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Copper(I)-Catalyzed Carbon–Halogen Bond-Selective Boryl Substitution of Alkenyl Halides

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1. Instrumentation and Chemicals

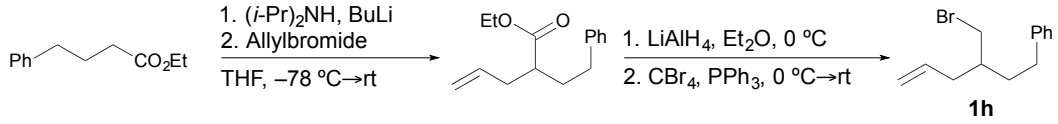
Materials were obtained from commercial suppliers and purified by standard procedures unless otherwise noted. Solvents were also purchased from commercial suppliers, degassed via three freeze-pump-thaw cycles, and further dried over molecular sieves (MS 4A). NMR spectra were recorded on JEOL JNM-ECX400P and JNM-ECS400 spectrometers (^{1}H: 400 MHz and ^{13}C: 100 MHz). Tetramethylsilane (^{1}H) and $CDCl_3$ (^{13}C) were employed as the external standards, respectively. CuCl (ReagentPlus® grade, 224332-25G, ≥99%) and K(O-*t*-Bu) / THF (1.0 M, 328650-50ML) were purchased from Sigma-Aldrich Co. and used as received. GLC analyses were conducted with a Shimadzu GC-2014 or GC-2025 equipped with a ULBON HR-1 glass capillary column (Shinwa Chemical Industries) and a FID detector. High-resolution mass spectra were recorded at the Center for Instrumental Analysis, Hokkaido University.

2. General Experimental Procedure.

Procedure for the Copper(I)-Catalyzed Chemoselective Borylation of 1a (Table 1).

Copper chloride (2.5 mg, 0.025 mmol) and bis(pinacolato)diboron (**2**) (152.4 mg, 0.60 mmol), *o*-diphenylphosphinophenol **L1** (7.0 mg, 0.025 mmol) were placed in an oven-dried reaction vial. After the vial was sealed with a screw cap containing a teflon-coated rubber septum, the vial was connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. Dry THF (0.4 mL) and K(O-*t*-Bu)/THF (1.0 M, 0.6 mL, 0.6 mmol) were added in the vial through the rubber septum using a syringe. After stirring for 30 min, **1a** (74.5. mg, 0.50 mmol) was added to the mixture at 0 °C. After the reaction was complete, the reaction mixture was passed through a silica gel column (radius: 10 mm, height of the column: 30 mm) eluting with Et_2O. The crude material was purified by flash column chromatography (SiO_2, Et_2O/pentane, typically 0:100–2:98) to give the corresponding borylation product **3a** as colorless oil.

3. Substrate Preparation



1h

Compounds **1a**–**1g** and **1i** were synthesized according to our previous publication.[1] In a oven-dried 200 mL round bottomed flask, a hexane solution of *n*-BuLi (1.55 M, 11.6 mL, 18.0 mmol) was added to a solution of (*i*-Pr)$_2$NH (3.05 mL, 21.8 mmol) in THF at 0 ºC. The reaction mixture was stirred for 15 min and then cooled to –78 ºC. The ethyl ester (2.88 g, 15.0 mmol) was added dropwise to the reaction mixture and the reaction mixture was further stirred for 30 min. Allylbromide (1.95 mL, 22.5 mmol) was then added dropwise into the mixture. It was warmed to room temperature and stirred for 4 h. The reaction mixture was quenched by addition of saturated NH_4Cl aq. and extracted with Et_2O three time. The combined organic layer was then dried over $MgSO_4$. After filtration, the solvents were removed by evaporation. The drude product was purified by flash column chromatography to obtain the corresponding ethyl ester (2.26 g, 9.8 mmol, 65%) as a colorless oil.

In a oven-dried round bottomed flask, a solution of the ethyl ester (2.09 g, 9.0 mmol) in Et_2O (10 mL) was added to a slurry of $LiAlH_4$ (512.3 mg, 13.5 mmol) in Et_2O (15 mL) at 0 ºC. After stirred for 9 h, the reaction mixture was quenched by addition of water and stirred until a white solid was formed. The mixture was filtered and dried over $MgSO_4$. The crude material was purified by flush column chromatography to obtain the corresponding alcohol (1.47 g, 7.7 mmol, 86%) as a colorless

oil.

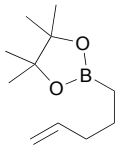
In a 100 mL round bottomed flask, CBr_4 (2.98 g, 9.0 mmol) and the alcohol (1.43 g, 7.5 mmol) were dissolved in dry THF (15 mL) and the mixture was cooled to 0 ºC. PPh_3 (2.36 g, 9.0 mmol) was then added portionwise and the reaction mixture was stirred for 12 h. The reaction mixture was quenched by addition of water and extracted three times with Et_2O. The combined organic layer was dried over $MgSO_4$. After filtration, the solvents were removed by evaporation. The crude product was purified by flush column chromatography to obtain **1h** (1.68 g, 6.6 mmol, 88%) as a colorless oil.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.67–1.79 (m, 3H), 2.19–2.23 (m, 2H), 2.57–2.71 (m, 2H), 3.45–3.52 (m, 2H), 5.06–5.15 (m, 2H), 5.67–5.78 (m, 1H), 7.18–7.21 (m, 3H), 7.26–7.31 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 32.8 (*C*H_2), 34.0 (*C*H_2), 36.6 (*C*H_2), 38.4 (*C*H_2), 38.6 (*C*H), 117.3 (*C*H_2), 125.8 (*C*H), 128.26 (*C*H), 128.35 (*C*H), 135.4 (*C*H), 141.8 (*C*). HRMS–EI (*m*/*z*): [M]+ calcd for $C_{13}H_{17}Br$, 252.05136; found, 252.05091.

4. Borylation Product Characterization

The ^{1}H and ^{13}C NMR spectra of product **4g** were identical to those we previously reported. [1]

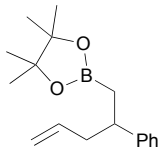
4,4,5,5-Tetramethyl-2-(pent-4-en-1-yl)-1,3,2-dioxaborolane (3a).[2]



3a

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.79 (t, *J* = 7.9 Hz, 2H), 1.25 (s, 12H), 1.51 (quin, *J* = 7.6 Hz, 2H), 2.02–2.08 (m, 2H), 4.91–5.02 (m, 2H), 5.75–5.85 (m, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 10.7 (br, s, B–*C*H_2), 23.3 (*C*H_2), 24.8 (*C*H_3), 36.3 (*C*H_2), 82.8 (*C*), 114.4 (*C*H_2), 138.9 (*C*H) HRMS–EI (*m*/*z*): [M]+ calcd for $C_{11}H_{21}BO_2$, 196.16346; found, 196.16381.

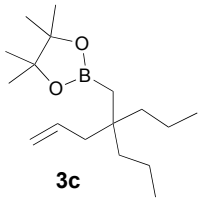
4,4,5,5-Tetramethyl-2-(2-phenylpent-4-en-1-yl)-1,3,2-dioxaborolane (3b).



3b

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.07–1.14 (m, 13H), 1.21–1.26 (m, 1H), 2.28–2.41 (m, 2H), 2.94 (dt, *J* = 7.1, 14.2 Hz, 1H), 4.90–4.98 (m, 2H), 5.62–5.73 (m, 1H), 7.12–7.27 (m, 5H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 18.7 (br, s, B–*C*H_2), 24.60 (*C*H_3), 24.65 (*C*H_3), 41.3 (*C*H), 43.7 (*C*H_2), 82.9 (*C*), 116.0 (*C*H_2), 125.8 (*C*H), 127.4 (*C*H), 128.0 (*C*H), 137.1 (*C*H), 146.7 (*C*). HRMS–EI (*m*/*z*): [M]+ calcd for $C_{17}H_{25}BO_2$, 272.19476; found, 272.19420.

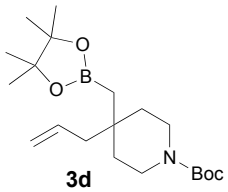
2-(2,2-Dipropylpent-4-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3c).



3c

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.75 (s, 2H), 0.83–0.88 (m, 6H), 1.23–1.25 (m, 20H), 2.06 (d, J = 7.6 Hz, 2H), 4.98–5.02 (m, 2H), 5.76–5.86 (m, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.9 (*C*H_3), 16.7 (*C*H_2), 24.8 (*C*H_3), 37.7 (*C*), 41.6 (*C*H_2), 43.5 (*C*H_2), 82.5 (*C*), 116.4 (*C*H_2), 136.1 (*C*H). The carbon directly attached to the boron atom was not detected, likely due to quadropolar relaxation. HRMS–EI (*m*/*z*): [M–Me]+ calcd for $C_{16}H_{30}BO_2$, 265.23388; found, 265.23362.

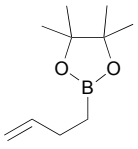
***tert*-Butyl 4-allyl-4-[(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl]piperidine-1-carboxylate (3d).**



3d

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.87 (s, 2H), 1.23 (s, 12 H), 1.39–14.9 (m, 13H), 2.16 (d, J = 7.5 Hz, 2H), 3.28–3.34 (m, 2H), 3.42–3.46 (m, 2H), 5.01–5.06 (m, 2H), 5.77–5.87 (m, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 19.7 (br, s, B–*C*H_2), 24.8 (*C*H_3), 28.4 (*C*H_3), 33.5 (*C*), 36.5 (*C*H_2), 39.7 (br, d, *C*H_2), 43.7 (*C*H_2), 79.0 (*C*), 82.8 (*C*), 117.5 (*C*H_2), 134.6 (*C*H), 155.0 (*C*). HRMS–EI (*m*/*z*): [M]+ calcd for $C_{20}H_{36}BNO_4$, 365.27374; found, 365.27327.

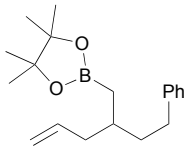
2-(But-3-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3e).[3,4]



3e

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.89 (t, J = 7.7 Hz, 2H), 1.24 (s, 12H), 2.14–2.20 (m, 2H), 4.88–5.03 (m, 2H), 5.84–5.94 (m, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 10.2 (br, s, B–*C*H_2), 24.8 (*C*H_3), 27.9 (*C*H_2), 83.0 (*C*), 113.1 (*C*H_2), 140.6 (*C*H). HRMS–EI (*m*/*z*): [M]+ calcd for $C_{10}H_{19}BO_2$, 182.14781; found, 182.14816.

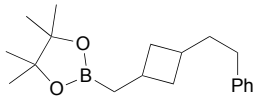
4,4,5,5-Tetramethyl-2-(2-phenethylpent-4-en-1-yl)-1,3,2-dioxaborolane (3h).



3h

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.85 (d, *J* = 6.7 Hz, 2H), 1.25 (s, 12H), 1.50–1.69 (m, 2H), 1.79 (septet, *J* = 6.7 Hz, 1H), 2.03–2.19 (m, 2H), 2.55–2.67 (m, 2H), 4.98–5.05 (m, 2H), 5.74–5.85 (m, 1H), 7.14–7.18 (m, 3H), 7.24–7.28 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 16.5 (br, s, B–*C*H_2), 24.8 (*C*H_3), 33.3 (*C*H_2), 33.9 (*C*H), 38.3 (*C*H_2), 40.8 (*C*H_2), 82.9 (*C*), 116.0 (*C*H_2), 125.5 (*C*H), 128.2 (*C*H), 128.3 (*C*H), 137.3 (*C*H), 143.1 (*C*). HRMS–EI (*m*/*z*): [M]+ calcd for $C_{19}H_{29}BO_2$, 300.22606; found, 300.22607.

4,4,5,5-Tetramethyl-2-[(3-phenethylcyclobutyl)methyl]-1,3,2-dioxaborolane (4h).

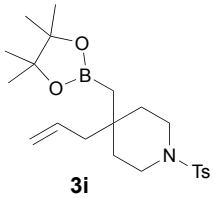


4h

The product **4h** was obtained as a diastereomeric mixture (1:1). The stereoselectivity was determined by ^{1}H NMR analysis of the crude reaction mixture.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.90 (d, *J* = 6.7 Hz, 2H), 1.00 (d, *J* = 7.9 Hz, 2H), 1.18–1.26 (m, 26H), 1.63 (dt, *J* = 7.8 Hz, 2H), 1.69–1.77 (m, 4H), 1.80–1.87 (m, 2H), 1.98–2.07 (m, 1H), 2.18–2.29 (m, 4H), 2.43–2.53 (m, 5H), 7.14–7.18 (m, 6H), 7.24–7.28 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 24.8 (*C*H_3), 27.9 (*C*H), 28.2 (*C*H), 30.7 (*C*H), 31.6 (*C*H), 33.6 (*C*H_2), 33.8 (*C*H_2), 35.0 (*C*H_2), 37.2 (*C*H_2), 38.3 (*C*H_2), 39.3 (*C*H_2), 82.8 (*C*), 125.5 (*C*H), 128.2 (*C*H), 128.3 (*C*H) 142.9 (*C*). The carbon directly attached to the boron atom was not detected, likely due to quadropolar relaxation. HRMS–EI (*m*/*z*): [M]+ calcd for $C_{19}H_{29}BO_2$, 300.22606; found, 300.22631.

4-Allyl-4-[(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl]-1-tosylpiperidine (3i).

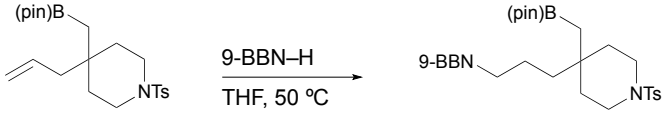


3i

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.72 (s, 2H), 1.21 (s, 12H), 1.57 (t, *J* = 5.6 Hz, 4H), 2.03 (d, *J* = 7.7 Hz, 2H), 2.44 (s, 3H), 2.85–2.91 (m, 2H), 3.10–3.15 (m, 2H), 4.94–5.04 (m, 2H), 5.65–5.79 (m, 1H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.64 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 19.2 (br, s, B–*C*H_2), 21.5 (*C*H_3), 24.8 (*C*H_3), 32.8 (*C*), 36.0 (*C*H_2), 42.0 (*C*H_2), 43.7 (*C*H_2), 82.9 (*C*), 117.8

(CH_2), 127.6 (*C*H), 129.5 (*C*H), 133.4 (*C*), 134.1 (*C*H), 143.2 (*C*). HRMS–ESI (*m*/*z*): [M+Na]+ calcd for $C_{22}H_{34}BNO_4SNa$, 442.21979; found, 442.22008.

5. Borylation Product Functionalization Procedure



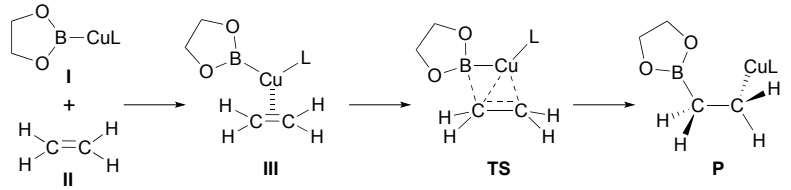
3i **5**

3i (62.9 mg, 0.15 mmol) was placed in an oven-dried reaction vial. After the vial was sealed with a screw cap containing a teflon-coated rubber septum, the vial was connected to a vacuum/nitrogen manifold through a needle. The reaction vial was evacuated and then backfilled with nitrogen. This cycle was repeated three times. 9-BBN–H/THF (0.5 M, 0.45 mL, 0.225 mmol) was added to the vial. The reaction mixture was stirred for 12 h at 50 ºC. Then, the NMR yield of **5** was measured with crude material under a nitrogen atmosphere.

6. Details of DFT Calculations

All calculations were performed with Gaussian 09W (revision C.01) program package.[5] Geometry optimizations were carried out with B3PW91/cc-pVDZ in the gas-phase. Frequency calculations were conducted on the gas-phase optimized geometries to check the all the stationary points as either minima or transition states.

Table S1 Results of DFT calculations of the alkene addition step in copper(I)-catalyzed borylation[1,6]



		ΔG (298 K, 1.0 atm, gas phase),[a] kcal mol^{-1}			
entry	ligand (L)	**I + II**	**III**	**TS**	**P**
1	Xantphos	0	7.1 (–6.5)	17.6 (2.1)	–11.4 (–24.9)
2	$P(C_6F_5)_3$	0	1.5 (–12.2)	19.3 (3.6)	–14.8 (–27.8)
3	PPh_3	0	3.5 (–10.4)	19.0 (3.6)	–16.2 (–30.5)
4	PCy_3	0	5.8 (–6.6)	21.1 (6.2)	–13.3 (–25.4)

[a]Electronic energies are shown in parenthese.

In the transition state, the activation free energy of borylcopper(I)/Xantphos was lower than those of borylcopper(I)/monophosphine ligand: $P(C_6F_5)_3$, PPh_3 and PCy_3 (entry 1). The

borylcopper(I)/monophosphine ligand exhibited high the activation free energies (entries 2–4). In particular, the activation free energy of borylcopper(I)/PCy_3 was higher than those of $P(C_6F_5)_3$ and PPh_3 (entry 4). These results supported the selectivity and yield of the borylation of alkenyl halide.

7. References

1 K. Kubota, E. Yamamoto and H. Ito, *J. Am. Chem. Soc.*, 2013, **135**, 2635–2640.

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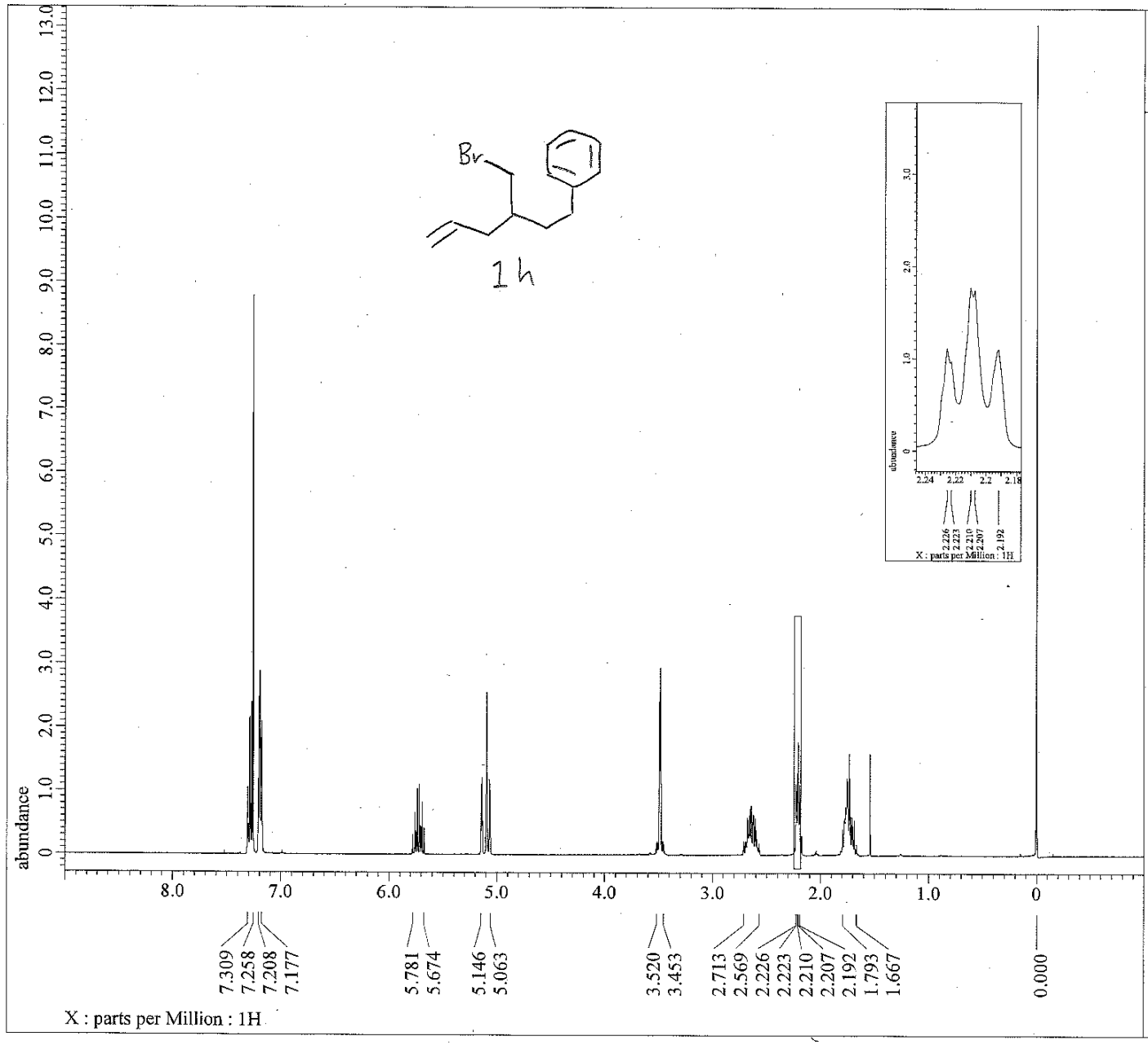
6 The results of entries 1 and 3 have been reported in our previous publication, see ref. 1.



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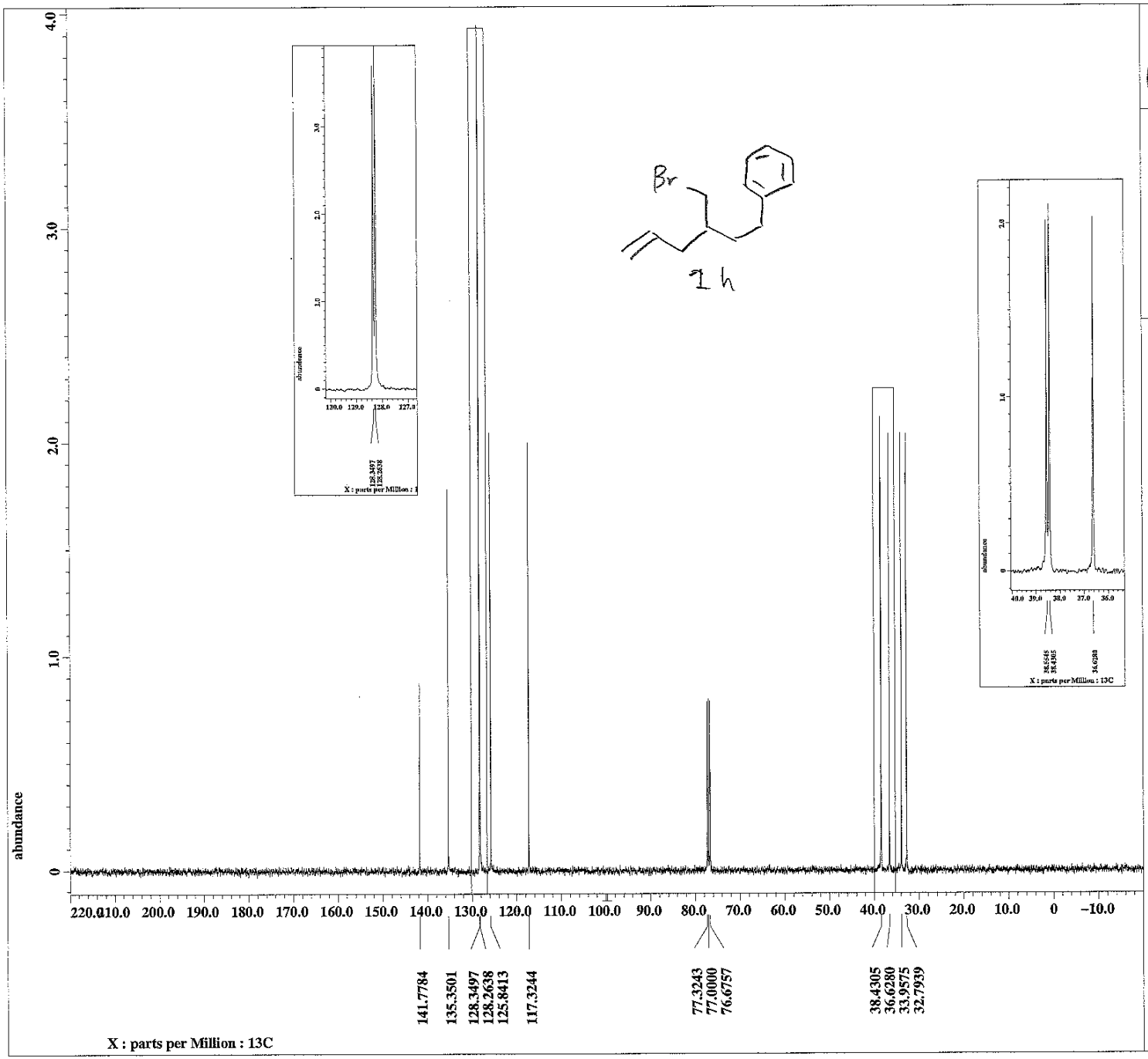

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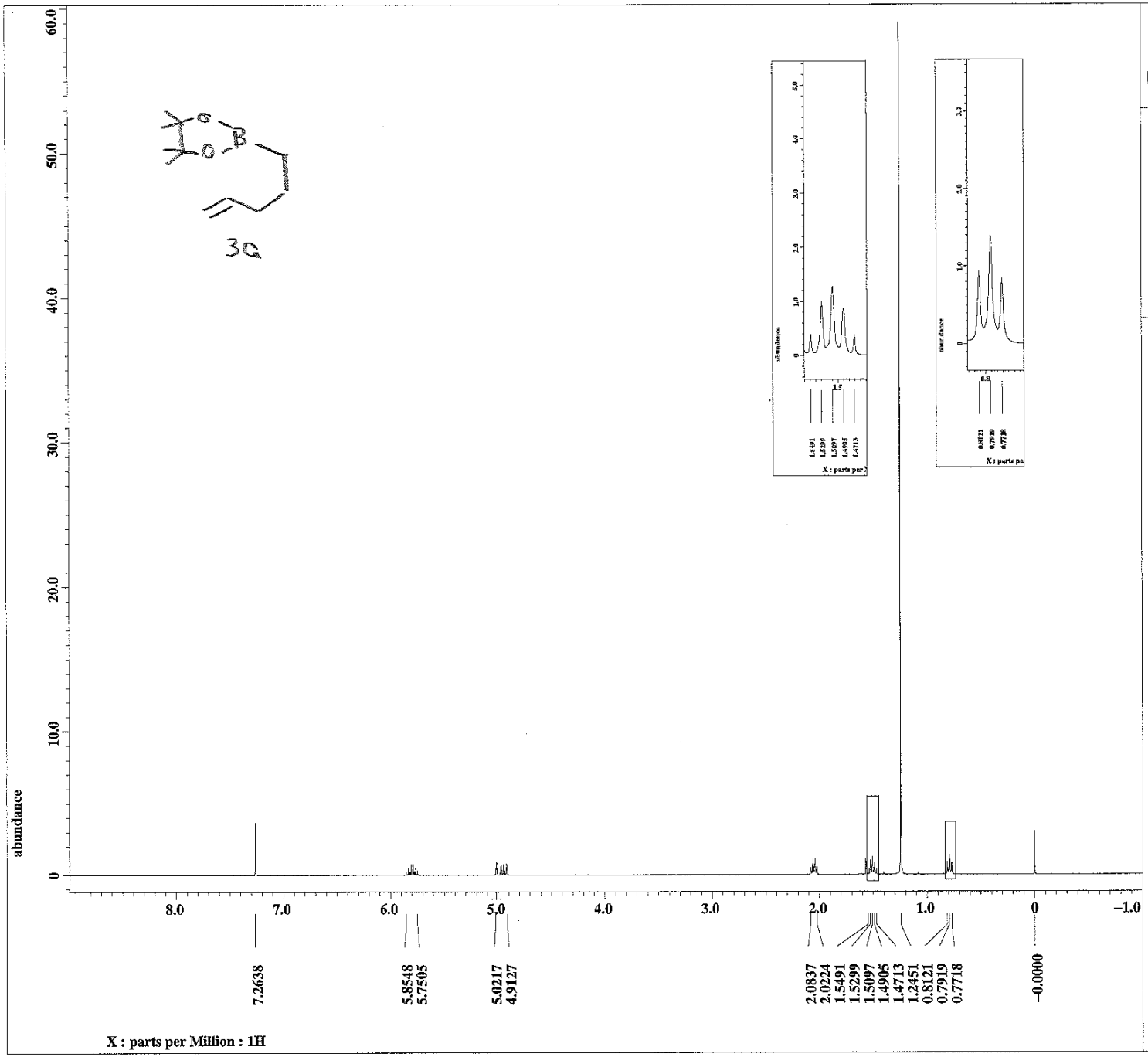
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

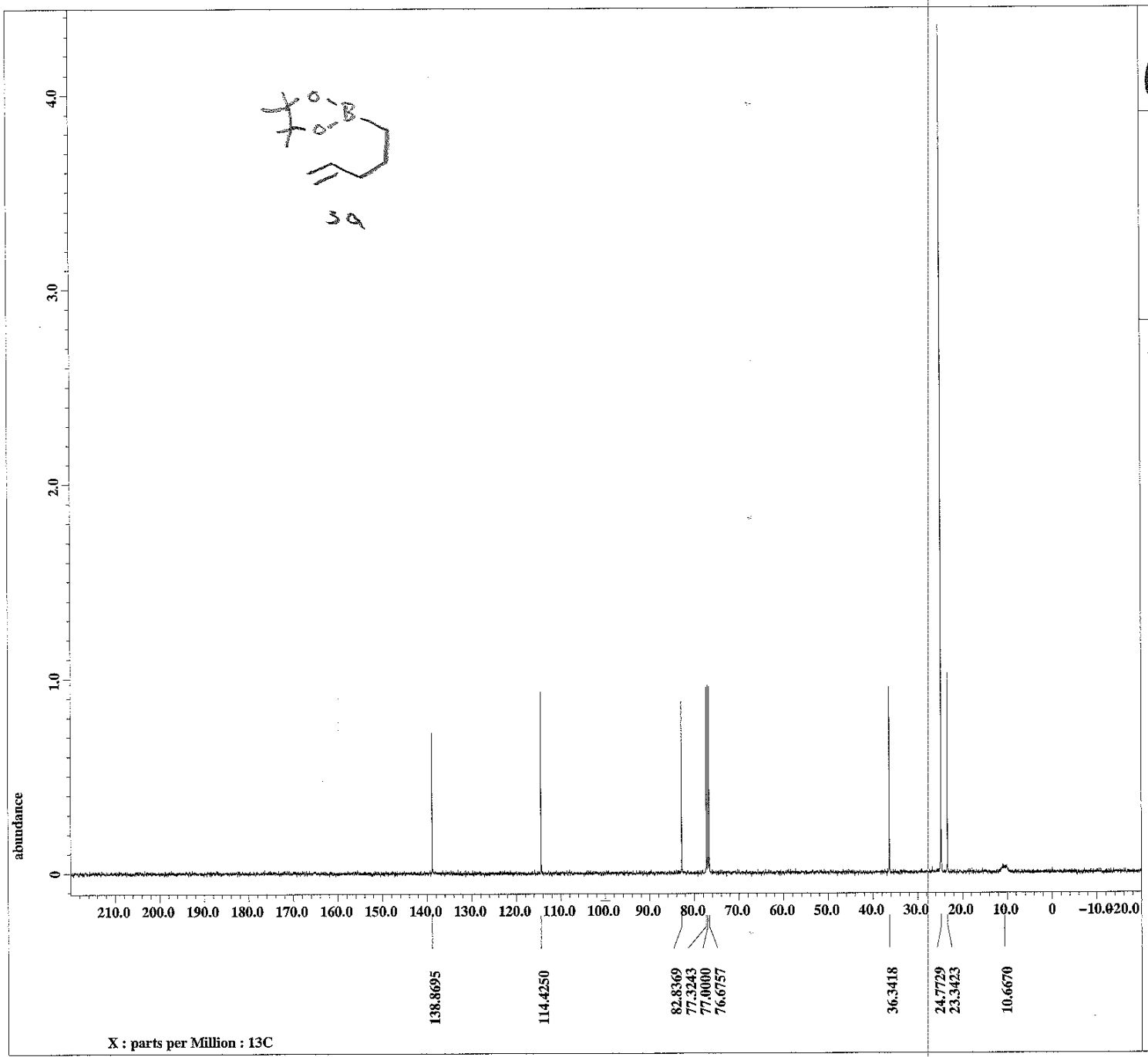
Derived from: IWA-575-carbon-1.jdf

Filename	= IWA-575-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#29256
Solvent	= CHLOROFORM-D
Creation_time	= 13-MAR-2015 00:30:58
Revision_time	= 13-MAR-2015 00:53:16
Current_time	= 13-MAR-2015 00:54:32
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 1.06430464[s]
X_domain	= 13C
X_freq	= 98.51479726[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.93958061[Hz]
X_sweep	= 30.78817734[kHz]
Irr_domain	= 1H
Irr_freq	= 391.78655441[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 60
Total_scans	= 60
X_90_width	= 8.8[us]
X_acq_time	= 1.06430464[s]
X_angle	= 30[deg]
X_atn	= 4.9[dB]
X_pulse	= 2.93333333[us]
Irr_atn_dec	= 22.52628[dB]
Irr_atn_noe	= 22.52628[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 3.06430464[s]
Temp_get	= 20.5[dC]




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: IWA-540-pure1-1.jdf
```

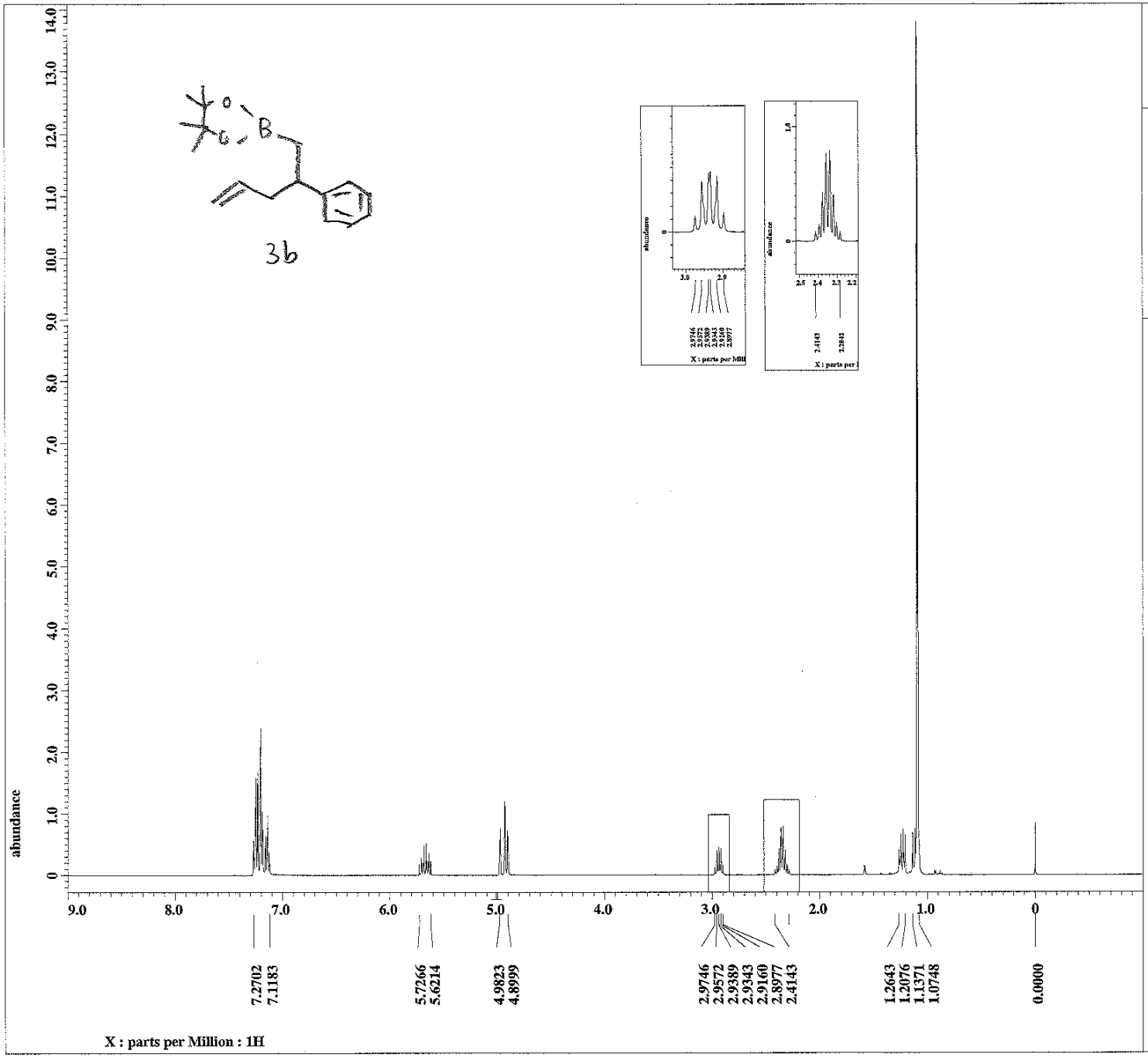
Filename	= IWA-540-pure1-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#432293
Solvent	= CHLOROFORM-D
Creation_time	= 11-MAR-2015 11:41:12
Revision_time	= 11-MAR-2015 12:11:47
Current_time	= 11-MAR-2015 12:11:50
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 16384
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.78790144[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.35869274[Hz]
X_sweep	= 5.87682181[kHz]
Irr_domain	= 1H
Irr_freq	= 391.78655441[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 391.78655441[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 10.7[us]
X_acq_time	= 2.78790144[s]
X_angle	= 45[deg]
X_atn	= 1.9[dB]
X_pulse	= 5.35[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 46
Relaxation_delay	= 4[s]
Repetition_time	= 6.78790144[s]
Temp_get	= 20.7[dC]



JEOL

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: IWA-540-carbon-1.jdf
```

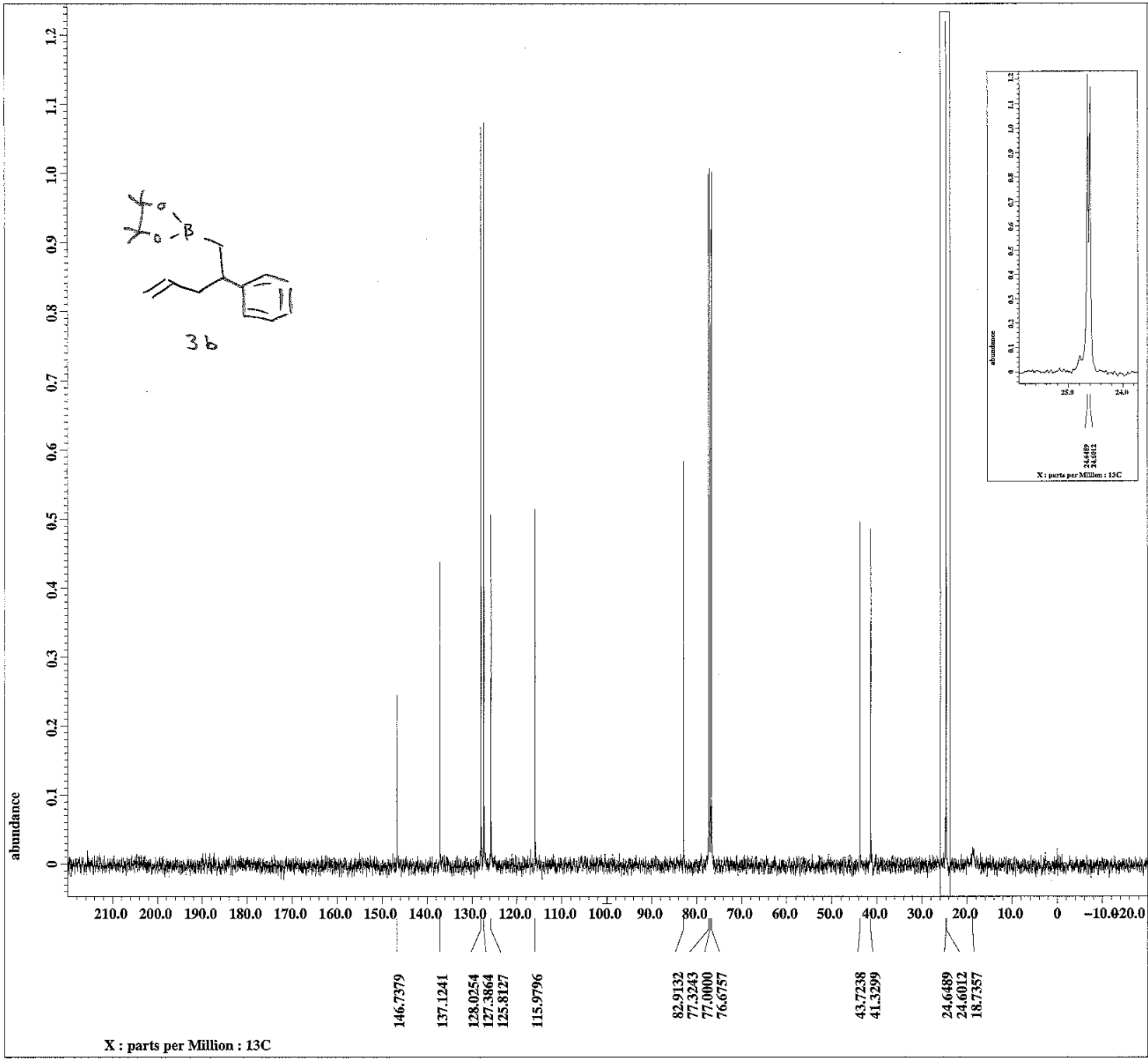
Filename	= IWA-540-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#436893
Solvent	= CHLOROFORM-D
Creation_time	= 11-MAR-2015 11:54:43
Revision_time	= 11-MAR-2015 12:16:58
Current_time	= 11-MAR-2015 12:19:34
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 1.06430464[s]
X_domain	= 13C
X_freq	= 98.51479726[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.93958061[Hz]
X_sweep	= 30.78817734[kHz]
Irr_domain	= 1H
Irr_freq	= 391.78655441[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 141
Total_scans	= 141
X_90_width	= 8.8[us]
X_acq_time	= 1.06430464[s]
X_angle	= 30[deg]
X_atn	= 4.9[dB]
X_pulse	= 2.93333333[us]
Irr_atn_dec	= 22.52628[dB]
Irr_atn_noe	= 22.52628[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 3.06430464[s]
Temp_get	= 20.9[dC]



JEOL

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: IWA-525-pure-1.jdf
```

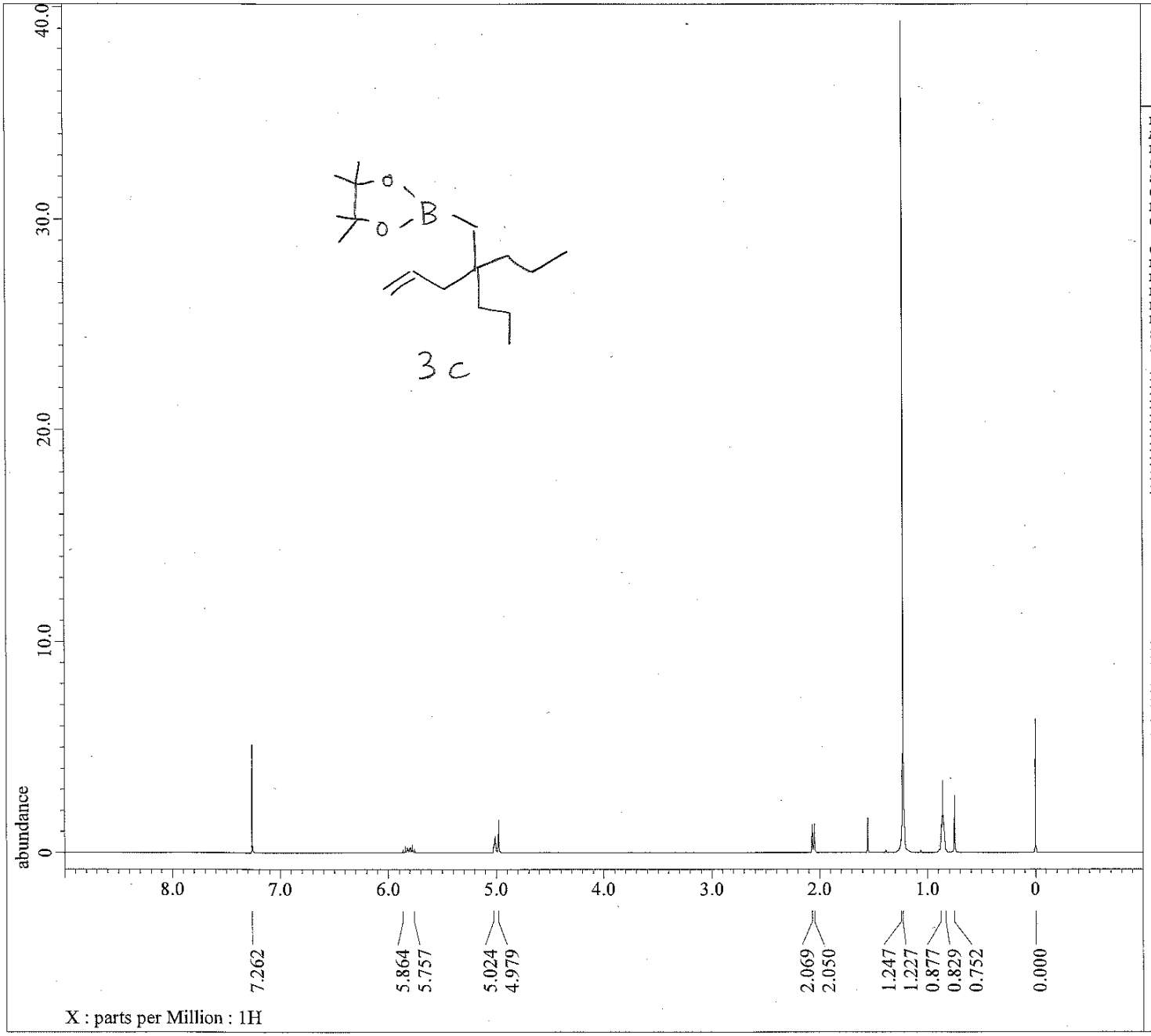
Filename	= IWA-525-pure-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#820667
Solvent	= CHLOROFORM-D
Creation_time	= 5-FEB-2015 22:18:05
Revision_time	= 15-MAR-2015 21:20:05
Current_time	= 15-MAR-2015 21:20:18
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 16384
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.78790144[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.35869274[Hz]
X_sweep	= 5.87682181[kHz]
Irr_domain	= 1H
Irr_freq	= 391.78655441[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 391.78655441[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 10.7[us]
X_acq_time	= 2.78790144[s]
X_angle	= 45[deg]
X_atn	= 1.9[dB]
X_pulse	= 5.35[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 4[s]
Repetition_time	= 6.78790144[s]
Temp_get	= 19.3[dC]



JEOL

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: IWA-525-carbon-1.jdf
```

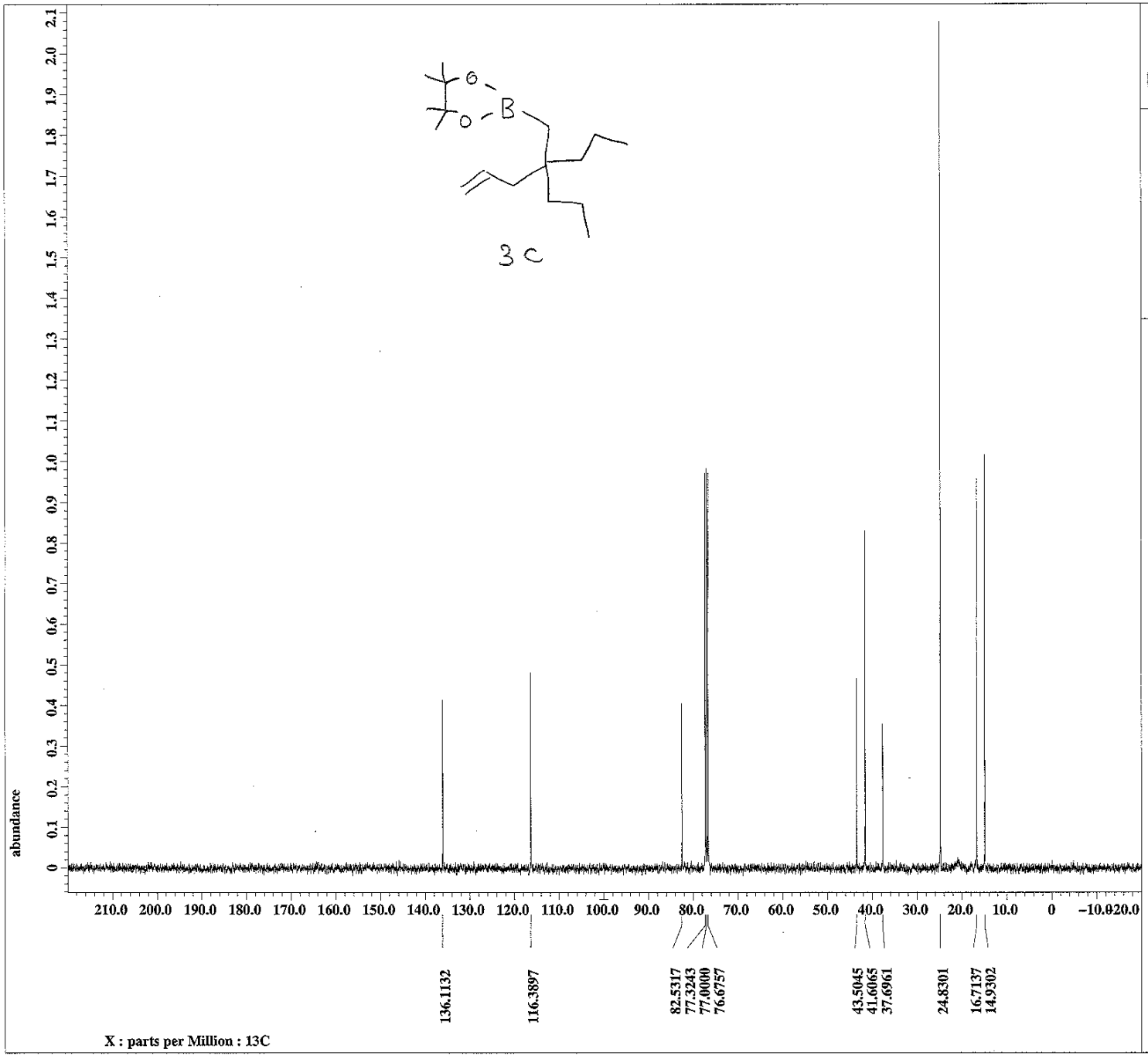
Filename	= IWA-525-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#524989
Solvent	= CHLOROFORM-D
Creation_time	= 14-MAR-2015 14:20:42
Revision_time	= 14-MAR-2015 14:44:25
Current_time	= 14-MAR-2015 14:45:58
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 1.06430464[s]
X_domain	= 13C
X_freq	= 98.51479726[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.93958061[Hz]
X_sweep	= 30.78817734[kHz]
Irr_domain	= 1H
Irr_freq	= 391.78655441[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 133
Total_scans	= 133
X_90_width	= 8.8[us]
X_acq_time	= 1.06430464[s]
X_angle	= 30[deg]
X_atn	= 4.9[dB]
X_pulse	= 2.93333333[us]
Irr_atn_dec	= 22.52628[dB]
Irr_atn_noe	= 22.52628[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 3.06430464[s]
Temp_get	= 20.6[dC]



3c

JEOL RESONANCE

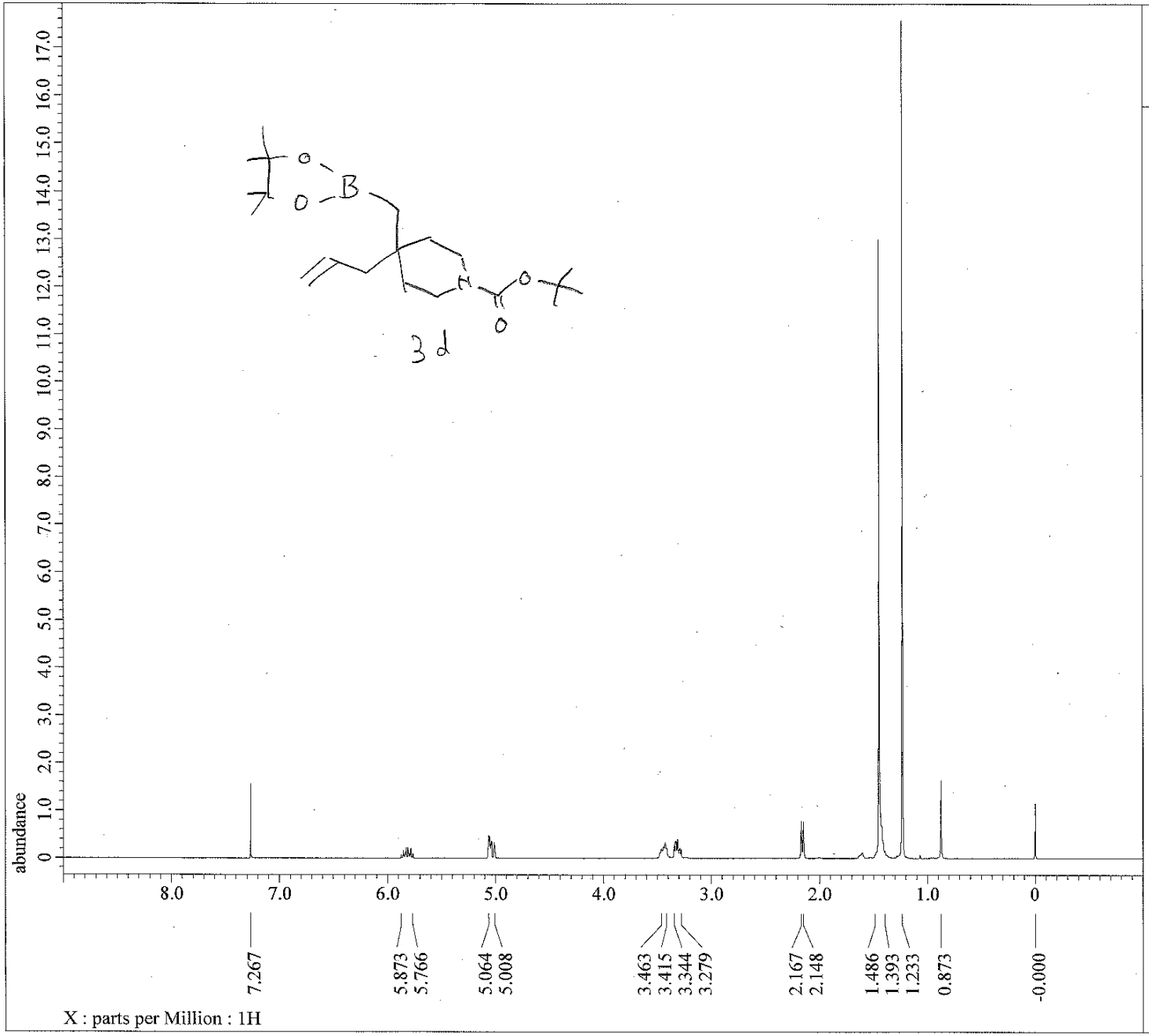
Filename	= IWA-572-pure1-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#350181
Solvent	= CHLOROFORM-D
Creation_Time	= 3-MAR-2015 09:26:36
Revision_Time	= 17-MAR-2015 04:41:06
Current_Time	= 17-MAR-2015 04:41:19
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 16384
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.78790144[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.35869274[Hz]
X_Sweep	= 5.87682181[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 20
Total_Scans	= 20
Relaxation_Delay	= 4[s]
Recvr_Gain	= 50
Temp_Get	= 20.5[dC]
X_90_Width	= 10.7[us]
X_Acq_Time	= 2.78790144[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 6.78790144[s]



---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

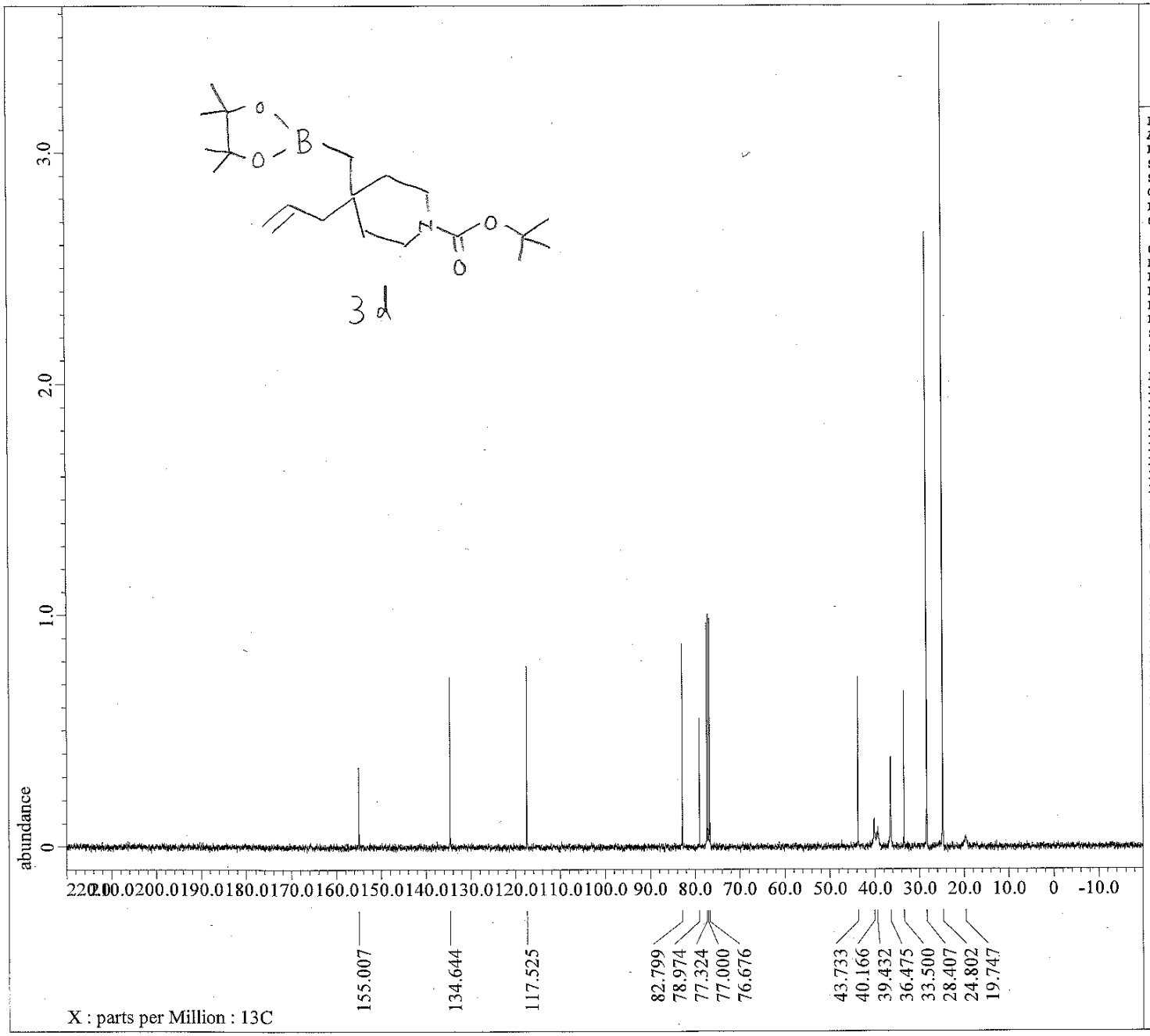
Derived from: IWA-572-carbon-1.jdf

Filename	= IWA-572-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#354959
Solvent	= CHLOROFORM-D
Creation_time	= 3-MAR-2015 09:38:51
Revision_time	= 3-MAR-2015 10:02:05
Current_time	= 3-MAR-2015 10:02:15
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 1.06430464[s]
X_domain	= 13C
X_freq	= 98.51479726[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.93958061[Hz]
X_sweep	= 30.78817734[kHz]
Irr_domain	= 1H
Irr_freq	= 391.78655441[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 133
Total_scans	= 133
X_90_width	= 8.8[us]
X_acq_time	= 1.06430464[s]
X_angle	= 30[deg]
X_atn	= 4.9[dB]
X_pulse	= 2.93333333[us]
Irr_atn_dec	= 22.52628[dB]
Irr_atn_noe	= 22.52628[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 3.06430464[s]
Temp_get	= 20.8[dC]



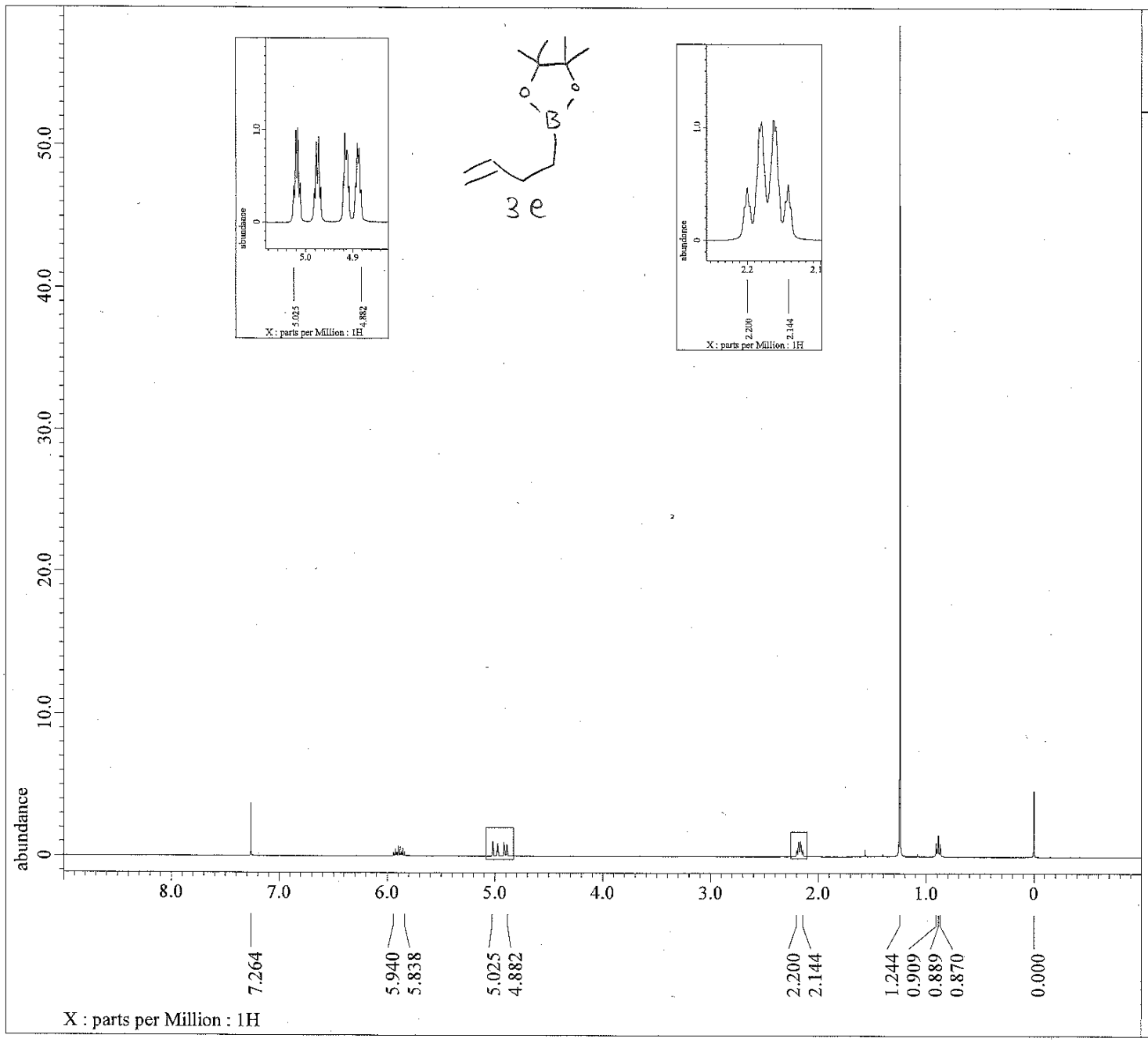
JEOL RESONANCE

Filename	= IWA-574-pure1-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#555195
Solvent	= CHLOROFORM-D
Creation_Time	= 3-MAR-2015 15:08:15
Revision_Time	= 17-MAR-2015 03:42:47
Current_Time	= 17-MAR-2015 03:43:06
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 16384
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.78790144[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.35869274[Hz]
X_Sweep	= 5.87682181[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 4[s]
Recvr_Gain	= 40
Temp_Get	= 20.9[dC]
X_90_Width	= 10.7[us]
X_Acq_Time	= 2.78790144[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 6.78790144[s]



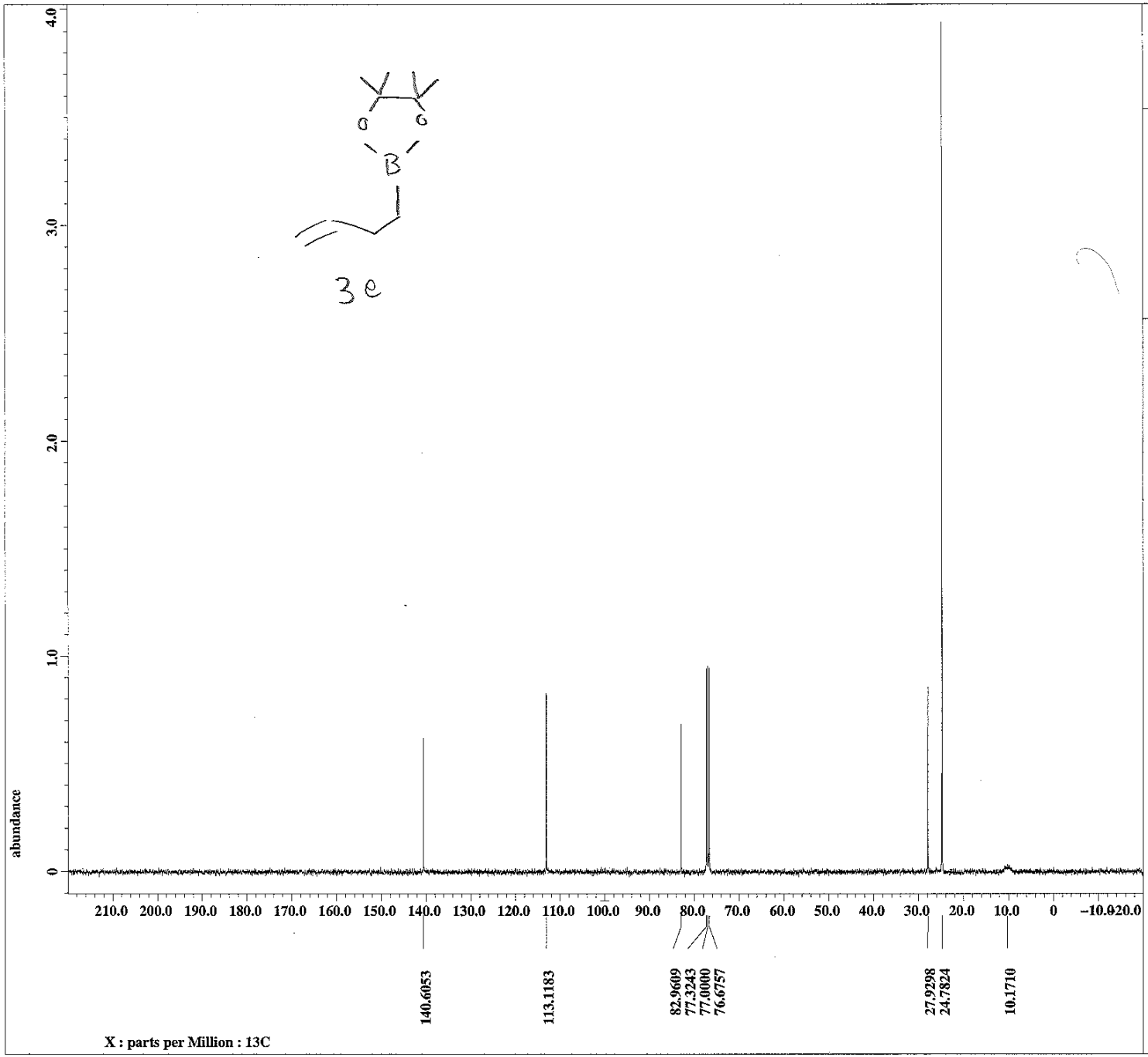
JEOL RESONANCE

Filename	= IWA-574-carbon-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#559960
Solvent	= CHLOROFORM-D
Creation_Time	= 3-MAR-2015 15:18:15
Revision_Time	= 17-MAR-2015 03:21:10
Current_Time	= 17-MAR-2015 03:22:47
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 89
Total_Scans	= 89
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.1[dC]
X_90_Width	= 8.8[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 2.93333333[us]
Irr_Atn_Dec	= 22.52628[dB]
Irr_Atn_Noe	= 22.52628[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



JEOL RESONANCE

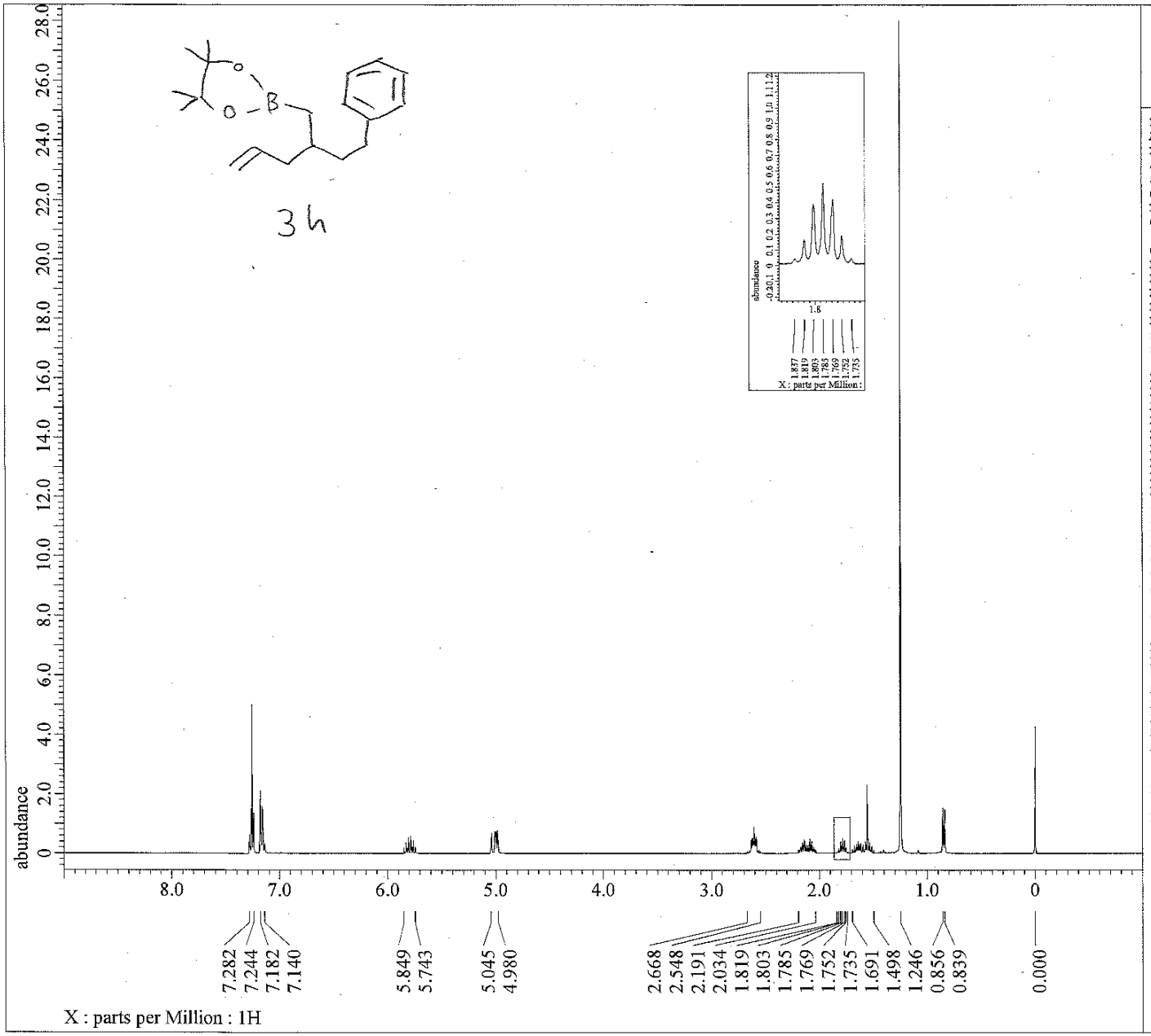
Filename	= IWA-554-pure1-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#3370
Solvent	= CHLOROFORM-D
Creation_Time	= 12-MAR-2015 23:46:08
Revision_Time	= 22-MAR-2015 17:11:51
Current_Time	= 22-MAR-2015 17:11:56
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 16384
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.78790144[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.35869274[Hz]
X_Sweep	= 5.87682181[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 46
Temp_Get	= 20.3[dC]
X_90_Width	= 10.7[us]
X_Acq_Time	= 2.78790144[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 6.78790144[s]



JEOL

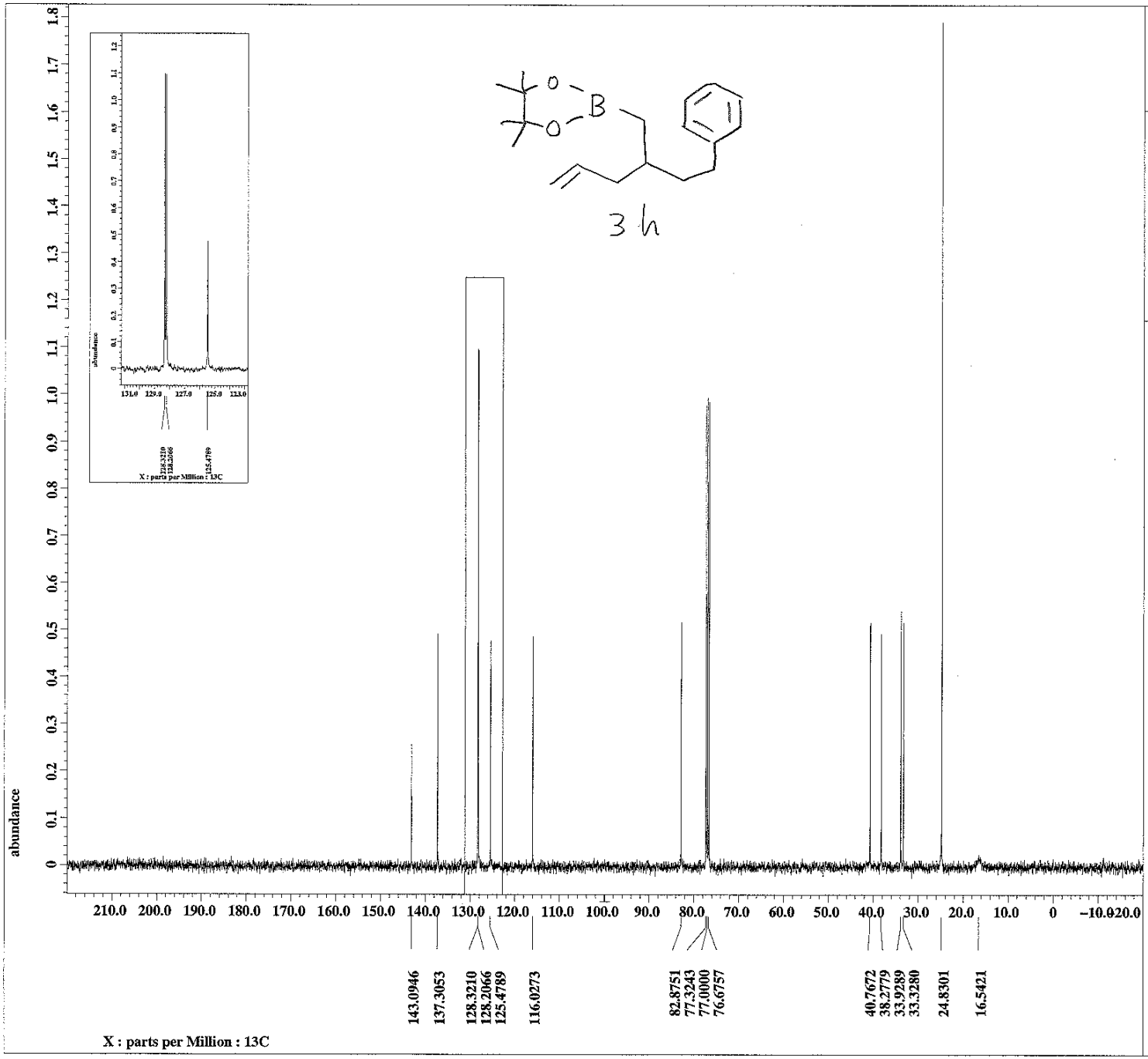
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: IWA-554-carbon-1.jdf
```

Filename	= IWA-554-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#7365
Solvent	= CHLOROFORM-D
Creation_time	= 12-MAR-2015 23:56:45
Revision_time	= 13-MAR-2015 00:19:14
Current_time	= 13-MAR-2015 00:22:19
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 1.06430464[s]
X_domain	= 13C
X_freq	= 98.51479726[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.93958061[Hz]
X_sweep	= 30.78817734[kHz]
Irr_domain	= 1H
Irr_freq	= 391.78655441[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 104
Total_scans	= 104
X_90_width	= 8.8[us]
X_acq_time	= 1.06430464[s]
X_angle	= 30[deg]
X_atn	= 4.9[dB]
X_pulse	= 2.93333333[us]
Irr_atn_dec	= 22.52628[dB]
Irr_atn_noe	= 22.52628[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 3.06430464[s]
Temp_get	= 20.5[dC]



JEOL RESONANCE

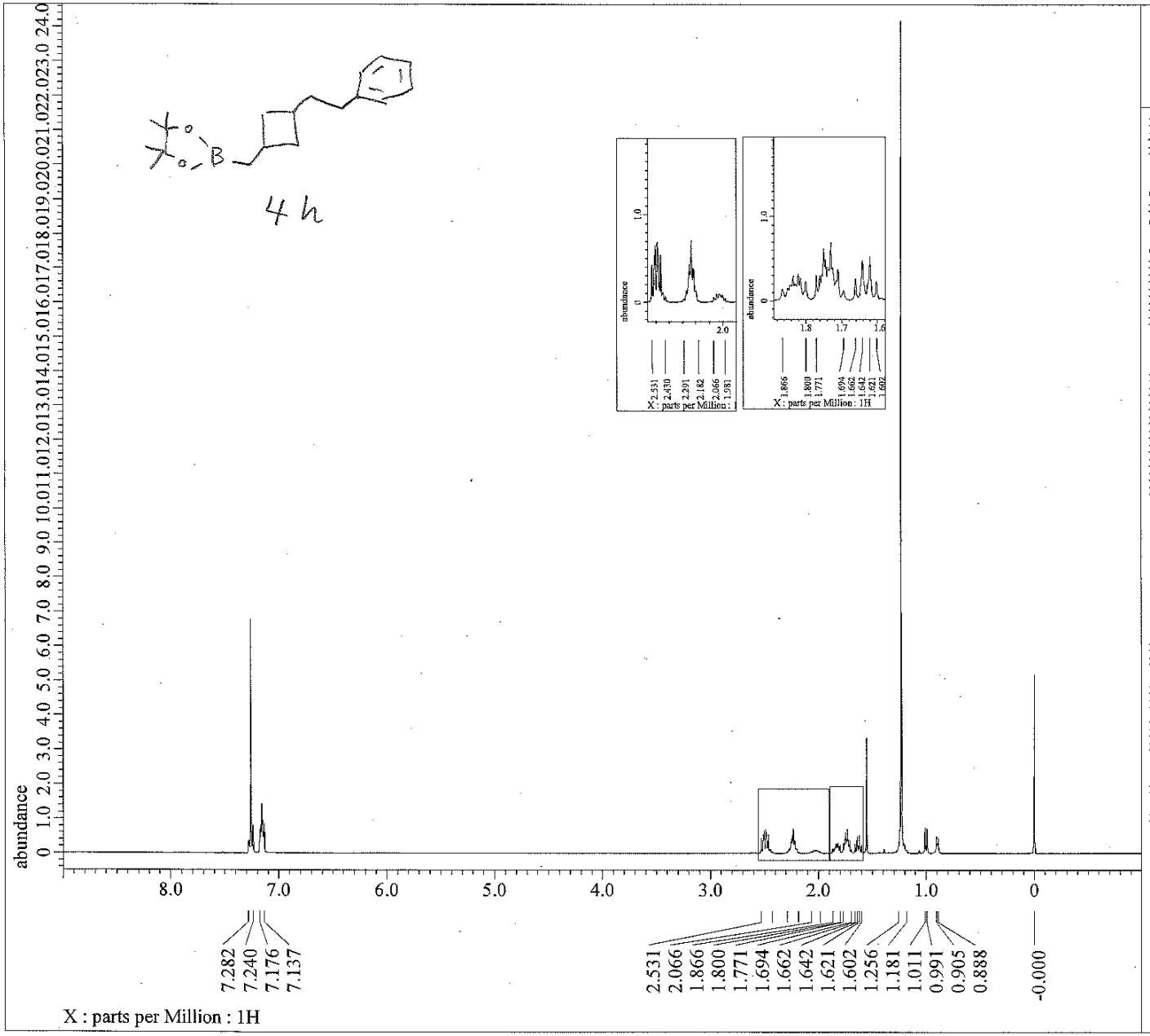
Filename	= IWA-580-pure1-14.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#755571
Solvent	= CHLOROFORM-D
Creation_Time	= 5-MAR-2015 20:40:49
Revision_Time	= 22-MAR-2015 18:19:59
Current_Time	= 22-MAR-2015 18:20:05
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 16384
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.78790144[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.35869274[Hz]
X_Sweep	= 5.87682181[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 48
Temp_Get	= 20.6[dC]
X_90_Width	= 10.7[us]
X_Acq_Time	= 2.78790144[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 6.78790144[s]



JEOL

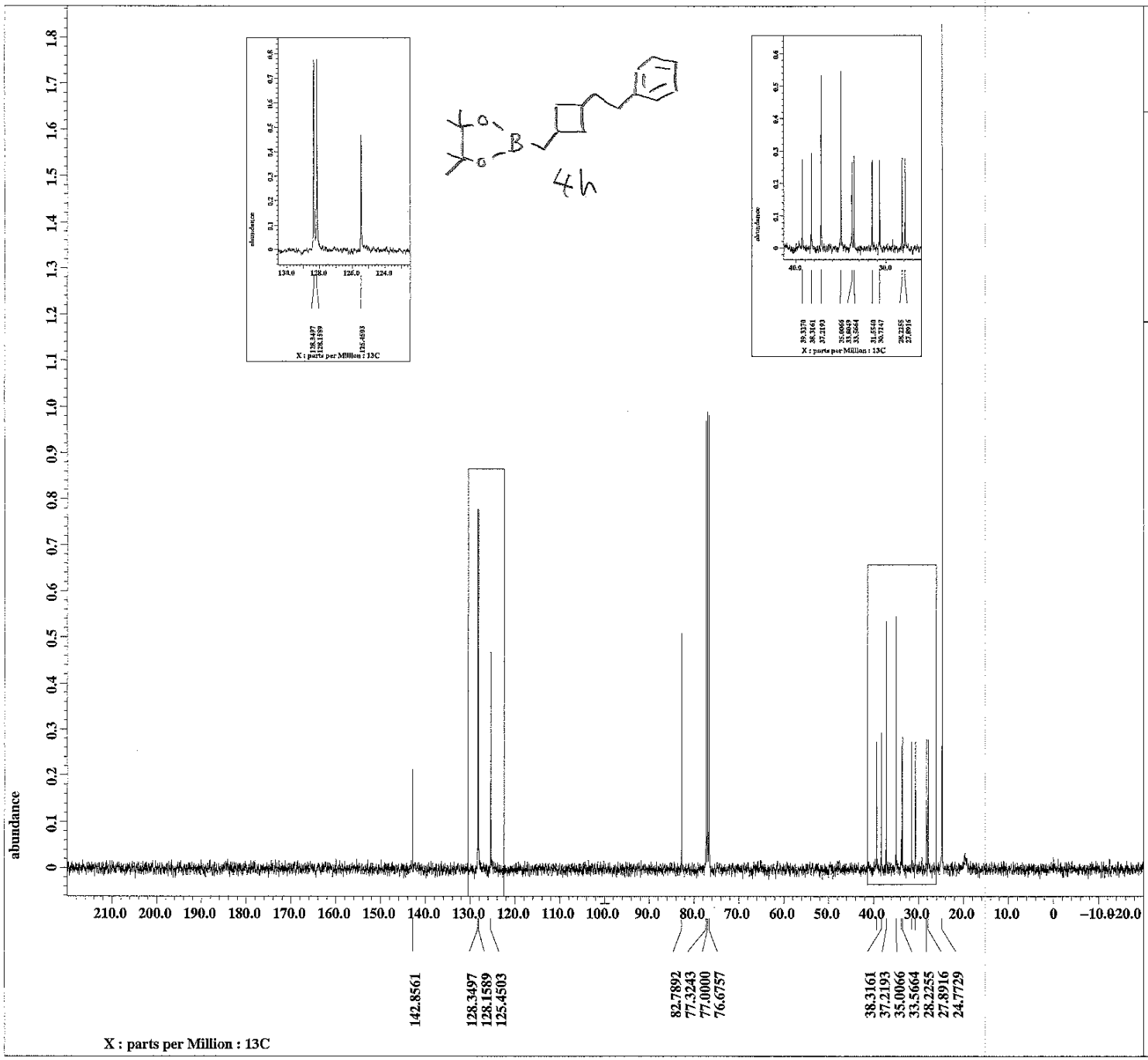
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: IWA-580-carbon-1.jdf
```

Filename	= IWA-580-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#759662
Solvent	= CHLOROFORM-D
Creation_time	= 5-MAR-2015 20:53:14
Revision_time	= 5-MAR-2015 21:28:09
Current_time	= 5-MAR-2015 21:30:49
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 1.06430464[s]
X_domain	= 13C
X_freq	= 98.51479726[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.93958061[Hz]
X_sweep	= 30.78817734[kHz]
Irr_domain	= 1H
Irr_freq	= 391.78655441[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 137
Total_scans	= 137
X_90_width	= 8.8[us]
X_acq_time	= 1.06430464[s]
X_angle	= 30[deg]
X_atn	= 4.9[dB]
X_pulse	= 2.93333333[us]
Irr_atn_dec	= 22.52628[dB]
Irr_atn_noe	= 22.52628[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 3.06430464[s]
Temp_get	= 20.9[dC]



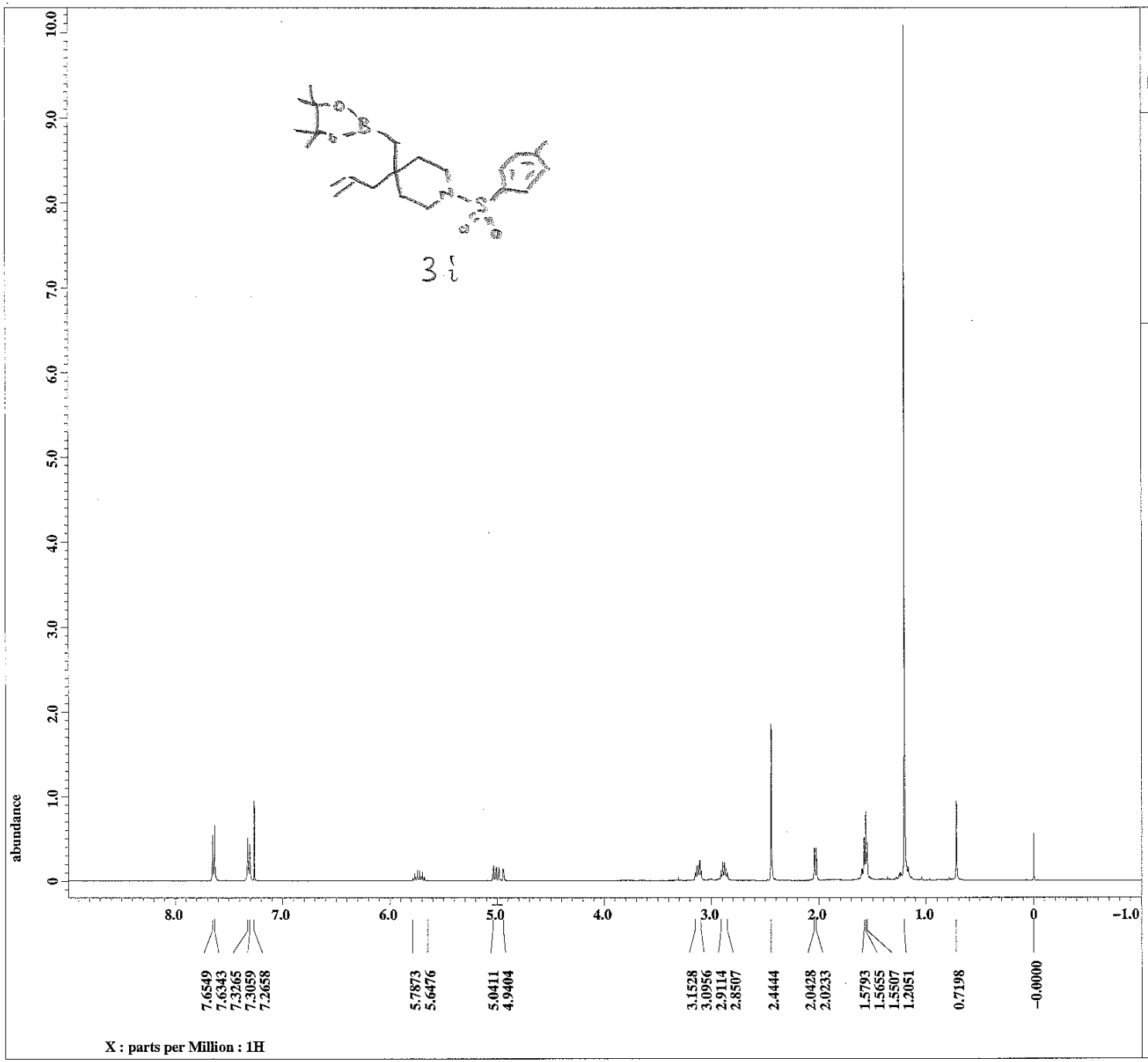
JEOL RESONANCE

Filename	= IWA-577-pure1-7.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#600371
Solvent	= CHLOROFORM-D
Creation_Time	= 7-MAR-2015 16:22:27
Revision_Time	= 22-MAR-2015 20:17:59
Current_Time	= 22-MAR-2015 20:20:45
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 16384
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.78790144[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.35869274[Hz]
X_Sweep	= 5.87682181[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 13
Total_Scans	= 13
Relaxation_Delay	= 4[s]
Recvr_Gain	= 52
Temp_Get	= 20.8[dC]
X_90_Width	= 10.7[us]
X_Acq_Time	= 2.78790144[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 6.78790144[s]



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: IWA-577-carbon-1.jdf
```

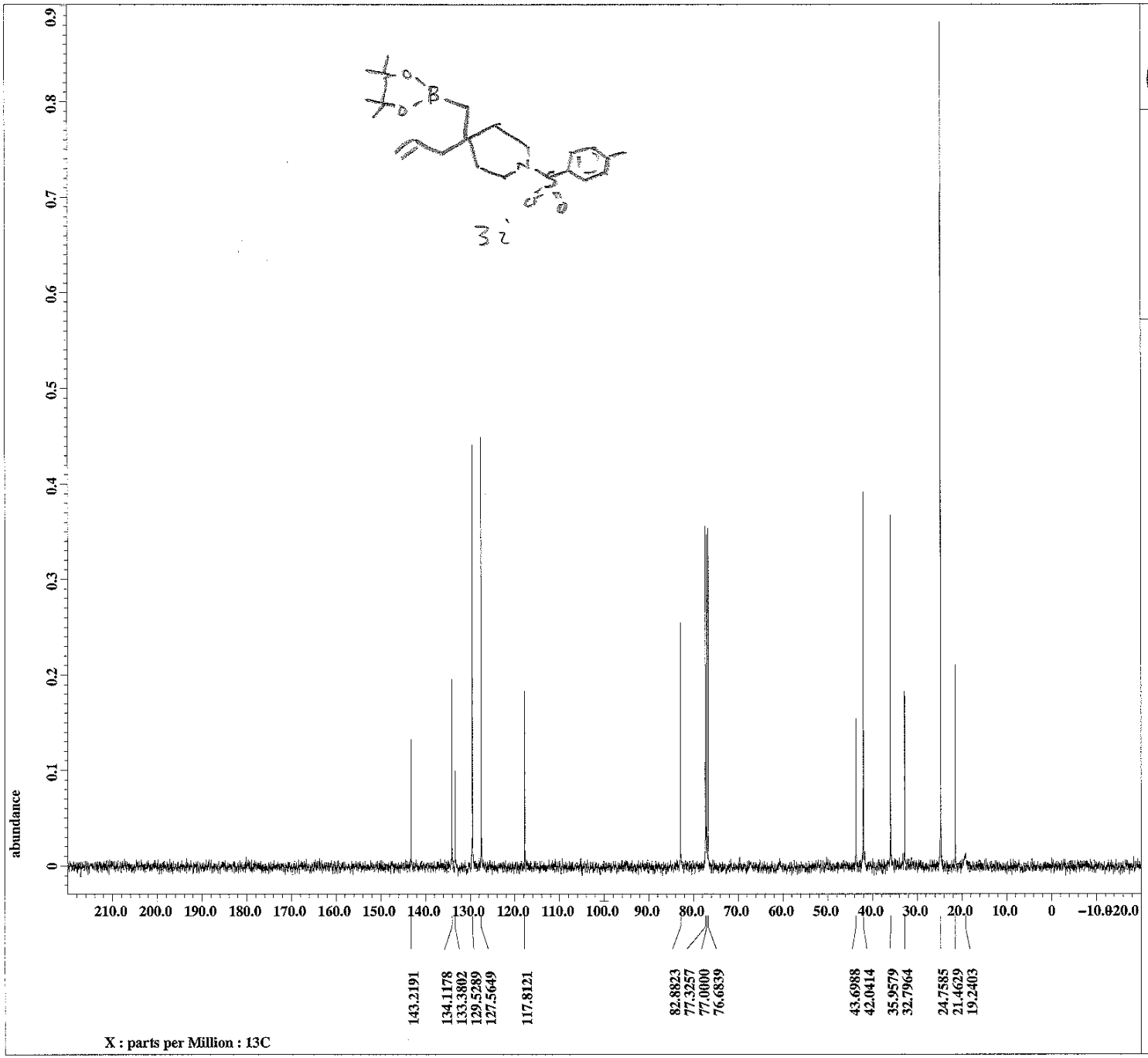
Filename	= IWA-577-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#604558
Solvent	= CHLOROFORM-D
Creation_time	= 7-MAR-2015 16:32:35
Revision_time	= 7-MAR-2015 16:55:55
Current_time	= 7-MAR-2015 16:57:13
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 1.06430464[s]
X_domain	= 13C
X_freq	= 98.51479726[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.93958061[Hz]
X_sweep	= 30.78817734[kHz]
Irr_domain	= 1H
Irr_freq	= 391.78655441[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 100
Total_scans	= 100
X_90_width	= 8.8[us]
X_acq_time	= 1.06430464[s]
X_angle	= 30[deg]
X_atn	= 4.9[dB]
X_pulse	= 2.93333333[us]
Irr_atn_dec	= 22.52628[dB]
Irr_atn_noe	= 22.52628[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 3.06430464[s]
Temp_get	= 21[dC]



---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: IWA-570-pure1-1.jdf

Filename	= IWA-570-pure1-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#596710
Solvent	= CHLOROFORM-D
Creation_time	= 11-MAR-2015 16:34:27
Revision_time	= 11-MAR-2015 16:48:56
Current_time	= 11-MAR-2015 16:48:59
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.20725248[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 12.6[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1[dB]
X_pulse	= 6.3[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 22.3[dC]



JEOL

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: IWA-570-carbon-1.jdf
```

Filename	= IWA-570-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#600739
Solvent	= CHLOROFORM-D
Creation_time	= 11-MAR-2015 16:45:16
Revision_time	= 11-MAR-2015 16:50:53
Current_time	= 11-MAR-2015 16:51:03
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 1.048576[s]
X_domain	= 13C
X_freq	= 99.54517646[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.95367432[Hz]
X_sweep	= 31.25[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 100
Total_scans	= 100
X_90_width	= 9.3[us]
X_acq_time	= 1.048576[s]
X_angle	= 30[deg]
X_atn	= 3.4[dB]
X_pulse	= 3.1[us]
Irr_atn_dec	= 20.20655[dB]
Irr_atn_noe	= 20.20655[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 50
Relaxation_delay	= 2[s]
Repetition_time	= 3.048576[s]
Temp_get	= 22.6[dC]