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Highly Selective Markovnikov Hydroboration of Alkyl-Substituted Terminal Alkenes with a Phosphine-Copper(I) Catalyst

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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, ^{13}C: 100 MHz and ^{11}B: 127 MHz). Tetramethylsilane (^{1}H), $CDCl_3$ (^{13}C) and $BF_3{\cdot}OEt_2$ (^{11}B) were employed as the external standards, respectively. Infrared (IR) spectra were recorded on a JASCO FT/IR-4600 spectrometer. 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 Global Facility Center, Hokkaido University.

2. General Experimental Procedure.

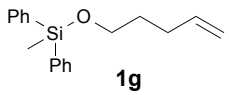
Procedure for the Copper(I)-Catalyzed Chemoselective Borylation of 1a (Table 1).

Copper chloride (2.5 mg, 0.025 mmol) and bis(pinacolato)diboron (**2**) (152.4 mg, 0.60 mmol), **L2** (12.6 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. The reaction mixture was stirred at room temperature and cooled down to –10 ºC. After stirring for 15 min, **1a** (74.5. mg, 0.50 mmol) and methanol were added dropwise to the mixture. 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, CH_2Cl_2/pentane, typically 0:100–40:60) to give the corresponding borylation product **3a** as a colorless oil.

3. Substrate Preparation

The substrates for asymmetric borylation **1a**–**1f** were purchased from commercial suppliers.

Methyl(pent-4-en-1-yloxy)diphenylsilane (1g).



1g

1g was prepared from 4-penten-1-ol according to the standard silylation procedure.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.64 (s, 3H), 1.67 (dt, *J* = 7.1, 14.4 Hz, 2H), 2.12 (q, *J* = 7.0 Hz, 2H), 3.71 (t, *J* = 6.5 Hz, 2H), 4.91–5.03 (m, 2H), 5.78 (ddt, *J* = 6.7, 10.3, 17.1 Hz, 1H), 7.35–7.43 (m, 6H), 7.59 (d, *J* = 7.2 Hz, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): –3.1 (*C*H_3), 30.0 (*C*H_2), 31.7 (*C*H_2), 62.8 (*C*H_2), 114.6 (*C*H_2), 127.8 (*C*H), 129.7 (*C*H), 134.3 (*C*H), 136.1 (*C*), 138.2 (*C*H). HRMS–EI (*m*/*z*): [M]+ calcd for $C_{18}H_{22}OSi$, 282.14399; found, 282.14461.

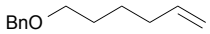
tert-Butyl(hex-5-en-1-yloxy)dimethylsilane (1h).[1]

1h

1h was prepared from 5-hexen-1-ol according to the standard silylation procedure.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.05 (s, 6H), 0.89 (s, 9H), 1.39–1.47 (m, 2H), 1.50–1.57 (m, 2H), 2.06 (q, *J* = 7.2 Hz, 2H), 3.61 (t, *J* = 6.5 Hz, 2H), 4.92–5.03 (m, 2H), 5.81 (ddt, *J* = 6.7, 10.3, 17.1 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): –5.3 (*C*H_3), 18.3 (*C*), 25.2 (*C*H_2), 25.9 (*C*H_3), 32.3 (*C*H_2), 33.6 (*C*H_2), 63.0 (*C*H_2), 114.4 (*C*H_2), 138.8 (*C*H). HRMS–EI (*m*/*z*): [M–CH_3]+ calcd for $C_{11}H_{23}OSi$, 199.15182; found, 199.15114.

[(Hex-5-en-1-yloxy)methyl]benzene (1i).[2]

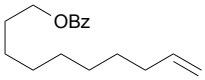


1i

1i was prepared from 5-hexen-1-ol according to the standard benzyl protection procedure.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.44–1.52 (m, 2H), 1.60–1.67 (m, 2H), 2.04–2.10 (m, 2H), 3.48 (t, *J* = 6.5 Hz, 2H), 4.50 (s, 2H), 4.93–5.03 (m, 2H), 5.81 (ddt, *J* = 6.7, 10.3, 17.1 Hz, 1H), 7.26–7.37 (m, 5H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 25.3 (*C*H_2), 29.1 (*C*H_2), 33.4 (*C*H_2), 70.0 (*C*H_2), 72.6 (*C*H_2), 114.4 (*C*H_2), 127.0 (*C*H), 127.3 (*C*H), 127.4 (*C*), 128.1 (*C*H), 138.5 (*C*H). HRMS–EI (*m*/*z*): [M]+ calcd for $C_{13}H_{18}O$, 190.13576; found, 190.13523.

Dec-9-en-1-yl benzoate (1j).[3]

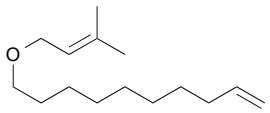


1j

1j was prepared from 9-decen-1-ol according to the standard benzoate protection procedure.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.31–1.48 (m, 10H), 1.76 (dt, *J* = 7.1 Hz, 14.4 Hz, 2H), 2.04 (q, *J* = 6.9 Hz, 2H), 4.32 (t, *J* = 6.7 Hz, 2H), 4.91–5.02 (m, 2H), 5.81 (ddt, *J* = 6.7, 10.2, 17.1 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.54–7.58 (m, 1H), 8.03–8.06 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 25.9 (*C*H_2), 28.6 (*C*H_2), 28.8 (*C*H_2), 28.9 (*C*H_2), 29.1 (*C*H_2), 29.3 (*C*H_2), 33.7 (*C*H_2), 65.0 (*C*H_2), 114.1 (*C*H_2), 128.2 (*C*H), 129.4 (*C*H), 130.4 (*C*), 132.7 (*C*H), 139.0 (*C*H), 166.5 (*C*). HRMS–EI (*m*/*z*): [M]+ calcd for $C_{17}H_{24}O_2$, 260.17763; found, 260.17723.

10-[(3-Methylbut-2-en-1-yl)oxy]dec-1-ene (1k).



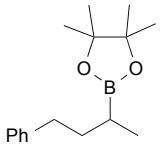
1k

1k was prepared from 9-decen-1-ol according to the standard etherification procedure.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.29–1.41 (m, 10H), 1.54–1.61 (m, 2H), 1.67 (s, 3H), 1.74 (s, 3H), 2.03 (q, *J* = 7.0 Hz, 2H), 3.40 (t, *J* = 6.9 Hz, 2H), 3.94 (d, *J* = 6.9 Hz, 2H), 4.91–5.02 (m, 2H), 5.33–5.38 (m, 1H), 5.81 (ddt, *J* = 6.9, 10.5, 17.1 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 17.9 (*C*H_3), 25.7 (*C*H_3), 26.1 (*C*H_2), 28.8 (*C*H_2), 29.0 (*C*H_2), 29.4 (*C*H_2), 29.7 (*C*H_2), 33.7 (*C*H_2), 67.1 (*C*H_2), 70.2 (*C*H_2), 114.0 (*C*H_2), 121.3 (*C*H), 136.4 (*C*), 139.0 (*C*H). HRMS–EI (*m*/*z*): [M]+ calcd for $C_{15}H_{28}O$, 224.21401; found, 224.21380.

4. Characterization of Borylation Products

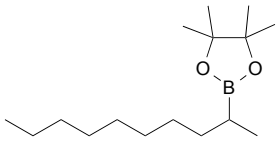
4,4,5,5-Tetramethyl-2-(4-phenylbutan-2-yl)-1,3,2-dioxaborolane (3a).[4]



3a

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.01–1.11 (m, 4H), 1.25 (s, 12H), 1.54–1.63 (m, 1H), 1.74–1.83 (m, 1H), 2.56–2.67 (m, 2H), 7.14–7.20 (m, 3H), 7.25–7.28 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 15.4 (*C*H_3), 16.8 (br, B–*C*H), 24.7 (*C*H_3), 24.8 (*C*H_3), 35.3 (*C*H_2), 82.9 (*C*), 125.5 (*C*H), 128.2 (*C*H), 128.4 (*C*H), 143.0 (*C*). ^{11}B NMR (127 MHz, $CDCl_3$, δ): 34.2. FT-IR (neat): ν_{max} = 2976, 1370, 1315, 1145, 699 cm^{-1}. HRMS–EI (*m*/*z*): [M]+ calcd for $C_{16}H_{25}BO_2$, 260.19476; found, 260.19437.

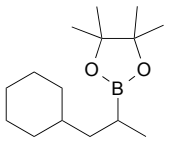
2-(Decan-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3b).



3b

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.88 (t, *J* = 6.7 Hz, 3H), 0.95–1.01 (m, 4H), 1.20–1.29 (m, 25H), 1.40–1.46 (m, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 15.5 (*C*H_3), 16.8 (br, B–*C*H), 22.7 (*C*H_2), 24.67 (*C*H_3), 24.71 (*C*H_3), 29.0 (*C*H_2), 29.3 (*C*H_2), 29.6 (*C*H_2), 29.8 (*C*H_2), 31.9 (*C*H_2), 33.2 (*C*H_2), 82.7 (*C*). ^{11}B NMR (127 MHz, $CDCl_3$, δ): 34.3. FT-IR (neat): ν_{max} = 2923, 1370, 1312, 1144, 860 cm^{-1}. HRMS–EI (*m*/*z*): [M]+ calcd for $C_{16}H_{33}BO_2$, 268.25736; found, 268.25827.

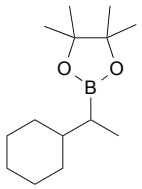
2-(1-Cyclohexylpropan-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3c).



3c

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.74–0.89 (m, 2H), 0.93 (d, *J* = 7.3 Hz, 3H), 1.06–1.40 (m, 20H), 1.60–1.70 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (br, B–*C*H), 15.7 (*C*H_3), 24.7 (*C*H_3), 26.4 (*C*H_2), 26.5 (*C*H_2), 26.7 (*C*H_2), 33.1 (*C*H_2), 33.6 (*C*H_2), 36.5 (*C*H), 40.8 (*C*H_2), 82.7 (*C*). ^{11}B NMR (127 MHz, $CDCl_3$, δ): 34.3. FT-IR (neat): ν_{max} = 2920, 1369, 1312, 1144, 861 cm^{-1}. HRMS–EI (*m*/*z*): [M]+ calcd for, $C_{15}H_{29}BO_2$, 252.22606; found, 252.22711.

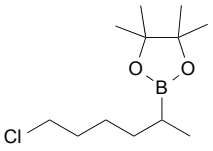
2-(1-Cyclohexylethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3d).[5]



3d

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.86–1.40 (m, 22H), 1.62–1.75 (m, 5H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 12.5 (*C*H_3), 24.7 (*C*H_3), 24.8 (*C*H_3), 26.69 (*C*H_2), 26.75 (*C*H_2), 31.8 (*C*H_2), 32.7 (*C*H_2), 40.4 (*C*H), 82.7 (*C*). The carbon directly attached to the boron atom was not detected, likely due to quadropolar relaxation. ^{11}B NMR (127 MHz, $CDCl_3$, δ): 34.1. FT-IR (neat): ν_{max} = 2921, 1358, 1310, 1143, 863 cm^{-1}. HRMS–EI (*m*/*z*): [M]+ calcd for, $C_{14}H_{27}BO_2$, 238.21041; found, 238.21127.

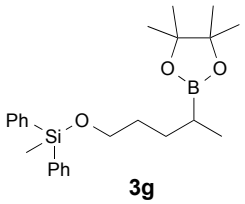
2-(6-Chlorohexan-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3f).[5]



3f

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.96–1.08 (m, 4H), 1.24–1.35 (m, 13H), 1.38–1.50 (m, 3H), 1.76 (dt, *J* = 7.1 Hz, 14.1 Hz, 2H), 3.53 (t, *J* = 6.7 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 15.4 (*C*H_3), 16.9 (br, B–*C*H), 24.67 (*C*H_3), 24.72 (*C*H_3), 26.2 (*C*H_2), 32.3 (*C*H_2), 32.8 (*C*H_2), 45.1 (*C*H_2), 82.8 (*C*). ^{11}B NMR (127 MHz, $CDCl_3$, δ): 34.2. FT-IR (neat): ν_{max} = 2931, 1370, 1313, 1143, 857 cm^{-1}. HRMS–EI (*m*/*z*): [M]+ calcd for $C_{12}H_{24}BClO_2$, 246.15579; found, 246.15550.

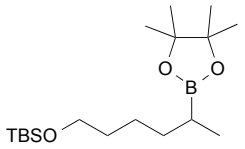
Methyldiphenyl{[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentyl]oxy}silane (3g).



3g

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.63 (s, 3H), 0.93–1.01 (m, 4H), 1.22–1.50 (m, 14H), 1.55–1.64 (m, 2H), 3.68 (t, *J* = 7.0 Hz, 2H), 7.34–7.43 (m, 6H), 7.58–7.60 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): –3.0 (*C*H_3), 15.5 (*C*H_3), 16.7 (br, B–*C*H), 24.6 (*C*H_3), 24.7 (*C*H_3), 29.2 (*C*H_2), 31.9 (*C*H_2), 63.8 (*C*H_2), 82.7 (*C*), 127.7 (*C*H), 129.6 (*C*H), 134.3 (*C*H), 136.2 (*C*). ^{11}B NMR (127 MHz, $CDCl_3$, δ): 34.1. FT-IR (neat): ν_{max} = 2928, 1315, 1145, 1118, 736 cm^{-1}. HRMS–EI (*m*/*z*): [M]+ calcd for, $C_{24}H_{35}BO_3Si$, 410.24485; found, 410.24413.

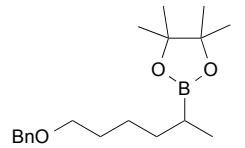
***tert*-Butyldimethyl{[5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexyl]oxy}silane (3h).**



3h

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.04 (s, 6H), 0.89 (s, 9H), 0.95–1.07 (m, 4H), 1.23–1.54 (m, 18H), 3.59 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): –5.3 (*C*H_3), 15.5 (*C*H_3), 16.9 (br, B–*C*H), 18.3 (*C*), 24.68 (*C*H_3), 24.72 (*C*H_3), 25.2 (*C*H_2), 26.0 (*C*H_3), 33.0 (*C*H_2), 33.1 (*C*H_2), 63.3 (*C*H_2), 82.7 (*C*). ^{11}B NMR (127 MHz, $CDCl_3$, δ): 34.2. FT-IR (neat): ν_{max} = 2929, 1313, 1145, 1097, 834 cm^{-1}. HRMS–EI (*m*/*z*): [M–CH_3]+ calcd for $C_{17}H_{36}BO_3Si$, 327.25268; found, 327.25236.

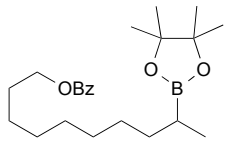
2-[6-(Benzyloxy)hexan-2-yl]-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3i).



3i

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.94–1.07 (m, 4H), 1.23–1.51 (m, 16H), 1.57–1.65 (m, 2H), 3.46 (t, *J* = 6.7 Hz, 2H), 4.50 (s, 2H), 7.25–7.34 (m, 5H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 15.4 (*C*H_3), 16.9 (br, B–*C*H), 24.61 (*C*H_3), 24.65 (*C*H_3), 25.4 (*C*H_2), 29.9 (*C*H_2), 32.9 (*C*H_2), 70.4 (*C*H_2), 72.7 (*C*H_2), 82.7 (*C*), 127.3 (*C*H), 127.4 (*C*H), 128.2 (*C*H), 138.7 (*C*). ^{11}B NMR (127 MHz, $CDCl_3$, δ): 34.2. FT-IR (neat): ν_{max} = 3064, 1369, 1313, 1144, 697 cm^{-1}. HRMS–EI (*m*/*z*): [M]+ calcd for, $C_{19}H_{31}BO_3$, 318.23662; found, 318.23709.

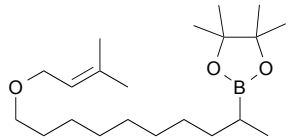
9-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)decyl benzoate (3j).



3j

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.95–1.01 (m, 4H), 1.23–1.47 (m, 24H), 1.76 (dt, *J* = 7.1 Hz, 14.4 Hz, 2H), 4.31 (t, *J* = 6.7 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.53–7.58 (m, 1H), 8.03–8.06 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 15.4 (*C*H_3), 16.8 (br, B–*C*H), 24.60 (*C*H_3), 24.64 (*C*H_3), 25.9 (*C*H_2), 28.6 (*C*H_2), 28.8 (*C*H_2), 29.2 (*C*H_2), 29.4 (*C*H_2), 29.7 (*C*H_2), 33.1 (*C*H_2), 65.0 (*C*H_2), 82.6 (*C*), 128.2 (*C*H), 129.4 (*C*H), 130.4 (*C*), 132.6 (*C*H), 166.5 (*C*). ^{11}B NMR (127 MHz, $CDCl_3$, δ): 34.2. FT-IR (neat): ν_{max} = 2924, 1720, 1273, 1145, 713 cm^{-1}. HRMS–EI (*m*/*z*): [M]+ calcd for, $C_{23}H_{37}BO_4$, 388.27849; found, 388.27830.

4,4,5,5-Tetramethyl-2-{10-[(3-methylbut-2-en-1-yl)oxy]decan-2-yl}-1,3,2-dioxaborolane (3k).

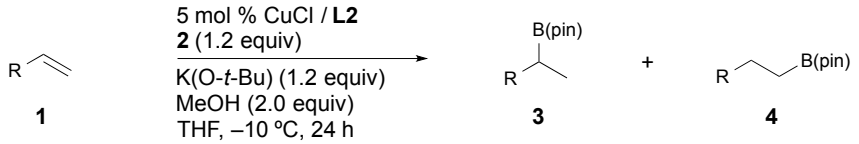


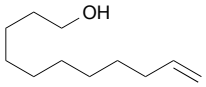
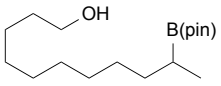
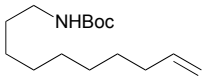
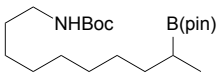
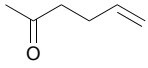
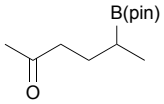
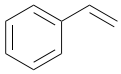
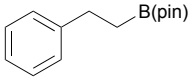
3k

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.95–1.03 (m, 4H), 1.24–1.46 (m, 24H), 1.53–1.60 (m, 2H), 1.67 (s, 3H), 1.74 (s, 3H), 3.39 (t, *J* = 7.0 Hz, 2H), 3.94 (d, *J* = 6.7 Hz, 2H), 5.33–5.38 (m, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 15.4 (*C*H_3), 16.8 (br, B–*C*H), 17.9 (*C*H_3), 24.58 (*C*H_3), 24.61 (*C*H_3), 25.7 (*C*H_3), 26.1 (*C*H_2), 28.8 (*C*H_2), 29.36 (*C*H_2), 29.45 (*C*H_2), 29.68 (*C*H_2), 29.72 (*C*H_2), 33.1 (*C*H_2), 67.1 (*C*H_2), 70.3 (*C*H_2), 82.6 (*C*), 121.3 (*C*H), 136.4 (*C*). ^{11}B NMR (127 MHz, $CDCl_3$, δ): 34.2. FT-IR (neat): ν_{max} = 2925, 1370, 1313, 1144, 859 cm^{-1}. HRMS–EI (*m*/*z*): [M]+ calcd for, $C_{21}H_{41}BO_3$, 352.31487; found, 352.31532.

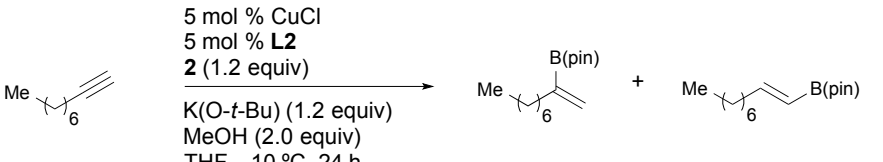
5. The results of substrates bearing various functionalities

Table S1 Copper(I)-catalyzed hydroboration of terminal alkenes bearing various functionalities[a]



entry	substrate	product	yield (%)[b]	3/4[c]
1	 **1l**	no reaction		
2	 **1m**	 **3m**	(<5)	-
3	 **1n**	 **3n**	(12)	90:10
4	 **1o**	 **3o**	75 (86)	96:4
5	 **1p**	 **4p**	39 (53)	<1:99

[a]Conditions: **1** (0.5 mmol), CuCl (0.025 mmol), **L2** (0.025 mmol), **2** (0.6 mmol) and K(O-*t*-Bu) (0.6 mmol) in THF (1.0 mL) at –10 ºC. [b]Isolated yield. The NMR yields are shown in parenthesis [c]Determined by GC analysis of the crude material.



6

7
40% (NMR yield)
7/**8** = 47:53

8
46% (NMR yield)

Scheme S1. Copper(I)-catalyzed hydroboration of alkyne.

6. References

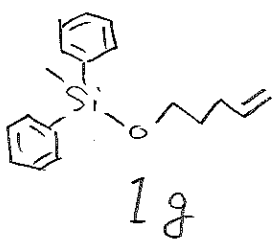
1 J. A. Marshall, J. J. Sabatini and F. Valeriote, *Bioorganic Med. Chem. Lett.*, 2007, **17**, 2434–2437.

2 V. Rawat, P. V. Chouthaiwale, G. Suryavanshi and A. Sudalai, *Tetrahedron Asymmetry*, 2009, **20**, 2173–2177.

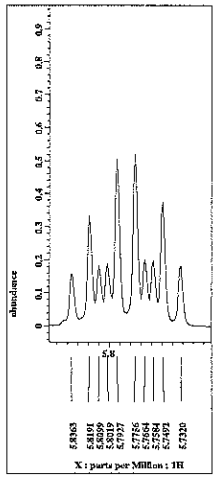
3 C. Luján and S. P. Nolan, *J. Organomet. Chem.*, 2011, **696**, 3935–3938.

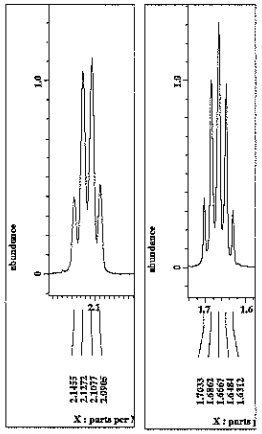
4 A. S. Dudnik and G. C. Fu, *J. Am. Chem. Soc.*, 2012, **134**, 10693–10697.

5 A. Ganić and A. Pfaltz, *Chem. - Eur. J.*, 2012, **18**, 6724–6728.



1g





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-818-pure1-1.jdf
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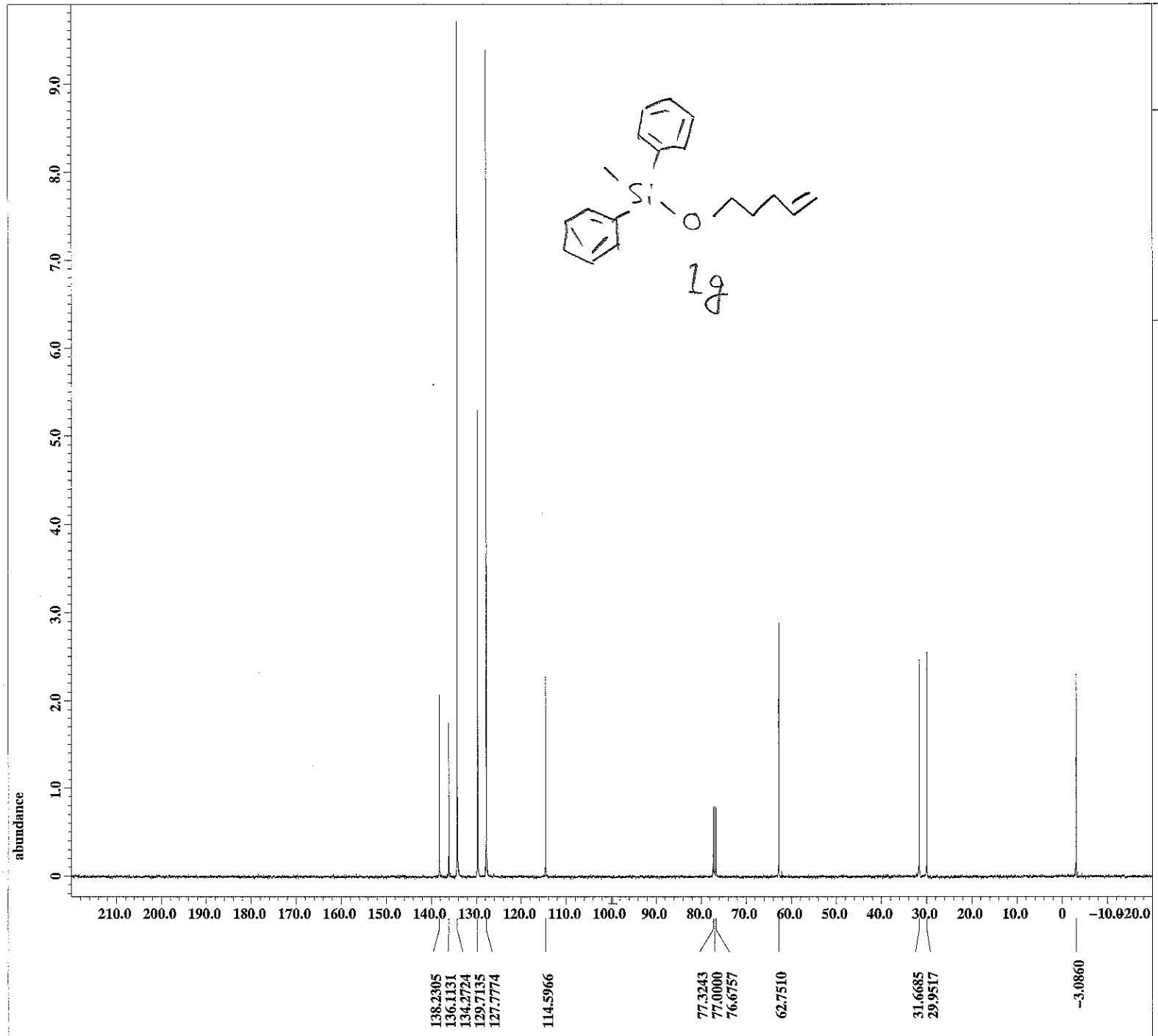
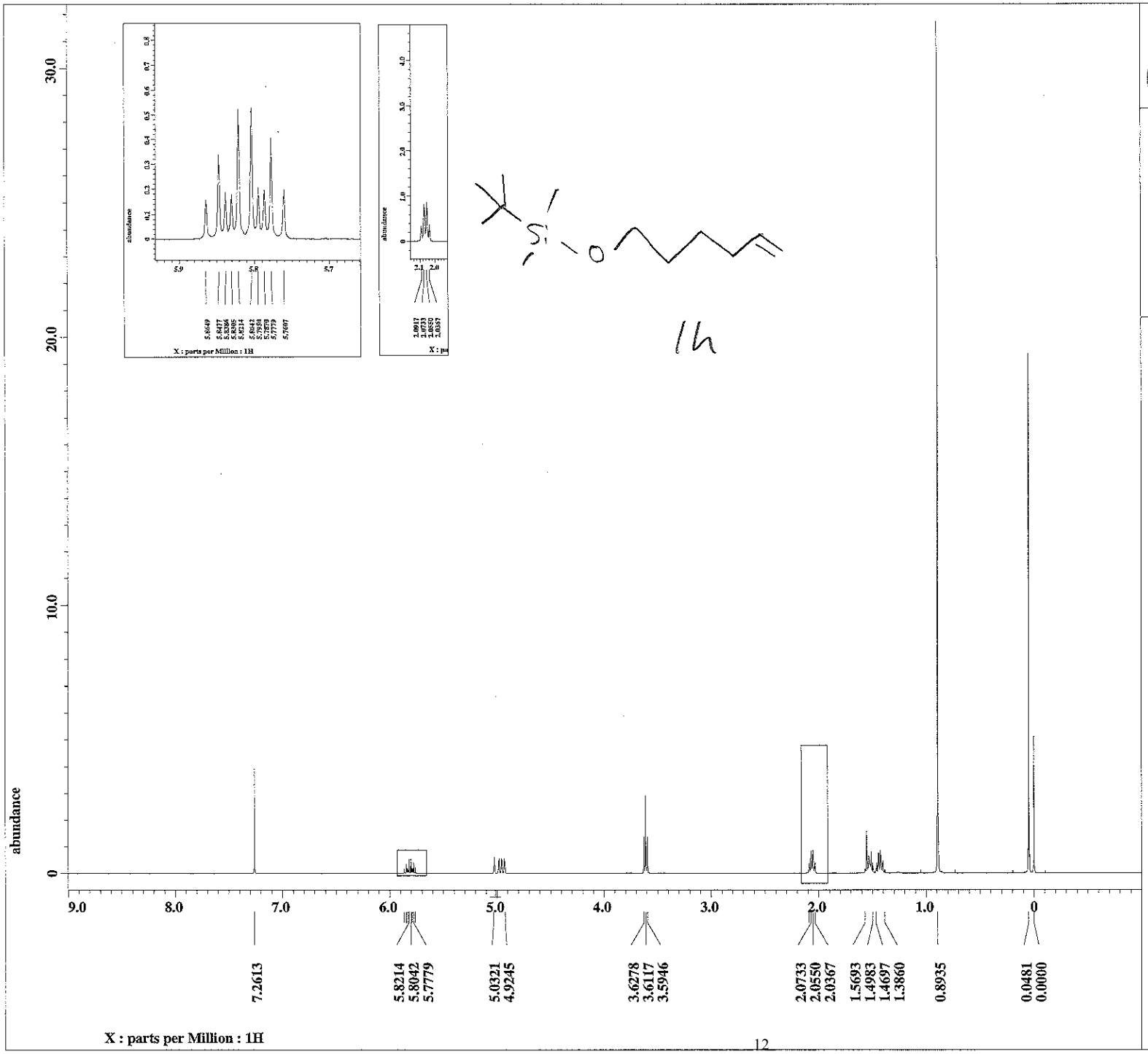
Filename	= IWA-818-pure1-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#712482
Solvent	= CHLOROFORM-D
Creation_time	= 24-OCT-2015 19:17:07
Revision_time	= 24-OCT-2015 19:55:34
Current_time	= 24-OCT-2015 19:55:38
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 38
Relaxation_delay	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 18.3[dC]



---- 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-818-carbon-1.jdf

Filename	= IWA-818-carbon-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#716322
Solvent	= CHLOROFORM-D
Creation_time	= 24-OCT-2015 19:25:18
Revision_time	= 24-OCT-2015 19:58:28
Current_time	= 24-OCT-2015 19:59:04
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	= 59
Total_scans	= 59
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	= 18.4[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-766-pure1-1.jdf
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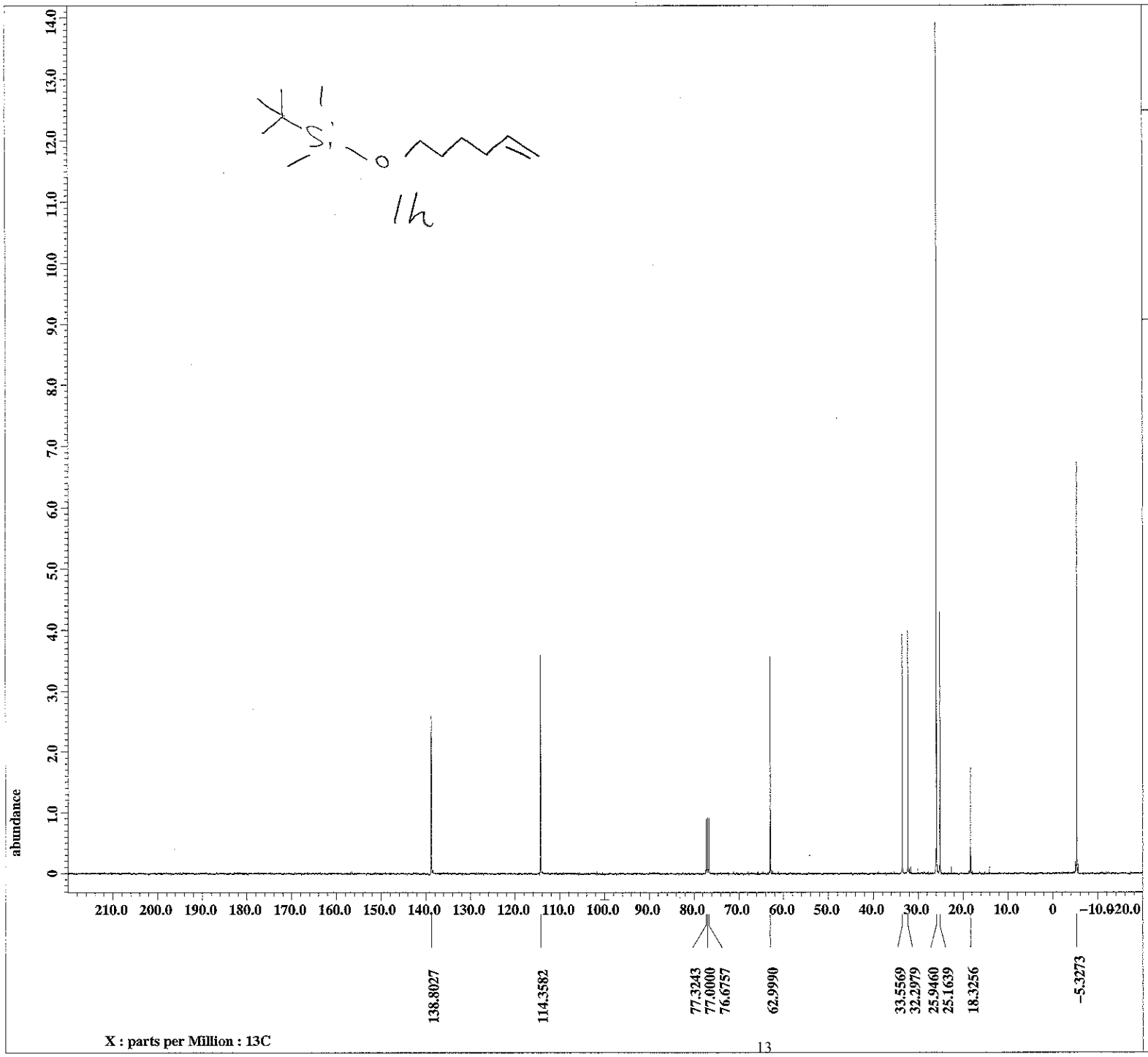
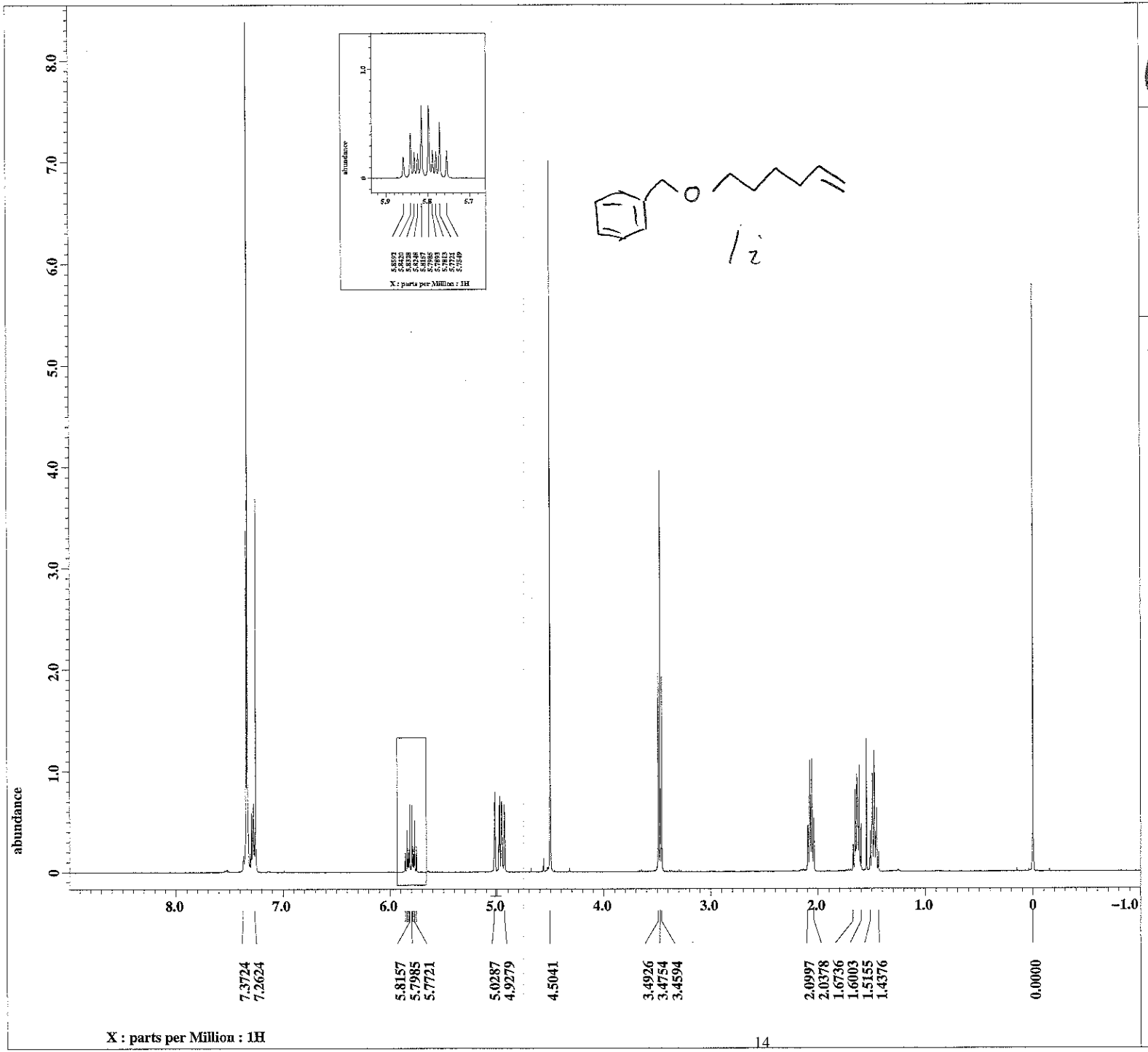
Filename	= IWA-766-pure1-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#684985
Solvent	= CHLOROFORM-D
Creation_time	= 24-OCT-2015 18:31:18
Revision_time	= 23-JAN-2016 19:54:09
Current_time	= 23-JAN-2016 19:54:11
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 44
Relaxation_delay	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 19.6[dC]



---- 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-766-carbon-1.jdf

Filename	= IWA-766-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#688551
Solvent	= CHLOROFORM-D
Creation_time	= 24-OCT-2015 18:39:13
Revision_time	= 24-OCT-2015 19:12:38
Current_time	= 24-OCT-2015 19:13:16
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	= 65
Total_scans	= 65
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	= 19.5[dC]

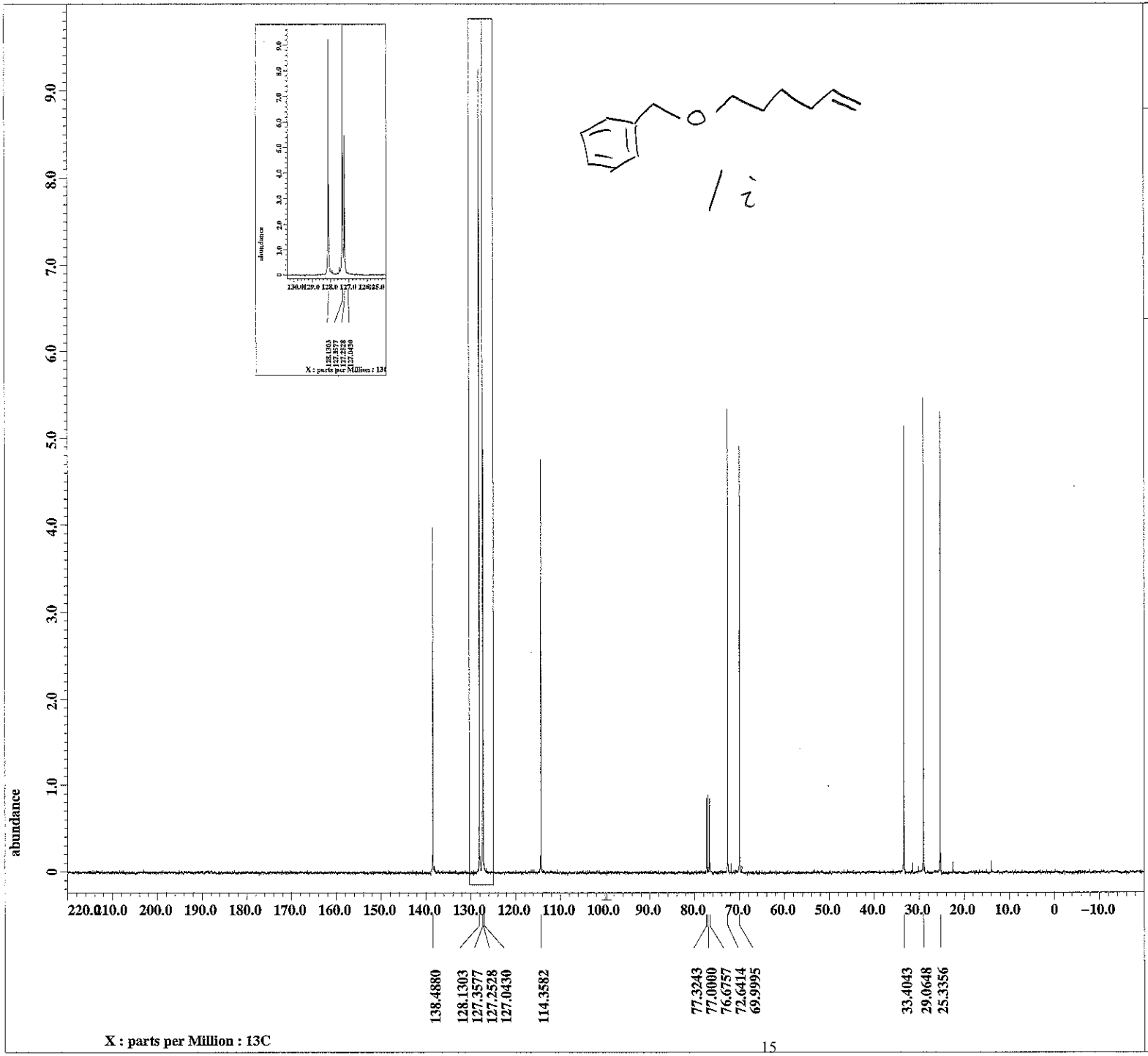


JEOL

```
---- 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-821-proton1-1.jdf
```

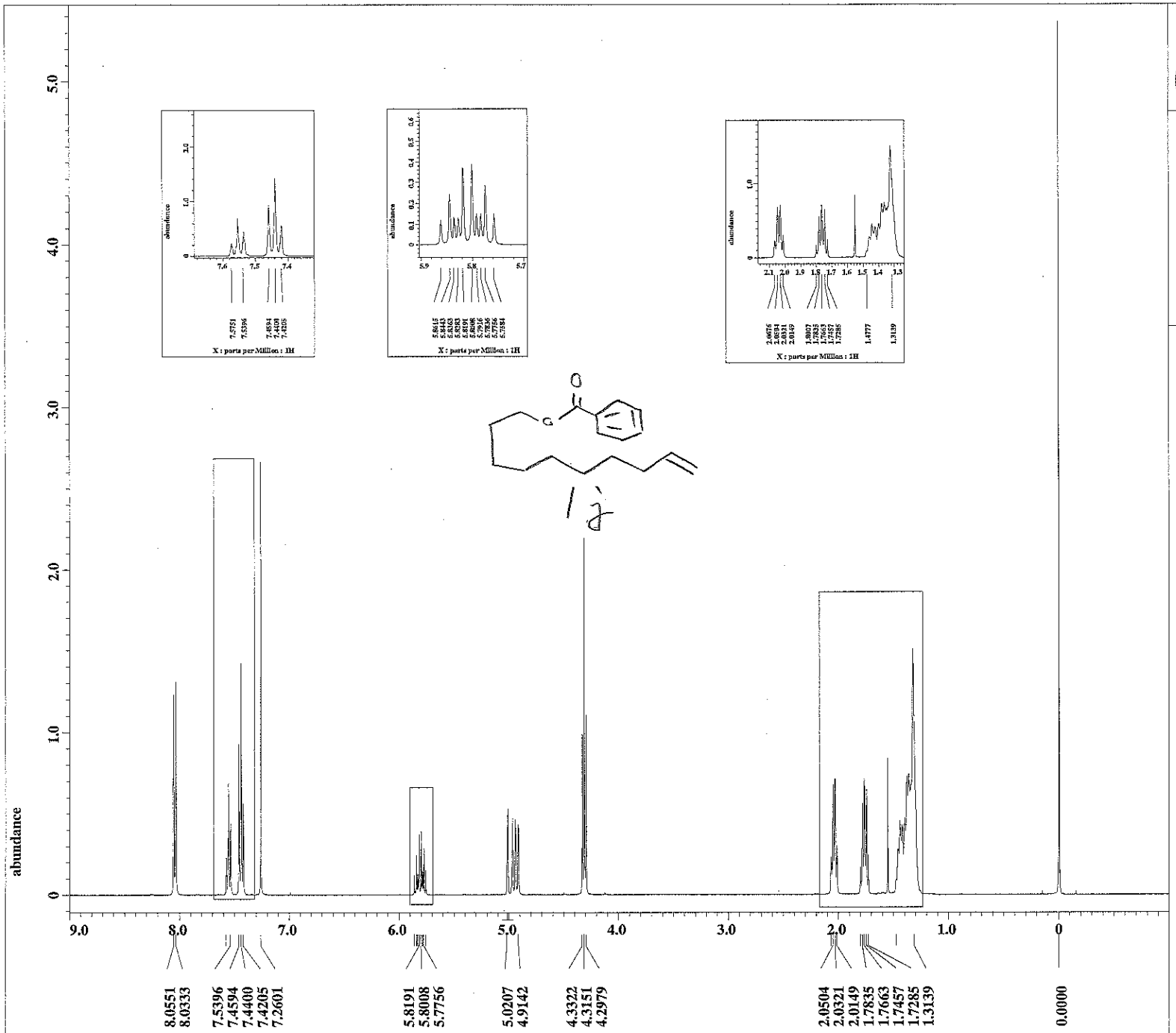
Filename	= IWA-821-proton1-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#768593
Solvent	= CHLOROFORM-D
Creation_time	= 6-DEC-2015 20:51:32
Revision_time	= 6-DEC-2015 21:26:40
Current_time	= 6-DEC-2015 21:26:43
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 44
Relaxation_delay	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 20.9[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
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
```

Filename	= IWA-826-carbon-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#721615
Solvent	= CHLOROFORM-D
Creation_time	= 25-OCT-2015 19:33:37
Revision_time	= 25-OCT-2015 20:07:30
Current_time	= 25-OCT-2015 20:08:30
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	= 52
Total_scans	= 52
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	= 20.2[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-845-proton-1.jdf
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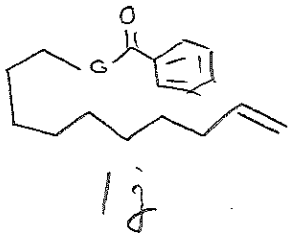
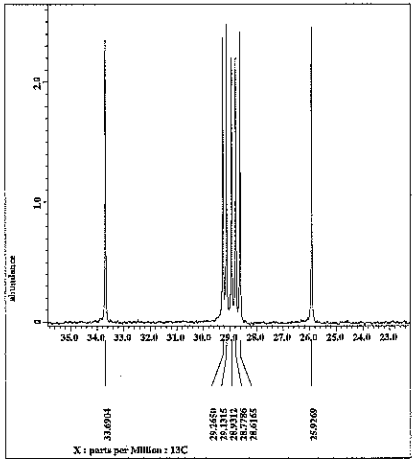
Filename	= IWA-845-proton-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#370976
Solvent	= CHLOROFORM-D
Creation_time	= 5-DEC-2015 09:49:03
Revision_time	= 5-DEC-2015 10:28:10
Current_time	= 5-DEC-2015 10:28:12
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 44
Relaxation_delay	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 21.4[dC]



12



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

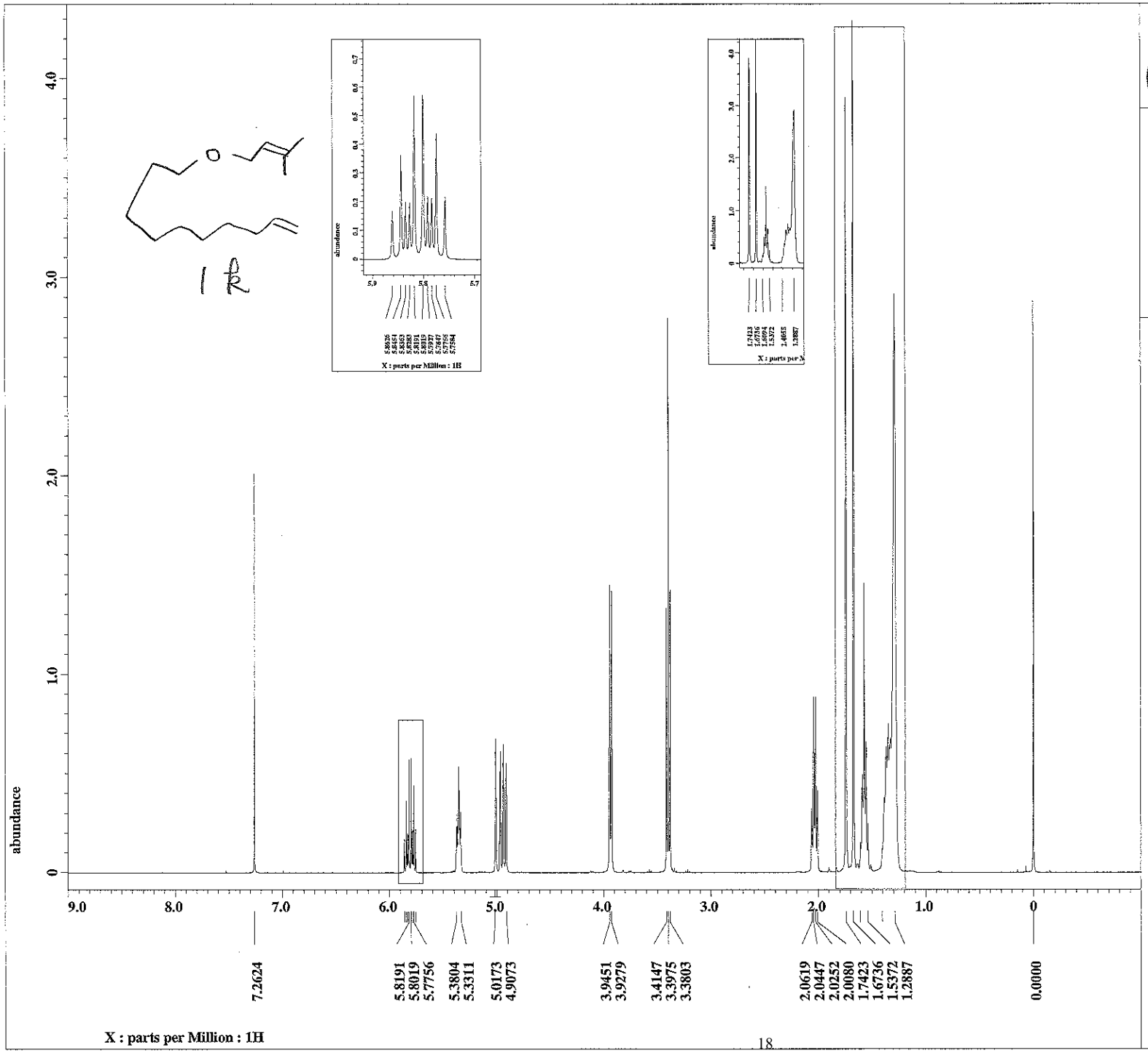
Derived from: IWA-845-carbon-2.jdf
```

```
Filename            = IWA-845-carbon-4.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_id           = S#374971
Solvent             = CHLOROFORM-D
Creation_time       =  5-DEC-2015 09:59:27
Revision_time       =  5-DEC-2015 10:31:09
Current_time        =  5-DEC-2015 10:32:15

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               = 95
Total_scans         = 95

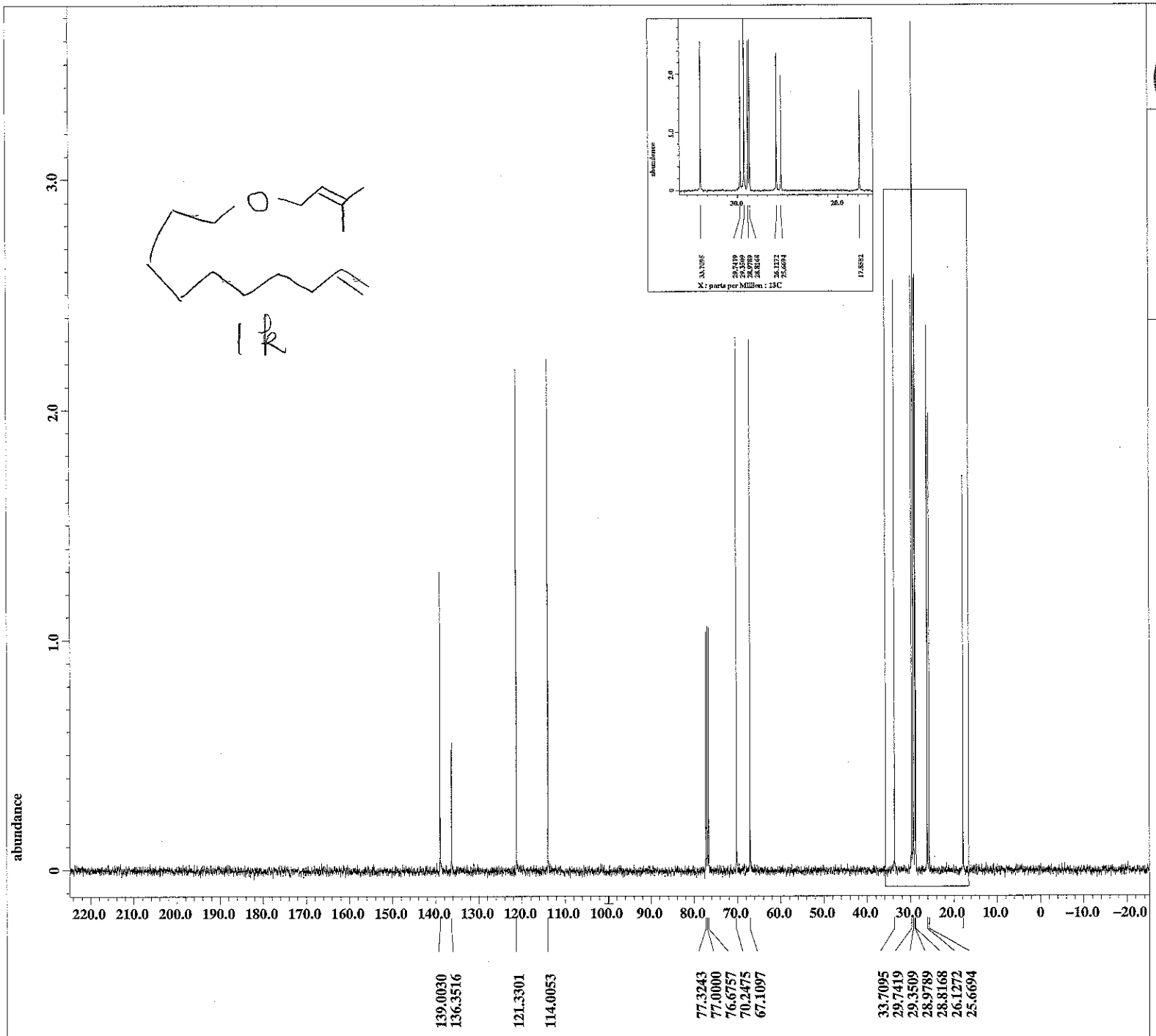
X_90_width          = 8.8[us]
X_acq_time          = 1.06430464[s]
X_angle             = 30[deg]
X_atn               = 4.9[dB]
X_pulse             = 2.93333333[us]
Irr_atn_dec         = 22.52628[dB]
Irr_atn_noe         = 22.52628[dB]
Irr_noise           = WALTZ
Decoupling          = TRUE
Initial_wait        = 1[s]
Noe                 = TRUE
Noe_time            = 2[s]
Recvr_gain          = 60
Relaxation_delay    = 2[s]
Repetition_time     = 3.06430464[s]
Temp_get            = 21.6[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-844-proton-1.jdf

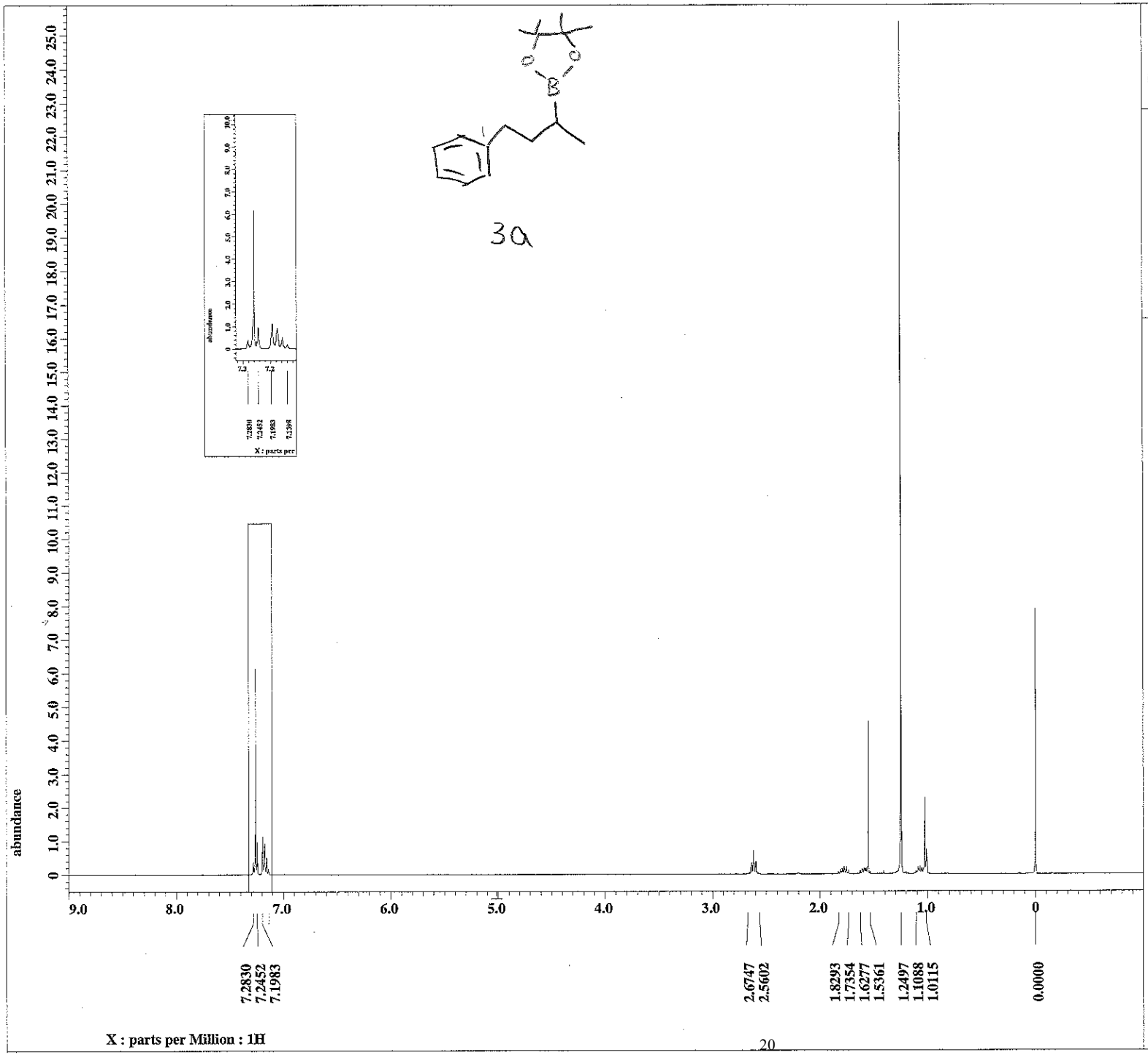
Filename	= IWA-844-proton-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#705234
Solvent	= CHLOROFORM-D
Creation_time	= 30-NOV-2015 19:07:02
Revision_time	= 30-NOV-2015 19:45:48
Current_time	= 30-NOV-2015 19:45:50
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 38
Relaxation_delay	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 20.8[dC]




```
---- 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-844-carbon-1.jdf
```

Filename	= IWA-844-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#709003
Solvent	= CHLOROFORM-D
Creation_time	= 30-NOV-2015 19:14:34
Revision_time	= 30-NOV-2015 19:46:36
Current_time	= 30-NOV-2015 19:49:26
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	= 51
Total_scans	= 51
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]



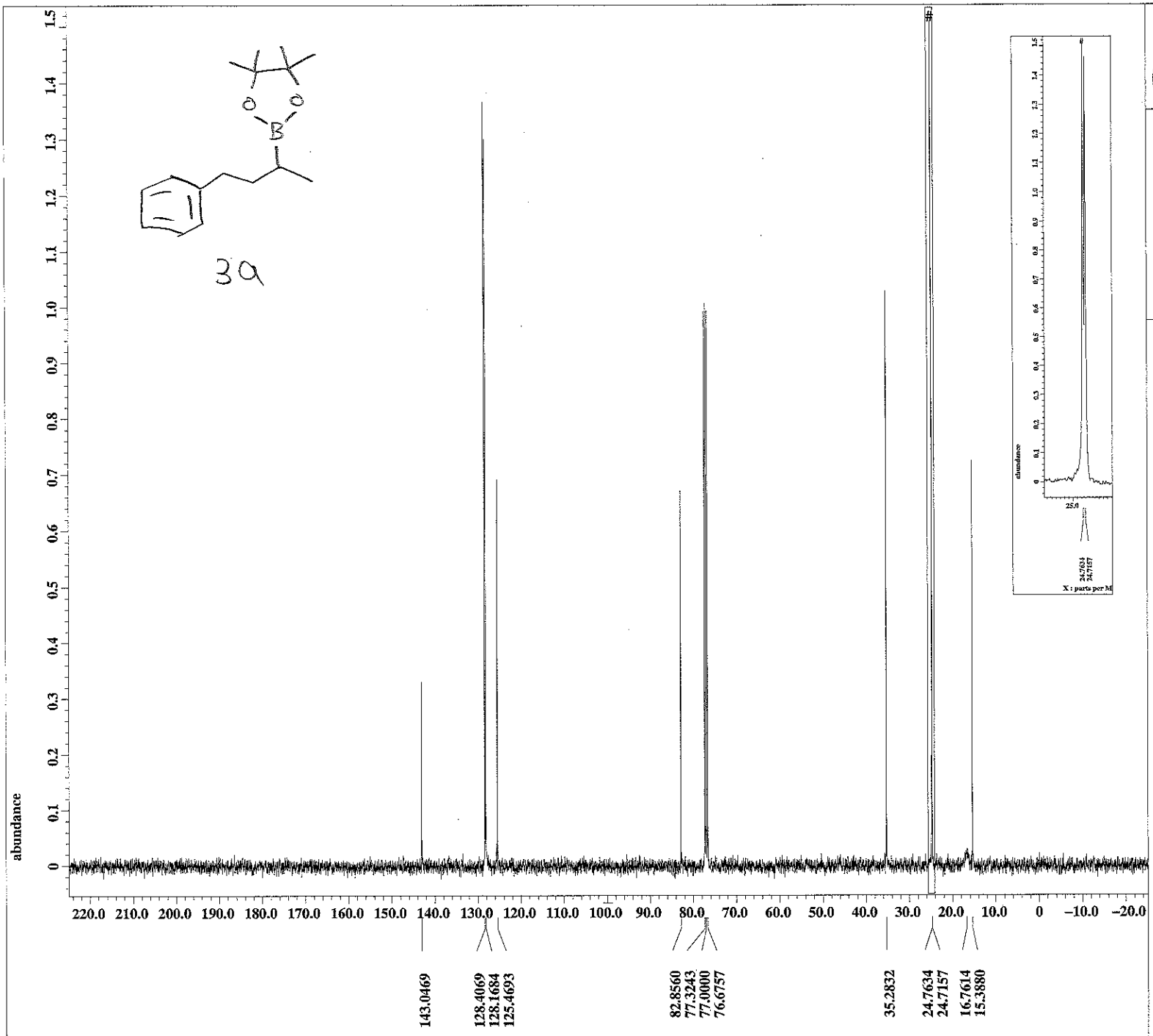
3a

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-776-pure1-1.jdf
```

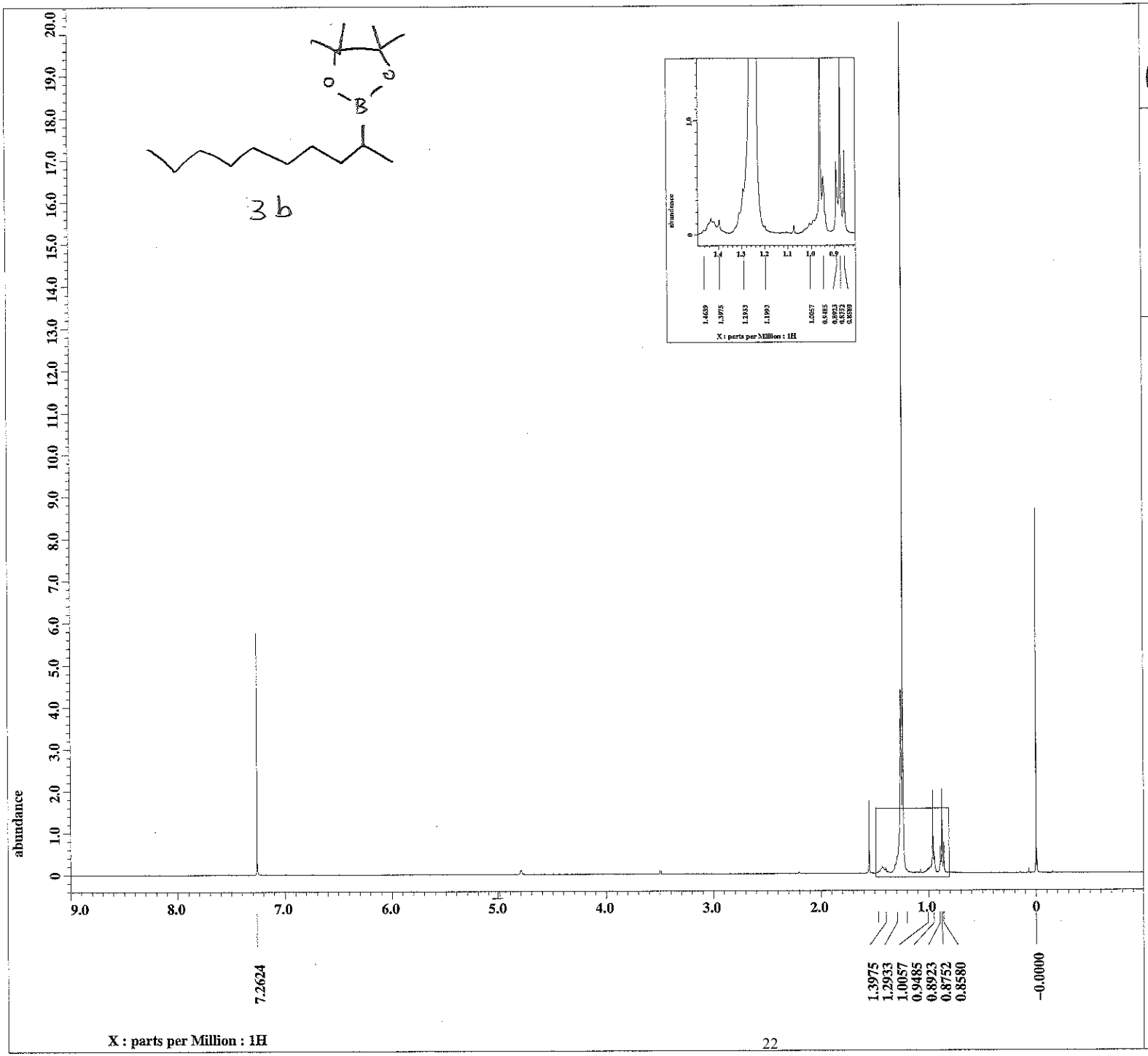
Filename	= IWA-776-pure1-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#649528
Solvent	= CHLOROFORM-D
Creation_time	= 3-NOV-2015 17:30:36
Revision_time	= 3-NOV-2015 18:10:29
Current_time	= 3-NOV-2015 18:10:31
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 20.2[dC]



---- 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-776-carbon-1.jdf

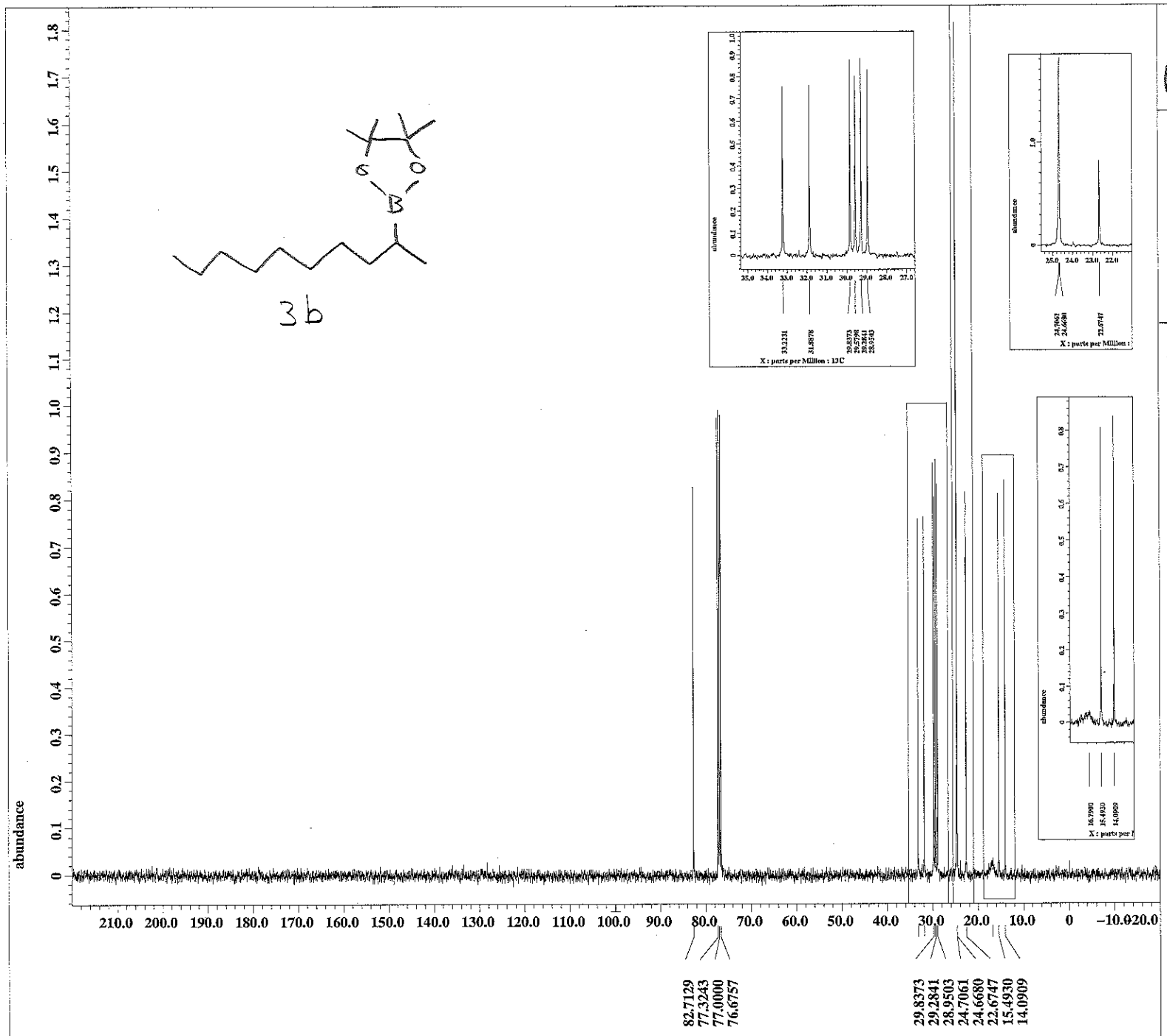
Filename	= IWA-776-carbon-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#653309
Solvent	= CHLOROFORM-D
Creation_time	= 3-NOV-2015 17:41:24
Revision_time	= 3-NOV-2015 18:16:31
Current_time	= 3-NOV-2015 18:17:53
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
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	= 110
Total_scans	= 110
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]



---- 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-845-pure1-1.jdf

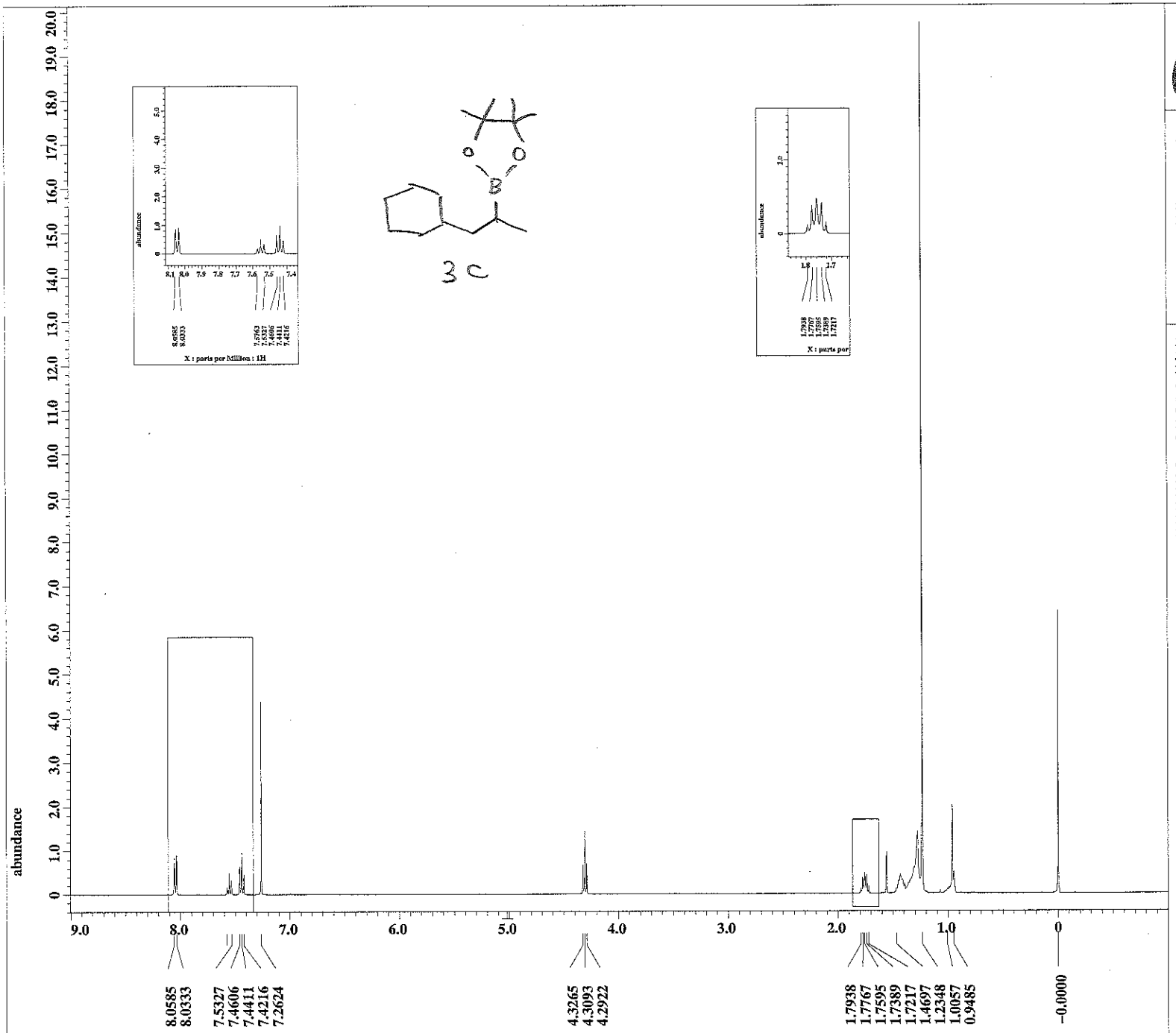
Filename	= IWA-845-pure1-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#740265
Solvent	= CHLOROFORM-D
Creation_time	= 26-NOV-2015 19:59:26
Revision_time	= 26-NOV-2015 20:43:39
Current_time	= 26-NOV-2015 20:43:42
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 20.9[dC]




```
---- 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-845-carbon-1.jdf
```

Filename	= IWA-845-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#744273
Solvent	= CHLOROFORM-D
Creation_time	= 26-NOV-2015 20:11:05
Revision_time	= 26-NOV-2015 20:48:16
Current_time	= 26-NOV-2015 20:51:06
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	= 119
Total_scans	= 119
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	= 21.2[dC]



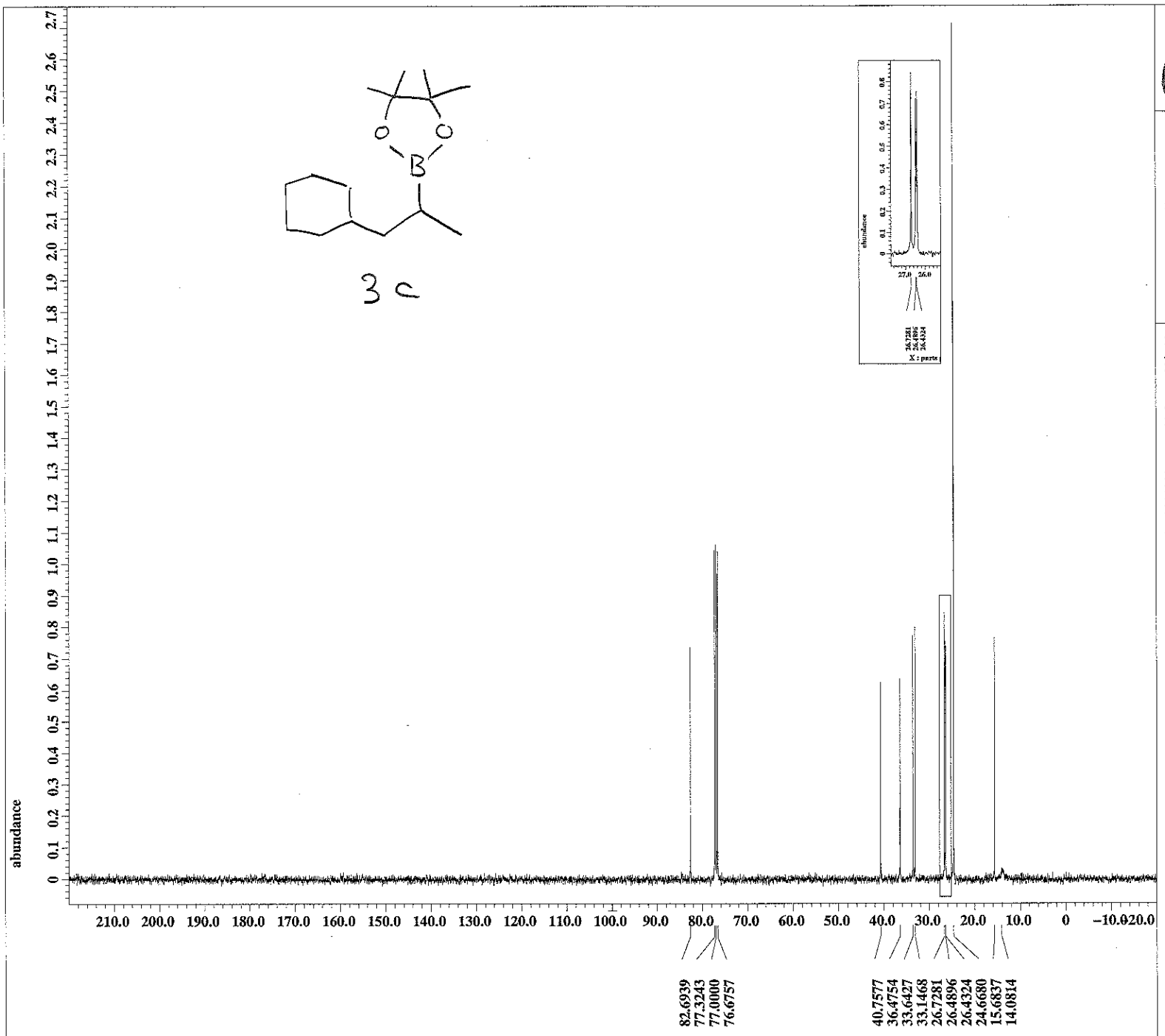
3c

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-859-pure-1.jdf
```

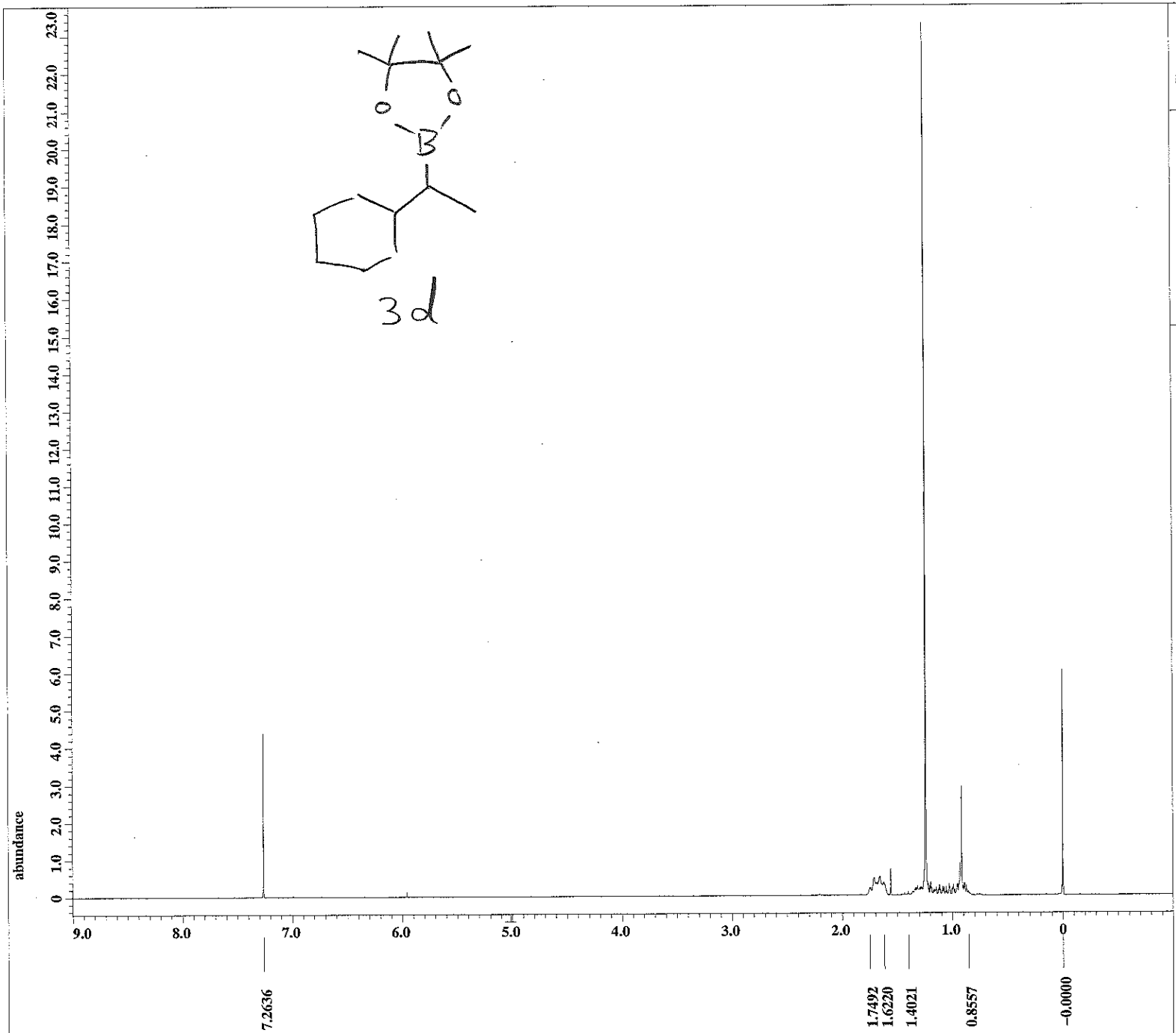
Filename	= IWA-859-pure-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#744326
Solvent	= CHLOROFORM-D
Creation_time	= 28-OCT-2015 20:09:24
Revision_time	= 4-DEC-2015 20:33:21
Current_time	= 4-DEC-2015 20:33:23
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 20.5[dC]




```
----- 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-872-carbon-1.jdf
```

Filename	= IWA-872-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#733739
Solvent	= CHLOROFORM-D
Creation_time	= 7-NOV-2015 19:54:49
Revision_time	= 7-NOV-2015 20:30:16
Current_time	= 7-NOV-2015 20:31:14
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	= 109
Total_scans	= 109
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	= 21.2[dC]

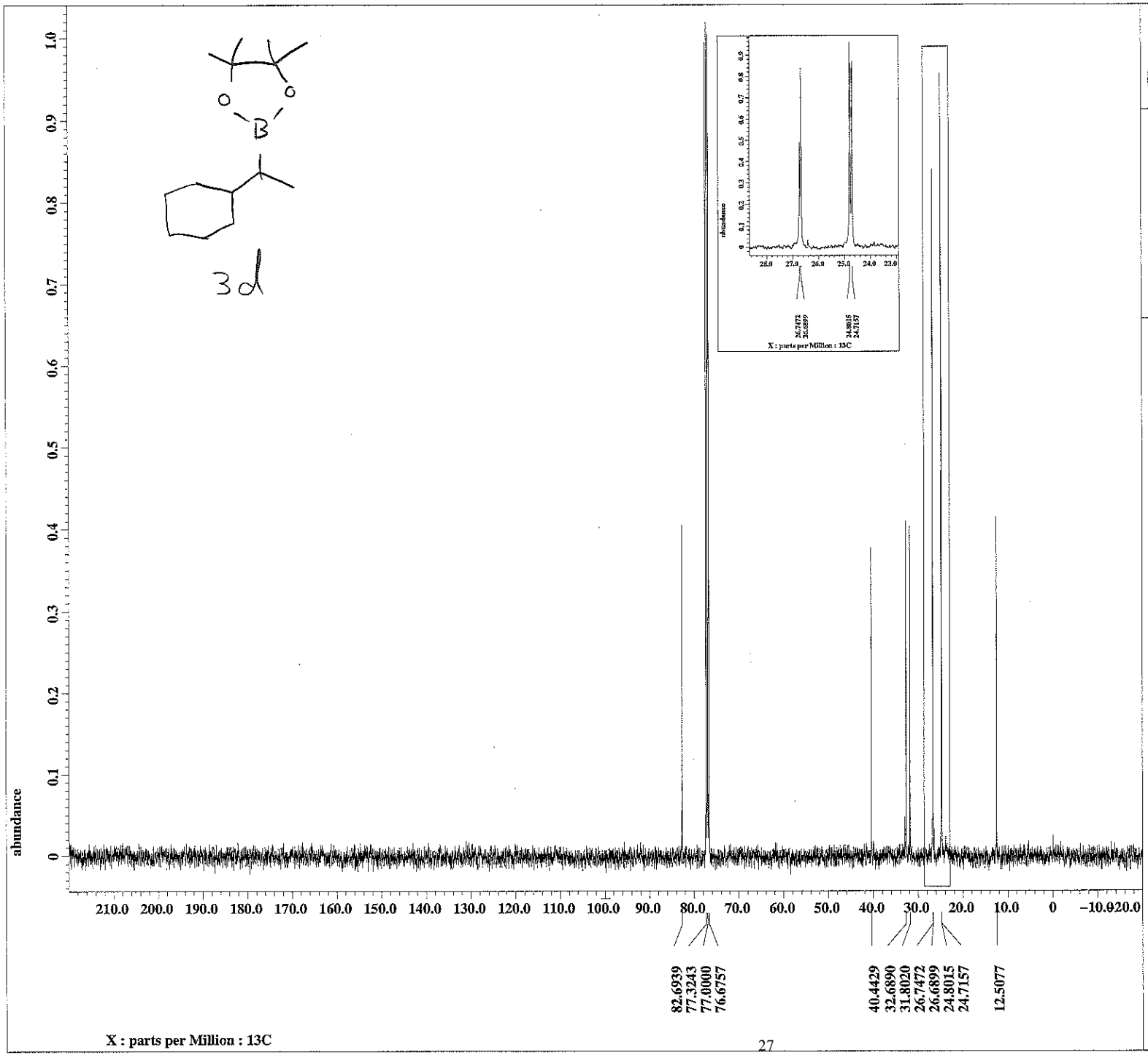


JEOL

```
----- 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-877-pure-1.jdf
```

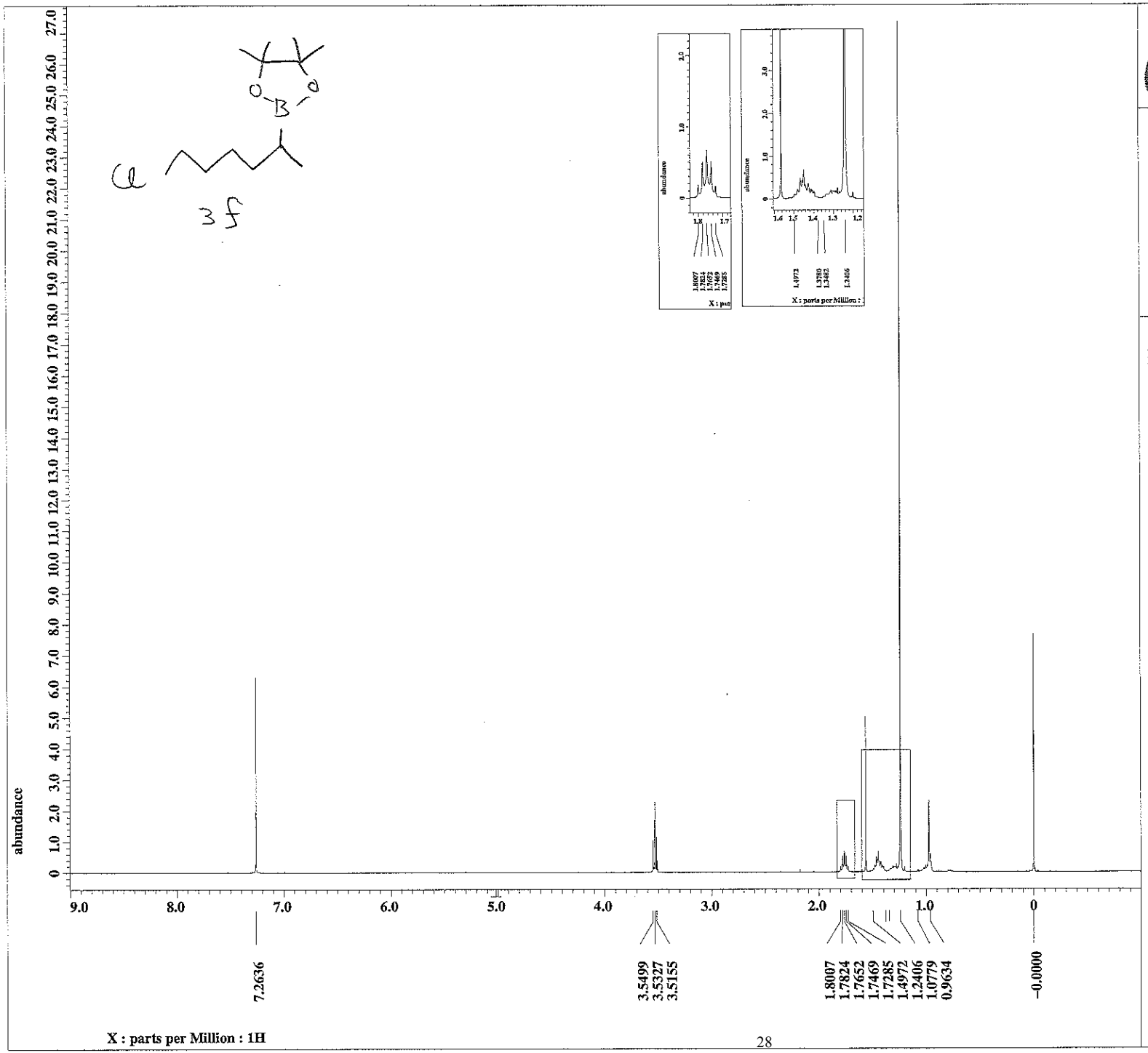
Filename	= IWA-877-pure-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#705530
Solvent	= CHLOROFORM-D
Creation_time	= 11-NOV-2015 19:03:17
Revision_time	= 11-NOV-2015 19:46:39
Current_time	= 11-NOV-2015 19:46:42
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 44
Relaxation_delay	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 18.6[dC]



---- 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-877-carbon-1.jdf

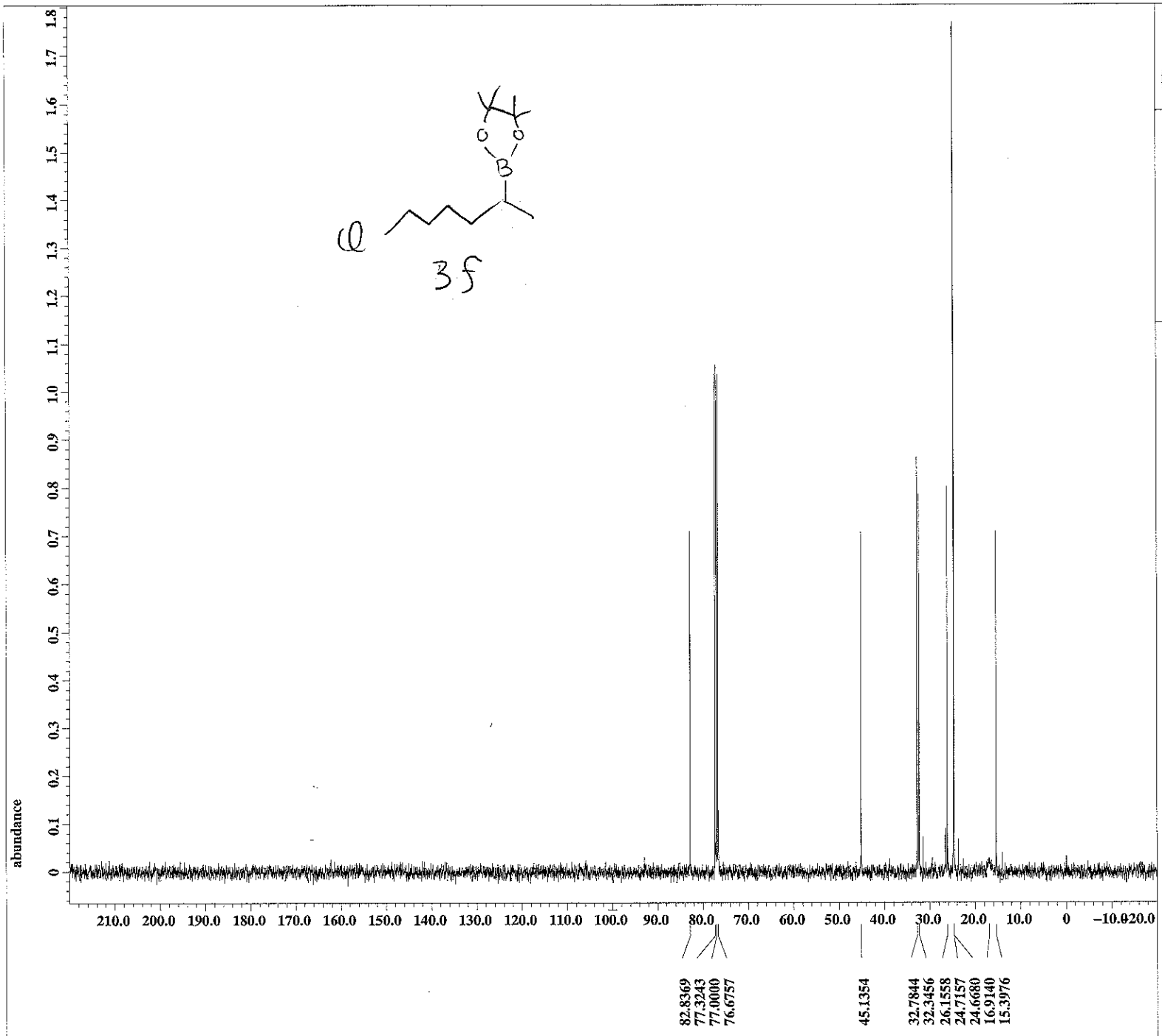
Filename	= IWA-877-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#709204
Solvent	= CHLOROFORM-D
Creation_time	= 11-NOV-2015 19:14:18
Revision_time	= 11-NOV-2015 19:50:36
Current_time	= 11-NOV-2015 20:01:03
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 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	= 127
Total_scans	= 127
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	= 19.5[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-874-pure-1.jdf
```

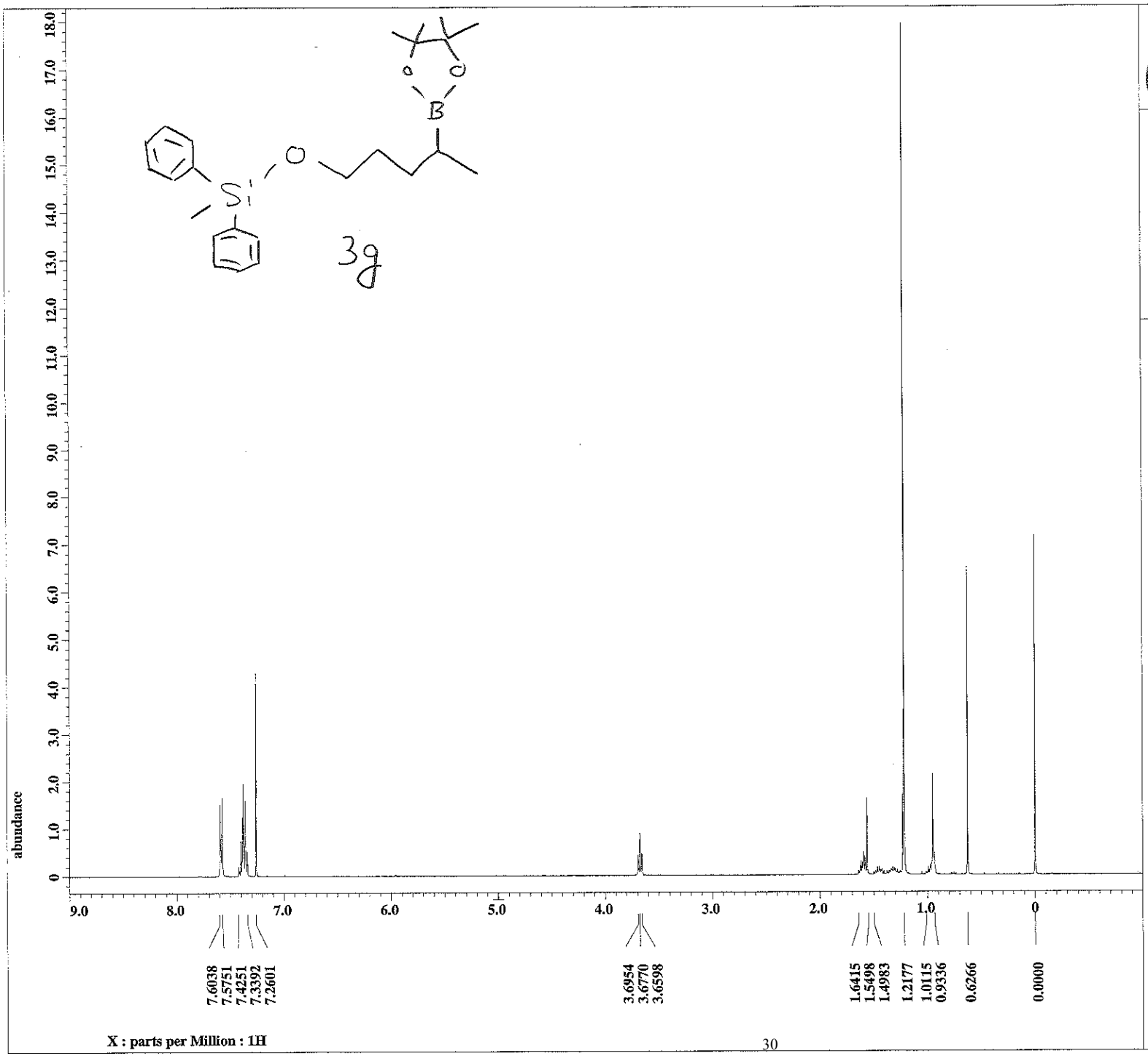
Filename	= IWA-874-pure-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#775787
Solvent	= CHLOROFORM-D
Creation_time	= 7-NOV-2015 21:00:26
Revision_time	= 23-JAN-2016 18:56:25
Current_time	= 23-JAN-2016 18:56:28
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 18.8[dC]



---- 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-874-carbon-1.jdf

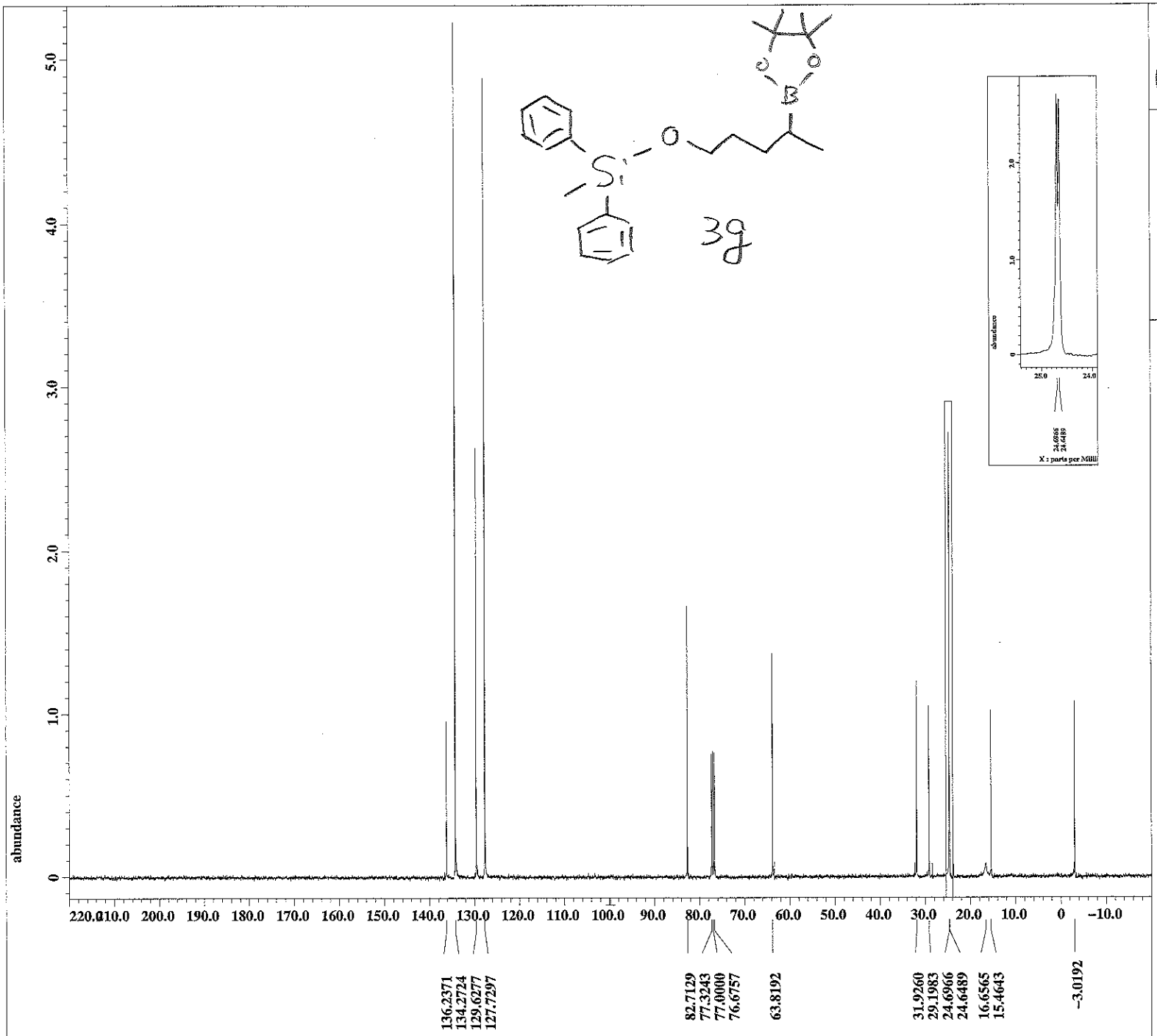
Filename	= IWA-874-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#779350
Solvent	= CHLOROFORM-D
Creation_time	= 7-NOV-2015 21:09:27
Revision_time	= 23-JAN-2016 19:46:13
Current_time	= 23-JAN-2016 19:46:58
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
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	= 81
Total_scans	= 81
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	= 18.9[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-851-pure1-1.jdf

Filename	= IWA-851-pure1-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#572854
Solvent	= CHLOROFORM-D
Creation_time	= 25-OCT-2015 15:24:03
Revision_time	= 25-OCT-2015 16:04:13
Current_time	= 25-OCT-2015 16:04:14
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 44
Relaxation_delay	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 18.1[dC]

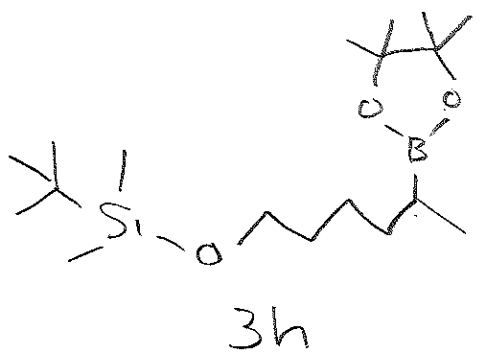


JEOL

```
---- 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-851-carbon-1.jdf
```

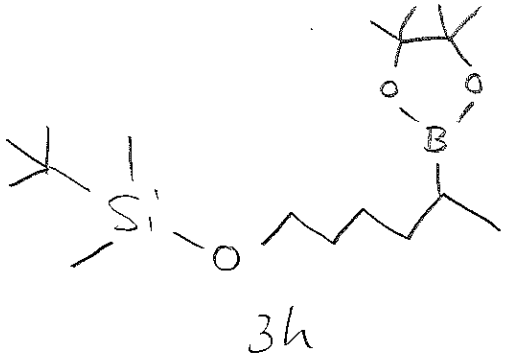
Filename	= IWA-851-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#576830
Solvent	= CHLOROFORM-D
Creation_time	= 25-OCT-2015 15:36:07
Revision_time	= 25-OCT-2015 16:09:48
Current_time	= 25-OCT-2015 16:10:41
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 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	= 128
Total_scans	= 128
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	= 19.2[dC]



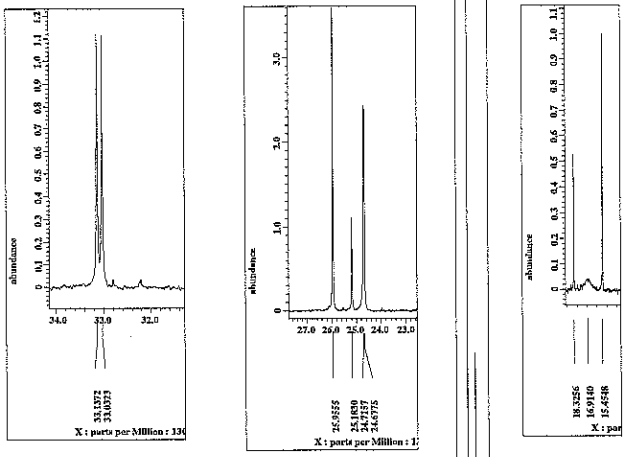
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: IWA-785-proton-1.jdf

Filename	= IWA-785-proton-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#726395
Solvent	= CHLOROFORM-D
Creation_time	= 3-NOV-2015 19:38:55
Revision_time	= 3-NOV-2015 20:16:39
Current_time	= 3-NOV-2015 20:16:40
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 44
Relaxation_delay	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 19.1[dC]



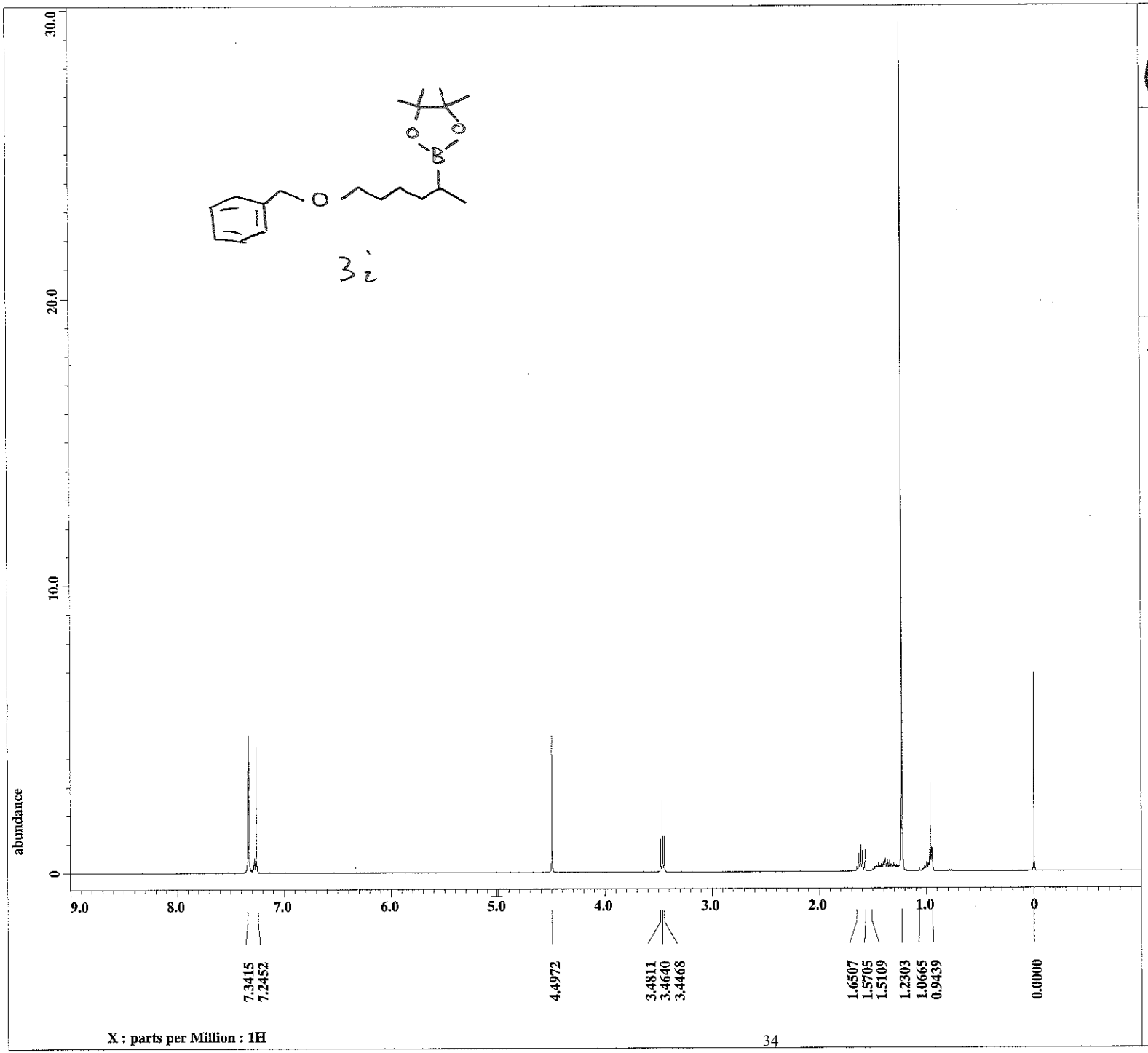
3h




```
---- 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-785-carbon-1.jdf
```

Filename	= IWA-785-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#730039
Solvent	= CHLOROFORM-D
Creation_time	= 3-NOV-2015 19:50:57
Revision_time	= 3-NOV-2015 20:25:50
Current_time	= 3-NOV-2015 20:27:38
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	= 143
Total_scans	= 143
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	= 19.8[dC]



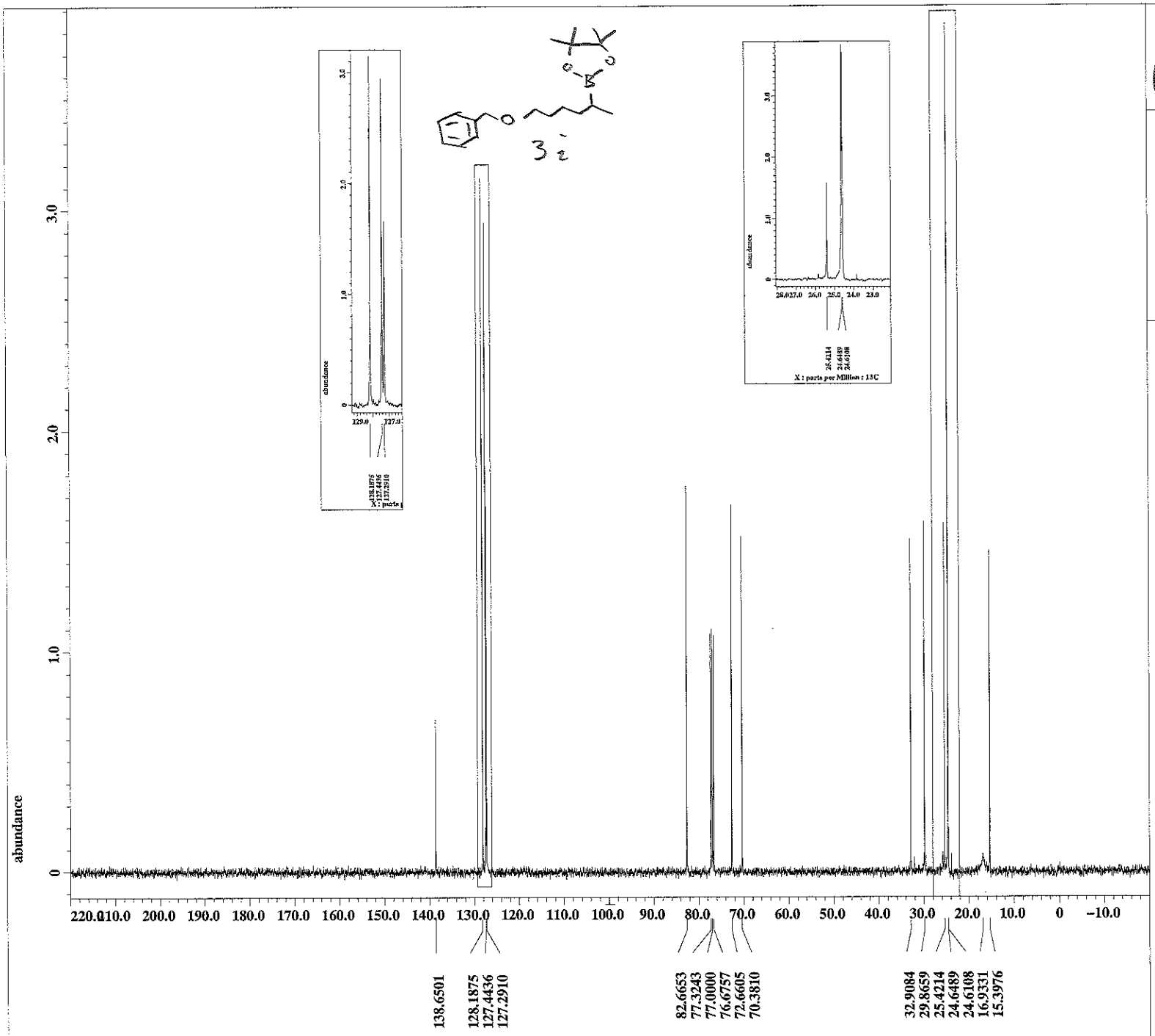
3i

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-853-pure-1.jdf
```

Filename	= IWA-853-pure-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#658283
Solvent	= CHLOROFORM-D
Creation_time	= 25-OCT-2015 17:46:39
Revision_time	= 25-OCT-2015 18:24:09
Current_time	= 25-OCT-2015 18:24:10
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 44
Relaxation_delay	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 18.8[dC]

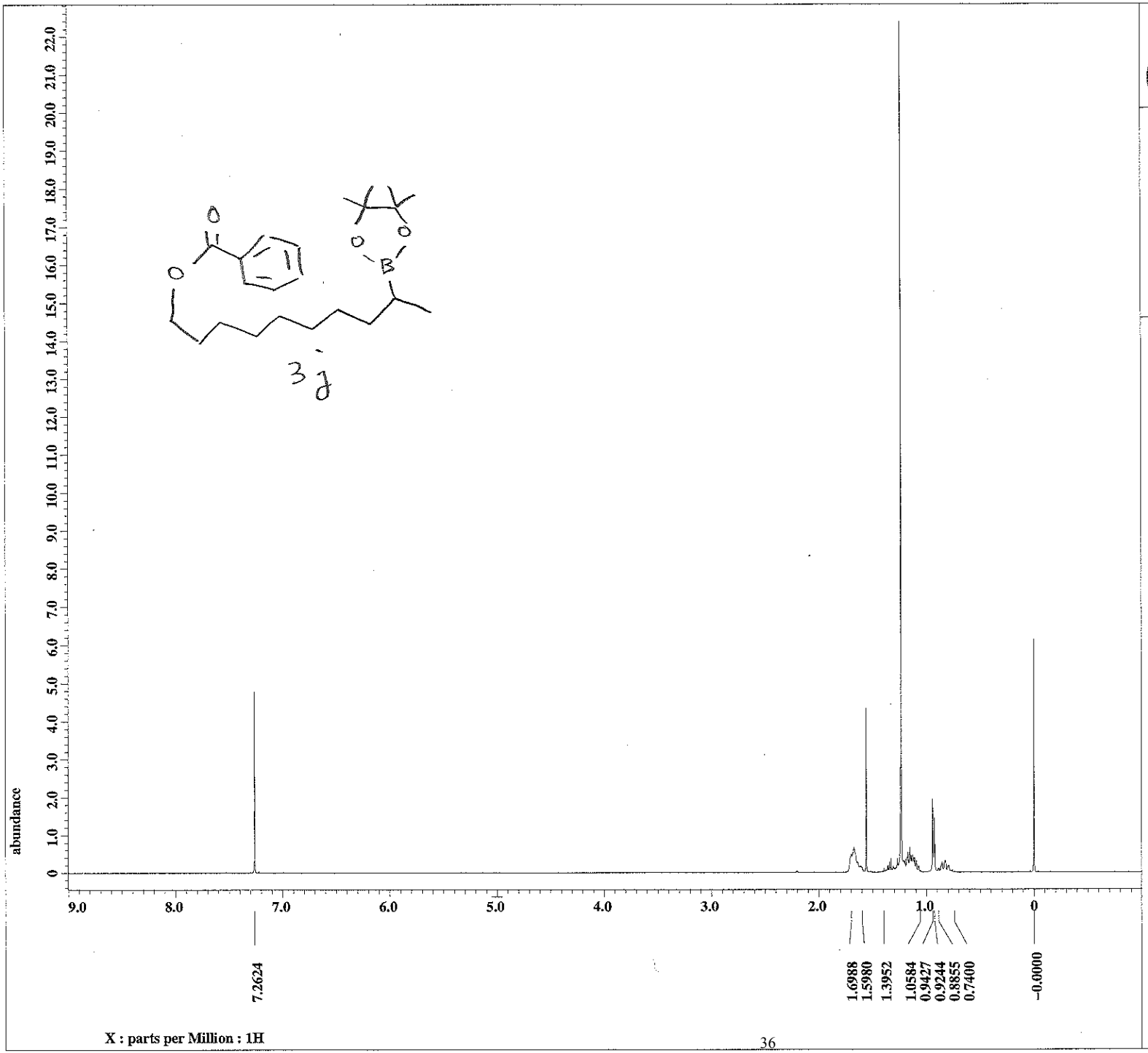


JEOL

```
---- 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-853-carbon-1.jdf
```

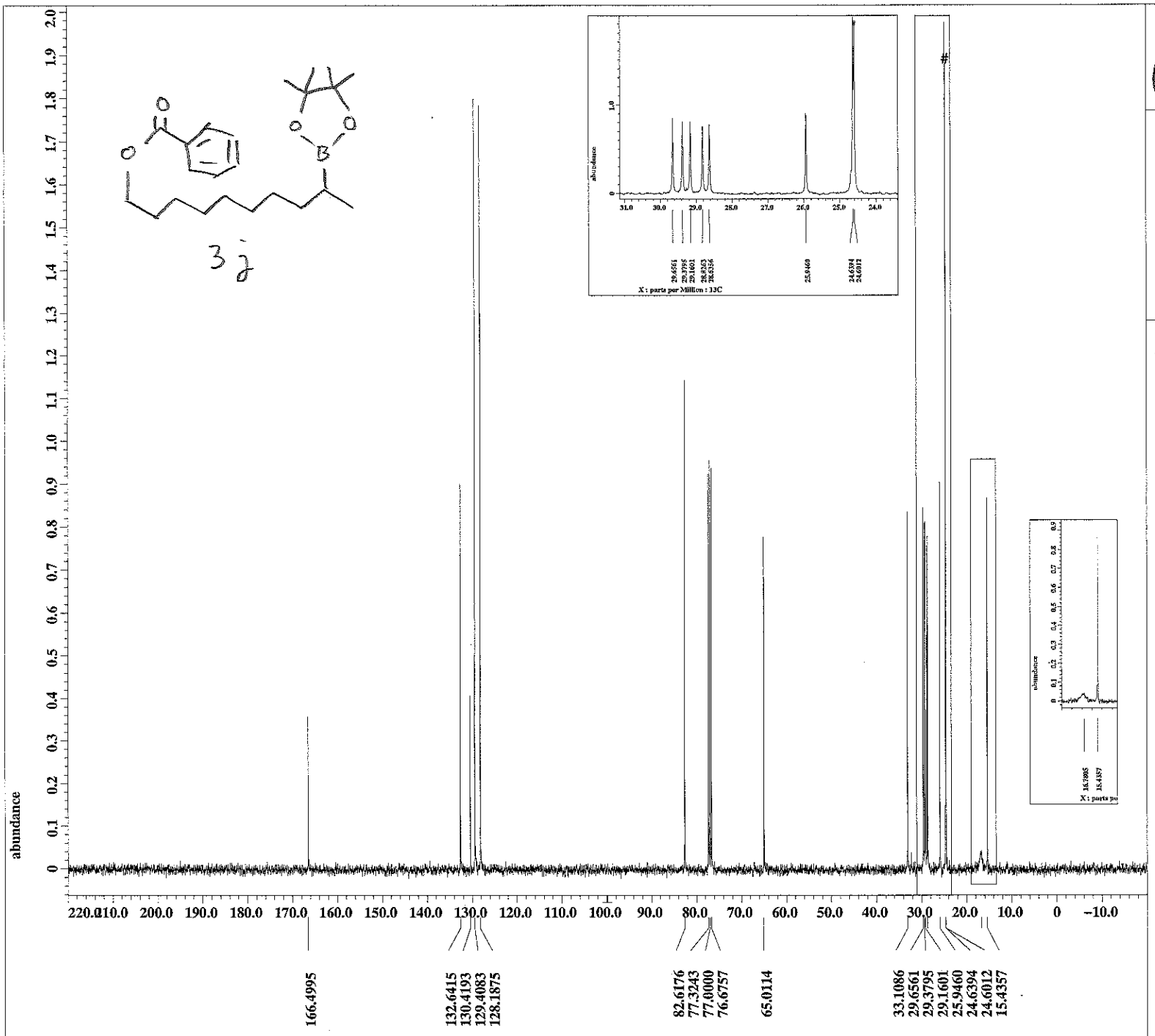
Filename	= IWA-853-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#661948
Solvent	= CHLOROFORM-D
Creation_time	= 25-OCT-2015 17:53:47
Revision_time	= 25-OCT-2015 18:28:19
Current_time	= 25-OCT-2015 18:29:42
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 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	= 46
Total_scans	= 46
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	= 18.8[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-872-pure-1.jdf
```

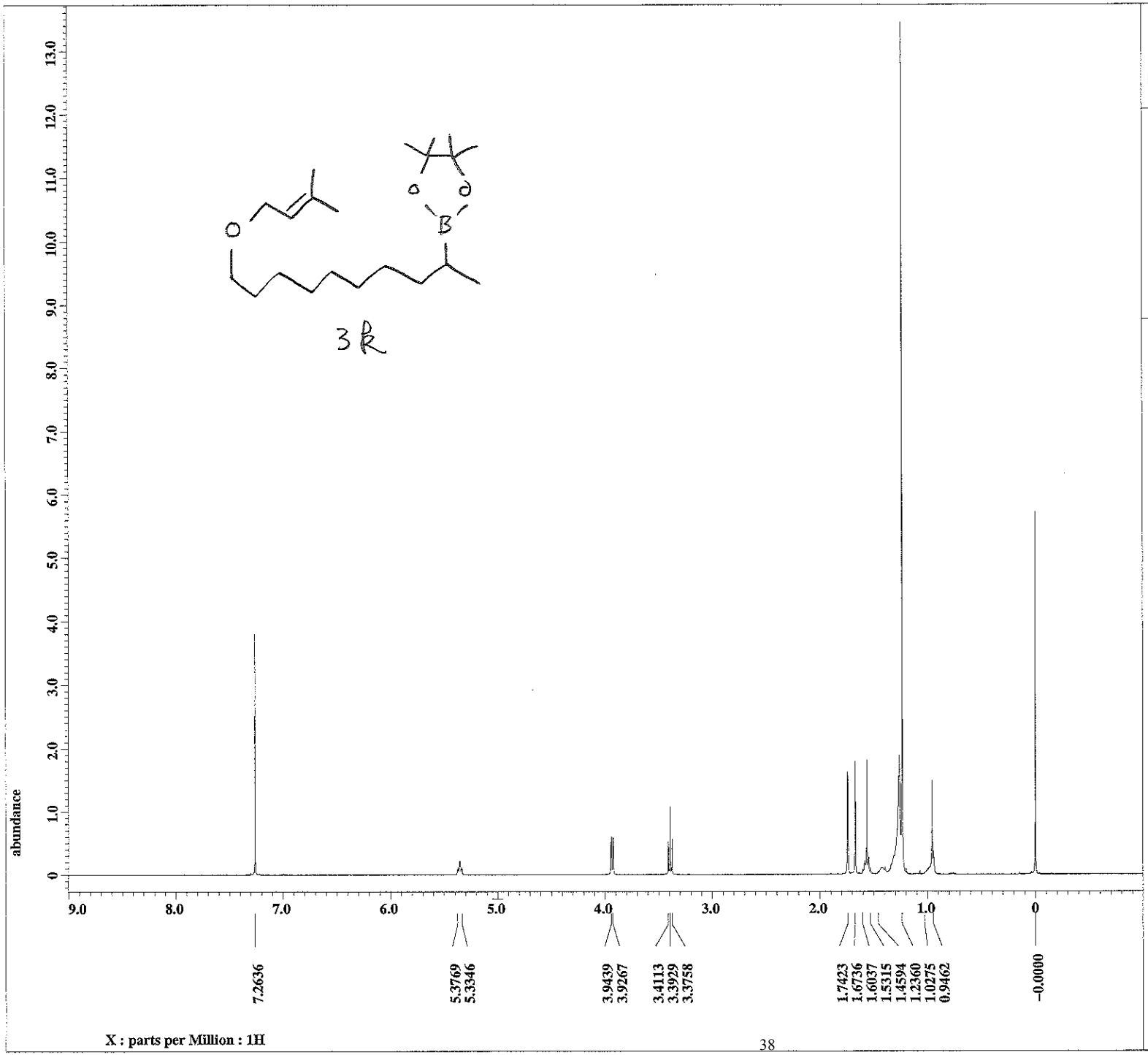
Filename	= IWA-872-pure-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#730205
Solvent	= CHLOROFORM-D
Creation_time	= 7-NOV-2015 19:44:29
Revision_time	= 4-DEC-2015 20:36:20
Current_time	= 4-DEC-2015 20:36:21
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 20.9[dC]



```
---- 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-859-carbon-1.jdf
```

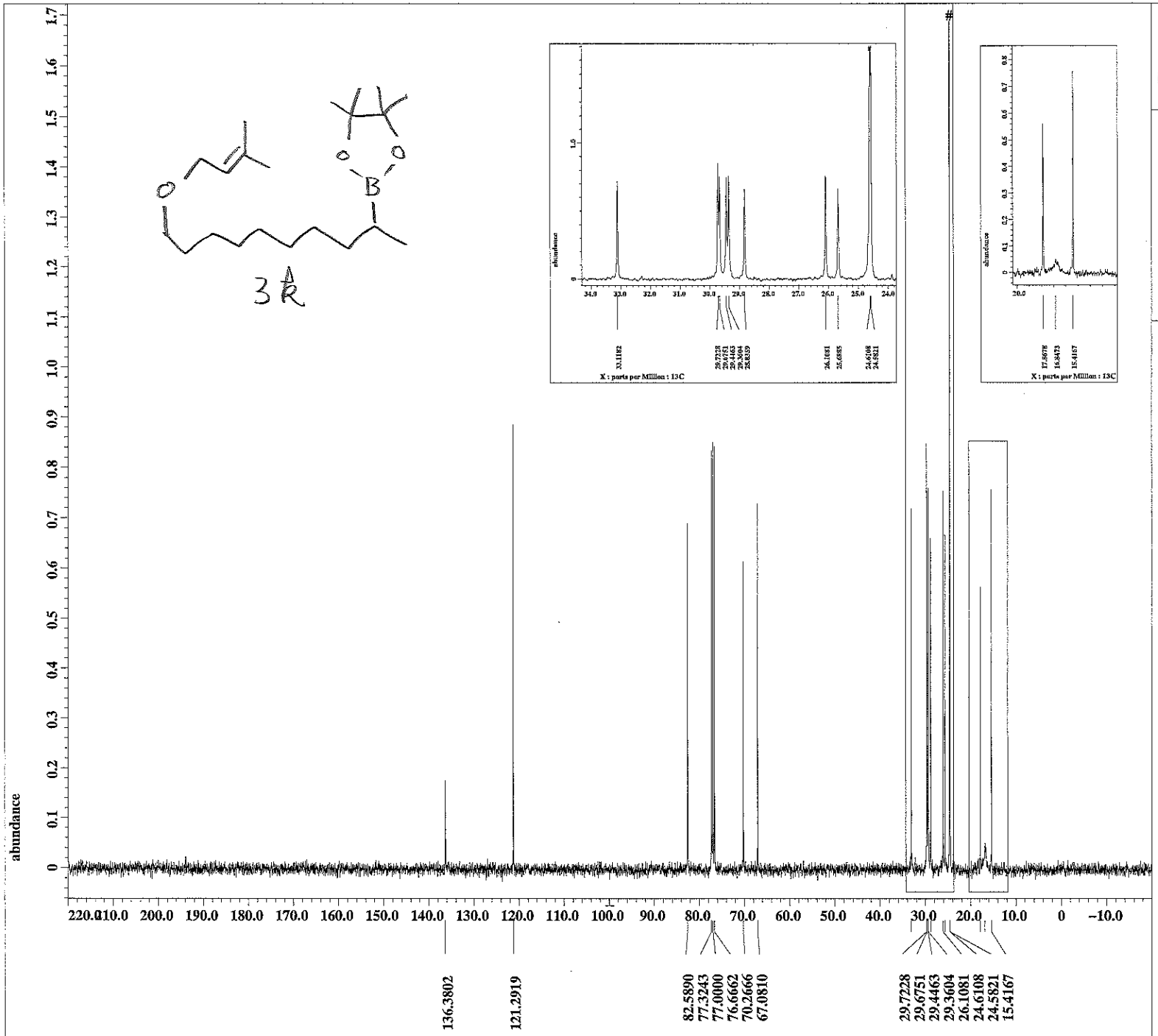
Filename	= IWA-859-carbon-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#747743
Solvent	= CHLOROFORM-D
Creation_time	= 28-OCT-2015 20:19:26
Revision_time	= 28-OCT-2015 20:53:34
Current_time	= 28-OCT-2015 20:55:18
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 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	= 107
Total_scans	= 107
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]



---- 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-857-pure-1.jdf

Filename	= IWA-857-pure-3.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#667969
Solvent	= CHLOROFORM-D
Creation_time	= 28-OCT-2015 18:02:09
Revision_time	= 28-OCT-2015 18:42:24
Current_time	= 28-OCT-2015 18:42:29
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.20197068[T] (390[MH
X_acq_duration	= 2.228224[s]
X_domain	= 1H
X_freq	= 391.78655441[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.44878791[Hz]
X_sweep	= 7.35294118[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	= 2.228224[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	= 44
Relaxation_delay	= 5[s]
Repetition_time	= 7.228224[s]
Temp_get	= 18.7[dC]




```
---- 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-857-carbon-1.jdf
```

Filename	= IWA-857-carbon-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#671432
Solvent	= CHLOROFORM-D
Creation_time	= 28-OCT-2015 18:11:56
Revision_time	= 28-OCT-2015 18:46:08
Current_time	= 28-OCT-2015 18:48:07
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	= 18.8[dC]