Mechanochemical Generation of Aryl Barium Nucleophiles from Unactivated Barium Metal

Koji Kubota[*a,b], Sota Kawamura[a], Julong Jiang[b,c], Satoshi Maeda[b,c], and Hajime Ito[*a,b]

[a]*Division of Applied Chemistry and Frontier Chemistry Center, Faculty of Engineering, Hokkaido University, Sapporo, Hokkaido, 060-8628, Japan.*
[b]*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Hokkaido 001-0021, Japan.*
[c]*Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Hokkaido, 060-0810, Japan*
e-mail: hajito@eng.hokudai.ac.jp, kbt@eng.hokudai.ac.jp

Table of contents

1. Chemicals and instrumentation

Materials were obtained from commercial suppliers and purified using standard procedures unless otherwise noted. Solvents were purchased from commercial suppliers and further dried over molecular sieve (MS 4Å). Barium pieces (> 99.99%, product no. 474711) were purchased from Aldrich and stored in a glovebox to prevent oxidation. All reactions were performed using grinding vessels in the Retsch MM 400 (Figure S1). Both jars and balls were made of stainless steel (SUS400B and SUS420J2, respectively, Figure S2). NMR spectra were recorded on JEOL JNM-EC X400P and JNM-ECS400 spectrometers (^{1}H: 392 or 396 or 399 or 401 MHz, ^{13}C: 99 or 100 MHz). Tetramethylsilane (^{1}H) and $CDCl_3$ (^{13}C) were employed as external standards, respectively. Multiplicity was recorded as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, and m = multiplet. 1,1,2,2-Tetrachloroethane, dibromomethane, and anisole were used as an internal standard to determine the NMR yields. Recycling preparative gel permeation chromatography (GPC) was conducted with a JAI LaboACE LC-5060 using $CHCl_3$ as the eluent with JAIGEL-1H. Preparative thin-layer chromatography (PTLC) was performed using Wakogel B5-F silica-coated plates (0.75 mm) prepared in our laboratory. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University.

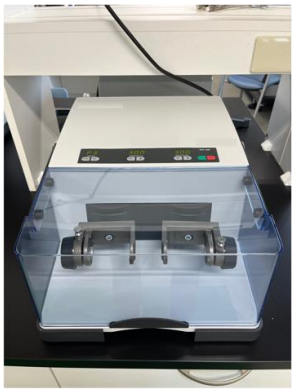


Figure S1. Retsch MM400 used in this study.

Figure S2. Stainless-steel jar (5 mL) and two stainless-steel balls (10 mm) used in this study.

2. List of substrates used in this study

Aryl halides, except **1k**, were obtained from commercial suppliers and were used as received. **1k** was synthesized according to the reported procedures.[1]

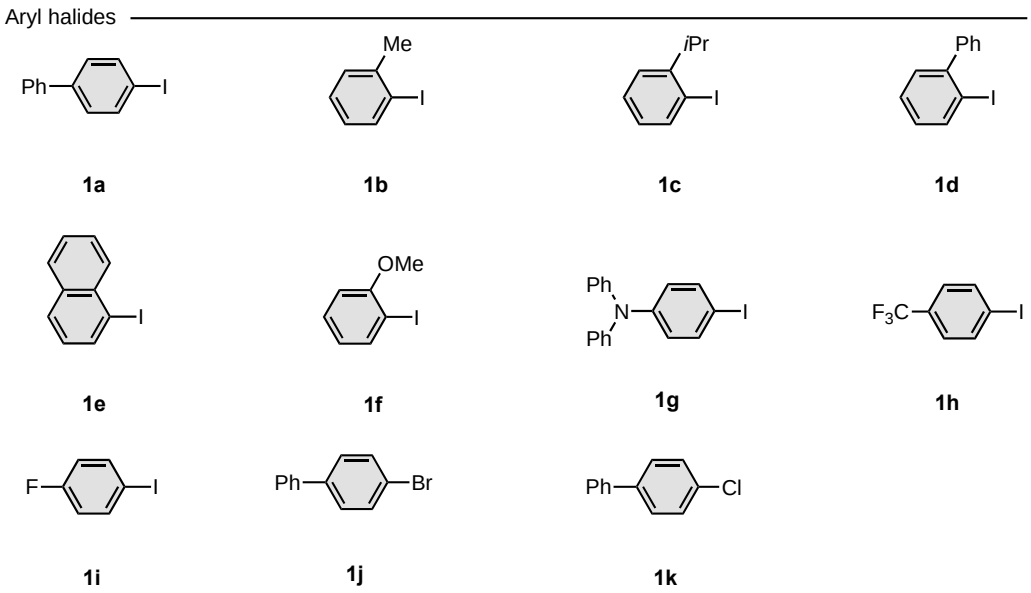


Figure S3. The list of aryl halides used in this study.

Electrophiles, except **3k**, were obtained from commercial suppliers. **3a**, **3b**, and **3d** were distilled before use. **3c**, **3e-3j**, and **5a-5e** were used as received. **3k** was synthesized according to the reported procedures.[2]

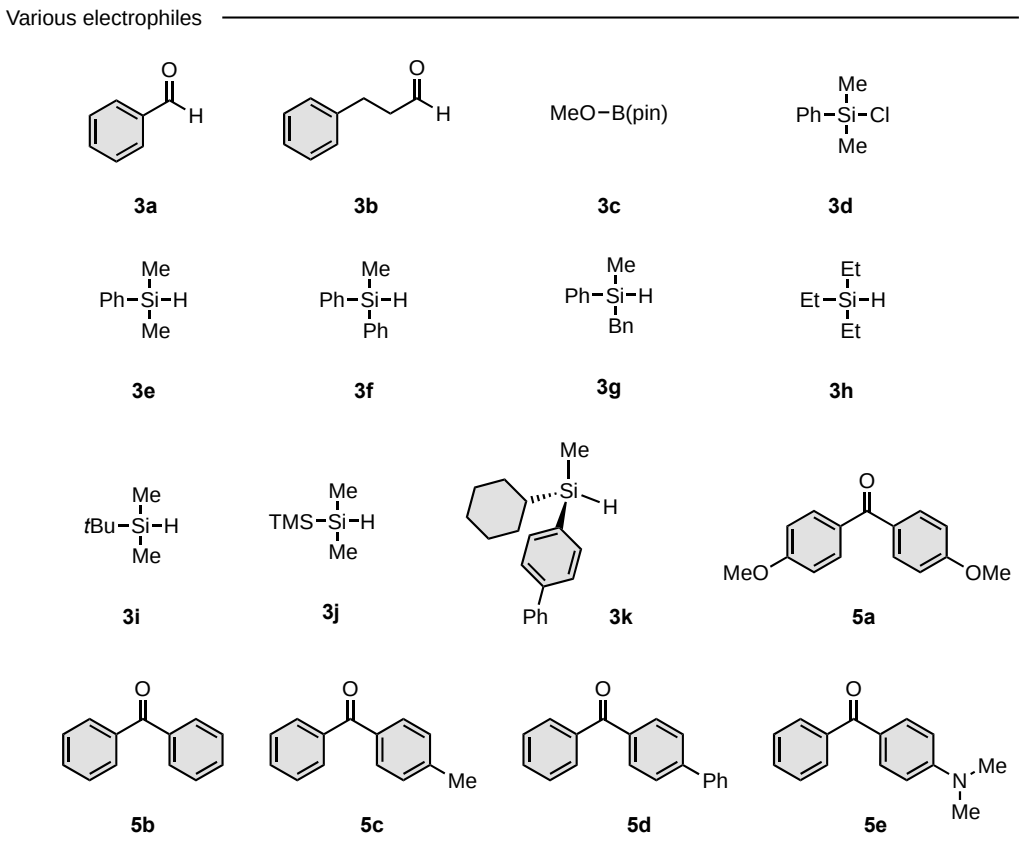
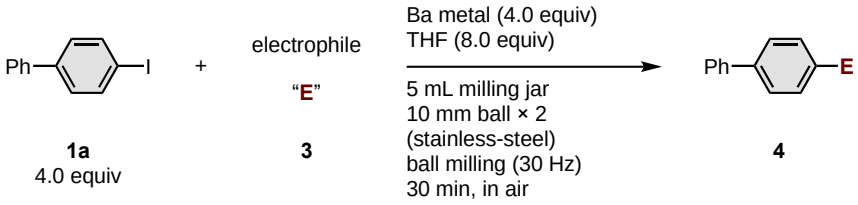


Figure S4. The list of electrophiles used in this study.

3. General procedure for the generation of aryl barium nucleophile and subsequent reactions with electrophiles

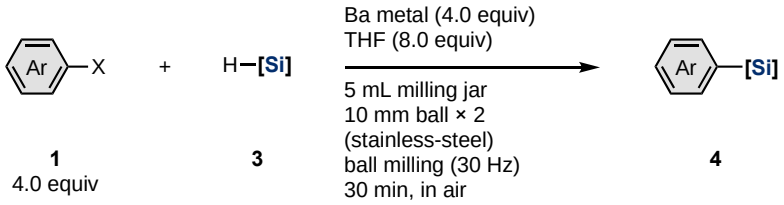
Caution: You should store barium metal in a glovebox, because barium metal is rapidly oxidated in air. If you use barium metal stored in air for a long time, reproducibility will become poor.

Procedure for nucleophilic addition to various electrophiles (A)



4-Iodobiphenyl (**1a**, 1.0 mmol, 4.0 equiv) was placed in a milling jar (stainless steel, 5 mL) loaded with two grinding balls (stainless-steel, diameter: 10 mm). The milling jar was then transferred to a glovebox. In a glovebox, Ba pieces (99.99 %, Aldrich) (137.3 mg, 1.0 mmol, 4.0 equiv) were placed in a milling jar. After the milling jar was removed from the glovebox, the jar was opened under air, and then an electrophile (**3a-d**, 0.25 mmol, 1.0 equiv) and THF (160 μL, 2.0 mmol, 8.0 equiv) were quickly added to the jar. After the jar was closed without purging with inert gas, the jar was placed in a ball mill (Retsch MM 400, 30 min, 30 Hz). After grinding for 30 min, the jar was opened in air, quenched with H_2O, and extracted with CH_2Cl_2 three times. The organic layer was washed with brine and dried over $MgSO_4$, and then filtrated. After the removal of the solvents under reduced pressure, yield of the corresponding products was determined by ^1H NMR analysis with tetrachloroethane or anisole as the internal standard.

Procedure for nucleophilic addition to hydrosilanes (B)

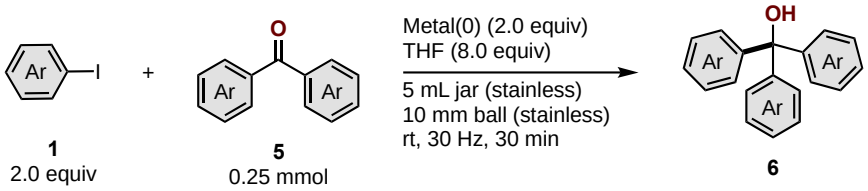


A solid organic halide (**1**, 1.0 mmol, 4.0 equiv) was placed in a milling jar (stainless steel, 5 mL) loaded with two grinding balls (stainless steel, diameter: 10 mm). The milling jar was then transferred to a glovebox. In a glovebox, Ba pieces (99.99 %, Aldrich) (137.3 mg, 1.0 mmol, 4.0 equiv) were placed in a milling jar. After the milling jar was removed from the glovebox, the jar was opened under air, then a hydrosilane (**3**, 0.25 mmol, 1.0 equiv) and THF (160 μL, 2.0 mmol, 8.0 equiv) were added to the jar. After the jar was closed without purging with inert gas, the jar was placed in a ball mill

(Retsch MM 400, 30 min, 30 Hz). After grinding for 30 min, the jar was opened in air, quenched with H_2O, and extracted with CH_2Cl_2 three times. The organic layer was washed with brine, dried over $MgSO_4$, and then filtrated. After the removal of the solvents under reduced pressure, the NMR yield of the corresponding products was determined by ^1H NMR analysis with tetrachloroethane or anisole as the internal standard. The crude material was purified by recycling gel permeation chromatography (GPC) using $CHCl_3$ as the eluent or flash column chromatography (SiO_2, only hexane) or preparative thin-layer chromatography (PTLC) to give the corresponding product.

When a liquid organic iodide **1** was used, **1** was added to the jar at the same time as a hydrosilane and THF.

Procedure for nucleophilic addition to diaryl ketones (C)



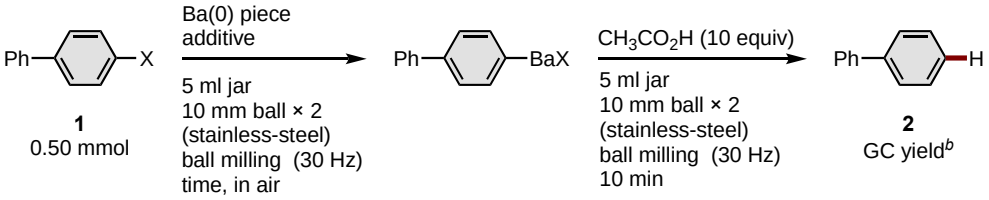
A solid organic halide (**1**, 0.50 or 0.375 mmol, 2.0 or 1.5 equiv) was placed in a milling jar (stainless steel, 5 mL) loaded with two grinding balls (stainless steel, diameter: 10 mm). The milling jar was then transferred to a glovebox. In a glovebox, Ba pieces (99.99 %, Aldrich) (0.50 or 0.375 mmol, 2.0 or 1.2 equiv) were placed in a milling jar. After the milling jar was removed from the glovebox, the jar was opened under air, then a diaryl ketone (**5**, 0.25 mmol, 1.0 equiv) and THF (160 μL, 2.0 mmol, 8.0 equiv) were added to the jar. After the jar was closed without purging with inert gas, the jar was placed in a ball mill (Retsch MM 400, 30 min, 30 Hz). After grinding for 30 min, the jar was opened in air, quenched with H_2O, and extracted with CH_2Cl_2 three times. The organic layer was washed with brine, dried over $MgSO_4$, and then filtrated. After the removal of the solvents under reduced pressure, the NMR yield of the corresponding products was determined by ^1H NMR analysis with dibromomethane as the internal standard. The crude material was purified by flash column chromatography (SiO_2, typically hexane/CH_2Cl_2 = 50/50, then hexane/Et_2O =95/5 to 75/25).

When a liquid organic iodide **1** was used, **1** was added to the jar at the same time as the hydrosilane and THF.

4. Protonation and deuteration experiments

Aryl barium species are highly unstable. Once formed under mechanochemical conditions, they can decompose rapidly. Therefore, the mass balance did not match in the following protonation experiments. The crude reaction mixture was carefully checked, but no byproducts were detected.

Table S1. Optimization study on protonation

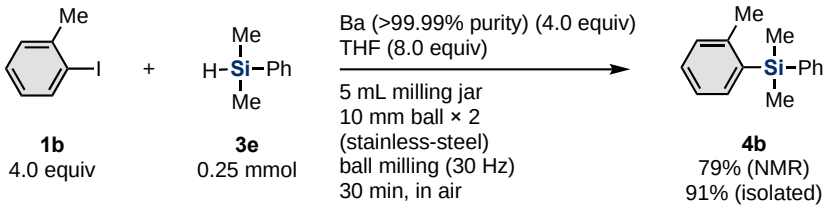


entry	halide	Ba (equiv)	additive	time	yield of **2** (%)	conversion of **1a, j** (%)
1	**1j** (X = Br)	1.0	THF (2.0 equiv)	60 min	29	63
2	**1j**	1.0	MTBE (2.0 equiv)	60 min	11	45
3	**1j**	1.0	2-MeTHF (2.0 equiv)	60 min	16	39
4	**1j**	1.0	1,4-dioxane (2.0 equiv)	60 min	13	29
5	**1j**	1.0	THP (2.0 equiv)	60 min	16	41
6	**1a** (X = I)	1.0	THF (2.0 equiv)	60 min	52	>99
7	**1a**	1.0	THF (2.0 equiv)	30 min	52	>99
8	**1a**	1.0	THP (2.0 equiv)	30 min	22	37
9	**1a**	1.0	none	30 min	33	>99
10[c]	**1a**	1.0	THF (2.0 equiv)	30 min	44	97
11[c]	**1a**	1.5	THF (2.0 equiv)	30 min	54	>99
12	**1a**	1.0	THF (4.0 equiv)	30 min	52	98
13	**1a**	2.0	THF (2.0 equiv)	30 min	50	>99
14	**1a**	2.0	THF (4.0 equiv)	30 min	29	>99
15	**1k** (X = Cl)	1.0	THF (2.0 equiv)	30 min	11	28

[a]Reactions were performed using Retsch MM400, a stainless-steel milling jar (5 mL), and a stainless-steel balls (10 mm × 2). Conditions: **1a** or **1j** (0.50 mmol), Barium (>99.99 %, Aldrich) (1.0–2.0 equiv), additive (2.0–4.0 equiv). [b]Yields were determined by GC analysis with dibenzyl as an internal standard. [c]Barium (>99.99%, Aldrich) that was stored under air for 1 month was used.

5. Reaction using barium metal with different purity

1. Dendritic pieces, purified by distillation, >99.99%, Aldrich-474711

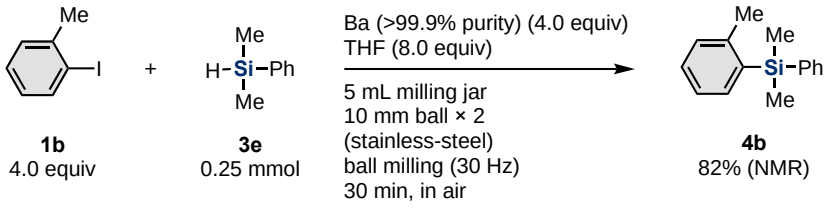


1b
4.0 equiv

3e
0.25 mmol

4b
79% (NMR)
91% (isolated)

2. Dendritic pieces, purified by distillation, >99.9%, Aldrich-441880



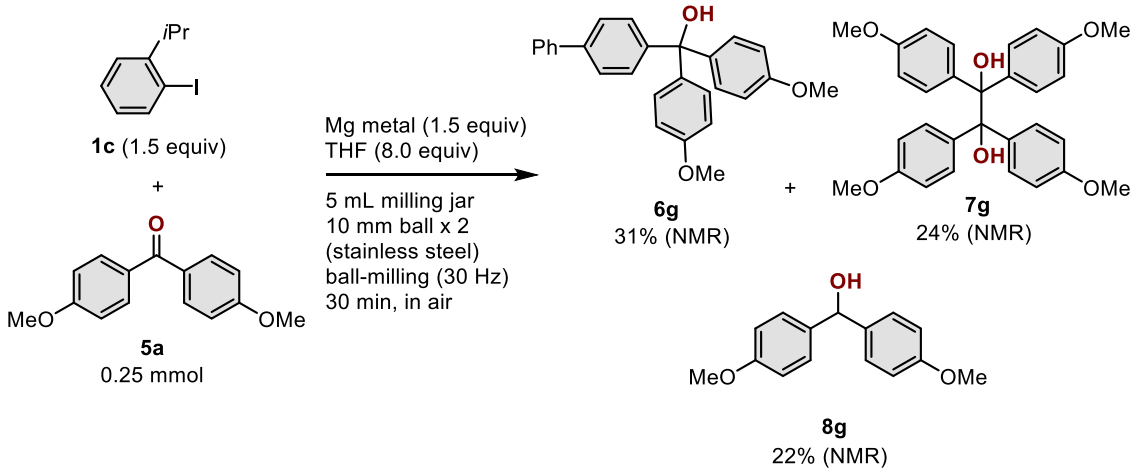
1b
4.0 equiv

3e
0.25 mmol

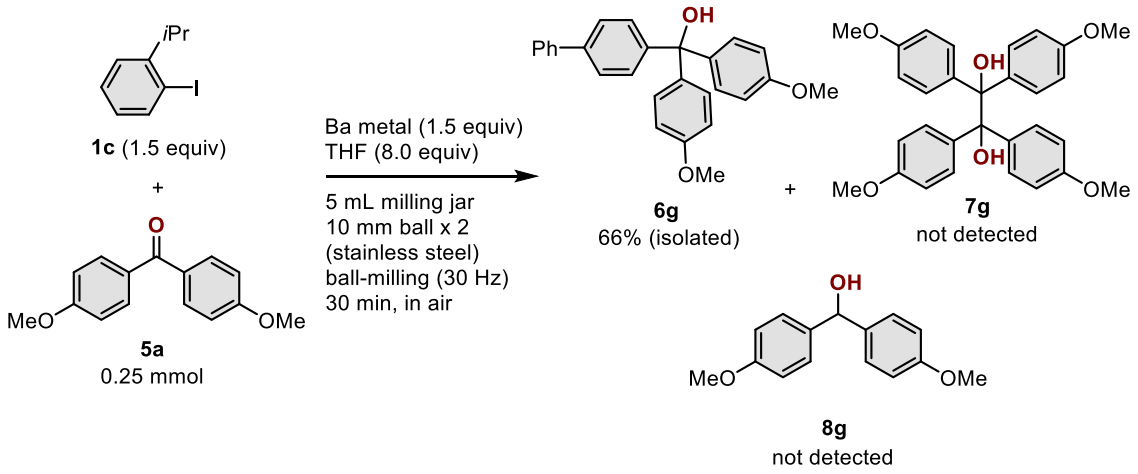
4b
82% (NMR)

6. Barbier-type ketone arylation with 1c and magnesium metal

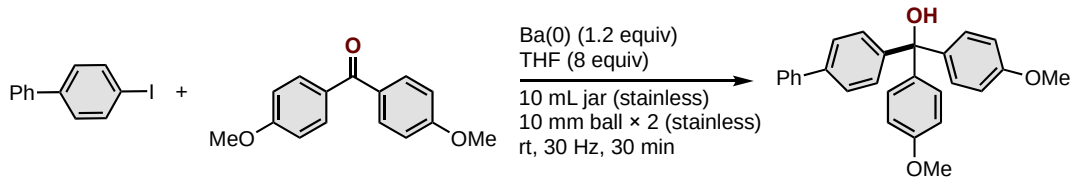
The reaction of sterically hindered **1c** in the presence of magnesium metal afforded the desired product **6g** in poor yield (31%), and significant amounts of other byproducts were formed (pinacol coupling byproduct **7g**: 24%; reduction byproduct **8g**: 22%).



In contrast, the reaction of **1c** with barium metal proceeded smoothly to give the desired tertiary alcohol **6g** in a better yield (66%) without the generation of these byproducts.



7. Details of scaled-up reaction



1d
1.2 equiv

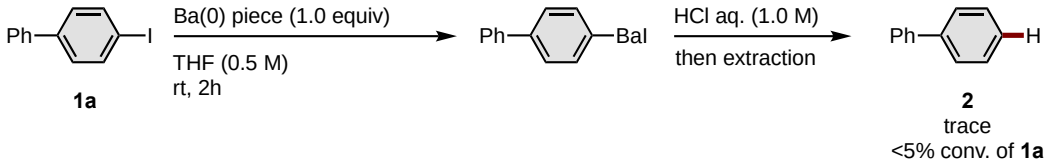
5a
2.5 mmol

6a
77% (isolated)
758 mg

1d (841.9 mg, 3.0 mmol, 1.2 equiv) was placed in a milling jar (stainless steel, 10 mL) loaded with two grinding balls (stainless steel, diameter: 10 mm). The milling jar was then transferred to a glovebox. In a glovebox, Ba pieces (99.99 %, Aldrich) (435.4 mg, 3.0 mmol, 1.2 equiv) were placed in a milling jar. After the milling jar was removed from the glovebox, the jar was opened under air, then a di(4-methoxyphenyl)ketone (**5a**, 605.6 mg 2.5 mmol, 1.0 equiv) and THF (1.6 mL, 20 mmol, 8.0 equiv) were added to the jar. After the jar was closed without purging with inert gas, the jar was placed in a ball mill (Retsch MM 400, 30 min, 30 Hz). After grinding for 30 min, the jar was opened in air, quenched with H_2O, and extracted with CH_2Cl_2 three times. The organic layer was washed with brine, dried over $MgSO_4$, and then filtrated. After the removal of the solvents under reduced pressure, the NMR yield of the corresponding products was determined by ^1H NMR analysis with dibromomethane (314.6 mg) as the internal standard. The crude material was purified by flash column chromatography (SiO_2, hexane/CH_2Cl_2 = 50/50, then hexane/Et_2O = 95/5 to 85/15) to give the corresponding product **6a** in 77% yield (757.8 mg, 1.91 mmol) as a white solid.

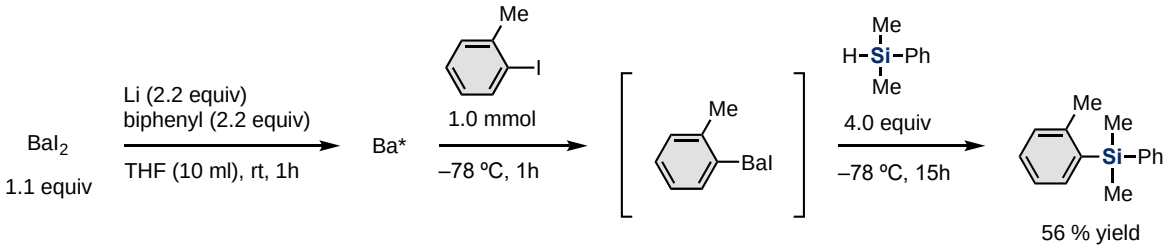
8. Details of solution-based reactions

Procedure for solution-based reaction with unactivated barium



Commercially available Ba pieces (99.99 %, Aldrich) 69.1 mg, 0.50 mmol, 1.0 equiv) were placed in an oven-dried reaction tube. After being sealed with a screw cap containing a Teflon™-coated rubber septum, the vial was connected to a nitrogen line through a needle. 4-Iodobiphenyl (**1a**, 141.9 mg, 0.50 mmol, 1.0 equiv) and THF (1.0 mL) were added to the vial, and then the reaction mixture was stirred at rt for 2 h. After 2 h, the reaction mixture was quenched with 1M HCl, and extracted with ethyl acetate three times. The organic layer was washed with brine, dried over $MgSO_4$, and then filtrated. Dibenzyl (51.4 mg) was added to the solution as the internal standard, followed by GC analysis. The yields of protonation compound **2** and the conversion of **1a** were determined by GC.

Procedure for solution-based substitution reaction with Rieke barium

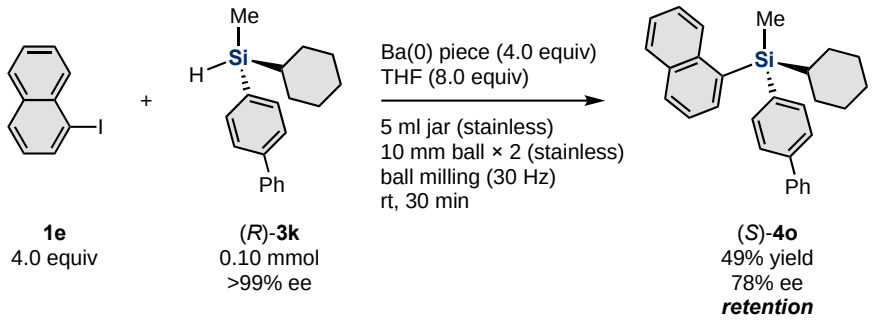


According to Rieke's method,[3] lithium (2.2 mmol, 15.0 mg) and biphenyl (2.2 mmol, 344.7 mg) in dry THF (5.0 mL) were stirred under N_2 for 2 h. To a well-suspended solution of BaI_2 (1.1 mmol) in dry THF (5.0 mL), the prepared lithium biphenylide was transferred via a disposable syringe at room temperature. The reaction mixture was stirred for 1 h at room temperature. Theoretically, 1.1 mmol Rieke barium should be generated in situ.

The above suspension was cooled to –78 ºC. Then, 2-iodotoluene (**1b**, 221.6 mg, 1.0 mmol) was added via a disposable syringe at –78 ºC under N_2, and the mixture was allowed to warm to rt and stirred for 1 h. Then, hydrosilane (**3e**, 610 μL, 4.0 mmol) was added at rt. The resulting mixture was stirred for 15 h. Finally, the mixture was quenched with NH_4Cl aq and extracted with Et_2O three times. The organic layer was washed with brine, dried over $MgSO_4$, and then filtrated. After the removal of the solvents under reduced pressure, the resulting crude mixture was analyzed by ^1H NMR with tetrachloroethane (27.5 mg) as an internal standard to obtain the NMR yield of **4b** in 56% yield.

9. Details of mechanistic study

Procedure for the reaction with chiral hydrosilanes (*R*)-3i



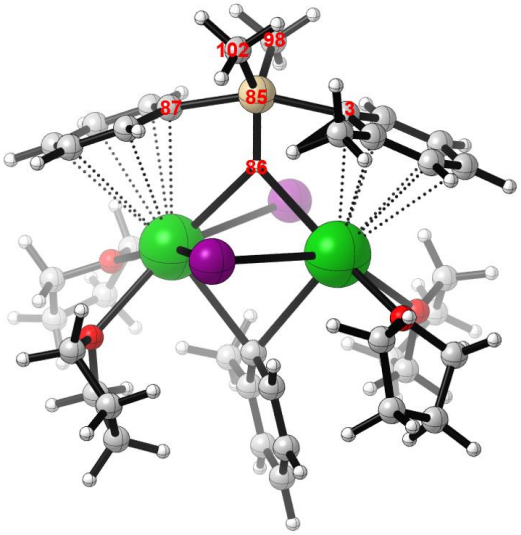
Two grinding balls (stainless, diameter: 10 mm) were placed in a milling jar (stainless, 5 mL). The milling jar was then transferred to a glovebox. In the glovebox, Ba pieces (99.99 %, Aldrich) (59.2 mg, 0.43 mmol, 4.3 equiv) were placed in a milling jar. After the milling jar was removed from glovebox, the jar was opened under air, then 1-iodonaphthalene (**1e**, 99.4 mg, 0.39 mmol, 3.9 equiv), a chiral hydrosilane [(*R*)-**3i**, 28.5 mg, 0.10 mmol, 1.0 equiv] and THF (65 μL, 0.8 mmol, 8.0 equiv) were added to the jar. After the jar was closed without purging with inert gas, the jar was placed in a ball mill (Retsch MM 400, 30 min, 30 Hz). After grinding for 30 min, the jar was opened in air, quenched with H_2O, and extracted with CH_2Cl_2 three times. The organic layer was washed with brine and dried over $MgSO_4$, and then filtrated. After the removal of the solvents under reduced pressure, the NMR yield of the corresponding products was determined by ^{1}H NMR analysis with tetrachloroethane (32.6 mg) as the internal standard. The crude material was purified by flash column chromatography (SiO_2, only hexane) and then purified by recycling gel permeation chromatography (GPC) using $CHCl_3$ as the eluent to give the corresponding product (*S*)-**4o** in 49% yield (20.1 mg, 0.05 mmol, 78% ee) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.68 (s, 3H), 1.07–1.43 (m, 5H), 1.47–1.62 (m, 1H), 1.62–1.80 (m, 4H), 1.94 (d, J = 10.4 Hz, 1H), 7.29–7.37 (m, 2H), 7.38–7.64 (m, 10H), 7.79 (d, J = 6.1 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): –4.4 (*C*H$_3$), 25.2 (*C*H), 27.0 (*C*H$_2$), 28.1 (*C*H$_2$), 28.35 (*C*H$_2$), 28.40 (*C*H$_2$), 125.2 (*C*H), 125.5 (*C*H), 125.7 (*C*H), 126.6 (*C*H), 127.2 (*C*H), 127.5 (*C*H), 128.9 (*C*H), 129.0 (*C*H), 129.1 (*C*H), 130.3 (*C*H), 133.6 (*C*), 134.5 (*C*), 135.2 (*C*H) 135.4 (*C*H), 136.4 (*C*), 137.4 (*C*), 141.1 (*C*), 141.6 (*C*). EI (m/z): $[M]^+$ calcd for $C_{29}H_{30}Si$: 406.2111, found: 406.2105. $[\alpha]_D^{26}$ –7.9 (c 1.61 in $CHCl_3$, 78% ee). Daicel CHIRALCEL® OD-3, hexane 100%, 0.5 mL/min, 40 °C, *S* isomer: t_S = 36.08 min; for the racemic compound: *R* isomer: t_R = 30.19 min, *S* isomer: t_S = 37.87 min.

10. Computational details

As it is difficult to determine the structure of ArBaI in a solid state, the AFIR method[4] is used to suggest the possible geometry of both the monomeric and dimeric species via a comprehensive and unbiased sampling calculation. This initial sampling calculation was conducted at the semi-empirical GFN-xTB level of theory[5] as implemented in ORCA 4.0, [6] and a collision energy of 200 kJ·mol^{-1} was applied to the entire molecule for any possible bond rearrangements.[4] The AFIR sampling calculation rendered in total 3729 possible isomers and conformers for dimeric ArBaI(THF)$_2$, of which the ones having the lowest energies were further reoptimized at the DFT level of theory with the B3LYP hybrid functional[7] as implemented in Gaussian 16.[8] Note that the energy profile shown in this study was generated with the geometries and energies derived from the following DFT calculations. In order to describe the dispersion properly, an explicit dispersion correction term called GD3,[9] was also employed in the DFT calculations. The polarized triple-ζ 6-311G(d,p) basis set[10] was used for C, H, O, and Si atoms during both the geometry optimization and the single-point calculation processes. The Stuttgart/Dresden pseudo-potential basis set SDD,[11] as well as a *d*-polarization function,[12] are used for Ba (ζ = 0.438) and I (ζ = 0.289) atoms. All the minima and transition states were fully optimized without any constraints. Frequency calculations were carried out to characterize all the optimized structures as minima or transition states. Transition states were identified by having one imaginary frequency. An intrinsic reaction coordinate (IRC) calculation[13] was performed for each transition state to ensure that it connected the correct reactants and products. The free energies were computed at 298.15 K and 1 atm. All the geometries shown in this article are visualized by the CYLview software.[14]

NBO Analysis on Intermediate II



Bonding orbitals involving Si atom

(Occupancy) Bond orbital/ Coefficients/ Hybrids

9. (1.62375) BD (1) C 3 -Si 85

(81.67%) 0.9037* C 3 s(21.09%)p 3.74(78.90%)d 0.00(0.01%)

(18.33%) 0.4281*Si 85 s(18.24%)p 2.83(51.58%)d 1.66(30.18%)

88. (1.81345) BD (1)Si 85 - H 86

(25.64%) 0.5064*Si 85 s(16.22%)p 3.90(63.34%)d 1.26(20.44%)

(74.36%) 0.8623* H 86 s(99.91%)p 0.00(0.09%)

89. (1.74000) BD (1)Si 85 - C 87

(17.89%) 0.4229*Si 85 s(18.03%)p 2.93(52.81%)d 1.62(29.16%)

(82.11%) 0.9062* C 87 s(26.74%)p 2.74(73.26%)d 0.00(0.01%)

90. (1.94672) BD (1)Si 85 - C 98

(26.62%) 0.5159*Si 85 s(23.66%)p 2.91(68.96%)d 0.31(7.37%)

(73.38%) 0.8566* C 98 s(32.03%)p 2.12(67.91%)d 0.00(0.05%)

91. (1.93477) BD (1)Si 85 - C 102

(26.07%) 0.5106*Si 85 s(24.05%)p 2.74(65.84%)d 0.42(10.11%)

(73.93%) 0.8598* C 102 s(32.14%)p 2.11(67.81%)d 0.00(0.05%)

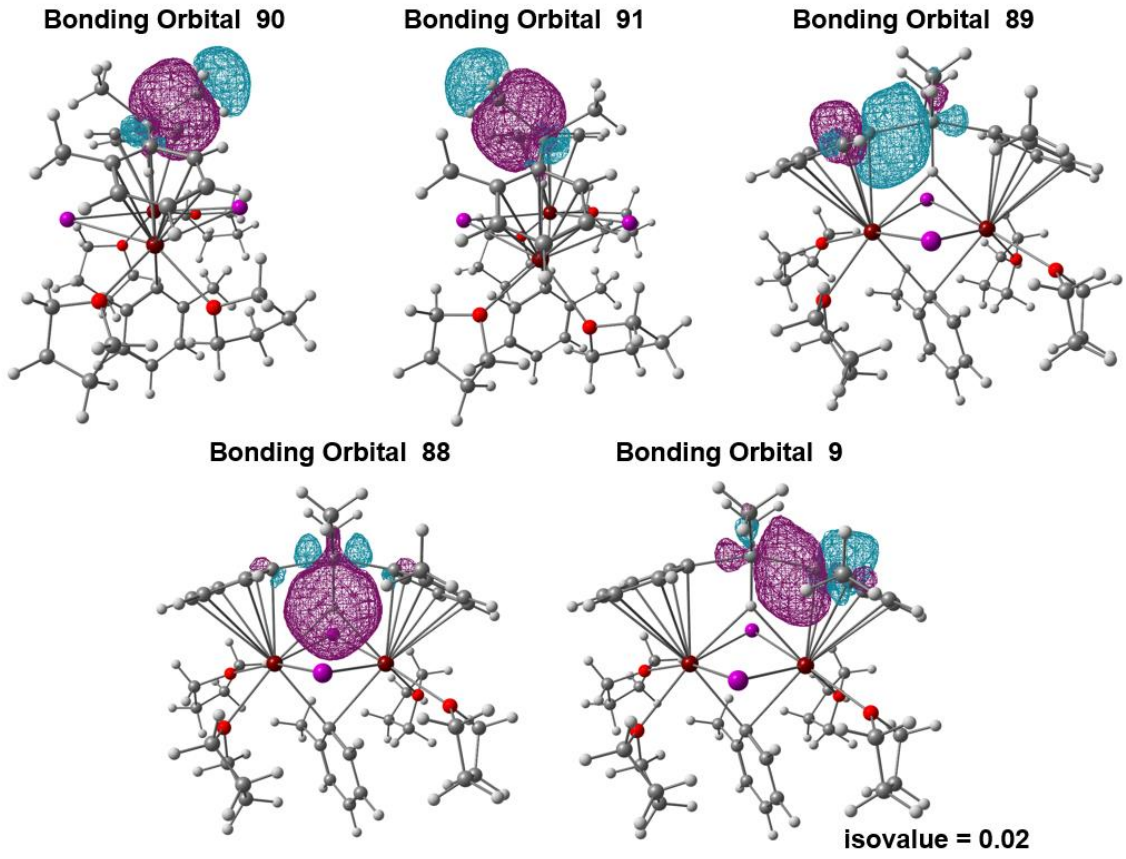


Figure S5. Visualised bonding orbitals involving the Si atom

Cartesian Coordinates of Optimized Structures

(**E**: Electronic Energy; **G**: Gibbs Free Energy at 298.15 Kelvin and under 1 atm)

M

(**E =** -773.13566312 a.u.; **G** = -772.84639608 a.u.)

0 1

C	-0.036517556013	-6.783214924819	4.427970938485
C	-0.893523270465	-5.705223841684	4.183202298798
C	-0.532921403465	-4.654590471228	3.306375160038
C	0.737354496103	-4.763339620861	2.708047068188
C	1.606373114511	-5.835568474701	2.945458051636
C	1.213988938233	-6.852313264665	3.810453641672
H	-0.339465405460	-7.578790654058	5.104977007953
H	1.079027879957	-3.986203222369	2.020439394793
H	2.577184358572	-5.876251076766	2.459606781025
H	1.871685538278	-7.692736937031	4.006936132036
Ba	-1.911405475589	-2.474663235208	2.466957356781
O	-0.624303017405	-1.286210744773	4.560818495655
C	0.283305138384	-0.177205627753	4.338839892670
C	0.024950699582	-2.113220585371	5.561409198964
C	1.668455536826	-0.825438569594	4.300288415703
H	0.177665568556	0.531741250052	5.169545537595
H	0.001577042112	0.304806843003	3.402519620451
C	1.522597688822	-2.072751394825	5.214771649866
H	-0.182242885887	-1.683468476888	6.548696157416
H	-0.402644817640	-3.112543170802	5.490057250075
H	1.896639269576	-1.120942293038	3.274922640002
H	2.445815316928	-0.138531217750	4.638397583615
H	2.130135126694	-1.998537221297	6.118371651410
H	1.808008903242	-2.980514631665	4.682855708679
O	-2.623907969352	-4.193749103827	0.463069241534
C	-2.509488029664	-5.625524460742	0.677433424141
C	-2.143550730519	-3.967944152956	-0.886915091443
C	-1.244807764868	-6.066037320055	-0.085830025254
H	-3.414762016201	-6.103742391581	0.286168189221
H	-2.435061436945	-5.791918596830	1.751139471527
C	-0.899573679502	-4.847709317213	-0.981560938686

H	-2.925357480696	-4.273270605387	-1.593953059752
H	-1.939759834721	-2.902813746001	-0.997686719397
H	-0.434101220310	-6.282066839714	0.609594329770
H	-1.443673096280	-6.962794335616	-0.675619965803
H	-0.669437023935	-5.125145195490	-2.011314761801
H	-0.046103476034	-4.300583523859	-0.576475146059
I	0.041614611162	-0.823421410377	0.387277455791
C	-2.245803399108	-5.658546059295	4.873526612416
H	-3.065430234129	-5.640507435292	4.143152384565
H	-2.415526728127	-6.517499394930	5.528467489149
H	-2.345489235476	-4.754844658738	5.488053842075

D

(**E** = -1546.33776865 a.u.; **G** = -1545.72917366 a.u.)

0 1

C	-6.821684757979	-0.922524167192	-0.477972356623
C	-5.477501328414	-1.284431286895	-0.332991848294
C	-4.429481067533	-0.463878073595	-0.817459009189
C	-4.841393300276	0.711704176674	-1.472850298194
C	-6.181013317308	1.085489931153	-1.638261288483
C	-7.178970866302	0.261582679489	-1.127759958181
H	-7.604758112356	-1.566556079050	-0.082709012924
H	-4.092927170800	1.402872347303	-1.880470989703
H	-6.441047162631	2.007246455506	-2.151924000349
H	-8.224933539996	0.531827559746	-1.232935650320
Ba	-1.735849652464	-0.202806306015	-0.340152420564
O	-1.710010225089	-2.380544213676	1.285473165325
C	-1.497576400031	-3.721891207963	0.772272882705
C	-1.498285142524	-2.356192004980	2.724114144769
C	-0.690665583483	-4.431150017878	1.852994554855
H	-0.977048351160	-3.636034978671	-0.183200024002
H	-2.474127278573	-4.191324853641	0.613325134963
C	-1.261549045559	-3.810271576668	3.137008086673
H	-0.627144648725	-1.730862065749	2.922207781972
H	-2.381118890409	-1.911331788341	3.189366395138
H	-0.803854457717	-5.515809823733	1.811431316200

H	0.367461622260	-4.181238496008	1.752419535182
H	-0.580493050174	-3.882232136616	3.986155564751
H	-2.204225463678	-4.295219268356	3.406256593713
O	-2.858911810760	1.210854914271	1.742378630198
C	-4.040908275687	0.689473040597	2.393652872448
C	-3.007020013835	2.647931807218	1.740309477902
C	-5.193989966994	1.628813145206	1.995293020814
H	-3.863374125467	0.688324459319	3.476482090430
H	-4.184056687235	-0.331276090057	2.042833952134
C	-4.483289665452	2.879905657137	1.415104196837
H	-2.740177580185	3.031001885388	2.734381571036
H	-2.307864894605	3.052037496777	1.007254315970
H	-5.824193019779	1.161961490404	1.239822415203
H	-5.811460764495	1.872329252262	2.862233933447
H	-4.849133470710	3.815133197039	1.842763044426
H	-4.626925512488	2.915192314466	0.335135748041
I	-0.093807556248	2.949187455923	-1.355549575069
C	-5.140438431351	-2.599301005557	0.347077813535
H	-4.249984449239	-2.498516332970	0.974402421670
H	-5.963040689967	-2.974937404295	0.964399313098
H	-4.911618439680	-3.370157998366	-0.398635841088
C	1.533816688045	-0.275991496492	3.789584645557
C	1.093069934775	0.291061576063	2.584109774693
C	1.270720199635	-0.372857712155	1.341294378511
C	1.877244454367	-1.645467210873	1.424583569922
C	2.319846838606	-2.223521073251	2.619502131963
C	2.154636367303	-1.525055894889	3.813427648073
H	1.388861644535	0.261790699516	4.724028089268
H	1.998783054401	-2.235621483868	0.512831317774
H	2.782251378056	-3.207036764885	2.622763728284
H	2.495565788330	-1.948137427265	4.752636322570
Ba	2.314427967602	0.554183859995	-1.062218901466
O	4.593897065662	-0.993527298210	-1.243223955235
C	4.525358818843	-2.434309122458	-1.404546381723
C	5.762616518233	-0.749896977932	-0.435737889328
C	5.046777390767	-3.025837650283	-0.077169462670

H	5.159926253565	-2.715678712540	-2.251545626820
H	3.491622817303	-2.687837780448	-1.638852506646
C	5.681831825680	-1.815930126152	0.656867620473
H	6.660140106789	-0.868257163203	-1.056519064706
H	5.707391823948	0.278730769260	-0.080443850061
H	4.235134005682	-3.452920249721	0.511527103362
H	5.775718727417	-3.815286850625	-0.266916977387
H	6.657798832361	-2.043066668011	1.088728123000
H	5.020902650030	-1.476540715688	1.456770587953
O	3.945776483217	1.999037677843	0.625089355037
C	3.908245213388	3.444803656625	0.622936556530
C	4.291972672842	1.574739853138	1.973252691857
C	3.290367015077	3.799555464972	1.969381099674
H	3.309464215111	3.763750737566	-0.232745552320
H	4.929160515623	3.833466518382	0.518631600501
C	3.879554573876	2.727312963846	2.912654333346
H	3.750409640061	0.649971545739	2.167659727467
H	5.369587386690	1.384830550143	2.012658887078
H	3.528667091580	4.817445229458	2.281448847061
H	2.206180266361	3.704745194179	1.903133665270
H	3.150833149944	2.390123711844	3.648888409896
H	4.749001363787	3.112500405642	3.449093946012
I	0.539031405096	-1.995073933120	-2.508629392686
C	0.368770152556	1.619649996563	2.638662006195
H	0.740549362044	2.267891276233	3.438264207050
H	0.445070880634	2.149053634276	1.687003779418
H	-0.698298994715	1.458736901151	2.821082706801

$PhSiMe_2H$

(**E =** -601.71921955 a.u.; **G** = -601.58370268 a.u.)

0 1

Si	-1.385363494180	-0.036329245336	-0.486558522759
H	-0.501285387209	1.093637542512	-0.079494572390
C	-0.394537337406	-1.639645766068	-0.378165537248
C	0.199922071347	-2.023478357081	0.835724437178
C	-0.236512105323	-2.493912079530	-1.479831767433

C	0.919842193304	-3.209966299574	0.946398792024
C	0.482902298984	-3.684087324700	-1.375563416319
C	1.062190699983	-4.044471879901	-0.161664457590
H	0.104147398918	-1.386690125407	1.710887099089
H	-0.678261149075	-2.232586761428	-2.436076992672
H	1.370710734949	-3.484113805454	1.894074920022
H	0.591350997937	-4.328294180441	-2.241487877401
H	1.622758506422	-4.969061647507	-0.078393353919
C	-1.985074559581	0.251189769698	-2.249595902819
H	-1.150486136264	0.307277728552	-2.953753215911
H	-2.650970000094	-0.552871393739	-2.576962635933
H	-2.541120414323	1.190619405427	-2.315523851868
C	-2.844074429282	-0.109262427739	0.707093351586
H	-3.407929483836	0.828224897107	0.700994506574
H	-3.526523679817	-0.919129048322	0.433122564008
H	-2.506496711564	-0.291266468859	1.731229820513

I

(**E** = -2148.08802654 a.u.; **G** = -2147.32014055 a.u.)

0 1

C	5.144042301993	-3.610564244093	0.030023444564
C	4.465189471114	-2.448350567362	-0.354405231232
C	3.934023531774	-1.541159469955	0.599898388235
C	4.142207714899	-1.897274503480	1.945728286844
C	4.830251545128	-3.048488875625	2.347607930955
C	5.333236259867	-3.913284910919	1.380446840423
H	5.534530315360	-4.288672965810	-0.726340537240
H	3.726103291814	-1.270923357799	2.737781012662
H	4.960738906099	-3.274604042924	3.402718921429
H	5.864442937995	-4.815190315987	1.668166153432
Ba	2.009761142274	0.278260633851	-0.172266671463
O	-4.328258486957	0.074001639952	1.341082872648
C	-4.304160910156	0.168434708946	2.785197187963
C	-5.661333336404	0.435440612512	0.938701503847
C	-5.232367739382	1.350388378421	3.136459952053
H	-3.265187479464	0.299424473422	3.086151545539

H	-4.675424477915	-0.775670432123	3.199475220614
C	-5.996852268959	1.642012731550	1.816999262902
H	-5.635051096188	0.636932629581	-0.131728059955
H	-6.337380911665	-0.407976799831	1.132695276022
H	-5.911079330360	1.080970337500	3.947199065787
H	-4.658361453025	2.219663822498	3.457294915567
H	-5.618656617312	2.553711746290	1.350131209307
H	-7.071424388331	1.759326918340	1.965212791134
O	2.984340746887	2.302506691242	1.388176883162
C	2.217592307009	3.495250665061	1.660022175926
C	3.672719939348	1.990653186695	2.619990569881
C	1.637829507380	3.262805493773	3.057355179253
H	1.469759629255	3.601973323936	0.876881149165
H	2.894301528579	4.359936668364	1.633061252911
C	2.672506436183	2.326973058995	3.741183223446
H	3.973440666788	0.944089924274	2.573240031270
H	4.574341935186	2.613533996081	2.678947574745
H	1.488160293006	4.200119645896	3.595571839667
H	0.676402489214	2.756008990806	2.972962853491
H	2.181593389996	1.423212211091	4.102739846114
H	3.175991111214	2.805272011575	4.583210557473
I	-0.141557187685	-0.464272351570	2.653020003553
C	4.260455673620	-2.171404253777	-1.835061271625
H	4.837911526716	-2.849592495506	-2.470164166478
H	3.207653958166	-2.287229482279	-2.125024516201
H	4.549218292353	-1.147302512247	-2.092993739164
C	-0.975243452515	4.703252691750	0.392471773002
C	-1.290246832684	3.349832822987	0.572659488244
C	-0.878438850106	2.347795592713	-0.351217624385
C	-0.134560648103	2.836503035842	-1.448123038522
C	0.202142792123	4.184504397342	-1.633828479758
C	-0.223964830681	5.128570992849	-0.704983684433
H	-1.313029128673	5.438617945776	1.119277737387
H	0.175848453176	2.135846041744	-2.224879468216
H	0.773278708693	4.495969250028	-2.504470640255
H	0.017198882669	6.179064286918	-0.829919216861

Ba	-2.114502910222	-0.244561986342	-0.228621909300
O	-3.872166234897	1.090128169415	-1.897376430867
C	-3.737777500988	0.898794269489	-3.326657872503
C	-4.105086870610	2.508446667875	-1.695058838072
C	-2.916945175726	2.099003196504	-3.784264334255
H	-4.737691087094	0.876679841187	-3.778848431304
H	-3.241064259456	-0.058842726002	-3.491153139787
C	-3.397566359889	3.238830972296	-2.854947071735
H	-5.187158444945	2.684555752603	-1.697178911602
H	-3.696133184281	2.770446496394	-0.720784528691
H	-1.859935233713	1.888704145912	-3.616705251323
H	-3.062592372979	2.319873566628	-4.842825600859
H	-4.093162156078	3.907835703105	-3.365692500735
H	-2.556321626810	3.826158598058	-2.488849734217
O	3.850893789993	1.523787739533	-1.773231190653
C	3.616452152390	2.706184695775	-2.556516613931
C	5.161199423734	1.697599535993	-1.189811706863
C	4.128497978950	3.854146448239	-1.677988199779
H	2.550704284082	2.751347014795	-2.778805954726
H	4.175365350406	2.627920001844	-3.497454737310
C	5.240288011579	3.190515306287	-0.817621174074
H	5.239681270909	1.005125448568	-0.350307067019
H	5.912771528451	1.425465738194	-1.940185714945
H	3.318916222793	4.221143709422	-1.044958240956
H	4.495624608291	4.690454048417	-2.275325101979
H	5.031973516004	3.327737457286	0.242492108998
H	6.229784441871	3.597729853040	-1.031788594724
I	-0.038135194403	-0.870871429964	-2.956412087358
C	-2.116758499659	2.960084835641	1.784249389115
H	-2.305381260663	3.807473629419	2.449495106790
H	-3.094138601118	2.559909724898	1.488309772850
H	-1.617663195023	2.176688109726	2.360835710619
Si	0.680630365966	-3.721686840117	0.123818219028
H	1.057565422171	-2.294825096926	-0.029160635744
C	-1.224936158258	-3.703318305734	0.064419384043
C	-1.917533098605	-3.734368506480	-1.160590998897

C	-1.989361486411	-3.564962585813	1.239022396534
C	-3.309359728287	-3.615789663070	-1.213329737599
C	-3.380429411422	-3.447936976057	1.192834245259
C	-4.044578443019	-3.469052730329	-0.034995394169
H	-1.365823756661	-3.824474195952	-2.088521448153
H	-1.492313750312	-3.520536682754	2.200585895326
H	-3.815874645431	-3.640101932531	-2.172183202176
H	-3.942223914368	-3.333041255560	2.113173104859
H	-5.124411961110	-3.375690746798	-0.073012411166
C	1.302328640990	-4.339105721264	1.775074838978
H	0.951220791325	-3.694165559191	2.584090189979
H	0.980426381646	-5.366146356202	1.971465299613
H	2.395079853066	-4.303120562207	1.780870152938
C	1.381574384222	-4.660884713984	-1.340044425332
H	2.472740742801	-4.658167948468	-1.269807540674
H	1.039120492545	-5.699499981717	-1.357348303837
H	1.102597857439	-4.181959544701	-2.281938832763

TS0

(**E** = -2148.07366180 a.u.; **G** = -2147.29749673 a.u.)

0 1

C	5.410619000000	-2.170763000000	-0.263557000000
C	4.069375000000	-2.364043000000	-0.637137000000
C	3.032484000000	-2.407635000000	0.333245000000
C	3.450747000000	-2.200466000000	1.669044000000
C	4.780006000000	-1.987441000000	2.045215000000
C	5.773121000000	-1.983773000000	1.067321000000
H	6.181686000000	-2.153828000000	-1.030971000000
H	2.701862000000	-2.196087000000	2.458072000000
H	5.038548000000	-1.836161000000	3.089711000000
H	6.813937000000	-1.831810000000	1.335201000000
Ba	1.777332000000	0.123815000000	-0.112639000000
O	-4.276730000000	0.086219000000	1.364710000000
C	-4.274172000000	0.193937000000	2.807234000000
C	-5.613340000000	0.415004000000	0.947985000000
C	-5.191649000000	1.391561000000	3.124880000000

H	-3.239126000000	0.312220000000	3.125258000000
H	-4.667404000000	-0.740420000000	3.223867000000
C	-5.981512000000	1.627275000000	1.807708000000
H	-5.584001000000	0.601908000000	-0.124710000000
H	-6.272189000000	-0.440092000000	1.148866000000
H	-5.852071000000	1.163851000000	3.962973000000
H	-4.606224000000	2.271717000000	3.391524000000
H	-5.644092000000	2.543463000000	1.319076000000
H	-7.058133000000	1.706910000000	1.965895000000
O	2.930969000000	1.977575000000	1.546813000000
C	2.373635000000	3.305663000000	1.668687000000
C	3.374875000000	1.572151000000	2.868868000000
C	1.630149000000	3.267710000000	2.996549000000
H	1.735444000000	3.484269000000	0.804261000000
H	3.191344000000	4.039357000000	1.673845000000
C	2.534976000000	2.381350000000	3.880278000000
H	3.222466000000	0.495285000000	2.944738000000
H	4.446021000000	1.783808000000	2.953683000000
H	1.465115000000	4.263094000000	3.412219000000
H	0.664704000000	2.784756000000	2.849093000000
H	1.940762000000	1.722610000000	4.513363000000
H	3.183117000000	2.985750000000	4.518708000000
I	-0.167010000000	-0.440411000000	2.889430000000
C	3.773840000000	-2.497422000000	-2.120144000000
H	3.911330000000	-3.528561000000	-2.462229000000
H	2.745418000000	-2.222797000000	-2.359562000000
H	4.438645000000	-1.863820000000	-2.714728000000
C	-0.838053000000	4.532199000000	0.305390000000
C	-1.114072000000	3.176471000000	0.531592000000
C	-0.632391000000	2.153854000000	-0.336883000000
C	0.106569000000	2.637406000000	-1.439803000000
C	0.400551000000	3.986843000000	-1.672638000000
C	-0.073283000000	4.946875000000	-0.785613000000
H	-1.221894000000	5.280289000000	0.995071000000
H	0.442208000000	1.929660000000	-2.199496000000
H	0.974333000000	4.282374000000	-2.546762000000

H	0.135058000000	6.000328000000	-0.940655000000
Ba	-2.099896000000	-0.428456000000	-0.198599000000
O	-3.778866000000	1.058718000000	-1.830447000000
C	-3.684349000000	0.921556000000	-3.269821000000
C	-4.006311000000	2.467823000000	-1.583702000000
C	-2.855190000000	2.126467000000	-3.704390000000
H	-4.697416000000	0.934770000000	-3.692388000000
H	-3.208501000000	-0.035800000000	-3.484281000000
C	-3.251936000000	3.228991000000	-2.690907000000
H	-5.086548000000	2.655184000000	-1.621509000000
H	-3.638885000000	2.690825000000	-0.584396000000
H	-1.797319000000	1.880625000000	-3.606666000000
H	-3.051795000000	2.406949000000	-4.740411000000
H	-3.896690000000	3.985625000000	-3.142517000000
H	-2.369092000000	3.723965000000	-2.288648000000
O	3.864696000000	1.140898000000	-1.553748000000
C	3.768089000000	2.229905000000	-2.489870000000
C	5.131293000000	1.318850000000	-0.885353000000
C	4.264923000000	3.447862000000	-1.703183000000
H	2.731699000000	2.295069000000	-2.819495000000
H	4.404357000000	2.011766000000	-3.356367000000
C	5.274233000000	2.839699000000	-0.689365000000
H	5.108267000000	0.742140000000	0.038435000000
H	5.921147000000	0.909735000000	-1.525208000000
H	3.426983000000	3.914279000000	-1.182069000000
H	4.716711000000	4.197725000000	-2.354587000000
H	5.009267000000	3.114636000000	0.330931000000
H	6.298176000000	3.166510000000	-0.877786000000
I	-0.113167000000	-0.854472000000	-3.094588000000
C	-1.977563000000	2.824988000000	1.727995000000
H	-2.177397000000	3.693916000000	2.361211000000
H	-2.951085000000	2.425922000000	1.419110000000
H	-1.506518000000	2.054052000000	2.340764000000
Si	0.625846000000	-3.420396000000	0.141023000000
H	0.349353000000	-1.938622000000	0.017203000000
C	-1.341981000000	-3.652451000000	0.045137000000

C	-2.020041000000	-3.698017000000	-1.190562000000
C	-2.149030000000	-3.520154000000	1.195765000000
C	-3.413304000000	-3.597922000000	-1.278824000000
C	-3.542269000000	-3.422868000000	1.120862000000
C	-4.181742000000	-3.453544000000	-0.120729000000
H	-1.450492000000	-3.781310000000	-2.109107000000
H	-1.680071000000	-3.460489000000	2.171781000000
H	-3.896062000000	-3.632608000000	-2.250247000000
H	-4.125744000000	-3.313819000000	2.029248000000
H	-5.261561000000	-3.374576000000	-0.184530000000
C	0.976659000000	-4.220209000000	1.811303000000
H	0.785090000000	-3.531211000000	2.636461000000
H	0.314521000000	-5.083610000000	1.929655000000
H	2.012109000000	-4.552702000000	1.876346000000
C	1.182454000000	-4.416639000000	-1.353843000000
H	2.227697000000	-4.706611000000	-1.252787000000
H	0.567500000000	-5.319404000000	-1.427117000000
H	1.067558000000	-3.850559000000	-2.279940000000

II

(**E** = -2148.08302027 a.u.; **G** = -2147.30648418 a.u.)

0 1

C	4.393249494904	-2.141258972647	-1.099387755135
C	3.156276211052	-2.690039149657	-1.484279522493
C	2.257180273889	-3.208266378529	-0.505860086407
C	2.717370278198	-3.160532305525	0.829960822834
C	3.953118338439	-2.625152018610	1.208674513968
C	4.798241934885	-2.095175838967	0.234952073264
H	5.048048355898	-1.733064993833	-1.863255480813
H	2.074617807013	-3.524508654761	1.621429709951
H	4.244671571214	-2.618849823571	2.253811805101
H	5.755592729727	-1.661517075808	0.502585008726
Ba	1.909558546545	-0.096737927287	0.131933014767
O	-4.022701570121	0.142239068977	1.692672694757
C	-4.035814233114	-0.172745651254	3.101908379396
C	-5.351314294845	0.595186231044	1.384224751926

C	-4.895957482644	0.930249712975	3.745185242133
H	-3.001730061322	-0.209085389942	3.440525790754
H	-4.483950258047	-1.165084889645	3.231464905042
C	-5.719491529248	1.508634354016	2.559467050500
H	-5.311967986480	1.085240220404	0.412541713169
H	-6.019144085262	-0.274084357214	1.322217709512
H	-5.532761875677	0.523224290993	4.532047120920
H	-4.265559128359	1.700225548285	4.191177779570
H	-5.413830921428	2.534625306581	2.345901366735
H	-6.793694521563	1.511866766803	2.750954527648
O	3.211953126475	1.162676093843	2.199371396950
C	2.856662500595	2.509014884238	2.601458520629
C	3.531703425604	0.398694896901	3.398332714264
C	2.142643649649	2.311832539974	3.928663605591
H	2.235661954341	2.941151576199	1.818548378046
H	3.773095974599	3.104159380287	2.712417976224
C	2.979661623566	1.202689230933	4.591833164533
H	3.048890583173	-0.574065239789	3.298985528083
H	4.616093706067	0.262900709914	3.444963588346
H	2.092974704743	3.227141776265	4.520630027776
H	1.128718524237	1.960391333890	3.738184142615
H	2.378933469242	0.574473824243	5.249898757595
H	3.796847774058	1.632102389703	5.176849266141
I	-0.072131650471	-1.329660803085	2.848682833349
C	2.836176995073	-2.700463444826	-2.963607655366
H	2.845199980125	-3.720216433276	-3.355532566375
H	1.852585026260	-2.278945564406	-3.168378278392
H	3.569360069121	-2.117491455331	-3.526355344518
C	-0.267459208394	4.299148442504	1.747993148641
C	-0.585244640935	2.939924833818	1.617362638946
C	-0.146580995011	2.165196795145	0.502919059076
C	0.596917242145	2.899297572581	-0.449111763187
C	0.926320715524	4.254813632519	-0.328337904272
C	0.494927076079	4.963294607585	0.787135167892
H	-0.617578998463	4.850523891831	2.617519419939
H	0.915272717416	2.406949285090	-1.367967916434

H	1.495785401635	4.754032853772	-1.106991323800
H	0.733728289471	6.014993365750	0.906453644080
Ba	-1.947325446102	-0.199543415714	-0.061401941341
O	-3.475132609307	1.862966378582	-1.122609426403
C	-3.410489646116	2.142983425362	-2.541815953257
C	-3.575190577275	3.152231205980	-0.472936790044
C	-2.481450447307	3.350103778758	-2.641865677293
H	-4.423288450041	2.362518649267	-2.904252113342
H	-3.026517668276	1.253081777864	-3.041133359474
C	-2.753038977703	4.132131707772	-1.331655063436
H	-4.634112962672	3.436466610367	-0.429293253136
H	-3.193367192587	3.042497964590	0.539970077691
H	-1.448867611865	3.000461828875	-2.670414460805
H	-2.672853165406	3.940133462374	-3.539689101555
H	-3.316515469929	5.049912406065	-1.511697263631
H	-1.820273728640	4.393695534414	-0.834613385543
O	3.834388458341	1.292439558796	-1.229545570466
C	3.750425794649	1.756248866676	-2.596014581545
C	4.857336852817	2.089676121830	-0.606890661368
C	3.990851237639	3.278566243118	-2.526571961715
H	2.772239373307	1.469362276257	-2.980861936455
H	4.526897729707	1.250143791373	-3.181270883816
C	4.572349883169	3.508180636494	-1.105281052101
H	4.768542744936	1.953669980475	0.470258510361
H	5.841397558404	1.731068400570	-0.937350018974
H	3.058528300575	3.827485775870	-2.661712839158
H	4.681324400690	3.598907244488	-3.308534533227
H	3.825936954930	3.978483115007	-0.463001674301
H	5.467317249306	4.132708164337	-1.107337201017
I	-0.012809603626	0.118195647158	-3.023352704433
C	-1.445366932701	2.317922221487	2.700209936513
H	-1.539164946920	2.968534137652	3.574372958297
H	-2.462698362650	2.119270028020	2.342721726421
H	-1.037569742070	1.359651351783	3.026064717999
Si	0.226284322743	-3.632885220214	-0.729748494338
H	0.165420416606	-2.056656304808	-0.467301051267

C	-1.802405024934	-3.325096641016	-0.823519538025
C	-2.406730239351	-2.815381860938	-1.993690398833
C	-2.635215410947	-3.382690962703	0.315817597624
C	-3.737647953260	-2.382880638669	-2.028833020749
C	-3.970109063144	-2.960766820924	0.296430509972
C	-4.528727042252	-2.450017603139	-0.877669791750
H	-1.818380413820	-2.724051401763	-2.899907247355
H	-2.229617610805	-3.746537170321	1.253445498809
H	-4.155522713033	-1.993870830642	-2.952314874087
H	-4.568854747451	-3.019877848235	1.199994372365
H	-5.560849005615	-2.117617343079	-0.898589574951
C	0.143332909335	-4.904217289921	0.687015198147
H	-0.006141866398	-4.444604537088	1.667565210049
H	-0.698645378743	-5.577802423500	0.504366039770
H	1.058892507224	-5.499247571072	0.728910578895
C	0.296407473875	-4.535053853599	-2.406554380076
H	1.229737147895	-5.094752610077	-2.505337621907
H	-0.540629570608	-5.238548249194	-2.448067080129
H	0.210008125828	-3.872274707145	-3.270070010808

TS1

(**E** = -2148.07832812 a.u.; **G** = -2147.30112882 a.u.)

0 1

C	-4.544499000000	2.101008000000	0.025066000000
C	-3.433441000000	2.436266000000	-0.768955000000
C	-2.343148000000	3.153789000000	-0.202541000000
C	-2.454290000000	3.492661000000	1.160062000000
C	-3.552962000000	3.145092000000	1.945029000000
C	-4.611436000000	2.443592000000	1.374661000000
H	-5.366618000000	1.555638000000	-0.428977000000
H	-1.643386000000	4.028804000000	1.637400000000
H	-3.573428000000	3.415666000000	2.995308000000
H	-5.477608000000	2.166726000000	1.965905000000
Ba	-1.832070000000	-0.113931000000	0.117549000000
O	4.116350000000	0.136566000000	1.168026000000
C	4.218833000000	0.501542000000	2.561605000000

C	5.444302000000	-0.242720000000	0.769857000000
C	5.199239000000	-0.519153000000	3.168059000000
H	3.214523000000	0.483136000000	2.981150000000
H	4.607920000000	1.524614000000	2.623910000000
C	5.959356000000	-1.091184000000	1.938139000000
H	5.363117000000	-0.767240000000	-0.180830000000
H	6.047952000000	0.664099000000	0.631709000000
H	5.870290000000	-0.041549000000	3.883610000000
H	4.659890000000	-1.308648000000	3.692390000000
H	5.699086000000	-2.139692000000	1.781274000000
H	7.043686000000	-1.026571000000	2.041518000000
O	-2.986781000000	-1.297105000000	2.314578000000
C	-2.503073000000	-2.566573000000	2.814991000000
C	-3.320811000000	-0.479708000000	3.468963000000
C	-1.669998000000	-2.180725000000	4.029339000000
H	-1.936153000000	-3.048490000000	2.019165000000
H	-3.362621000000	-3.194787000000	3.084925000000
C	-2.460420000000	-1.002259000000	4.638908000000
H	-3.102447000000	0.555939000000	3.207124000000
H	-4.393503000000	-0.580003000000	3.664847000000
H	-1.532561000000	-3.011495000000	4.723338000000
H	-0.691458000000	-1.839885000000	3.693550000000
H	-1.788136000000	-0.227331000000	5.006912000000
H	-3.095704000000	-1.332690000000	5.463633000000
I	0.189606000000	1.339515000000	2.644556000000
C	-3.459597000000	1.989751000000	-2.218311000000
H	-3.688893000000	2.826150000000	-2.882589000000
H	-2.502585000000	1.585798000000	-2.556893000000
H	-4.223530000000	1.223847000000	-2.370520000000
C	0.653443000000	-4.268105000000	1.730591000000
C	0.893653000000	-2.903091000000	1.520163000000
C	0.319756000000	-2.199075000000	0.421402000000
C	-0.468471000000	-3.004898000000	-0.430820000000
C	-0.718558000000	-4.367886000000	-0.231241000000
C	-0.156405000000	-5.006702000000	0.867740000000
H	1.104273000000	-4.765712000000	2.585926000000

H	-0.885215000000	-2.568272000000	-1.340045000000
H	-1.327434000000	-4.925253000000	-0.937344000000
H	-0.331364000000	-6.062120000000	1.048593000000
Ba	1.869380000000	0.268229000000	-0.408735000000
O	3.477294000000	-1.740651000000	-1.494610000000
C	3.382248000000	-2.112451000000	-2.891101000000
C	3.722414000000	-2.976799000000	-0.785204000000
C	2.566799000000	-3.405169000000	-2.886036000000
H	4.396878000000	-2.260751000000	-3.283548000000
H	2.896528000000	-1.294035000000	-3.422074000000
C	2.910604000000	-4.056905000000	-1.520914000000
H	4.799768000000	-3.185639000000	-0.815000000000
H	3.415877000000	-2.833377000000	0.248358000000
H	1.506229000000	-3.156783000000	-2.935151000000
H	2.813118000000	-4.042382000000	-3.737087000000
H	3.497849000000	-4.970308000000	-1.634397000000
H	2.004309000000	-4.298506000000	-0.967785000000
O	-3.927108000000	-1.387194000000	-1.117745000000
C	-3.901179000000	-1.879861000000	-2.477849000000
C	-4.801789000000	-2.280678000000	-0.401175000000
C	-3.894610000000	-3.413540000000	-2.346923000000
H	-3.017039000000	-1.467510000000	-2.963463000000
H	-4.799320000000	-1.519627000000	-2.993263000000
C	-4.415101000000	-3.675852000000	-0.905968000000
H	-4.635302000000	-2.118791000000	0.663634000000
H	-5.841883000000	-2.031721000000	-0.648234000000
H	-2.883712000000	-3.803135000000	-2.471848000000
H	-4.526025000000	-3.875326000000	-3.107485000000
H	-3.618487000000	-4.088308000000	-0.284775000000
H	-5.259833000000	-4.366211000000	-0.879285000000
I	-0.137994000000	-0.415524000000	-3.270061000000
C	1.813931000000	-2.196339000000	2.495909000000
H	2.044706000000	-2.817628000000	3.365847000000
H	2.770088000000	-1.932910000000	2.029542000000
H	1.374375000000	-1.261035000000	2.845963000000
Si	-0.632187000000	3.595987000000	-1.102927000000

H	-0.421299000000	1.830617000000	-0.863255000000
C	1.327789000000	3.431543000000	-0.979460000000
C	2.077101000000	3.003909000000	-2.096854000000
C	2.048813000000	3.658922000000	0.208895000000
C	3.462117000000	2.813132000000	-2.033146000000
C	3.429556000000	3.452933000000	0.287957000000
C	4.146006000000	3.030278000000	-0.833635000000
H	1.571829000000	2.793955000000	-3.032745000000
H	1.523095000000	3.980929000000	1.100236000000
H	4.003819000000	2.496839000000	-2.919127000000
H	3.944427000000	3.622302000000	1.227863000000
H	5.217991000000	2.877764000000	-0.776197000000
C	-0.634481000000	5.449109000000	-0.529765000000
H	-0.344797000000	5.589007000000	0.517454000000
H	0.087446000000	6.011497000000	-1.132185000000
H	-1.622811000000	5.904084000000	-0.654293000000
C	-0.915518000000	3.728908000000	-2.972633000000
H	-1.892444000000	4.170663000000	-3.180416000000
H	-0.162141000000	4.410664000000	-3.378528000000
H	-0.840614000000	2.779489000000	-3.505426000000

III

(**E** = -2148.09843225 a.u.; **G** = -2147.32398791 a.u.)

0 1

C	4.259212508740	-2.751477948762	0.114498843432
C	3.256141159222	-2.936305441267	-0.848945414913
C	2.112614722629	-3.709495413788	-0.522348922311
C	2.064888485804	-4.287367382789	0.760407178852
C	3.056008069263	-4.079967467848	1.719057782954
C	4.164113236507	-3.304403407592	1.393194358977
H	5.129619368115	-2.157825115399	-0.146856661697
H	1.222906218960	-4.911897925594	1.036698241626
H	2.950903131175	-4.507921912245	2.708041940835
H	4.951050456076	-3.135536027124	2.120058674911
Ba	1.930434741861	-0.363725291211	1.122266569653
O	-3.628732486442	0.172019872162	1.308596968681

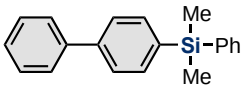
C	-3.604215298461	-0.342897914458	2.661787727275
C	-4.872026628687	0.882188292974	1.172097129056
C	-4.404689709909	0.665467556572	3.518225332233
H	-2.561009293423	-0.459837045342	2.953379130546
H	-4.083732526042	-1.326990096348	2.668760289731
C	-4.991281054139	1.655577091964	2.482879343976
H	-4.799740287583	1.497560251377	0.276870208478
H	-5.694378520305	0.161565652671	1.055696457738
H	-5.196382576123	0.153319023512	4.068202414076
H	-3.769872756089	1.169155895345	4.247054238366
H	-4.381101350872	2.560039596248	2.425812714894
H	-6.018102066592	1.949810753488	2.706940990816
O	3.303952619836	1.455219717122	2.736678281625
C	3.154515281795	2.900600195122	2.660078337471
C	3.415494447111	1.096102868420	4.134077042579
C	2.684332723569	3.366766806683	4.053943853873
H	2.427939635923	3.108298460865	1.875965836844
H	4.119262127601	3.338628825140	2.384501416683
C	2.459840992355	2.053807523249	4.830315713882
H	3.132389911921	0.046564306087	4.237886715238
H	4.453778490463	1.232309916174	4.463470354630
H	3.455820137616	3.972291158973	4.535520296090
H	1.776975231340	3.965559620909	3.983306525488
H	1.439056448795	1.689239113524	4.702084832817
H	2.661090158352	2.148078731649	5.898577456530
I	0.330823580569	-1.769932101768	3.798085792058
C	3.438762280259	-2.293889963915	-2.201351666542
H	3.558305484370	-3.046219156886	-2.984356387764
H	2.577211246825	-1.677038035783	-2.459540328208
H	4.327246429088	-1.662122015114	-2.206752752276
C	-0.169720721196	4.117878954174	1.932195159762
C	-0.330937423958	2.725404496226	1.941547448094
C	0.036783220266	1.922951178284	0.826136714210
C	0.540624261489	2.643308599814	-0.280238855990
C	0.700093021035	4.034095342056	-0.305365585449
C	0.350881659284	4.776867142280	0.817534756629

H	-0.461570425045	4.700488947873	2.803188098616
H	0.808933444958	2.105528050356	-1.189396880829
H	1.085018074758	4.529877506112	-1.191488748070
H	0.469028544406	5.855539606658	0.826175382912
Ba	-1.656155833241	0.062796493520	-0.722230505117
O	-3.192533198891	2.382548340758	-1.244207129826
C	-3.606587115054	2.762669726435	-2.577090354928
C	-2.997886244895	3.608453799971	-0.489687388468
C	-2.757095565883	3.987929581351	-2.879785351319
H	-4.681071676478	2.993334936649	-2.569702128053
H	-3.406869778872	1.920566795243	-3.239124589340
C	-2.734250192351	4.724327424714	-1.524082772903
H	-3.901672371524	3.804145590111	0.099001974125
H	-2.162316915656	3.444722716025	0.186734650525
H	-1.758166615723	3.650981422768	-3.164299742962
H	-3.165335000588	4.594599843832	-3.689996057963
H	-3.519664494649	5.482569856196	-1.477487057732
H	-1.778477507369	5.213098807373	-1.338423316189
O	3.592324218841	0.784520223885	-0.803713297096
C	3.210297106440	1.088798245231	-2.172618585652
C	4.655968119834	1.693344590390	-0.472320319296
C	3.468326167055	2.598603079569	-2.360304144778
H	2.172463342014	0.783652539004	-2.304176174096
H	3.835250902921	0.495355962109	-2.845722921797
C	4.201610476429	3.026106043454	-1.065399847676
H	4.766812700401	1.690942661155	0.612861705105
H	5.591525219202	1.343070051983	-0.930133625707
H	2.536902485591	3.146689243533	-2.495879683189
H	4.083614583312	2.771665015883	-3.244857826209
H	3.504049472473	3.511002133318	-0.380626359701
H	5.034858639445	3.706547072077	-1.250252721650
I	-0.661763504699	0.629867373071	-3.924803220865
C	-0.979418631651	2.089511102095	3.150102342110
H	-0.857833628562	2.692060361729	4.055536070550
H	-2.053612058752	1.983861054290	2.973049086764
H	-0.590513320397	1.088338342731	3.341160757862

Si	0.634411670413	-4.108145325353	-1.667999152232
H	0.562561718820	-0.968227563027	-0.758919376833
C	-1.018989263651	-3.579048126825	-0.882300363533
C	-2.147390749355	-3.415314637549	-1.707149752530
C	-1.205421247905	-3.404057339394	0.500104606181
C	-3.404181763588	-3.104252090540	-1.176040385862
C	-2.455547206065	-3.105633329493	1.038251500735
C	-3.564451005060	-2.957693942619	0.202116097311
H	-2.055399242796	-3.513915704720	-2.782787584312
H	-0.371773108092	-3.463522334143	1.187457324358
H	-4.253041057355	-2.983004177580	-1.840692334397
H	-2.540244637872	-2.975328561578	2.109929982954
H	-4.536931741117	-2.718685784835	0.617085313766
C	0.580260933975	-5.997383066902	-1.776703261666
H	0.489482832331	-6.457889381830	-0.789348700628
H	-0.276475789842	-6.320460342712	-2.375681631148
H	1.489548219623	-6.385804253739	-2.245521448499
C	0.692216777912	-3.420601588062	-3.414344628052
H	1.606895875051	-3.707074566645	-3.936668738312
H	-0.141119663531	-3.845420798260	-3.982643301841
H	0.589991893906	-2.333539412461	-3.444007381087

11. Characterization of products

[1,1'-Biphenyl]-4-yldimethyl(phenyl)silane (4a).

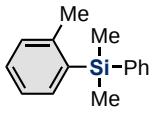


4a

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1a** (281.4 mg, 1.0 mmol) and hydrosilane **3e** (33.9 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with anisole (25.2 mg) as an internal standard to obtain the NMR yield of **4a** in 79% yield. The product **4a** was purified by GPC and obtained in 84% yield (60.1 mg, 0.21 mmol) as a colorless liquid. ^{1}H and ^{13}C NMR of the product **4a** were in agreement with the literature.[15]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.59 (s, 6H), 7.31–7.40 (m, 4H), 7.40–7.47 (m, 2H), 7.54–7.62 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –2.2 (*C*H$_3$), 126.7 (*C*H), 127.3 (*C*H), 127.5 (*C*H), 128.0 (*C*H), 128.9 (*C*H), 129.3 (*C*H), 134.3 (*C*H), 134.8 (*C*H), 137.1 (*C*), 138.3 (*C*), 141.2 (*C*), 142.0 (*C*). EI (m/z): $[M]^+$ calcd for $C_{20}H_{20}Si$: 288.1329, found: 288.1327.

Dimethyl(phenyl)(*o*-tolyl)silane (4b).

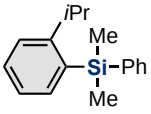


4b

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1b** (216.4 mg, 1.0 mmol) and hydrosilane **3e** (34.3 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with tetrachloroethane (47.8 mg) as an internal standard to obtain the NMR yield of **4b** in 79% yield. The product **4b** was purified by PTLC and obtained in 91% yield (51.6 mg, 0.23 mmol) as a colorless liquid. ^{1}H and ^{13}C NMR of the product **4b** were in agreement with the literature.[16]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.58 (s, 6H), 2.27 (s, 3H), 7.12–7.23 (m, 2H), 7.27–7.39 (m, 4H), 7.45–7.51 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –1.3 (*C*H$_3$), 23.3 (*C*H$_3$), 125.1 (*C*H), 128.0 (*C*H), 129.0 (*C*H), 129.7 (*C*H), 130.0 (*C*H), 134.1 (*C*H), 135.5 (*C*H), 136.3 (*C*), 139.0 (*C*), 144.2 (*C*). EI (m/z): $[M]^+$ calcd for $C_{15}H_{18}Si$: 226.1172, found: 226.1172.

(2-Isopropylphenyl)dimethyl(phenyl)silane (4c).

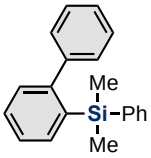


4c

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1c** (247.2 mg, 1.0 mmol) and hydrosilane **3e** (33.9 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with anisole (25.4 mg) as an internal standard to obtain the NMR yield of **4c** in 80% yield. The product **4c** was purified by GPC and obtained in 82% yield (51.9 mg, 0.20 mmol) as a colorless liquid.

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.58 (s, 6H), 1.03 (d, J = 6.8 Hz, 6H), 2.97 (sept, J = 6.7Hz, 1H), 7.15–7.22 (m, 1H), 7.27–7.43 (m, 5H), 7.43–7.56 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –0.7 (*C*H_3), 24.4 (*C*H_3), 34.1 (*C*H), 125.3 (*C*H), 125.5 (*C*H), 127.8 (*C*H), 129.0 (*C*H), 130.1 (*C*H), 134.1 (*C*H), 135.2 (*C*), 135.4 (*C*), 139.6 (*C*), 155.6 (*C*). EI (m/z): $[M]^+$ calcd for $C_{17}H_{22}Si$: 254.1485, found: 254.1489

[1,1'-Biphenyl]-2-yldimethyl(phenyl)silane (4d).

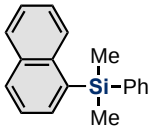


4d

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1d** (281.8 mg, 1.0 mmol) and hydrosilane **3e** (34.1 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with anisole (25.2 mg) as an internal standard to obtain the NMR yield of **4d** in 76% yield. The product **4d** was purified by GPC and obtained in 82% yield (59.4 mg, 0.21 mmol) as a colorless liquid by GPC separation. ^{1}H and ^{13}C NMR of the product **4d** were in agreement with the literature.[17]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.17 (s, 6H), 7.06–7.11 (m, 2H), 7.19–7.25 (m, 3H), 7.25–7.44 (m, 8H), 7.62 (dd, J = 7.5, 1.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –1.0 (*C*H_3), 126.4 (*C*H), 127.1 (*C*H), 127.7 (*C*H), 127.8 (*C*H), 128.8 (*C*H), 129.0 (*C*H), 129.5 (*C*H), 129.8 (*C*H), 134.1 (*C*H), 135.9 (*C*H), 136.5 (*C*), 140.1 (*C*), 144.2 (*C*), 149.7 (*C*). EI (m/z): $[M]^+$ calcd for $C_{20}H_{20}Si$: 288.1329, found: 288.1332.

Dimethyl(naphthalen-1-yl)(phenyl)silane (4e).

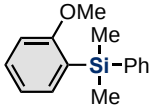


4e

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1e** (255.6 mg, 1.0 mmol) and hydrosilane **3e** (33.6 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with anisole (25.0 mg) as an internal standard to obtain the NMR yield of **4e** in 76% yield. The product **4e** was purified by GPC and obtained in 82% yield (53.1 mg, 0.20 mmol) as a colorless liquid. ^{1}H and ^{13}C NMR of the product **4e** were in agreement with the literature.[15]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.70 (s, 6H), 7.30–7.58 (m, 8H), 7.72 (dd, J = 7.0, 1.0 Hz, 1H), 7.86 (dd, J = 8.0, 1.2 Hz, 1H), 7.91 (t, J = 8.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –0.81 (*CH*$_3$), 125.2 (*CH*), 125.5 (*CH*), 125.8 (*CH*), 128.0 (*CH*), 128.7 (*CH*), 129.1 (*CH*), 129.2 (*CH*), 130.4 (*CH*), 133.5 (*C*), 134.3 (*CH*), 134.8 (*CH*), 135.8 (*C*), 137.1 (*C*), 139.0 (*C*). EI (m/z): $[M]^+$ calcd for $C_{18}H_{18}Si$: 262.1172, found: 262.1172.

(2-Methoxyphenyl)dimethyl(phenyl)silane (4f).

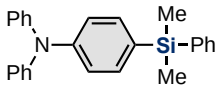


4f

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1f** (235.7 mg, 1.0 mmol) and hydrosilane **3e** (34.3 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with tetrachloroethane (45.4 mg) as an internal standard to obtain the NMR yield of **4f** in 94% yield. The product **4f** was purified by GPC and obtained in 61% yield (37.3 mg, 0.15 mmol) as a colorless liquid. ^{1}H and ^{13}C NMR of product **4f** were in agreement with the literature.[17]

^{1}H NMR (400 MHz, $CDCl_3$, δ): 0.55 (s, 6H), 3.74 (s, 3H), 6.83 (d, J = 8.4 Hz, 1H), 6.91 (dt, J = 9.9, 7.2 Hz, 1H), 7.24–7.28 (m, 1H) 7.30–7.39 (m, 4H), 7.50–7.60 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –2.1 (*C*H_3), 55.1 (*C*H_3), 109.8 (*C*H), 120.6 (*C*H), 126.2 (*C*), 127.7 (*C*H), 128.8 (*C*H), 131.2 (*C*H), 134.3 (*C*H), 136.1 (*C*H), 139.1 (*C*), 164.6 (*C*). EI (m/z): $[M]^+$ calcd for $C_{15}H_{18}OSi$: 242.1121, found: 242.1123.

4-[Dimethyl(phenyl)silyl]-*N*,*N*-diphenylaniline (4g).

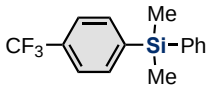


4g

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1g** (370.4 mg, 1.0 mmol) and hydrosilane **3e** (33.9 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with tetrachloroethane (47.3 mg) as an internal standard to obtain the NMR yield of **4g** in 48% yield. The product **4g** was purified by GPC and obtained in 56% yield (53.1 mg, 0.14 mmol) as a colorless liquid. ^{1}H and ^{13}C NMR of the product **4g** were in agreement with the literature.[18]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.53 (s, 6H), 6.99–7.05 (m, 4H), 7.08–7.13 (m, 4H), 7.22–7.29 (m, 4H), 7.32–7.39 (m, 5H), 7.51–7.58 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –2.1 (*C*H$_3$), 122.4 (*C*H), 123.2 (*C*H), 124.9 (*C*H), 127.9 (*C*H), 129.1 (*C*H), 129.4 (*C*H), 130.8 (*C*), 134.3 (*C*H), 135.2 (*C*H), 138.7 (*C*), 147.6 (*C*), 148.7 (*C*). EI (m/z): $[M]^+$ calcd for $C_{26}H_{25}NSi$: 379.1751, found: 379.1750.

Dimethyl(phenyl)(4-(trifluoromethyl)phenyl)silane (4h).

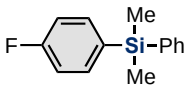


4h

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1h** (271.8 mg, 1.0 mmol) and hydrosilane **3e** (34.4 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with anisole (47.6 mg) as an internal standard to obtain the NMR yield of **4h** in 57% yield. The product **4h** was purified by GPC and obtained in 48% yield (33.7 mg, 0.208 mmol) as a colorless liquid. ^{1}H and ^{13}C NMR of the product **4h** were in agreement with the literature.[15]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.58 (s, 6H), 7.32–7.44 (m, 3H), 7.46–7.55 (m, 2H), 7.55–7.66 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –2.5 (*C*H$_3$), 124.5 (q, $J_{C–F}$ = 3.8 Hz, *C*H), 126.6 (q, $J_{C–F}$ = 223.0 Hz, *C*), 128.1 (*C*H), 129.6 (*C*H), 131.2 (q, $J_{C–F}$ = 32.3 Hz, *C*), 134.3 (*C*H), 134.6 (*C*H), 137.2 (*C*), 143.5 (*C*). EI (m/z): $[M]^+$ calcd for $C_{15}H_{15}F_3Si$: 280.0890, found: 280.0891.

(4-Fluorophenyl)dimethyl(phenyl)silane (4i).

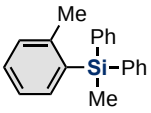


4i

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1i** (223.7 mg, 1.0 mmol) and hydrosilane **3e** (33.5 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with tetrachloroethane (28.5 mg) as an internal standard to obtain the NMR yield of **4i** in 58% yield. The product **4i** was purified by flash column chromatography (SiO_2, only hexane) and obtained in 36% yield (20.2 mg, 0.09 mmol) as a colorless liquid. ^{1}H and ^{13}C NMR of the product **4i** were in agreement with the literature.[16]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.54 (s, 6H), 6.99–7.09 (m, 2H), 7.31–7.39 (m, 3H), 7.45–7.54 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –2.2 (*C*H$_3$), 115.1 (d, $J_{C–F}$ = 19.2 Hz, *C*H$_2$), 128.0 (*C*H), 129.4 (*C*H), 133.8 (d, $J_{C–F}$ = 2.8 Hz, *C*), 134.2 (*C*H), 136.2 (d, $J_{C–F}$ = 7.7 Hz, *C*H), 138.1 (*C*), 163.9 (d, $J_{C–F}$ = 248.1 Hz, *C*). EI (m/z): $[M]^+$ calcd for $C_{14}H_{15}FSi$: 230.0922, found: 230.0924.

Methyldiphenyl(*o*-tolyl)silane (4j).

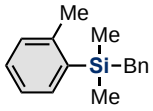


4j

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1b** (221.0 mg, 1.0 mmol) and hydrosilane **3f** (50.2 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with tetrachloroethane (42.8 mg) as an internal standard to obtain the NMR yield of **4j** in 79% yield. The product **4j** was purified by PTLC (hexane/ethyl acetate, 98:2) and obtained in 87% yield (63.5 mg, 0.22 mmol) as a colorless liquid.

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.87 (s, 3H), 2.22 (s, 3H), 7.12 (t, J = 7.6 Hz, 1H), 7.18 (d, J = 8.0 Hz, 1H), 7.26–7.42 (m, 8H), 7.46–7.53 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –2.2 (*C*H$_3$), 23.7 (*C*H$_3$), 125.1 (*C*H), 128.0 (*C*H), 129.4 (*C*H), 130.0 (*C*H), 130.1 (*C*H), 134.5 (*C*), 135.3 (*C*H), 136.7 (*C*), 137.1 (*C*H), 144.7 (*C*). EI (m/z): $[M]^+$ calcd for $C_{20}H_{20}Si$: 288.1329, found: 288.1337.

Benzyldimethyl(*o*-tolyl)silane (4k).

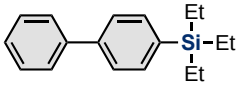


4k

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1b** (219.1 mg, 1.0 mmol) and hydrosilane **3g** (38.1 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with tetrachloroethane (47.3 mg) as an internal standard to obtain the NMR yield of **4k** in 68% yield. The product **4k** was purified by PTLC (hexane/ethyl acetate, 98:2) and GPC and obtained in 69% yield (60.1 mg, 0.18 mmol) as a colorless liquid. ^{1}H NMR of the product **4k** was in agreement with the literature.[19]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.28 (s, 6H), 2.38 (s, 2H), 2.44 (s, 3H), 6.94 (d, J = 8.0 Hz, 2H), 7.03–7.09 (m, 1H), 7.12–7.33 (m, 5H), 7.41 (d, J = 7.6Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –2.0 (*C*H$_3$), 23.4 (*C*H$_3$), 26.3 (*C*H$_2$), 124.2 (*C*H), 125.1 (*C*H), 128.2 (*C*H), 128.4 (*C*H), 129.5 (*C*H), 130.0 (*C*H), 134.9 (*C*H), 136.8 (*C*), 140.0 (*C*), 143.8 (*C*). EI (m/z): $[M]^+$ calcd for $C_{16}H_{20}Si$: 240.1329, found: 240.1326.

(1,1'-Biphenyl)-4-yltriethylsilane (4l).

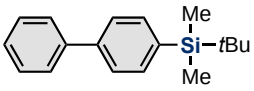


4l

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1a** (280.4 mg, 1.0 mmol) and hydrosilane **3h** (28.8 mg, 0.25 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with tetrachloroethane (24.6 mg) as an internal standard to obtain the NMR yield of **4l** in 48% yield. The product **4l** was purified by GPC and obtained in 43% yield (28.4 mg, 0.11 mmol) as a colorless liquid. ^{1}H and ^{13}C NMR of the product **4l** were in agreement with the literature.[20]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.82 (q, J = 7.8 Hz, 6H), 0.99 (t, J = 8.0 Hz, 9H), 7.33 (t, J = 6.6 Hz, 1H), 7.43 (t, J = 7.8 Hz, 2H), 7.54–7.63 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 3.5 (*C*H$_2$), 7.6 (*C*H$_3$), 126.5 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 128.9 (*C*H), 134.8 (*C*H), 136.4 (*C*), 141.3 (*C*), 141.5 (*C*). EI (m/z): $[M]^+$ calcd for $C_{18}H_{24}Si$: 268.1642, found: 268.1641.

(1,1'-Biphenyl)-4-yl(*tert*-butyl)dimethylsilane (4m).

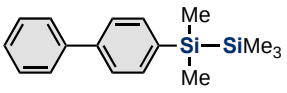


4m

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1a** (279.0 mg, 1.0 mmol) and hydrosilane **3i** (28.3 mg, 0.24 mmol). The resulting crude mixture was analyzed by ^{1}H NMR with tetrachloroethane (20.2 mg) as an internal standard to obtain the NMR yield of **4m** in 59% yield. The product **4m** was purified by GPC and obtained in 46% yield (30.0 mg, 0.11 mmol) as a colorless liquid. ^{1}H and ^{13}C NMR of the product **4m** were in agreement with the literature.[21]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.30 (s, 6H), 0.91 (s, 9H), 7.34 (t, J = 7.2 Hz, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.56–7.63 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –6.0 (*C*H_3), 17.1 (*C*), 26.7 (*C*H_3), 126.3 (*C*H), 127.3 (*C*H), 127.5 (*C*H), 128.9 (*C*H), 135.1 (*C*H), 136.7 (*C*), 141.2 (*C*), 141.6 (*C*). EI (m/z): $[M]^+$ calcd for $C_{18}H_{24}Si$: 268.1642, found: 268.1642.

1-[(1,1'-biphenyl)-4-yl]-1,1,2,2,2-pentamethyldisilane (4n).

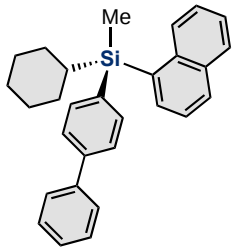


4n

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1a** (279.5 mg, 1.0 mmol) and hydrosilane **3j** (32.7 mg, 0.25 mmol). The product **4n** was purified by flash column chromatography (SiO_2, only hexane) and GPC and obtained in 17% yield (11.7 mg, 0.04 mmol) as a yellow oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.08 (s, 9H), 0.36 (s, 6H), 7.31–7.38 (m, 1H), 7.40–7.48 (m, 2H), 7.49–7.64 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –3.8 (*C*H_3), –2.1 (*C*H_3), 126.6 (*C*H), 127.2 (*C*H), 127.4 (*C*H), 128.9 (*C*H), 134.4 (*C*H), 138.6 (*C*H), 141.1 (*C*), 141.3 (*C*). EI (m/z): $[M]^+$ calcd for $C_{17}H_{24}Si_2$: 284.1411, found: 284.1411.

(*S*)-(1,1'-biphenyl)-4-yl(cyclohexyl)(methyl)(naphthalen-1-yl)silane [(*S*)-4o].

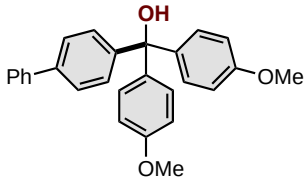


(*S*)-**4o**

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1e** (99.4 mg, 0.39 mmol) and hydrosilane (*R*)-**3k** (28.5 mg, 0.10 mmol). The product (*S*)-**4o** was purified by flash column chromatography (SiO_2, only hexane) and GPC and obtained in 49% yield (20.1 mg, 0.05 mmol, 78% ee) as a white solid. ^{1}H and ^{13}C NMR of the product (*S*)-**4o** were in agreement with the literature.[2]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.68 (s, 3H), 1.07–1.43 (m, 5H), 1.47–1.62 (m, 1H), 1.62–1.80 (m, 4H), 1.94 (d, J = 10.4 Hz, 1H), 7.29–7.37 (m, 2H), 7.38–7.64 (m, 10H), 7.79 (d, J = 6.1 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): –4.4 (*C*H_3), 25.2 (*C*H), 27.0 (*C*H_2), 28.1 (*C*H_2), 28.35 (*C*H_2), 28.40 (*C*H_2), 125.2 (*C*H), 125.5 (*C*H), 125.7 (*C*H), 126.6 (*C*H), 127.2 (*C*H), 127.5 (*C*H), 128.9 (*C*H), 129.0 (*C*H), 129.1 (*C*H), 130.3 (*C*H), 133.6 (*C*), 134.5 (*C*), 135.2 (*C*H) 135.4 (*C*H), 136.4 (*C*), 137.4 (*C*), 141.1 (*C*), 141.6 (*C*). EI (m/z): $[M]^+$ calcd for $C_{29}H_{30}Si$: 406.2111, found: 406.2105. $[\alpha]_D^{26}$ –7.9 (c 1.61 in $CHCl_3$, 78% ee). Daicel CHIRALCEL® OD-3, hexane 100%, 0.5 mL/min, 40 °C, *S* isomer: t_S = 36.08 min; for the racemic compound: *R* isomer: t_R = 30.19 min, *S* isomer: t_S = 37.87 min. The absolute configuration of **4o** was determined by the retention time of the reported HPLC trace.[2]

[1,1'-Biphenyl]-4-ylbis(4-methoxyphenyl)methanol (6a)

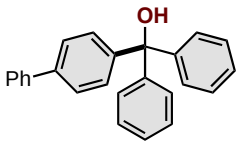


6a

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1a** (142.1 mg, 0.50 mmol) and diaryl ketone **5a** (61.1 mg, 0.25 mmol). The product **6a** was purified by flash column chromatography (SiO_2, hexane/CH_2Cl_2 = 50/50 then hexane/Et_2O = 95/5 to 80/20) and obtained in 83% yield (82.9 mg, 0.21 mmol) as a white solid.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.74 (s, 1H, OH), 3.81 (s, 6H), 6.83–6.88 (m, 4H), 7.18–7.25 (m, 4H), 7.33–7.38 (m, 3H), 7.40–7.46 (m, 2H), 7.51–7.56 (m, 2H), 7.56–7.62 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 55.4 (*C*H_3), 81.4 (*C*), 113.3 (*C*H), 126.7 (*C*H), 127.2 (*C*H), 127.4 (*C*H), 128.3 (*C*H), 128.9 (*C*H), 129.3 (*C*H), 139.5 (*C*), 140.0 (*C*), 140.8 (*C*), 146.5 (*C*), 158.8 (*C*). EI (m/z): $[M]^+$ calcd for $C_{27}H_{24}O_3$: 396.1720, found: 396.1706.

[1,1'-Biphenyl]-4-yldiphenylmethanol (6b)

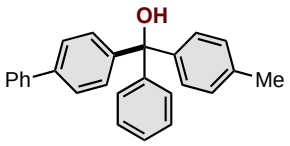


6b

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1a** (141.2 mg, 0.50 mmol) and diaryl ketone **5b** (46.0 mg, 0.25 mmol). The product **6b** was purified by flash column chromatography (SiO_2, hexane/CH_2Cl_2 = 50/50 then hexane/Et_2O = 90/10) and obtained in 94% yield (80.1 mg, 0.24 mmol) as a colorless oil.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.83 (s, 1H, OH), 7.28–7.38 (m, 13H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.54 (d, *J* = 7.9 Hz, 2H), 7.59 (d, *J* = 8.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 82.0 (*C*), 126.8 (*C*H), 127.2 (*C*H), 127.5 (*C*H), 128.05 (*C*H), 128.13 (*C*H), 128.5 (*C*H), 128.9 (*C*H), 140.2 (*C*), 140.7 (*C*), 146.0 (*C*), 146.9 (*C*). EI (m/z): $[M]^+$ calcd for $C_{25}H_{20}O$: 336.1509, found: 336.1500.

[1,1'-Biphenyl]-4-yl(phenyl)(p-tolyl)methanol (6c)

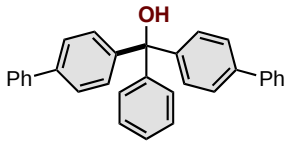


6c

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1a** (141.3 mg, 0.50 mmol) and diaryl ketone **5c** (50.0 mg, 0.25 mmol). The product **6c** was purified by flash column chromatography (SiO_2, hexane/CH_2Cl_2 = 50/50 then hexane/Et_2O = 90/10 to 80/20) and obtained in 86% yield (76.3 mg, 0.21 mmol) as a colorless oil.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.35 (s, 3H), 2.79 (s, 1H, OH), 7.11–7.16 (m, 2H), 7.17–7.22 (m, 2H), 7.27–7.38 (m, 8H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.51–7.56 (m, 2H), 7.56–7.61 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 21.2 (*C*H$_3$), 81.9 (*C*), 126.7 (*C*H), 127.2 (*C*H), 127.38 (*C*H), 127.44 (*C*H), 128.0 (*C*H), 128.1 (*C*H), 128.5 (*C*H), 128.8 (*C*H), 128.9 (*C*H), 137.2 (*C*), 140.1 (*C*), 140.8 (*C*), 144.1 (*C*), 146.2 (*C*) 147.1 (*C*). EI (m/z): $[M]^+$ calcd for $C_{26}H_{22}O$: 350.1665, found: 350.1648.

Di([1,1'-biphenyl]-4-yl)(phenyl)methanol (6d)

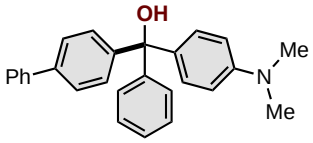


6d

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1a** (140.2 mg, 0.50 mmol) and diaryl ketone **5d** (66.0 mg, 0.25 mmol). The product **6d** was purified by flash column chromatography (SiO_2, hexane/CH_2Cl_2 = 50/50 then hexane/Et_2O = 90/10 to 80/20) and obtained in 86% yield (90.1 mg, 0.21 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 2.86 (s, 1H, OH), 7.28–7.49 (m, 15H), 7.52–7.66 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 81.9 (*C*), 126.8 (*C*H), 127.2 (*C*H), 127.50 (*C*H), 127.53 (*C*H), 128.1 (*C*H), 128.2 (*C*H), 128.5 (*C*H), 128.9 (*C*H), 140.2 (*C*), 140.7 (*C*), 145.9 (*C*), 146.9 (*C*). EI (m/z): $[M]^+$ calcd for $C_{31}H_{24}O$: 412.1822, found: 412.1807.

[1,1'-Biphenyl]-4-yl(4-(dimethylamino)phenyl)(phenyl)methanol (6e)

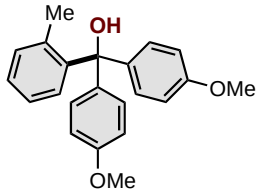


6e

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1a** (141.1 mg, 0.50 mmol) and diaryl ketone **5e** (58.4 mg, 0.25 mmol). The product **6e** was purified by flash column chromatography (SiO_2, hexane/CH_2Cl_2 = 50/50 then hexane/Et_2O = 80/20 to 75/25) and obtained in 69% yield (67.9 mg, 0.17 mmol) as a orange oil.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.74 (s, 1H, OH), 2.95 (s, 6H), 6.68 (d, *J* = 9.1 Hz, 2H), 7.10–7.15 (m, 2H), 7.26–7.46 (m, 10H), 7.51–7.56 (m, 2H), 7.57–7.62 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 40.6 (*C*H_3), 81.8 (*C*), 111.9 (*C*H), 126.6 (*C*H), 127.1 (*C*H), 127.2 (*C*H), 127.4 (*C*H), 128.0 (*C*H), 128.4 (*C*H), 128.9 (*C*H), 129.0 (*C*H), 134.9 (*C*), 139.8 (*C*), 140.9 (*C*), 146.6 (*C*), 147.5 (*C*) 149.8 (*C*). EI (m/z): $[M]^+$ calcd for $C_{27}H_{25}NO$: 379.1931, found: 379.1915.

Bis(4-methoxyphenyl)(o-tolyl)methanol (6f)

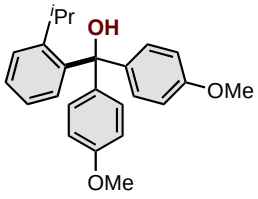


6f

The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1b** (82.5 mg, 0.375 mmol) and diaryl ketone **5a** (61.0 mg, 0.25 mmol). The product **6f** was purified by flash column chromatography (SiO_2, hexane/CH_2Cl_2 = 50/50 then hexane/Et_2O = 90/10 to 85/15) and obtained in 72% yield (60.9 mg, 0.18 mmol) as a colorless oil.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.15 (s, 3H), 2.90 (s, 1H, OH), 3.80 (s, 6H), 6.76 (d, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 9.1 Hz, 4H), 6.98–7.07 (m, 1H), 7.08–7.23 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 22.3 (*C*H_3), 55.4 (*C*H_3), 82.7 (*C*), 113.3 (*C*H), 125.0 (*C*H), 127.8 (*C*H), 129.0 (*C*H), 129.5 (*C*H), 132.6 (*C*H), 138.0 (*C*), 139.3 (*C*), 145.0 (*C*), 158.6 (*C*). EI (m/z): $[M]^+$ calcd for $C_{22}H_{22}O_3$: 334.1564, found: 334.1557.

(2-Isopropylphenyl)bis(4-methoxyphenyl)methanol (6g)



6g

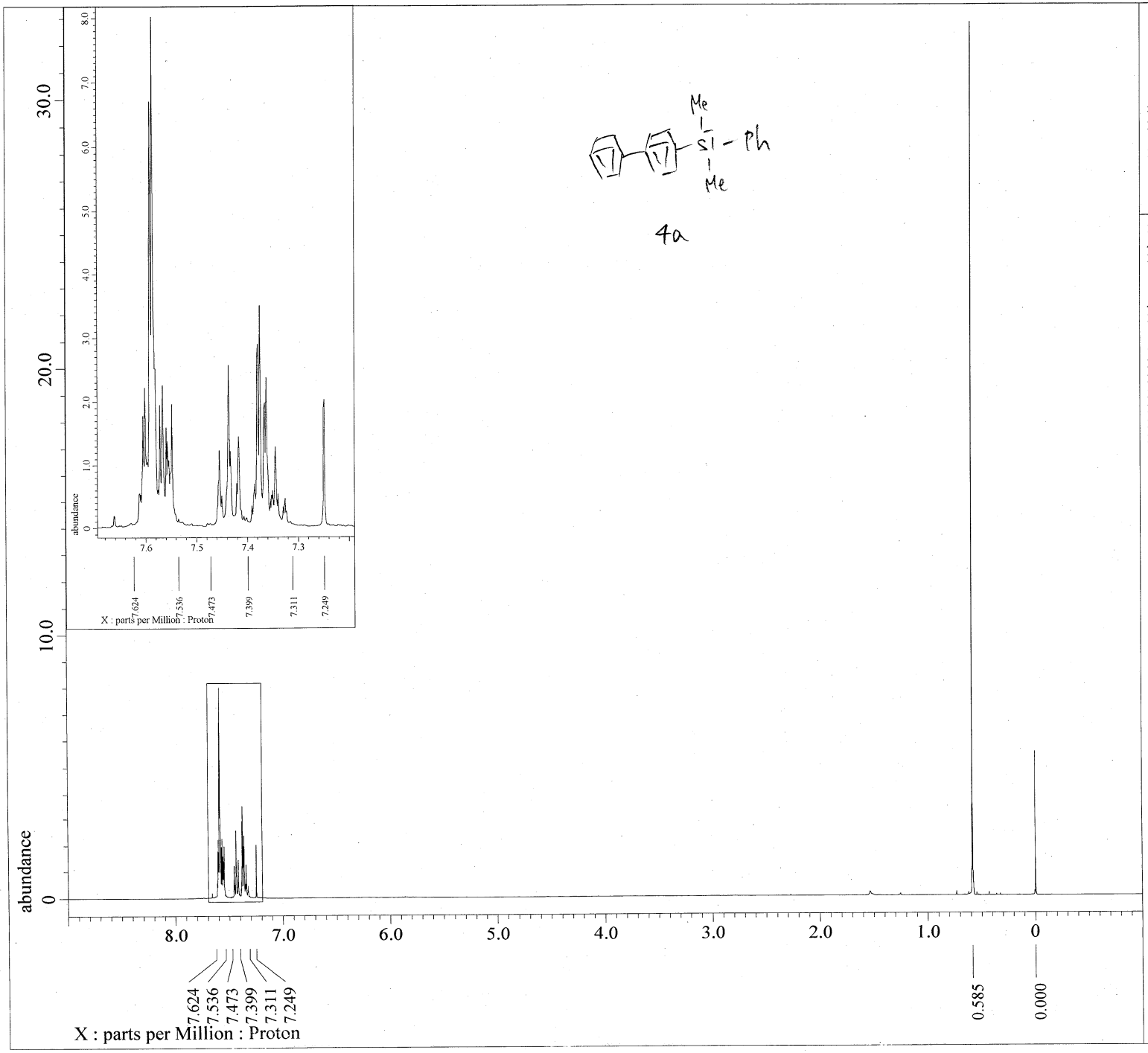
The reaction was performed according to the general procedure. The reaction was conducted with aryl iodide **1c** (91.7 mg, 0.375 mmol) and diaryl ketone **5a** (60.7 mg, 0.25 mmol). The product **6g** was purified by flash column chromatography (SiO_2, hexane/CH_2Cl_2 = 50/50 then hexane/Et_2O = 90/10 to 80/20) and obtained in 66% yield (59.8 mg, 0.16 mmol) as a colorless oil.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 0.96 (d, J = 6.7 Hz, 6H), 2.89 (s, 1H, OH), 3.28 (sept, J = 6.7 Hz, 1H), 3.81 (s, 6H), 6.71 (d, J = 8.3 Hz, 1H), 6.84 (d, J = 8.7 Hz, 4H), 6.99 (t, J = 7.3 Hz, 1H), 7.14 (d, J = 9.1 Hz, 4H), 7.29 (t, J = 7.5 Hz, 1H), 7.38 (d, J = 7.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.3 (CH_3), 30.1 (CH), 55.4 (CH_3), 82.6 (C), 113.2 (CH), 124.6 (CH), 128.1 (CH), 128.2 (CH), 129.1 (CH), 129.2 (CH), 140.0 (C), 144.0 (C), 149.4 (C), 158.6 (C). EI (m/z): $[M]^+$ calcd for $C_{24}H_{26}O_3$: 362.1877, found: 362.1871.

13. References

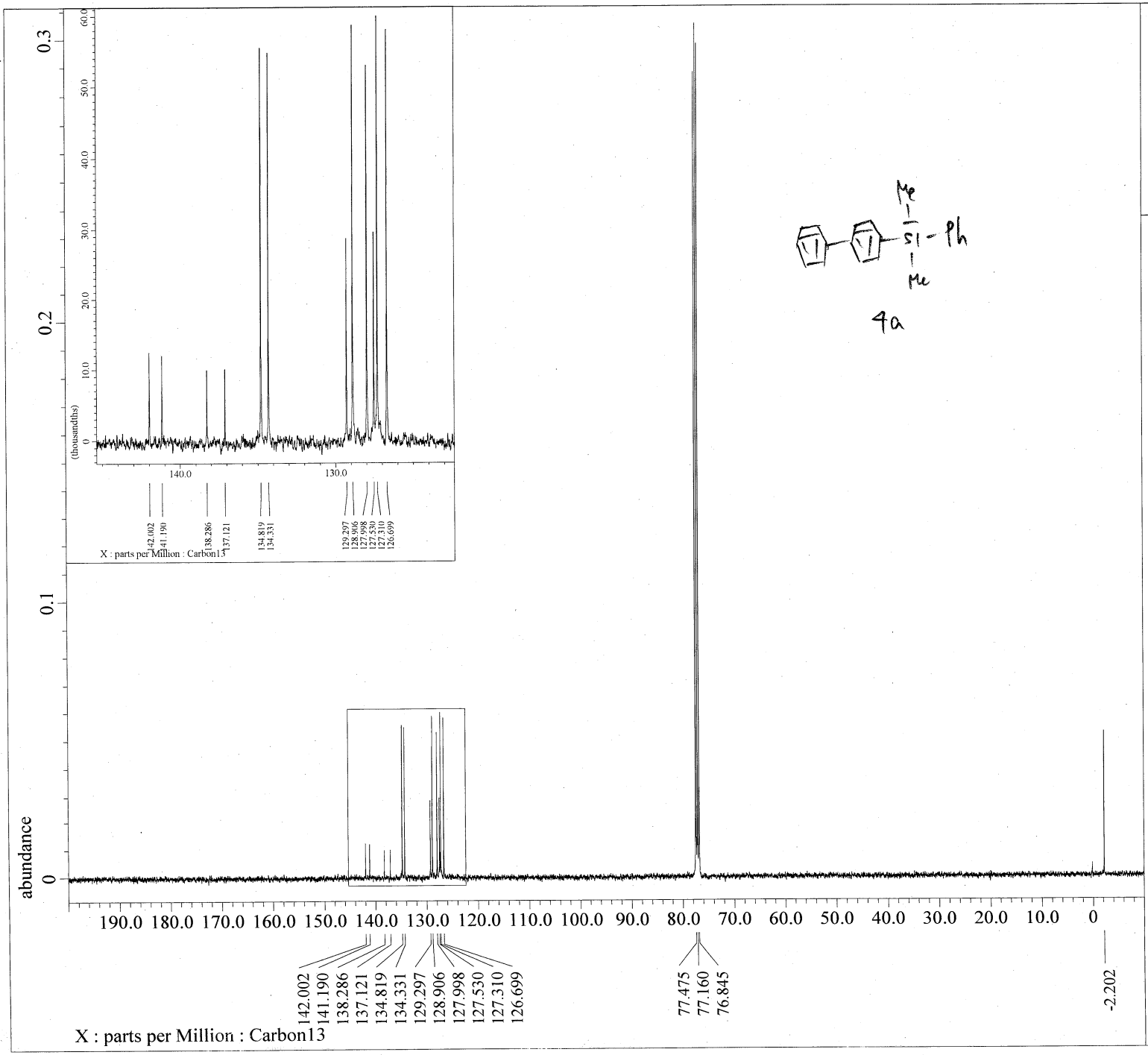
1. J.-H. Li and W.-J. Liu, *Org. Lett.,* **2004**, *6*, 2809–2811.
2. X. Wang, C. Feng, J. Jiang, S. Maeda, K. Kubota and H. Ito, *Nat. Commun*., **2023**, *14*, 5561–5571.
3. A. Yanagisawa, S. Habaue, K. Yasue and H. Yamamoto, *J. Am. Chem. Soc.,* **1994**, *116*, 6130–6141.
4. (a) S. Maeda, K. Ohno and K. Morokuma, *Phys. Chem. Chem. Phys.* 2013, **15**, 3683–3701. (b) S. Maeda, Y. Harabuchi, M. Takagi, T. Taketsugu and K. Morokuma, *Chem. Rec.* 2016, **16**, 2232–2248. (c) S. Maeda, Y. Harabuchi, M. Takagi, K. Saita, K. Suzuki, T. Ichino, Y. Sumiya, K. Sugiyama and Y. Ono, *J. Comput. Chem.* 2018, **39**, 233–251. (d) S. Maeda and Y. Harabuchi, *WIREs Comput. Mol. Sci.* 2021, **11**, e1538.
5. S. Grimme, C. Bannwarth and P. Shushkov, *J. Chem. Theory Comput.* 2017, **13**, 1989–2009.
6. F. Neese, *WIREs Comput. Mol. Sci.* 2018, **8**, e1327.
7. (a) A. D. Becke, *Phys. Rev. A* 1988, **38**, 3098–3100. (b) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 1372–1377. (c) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648–5652. (d) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B* 1988, **37**, 785–789.
8. Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
9. (a) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104. (b) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.* 2011, **32**, 1456–1465.
10. (a) A. D. McLean and G. S. Chandler, *J. Chem. Phys.* 1980, **72**, 5639–5648. (b) R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.* 1980, **72**, 650–654.
11. (a) M. Dolg, U. Wedig, H. Stoll and H. Preuss, *J. Chem. Phys.* 1987, **86**, 866–872. (b) G. Igel-Mann, H. Stoll and H. Preuss, *Mol. Phys.* 1988, **65**, 1321–1328. (c) A. Bergner, M. Dolg, W. Kuechle, H. Stoll and H. Preuss, *Mol. Phys.* 1993, **80**, 1431–1441.
12. A. Höllwarth, M. Böhme, S. Dapprich, A. W. Ehlers, A. Gobbi, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp and G. Frenking, G. *Chem. Phys. Lett.* 1993, **208**, 237–240.
13. K. Fukui, *Acc. Chem. Res.* 1981, **14**, 363–368.
14. CYLview, 1.0b; C. Y. Legault, Université de Sherbrooke, 2009.

15. W.-Y. Qi, J.-S. Zhen, X. Xu, X. Du, Y. Li, H. Yuan, Y.-S. Guan, X. Wei, Z.-Y. Wang, G. Liang and Y. Luo, *Org. Lett*., **2021**, *23*, 5988–5992.
16. K. Murakami, K. Harano, H. Yorimitsu and K. Oshima, *Angew. Chem. Int. Ed.*, **2008**, *47*, 5833–5835.
17. Y.-Y. Kong and Z.-X. Wang, *Adv. Synth. Catal.*, **2019**, *361*, 5440–5448.
18. S. Mallick, P. Xu, E.-U. Würthwein, and A. Studer, *Angew. Chem. Int. Ed.*, **2019**, *58*, 283–287.
19. W. Kirmse, W. Konrad and I. S. Özkir, *Tetrahedron*, **1997**, *53*, 9935–9964.
20. S. Chen, X. Guo, H. Hou, S. Geng, Z. Liu, Y. He, X.-S. Xue and Z. Feng, *Angew. Chem. Int. Ed.*, **2023**, *62*, e202303470.
21. G. Pandey, S. K. Tiwari, P. Singh and P. K. Mondal, *Org. Lett.*, **2021**, *23*, 7730–7734.



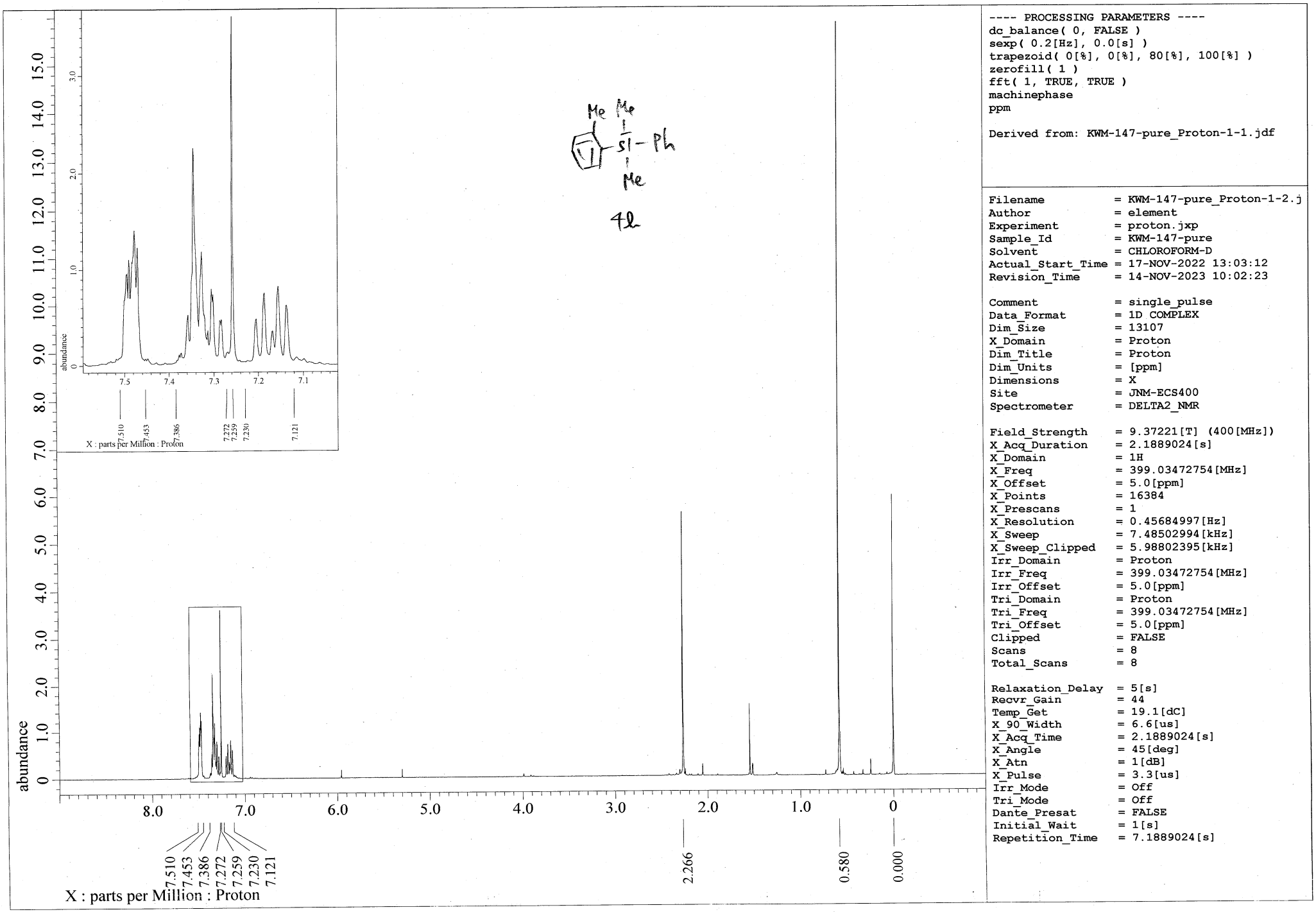

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-136-pure_Proton-1-1.jdf
```

Filename	= KWM-136-pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KWM-136-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-NOV-2022 22:52:13
Revision_Time	= 14-NOV-2023 09:55:39
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 19.6[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



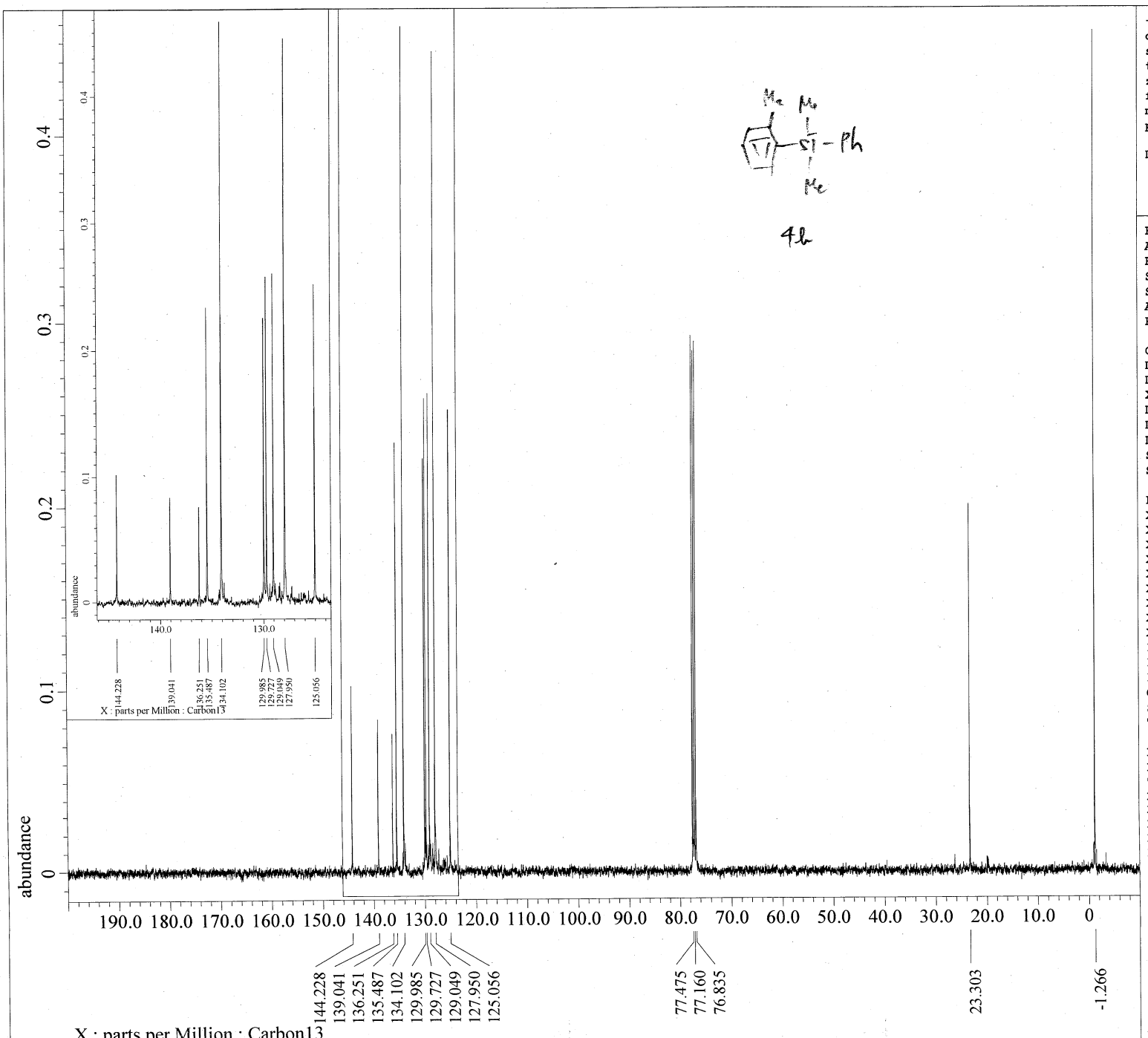

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-136-pure_Carbon-1-1.jdf
```

Filename	= KWM-136-pure_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KWM-136-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-NOV-2022 22:53:33
Revision_Time	= 14-NOV-2023 09:57:12
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 2048
Total_Scans	= 2048
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.8[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



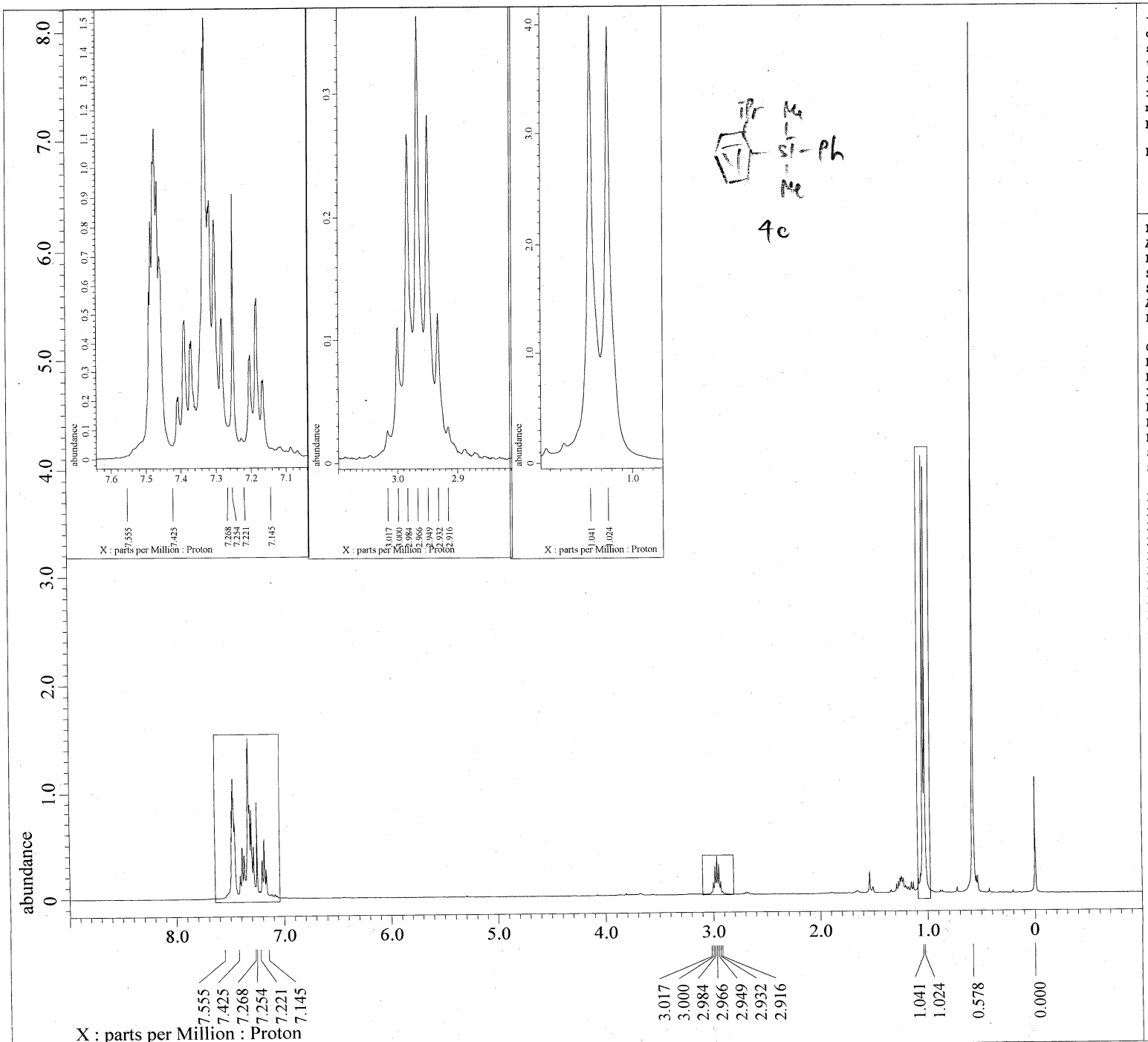

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-147-pure_Proton-1-1.jdf
```

Filename	= KWM-147-pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KWM-147-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-NOV-2022 13:03:12
Revision_Time	= 14-NOV-2023 10:02:23
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 19.1[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-147-pure_Carbon-1-1.jdf
```

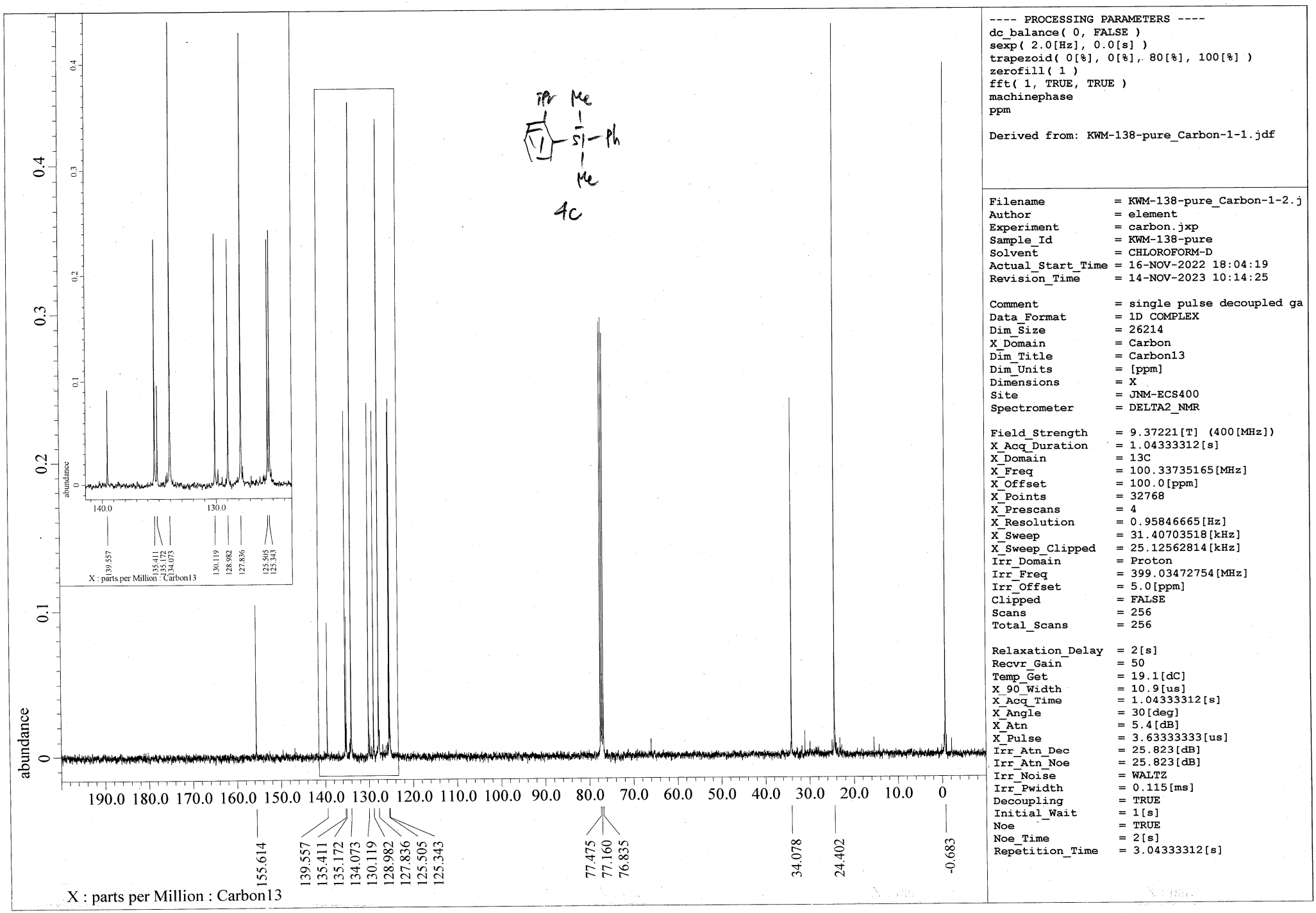
Filename	= KWM-147-pure_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KWM-147-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-JAN-2023 15:16:25
Revision_Time	= 14-NOV-2023 10:03:58
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.8[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



4c

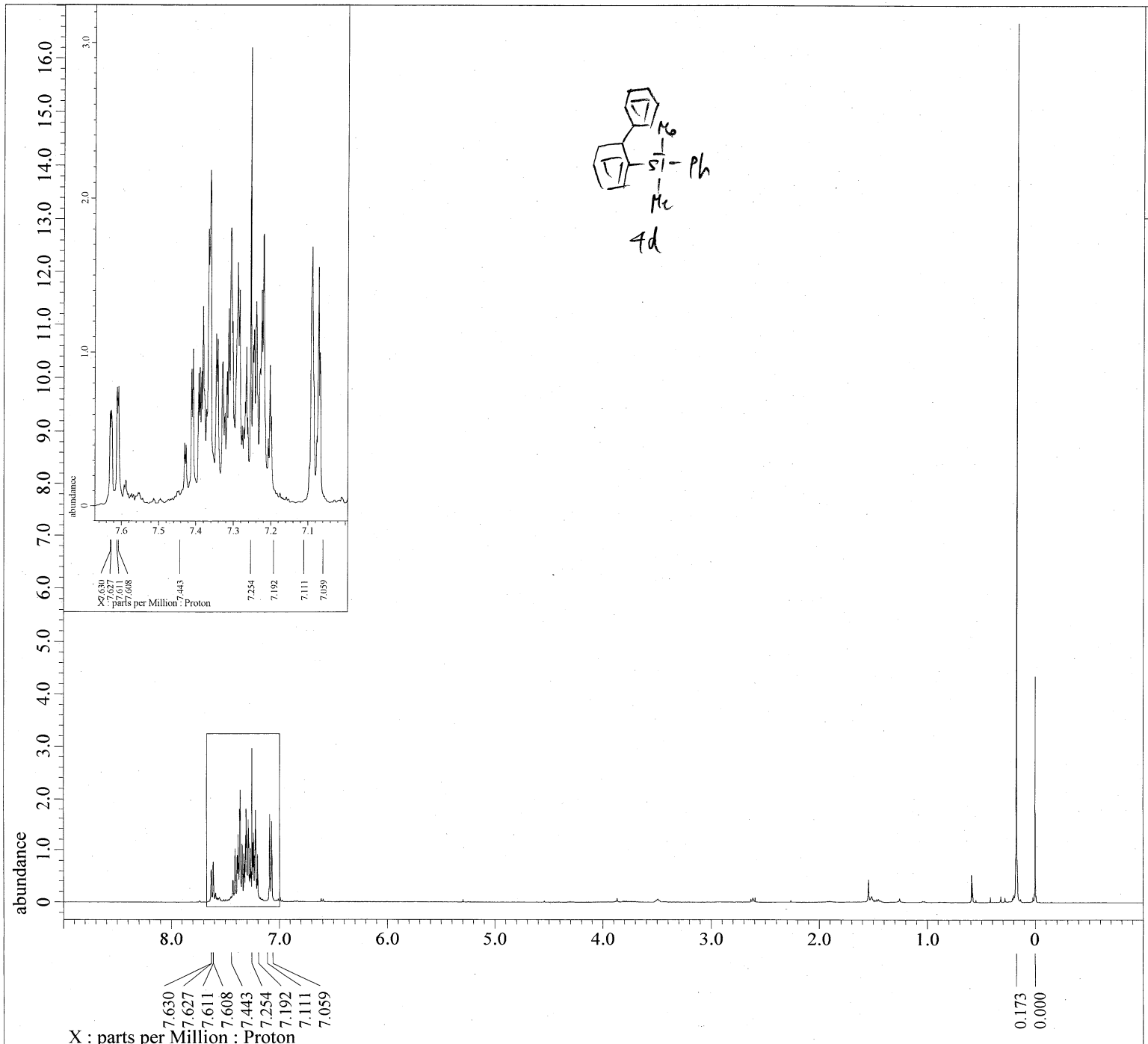
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-138-pure_Proton-1-1.jdf
```

Filename	= KWM-138-pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KWM-138-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 10-NOV-2022 22:43:29
Revision_Time	= 14-NOV-2023 10:12:32
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 19.5[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-138-pure_Carbon-1-1.jdf
```

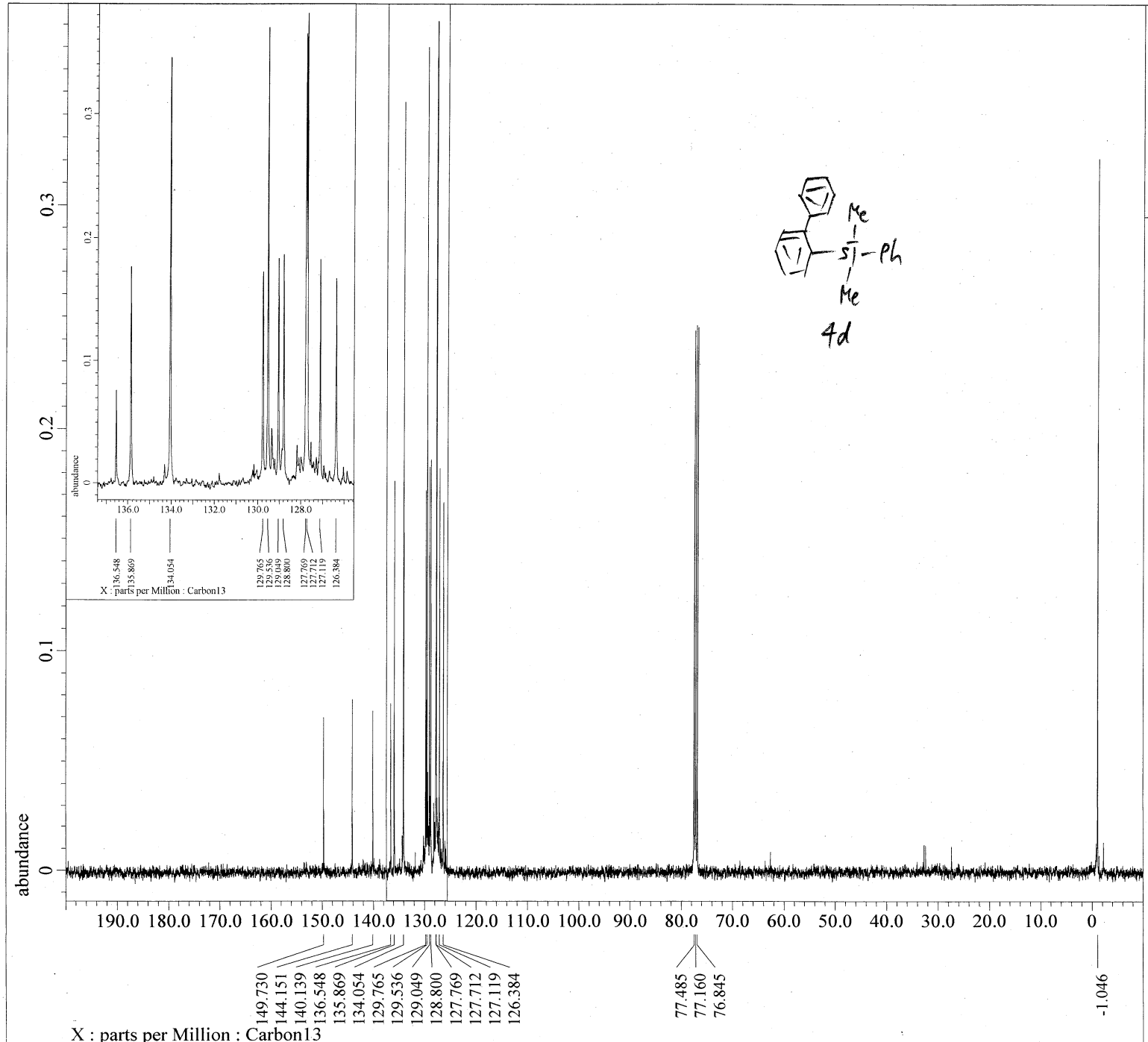
Filename	= KWM-138-pure_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KWM-138-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-NOV-2022 18:04:19
Revision_Time	= 14-NOV-2023 10:14:25
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.1[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



4d

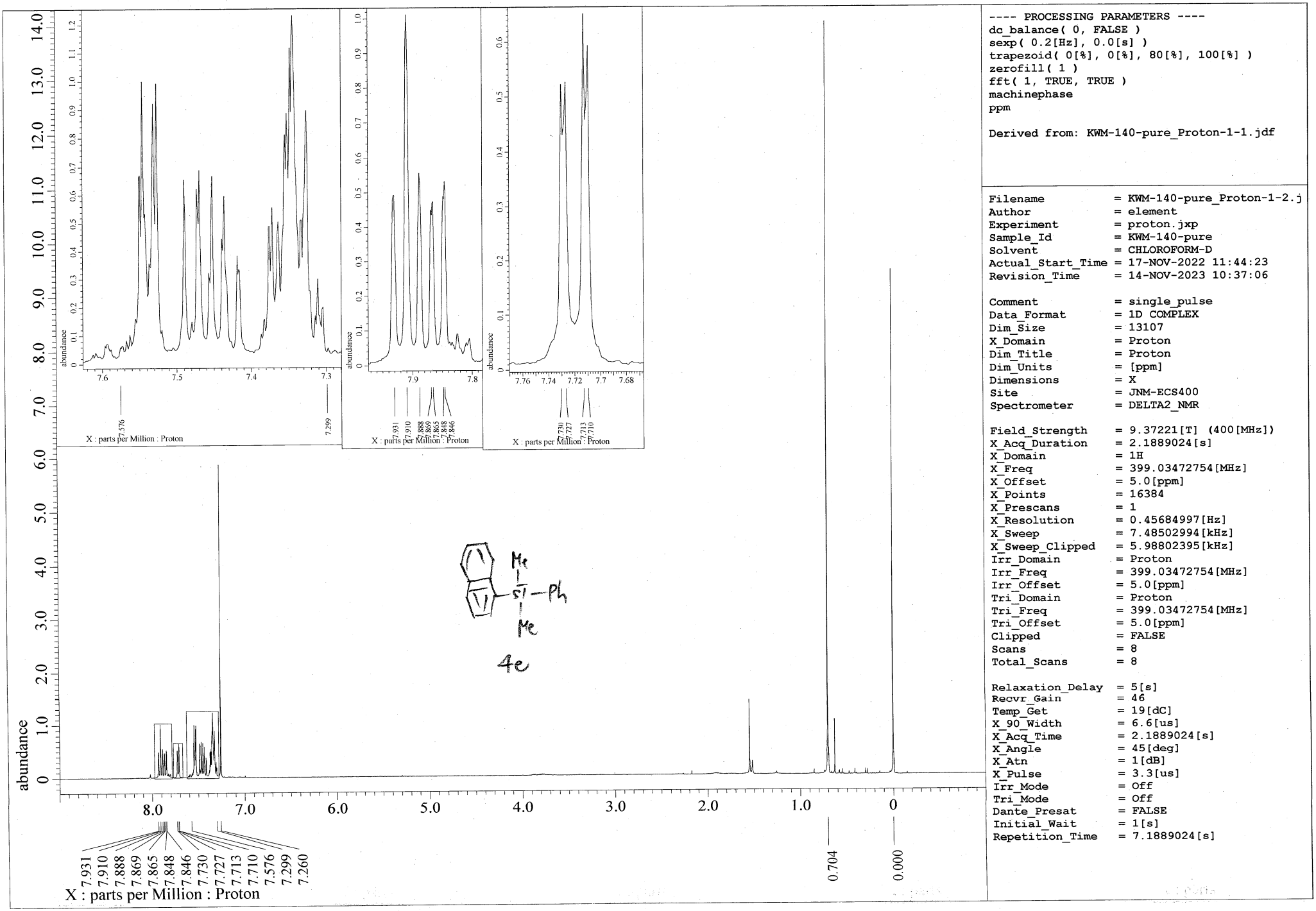
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-139-pure_Proton-1-1.jdf
```

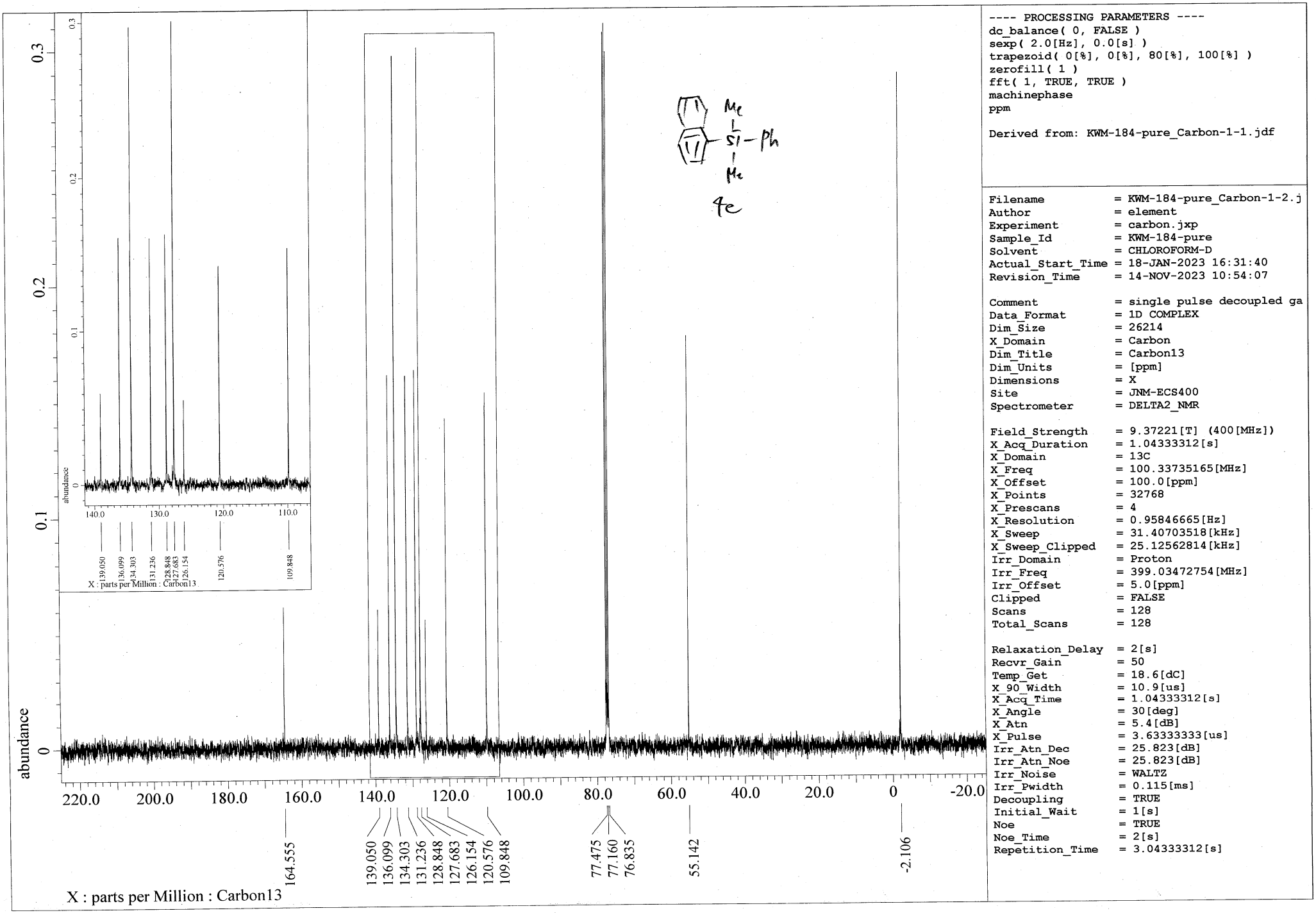
Filename	= KWM-139-pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KWM-139-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 10-NOV-2022 22:51:17
Revision_Time	= 14-NOV-2023 10:31:37
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 19.7[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]

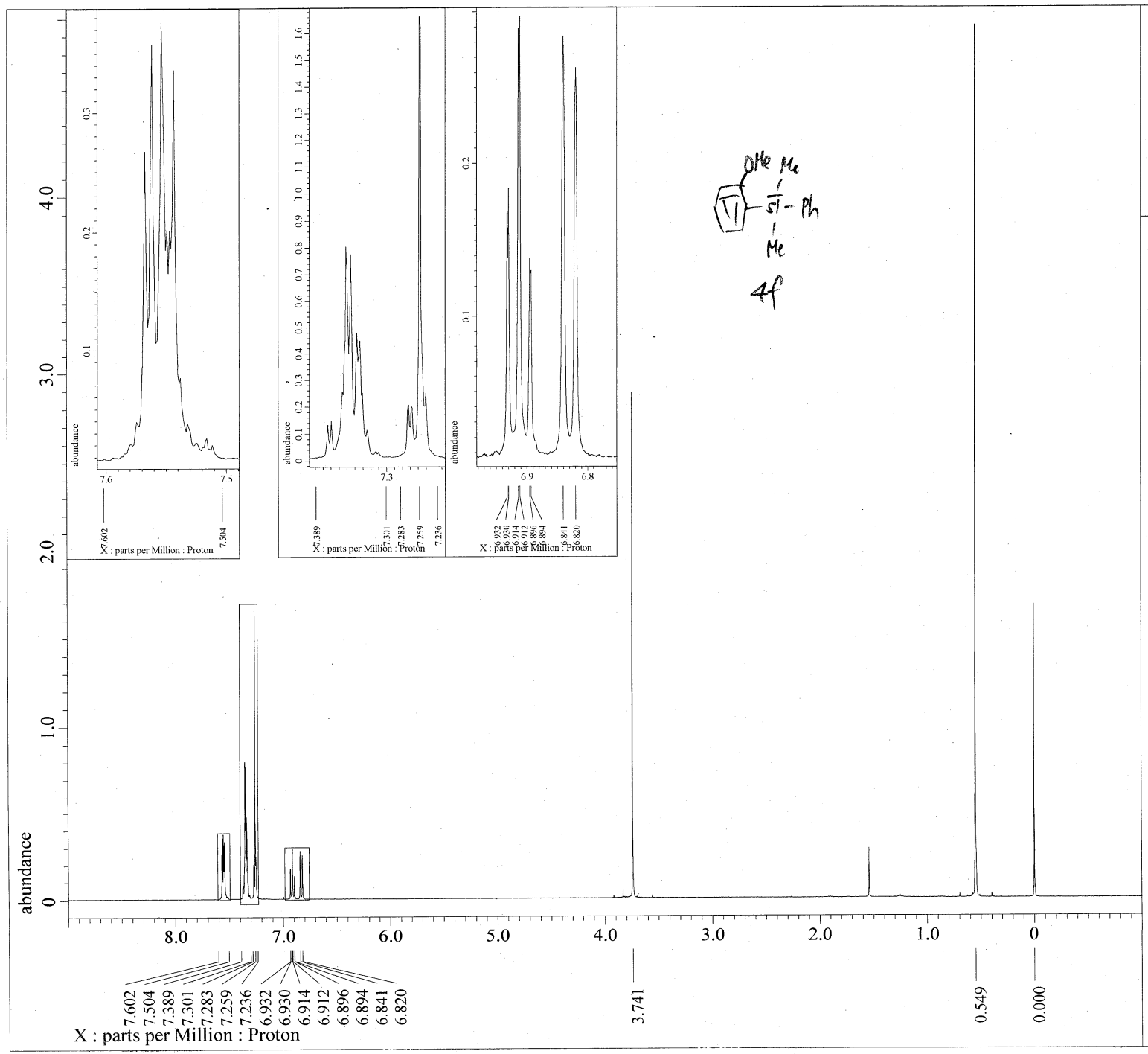



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-139-pure_Carbon-1-1.jdf
```

Filename	= KWM-139-pure_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KWM-139-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-NOV-2022 18:36:59
Revision_Time	= 14-NOV-2023 10:33:29
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.8[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]


---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KWM-140-pure_Proton-1-1.jdf
Filename = KWM-140-pure_Proton-1-2.j
Author = element
Experiment = proton.jxp
Sample_Id = KWM-140-pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-NOV-2022 11:44:23
Revision_Time = 14-NOV-2023 10:37:06
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.37221[T] (400[MHz])
X_Acq_Duration = 2.1889024[s]
X_Domain = 1H
X_Freq = 399.03472754[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45684997[Hz]
X_Sweep = 7.48502994[kHz]
X_Sweep_Clipped = 5.98802395[kHz]
Irr_Domain = Proton
Irr_Freq = 399.03472754[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 399.03472754[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 19[dC]
X_90_Width = 6.6[us]
X_Acq_Time = 2.1889024[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 3.3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.1889024[s]
abundance
X : parts per Million : Proton
7.931
7.910
7.888
7.869
7.865
7.848
7.846
7.730
7.727
7.713
7.710
7.576
7.299
7.260
0.704
0.000
Me
Si
Ph
Me
4e

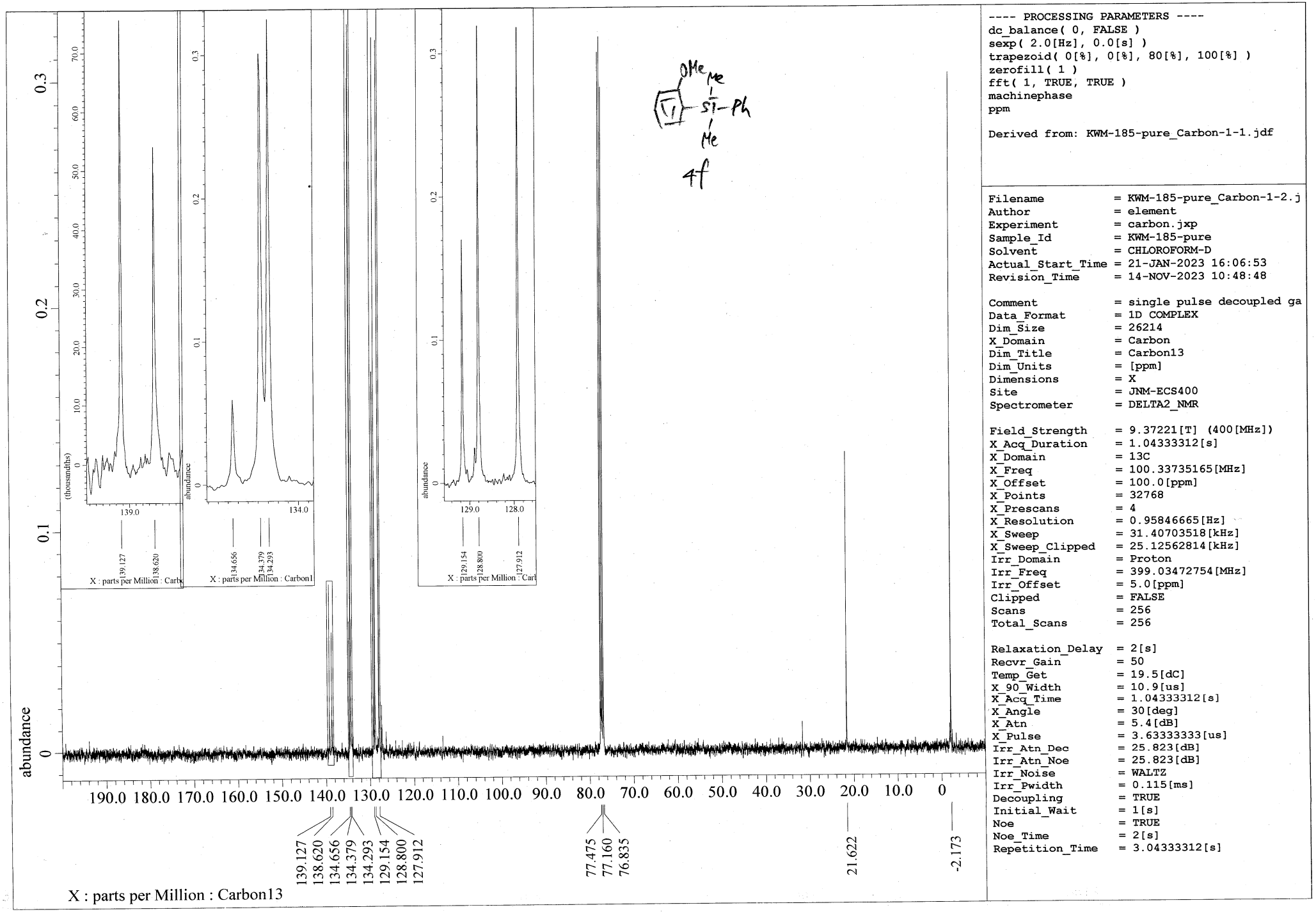

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KWM-184-pure_Carbon-1-1.jdf
Filename = KWM-184-pure_Carbon-1-2.j
Author = element
Experiment = carbon.jxp
Sample_Id = KWM-184-pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-JAN-2023 16:31:40
Revision_Time = 14-NOV-2023 10:54:07
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.37221[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.33735165[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.03472754[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 18.6[dC]
X_90_Width = 10.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 5.4[dB]
X_Pulse = 3.63333333[us]
Irr_Atn_Dec = 25.823[dB]
Irr_Atn_Noe = 25.823[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Me
Si
Ph
Me
4e
abundance
X : parts per Million : Carbon13
164.555
139.050
136.099
134.303
131.236
128.848
127.683
126.154
120.576
109.848
77.475
77.160
76.835
55.142
-2.106

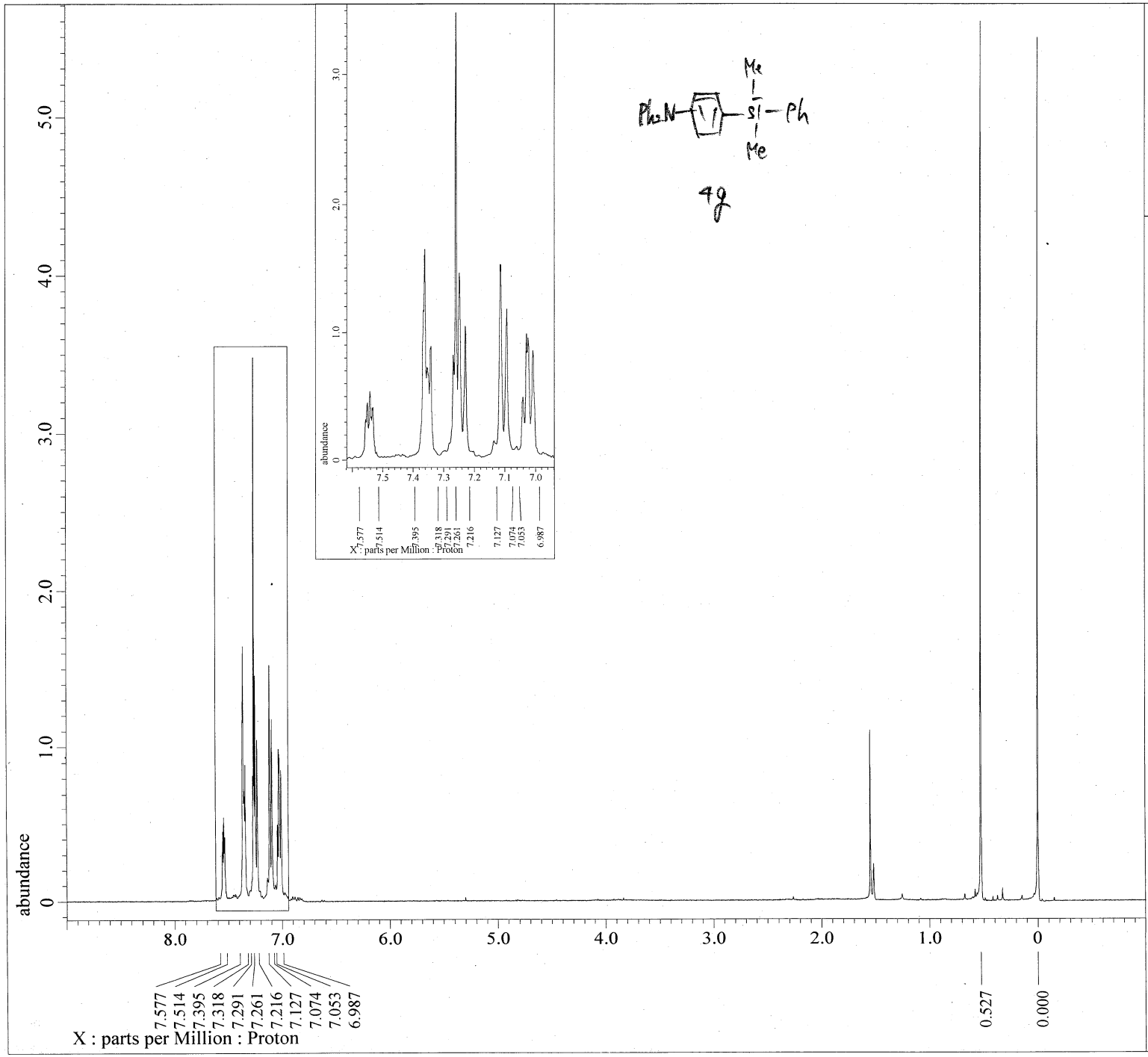


4f

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-184-pure_Proton-1-1.jdf
```

Filename	= KWM-184-pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KWM-184-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-DEC-2022 09:50:09
Revision_Time	= 16-NOV-2023 13:23:30
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 19[dC]
X_90_Width	= 11.25[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 5.625[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

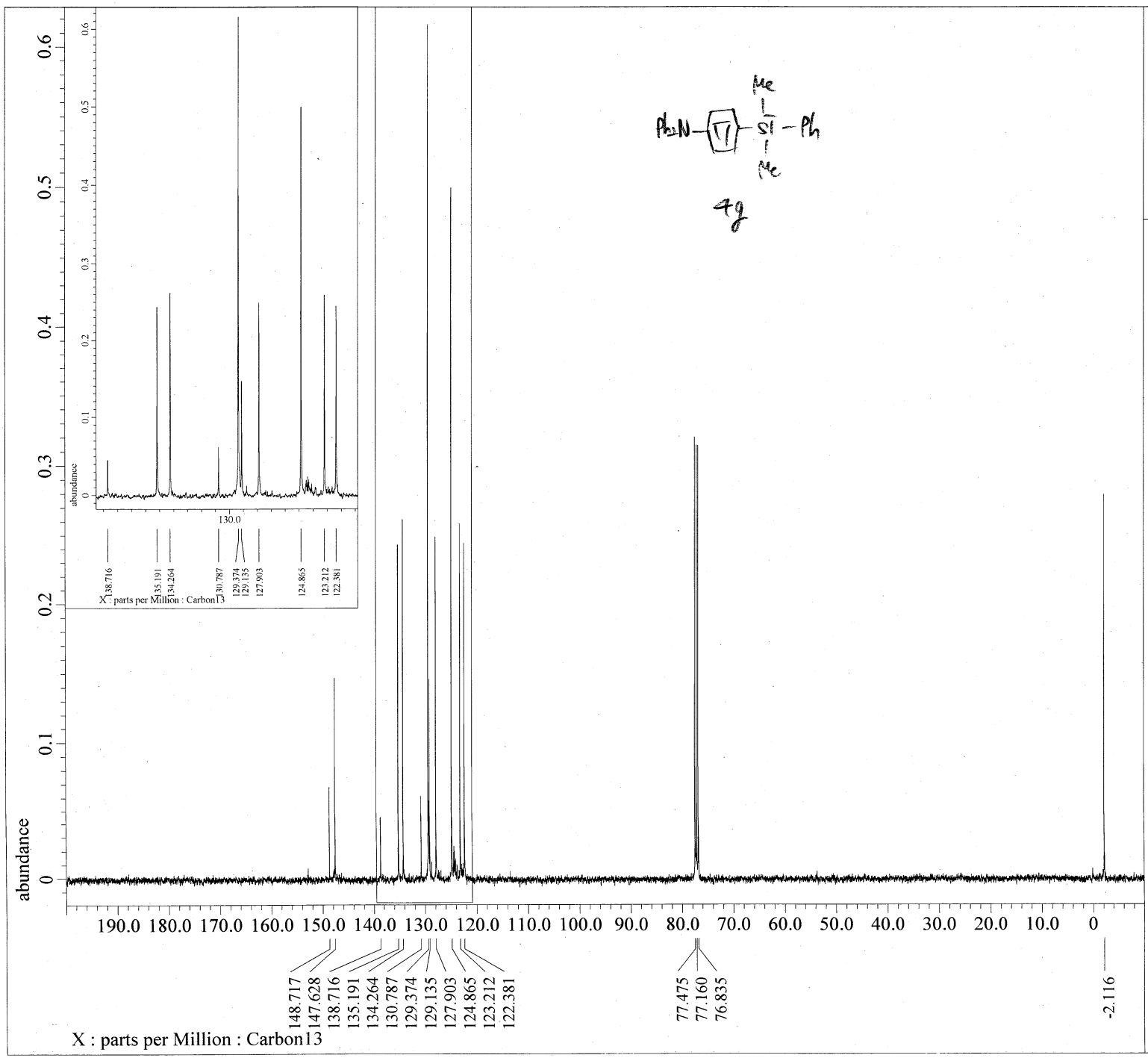

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KWM-185-pure_Carbon-1-1.jdf
Filename = KWM-185-pure_Carbon-1-2.j
Author = element
Experiment = carbon.jxp
Sample_Id = KWM-185-pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-JAN-2023 16:06:53
Revision_Time = 14-NOV-2023 10:48:48
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.37221[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.33735165[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.03472754[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.5[dC]
X_90_Width = 10.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 5.4[dB]
X_Pulse = 3.63333333[us]
Irr_Atn_Dec = 25.823[dB]
Irr_Atn_Noe = 25.823[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
OMe
Me
Si
Ph
Me
4f
abundance
(thousandths)
X : parts per Million : Carbon
X : parts per Million : Carbon1
X : parts per Million : Carbon
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
139.127
138.620
134.656
134.379
134.293
129.154
128.800
127.912
77.475
77.160
76.835
21.622
-2.173
X : parts per Million : Carbon13



4g

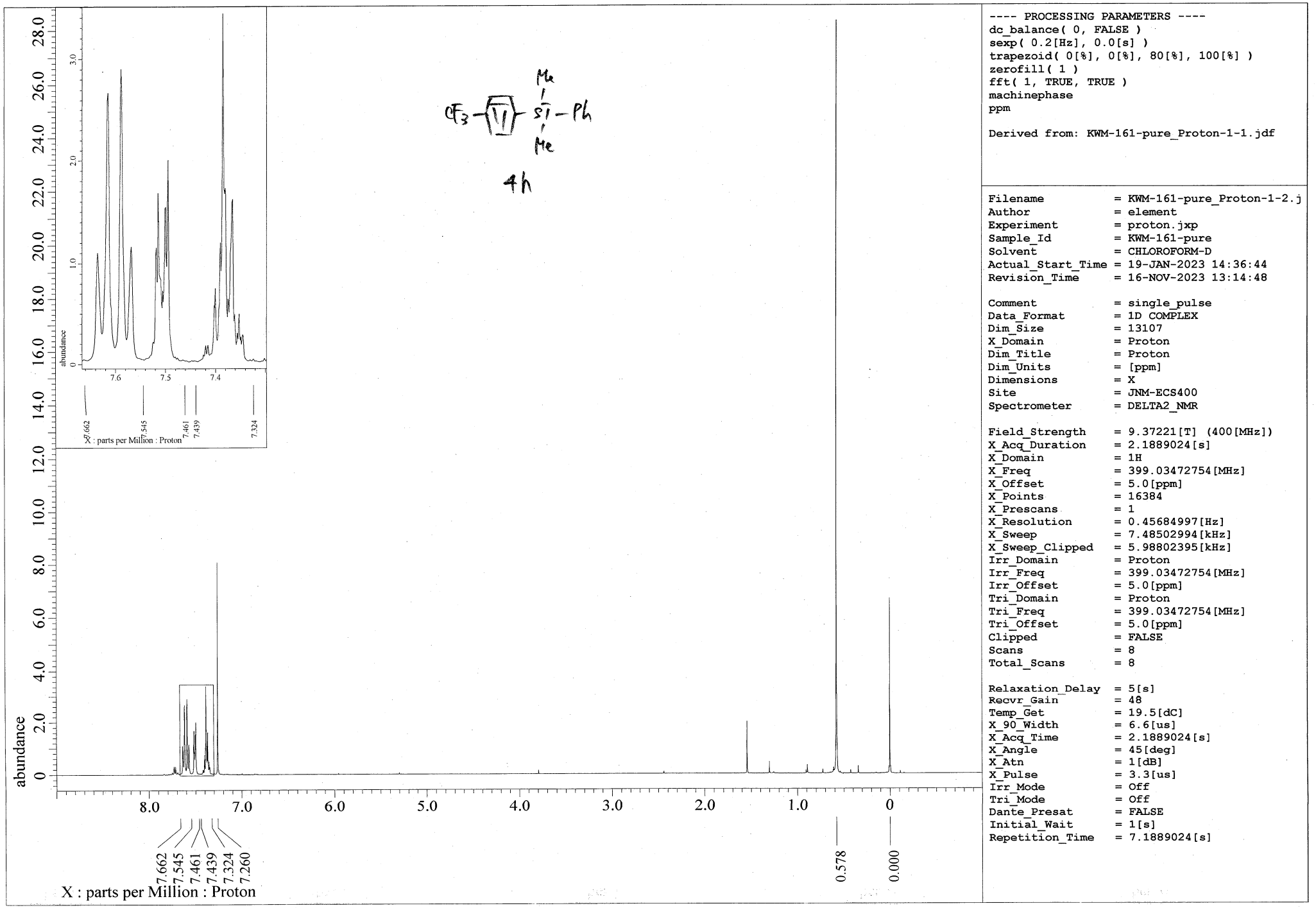
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-146-pure_Proton-1-1.jdf
```

```
Filename            = KWM-146-pure_Proton-1-2.j
Author              = element
Experiment          = proton.jxp
Sample_Id           = KWM-146-pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 17-NOV-2022 11:50:41
Revision_Time       = 14-NOV-2023 11:03:39

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Proton
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 2.1889024[s]
X_Domain            = 1H
X_Freq              = 399.03472754[MHz]
X_Offset            = 5.0[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.45684997[Hz]
X_Sweep             = 7.48502994[kHz]
X_Sweep_Clipped     = 5.98802395[kHz]
Irr_Domain          = Proton
Irr_Freq            = 399.03472754[MHz]
Irr_Offset          = 5.0[ppm]
Tri_Domain          = Proton
Tri_Freq            = 399.03472754[MHz]
Tri_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 46
Temp_Get            = 19[dC]
X_90_Width          = 6.6[us]
X_Acq_Time          = 2.1889024[s]
X_Angle             = 45[deg]
X_Atn               = 1[dB]
X_Pulse             = 3.3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.1889024[s]
```



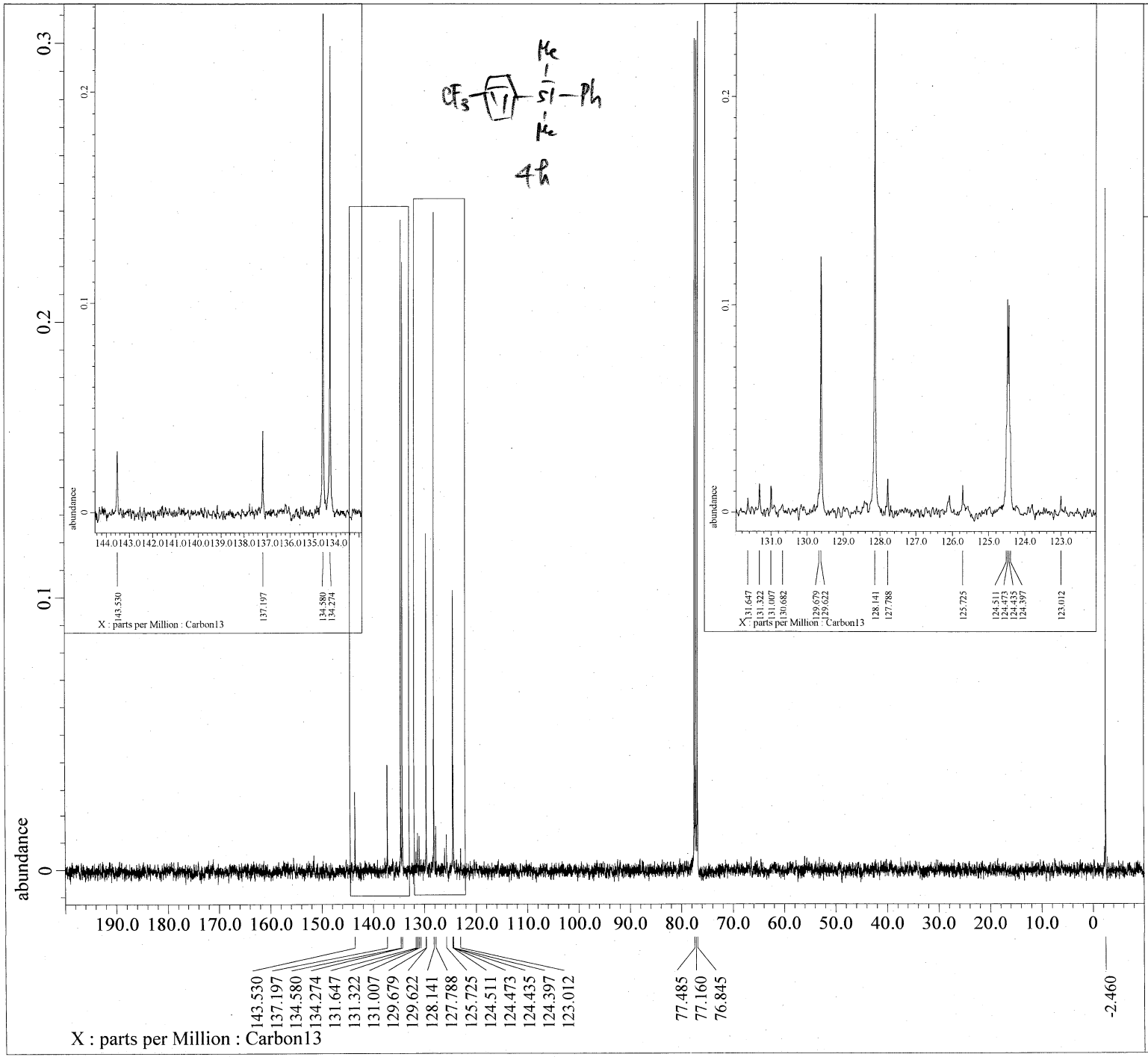

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-146-pure_Carbon-1-1.jdf
```

```
Filename            = KWM-146-pure_Carbon-1-2.j
Author              = element
Experiment          = carbon.jxp
Sample_Id           = KWM-146-pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 19-NOV-2022 09:46:32
Revision_Time       = 14-NOV-2023 11:04:50

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = Carbon
Dim_Title           = Carbon13
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 1.04333312[s]
X_Domain            = 13C
X_Freq              = 100.33735165[MHz]
X_Offset            = 100.0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.95846665[Hz]
X_Sweep             = 31.40703518[kHz]
X_Sweep_Clipped     = 25.12562814[kHz]
Irr_Domain          = Proton
Irr_Freq            = 399.03472754[MHz]
Irr_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 256
Total_Scans         = 256

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 20.1[dC]
X_90_Width          = 10.9[us]
X_Acq_Time          = 1.04333312[s]
X_Angle             = 30[deg]
X_Atn               = 5.4[dB]
X_Pulse             = 3.63333333[us]
Irr_Atn_Dec         = 25.823[dB]
Irr_Atn_Noe         = 25.823[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 0.115[ms]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 3.04333312[s]
```



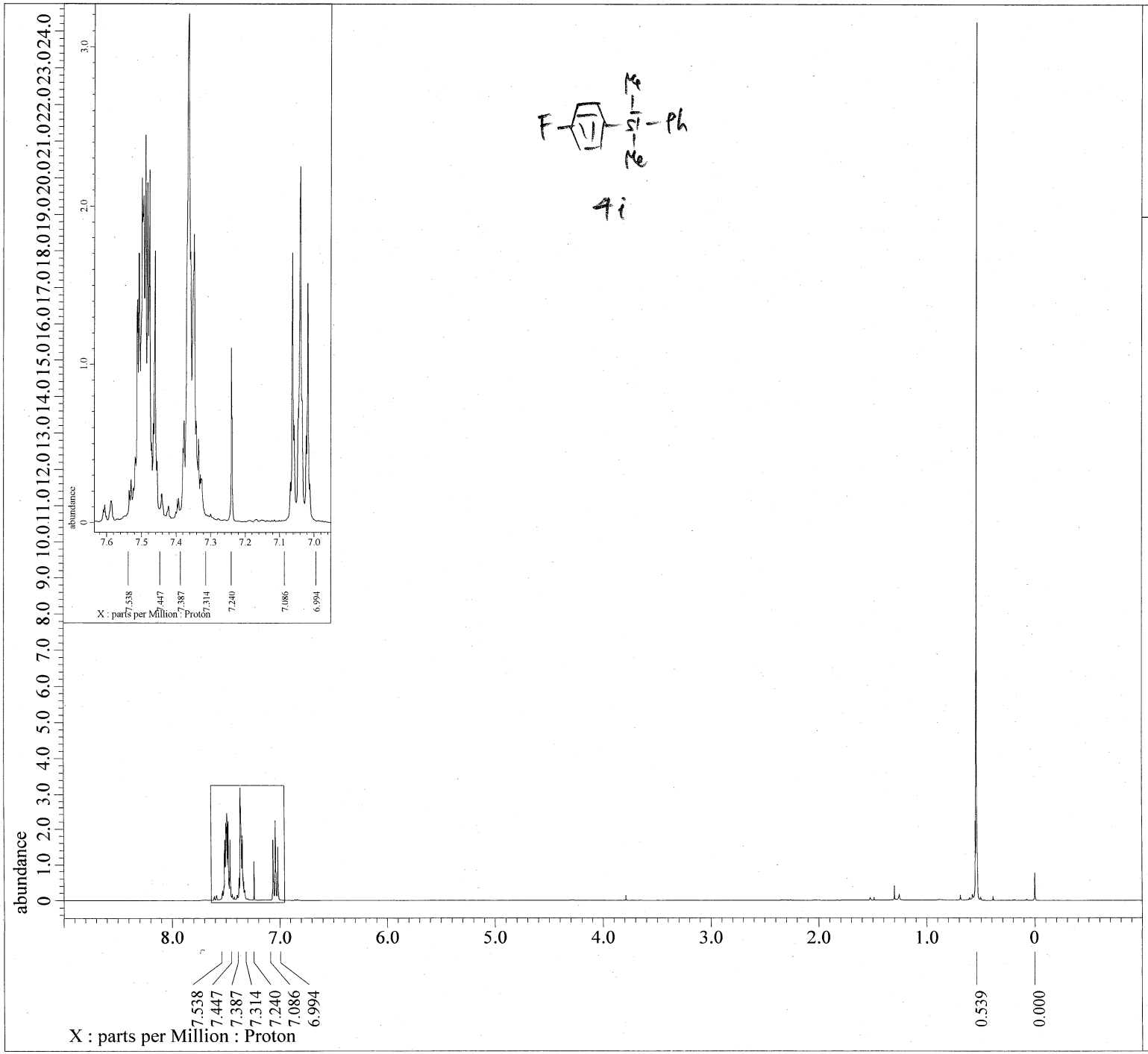

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-161-pure_Proton-1-1.jdf
```

Filename	= KWM-161-pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KWM-161-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-JAN-2023 14:36:44
Revision_Time	= 16-NOV-2023 13:14:48
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 48
Temp_Get	= 19.5[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



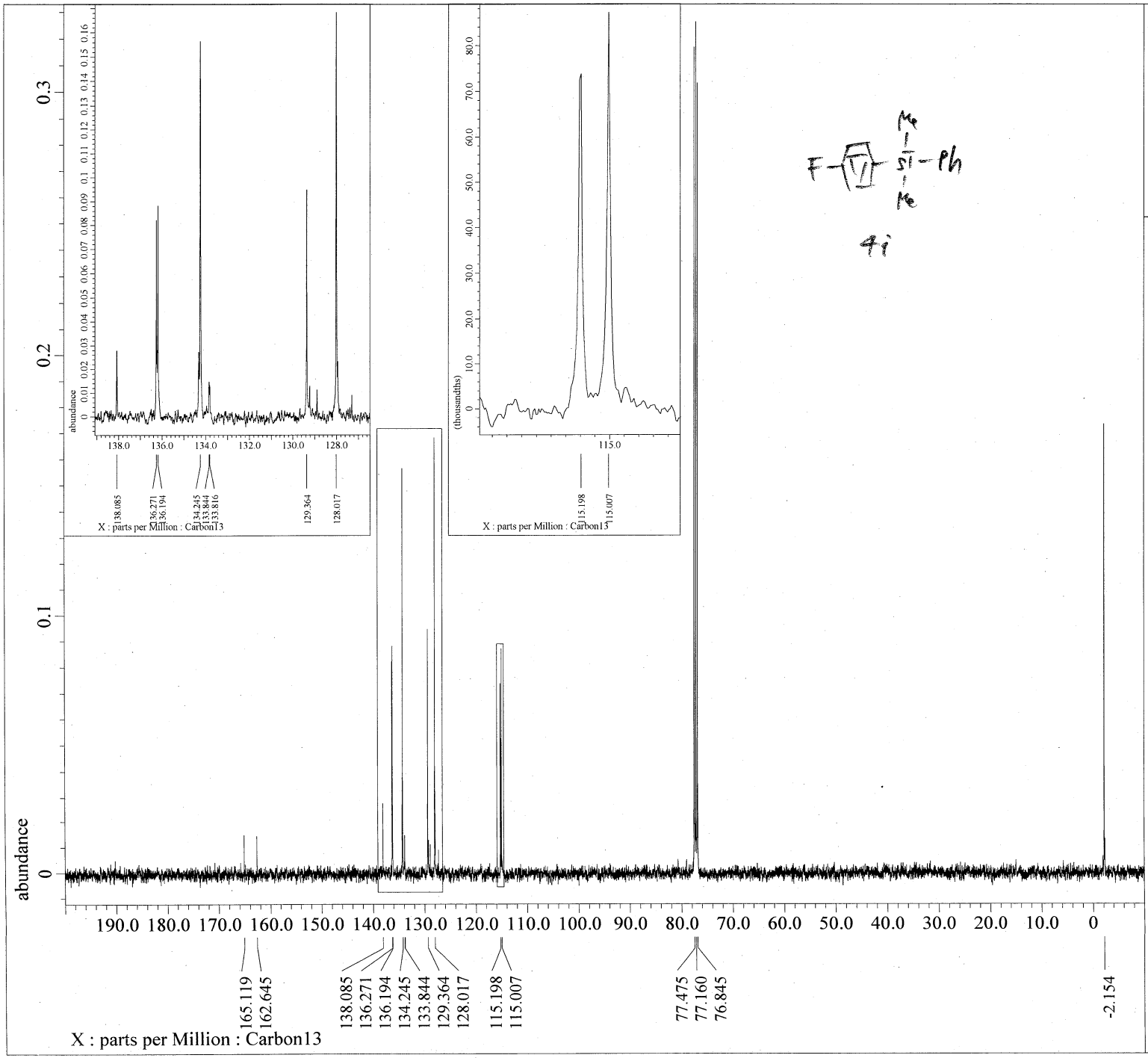

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-161-pure_Carbon-1-1.jdf
```

Filename	= KWM-161-pure_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KWM-161-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-JAN-2023 15:40:08
Revision_Time	= 14-NOV-2023 11:13:24
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.2[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



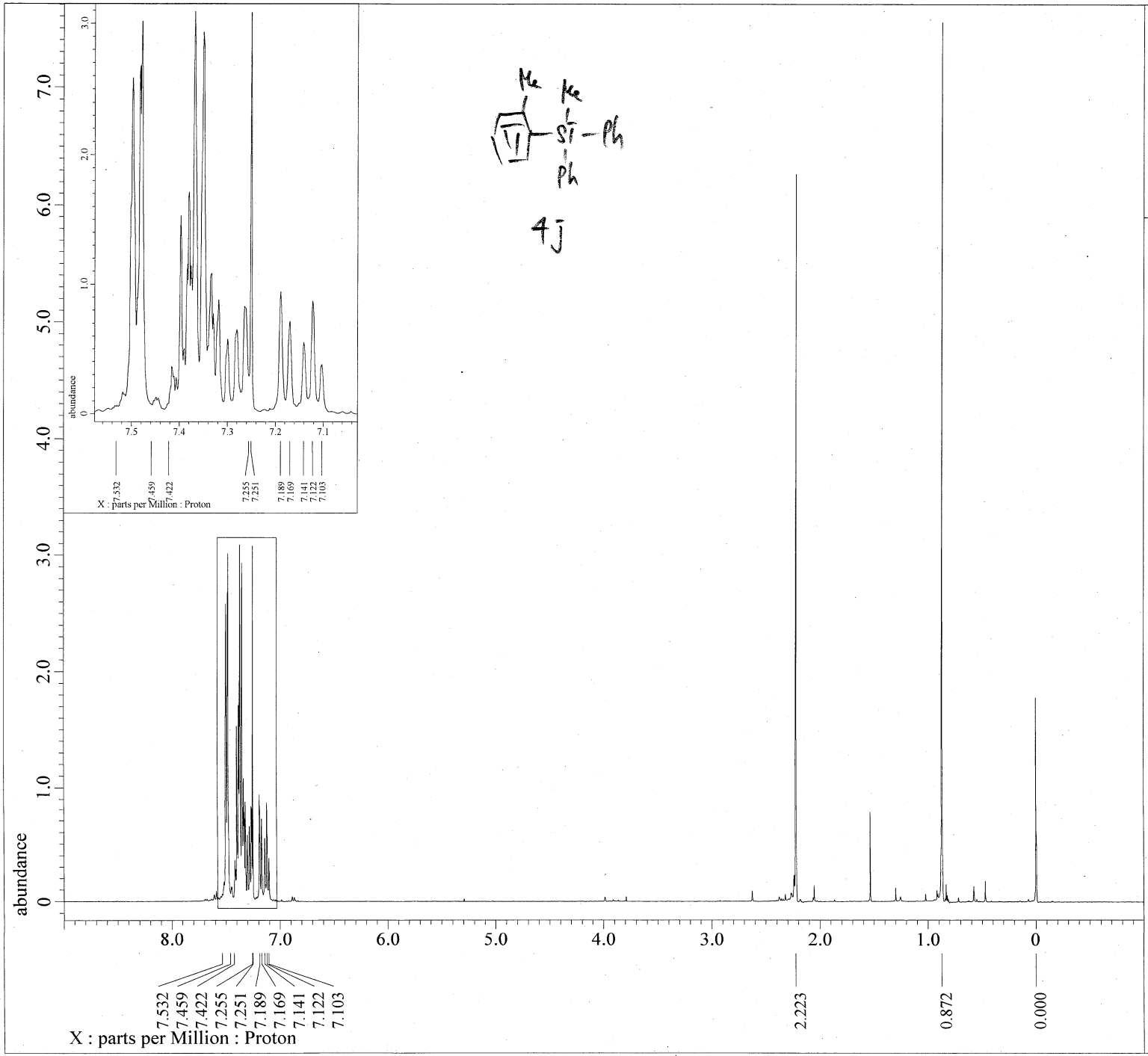

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-189-pure_Proton-1-1.jdf
```

Filename	= KWM-189-pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KWM-189-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-JAN-2023 17:06:50
Revision_Time	= 14-NOV-2023 11:16:41
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 32
Temp_Get	= 19.2[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



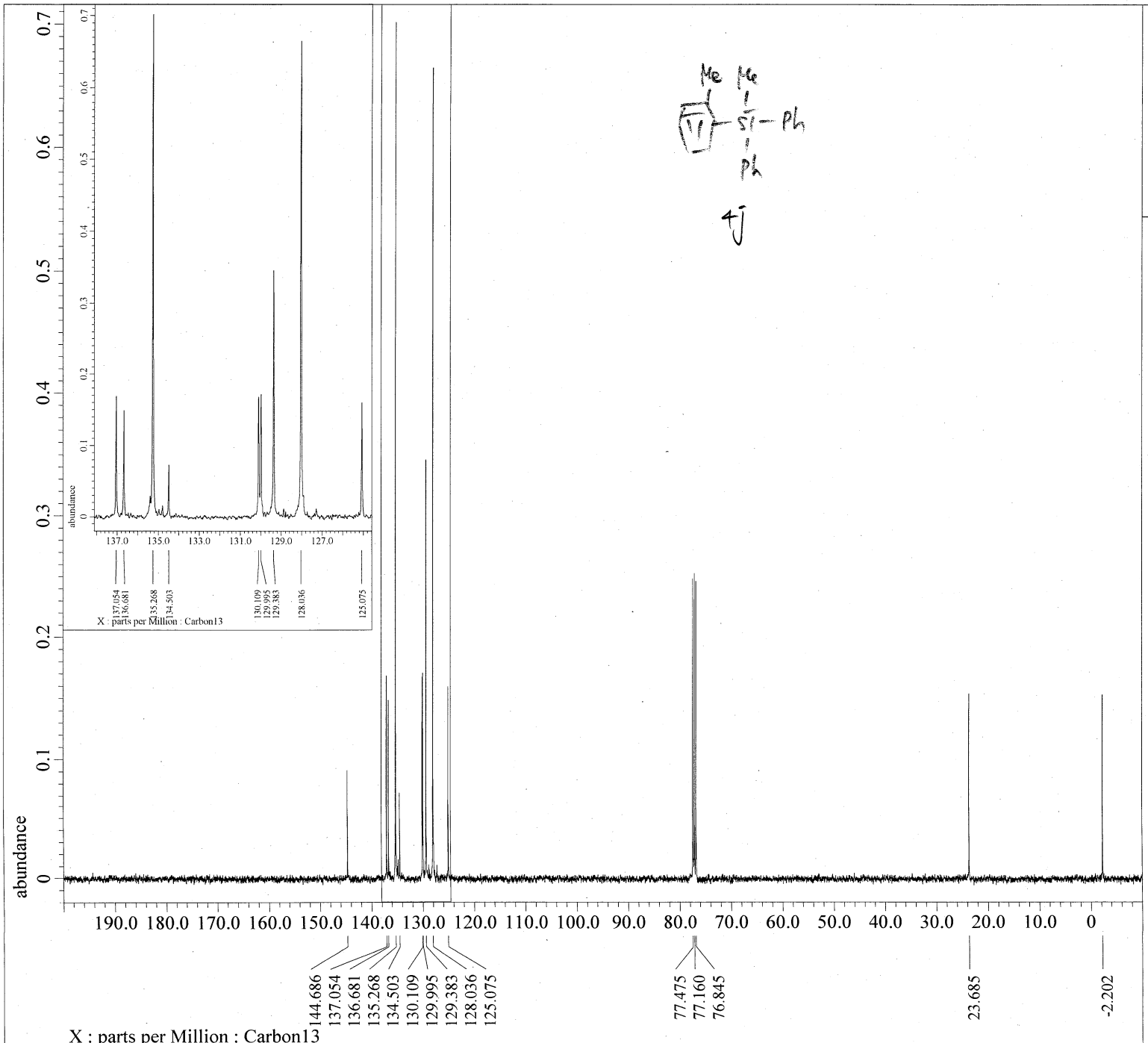

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-189-pure_Carbon-1-1.jdf
```

```
Filename            = KWM-189-pure_Carbon-1-2.j
Author              = element
Experiment          = carbon.jxp
Sample_Id           = KWM-189-pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 24-JAN-2023 17:08:09
Revision_Time       = 14-NOV-2023 11:20:25

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = Carbon
Dim_Title           = Carbon13
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 1.04333312[s]
X_Domain            = 13C
X_Freq              = 100.33735165[MHz]
X_Offset            = 100.0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.95846665[Hz]
X_Sweep             = 31.40703518[kHz]
X_Sweep_Clipped     = 25.12562814[kHz]
Irr_Domain          = Proton
Irr_Freq            = 399.03472754[MHz]
Irr_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 256
Total_Scans         = 256

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.2[dC]
X_90_Width          = 10.9[us]
X_Acq_Time          = 1.04333312[s]
X_Angle             = 30[deg]
X_Atn               = 5.4[dB]
X_Pulse             = 3.63333333[us]
Irr_Atn_Dec         = 25.823[dB]
Irr_Atn_Noe         = 25.823[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 0.115[ms]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 3.04333312[s]
```



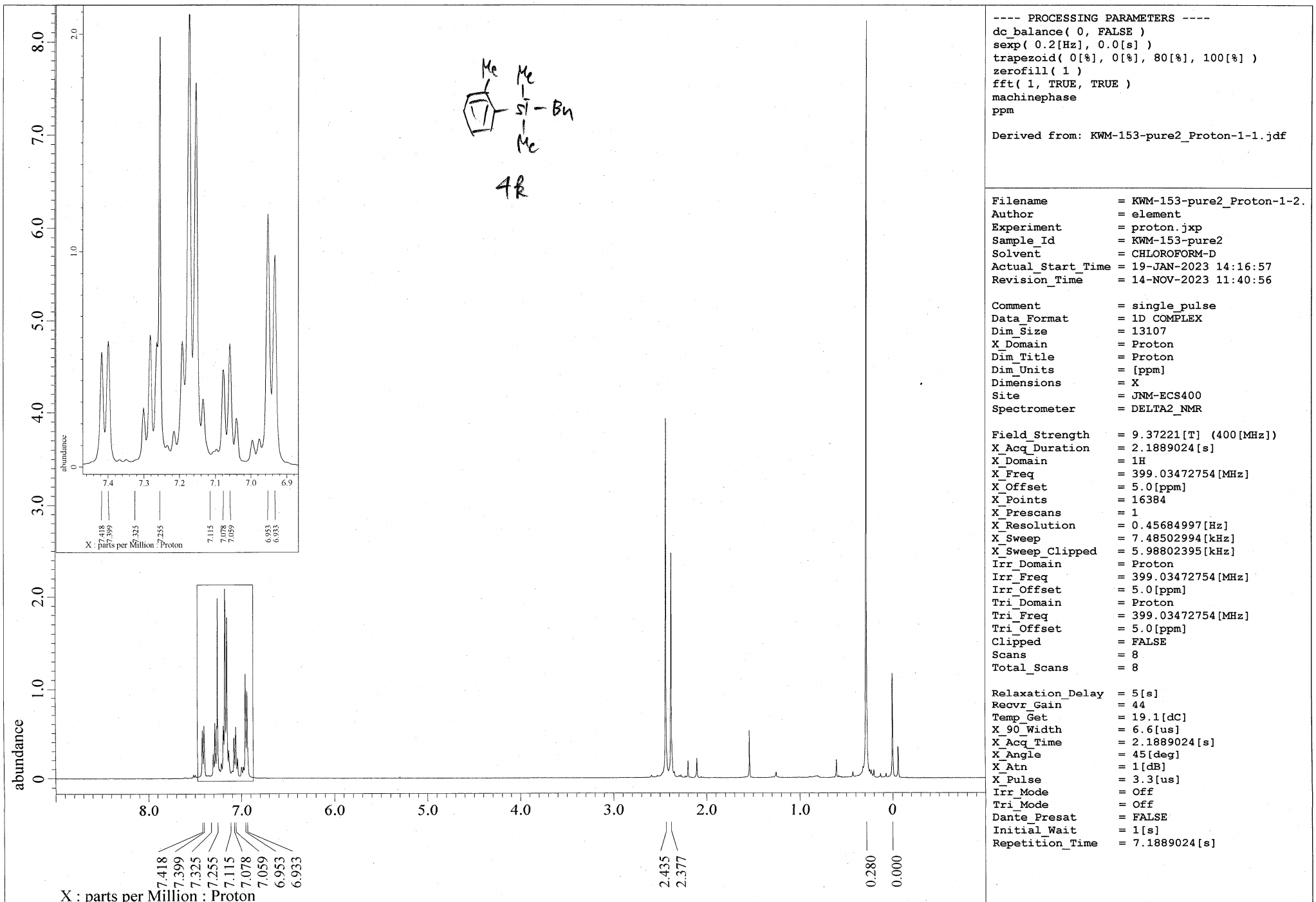

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-151-pure2_Proton-1-1.jdf
```

Filename	= KWM-151-pure2_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KWM-151-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-JAN-2023 14:09:33
Revision_Time	= 14-NOV-2023 11:36:23
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 18.8[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



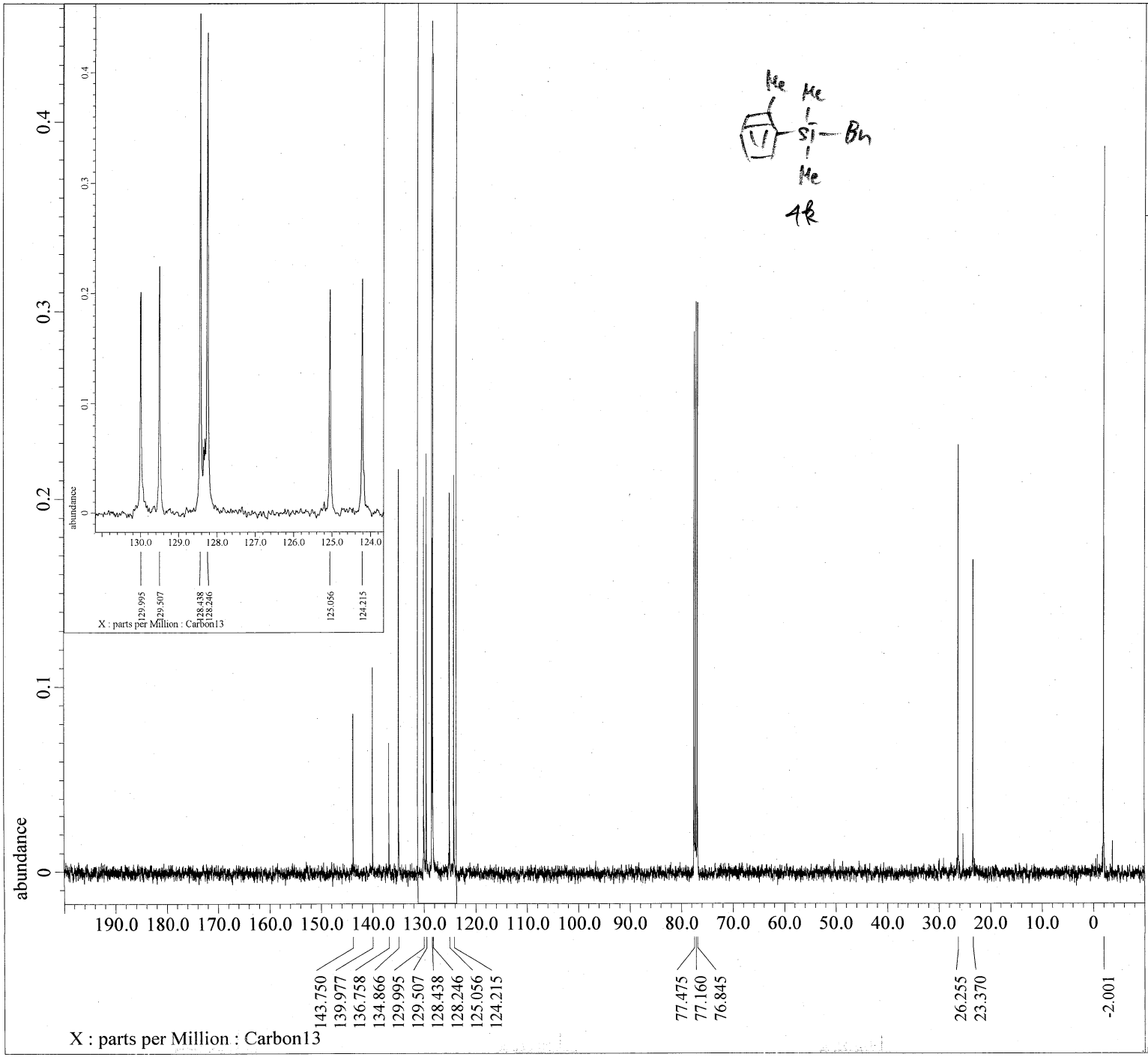

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-151-pure_Carbon-1-1.jdf
```

Filename	= KWM-151-pure_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KWM-151-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-JAN-2023 15:43:52
Revision_Time	= 14-NOV-2023 11:37:31
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.2[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



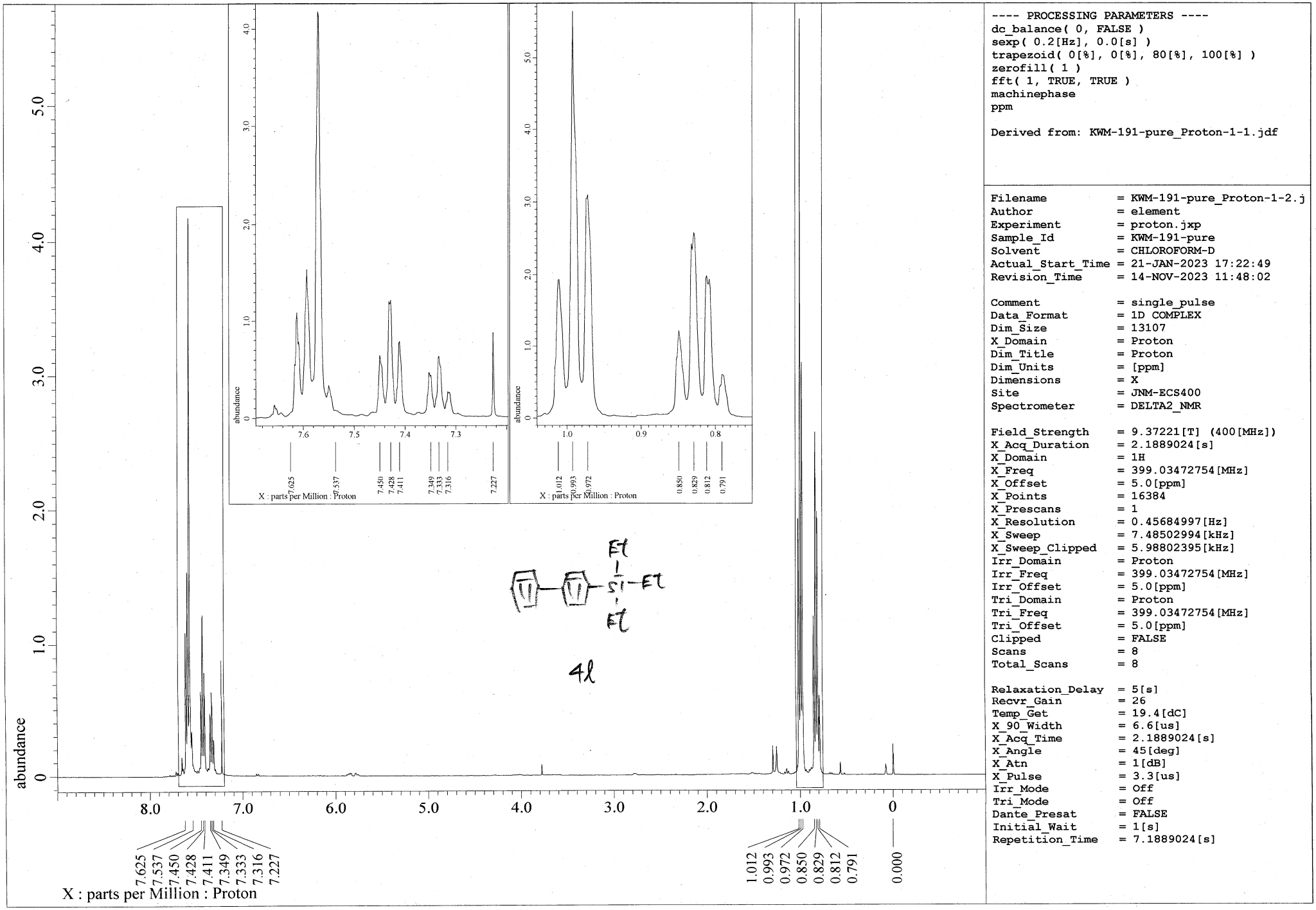

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-153-pure2_Proton-1-1.jdf
```

Filename	= KWM-153-pure2_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KWM-153-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-JAN-2023 14:16:57
Revision_Time	= 14-NOV-2023 11:40:56
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 19.1[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



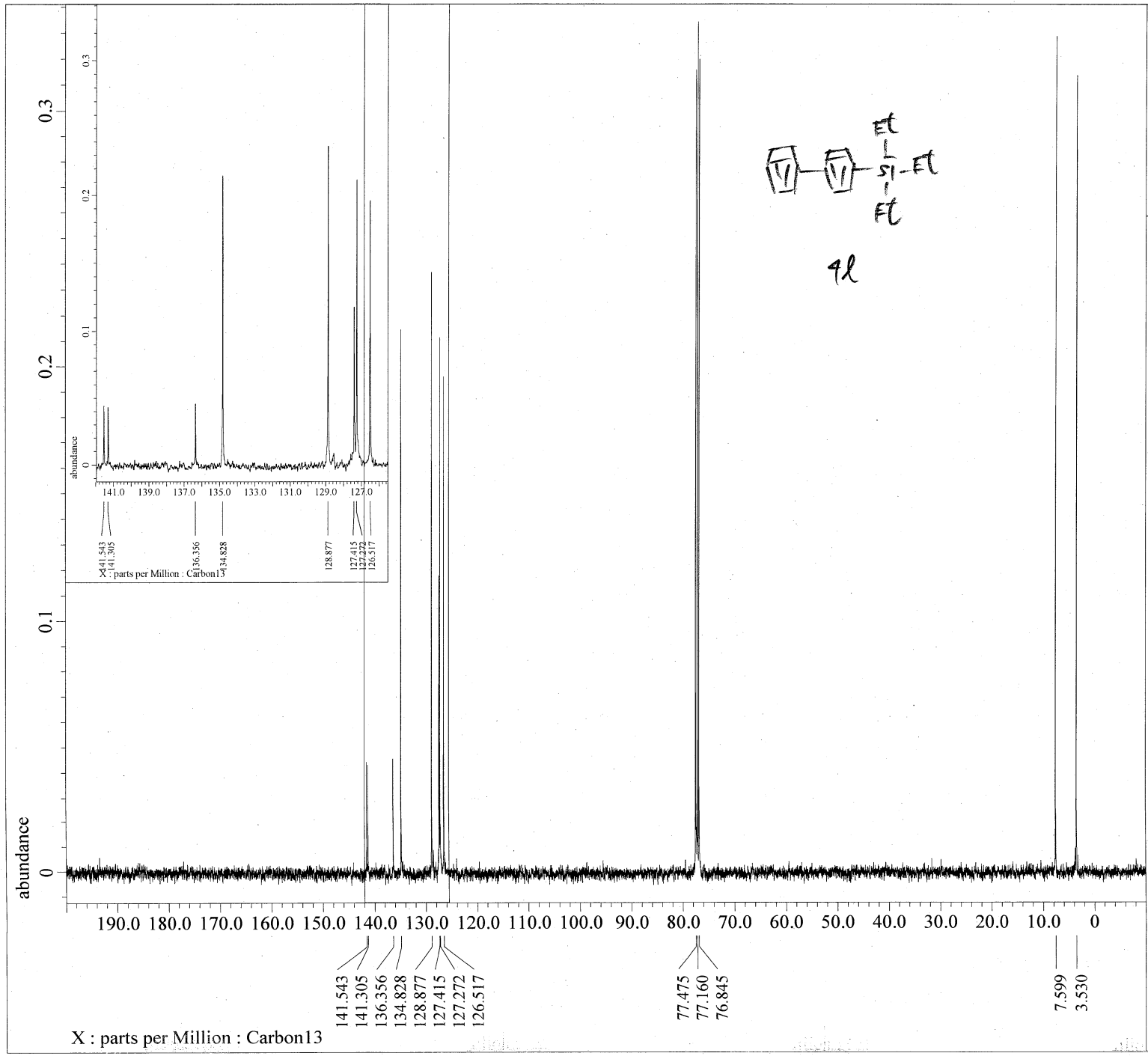

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-153-pure_Carbon-1-1.jdf
```

Filename	= KWM-153-pure_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KWM-153-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-JAN-2023 16:12:31
Revision_Time	= 14-NOV-2023 11:41:28
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.8[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



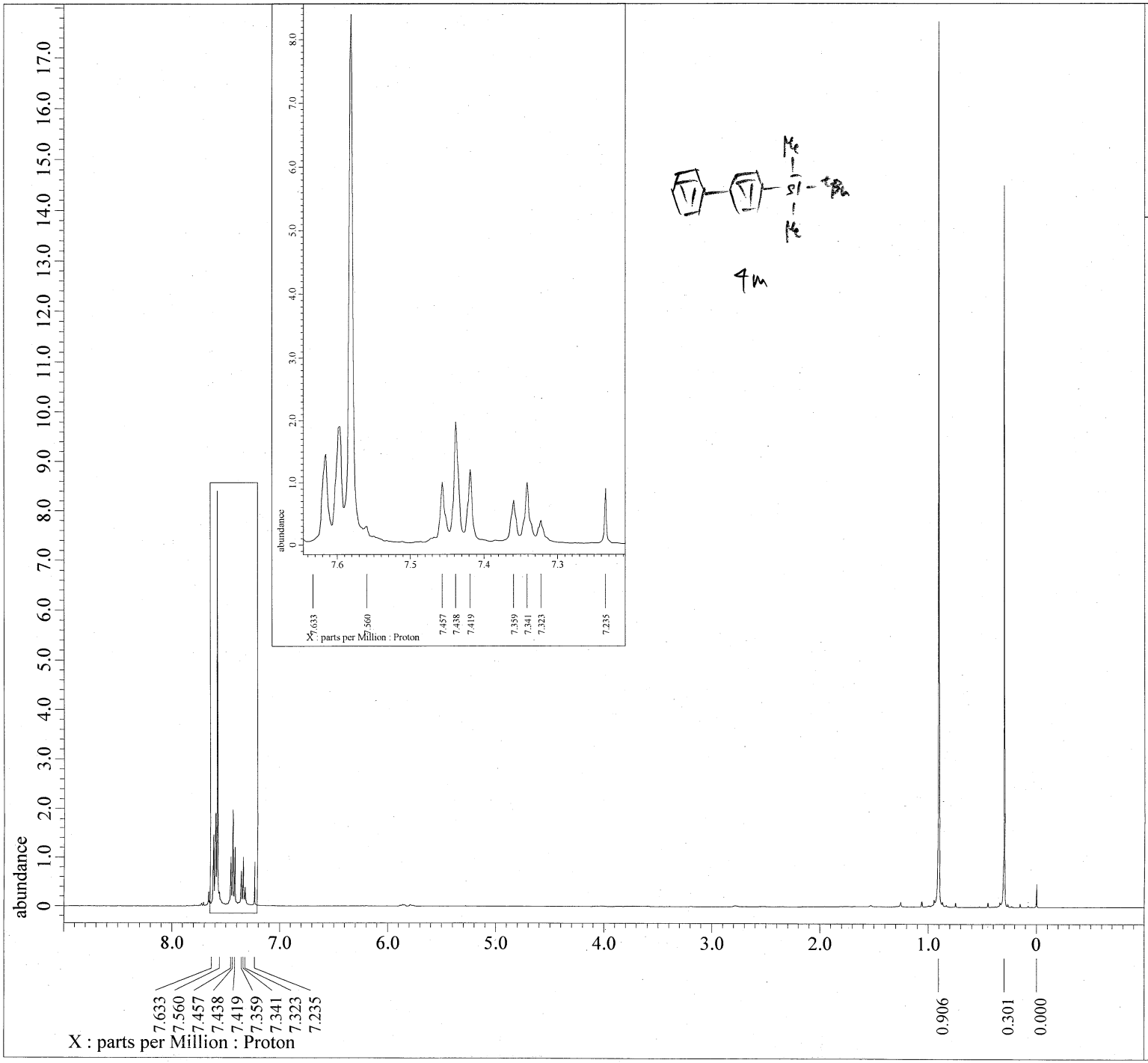

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-191-pure_Proton-1-1.jdf
```

Filename	= KWM-191-pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KWM-191-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-JAN-2023 17:22:49
Revision_Time	= 14-NOV-2023 11:48:02
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 26
Temp_Get	= 19.4[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-191-pure_Carbon-1-1.jdf
```

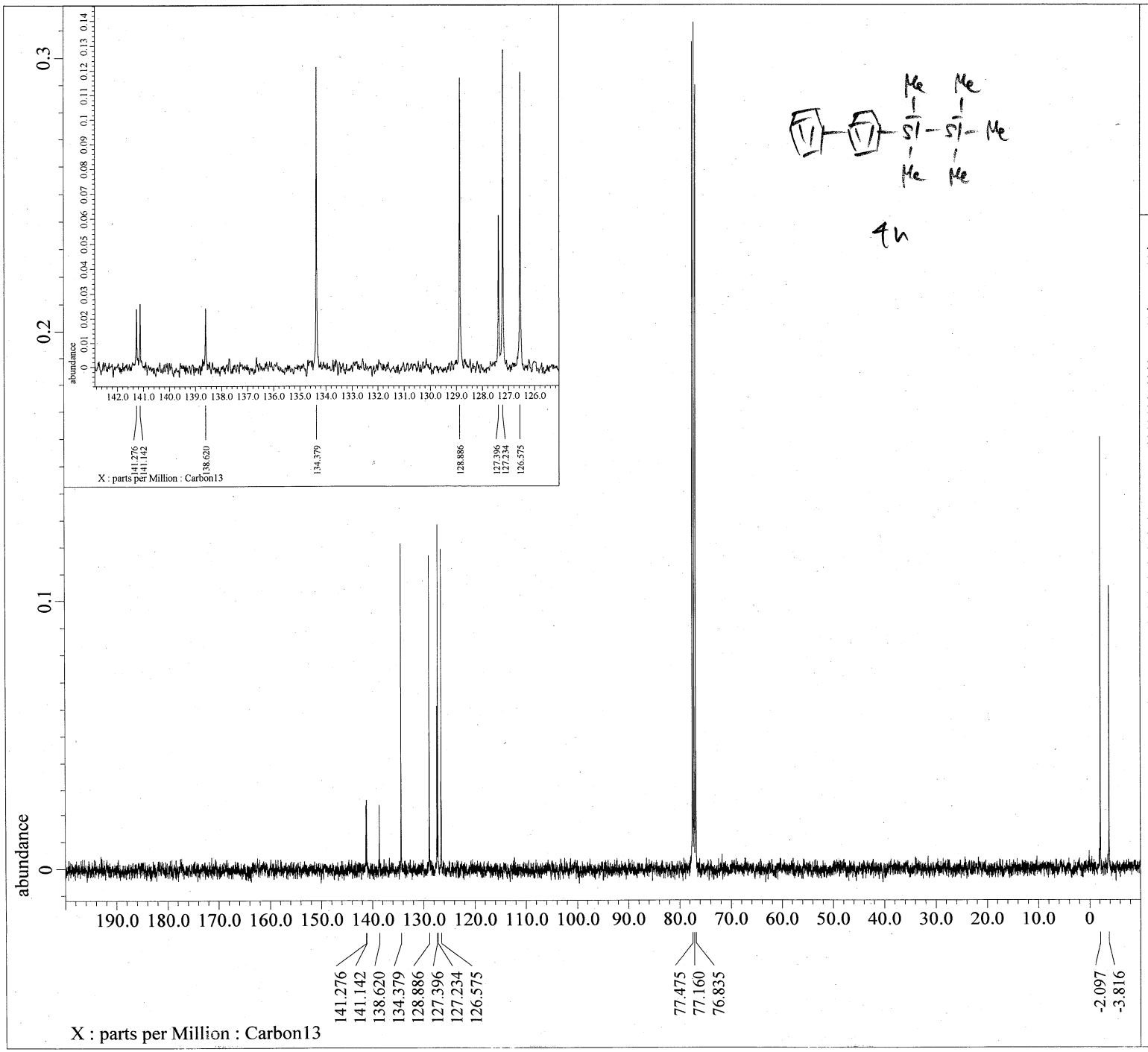
Filename	= KWM-191-pure_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KWM-191-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-JAN-2023 17:01:35
Revision_Time	= 14-NOV-2023 11:49:33
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.5[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



4m

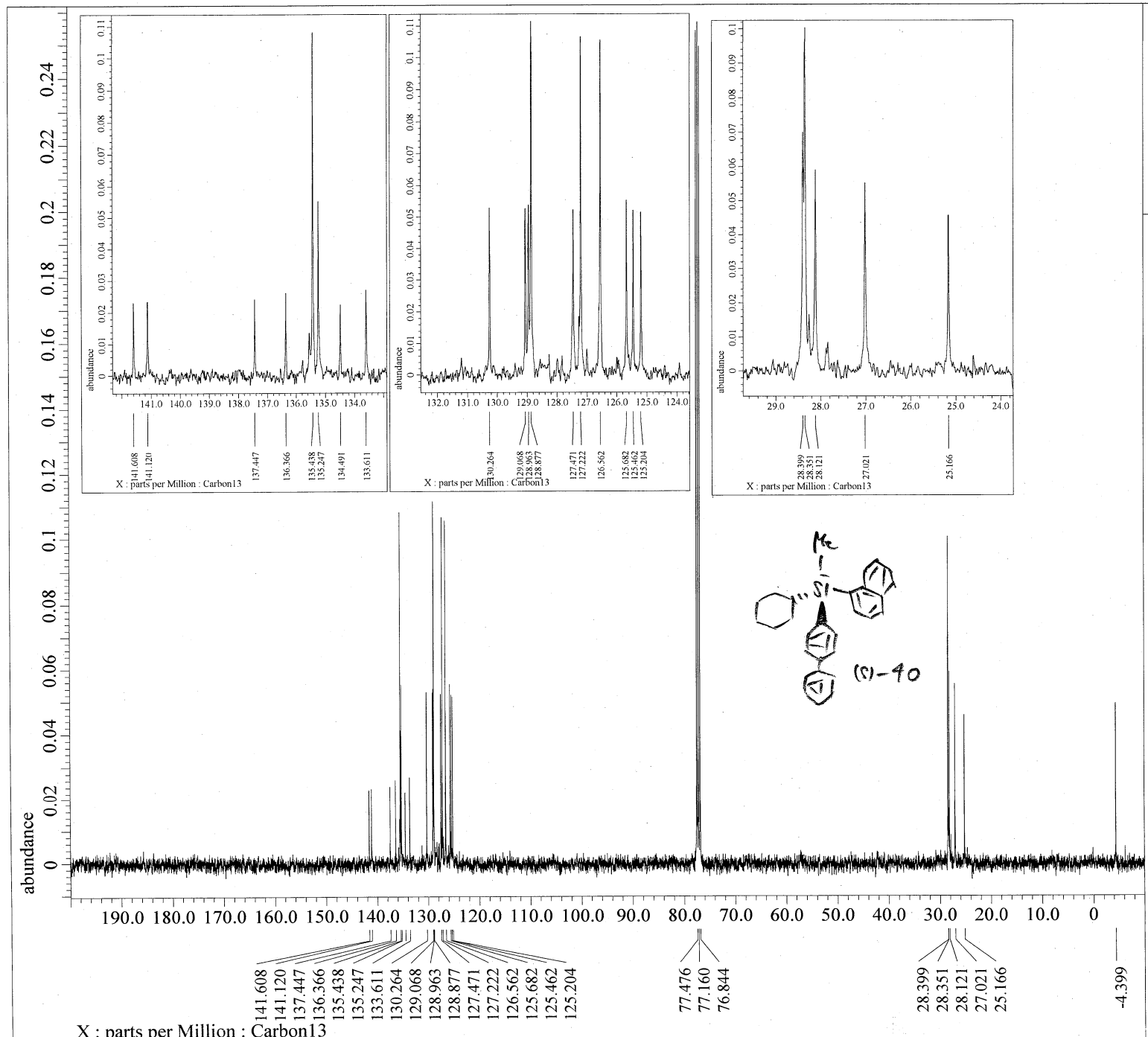
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-188-pure2_Proton-1-1.jdf
```

```
Filename            = KWM-188-pure2_Proton-1-2.
Author              = element
Experiment          = proton.jxp
Sample_Id           = KWM-188-pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 19-JAN-2023 15:12:41
Revision_Time       = 14-NOV-2023 11:51:44

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Proton
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 2.1889024[s]
X_Domain            = 1H
X_Freq              = 399.03472754[MHz]
X_Offset            = 5.0[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.45684997[Hz]
X_Sweep             = 7.48502994[kHz]
X_Sweep_Clipped     = 5.98802395[kHz]
Irr_Domain          = Proton
Irr_Freq            = 399.03472754[MHz]
Irr_Offset          = 5.0[ppm]
Tri_Domain          = Proton
Tri_Freq            = 399.03472754[MHz]
Tri_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 30
Temp_Get            = 17.8[dC]
X_90_Width          = 6.6[us]
X_Acq_Time          = 2.1889024[s]
X_Angle             = 45[deg]
X_Atn               = 1[dB]
X_Pulse             = 3.3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.1889024[s]
```



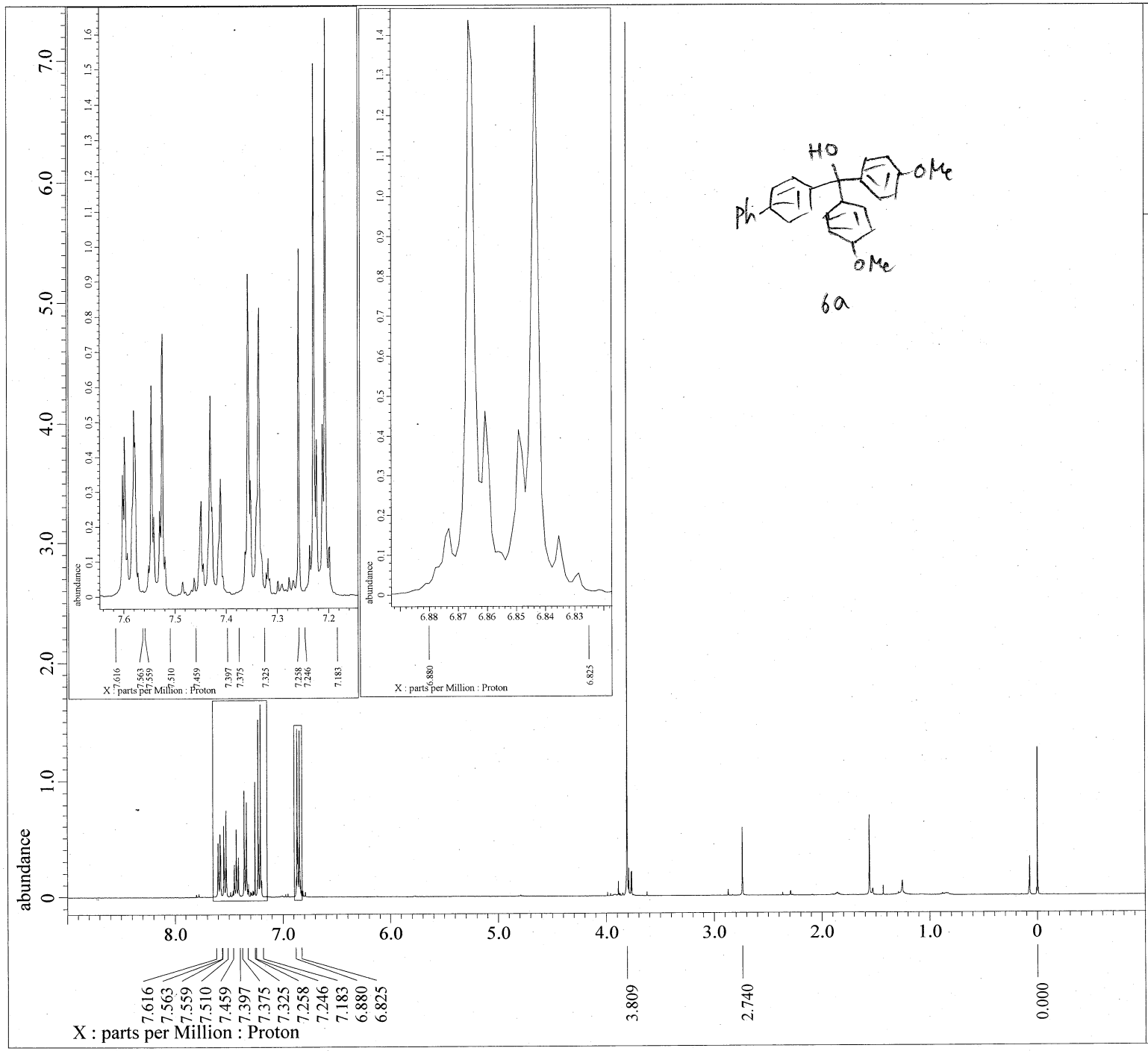

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-449-pure_Carbon-1-1.jdf
```

Filename	= KWM-449-pure_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KWM-449-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-OCT-2023 11:30:33
Revision_Time	= 13-OCT-2023 11:10:04
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-230-pure_Carbon-1-1.jdf
```

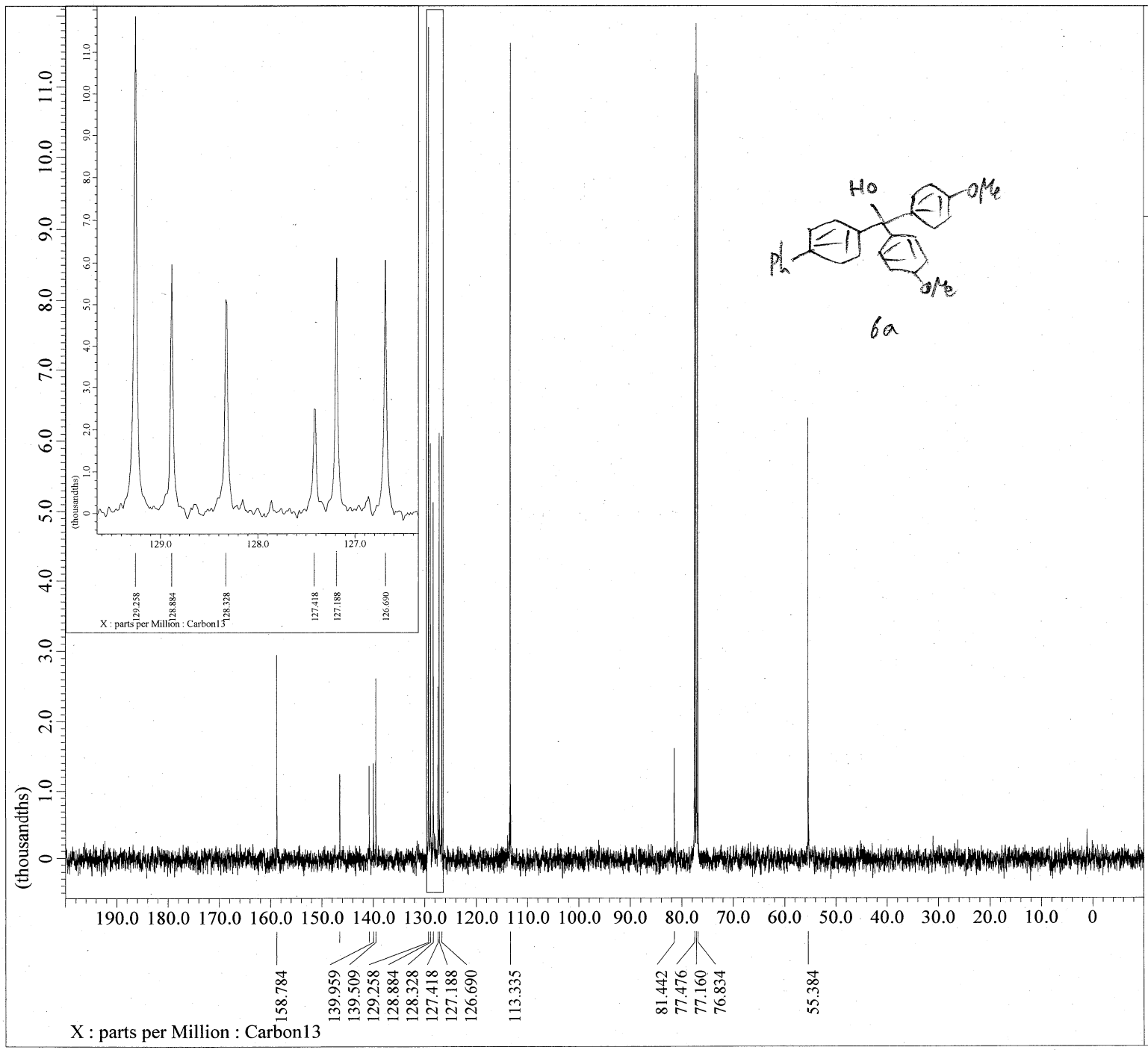
Filename	= KWM-230-pure_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KWM-230-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-MAR-2023 09:19:07
Revision_Time	= 13-NOV-2023 14:06:41
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 1.03809024[s]
X_Domain	= 13C
X_Freq	= 100.71389092[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19[dC]
X_90_Width	= 12.68[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 4[dB]
X_Pulse	= 4.22666667[us]
Irr_Atn_Dec	= 26.45[dB]
Irr_Atn_Noe	= 26.45[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.03809024[s]



6a

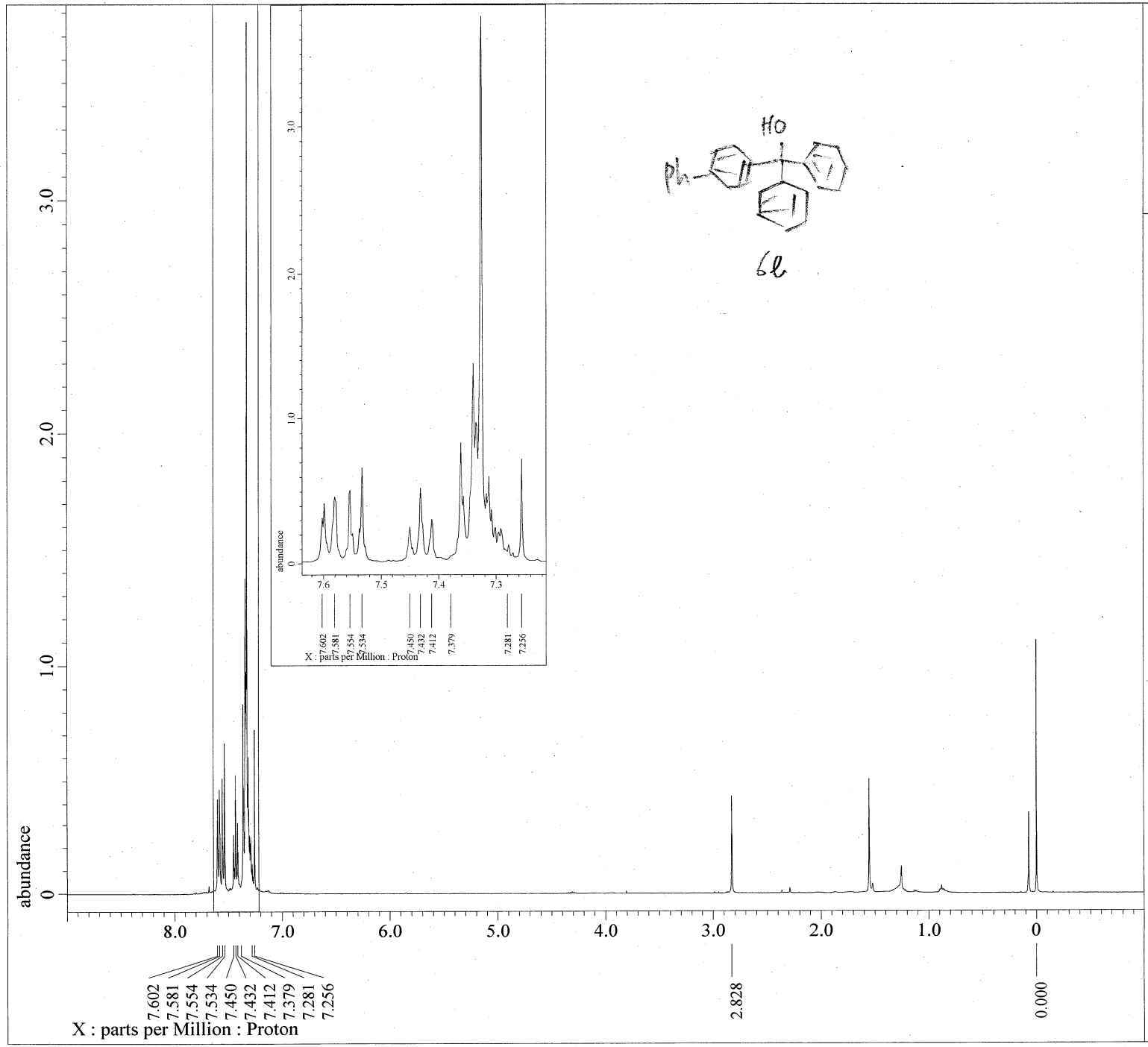
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-611-pure-re_Proton-1-1.jdf
```

Filename	= KWM-611-pure-re_Proto
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= KWM-611-pure-re
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-JUN-2024 12:29:33
Revision_Time	= 9-JUL-2024 11:20:54
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.1[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



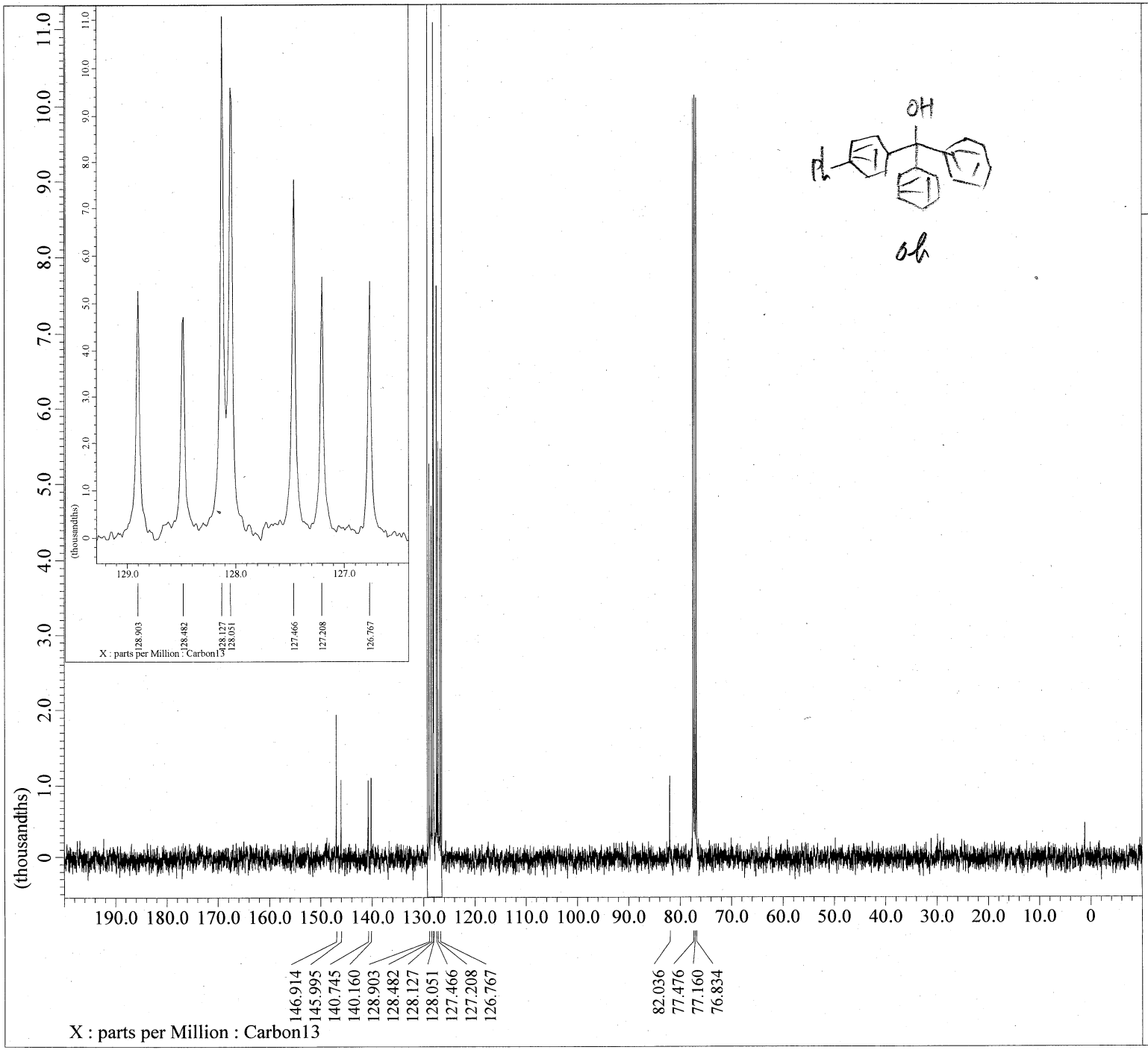

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-611-pure_Carbon-1-1.jdf
```

Filename	= KWM-611-pure_Carbo
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= KWM-611-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2024 17:38:
Revision_Time	= 6-JUL-2024 21:04:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
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]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.2[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



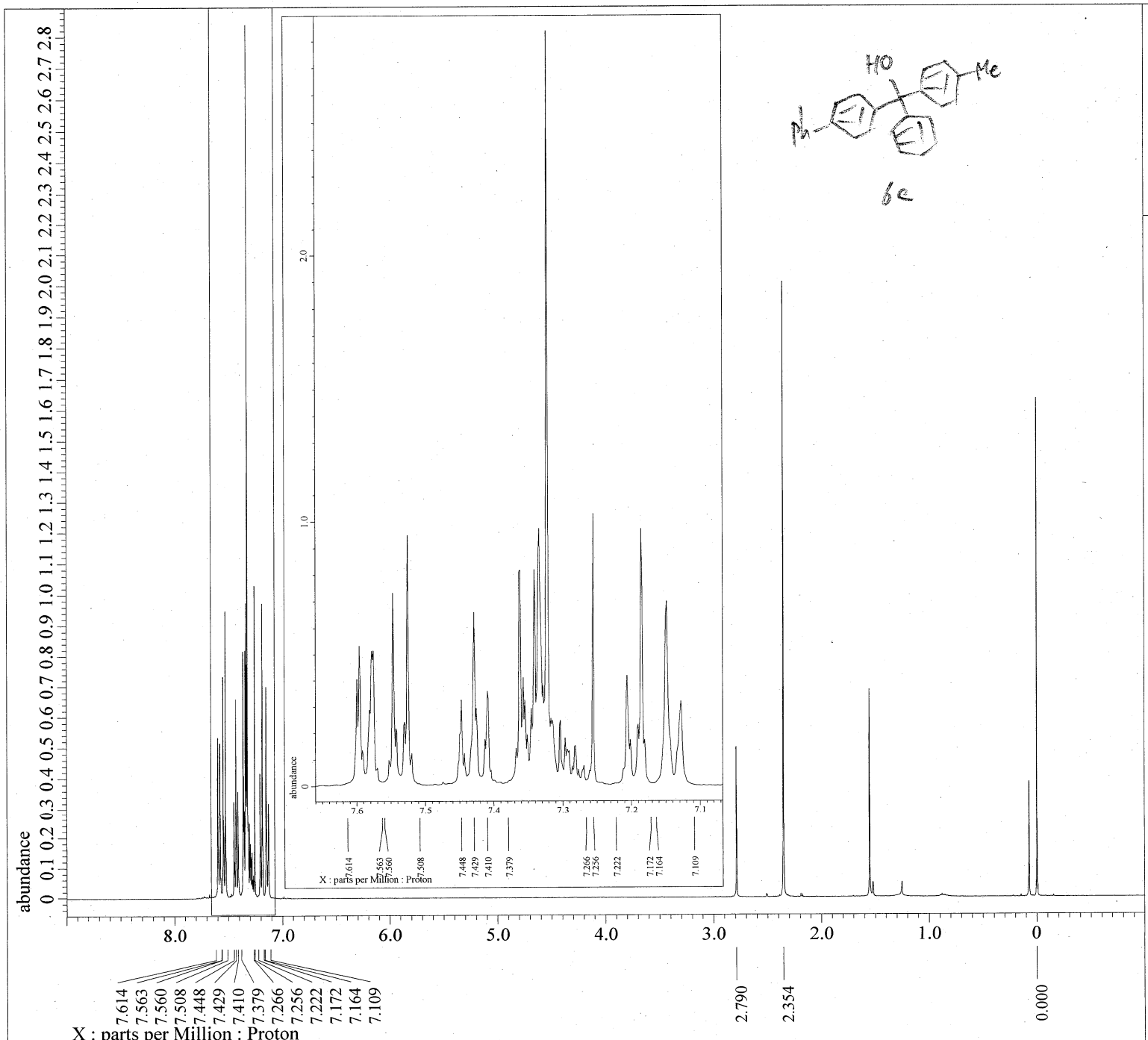

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-613-pure-re_Proton-1-1.jdf
```

Filename	= KWM-613-pure-re_Proto
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= KWM-613-pure-re
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-JUN-2024 12:39:21
Revision_Time	= 6-JUL-2024 21:08:58
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.2[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-613-pure_Carbon-1-1.jdf
```

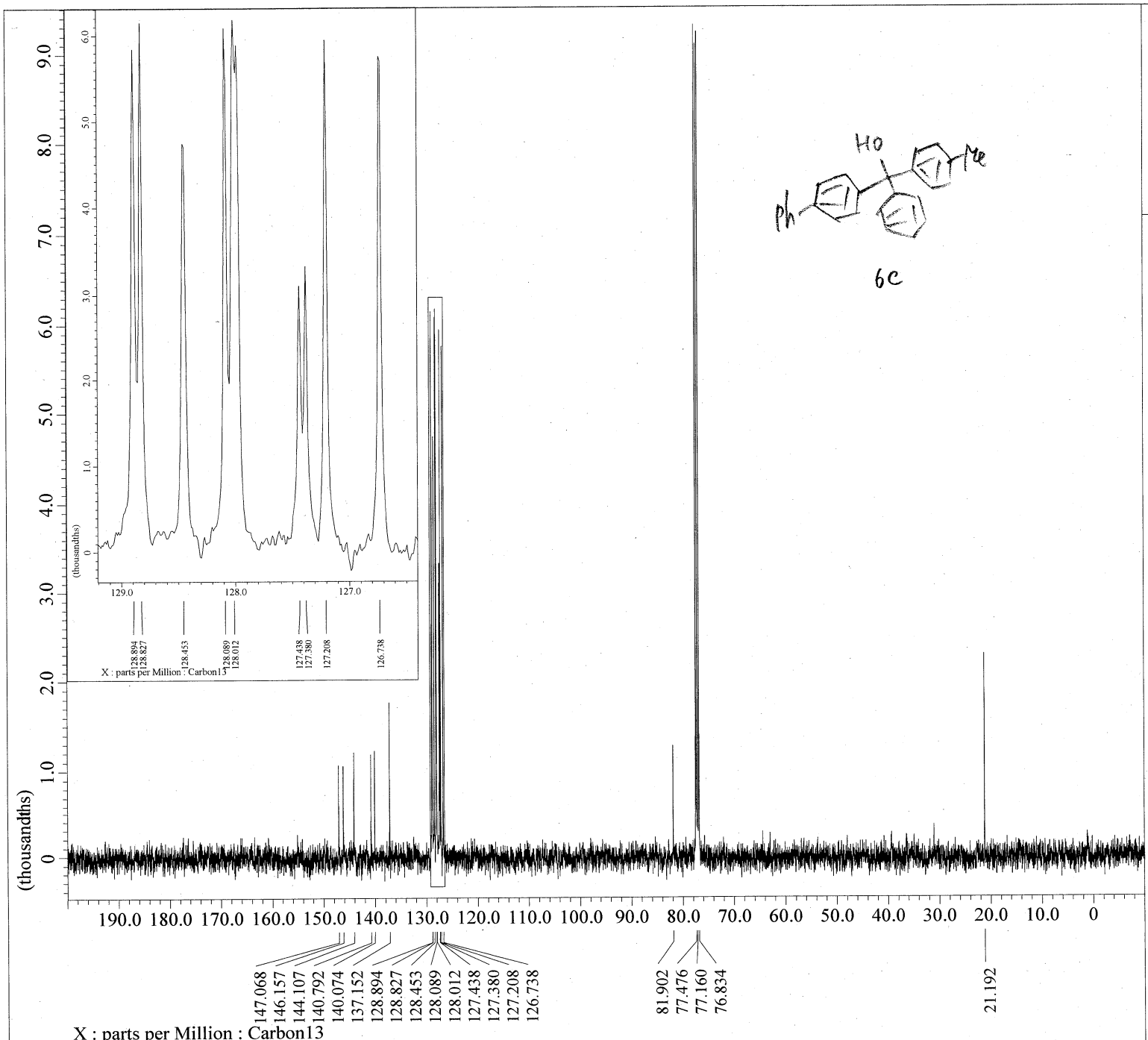
Filename	= KWM-613-pure_Carbo
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= KWM-613-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2024 18:16:
Revision_Time	= 6-JUL-2024 21:10:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
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]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.8[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



6e

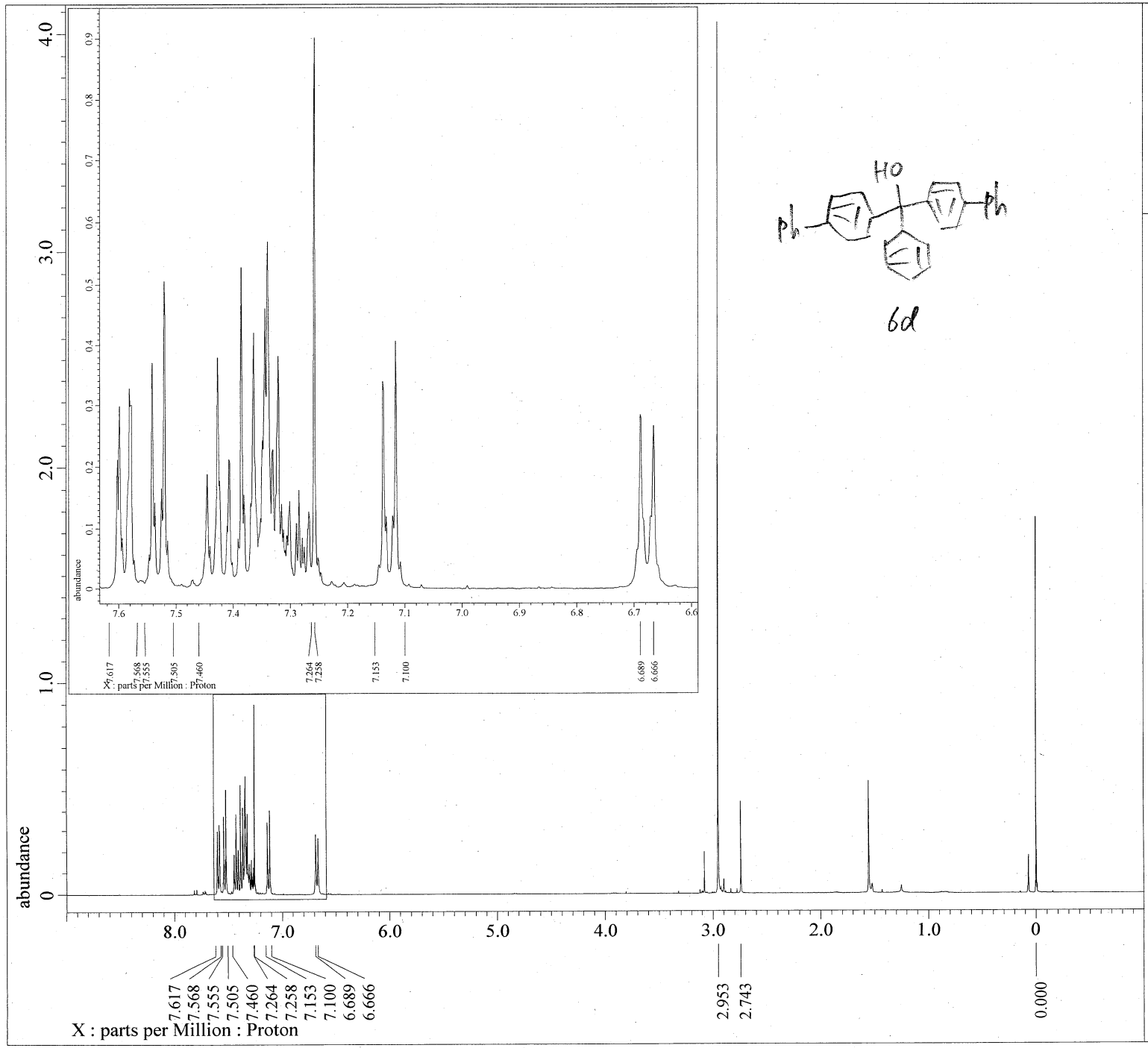
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-609-pure-re_Proton-1-1.jdf
```

Filename	= KWM-609-pure-re_Proto
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= KWM-609-pure-re
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-JUN-2024 12:24:54
Revision_Time	= 9-JUL-2024 11:17:41
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.2[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-609-pure_Carbon-1-1.jdf
```

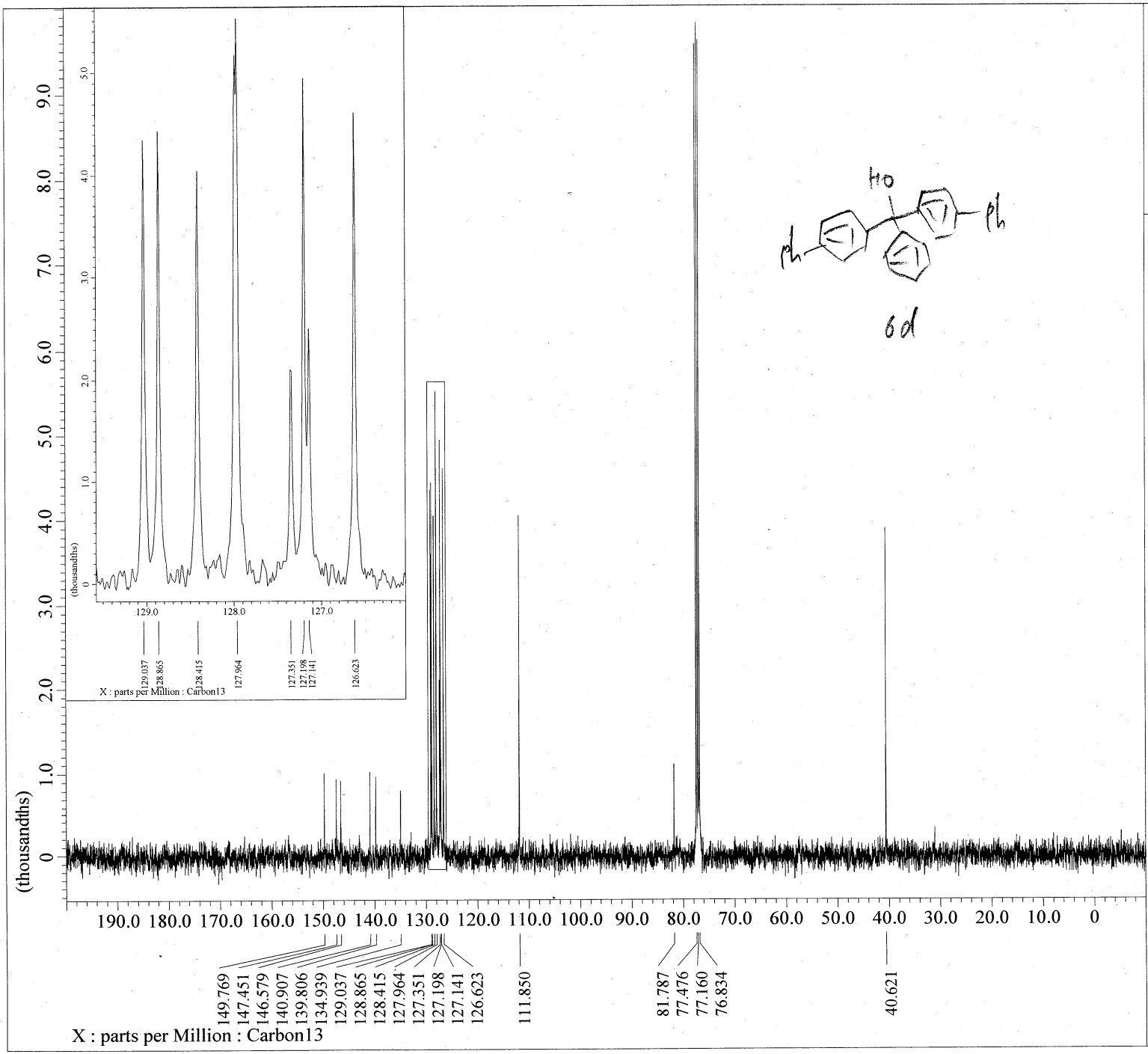
Filename	= KWM-609-pure_Carbo
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= KWM-609-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2024 17:20:
Revision_Time	= 6-JUL-2024 21:12:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
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]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.4[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



6d

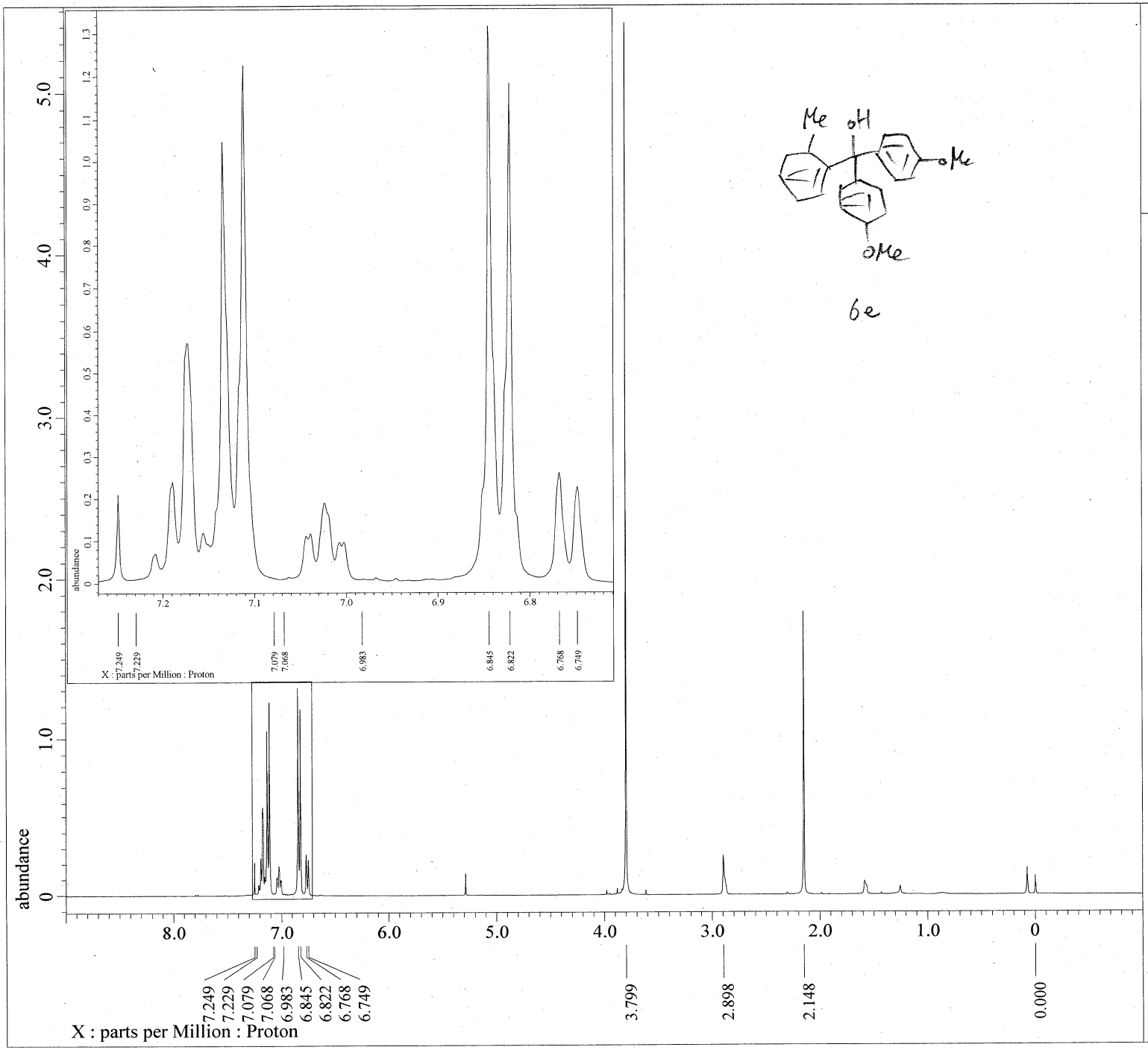
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-612-pure-re_Proton-1-1.jdf
```

Filename	= KWM-612-pure-re_Proto
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= KWM-612-pure-re
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-JUN-2024 12:34:10
Revision_Time	= 9-JUL-2024 11:11:31
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.2[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-612-pure_Carbon-1-1.jdf
```

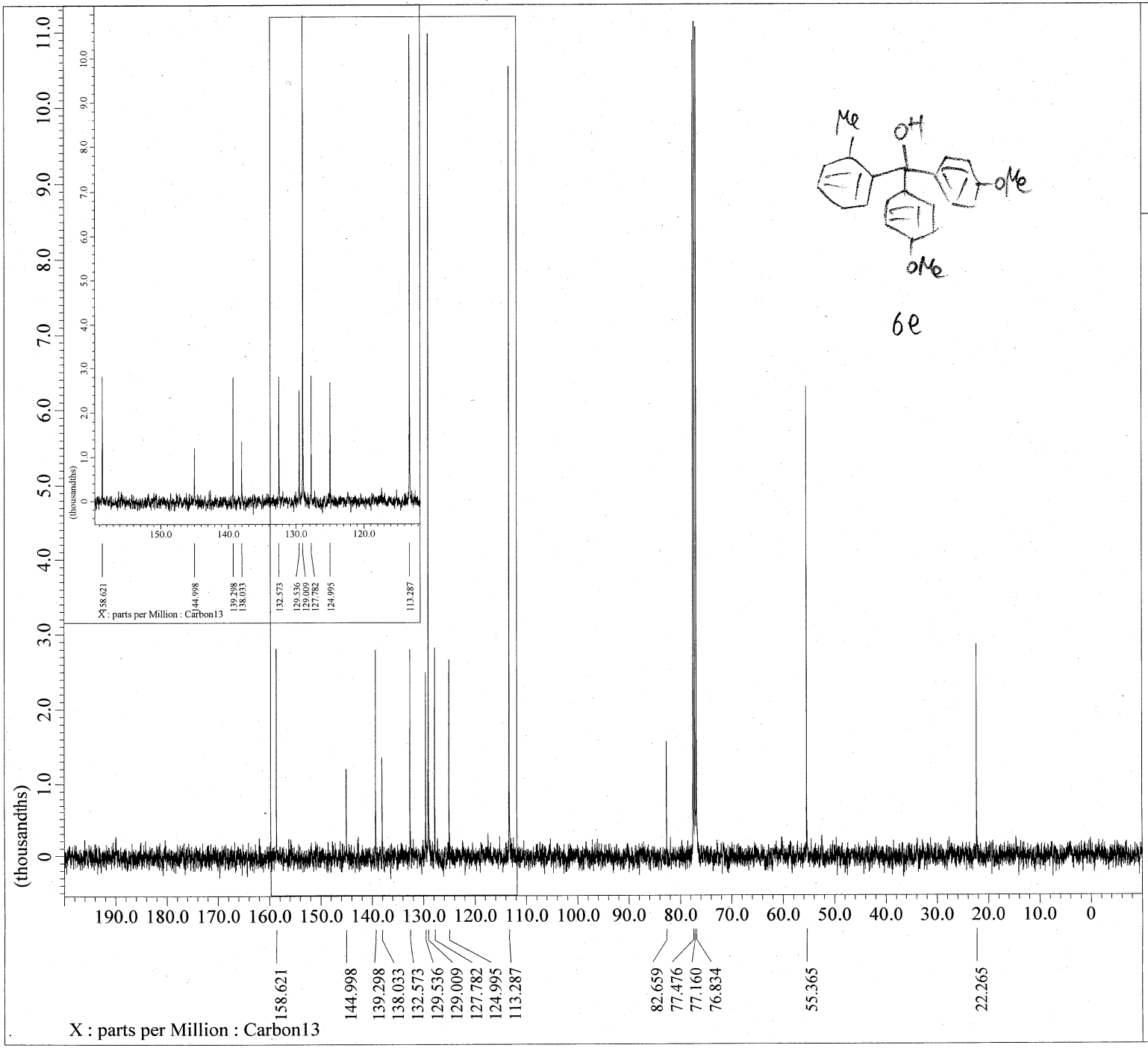
Filename	= KWM-612-pure_Carbo
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= KWM-612-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2024 17:57:
Revision_Time	= 6-JUL-2024 21:25:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
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]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



6e

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-Me-Pure_Proton-1-1.jdf
```

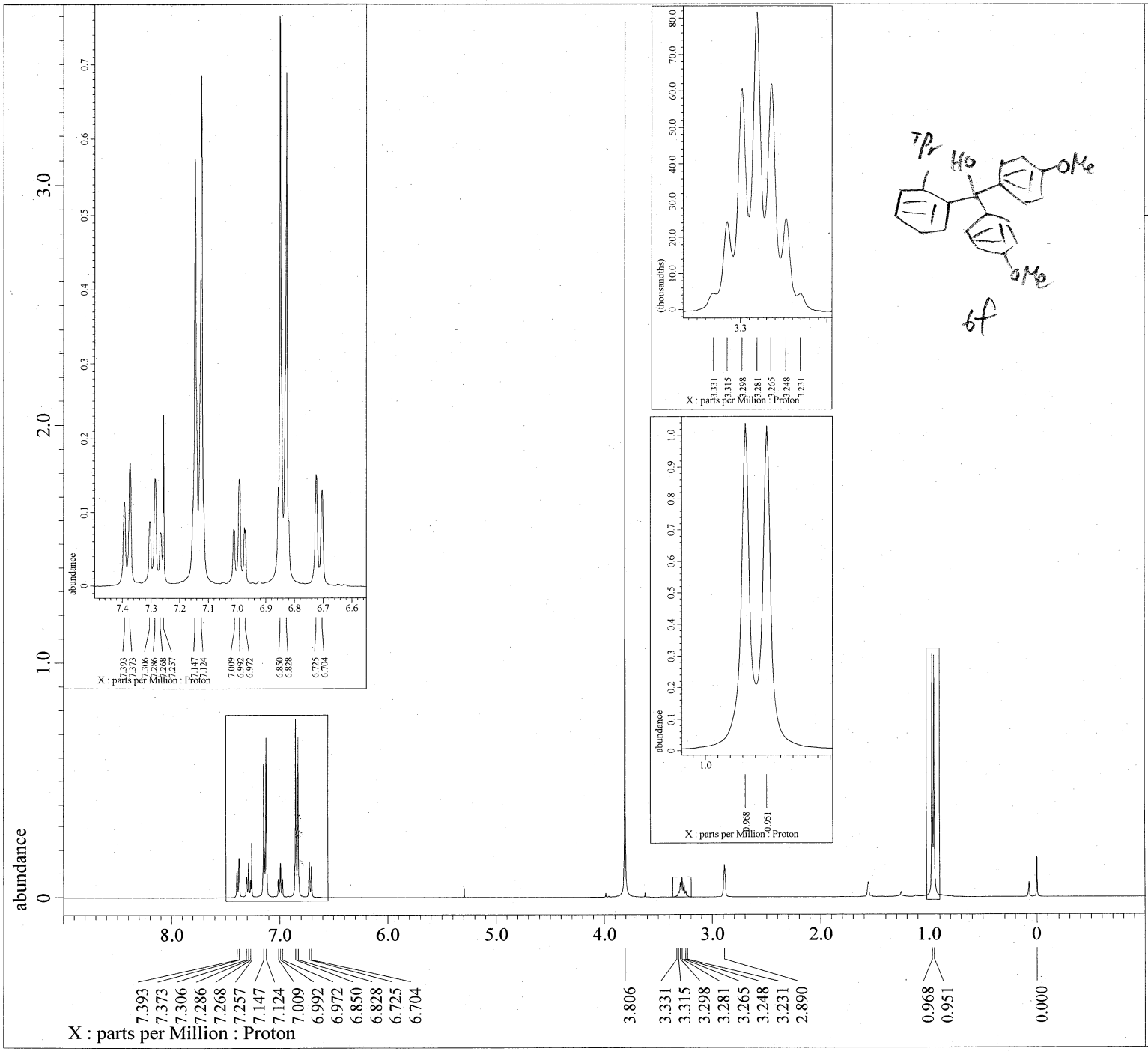
Filename	= KWM-Me-Pure_Proton-1-
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= KWM-Me-Pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2024 11:42:28
Revision_Time	= 9-JUL-2024 11:07:38
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 18.7[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



6e

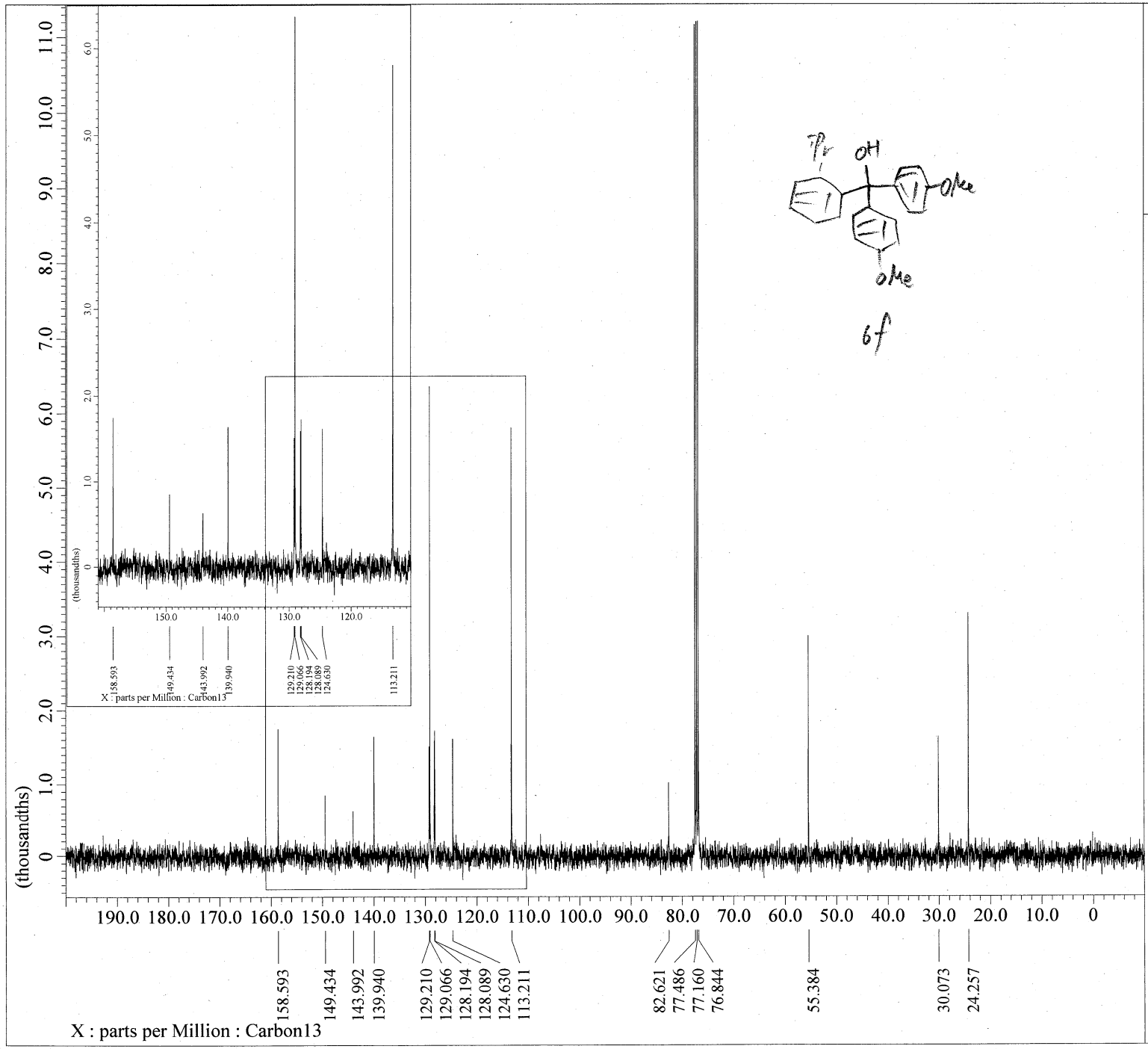
```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-Me-Pure_Carbon-1-1.jdf
```

Filename	= KWM-Me-Pure_Carbon
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= KWM-Me-Pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2024 11:43:
Revision_Time	= 6-JUL-2024 21:38:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
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]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.8[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-iPr-Pure_Proton-1-1.jdf
```

Filename	= KWM-iPr-Pure_Proton-1
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= KWM-iPr-Pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2024 12:01:46
Revision_Time	= 6-JUL-2024 21:43:39
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 18.8[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



6f

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KWM-iPr-Pure_Carbon-1-1.jdf
```

Filename	= KWM-iPr-Pure_Carbo
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= KWM-iPr-Pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2024 12:03:
Revision_Time	= 6-JUL-2024 21:41:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
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]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.7[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2023/03/01 18:32 Reported Date and Time: 2023/03/02 10:56

Processed Date and Time: 2023/03/01 20:21

Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\4202\

Processing Method: 0.0/100.0 iPrOH/Hexane

System (acquisition): Sys 1 Series: 4202

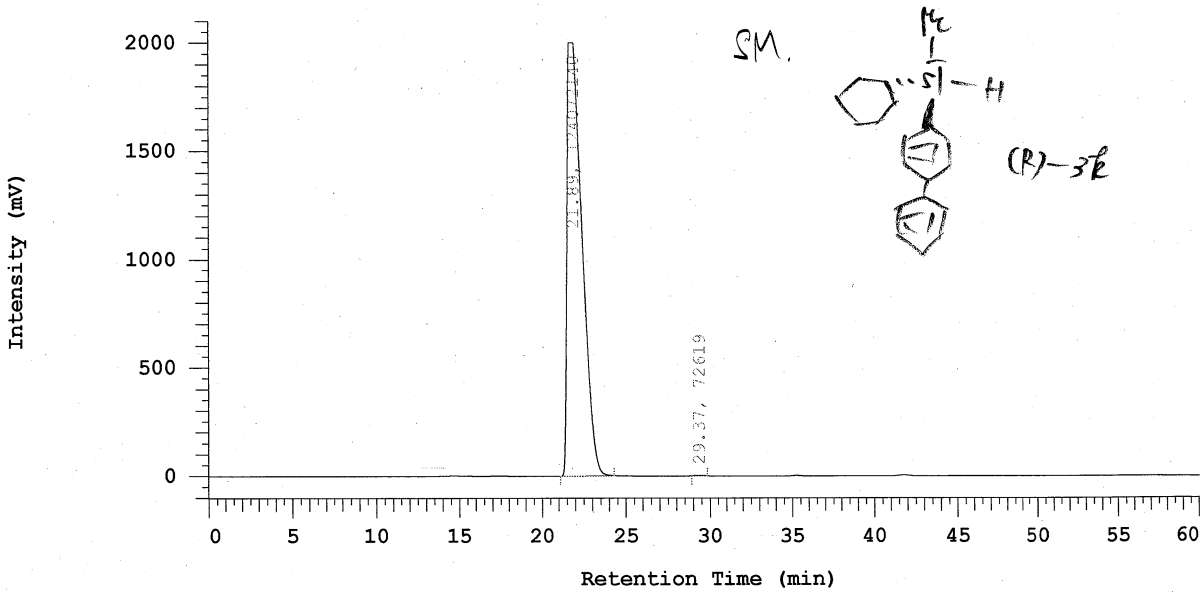
Application(data): Isocratic HPLC Vial Number: 153

Sample Name: KWM-230-SM Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 0.0/100.0 iPrOH/Hexane

Column Type: OD-H 2 Method Developer: Administrator

Pump A: L-2130

Pump A Solvent A: Hexane Pump A Solvent B: 10/90 iPrOH/Hexane

Pump A Solvent C: iPrOH Pump A Solvent D: EtOH

Method Description:

Chrom Type: HPLC Channel : 1

Peak Quantitation: AREA

Calculation Method: AREA%

No.	RT	Area	Area %
1	21.89	1.240E+08	99.942
2	29.37	72619	0.058
		1.241E+08	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2023/03/01 23:40 Reported Date and Time: 2023/03/02 10:56

Processed Date and Time: 2023/03/02 10:27

Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\4204\

Processing Method: 0.0/100.0 iPrOH/Hexane

System (acquisition): Sys 1 Series: 4204

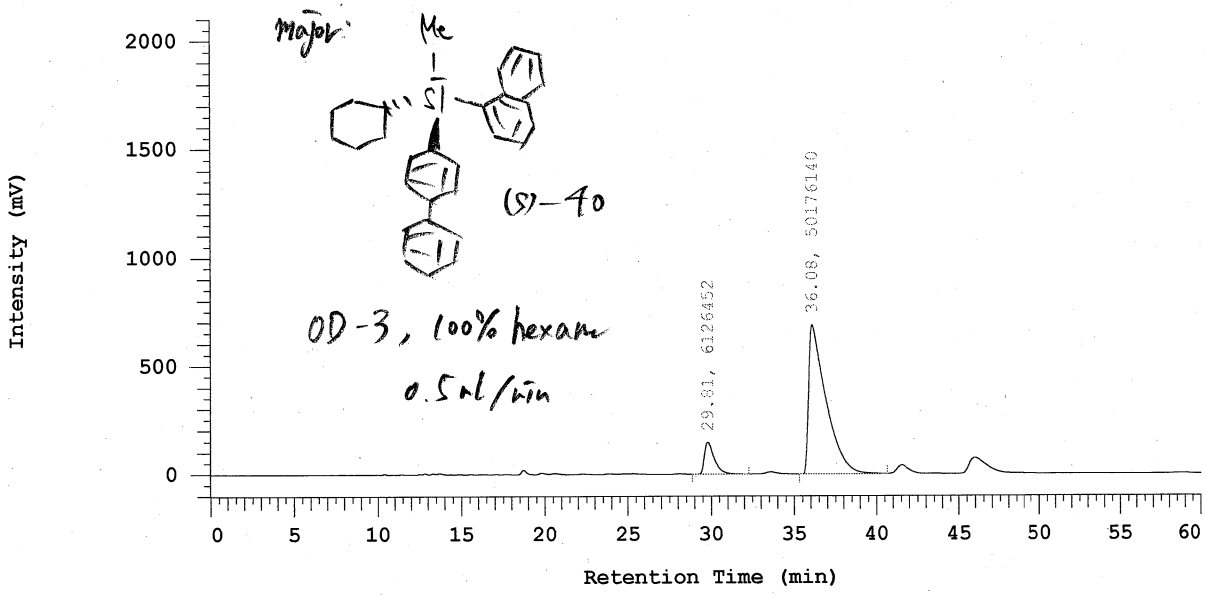
Application(data): Isocratic HPLC Vial Number: 152

Sample Name: KWM-230-pure2 Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 0.0/100.0 iPrOH/Hexane

Column Type: OD-H 2 Method Developer: Administrator

Pump A: L-2130

Pump A Solvent A: Hexane Pump A Solvent B: 10/90 iPrOH/Hexane

Pump A Solvent C: iPrOH Pump A Solvent D: EtOH

Method Description:

Chrom Type: HPLC Channel : 1

Peak Quantitation: AREA

Calculation Method: AREA%

No.	RT	Area	Area %
1	29.81	6126452	10.881
2	36.08	50176140	89.119
		56302592	100.000

Peak rejection level: 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 2023/03/01 22:39 Reported Date and Time: 2023/03/02 10:55

Processed Date and Time: 2023/03/02 10:24

Data Path: C:\WIN32APP\D2000HSM\Isocratic\DATA\4203\

Processing Method: 0.0/100.0 iPrOH/Hexane

System (acquisition): Sys 1 Series: 4203

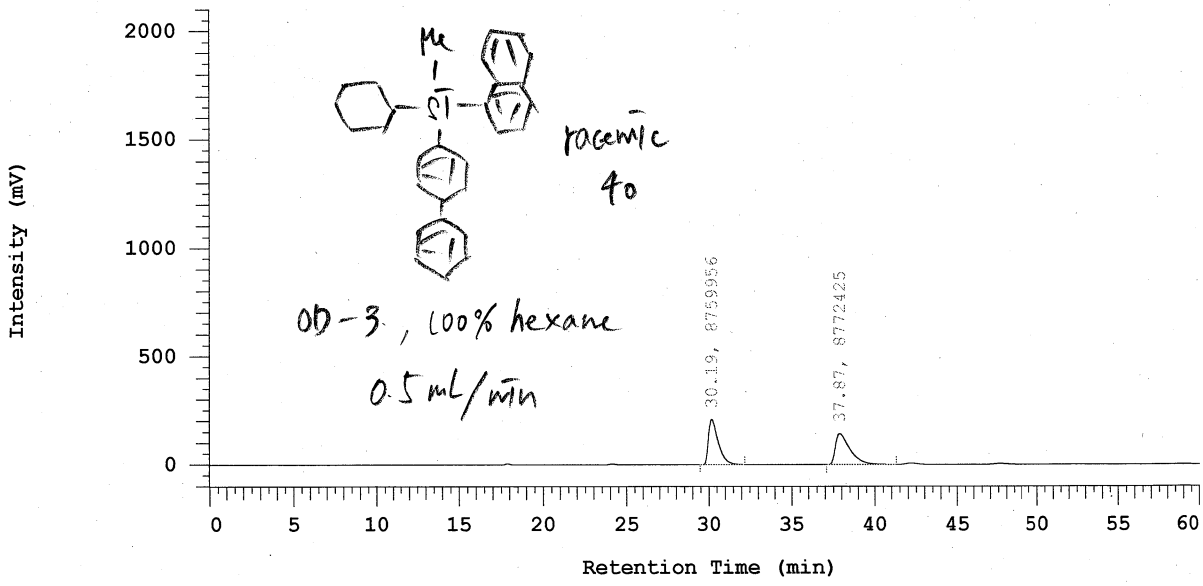
Application(data): Isocratic HPLC Vial Number: 151

Sample Name: KWM-230-Rac2 Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:

Chrom Type: HPLC Channel : 1



Processing Method: 0.0/100.0 iPrOH/Hexane

Column Type: OD-H 2 Method Developer: Administrator

Pump A: L-2130

Pump A Solvent A: Hexane Pump A Solvent B: 10/90 iPrOH/Hexane

Pump A Solvent C: iPrOH Pump A Solvent D: EtOH

Method Description:

Chrom Type: HPLC Channel : 1

Peak Quantitation: AREA

Calculation Method: AREA%

No.	RT	Area	Area %
1	30.19	8759956	49.964
2	37.87	8772425	50.036
		17532381	100.000

Peak rejection level: 0