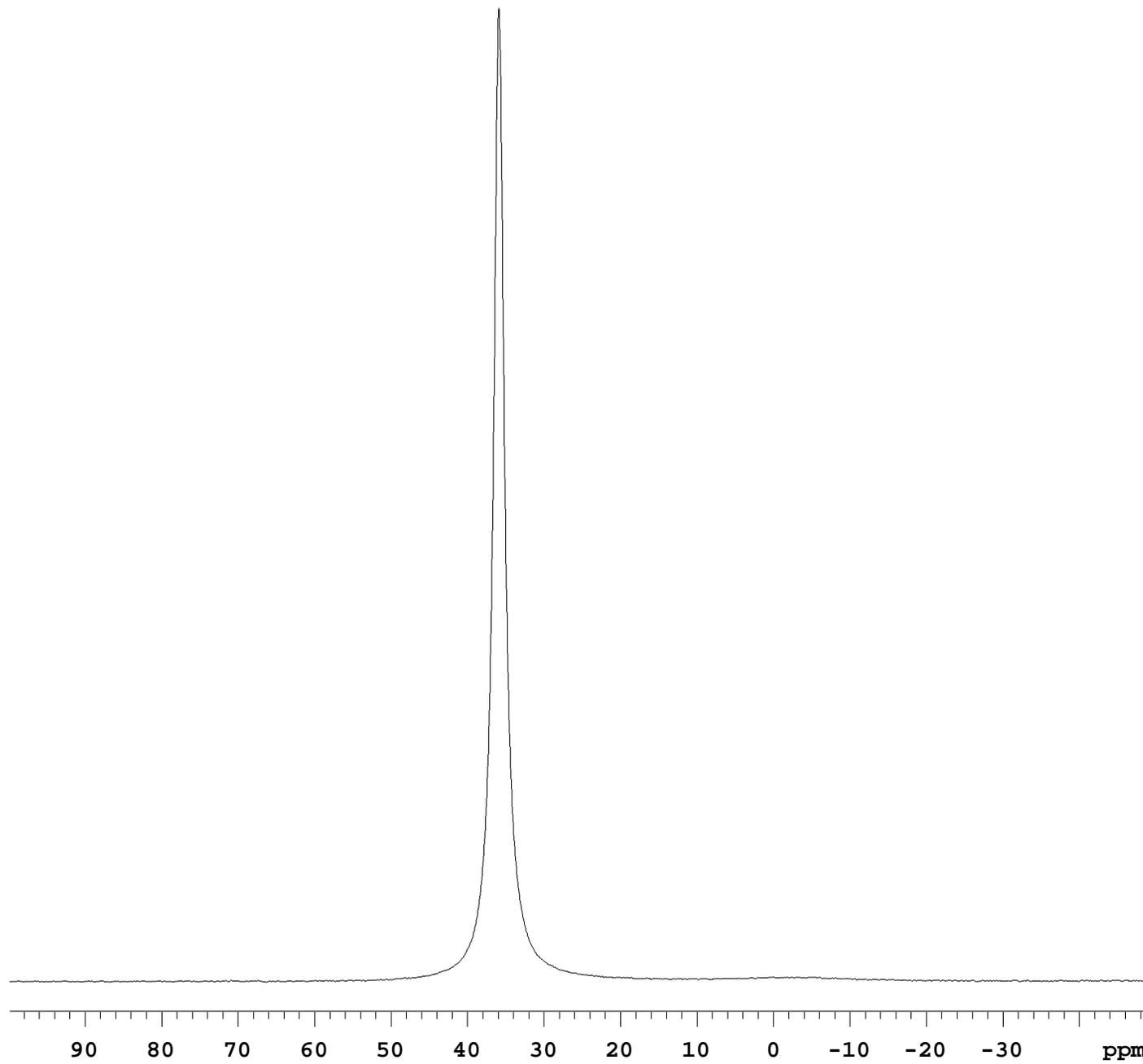
INDEX	FREQUENCY	PPM	HEIGHT
1	3452.2	35.860	159.0

UO Inova-300-North  
Boron-11  
  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: B  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
40 repetitions

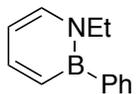
OBSERVE B11, 96.2682868

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute



Archive dir:

File: B



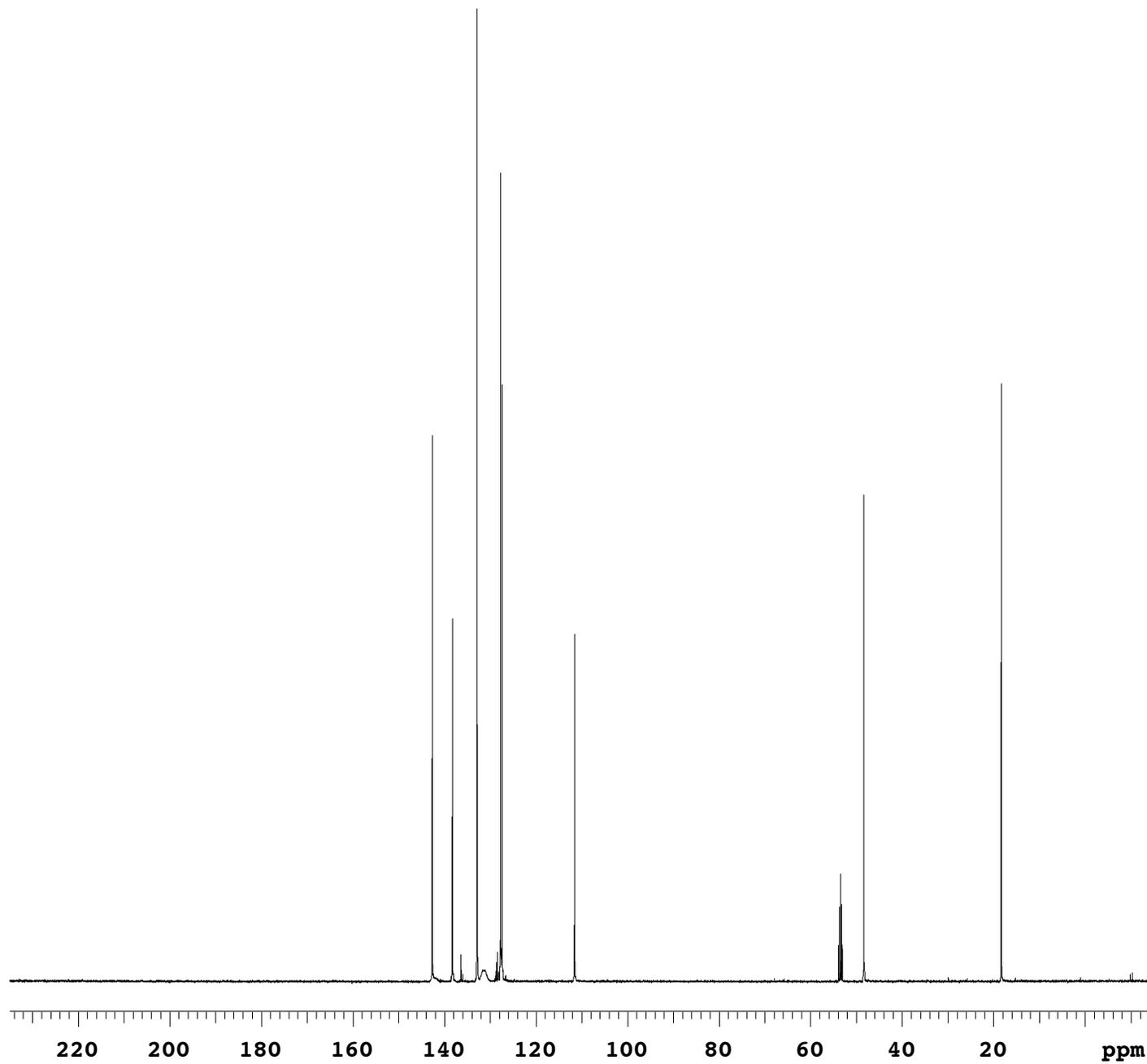
2a

UO Inova-500 standard 1H  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: C  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.000 sec  
Width 31434.2 Hz  
284 repetitions

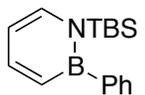
OBSERVE C13, 125.7515537  
DECOUPLE H1, 500.1077051  
Power 39 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 65536  
Total time 9 minutes



Archive dir:

File: C



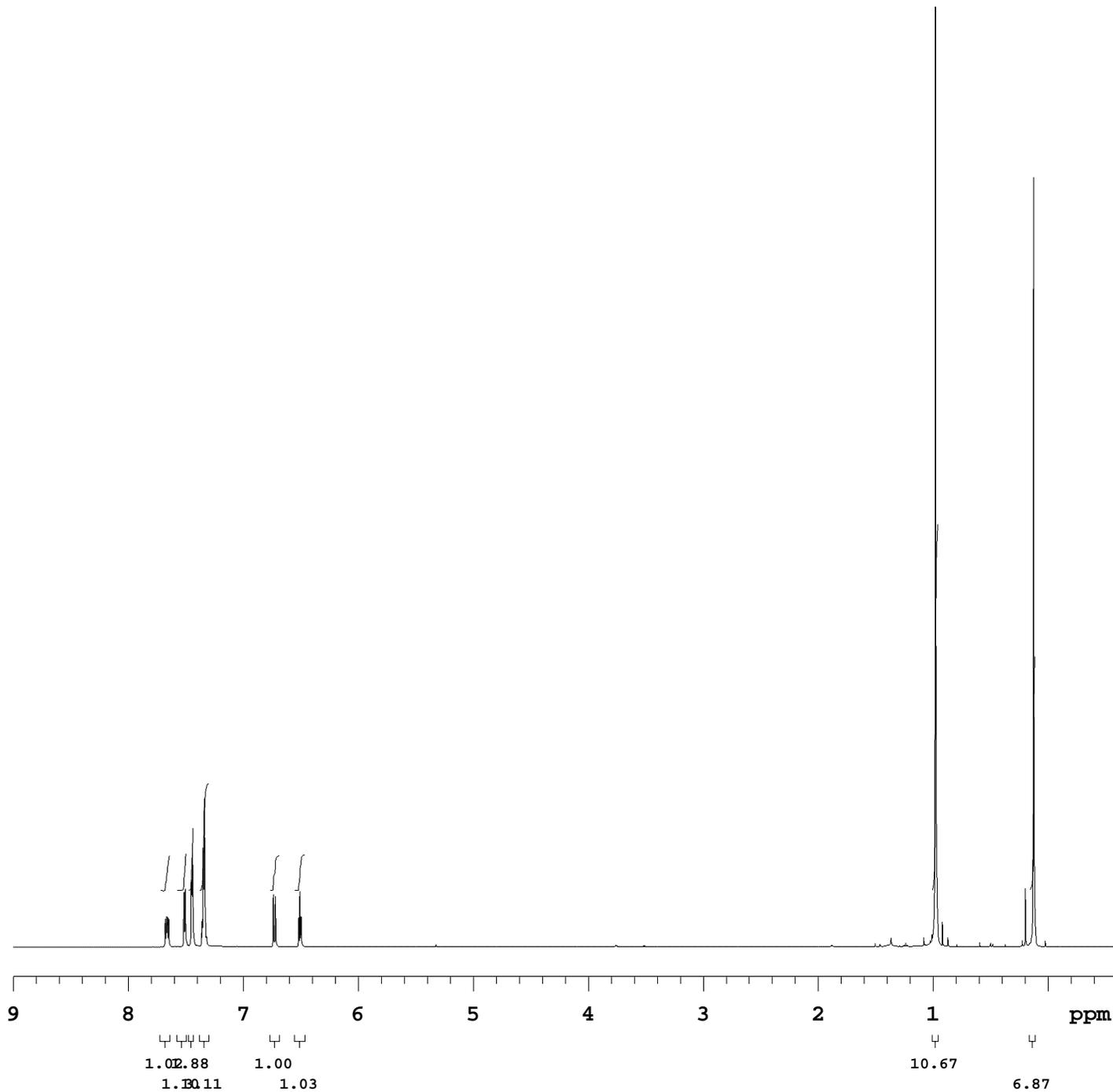
2b

UO VNMR5-600  
{CH-ColdProbe} 1H-observe  
  
Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: NTBS\_BPh\_H  
VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 9615.4 Hz  
8 repetitions

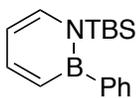
OBSERVE H1, 599.9795419

DATA PROCESSING  
FT size 65536  
Total time 1 minute



Archive dir:

File: NTBS\_BPh\_H



2b

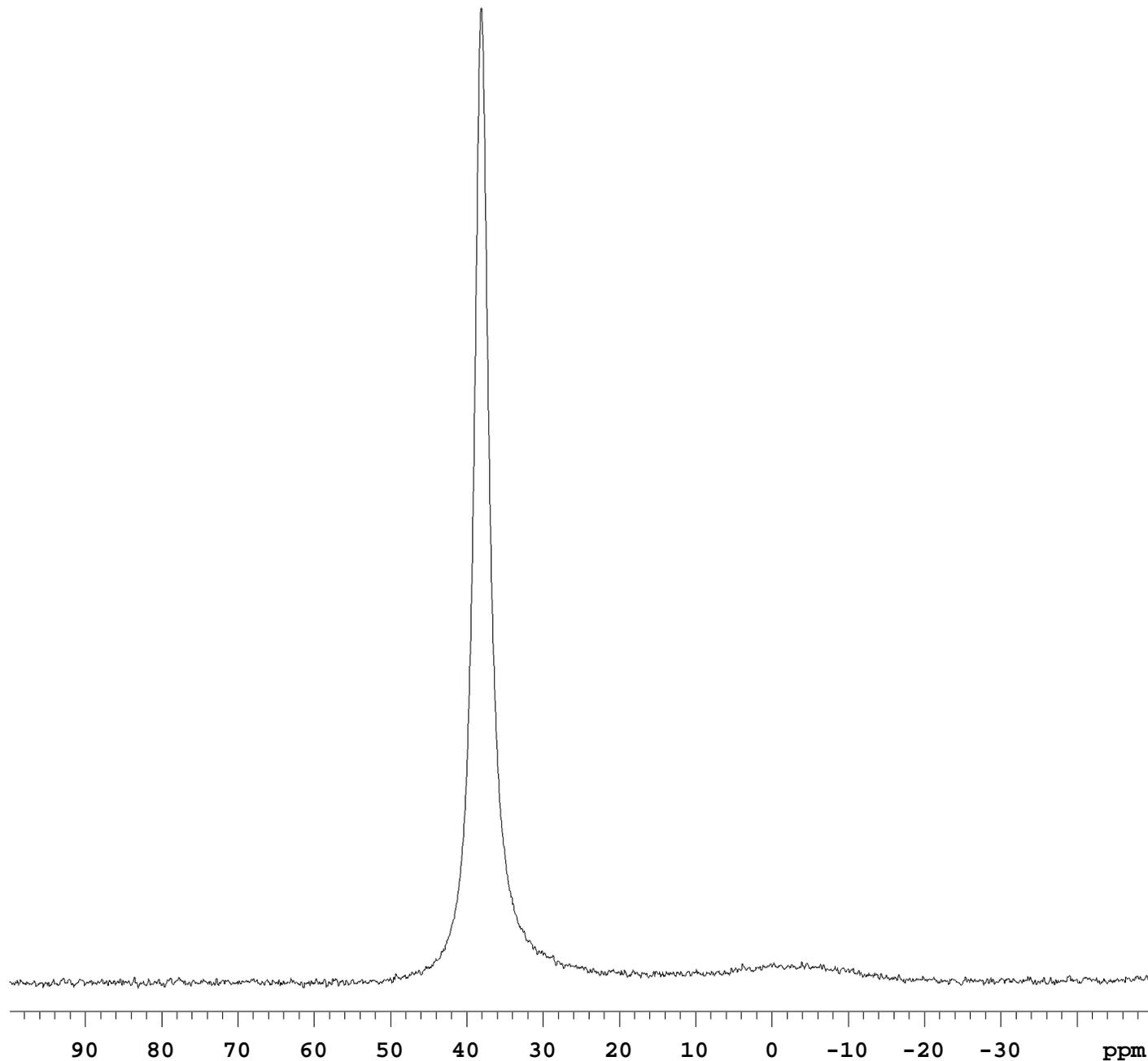
INDEX	FREQUENCY	PPM	HEIGHT
1	3662.2	38.041	159.0

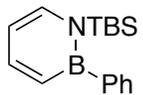
UO Inova-300-North  
Boron-11  
  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: NTBS\_BPh\_B  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
80 repetitions

OBSERVE B11, 96.2682868

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute





2b

UO Inova-500 standard 1H

Solvent: cd2cl2

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

284 repetitions

OBSERVE C13, 125.7515537

DECOUPLE H1, 500.1077051

Power 39 dB

continuously on

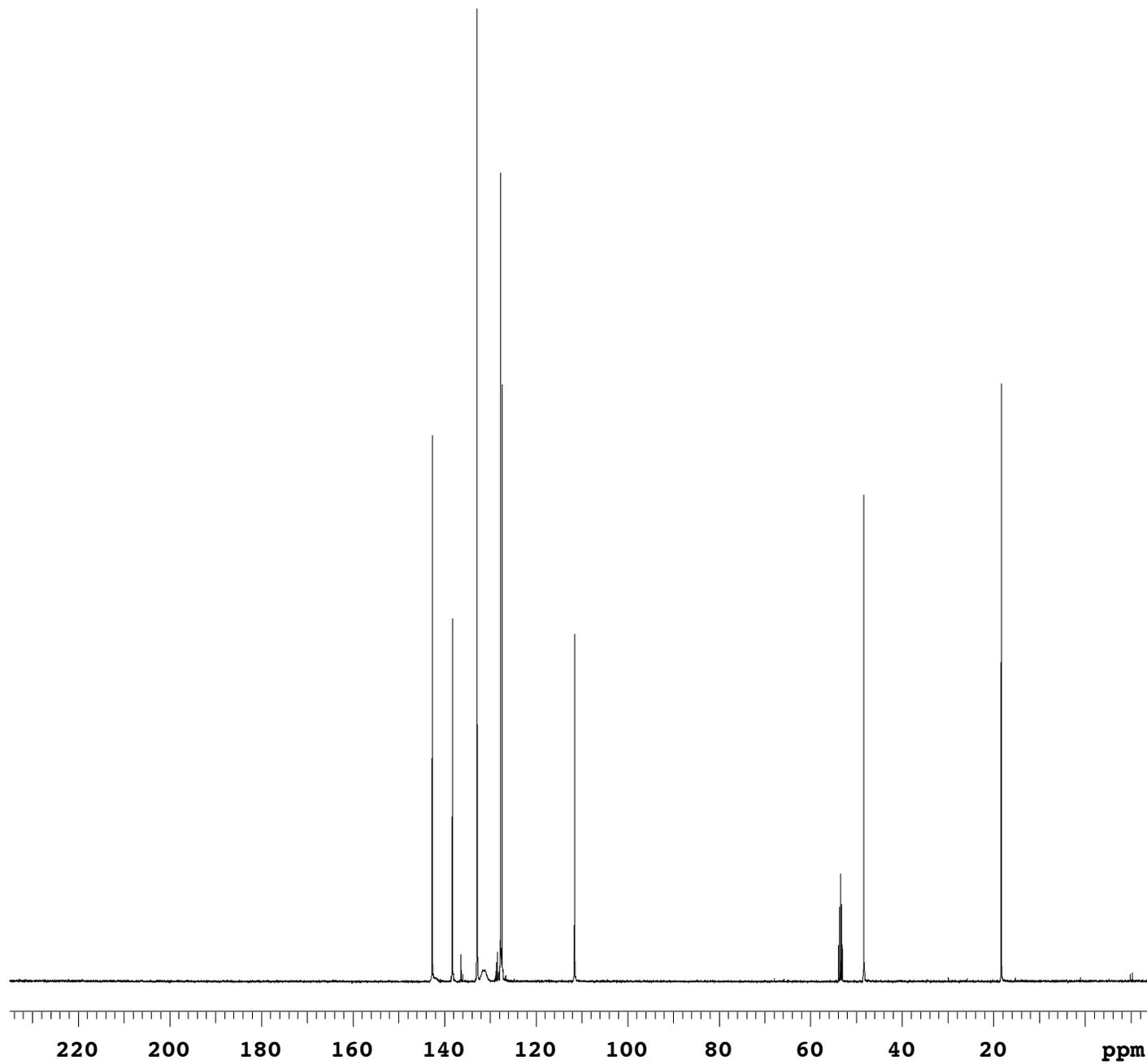
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

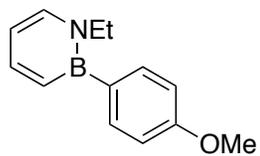
FT size 65536

Total time 9 minutes



Archive dir:

File: C



2c

UO Inova-300-North  
Boron-11

Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-OMe\_H\_300  
INOVA-500 "sunofnmr.uoregon.edu"

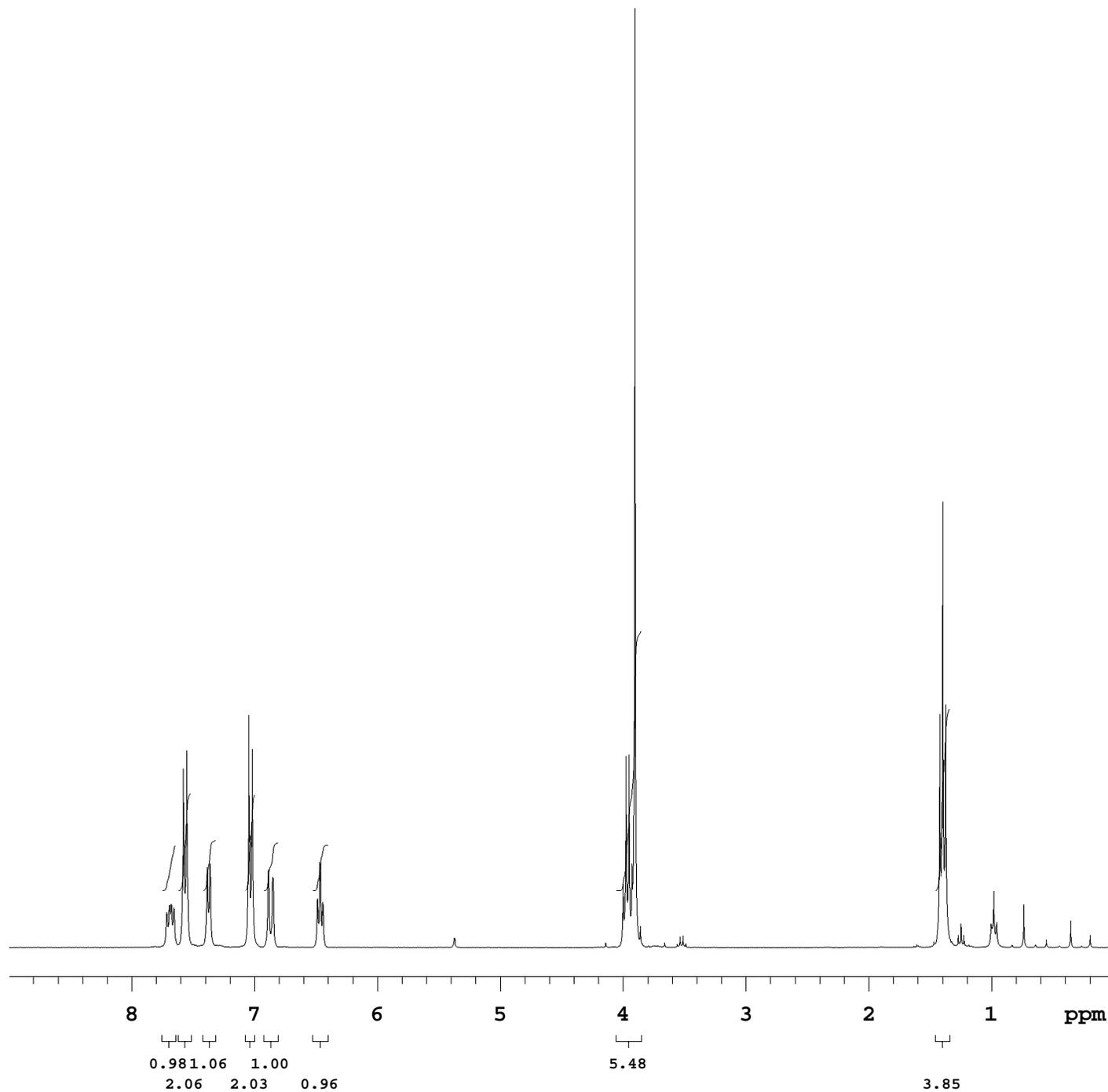
PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 4800.8 Hz  
8 repetitions

OBSERVE H1, 300.0510060

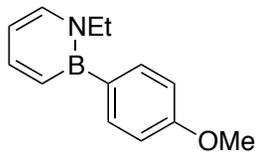
DATA PROCESSING

FT size 32768  
Total time 1 minute



Archive dir:

File: 4-OMe\_H\_300



2c

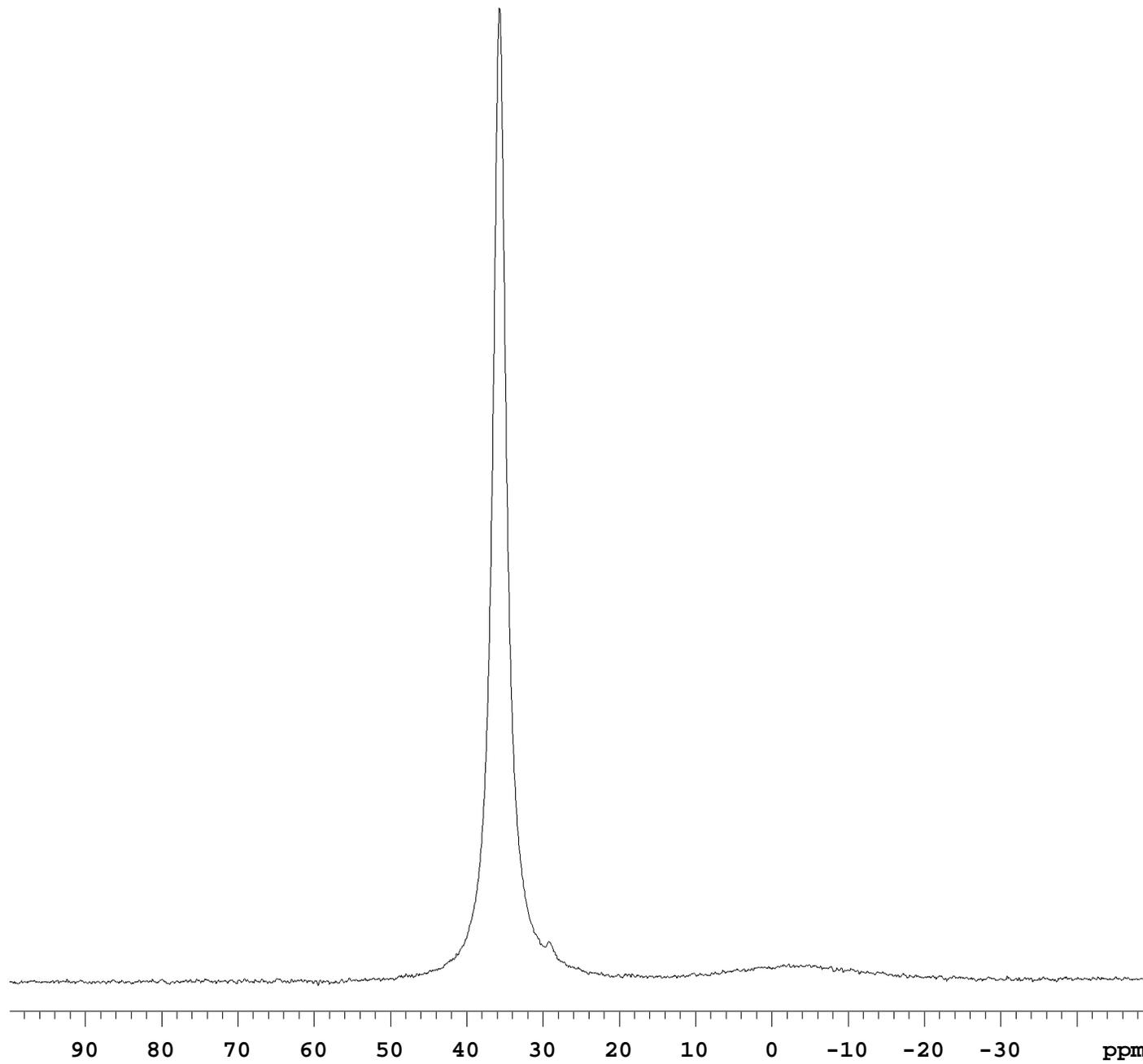
INDEX	FREQUENCY	PPM	HEIGHT
1	3437.5	35.708	159.0

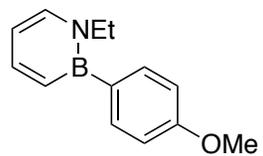
UO Inova-300-North  
Boron-11  
  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-OMe\_B  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
88 repetitions

OBSERVE B11, 96.2682868

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute





2c

STANDARD 1H OBSERVE -  
profile

Solvent: d2o  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-OMe\_C  
VNMRS-500 "sunofnmr.uoregon.edu"

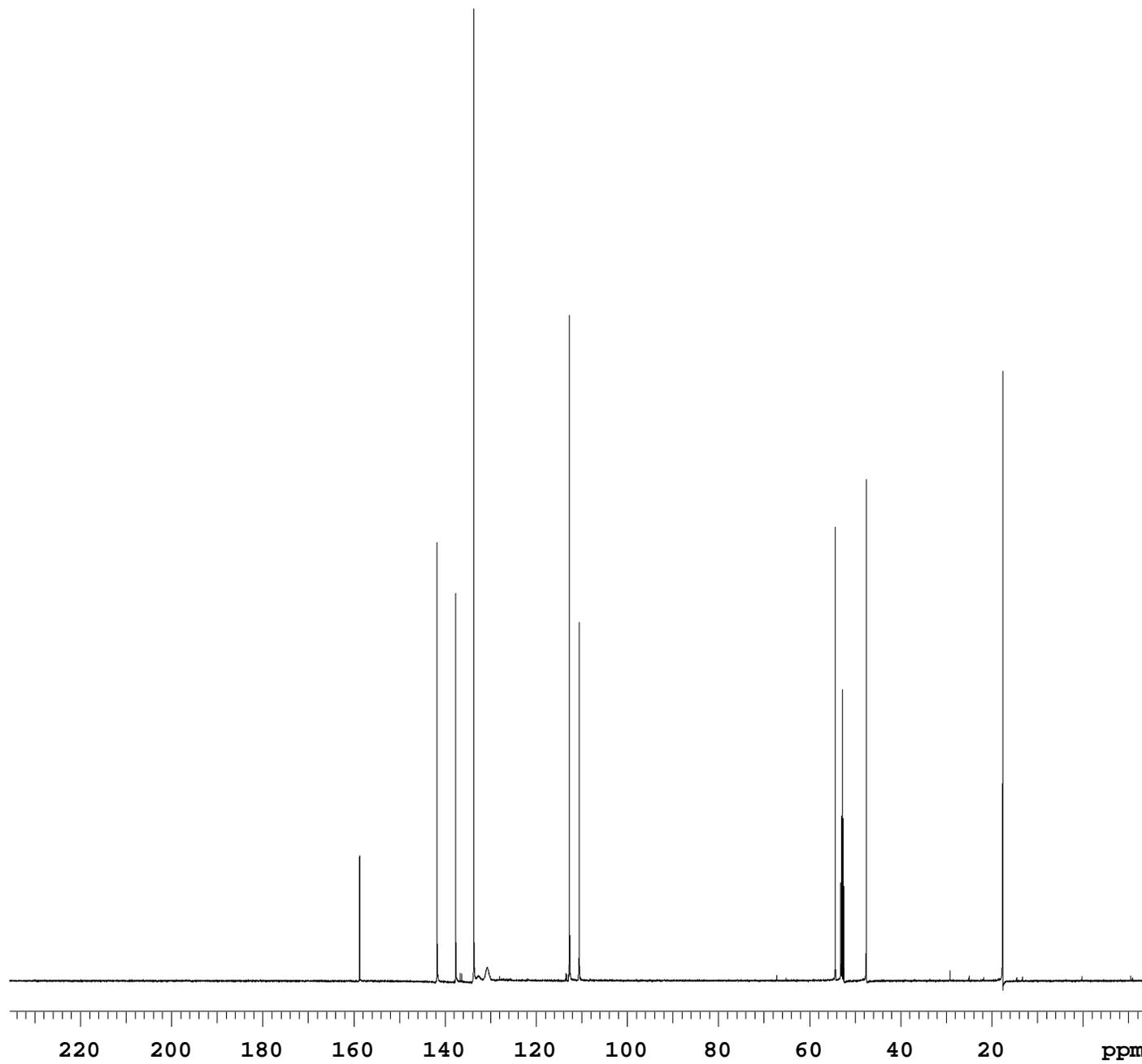
PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
48 repetitions

OBSERVE C13, 150.8650739  
DECOUPLE H1, 599.9829318  
Power 41 dB  
continuously on  
WALTZ-16 modulated

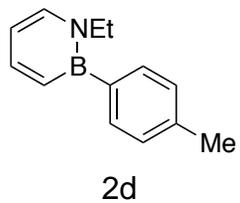
DATA PROCESSING

Line broadening 0.5 Hz  
FT size 65536  
Total time 1 minutes



Archive dir:

File: 4-OMe\_C



STANDARD 1H OBSERVE -  
profile

Solvent: d2o  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-Me\_H  
VNMRS-500 "sunofnmr.uoregon.edu"

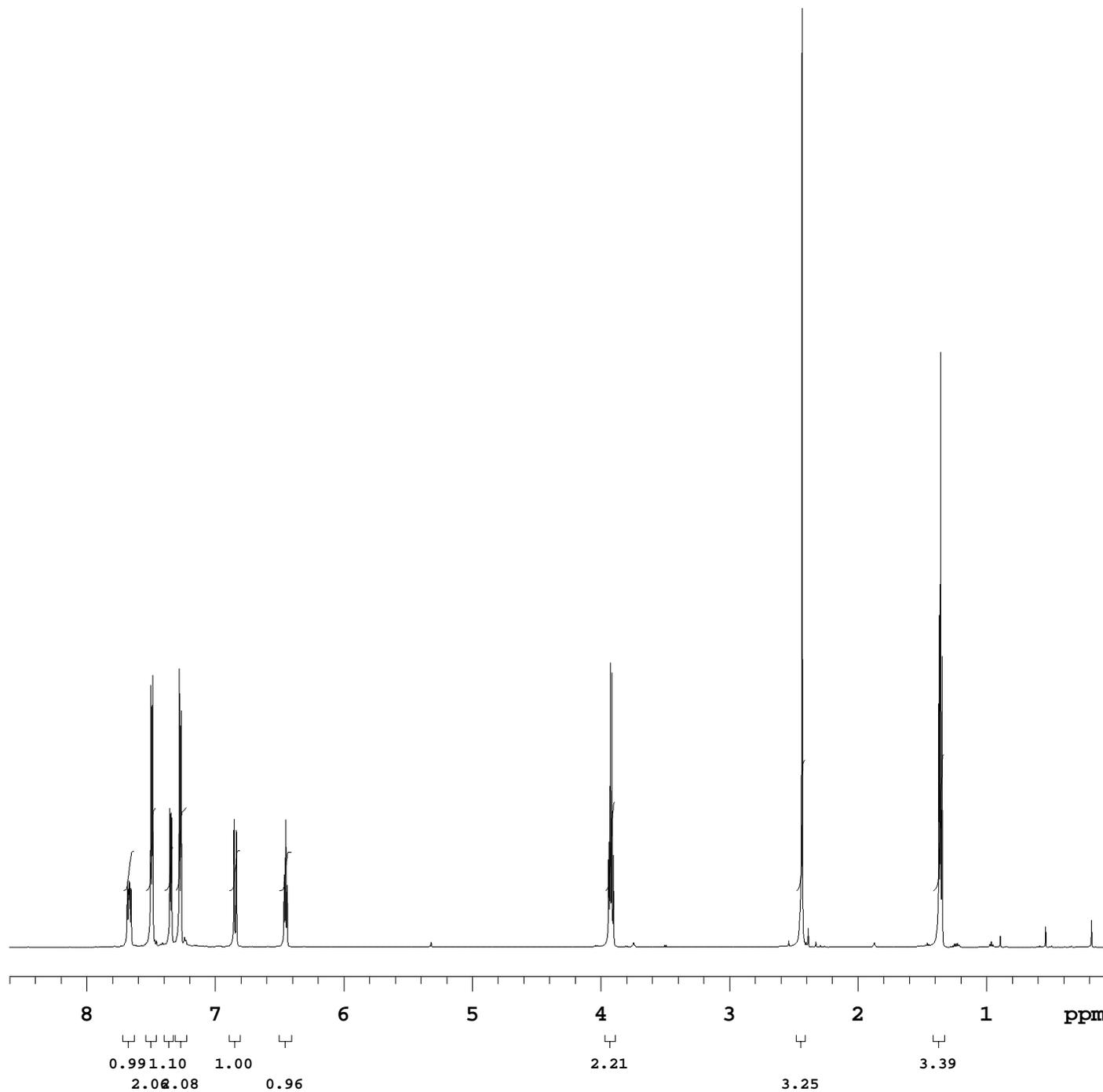
PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 9615.4 Hz  
8 repetitions

OBSERVE H1, 599.9795438

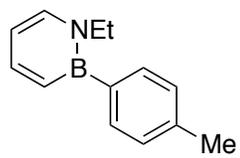
DATA PROCESSING

FT size 65536  
Total time 1 minute



Archive dir:

File: 4-Me\_H



2d

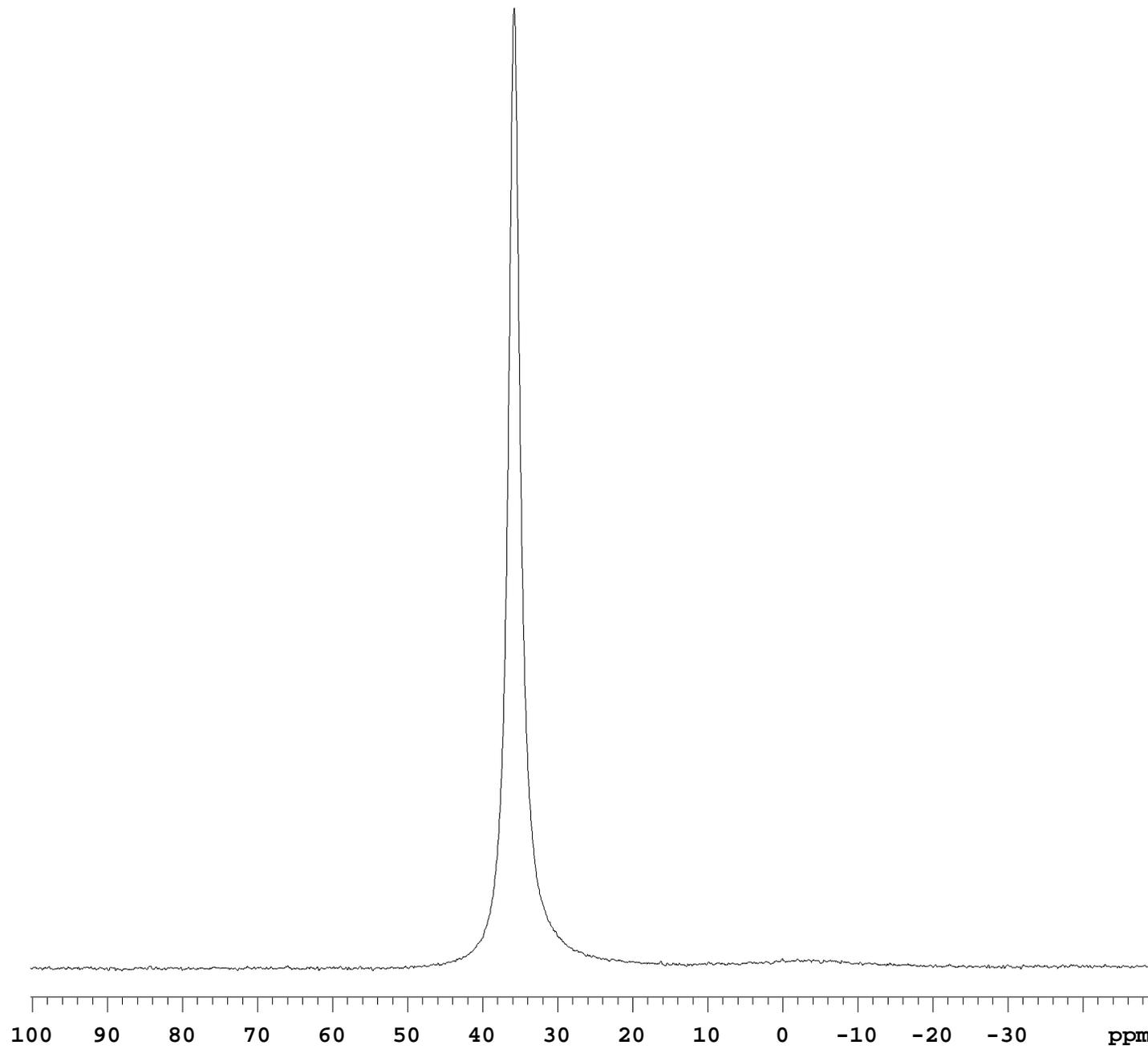
INDEX	FREQUENCY	PPM	HEIGHT
1	3442.4	35.759	159.0

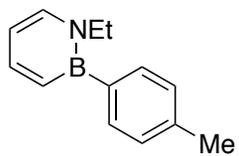
UO Inova-300-North  
Boron-11  
  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-Me\_B  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
80 repetitions

OBSERVE B11, 96.2682868

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute





2d

STANDARD 1H OBSERVE -  
profile

Solvent: d2o  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-Me\_C  
VNMRS-500 "sunofnmr.uoregon.edu"

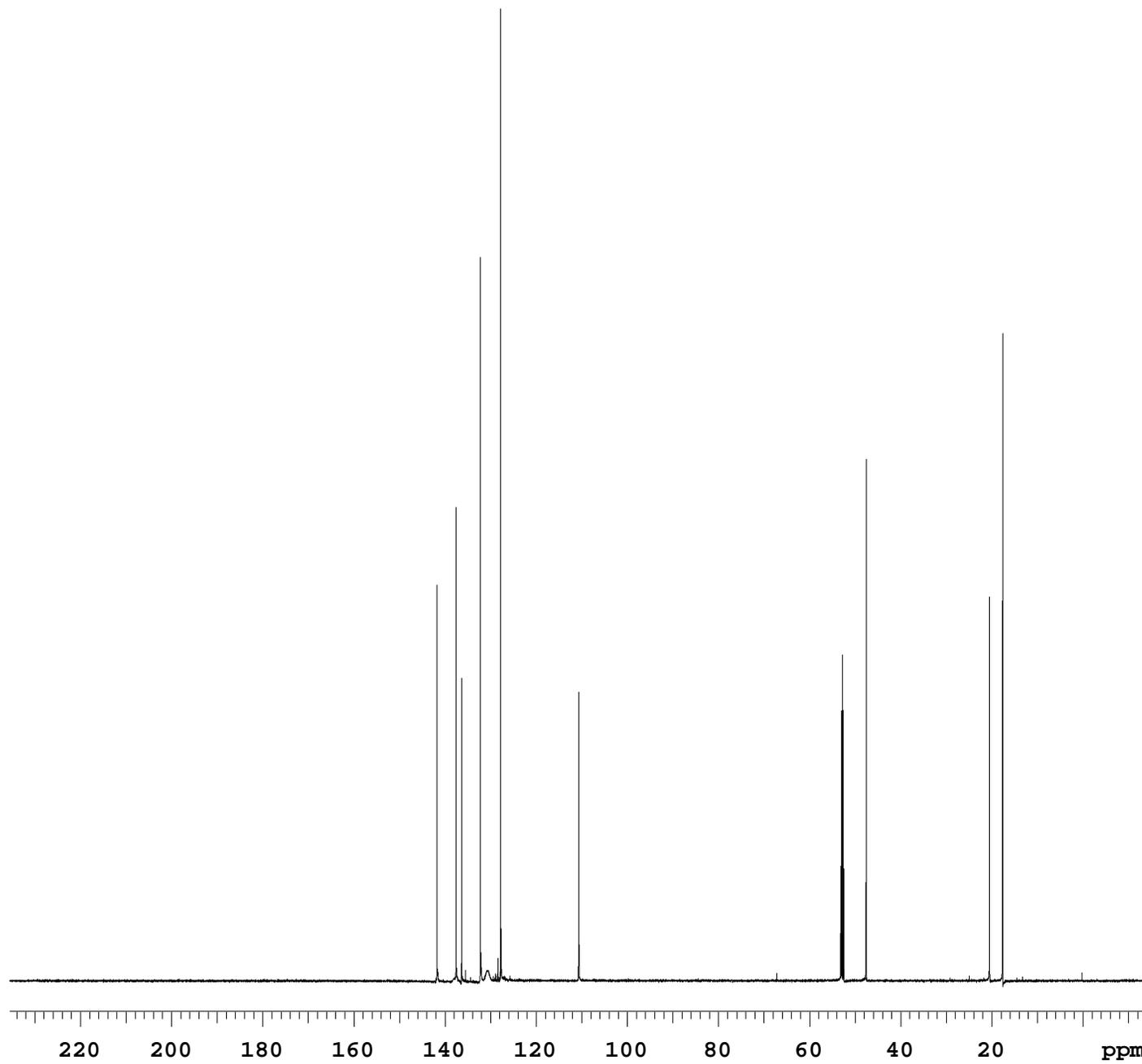
PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
52 repetitions

OBSERVE C13, 150.8650739  
DECOUPLE H1, 599.9829318  
Power 41 dB  
continuously on  
WALTZ-16 modulated

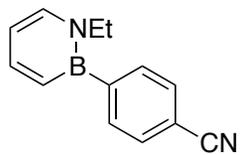
DATA PROCESSING

Line broadening 0.5 Hz  
FT size 65536  
Total time 1 minutes



Archive dir:

File: 4-Me\_C



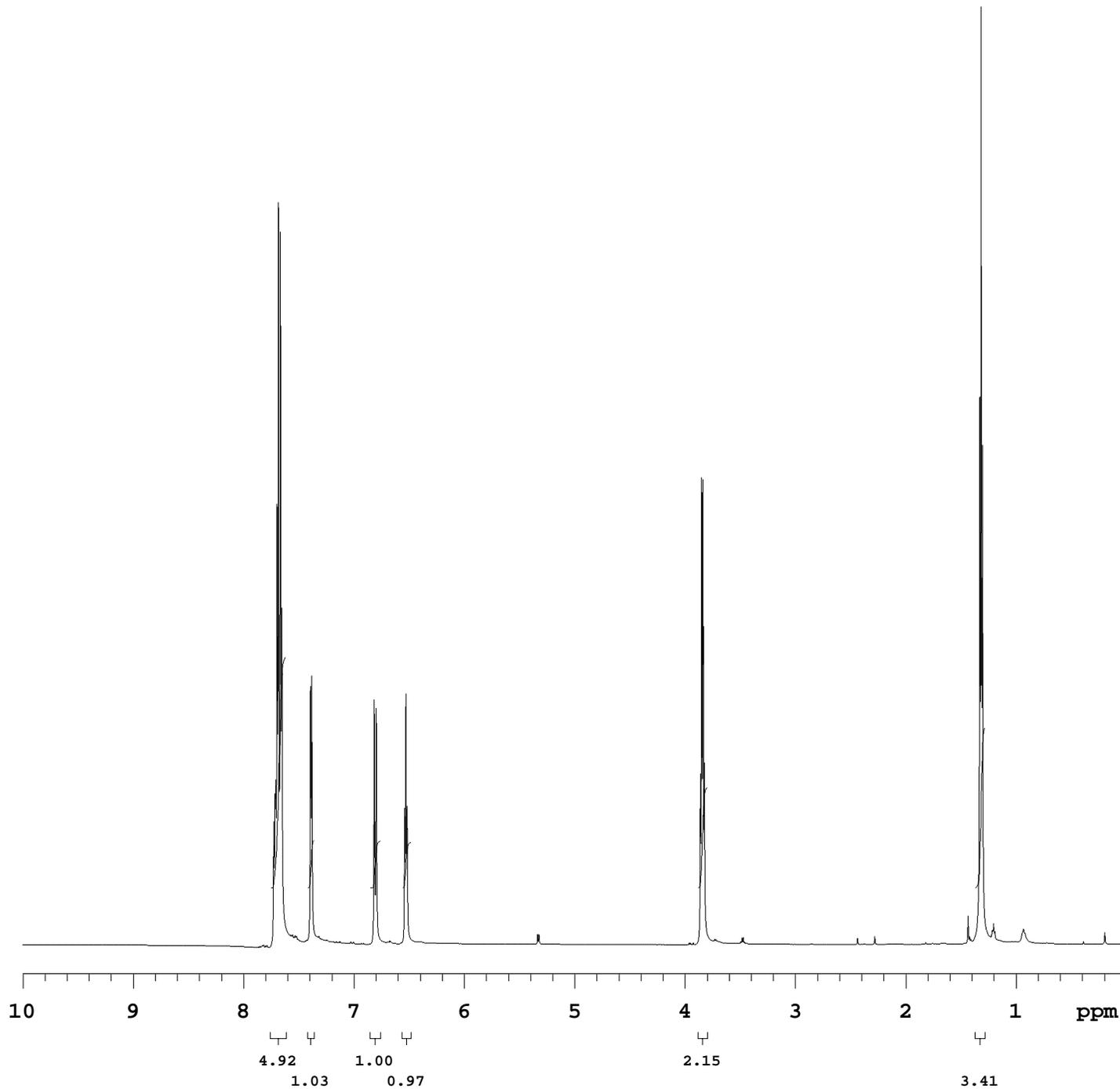
2e

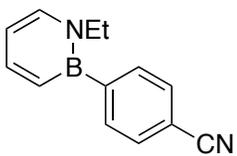
UO VNMR5-600  
\_CH-ColdProbe\_ 1H-observe  
  
Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-CN\_H  
VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 9615.4 Hz  
8 repetitions

OBSERVE H1, 599.9795419

DATA PROCESSING  
FT size 65536  
Total time 1 minute





2e

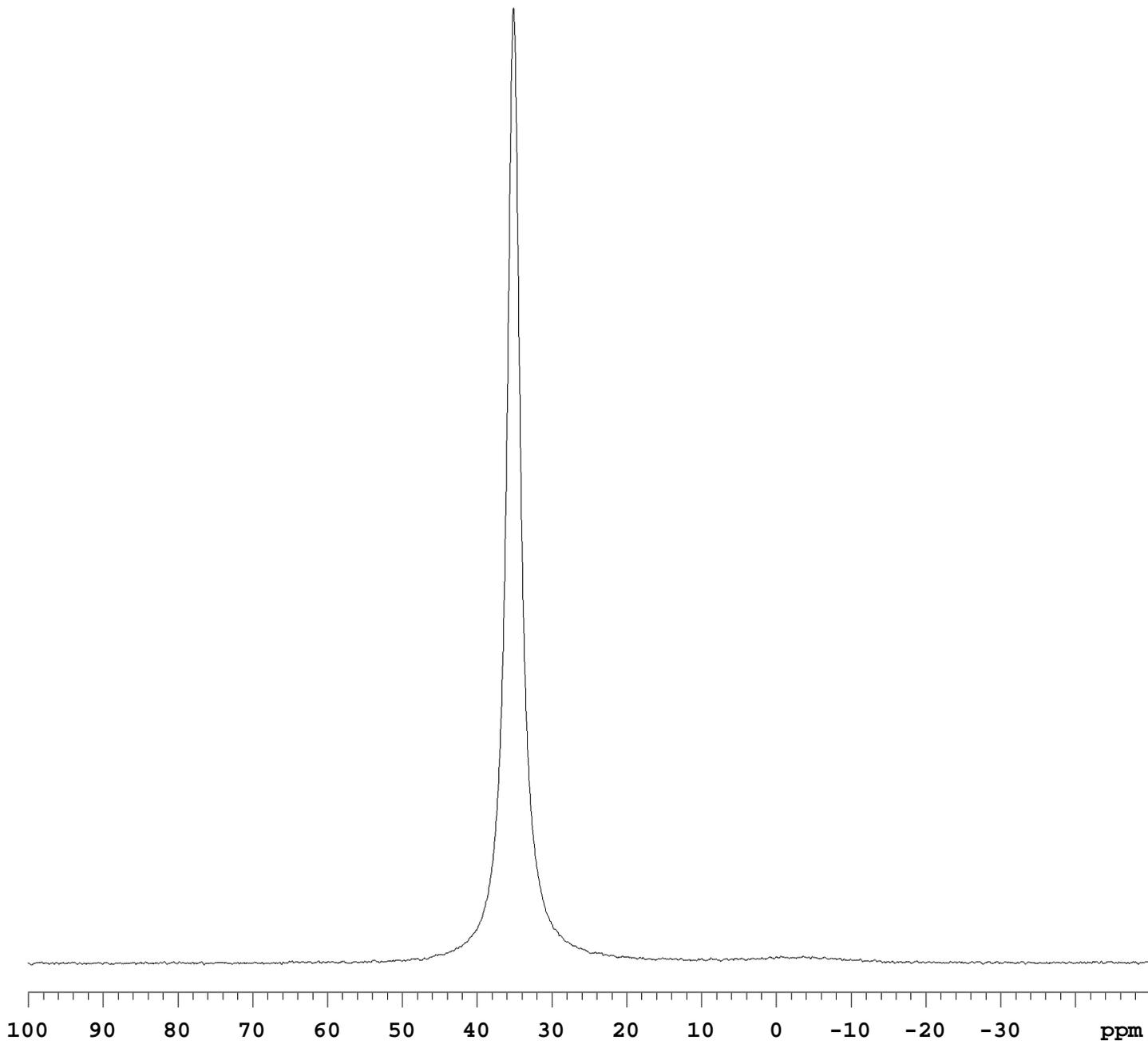
INDEX	FREQUENCY	PPM	HEIGHT
1	3379.0	35.099	159.0

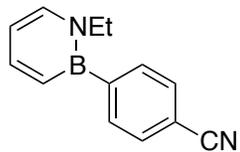
UO Inova-300-North  
Boron-11  
  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-CN\_B  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
80 repetitions

OBSERVE B11, 96.2682868

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute





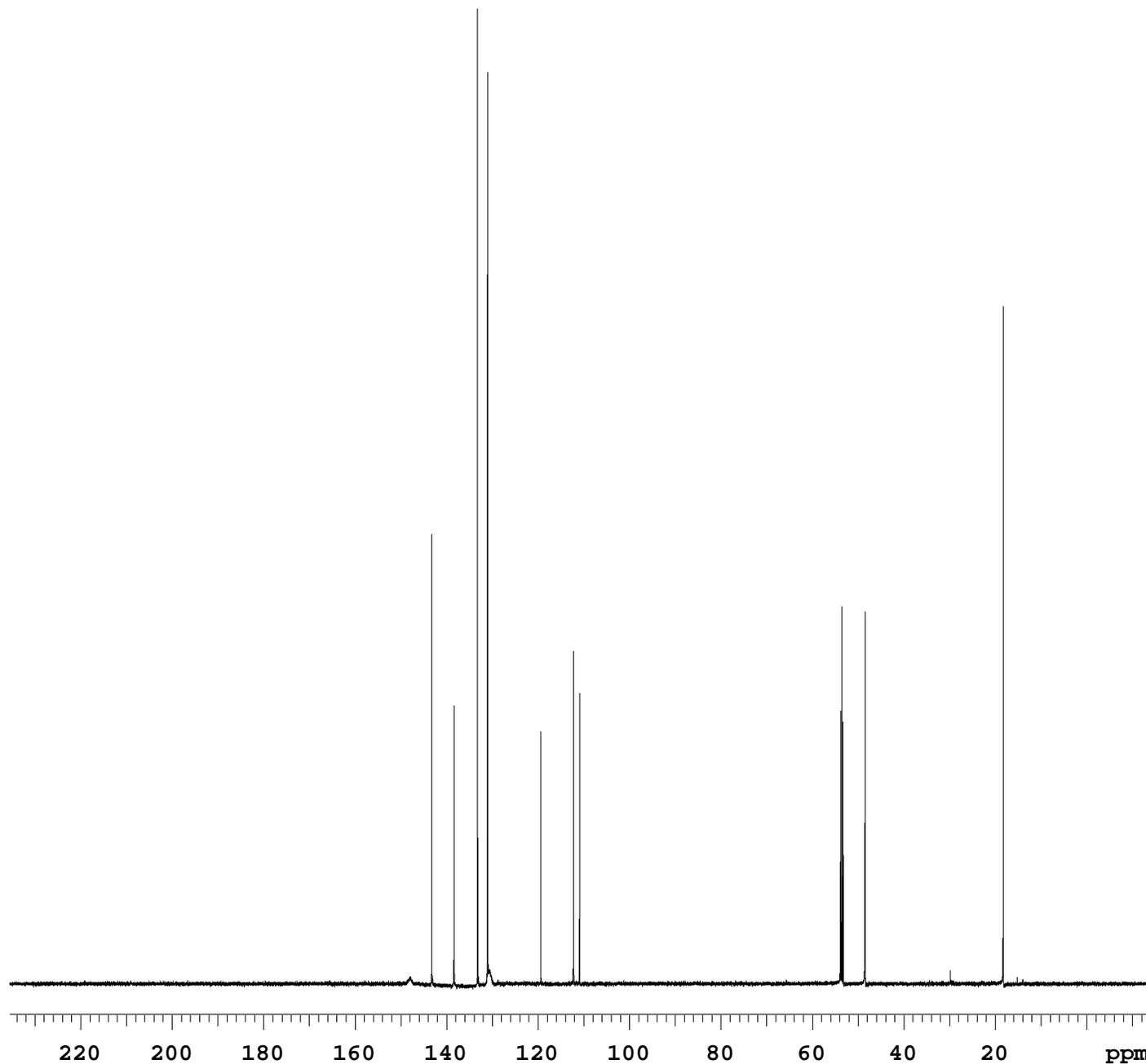
2e

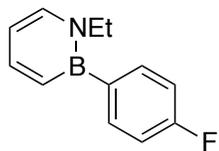
UO VNMR5-600  
\_CH-ColdProbe\_ 1H-observe  
  
Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-CN\_C  
VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
40 repetitions

OBSERVE C13, 150.8649758  
DECOUPLE H1, 599.9825418  
Power 41 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 minute





2f

UO Inova-300-North  
Fluorine-19

Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-fluoro\_H\_300  
INOVA-500 "sunofnmr.uoregon.edu"

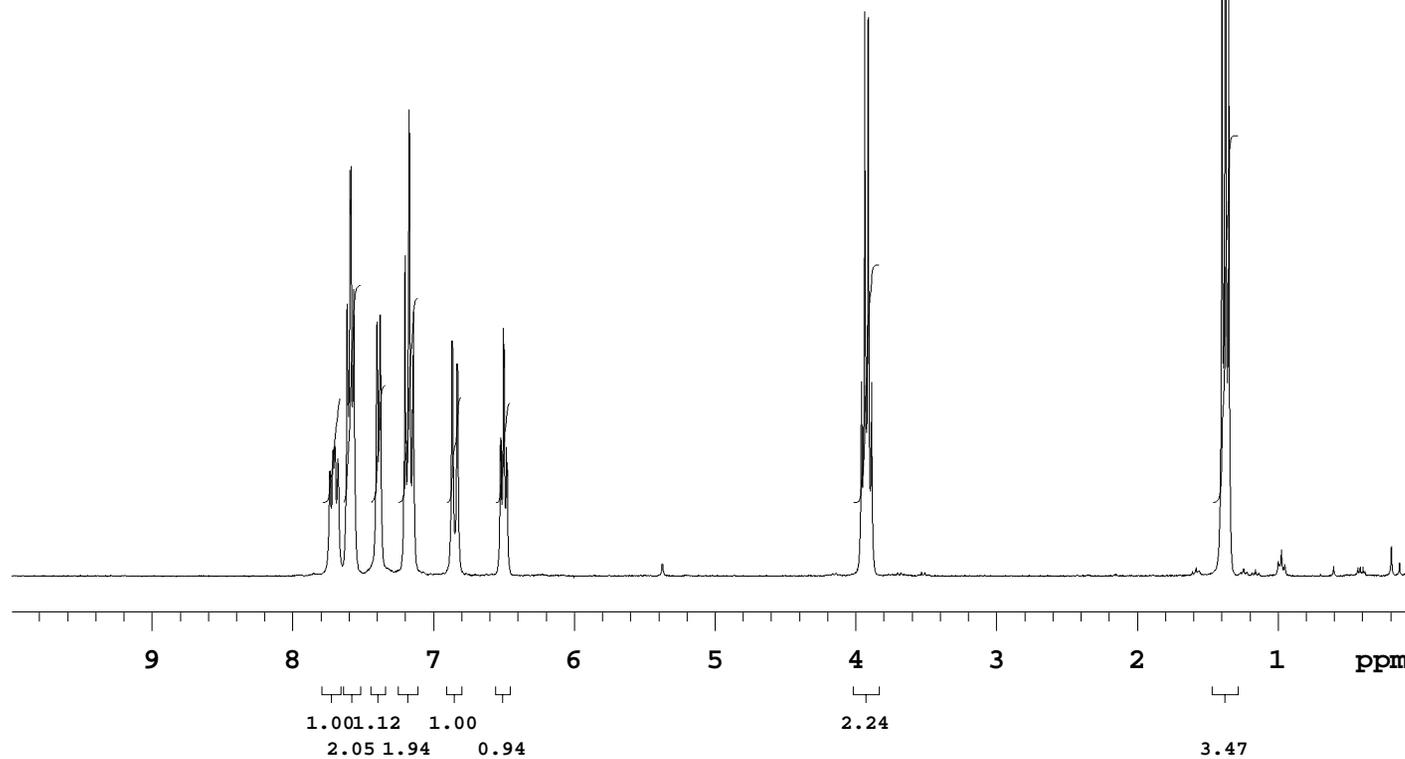
PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 4800.8 Hz  
8 repetitions

OBSERVE H1, 300.0510060

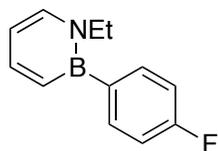
DATA PROCESSING

FT size 32768  
Total time 1 minute



Archive dir:

File: 4-fluoro\_H\_300



2f

INDEX	FREQUENCY	PPM	HEIGHT
1	3413.1	35.454	159.0

UO Inova-300-North  
Boron-11

Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-fluoro\_B  
INOVA-500 "sunofnmr.uoregon.edu"

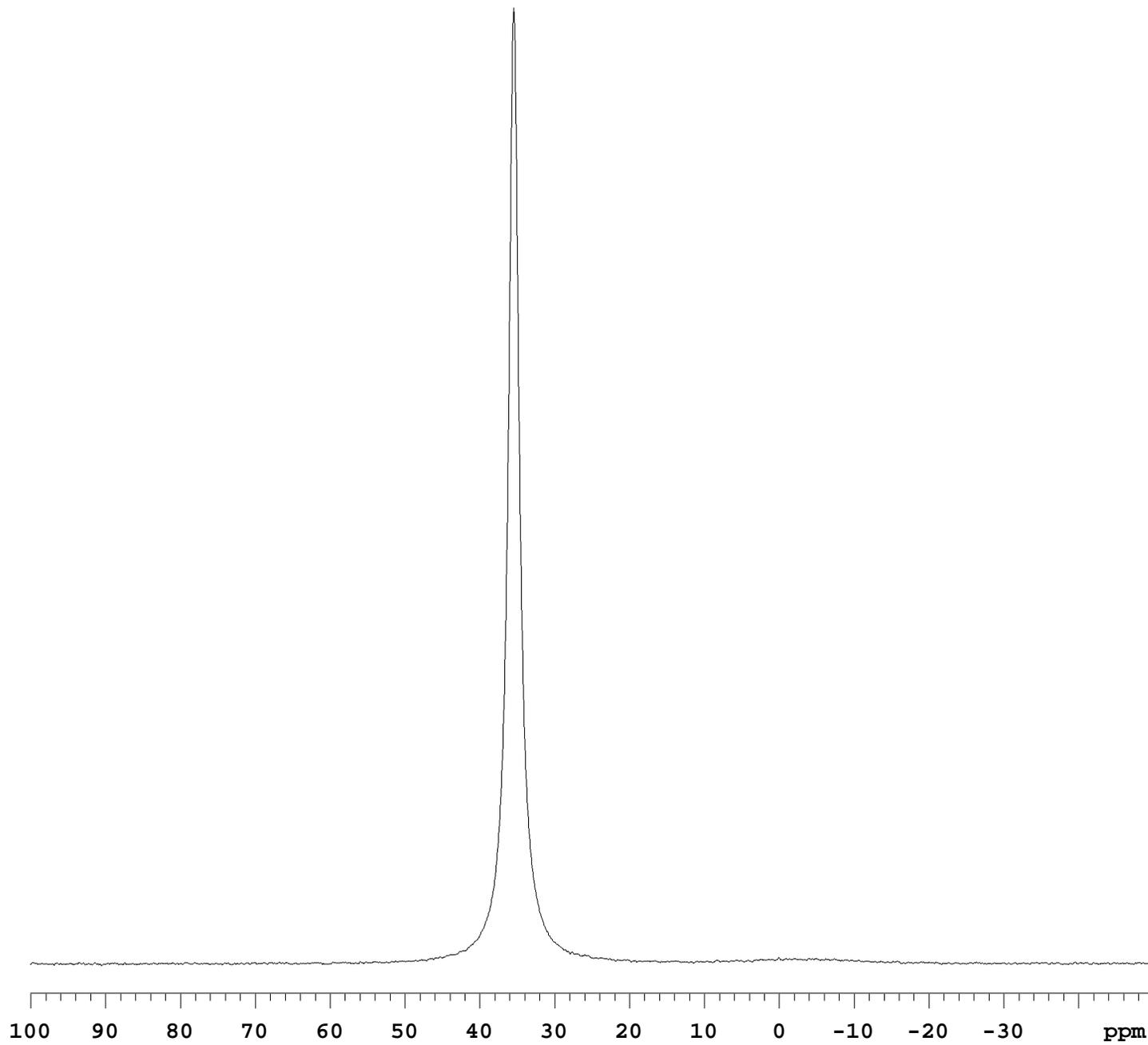
PULSE SEQUENCE

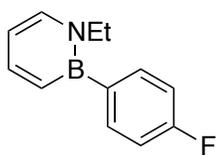
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
96 repetitions

OBSERVE B11, 96.2681019

DATA PROCESSING

Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute





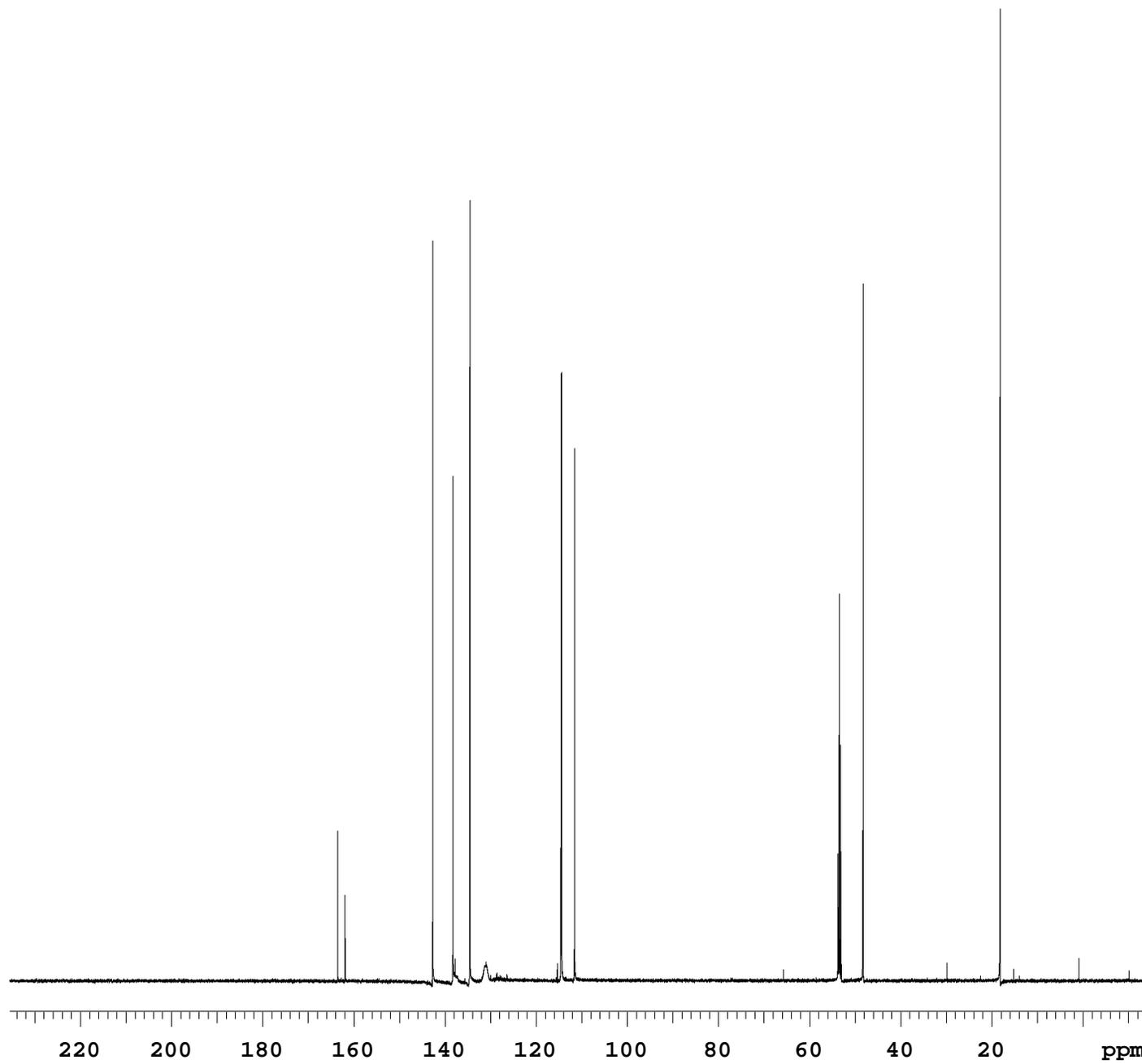
2f

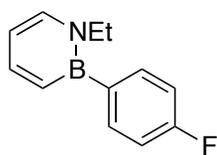
UO VNMR5-600  
\_CH-ColdProbe\_ 1H-observe  
  
Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-fluoro\_C  
VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
40 repetitions

OBSERVE C13, 150.8649758  
DECOUPLE H1, 599.9825418  
Power 41 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 minute





2f

INDEX	FREQUENCY	PPM	HEIGHT
1	-32634.4	-115.589	41.9
2	-32640.5	-115.611	91.9
3	-32643.5	-115.622	105.1
4	-32650.4	-115.646	167.4
5	-32656.5	-115.668	109.1
6	-32659.5	-115.679	99.5
7	-32665.6	-115.700	46.4

UO Inova-300-North  
Fluorine-19

Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-fluoro\_F  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.000 sec  
Width 100.0 kHz  
8 repetitions

OBSERVE F19, 282.3300125

DATA PROCESSING

Line broadening 1.0 Hz  
FT size 262144  
Total time 1 minute

150

100

50

0

-50

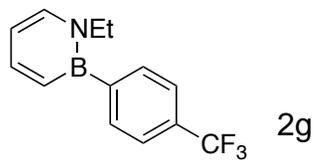
-100

-150

ppm

Archive dir:

File: 4-fluoro\_F



UO Inova-300-North  
Boron-11

Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-CF3\_H\_300  
INOVA-500 "sunofnmr.uoregon.edu"

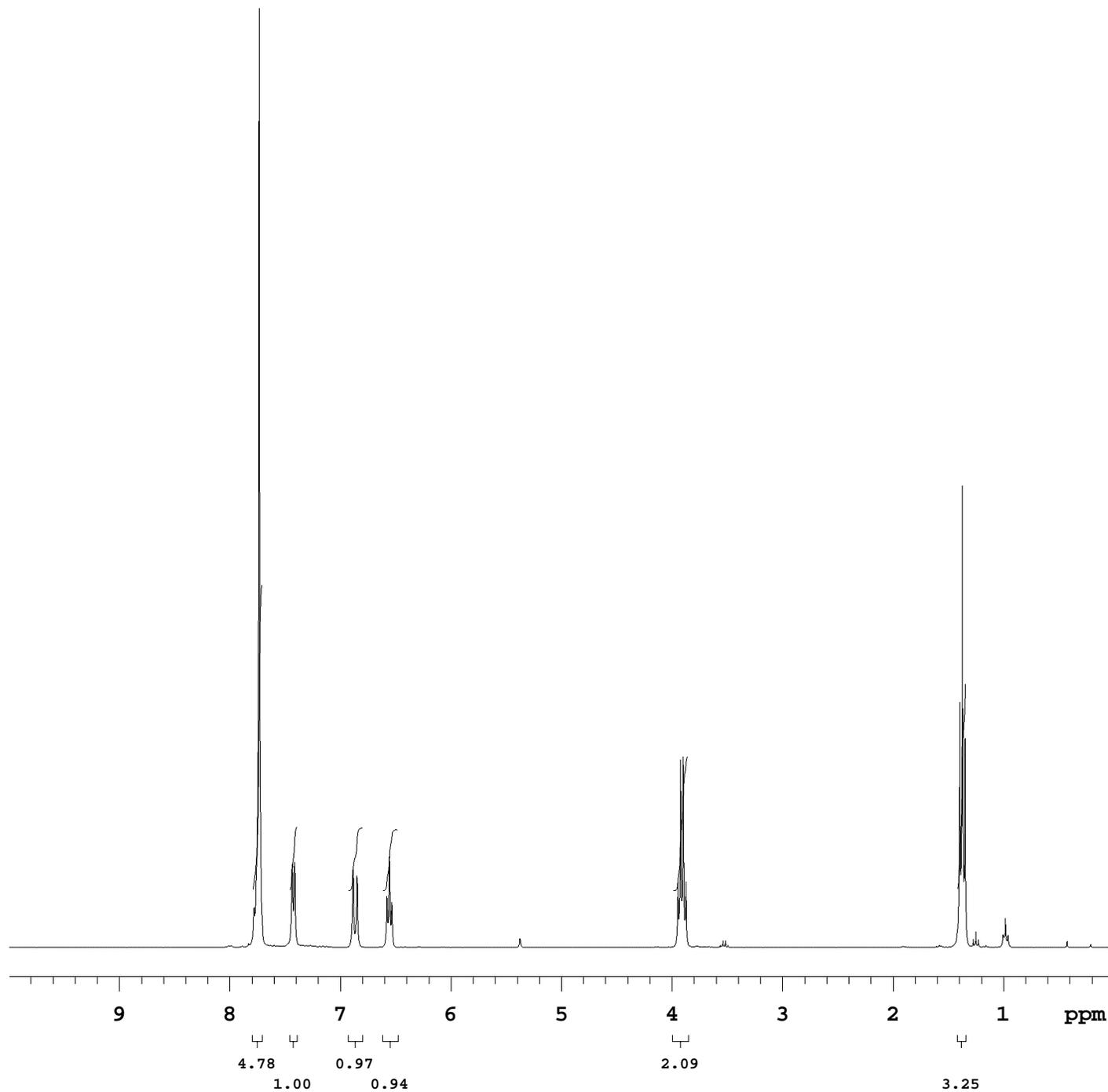
PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 4800.8 Hz  
8 repetitions

OBSERVE H1, 300.0510060

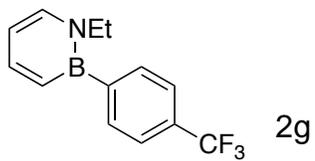
DATA PROCESSING

FT size 32768  
Total time 1 minute



Archive dir:

File: 4-CF3\_H\_300



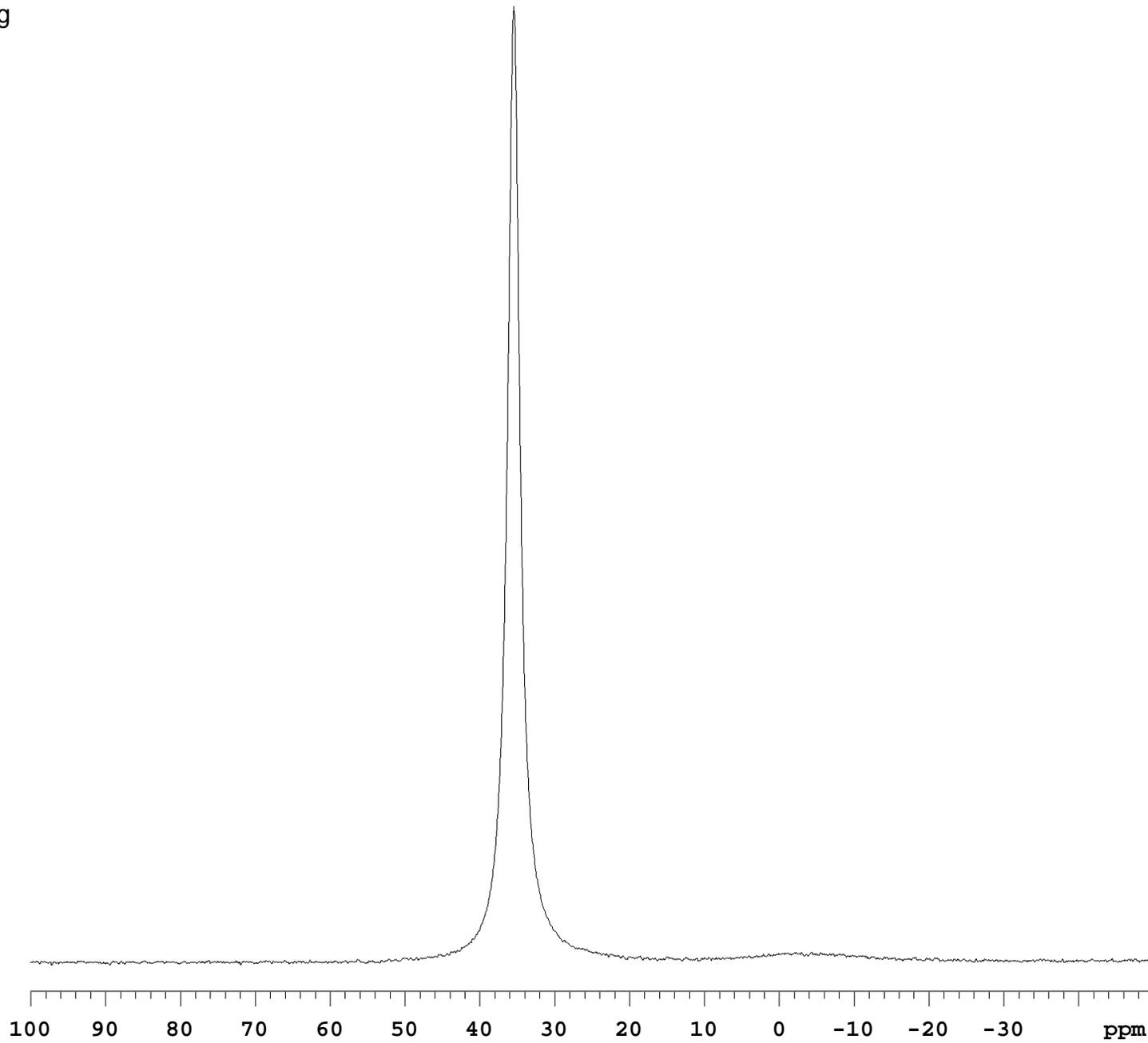
INDEX	FREQUENCY	PPM	HEIGHT
1	3413.1	35.454	159.0

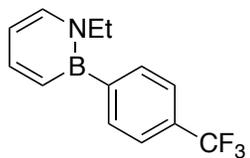
UO Inova-300-North  
Boron-11  
  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-CF3\_B  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
80 repetitions

OBSERVE B11, 96.2682868

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute





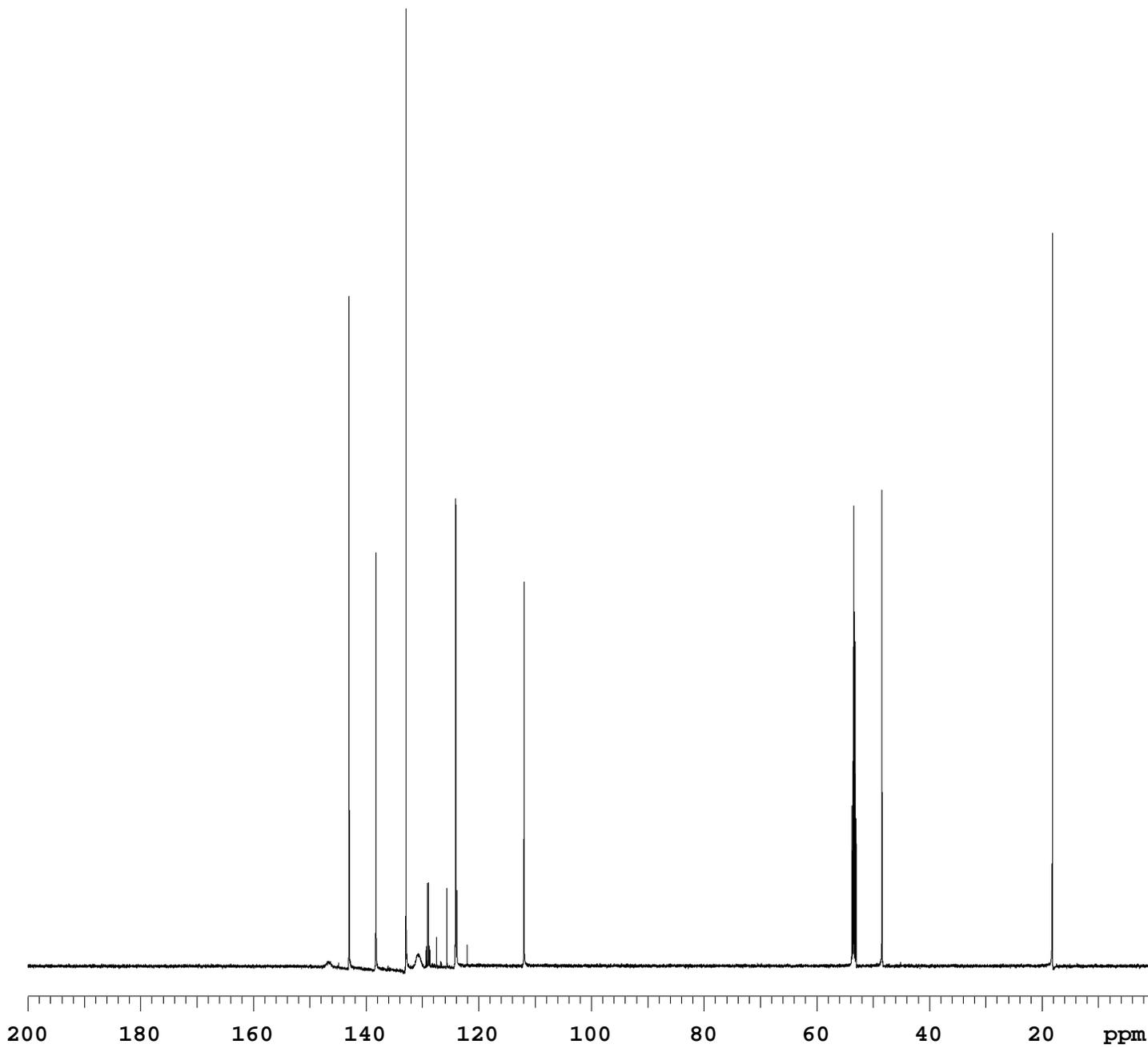
2g

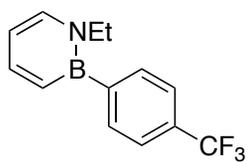
UO VNMR5-600  
\_CH-ColdProbe\_ 1H-observe  
  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-CF3\_C  
VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
56 repetitions

OBSERVE C13, 150.8649758  
DECOUPLE H1, 599.9825418  
Power 41 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 minutes





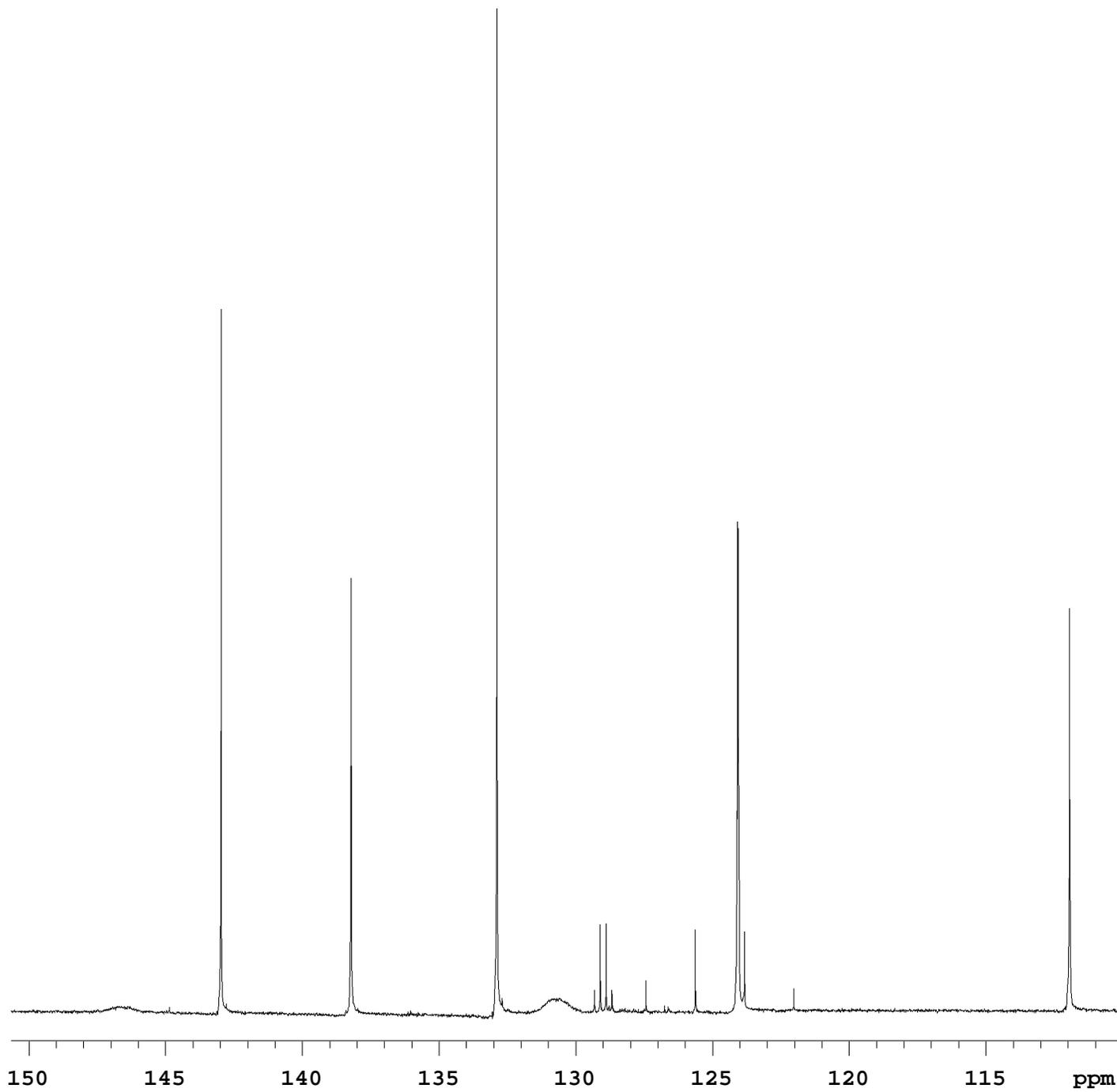
2g

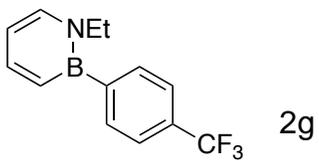
UO VNMR5-600  
\_CH-ColdProbe\_ 1H-observe  
  
Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-CF3\_C  
VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
56 repetitions

OBSERVE C13, 150.8649758  
DECOUPLE H1, 599.9825418  
Power 41 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 minutes





INDEX	FREQUENCY	PPM	HEIGHT
1	-17716.6	-62.751	167.4

UO Inova-300-North  
Fluorine-19

Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-CF3\_F  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.000 sec  
Width 100.0 kHz  
8 repetitions

OBSERVE F19, 282.3300125

DATA PROCESSING

Line broadening 1.0 Hz  
FT size 262144  
Total time 1 minute

150

100

50

0

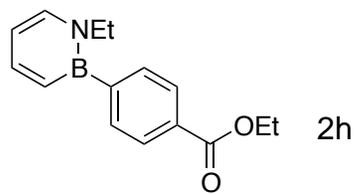
-50

-100

-150

ppm

Archive dir: File: 4-CF3\_F

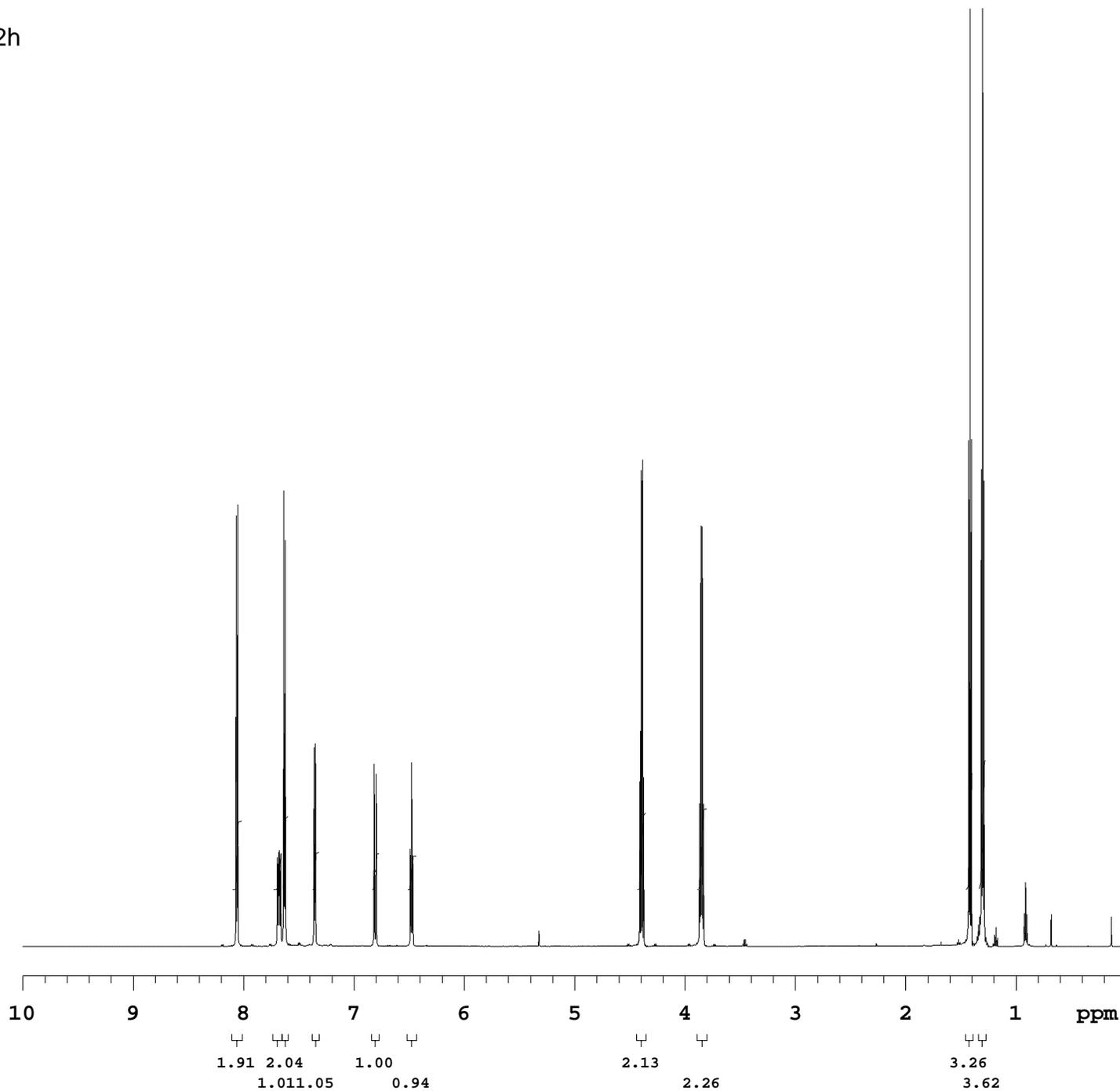


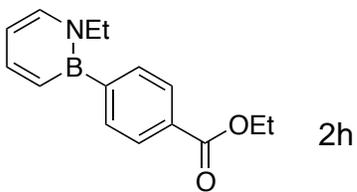
UO VNMRS-600  
 {CH-ColdProbe} 1H-observe  
 Solvent: cd2c12  
 Temp. 25.0 C / 298.1 K  
 Operator: ger  
 File: 4-CO2Et\_H  
 VNMRS-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 3.000 sec  
 Width 9615.4 Hz  
 8 repetitions

OBSERVE H1, 599.9795419

DATA PROCESSING  
 FT size 65536  
 Total time 1 minute





INDEX	FREQUENCY	PPM	HEIGHT
1	3398.5	35.302	159.0

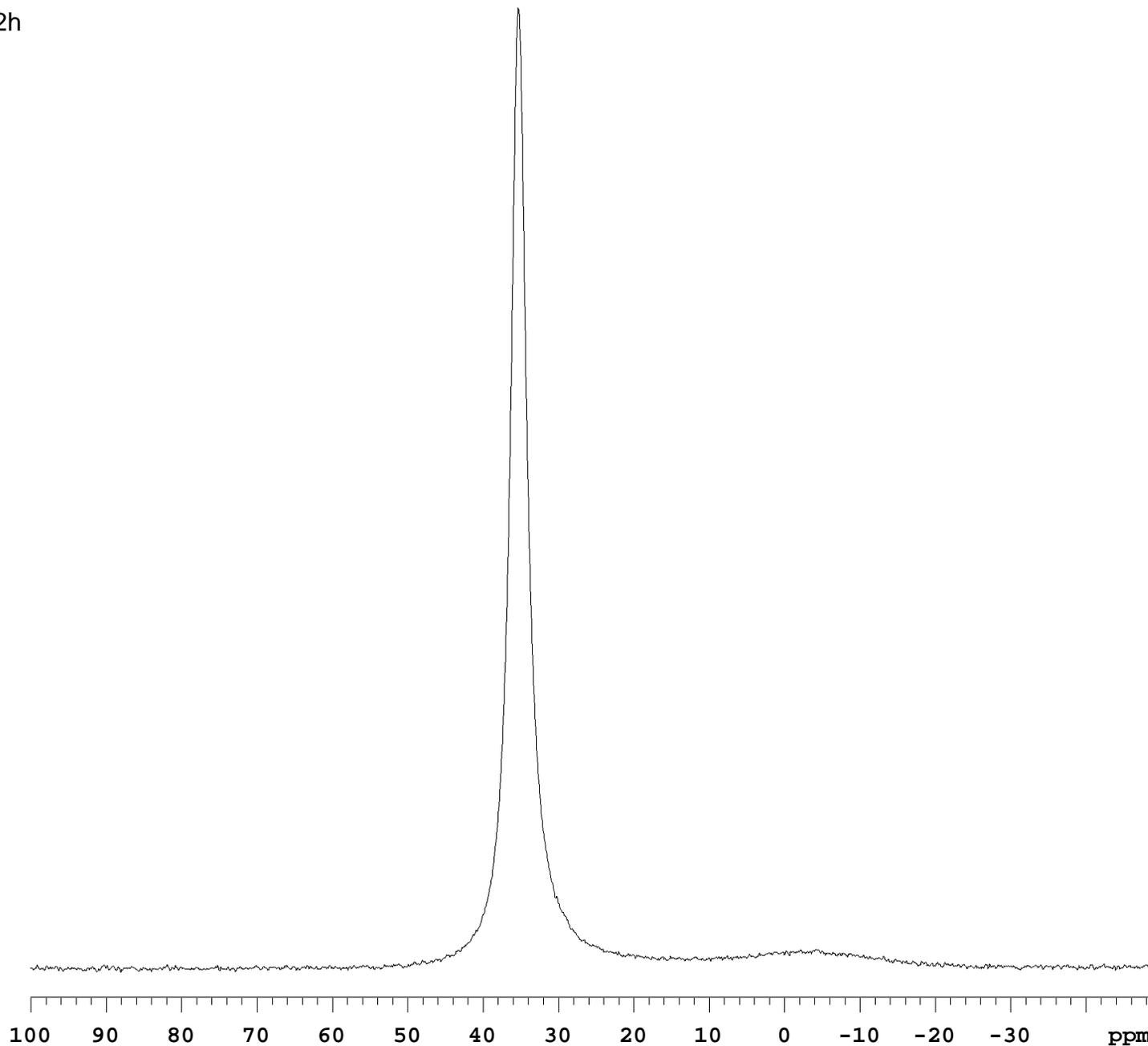
UO Inova-300-North  
Boron-11

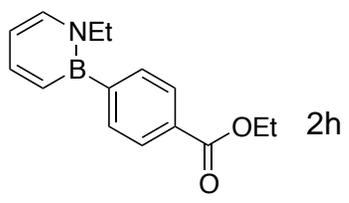
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-CO2Et\_B  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
96 repetitions

OBSERVE B11, 96.2682868

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute



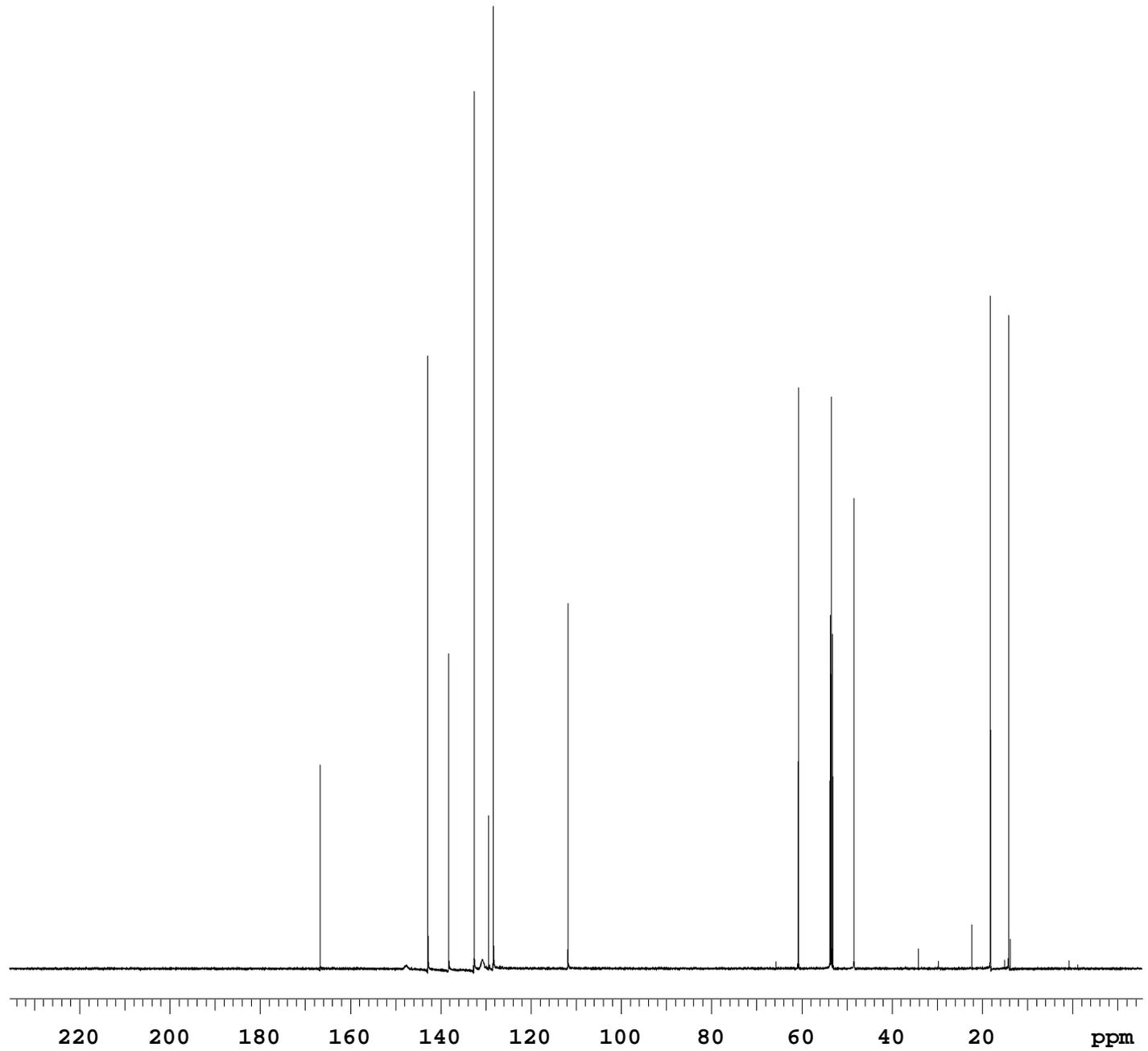


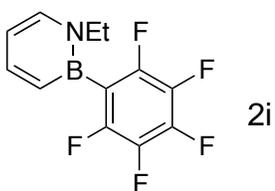
UO VNMR5-600  
\_CH-ColdProbe\_ 1H-observe  
  
Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-CO2Et\_C  
VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
52 repetitions

OBSERVE C13, 150.8649758  
DECOUPLE H1, 599.9825418  
Power 41 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 minutes



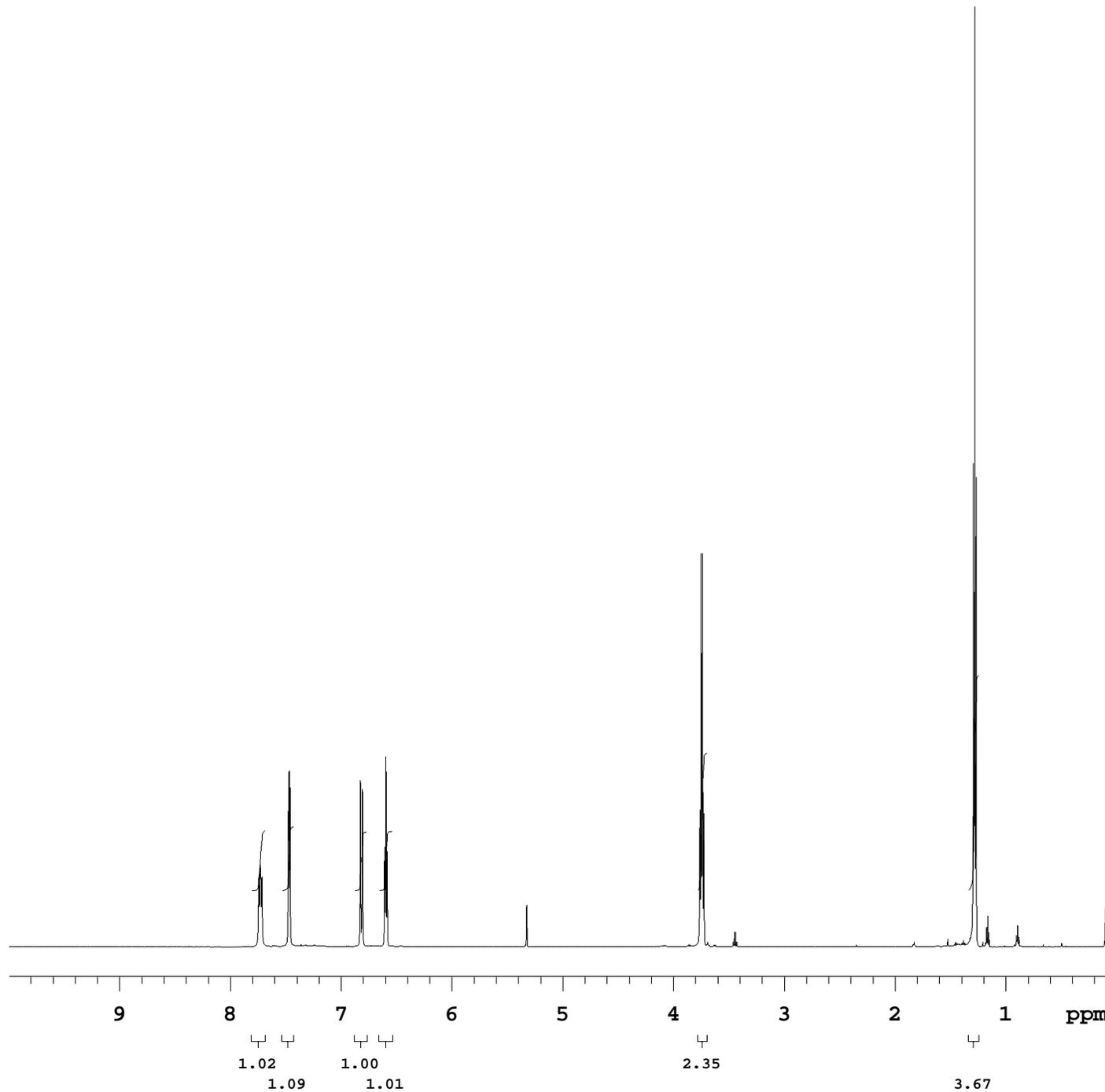


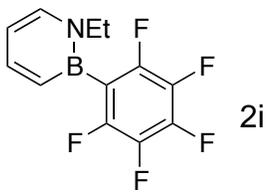
UO VNMR5-600  
 {CH-ColdProbe} 1H-observe  
 Solvent: cd2c12  
 Temp. 25.0 C / 298.1 K  
 Operator: ger  
 File: C6F5\_H  
 VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 3.000 sec  
 Width 9615.4 Hz  
 8 repetitions

OBSERVE H1, 599.9795419

DATA PROCESSING  
 FT size 65536  
 Total time 1 minute





INDEX	FREQUENCY	PPM	HEIGHT
1	3027.4	31.447	159.0

UO Inova-300-North  
Boron-11

Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: C6F5\_B  
INOVA-500 "sunofnmr.uoregon.edu"

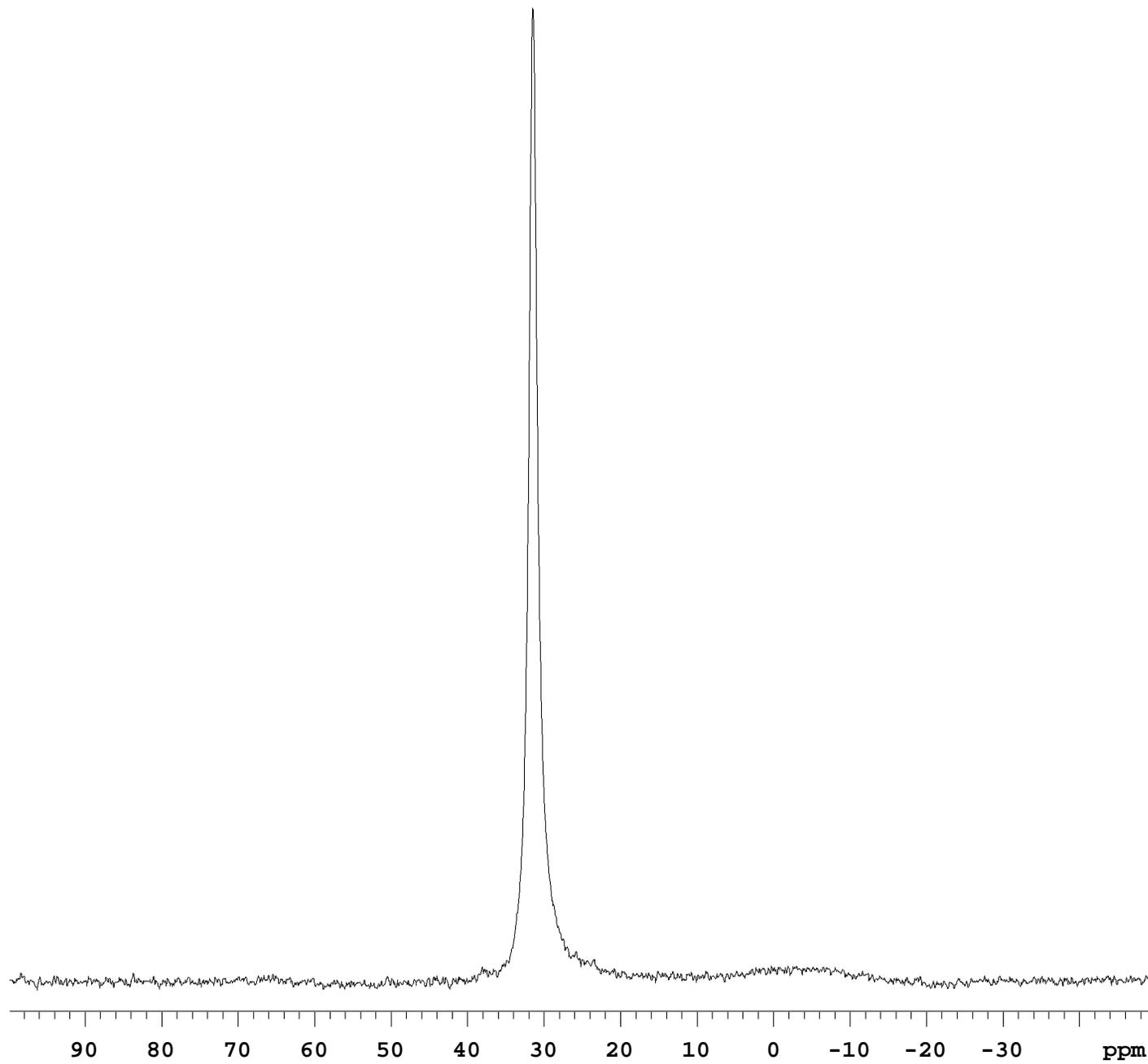
PULSE SEQUENCE

Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
24 repetitions

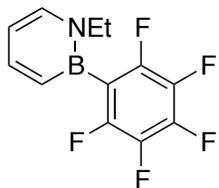
OBSERVE B11, 96.2682868

DATA PROCESSING

Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute



Archive dir: File: C6F5\_B



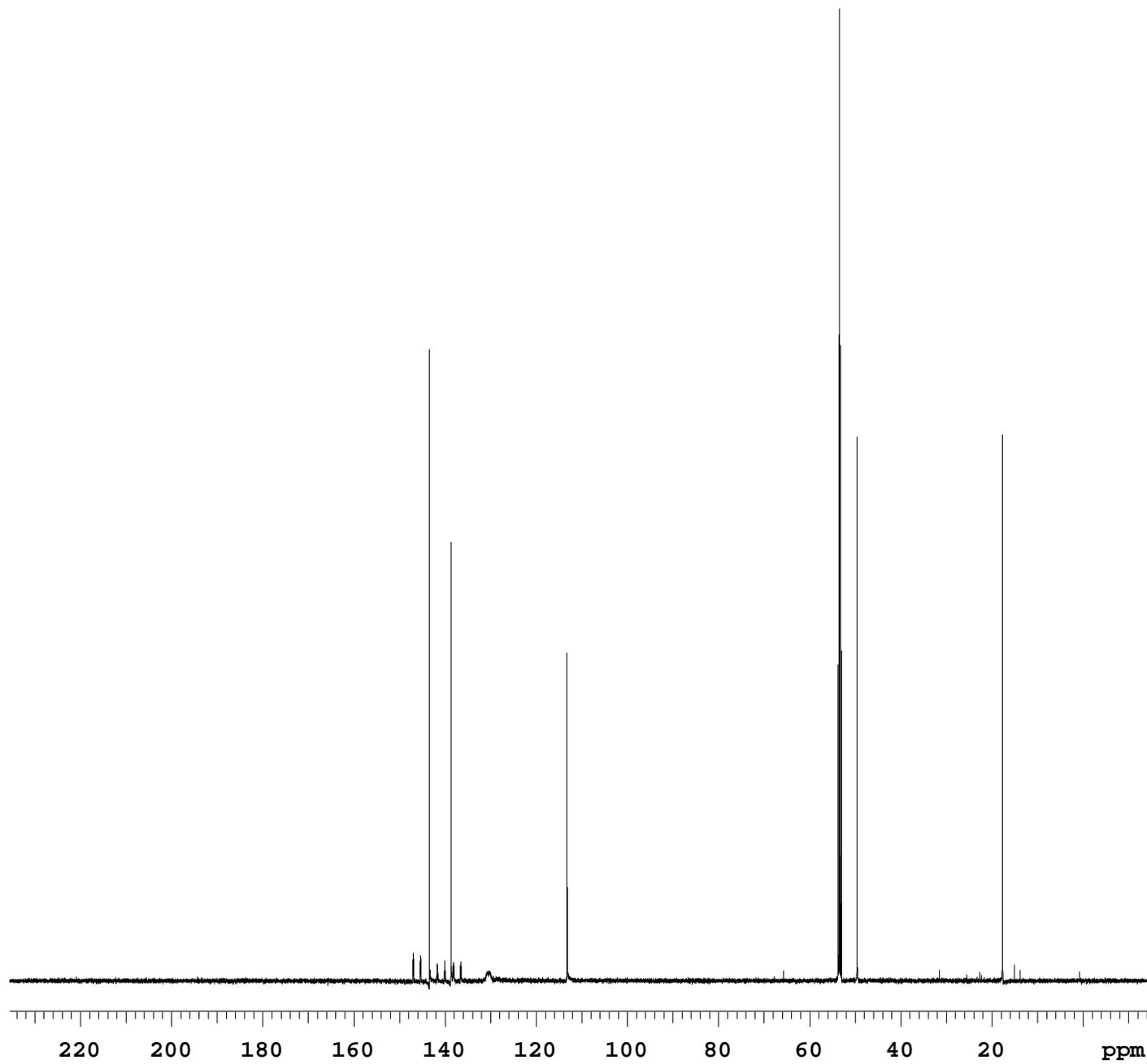
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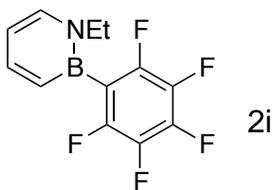
UO VNMR5-600  
\_CH-ColdProbe\_ 1H-observe  
  
Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: C6F5\_C  
VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
80 repetitions

OBSERVE C13, 150.8649758  
DECOUPLE H1, 599.9825418  
Power 41 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 2 minutes





UO VNMR5-600  
\_CH-ColdProbe\_ 1H-observe  
  
Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: C6F5\_C  
VNMR5-500 "sunofnmr.uoregon.edu"

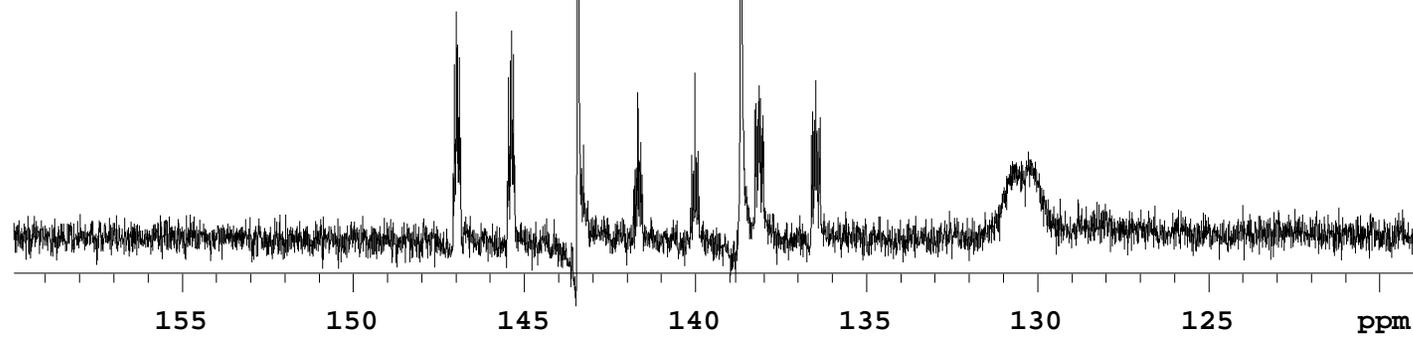
PULSE SEQUENCE

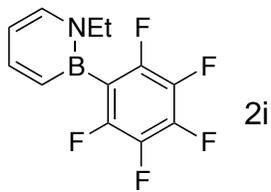
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
80 repetitions

OBSERVE C13, 150.8649758  
DECOUPLE H1, 599.9825418  
Power 41 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz  
FT size 65536  
Total time 2 minutes





UO Inova-300 Fluorine-19

Solvent: cd2cl2

Temp. 25.0 C / 298.1 K

Operator: ger

File: C6F5\_F

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 100.0 kHz

8 repetitions

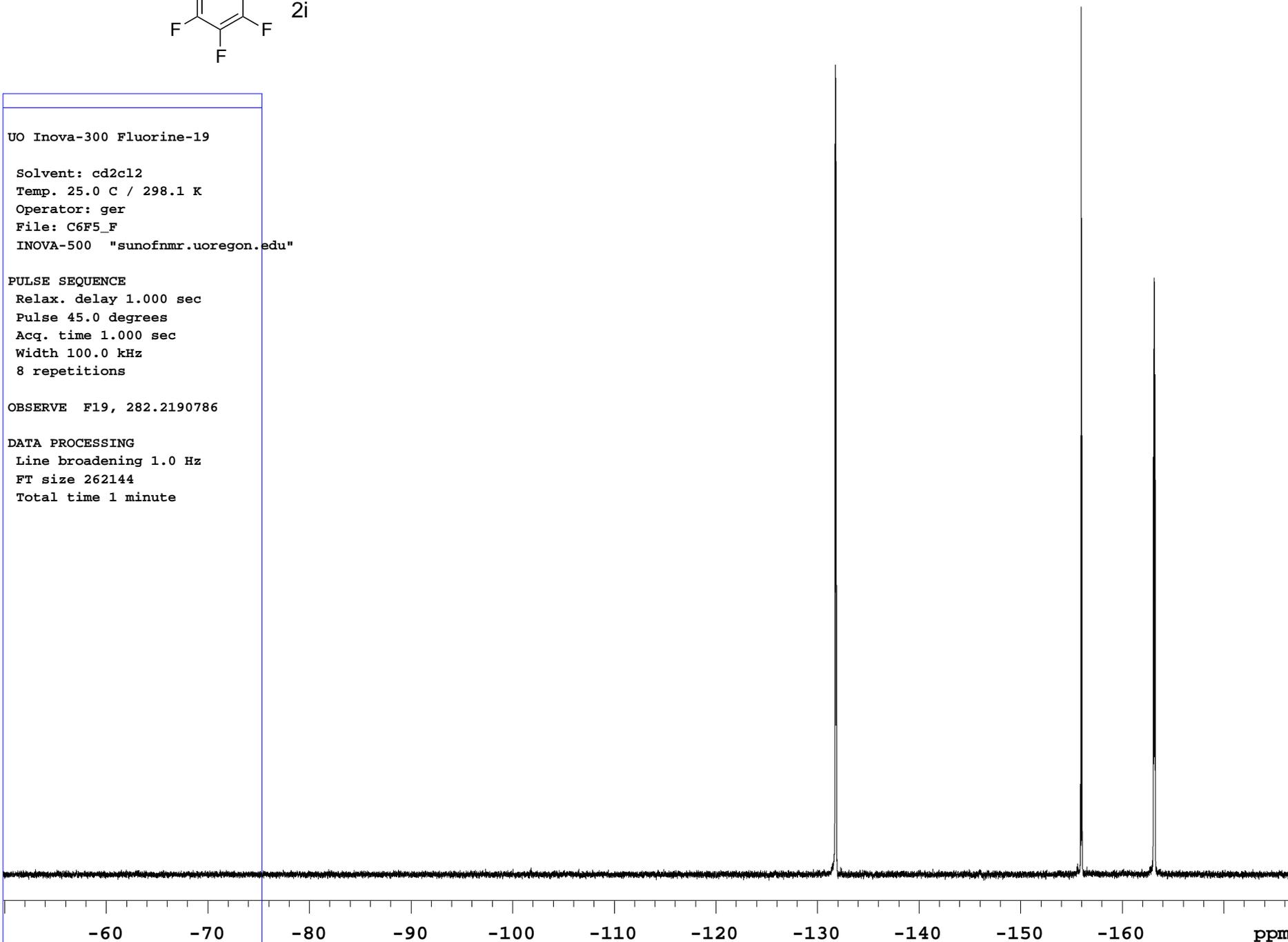
OBSERVE F19, 282.2190786

DATA PROCESSING

Line broadening 1.0 Hz

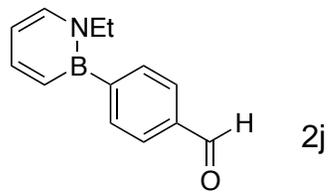
FT size 262144

Total time 1 minute



Archive dir:

File: C6F5\_F



UO Inova-300-North  
Boron-11

Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-formyl\_H\_300  
INOVA-500 "sunofnmr.uoregon.edu"

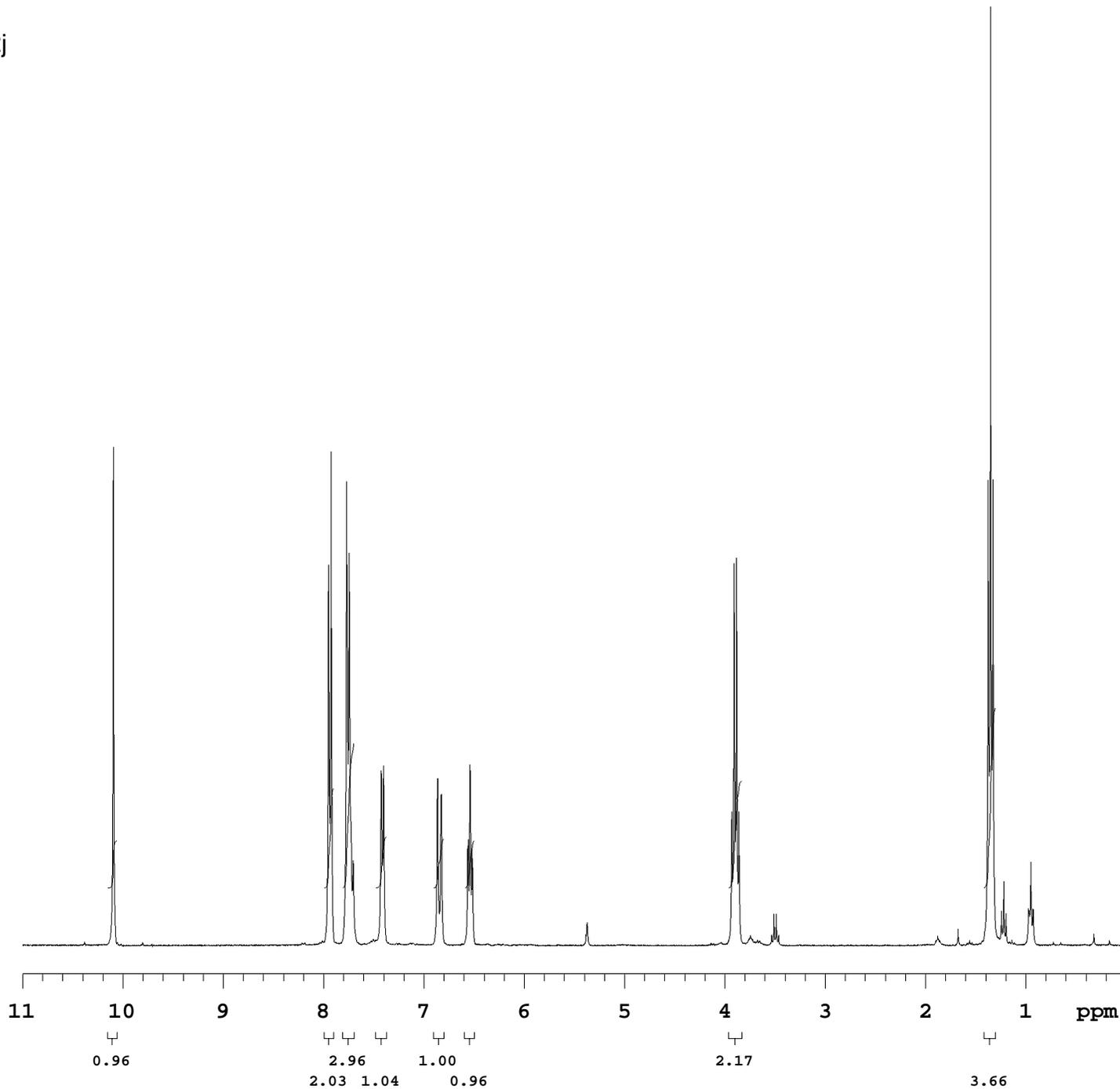
PULSE SEQUENCE

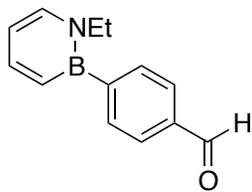
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 4800.8 Hz  
8 repetitions

OBSERVE H1, 300.0510060

DATA PROCESSING

FT size 32768  
Total time 1 minute





2j

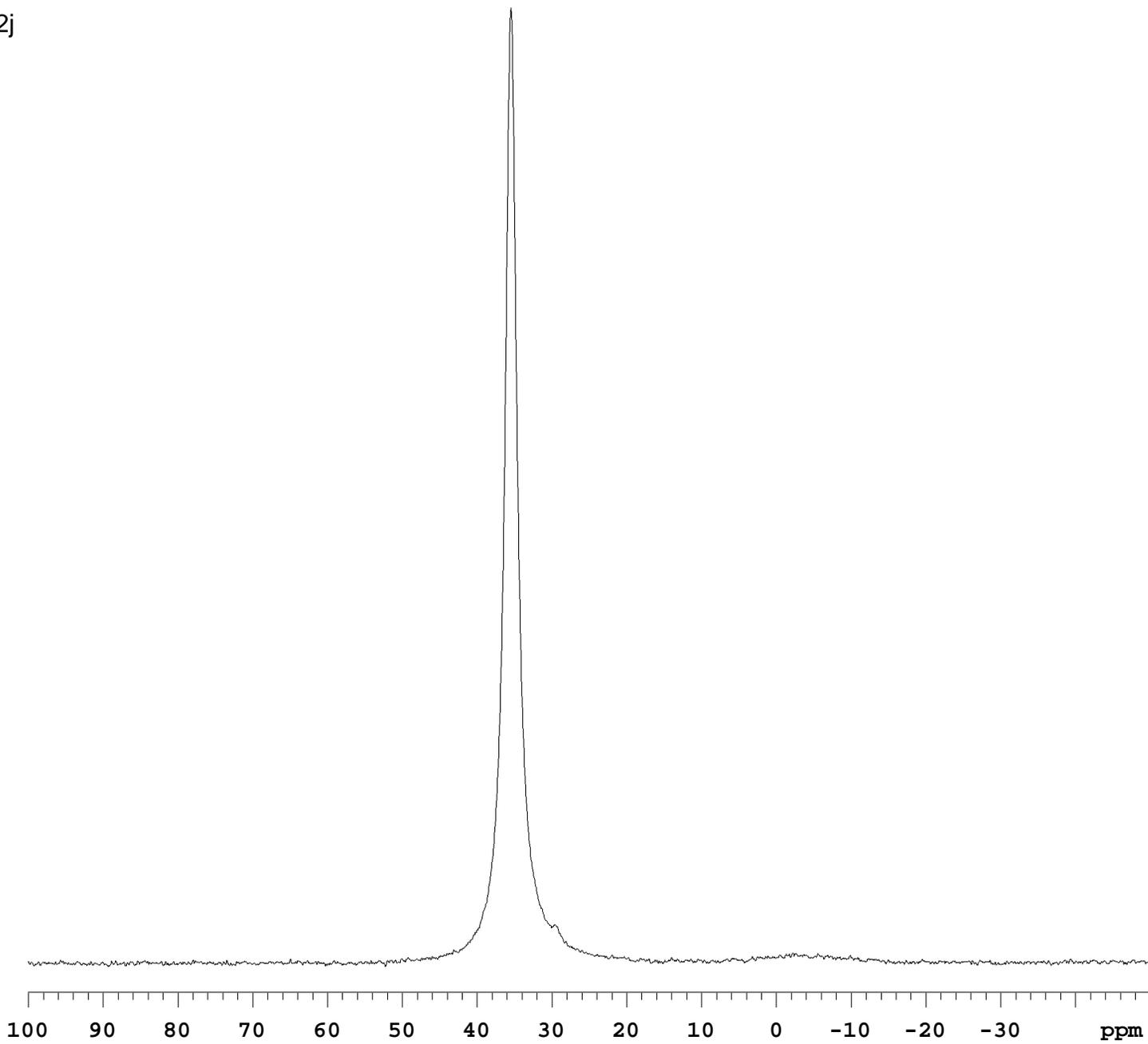
INDEX	FREQUENCY	PPM	HEIGHT
1	3413.1	35.454	159.0

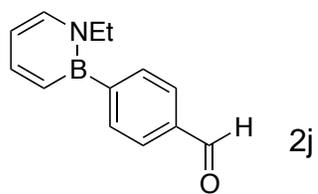
UO Inova-300-North  
Boron-11  
  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-formyl\_B  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
96 repetitions

OBSERVE B11, 96.2682868

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute





STANDARD 1H OBSERVE -  
profile

Solvent: d2o  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-formyl\_C  
VNMRS-500 "sunofnmr.uoregon.edu"

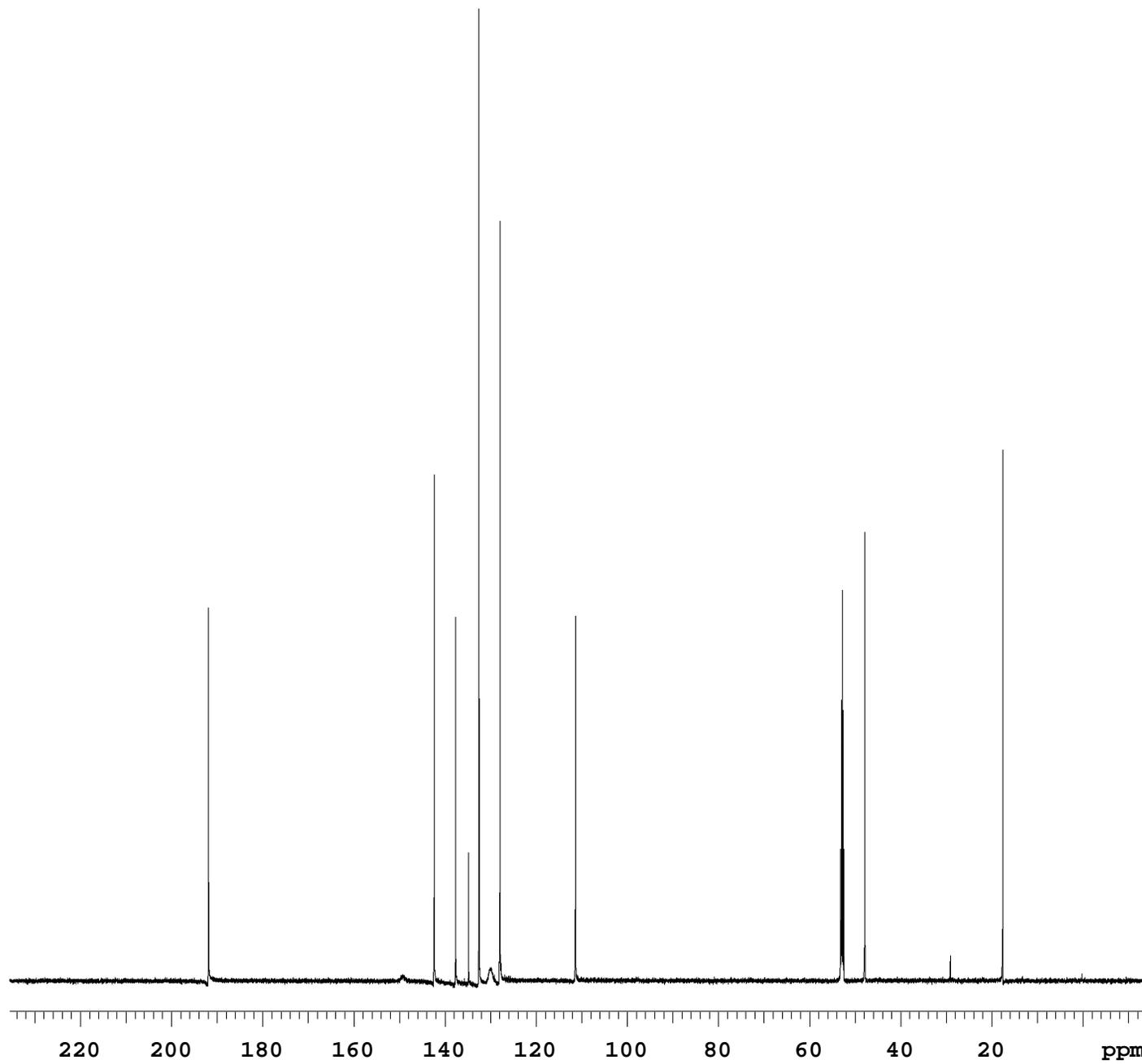
PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
40 repetitions

OBSERVE C13, 150.8650739  
DECOUPLE H1, 599.9829318  
Power 41 dB  
continuously on  
WALTZ-16 modulated

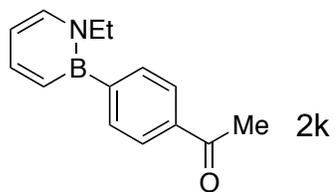
DATA PROCESSING

Line broadening 0.5 Hz  
FT size 65536  
Total time 1 minute



Archive dir:

File: 4-formyl\_C

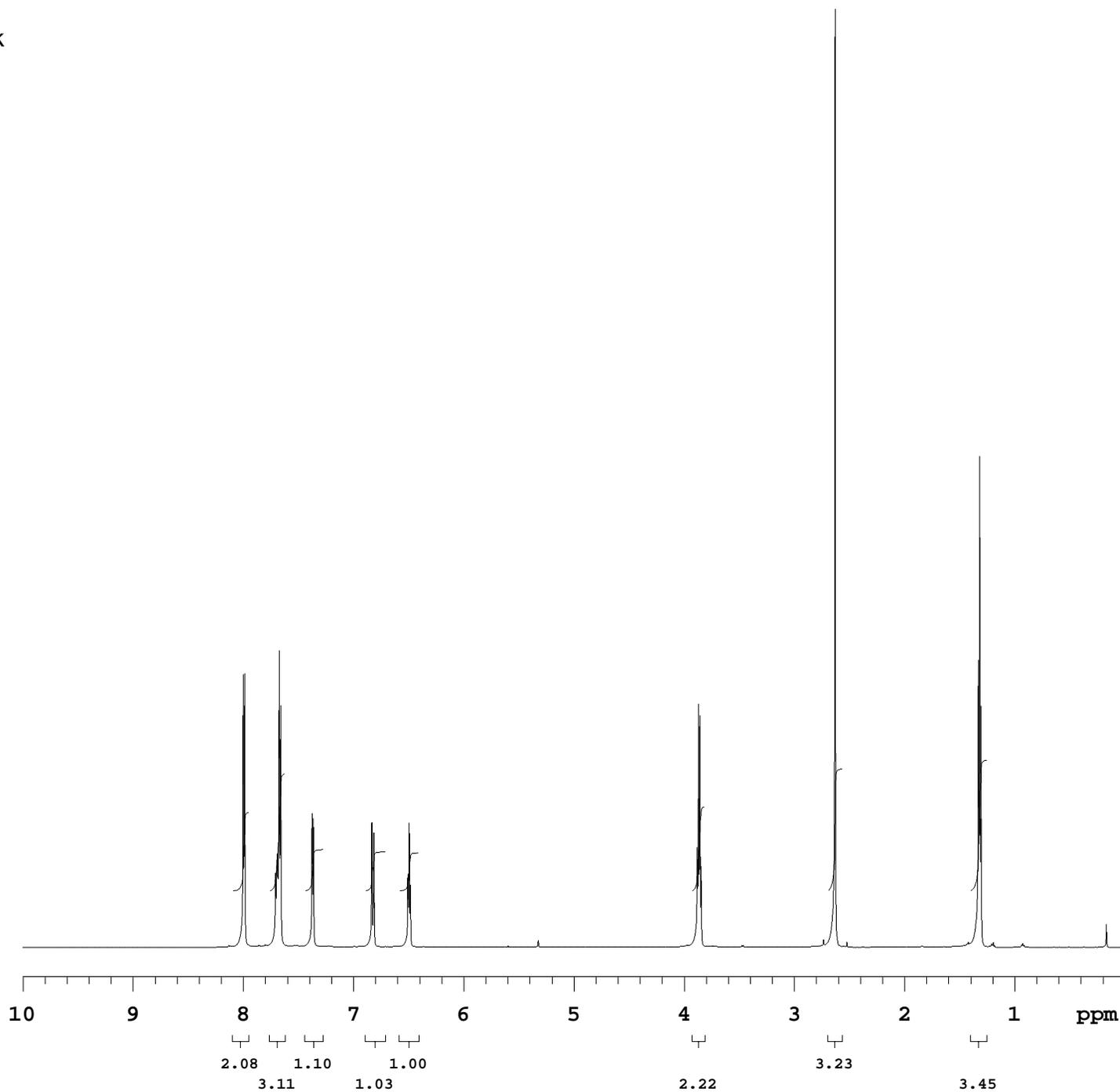


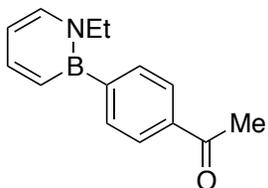
UO VNMR5-600  
{CH-ColdProbe} 1H-observe  
  
Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-Ac\_H  
VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 9615.4 Hz  
8 repetitions

OBSERVE H1, 599.9795419

DATA PROCESSING  
FT size 65536  
Total time 1 minute





2k

INDEX	FREQUENCY	PPM	HEIGHT
1	3413.1	35.454	159.0

UO Inova-300-North  
Boron-11

Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-Ac\_B  
INOVA-500 "sunofnmr.uoregon.edu"

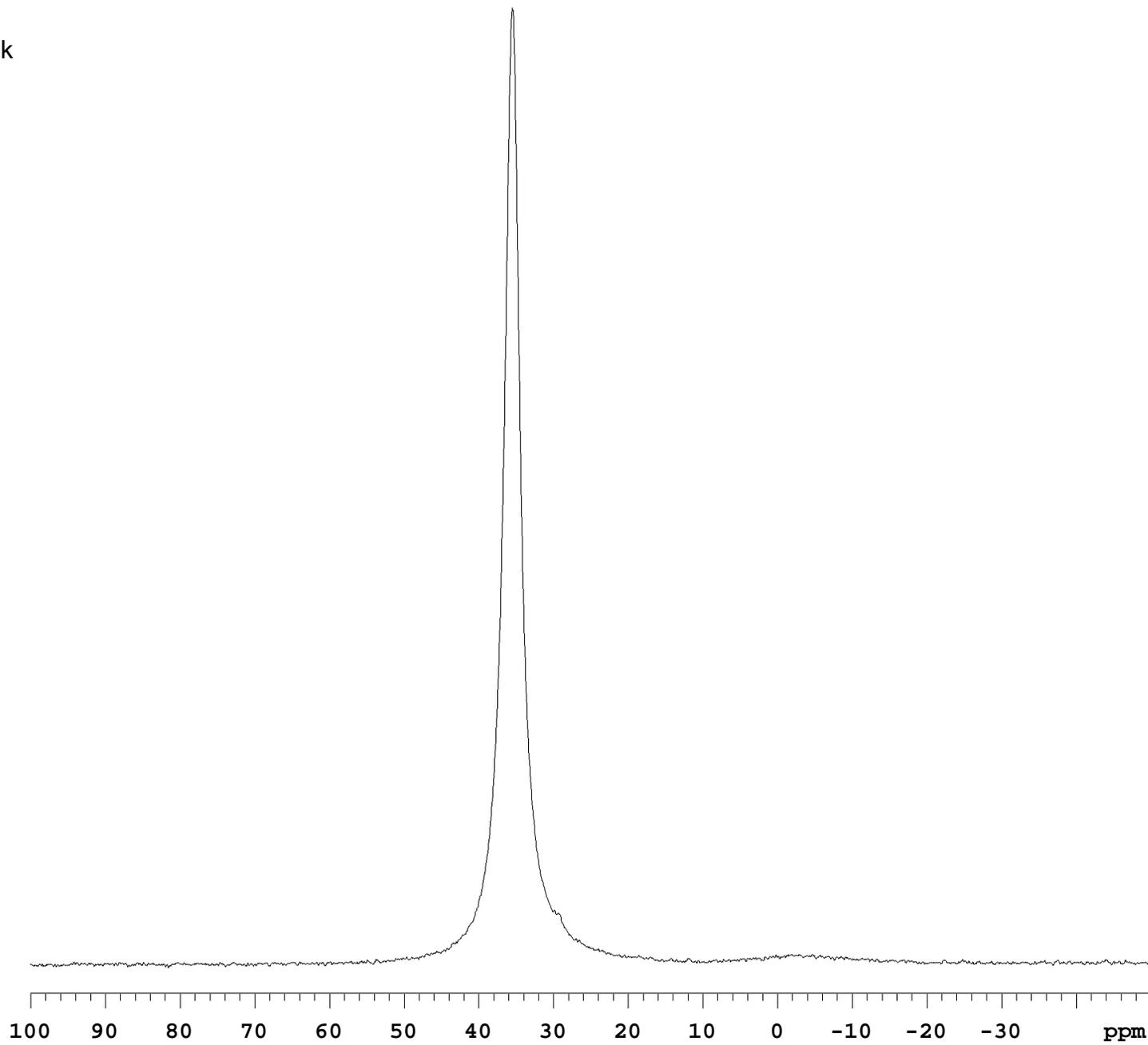
PULSE SEQUENCE

Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
88 repetitions

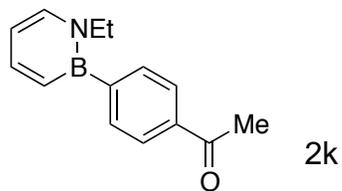
OBSERVE B11, 96.2682868

DATA PROCESSING

Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute



Archive dir: File: 4-Ac\_B

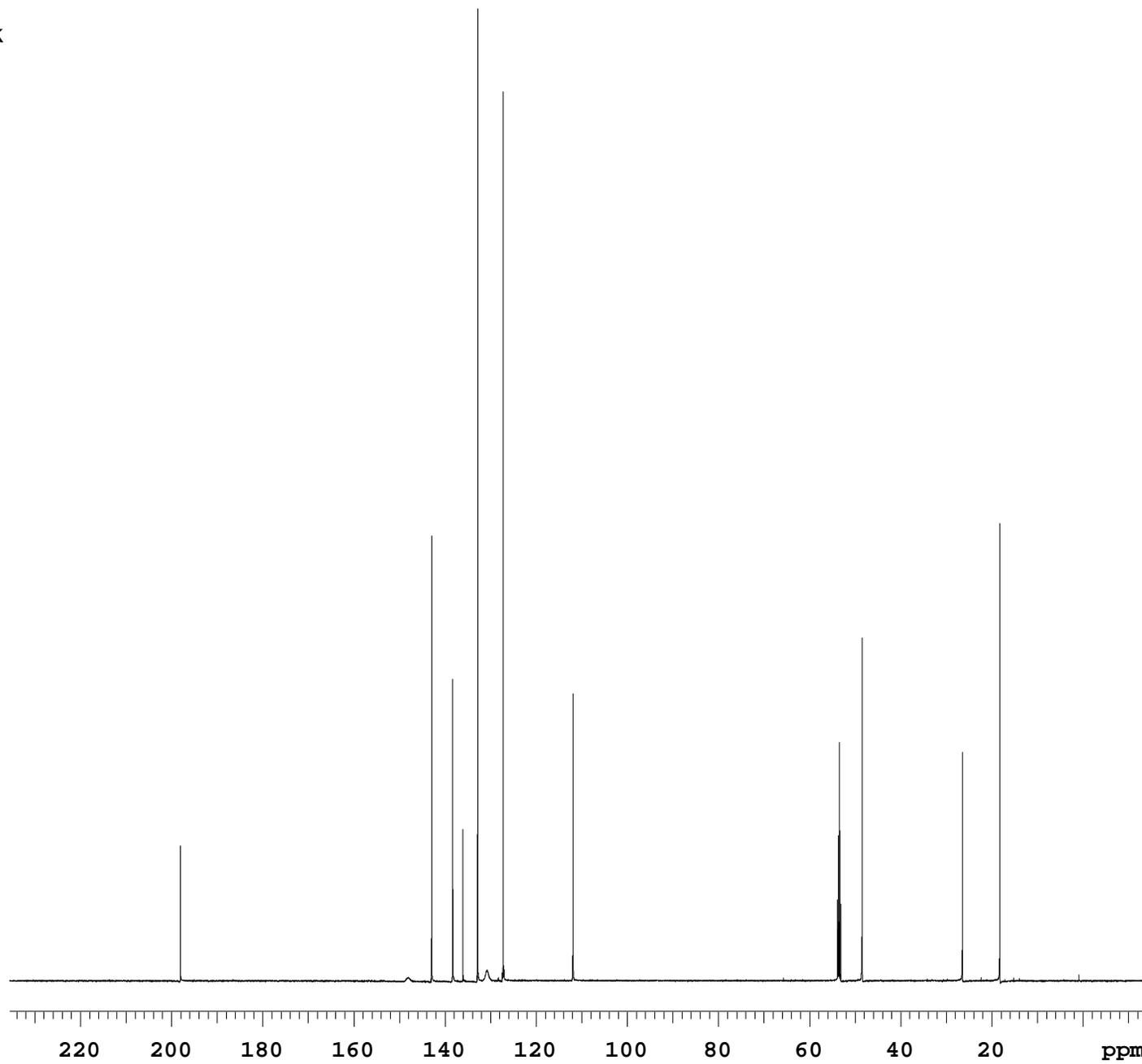


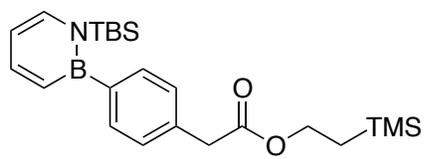
UO VNMR5-600  
{CH-ColdProbe}  
13C-observe  
  
Solvent: cd2c12  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: 4-Ac\_C  
VNMR5-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37878.8 Hz  
60 repetitions

OBSERVE C13, 150.8649758  
DECOUPLE H1, 599.9825418  
Power 41 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 minutes





4

UO Inova-500 Carbon-13

Solvent: cd2cl2

Temp. 25.0 C / 298.1 K

Operator: ger

File: H

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 8001.6 Hz

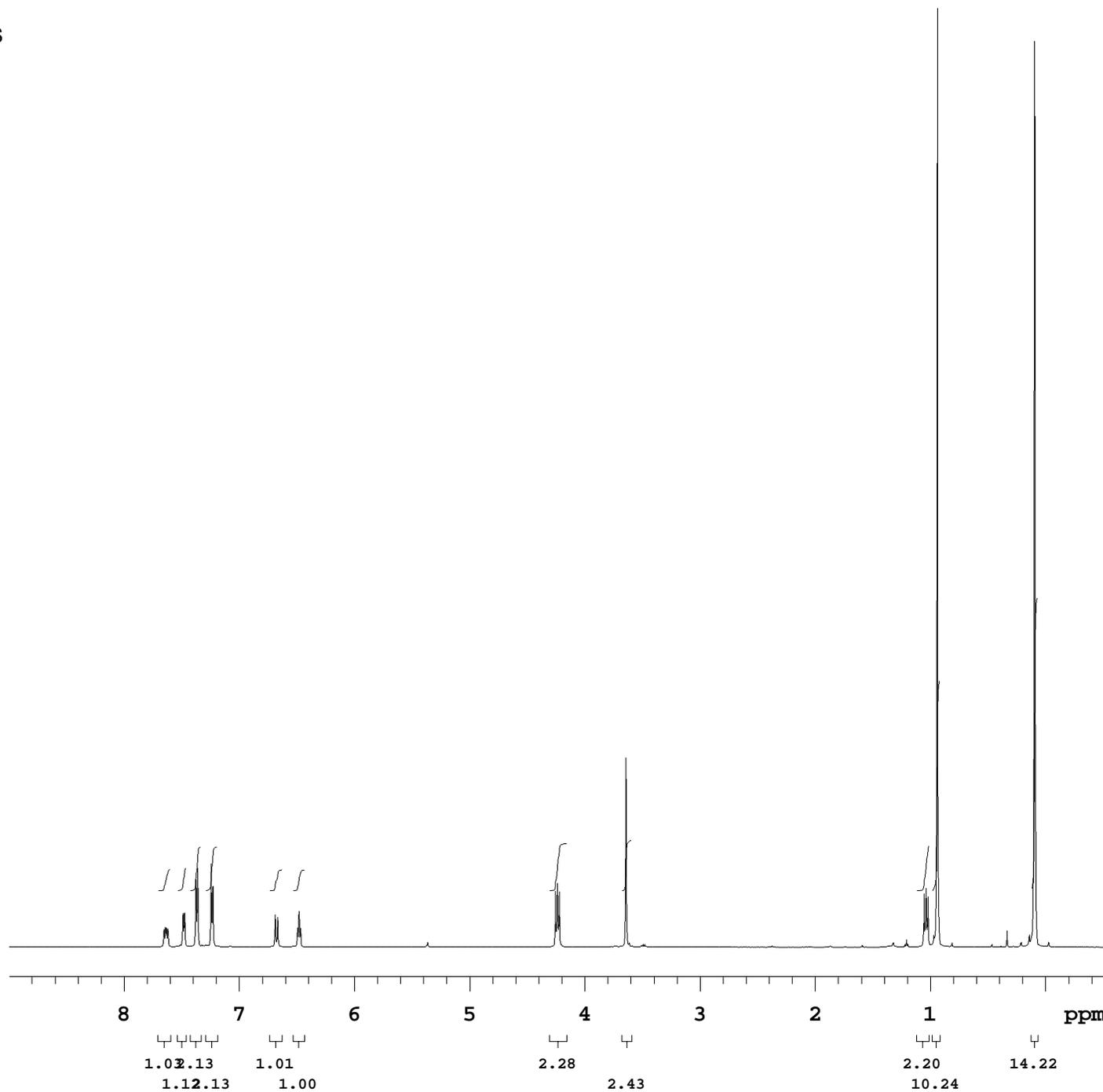
8 repetitions

OBSERVE H1, 500.1052045

DATA PROCESSING

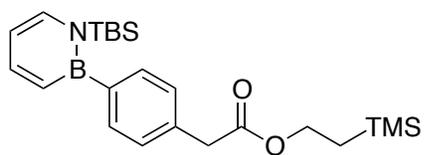
FT size 32768

Total time 1 minute



Archive dir:

File: H



4

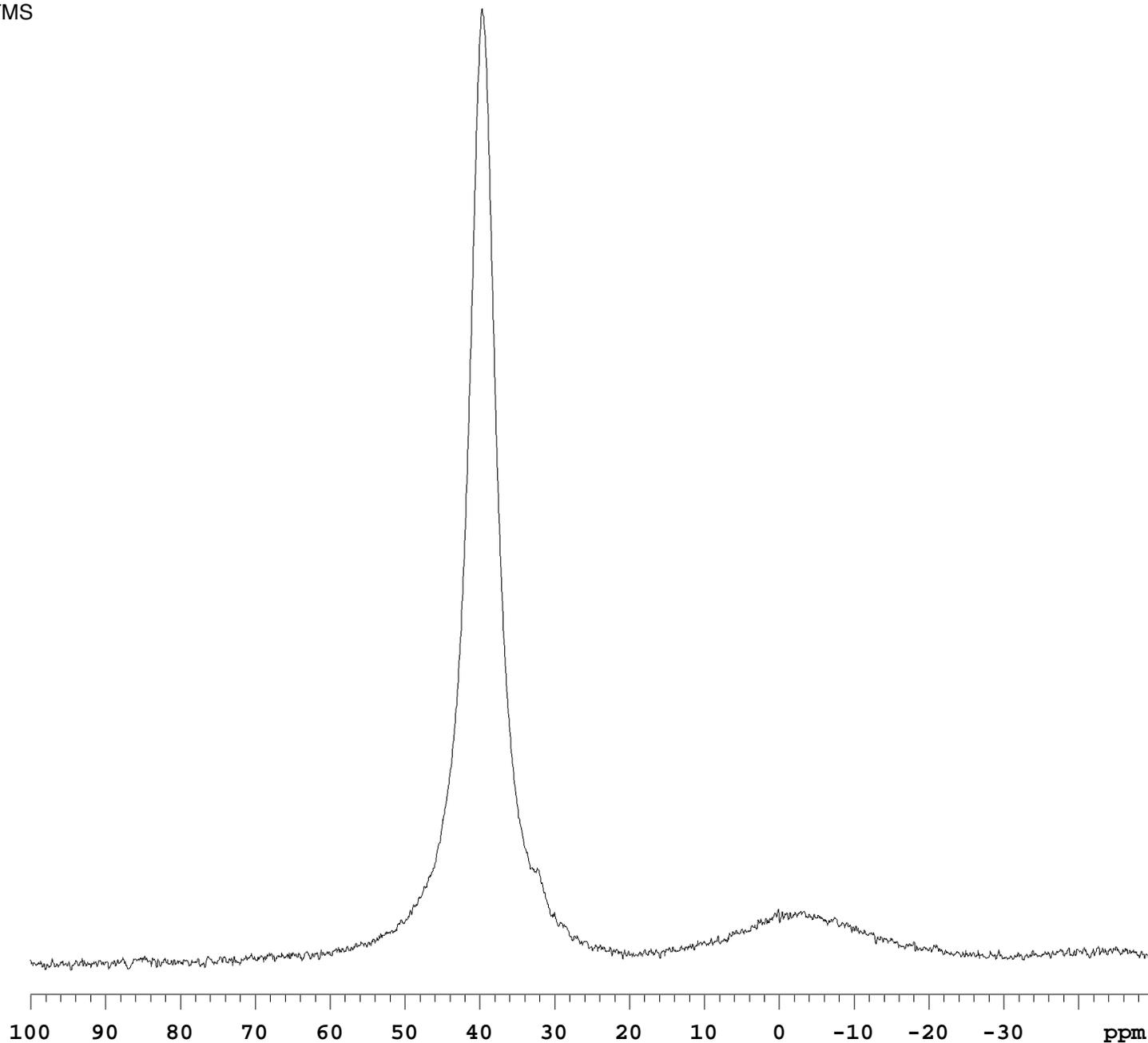
INDEX	FREQUENCY	PPM	HEIGHT
1	3818.4	39.664	159.0

UO Inova-300-North  
Boron-11  
  
Solvent: c6d6  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File:  
INOVA-500 "sunofnmr.uoregon.edu"

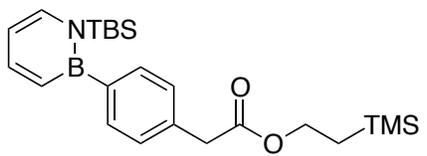
PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
128 repetitions

OBSERVE B11, 96.2681106

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute



Archive dir: File:



4

UO Inova-500 Carbon-13

Solvent: cd2cl2

Temp. 25.0 C / 298.1 K

Operator: ger

File: C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

2188 repetitions

OBSERVE C13, 125.7515537

DECOUPLE H1, 500.1077051

Power 39 dB

continuously on

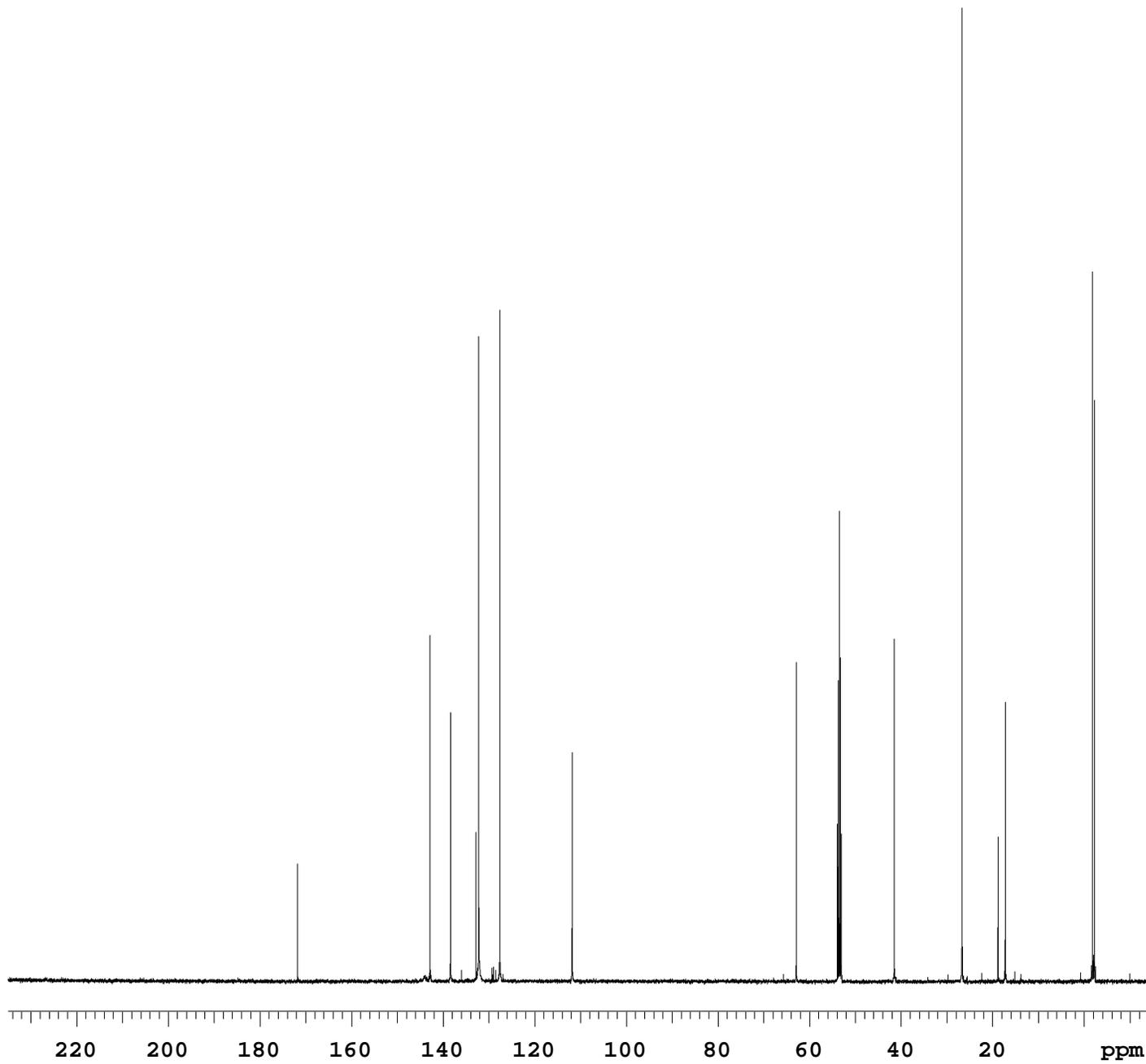
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

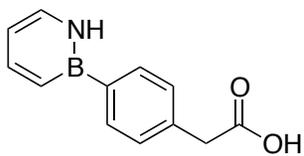
FT size 65536

Total time 109 minutes



Archive dir:

File: C



5

UO Inova-300 Standard-1H

Solvent: acetone  
Ambient temperature  
Operator: ger  
File: H  
INOVA-500 "hotwax.uoregon.edu"

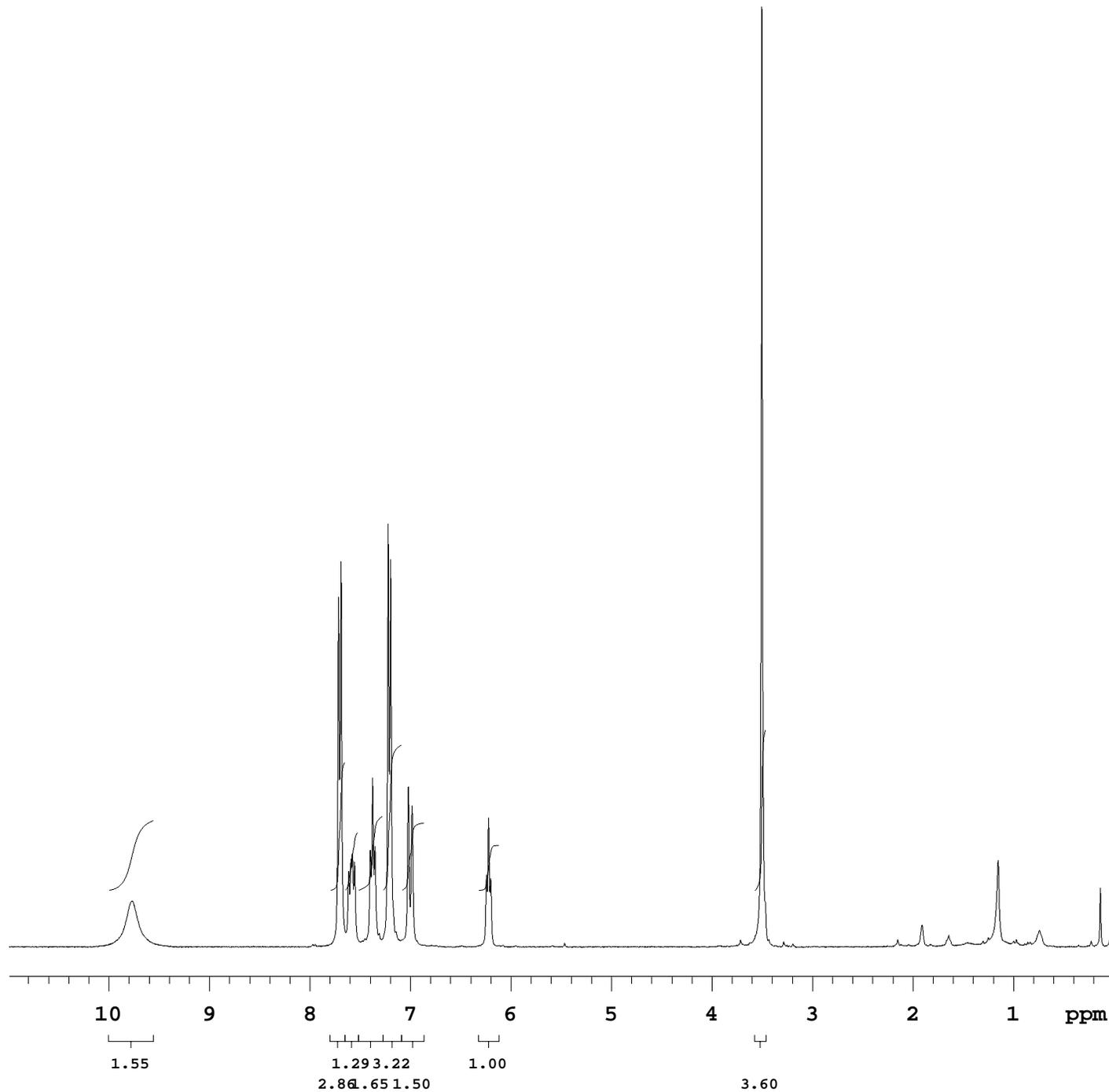
PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.000 sec  
Width 4799.0 Hz  
8 repetitions

OBSERVE H1, 299.9341266

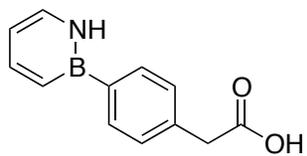
DATA PROCESSING

Line broadening 0.2 Hz  
FT size 32768  
Total time 1 minute



Archive dir:

File: H



5

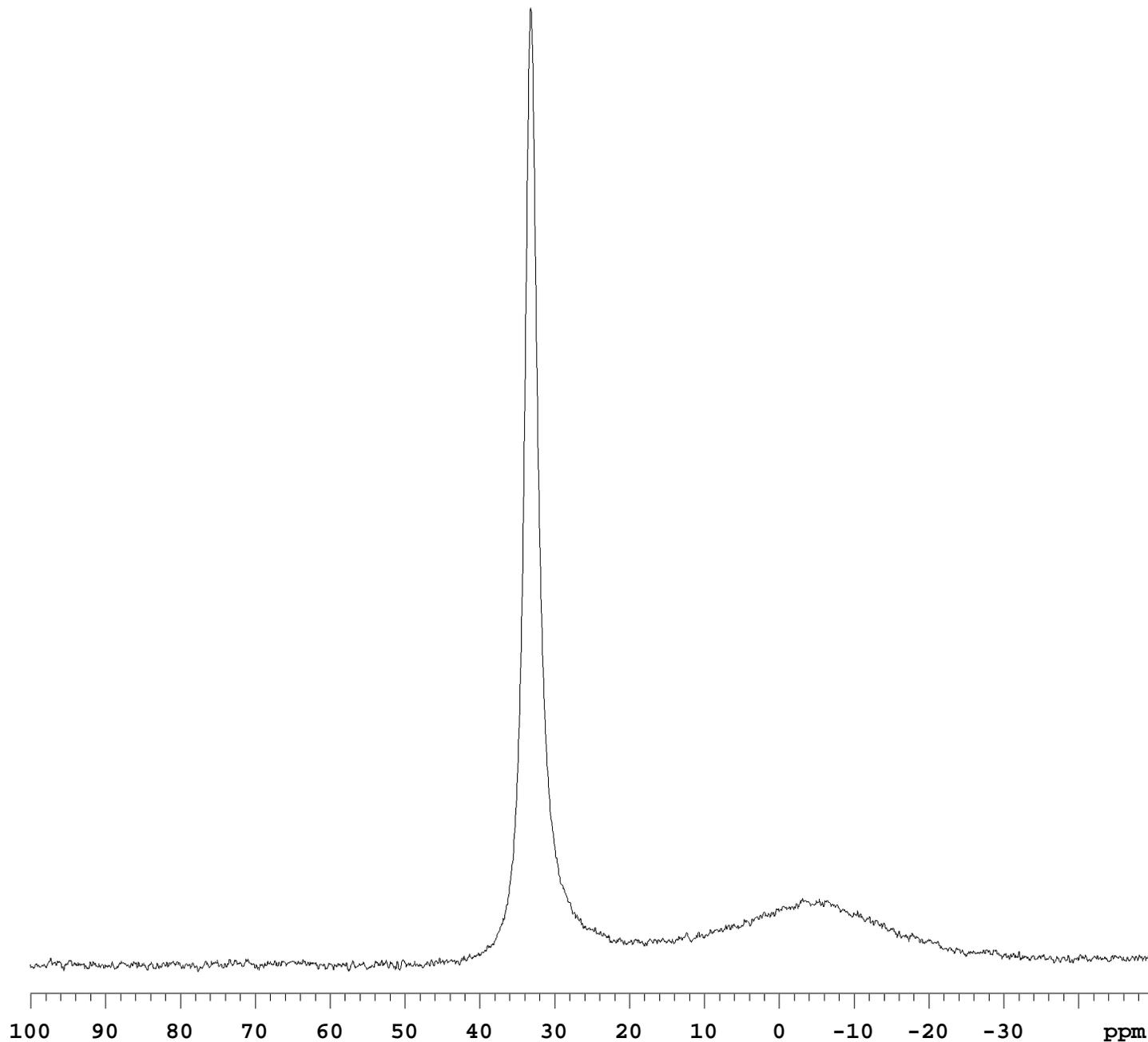
INDEX	FREQUENCY	PPM	HEIGHT
1	3193.4	33.172	159.0

UO Inova-300-North  
Boron-11  
  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: B  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 100.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
120 repetitions

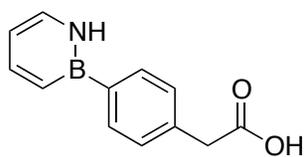
OBSERVE B11, 96.2682868

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute



Archive dir:

File: B



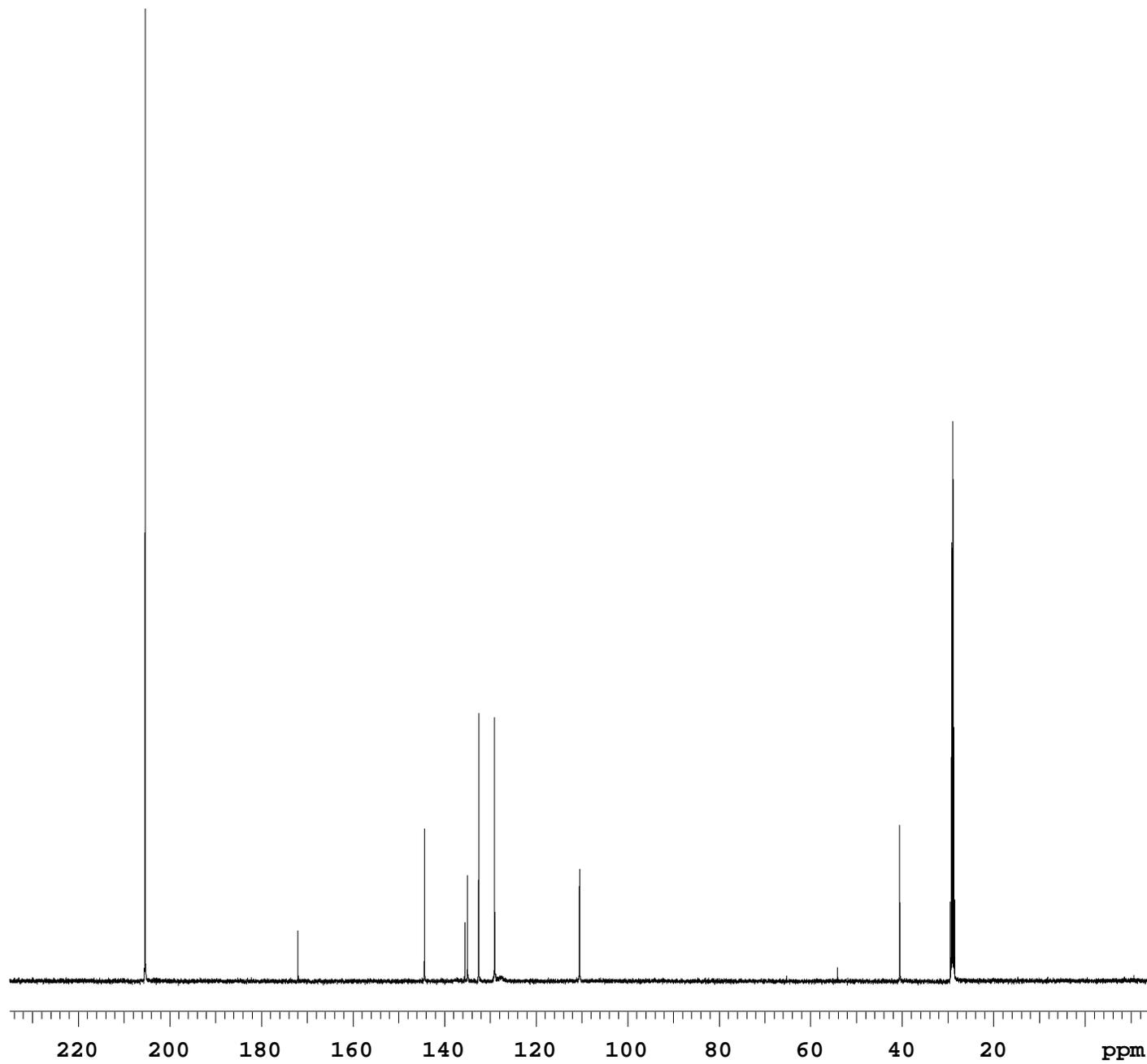
5

UO Inova-500 standard 1H  
Solvent: acetone  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: C  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.000 sec  
Width 31434.2 Hz  
600 repetitions

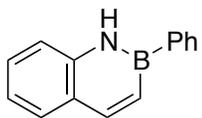
OBSERVE C13, 125.7519649  
DECOUPLE H1, 500.1093404  
Power 39 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 65536  
Total time 20 minutes



Archive dir:

File: C



7

UO Inova-500 standard 1H

Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: GER-3-191-3\_H  
INOVA-500 "sunofnmr.uoregon.edu"

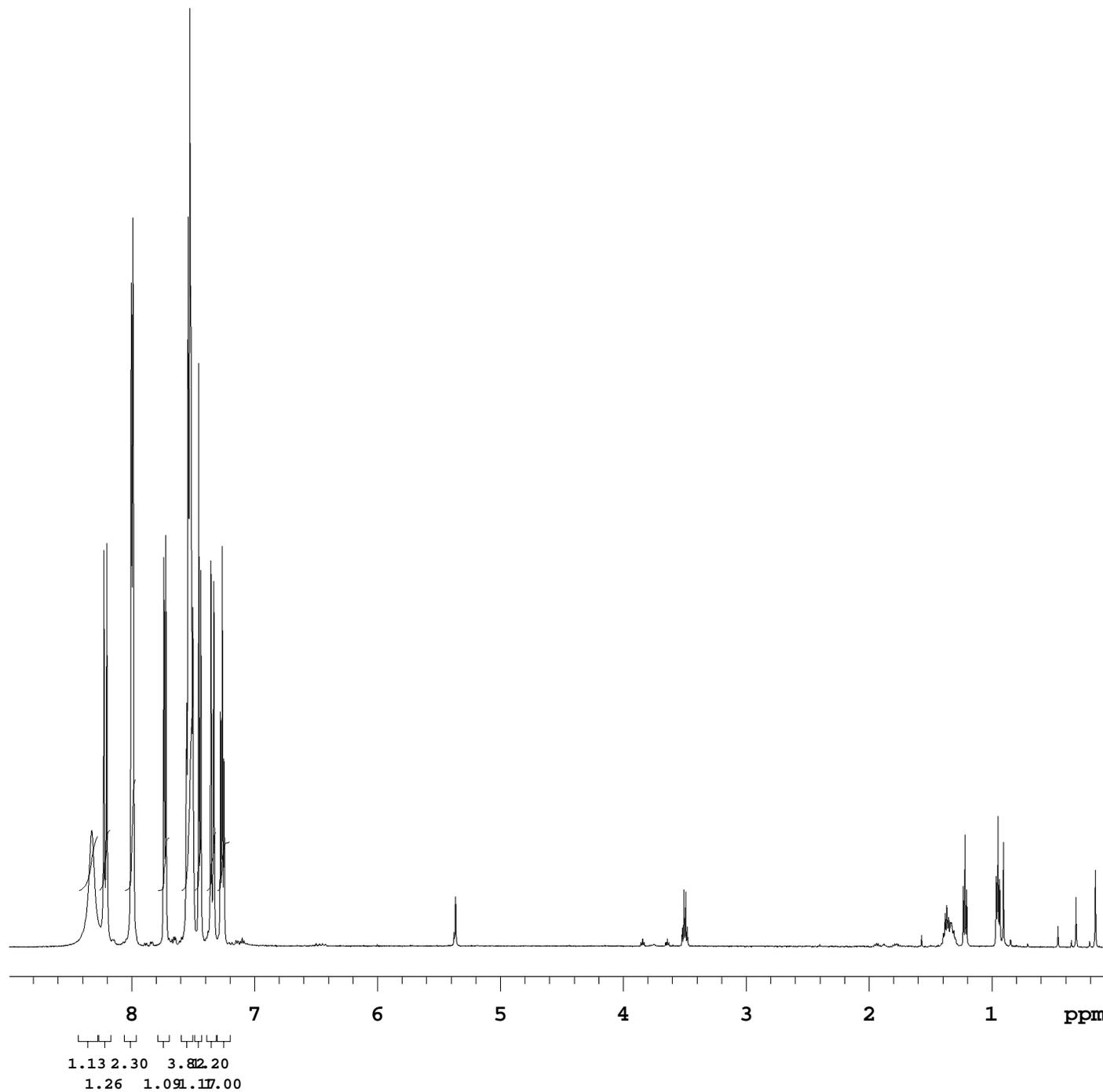
PULSE SEQUENCE

Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8001.6 Hz  
8 repetitions

OBSERVE H1, 500.1052045

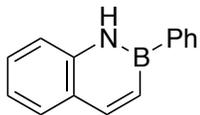
DATA PROCESSING

FT size 32768  
Total time 1 minute



Archive dir:

File: GER-3-191-3\_H



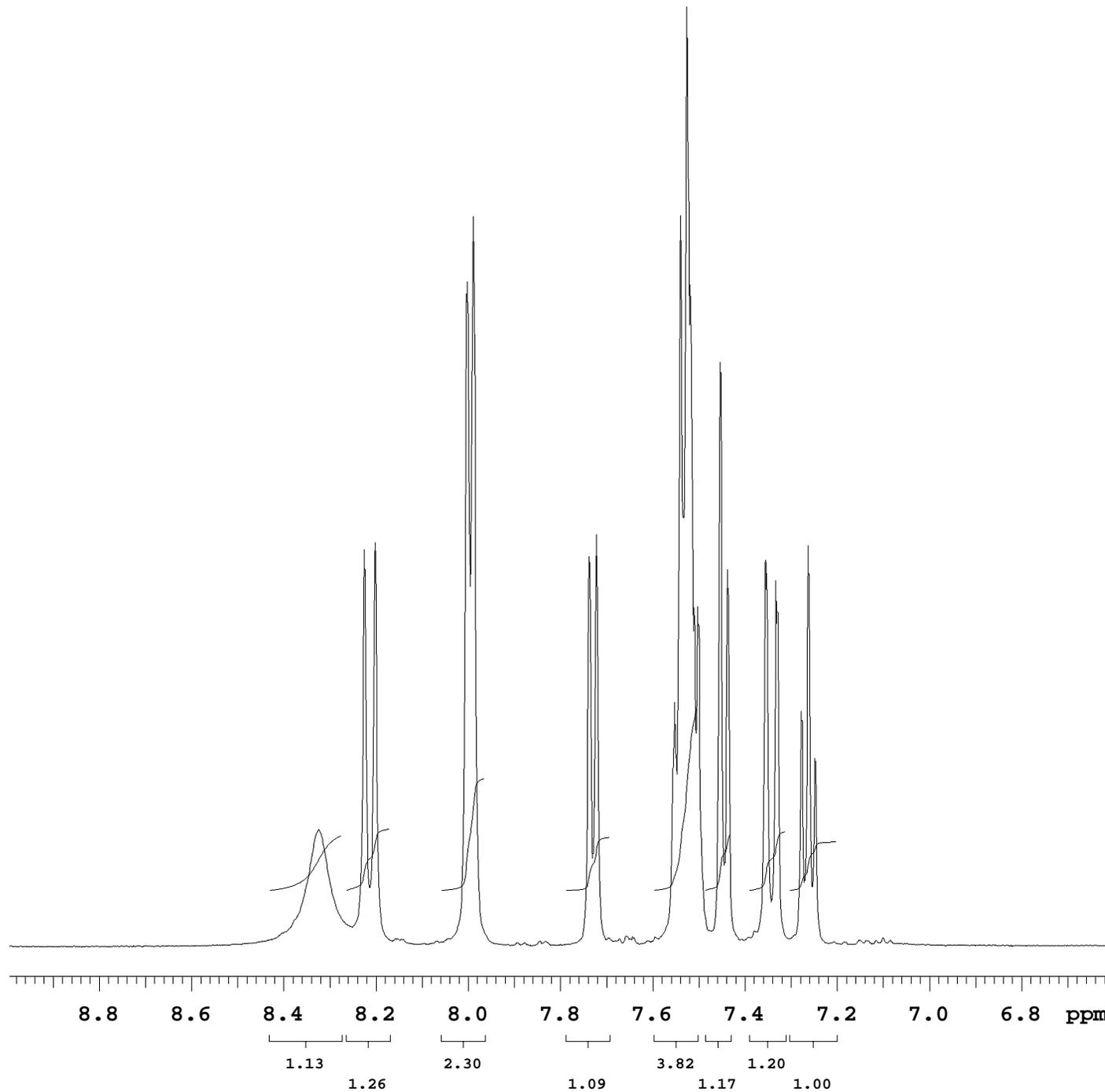
7

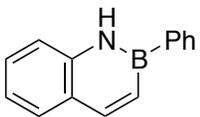
UO Inova-500 standard 1H  
Solvent: cd2cl2  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: GER-3-191-3\_H  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8001.6 Hz  
8 repetitions

OBSERVE H1, 500.1052045

DATA PROCESSING  
FT size 32768  
Total time 1 minute





7

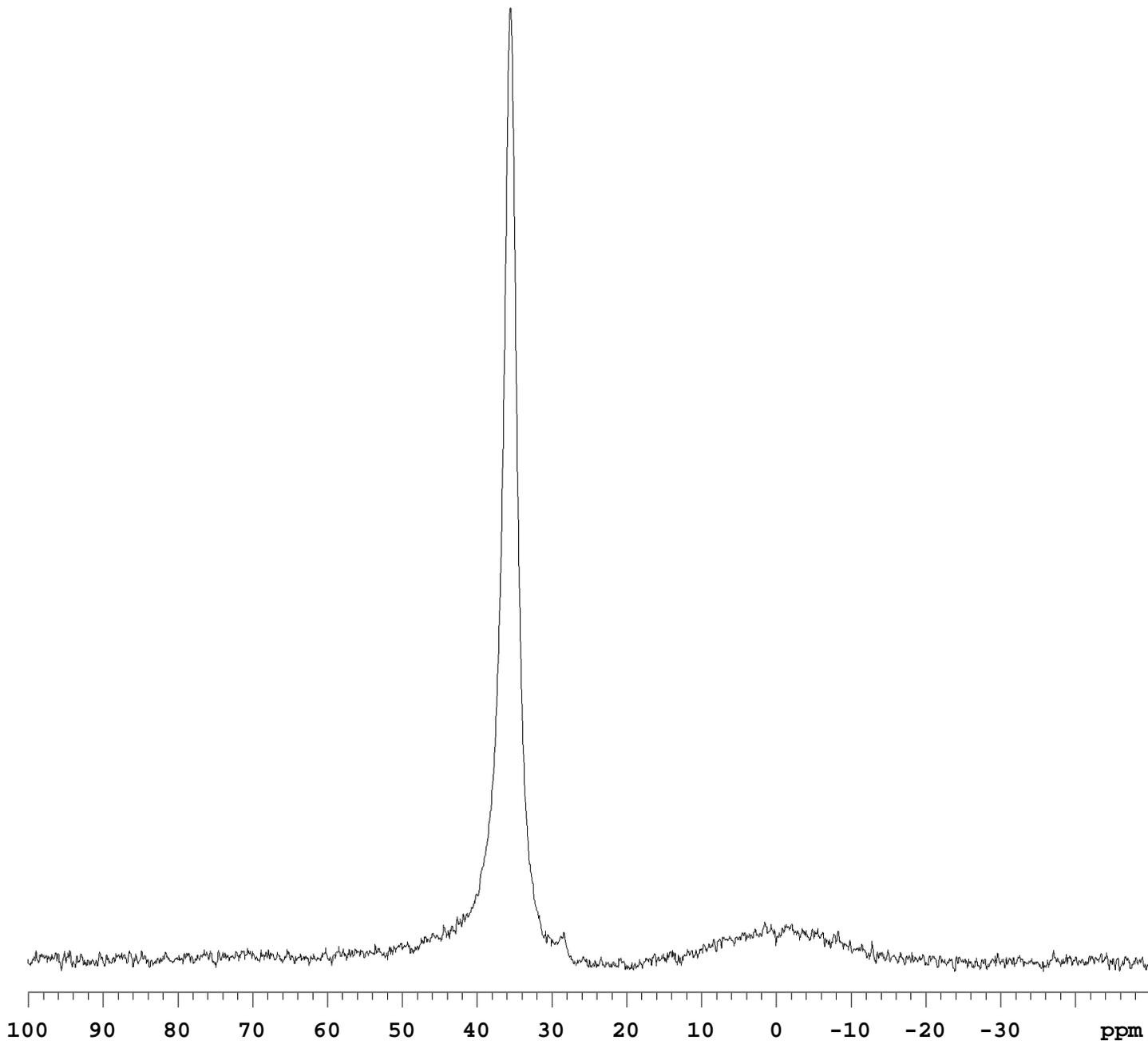
INDEX	FREQUENCY	PPM	HEIGHT
1	3418.0	35.505	159.0

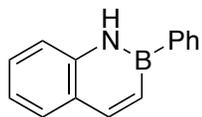
UO Inova-300-North  
Boron-11  
  
Solvent: toluene  
Temp. 25.0 C / 298.1 K  
Operator: ger  
File: GER-3-191-2\_B  
INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
Relax. delay 0.200 sec  
Pulse 90.0 degrees  
Acq. time 0.200 sec  
Width 40000.0 Hz  
80 repetitions

OBSERVE B11, 96.2681164

DATA PROCESSING  
Line broadening 10.0 Hz  
FT size 16384  
Total time 1 minute





7

UO Inova-500 Carbon-13

Solvent: cd2cl2

Temp. 25.0 C / 298.1 K

Operator: ger

File: GER-3-191-3\_C

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 31434.2 Hz

1436 repetitions

OBSERVE C13, 125.7515537

DECOUPLE H1, 500.1077051

Power 39 dB

continuously on

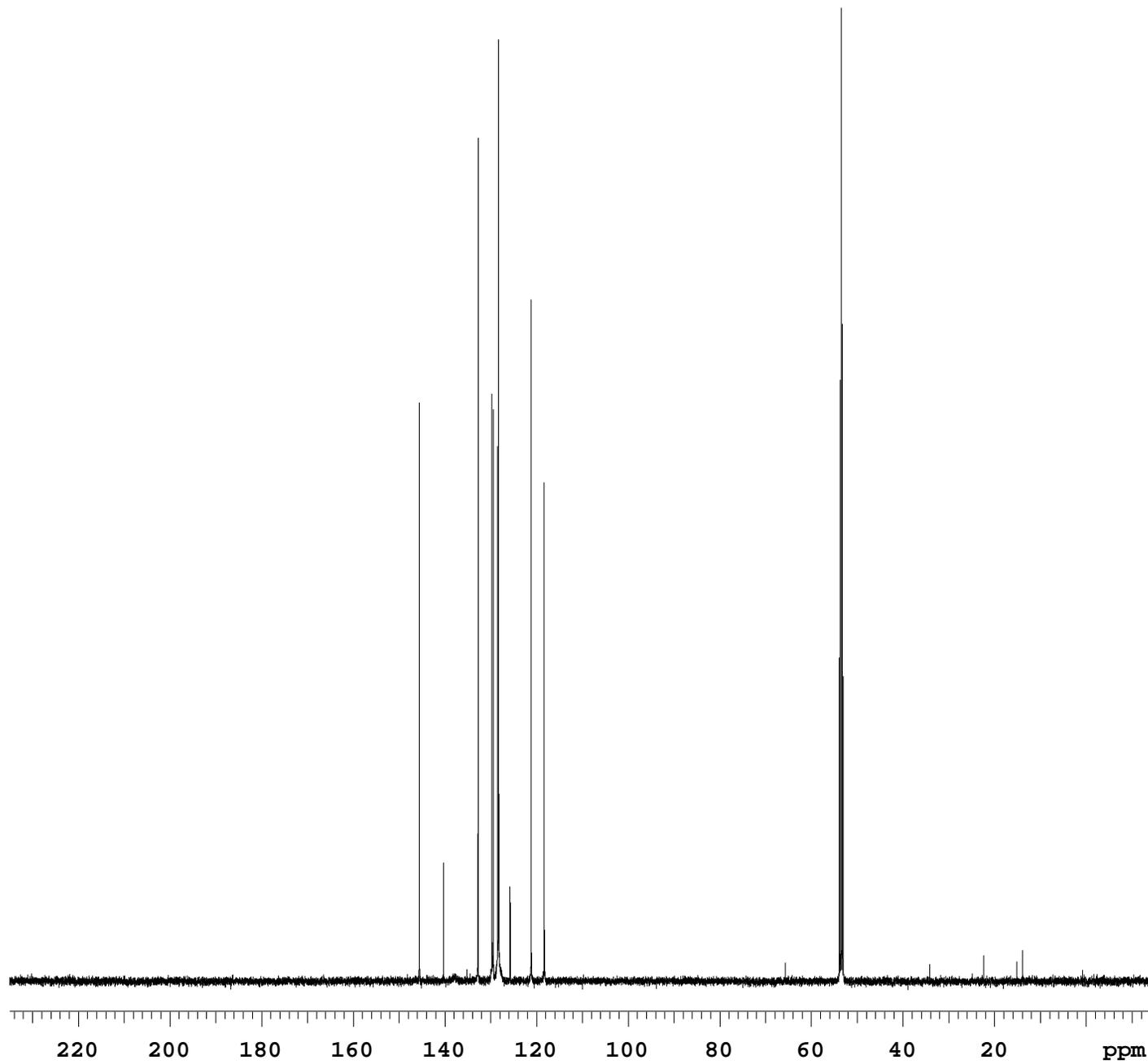
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

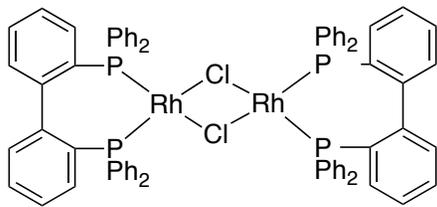
FT size 65536

Total time 47 minutes



Archive dir:

File: GER-3-191-3\_C



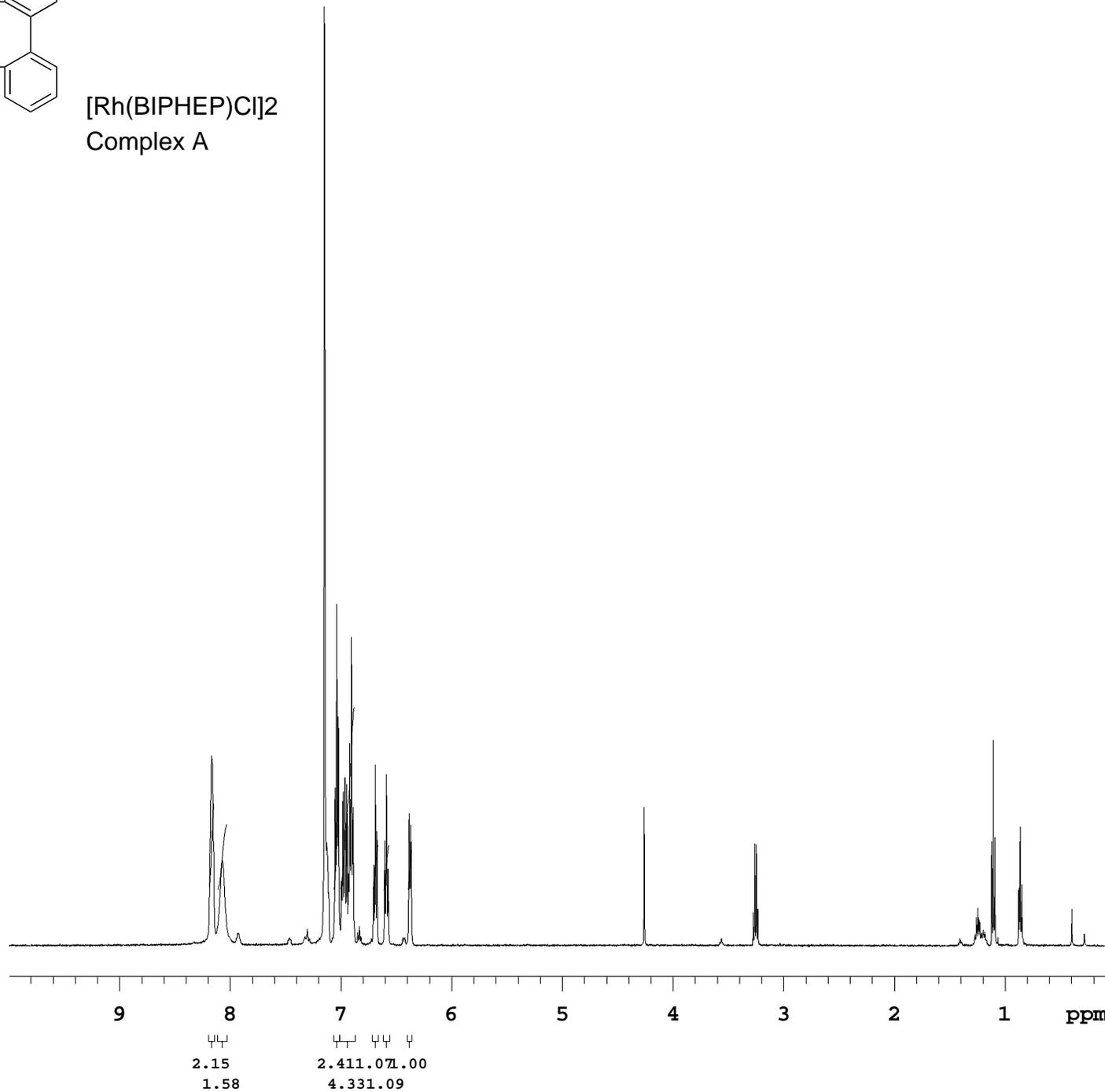
[Rh(BIPHEP)Cl]<sub>2</sub>  
Complex A

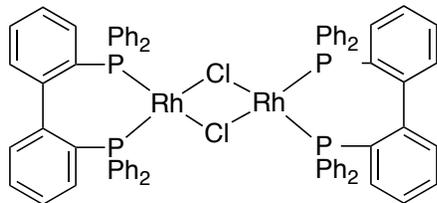
UO Inova-500 standard 1H  
 Solvent: c6d6  
 Temp. 25.0 C / 298.1 K  
 Operator: ger  
 File:  
 INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.048 sec  
 Width 8001.6 Hz  
 8 repetitions

OBSERVE H1, 500.1042894

DATA PROCESSING  
 FT size 32768  
 Total time 1 minute





[Rh(BIPHEP)Cl]<sub>2</sub>  
Complex A

INDEX	FREQUENCY	PPM	HEIGHT
1	9503.7	46.945	84.7
2	9310.7	45.991	87.1

UO Inova-500 P31

Solvent: c6d6

Temp. 25.0 C / 298.1 K

Operator: ger

File:

INOVA-500 "sunofnmr.uoregon.edu"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.000 sec

Width 50000.0 Hz

64 repetitions

OBSERVE P31, 202.4459271

DECOUPLE H1, 500.1067899

Power 39 dB

on during acquisition

off during delay

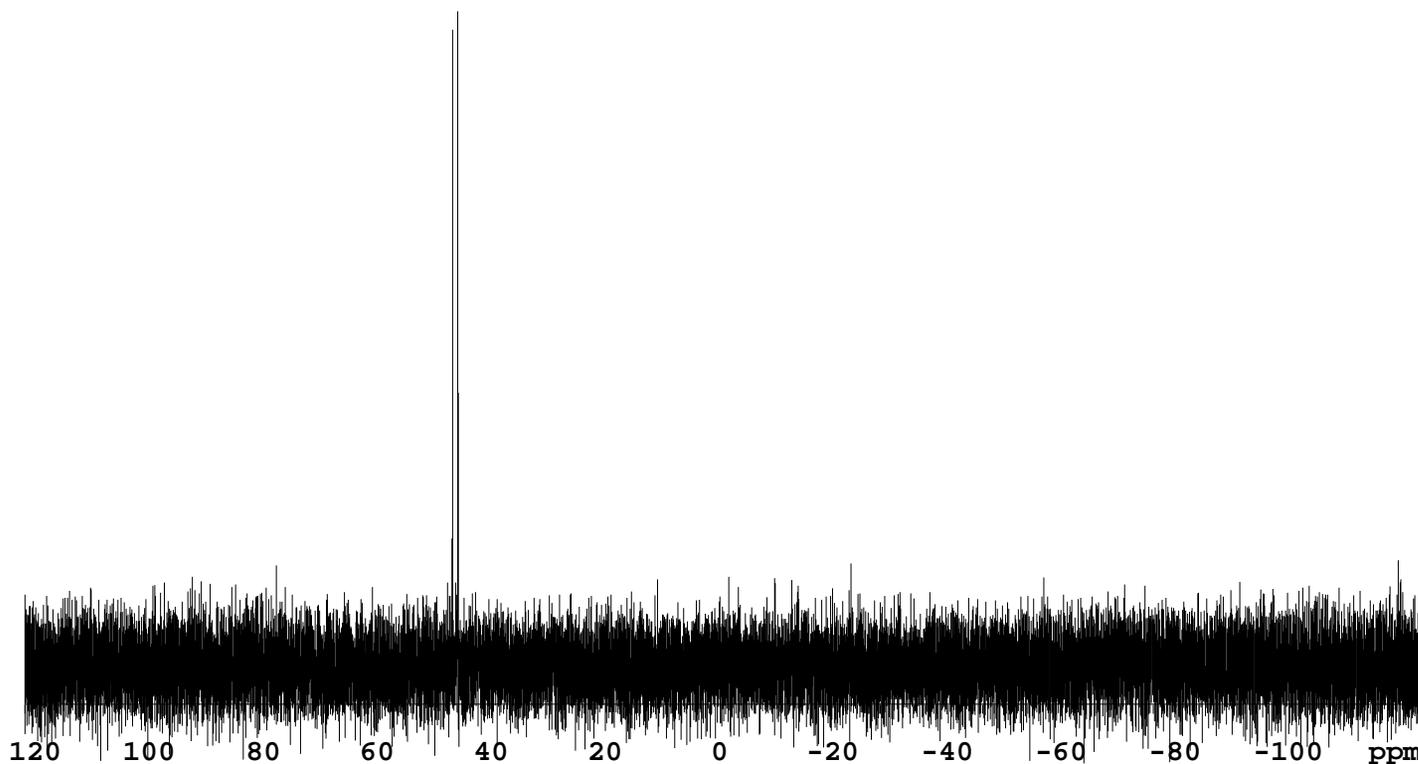
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 2 minutes



Archive dir:

File: