Supplementary Information for

Sonogashira Coupling of the Ethynyl Monocarborane $[CB_{11}H_{11}$-12-C≡CH$]^-$

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I General Information

Chemicals

Bromoarenes, $Pd(PPh_3)_4$, CuI, anhydrous Et_3N, anhydrous THF, and solvents for purification were purchased from Energy Chemicals. All liquid reagents were degassed by bubbling N_2 through them for several minutes. Et_3N and THF were degassed, dried by passage through basic aluminum oxide and stored over 3 Å molecular sieves. Acetone-d_6 was purchased from Cambridge Isotope Laboratories. The anions $[CB_{11}H_{12}]^-$ and $[CB_{11}H_{11}\text{-}12\text{-}CCH]^-$ were prepared according to the literature.[1]

Reaction Conditions

Glassware for air-sensitive reactions was dried at 150 °C for 12 h and allowed to cool under nitrogen atmosphere. All experiments were carried out under nitrogen atmosphere; see the procedures for details.

Characterization

Thin-layer chromatography (TLC) was carried out using silica gel 60, F254 with a thickness of 0.25 mm. Preparative TLC was carried out using silica gel 60, F254 with a thickness of 1.0 mm. Column chromatography was performed on silica gel 60 (200-300 mesh).

NMR spectra were recorded on a Bruker AVANCE III 500 spectrometer (^{1}H NMR 500.13 MHz, ^{13}C NMR 125.77 MHz, ^{11}B NMR 160.46 MHz) or a Bruker AVANCE III 400 spectrometer (^{1}H NMR 400.13 MHz, ^{13}C NMR 100.62 MHz, ^{11}B NMR 128.38 MHz) at the temperature indicated. Data are reported as follows: Chemical shift in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, etc.), coupling constant *J* in Hz, integration, and (where applicable) interpretation. Signals were referenced against solvent peaks (^{1}H: residual $CD_3C(O)CD_2H$ = 2.05 ppm; ^{13}C: $CD_3C(O)CD_3$ = 29.84 ppm). ^{11}B and ^{11}B{^{1}H} NMR spectra were calibrated against external BF_3*Et_2O = 0 ppm (BF_3*Et_2O capillary in C_6D_6).

Additional remark about the NMR spectra:

a) In certain ^{1}H and $^{1}H\{^{11}B\}$ NMR spectra measured in acetone-d_6, double water peaks were observed. This is a result of different resonances from H_2O and HOD and has been described in the literature.[2] In our experience, the appearance of double water peaks depends on the temperature, water content and compound being measured. A spectrum of acetone-d_6 in which the distinct resonances from H_2O and HOD are visible is shown in Figure S1.

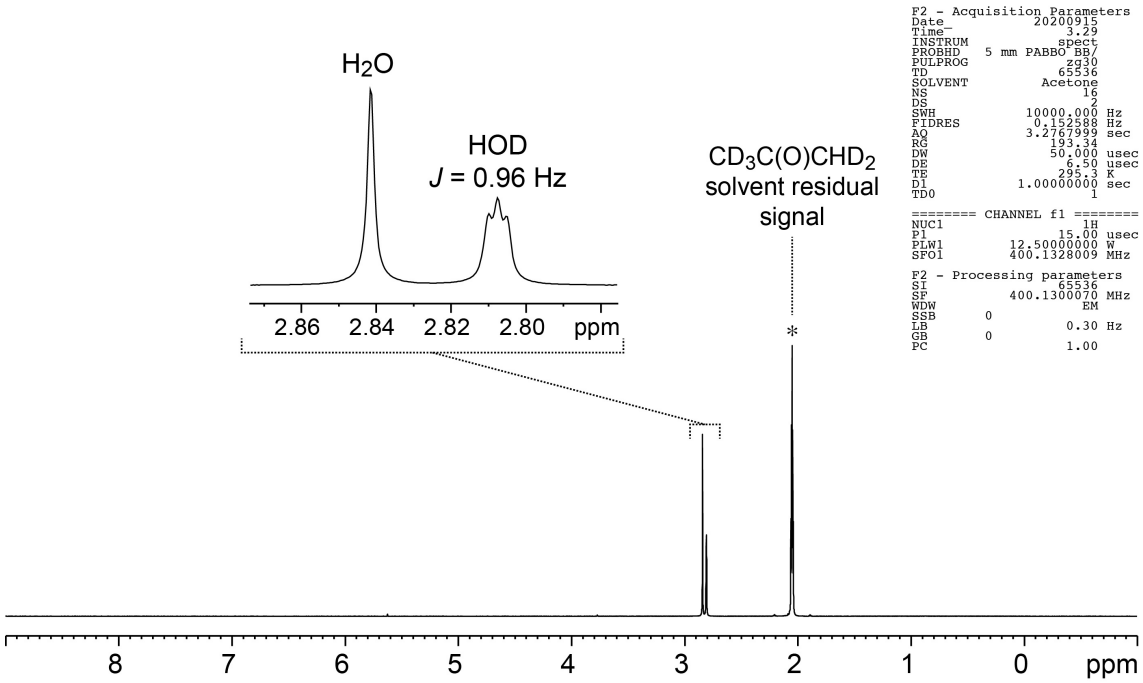


Figure S1. ^{1}H NMR spectrum of acetone-d_6 solvent as received from Cambridge Isotope Laboratories (400 MHz, 22 °C).

b) Integration of the B–H signals in the $^{1}H\{^{11}B\}$ spectra gave numbers of *ca.* 3.5-4 instead of 5 for the upper-belt and lower-belt hydrogen atoms. This is because coupling to ^{10}B ($I = 3$, 20% abundance) is still present and leads to severe broadening of the ^{10}B–H resonances.

c) Some products with an aryl 1,4-substitution [$CB_{11}H_{11}$-CC-C_6H_4-4-R] gave complicated ^{1}H signals for the *ortho* and *meta* positions because of magnetic inequivalence of the Ar-H hydrogen atoms ($H_AH_{A'}H_BH_{B'}$ system). Resonances are reported as doublets when they appeared as doublets, otherwise as multiplets.

d) For the $[Et_4N]^+$ cation, coupling to ^{14}N (I = 1) was observed in many of the ^1H and $^{13}C\{^1H\}$ spectra, leading to triplet-like splitting.

d) For all of the products, $^{13}C\{^1H\}$ NMR spectra showed weak signals for the alkyne B-C and B-C-***C*** carbon atoms. This is caused by severe broadening and splitting by the quadrupolar nuclei ^{10}B (I = 3, 20% abundance) and ^{11}B (I = 3/2, 80% abundance). In some cases, the ^{13}C NMR signals could be observed, but in others they could not, even with a high number of scans and at concentrations of 30 mg/0.6 mL. An example where detection of the alkyne resonances was successful is shown in Figures S2 and S3 for $[Et_4N][CB_{11}H_{11}\text{-}CC\text{-}C_6H_4\text{-}4\text{-}NO_2]$. The quartet-like signals for B-C and B-C-***C*** appear at 111 ppm and 92 ppm, respectively.
Indirect detection of the B-C-***C*** carbon atom can successfully be achieved using ^1H-^{13}C HMBC NMR spectroscopy. In these spectra, the correlation signal caused by $^3J_{H,C}$ coupling between ^1H(*ortho*) and B-C-***^{13}C*** revealed the chemical shift of the B-C-***C*** position. Examples for this kind of detection are shown for $[Et_4N][CB_{11}H_{11}\text{-}CC\text{-}C_6H_4\text{-}4\text{-}NO_2]$, $[Et_4N][CB_{11}H_{11}\text{-}CC\text{-}C_6H_4\text{-}4\text{-}F]$ and $[Et_4N][CB_{11}H_{11}\text{-}CC\text{-}C_6H_4\text{-}4\text{-}Me]$ in Figures S4–S6. Indirect detection was not applied to all of the compounds.

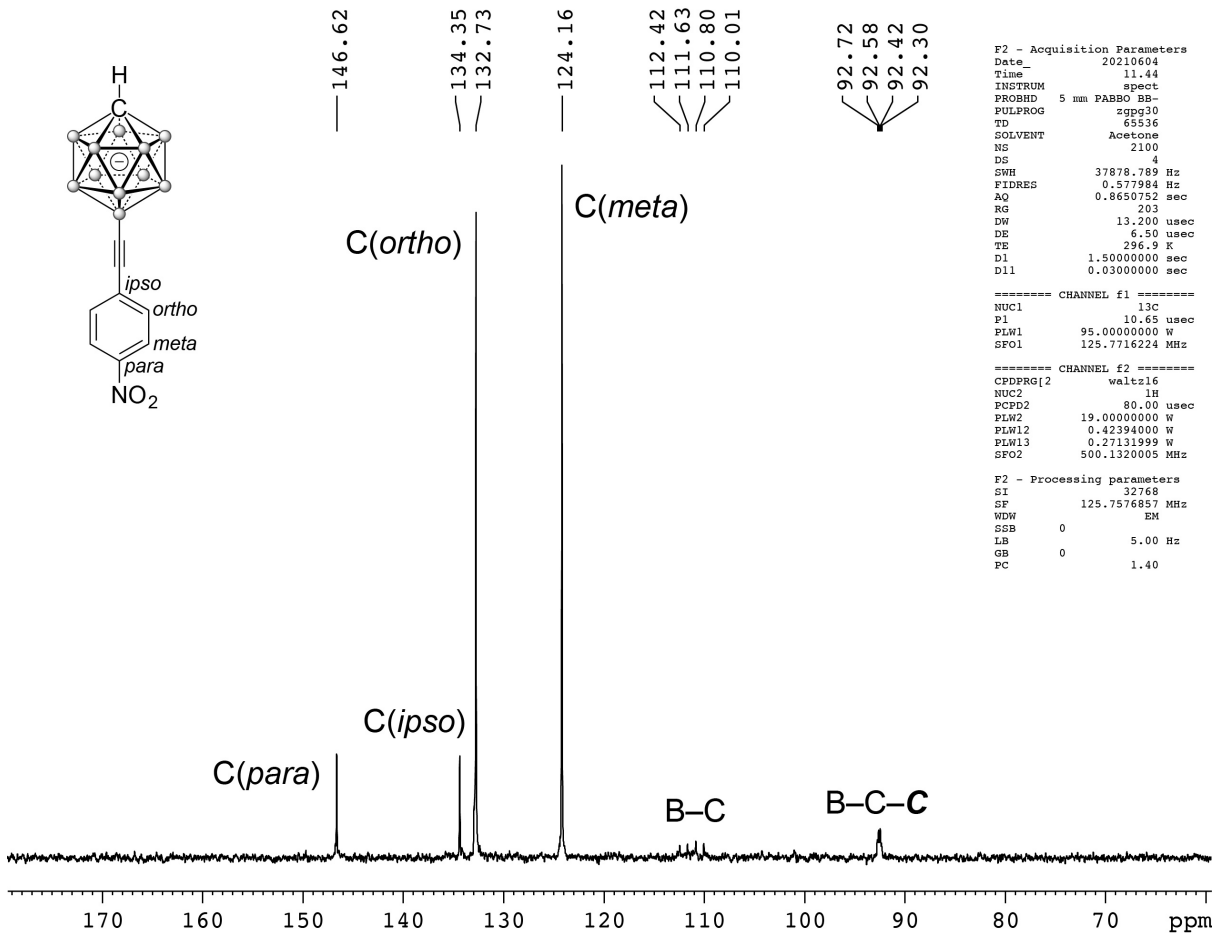


Figure S2. Aromatic and alkyne region of the $^{13}C\{^{1}H\}$ NMR spectrum of $[Et_4N][CB_{11}H_{11}$-CC-C_6H_4-4-$NO_2]$ (acetone-d_6,126 MHz, 24 °C). Assignments based on HSQC and HMBC spectra.

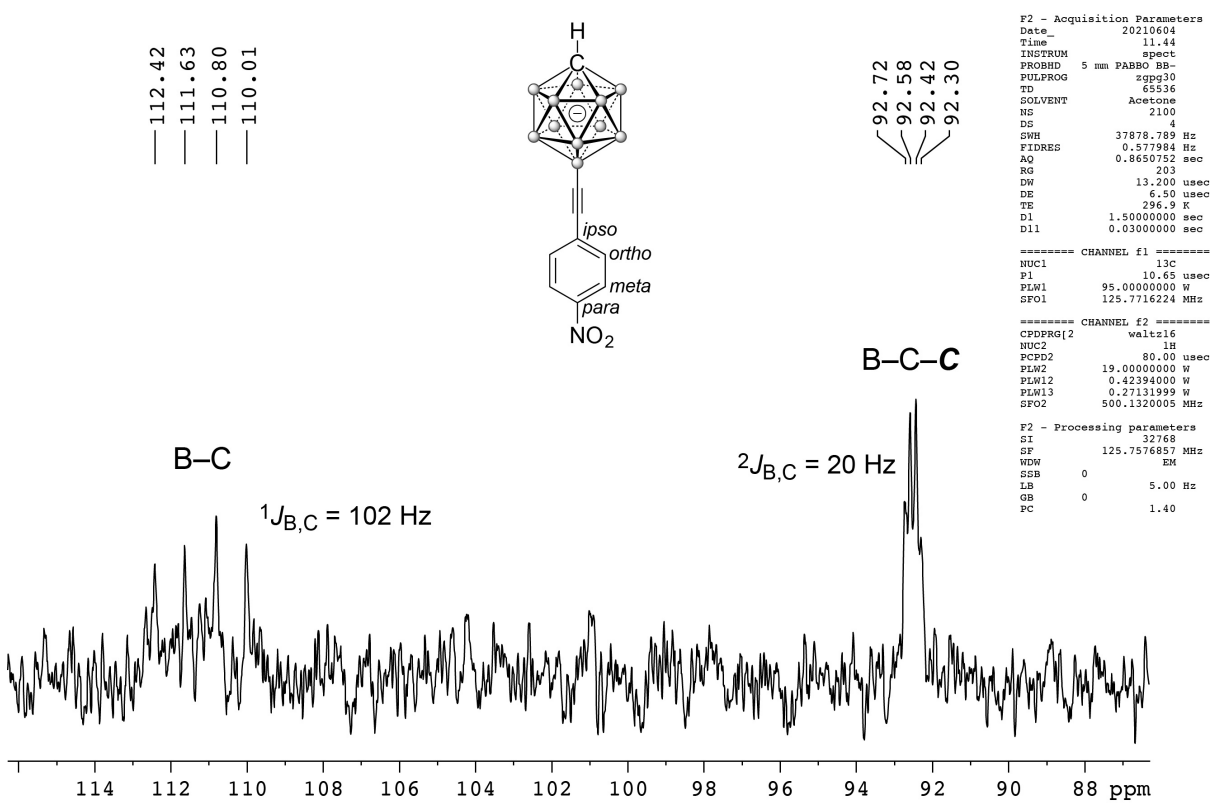


Figure S3. Detail of Figure S2: Alkyne region of the $^{13}C\{^{1}H\}$ NMR spectrum of $[Et_4N][CB_{11}H_{11}\text{-}CC\text{-}C_6H_4\text{-}4\text{-}NO_2]$ (acetone-d_6,126 MHz, 24 °C).

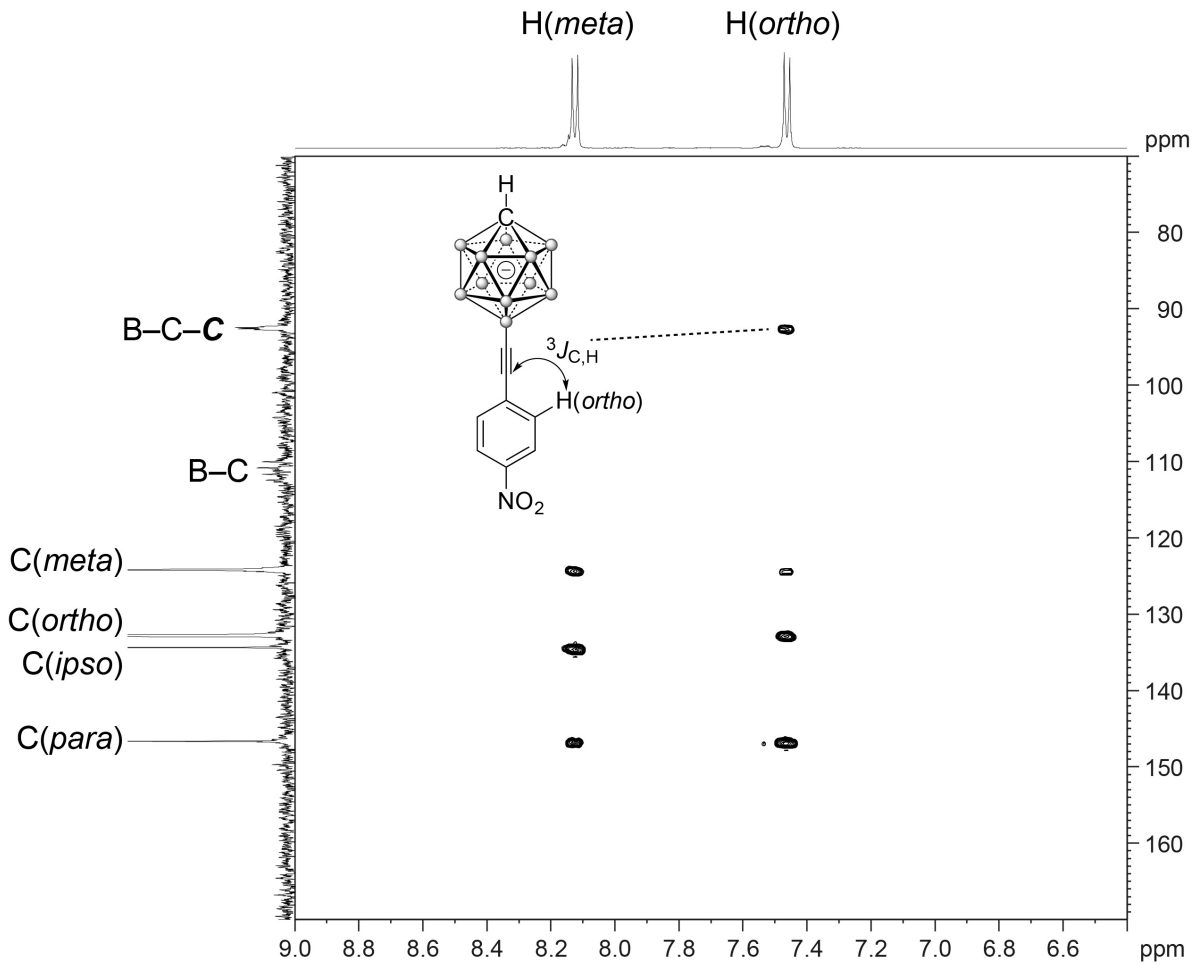


Figure S4. Aromatic and alkyne region of the ^{13}C-^{1}H HMBC NMR spectrum of $[Et_4N][CB_{11}H_{11}$-CC-C_6H_4-4-$NO_2]$ (acetone-d_6, 24 °C). The assignments of the signals are based on HSQC and HMBC spectra.

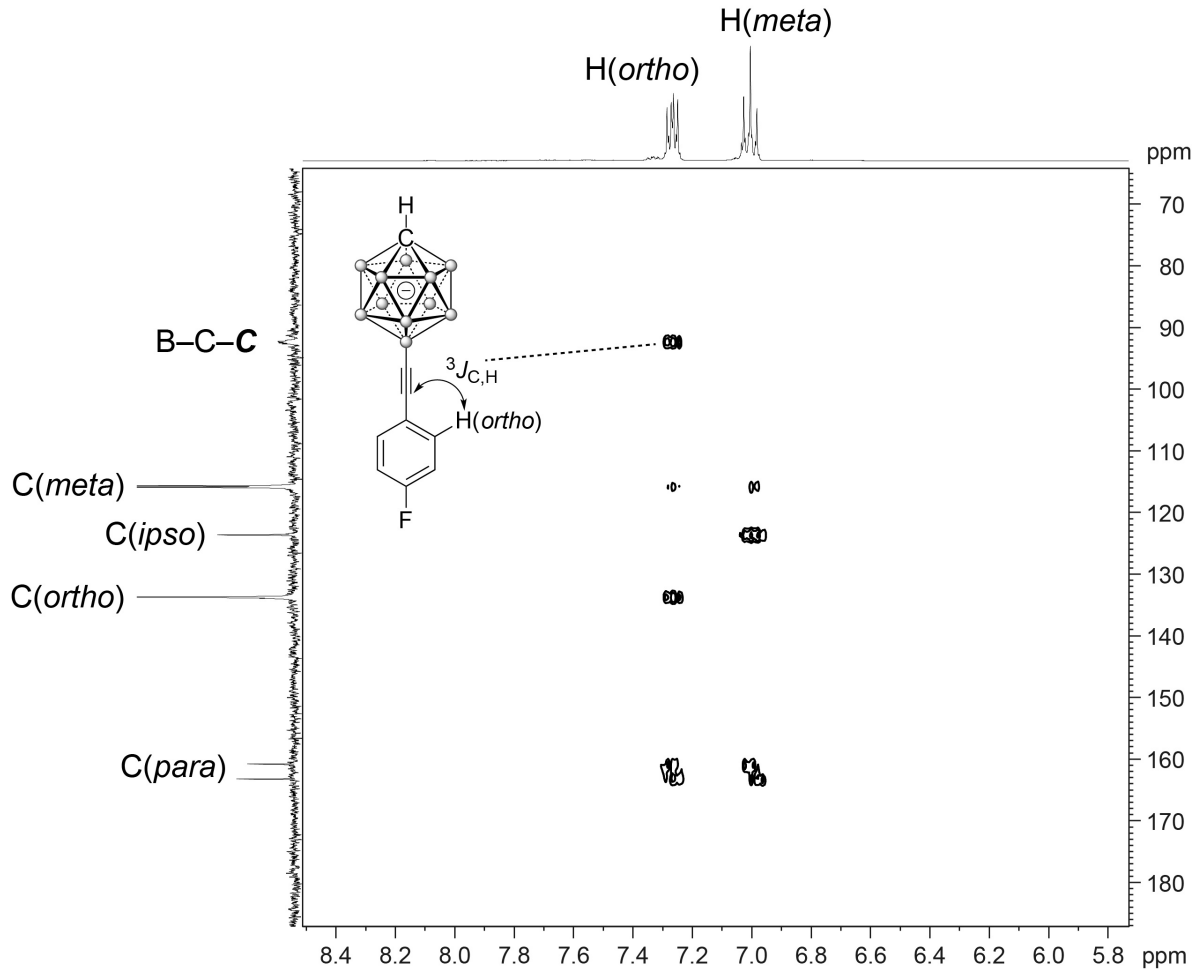


Figure S5. Aromatic and alkyne region of the ^{13}C-^{1}H HMBC NMR spectrum of $[Et_4N][CB_{11}H_{11}$-CC-C_6H_4-4-F] (acetone-d_6, 24 °C); the C(*para*), C(*meta*) and C(*ortho*) ^{13}C signals appear as doublets because of splitting by ^{19}F with I = 1/2. The assignments of the signals are based on HSQC and HMBC spectra.

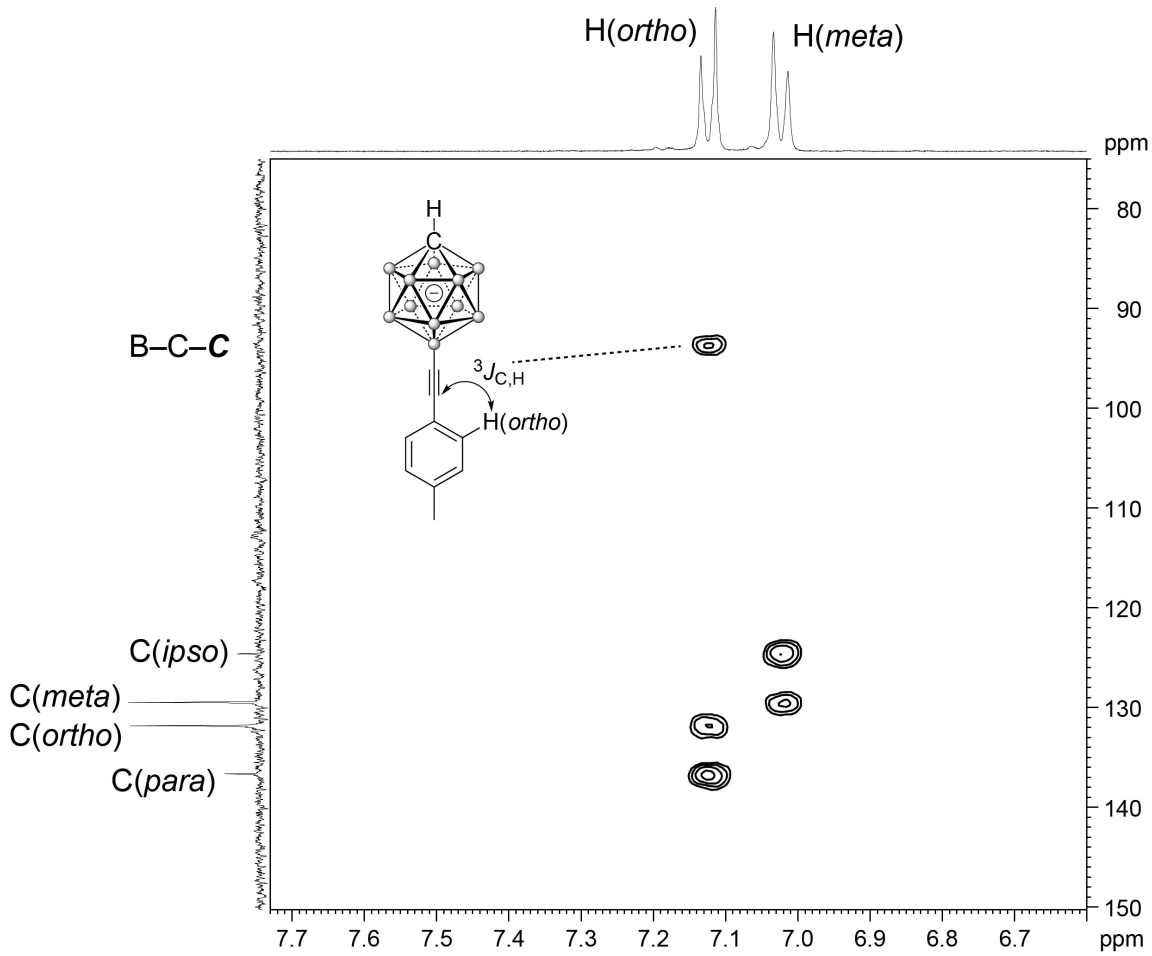


Figure S6. Aromatic and alkyne region of the ^{13}C-^{1}H HMBC NMR spectrum of $[Et_4N][CB_{11}H_{11}$-CC-C_6H_4-4-Me] (acetone-d_6, 24 °C). The assignments of the signals are based on HSQC and HMBC spectra.

Low-resolution ESI-MS data were recorded on an Advion Expression CMS instrument, and high-resolution MS data were recorded using an Agilent Technologies 6545 Q-TOF LC/MS instrument.

The plots with a large *m/z* range demonstrate bulk purity, in particular the absence of clusters that would be difficult to detect by NMR spectroscopy, such as starting material or homo-coupling product. The zoomed-in plots show the observed isotopic pattern from the HRMS measurements.

Single-crystal X-ray diffraction studies were performed on an Oxford Diffraction Gemini A Ultra diffractometer equipped with a 135mm Atlas CCD detector and using Cu or Mo K-α radiation.

II Experimental Section

Mono-iodination of $[CB_{11}H_{12}]^-$

$[Cs][CB_{11}H_{12}]$ (1.02 g, 3.7 mmol) was suspended in CH_3COOH (25 mL). The white solid was suspended at 25 °C and gave a clear solution after 15 min of stirring. The flask was heated to 80 °C in an oil bath. I_2 (1.22 g, 4.4 mmol, 1.2 equiv) was added, and the mixture was stirred for 5 hours. ESI-MS analysis showed only a signal at *m/z* 269, indicating clean formation of mono-iodinated B(12)-I and B(7)-I products.

To the purple-red solution, Na_2SO_3 was added carefully to quench excess I_2. A sample for ^{11}B NMR analysis in order to evaluate the crude ratio of B(12)-I to B(7)-I can be taken at this point. The solution was concentrated on a rotary evaporator, and a yellow solid was obtained. H_2O (25 mL) was added to the solid. $CsOH \cdot H_2O$ was added to adjust the pH value to 12, and the mixture became almost colorless. It was heated to boiling temperature and filtered while hot. The filtrate was concentrated on a rotary evaporator and recrystallized from H_2O to afford $[Cs][12\text{-}I\text{-}CB_{11}H_{11}]$ as colorless crystals (1.19 g, 80%).

Additional remarks about the isomeric purity:

$^{11}B\{^1H\}$ NMR spectra of crude samples after quenching with Na_2SO_3 typically indicated a ratio of B(12)-I to B(7)-I of approximately 85:15 (Figure S7a). Recrystallization from H_2O afforded B(12)-I enrichment to a ratio of 95:5 or higher (Figure S7b). The purity can be further increased by a second recrystallization, resulting in spectra which indicate a ratio of 98:2 or higher (Figure S7c).

Small ^{11}B NMR signals (in addition to those of the 12-isomer) in some of the spectra of the compounds **5** stem from small amounts of 7-isomer.

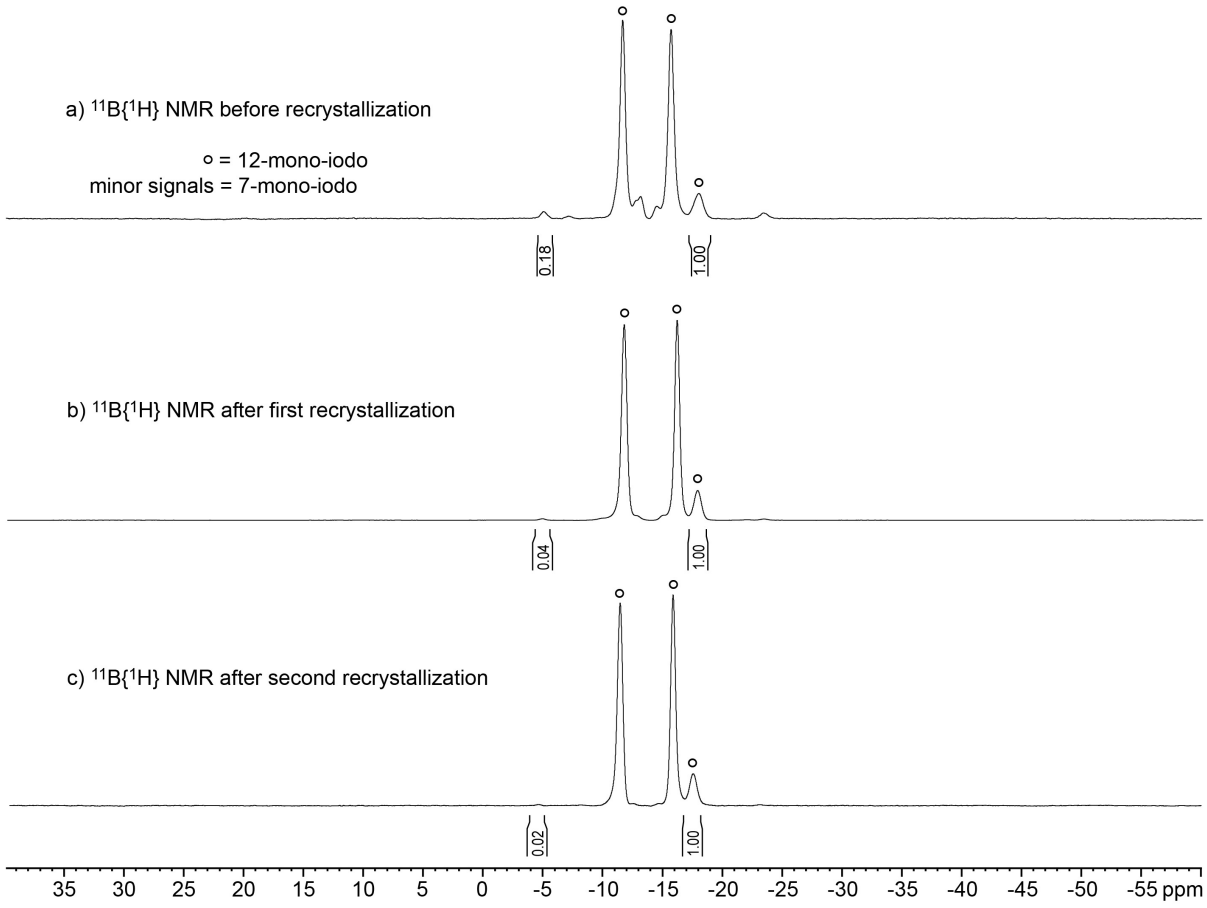
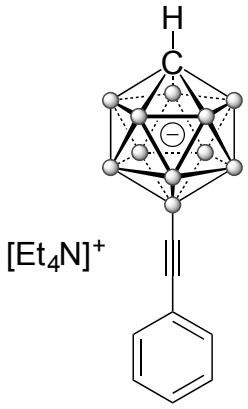


Figure S7. $^{11}B\{^{1}H\}$ NMR spectra showing a) the crude product of the mono-iodination of $[CB_{11}H_{12}]^{-}$, b) the product after the first recrystallization from water, and c) the product after the second recrystallization from water (128 MHz for ^{11}B, acetone-d_6, 24 °C).

General procedure for the Sonogashira coupling

In a glovebox under N_2 atmosphere, a 30 mL high pressure tube was charged with a magnetic stir bar, [Cs][$CB_{11}H_{11}$-12-CCH] (30 mg, 0.1 mmol), $Pd(PPh_3)_4$ (5.78 mg, 0.05 mmol) and CuI (1.9 mg, 0.1 mmol). Anhydrous THF (2 mL) and anhydrous Et_3N (0.5 mL) were added. This suspension was stirred for 10 minutes at 500 rpm. Bromobenzene (degassed, 21 µL, 31 mg, 0.2 mmol) was added using an Eppendorf pipet. The tube then was sealed tightly, taken out of the glovebox and heated to 60 °C for 12 hours. The reaction mixture was quenched with deionized water (4 mL), and the resulting suspension was evaporated to dryness on a rotary evaporator. The yellow-brownish solid that was obtained was dissolved in CH_2Cl_2 (15 mL) and H_2O (10 mL), and Et_4NBr (84 mg, 0.4 mmol) was added for cation exchange. This mixture was stirred vigorously for an hour. The organic layer was separated, and the aqueous layer was extracted with CH_2Cl_2 (3 x 10 mL). All organic layers were combined and dried over $MgSO_4$. Filtration afforded a clear yellow solution, which was concentrated on a rotary evaporator and purified by silica gel column chromatography (eluent CH_2Cl_2/MeCN 10:1, fraction size 5 mL).

For products **5a**, **5k** and **5r** the coupling was performed with 1.1 mmol of [Cs][$CB_{11}H_{11}$-12-CCH] starting material in order to demonstrate scalability. The reaction was carried out in a 200 mL glass pressure tube under identical conditions to the general procedure. Purification of the products by silica gel chromatography afforded yields of 68%, 74% and 87%, respectively.



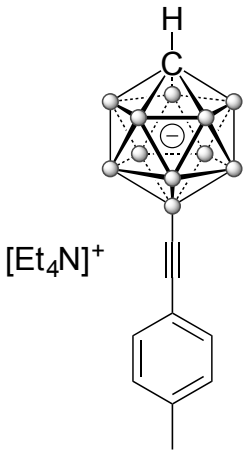
5a (70% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 7.28-7.14 (overlapping m, 5H, Ar-H), 3.44(q, *J* = 7.2 Hz, 8H, CH_2 of cation), 2.22 (broad signal, 1H, cage CH), 1.79 (broad signal, 5H, BH), 1.68 (broad signal, 5H, BH), 1.36 (tt, *J* = 7.2 Hz, 1.8 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -6.92 (1B, B12), -12.25 (5B, B7-11), -16.65 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 131.89, 128.85, 127.47, 127.10 (Ar-C), 52.98 (CH_2 of cation), 49.01 (cage C), 7.64 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_9H_{16}B_{11}]^-$: 243.2354. Found: 243.2352.



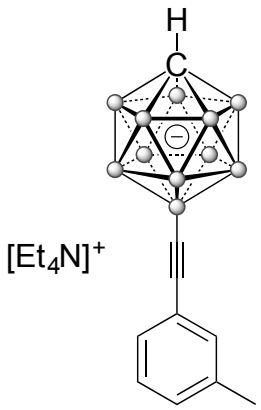
5b (83% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 7.13 (d, J = 8.1 Hz, 2H, Ar-H), 7.02 (d, J = 8.1 Hz, 2H, Ar-H), 3.49 (q, J = 7.1 Hz, 8H, CH_2 of cation), 2.25 (s, 3H, Ar-CH_3), 2.20 (broad signal, 1H, cage CH), 1.79 (broad signal, 5H, BH), 1.67 (broad signal, 5H, BH), 1.39 (tt, J = 7.1 Hz, 1.8 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -6.82 (1B, B12), -12.27 (5B, B7-11), -16.73 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 136.64, 131.83, 129.47, 124.61(Ar-C), 52.96 (CH_2 of cation), 48.85 (cage C), 21.22 (methyl group on the benzene), 7.64 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{10}H_{18}B_{11}]^-$: 257.2510. Found: 257.2513.



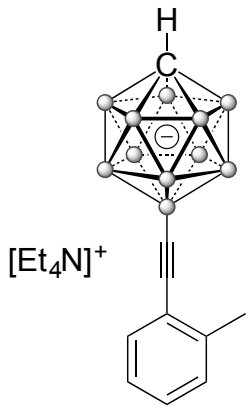
5c (87% yield)

^{1}H{^{11}B} NMR (500 MHz, acetone-d_6, 23 °C): 7.11-6.97 (overlapping m, 4H, Ar-H), 3.48 (q, *J* = 7.1 Hz, 8H, CH_2 of cation), 2.21 (s, 3H, Ar-CH_3), 2.05 (broad signal, 1H, cage CH), 1.79 (broad signal, 5H, BH), 1.67 (broad signal, 5H, BH), 1.39 (tt, *J* = 7.1 Hz, 1.7 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (160 MHz, acetone-d_6, 23 °C): -6.87 (1B, B12), -12.25 (5B, B7-11), -16.67 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 138.24, 132.64, 128.94, 128.69, 127.82, 127.46 (Ar-C), 53.01 (CH_2 of cation), 48.93 (cage C), 21.14 (CH_3), 7.66 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{10}H_{18}B_{11}]^-$: 257.2510. Found: 257.2535.



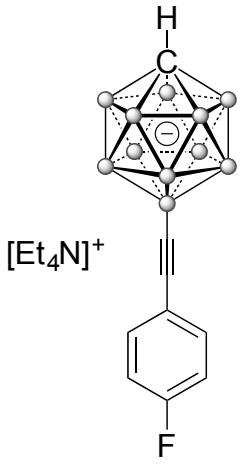
5d (85% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 7.28-6.99 (overlapping m, 4H, Ar-H), 3.44 (q, *J* = 7.1 Hz, 8H, CH_2 of cation), 2.32 (s, 3H, Ar-CH_3), 2.21 (broad signal, 1H, cage CH), 1.80 (broad signal, 5H, BH), 1.68 (broad signal, 5H, BH), 1.36 (tt, *J* = 7.1 Hz, 1.8 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (160 MHz, acetone-d_6, 23 °C): -6.71 (1B, B12), -12.19 (5B, B7-11), -16.67 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 140.37, 131.82, 131.64, 129.78, 127.25, 126.06 (Ar-C), 52.97 (CH_2 of cation), 48.83 (cage C), 20.79 (CH_3), 7.63 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{10}H_{18}B_{11}]^-$: 257.2510. Found: 257.2535.



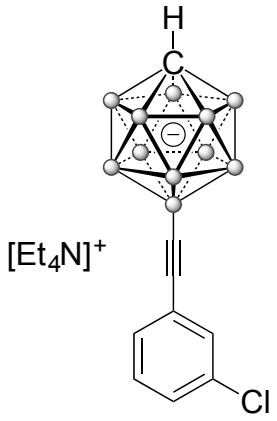
5e (73% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 7.35-7.20 (m, 2H, Ar-H), 7.10-6.93 (m, 2H, Ar-H), 3.43 (q, J = 7.1 Hz, 8H, CH_2 of cation), 2.22 (broad signal, 1H, cage CH), 1.77 (broad signal, 5H, BH), 1.66 (broad signal, 5H, BH), 1.35 (t, J = 7.1 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -6.99 (1B, B12), -12.26 (5B, B7-11), -16.64 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 162.03 (d, J = 245 Hz, C-F), 133.75 (d, J = 8.1 Hz, Ar-C(*ortho*)), 123.74 (Ar-C(*ipso*)), 115.79 (d, J = 21.9 Hz, Ar-C(*meta*)), 52.98 (CH_2 of cation), 49.05 (cage C), 7.64 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_9H_{15}B_{11}F]^-$: 261.2254. Found: 261.2258.



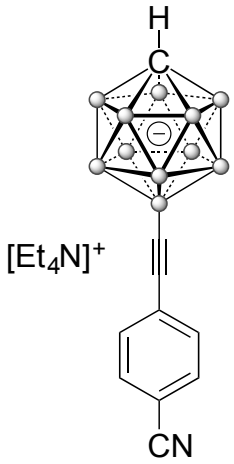
5f (81% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 7.25-7.17 (overlapping m, 4H, Ar-H), 3.47 (q, *J* = 7.1 Hz, 8H, CH_2 of cation), 2.23 (broad signal, 1H, cage CH), 1.78 (broad signal, 5H, BH), 1.68 (broad signal, 5H, BH), 1.38 (tt, *J* = 7.1 Hz, 1.7 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -7.23 (1B, B12), -12.26 (5B, B7-11), -16.60 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 134.17, 131.45, 130.55, 130.39, 129.36, 127.25 (Ar-C), 53.01 (CH_2 of cation), 49.37 (cage C), 7.66 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_9H_{15}B_{11}Cl]^-$: 279.1922. Found: 278.1959.



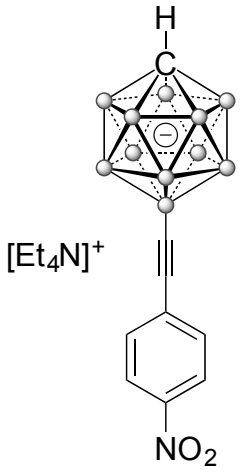
5g (73% yield)

^{1}H{^{11}B} NMR (500 MHz, acetone-d_6, 23 °C): 7.63-7.62 (m, 2H, Ar-H), 7.40-7.39 (m, 2H, Ar-H), 3.49 (q, J = 7.2 Hz, 8H, CH_2 of cation), 2.23 (broad signal, 1H, cage CH), 1.79 (broad signal, 5H, BH), 1.69 (broad signal, 5H, BH), 1.39 (tt, J = 7.2 Hz, 1.8 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (160 MHz, acetone-d_6, 23 °C): -7.44 (1B, B12), -12.27 (5B, B7-11), -16.56 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 132.69, 132.66, 119.38,110.17 (Ar-C), 52.94 (CH_2 of cation), 49.78 (cage C), 7.64 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{10}H_{15}B_{11}N]^-$: 268.2301. Found: 268.2297.



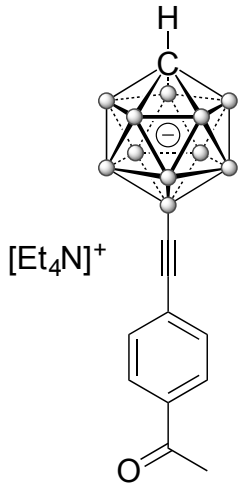
5h (65% yield)

^{1}H{^{11}B} NMR (500 MHz, acetone-d_6, 23 °C): 8.13 (d, J = 8.8 Hz, 2H, Ar-H), 7.46 (d, J = 8.8 Hz, 2H, Ar-H), 3.47 (q, J = 7.1 Hz, 8H, CH_2 of cation), 2.27 (broad signal, 1H, cage CH), 1.70 (broad signal, 5H, BH), 1.69 (broad signal, 5H, BH), 1.38 (tt, J = 7.1 Hz, 1.7 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (160 MHz, acetone-d_6, 23 °C): -7.53 (1B, B12), -12.27 (5B, B7-11), -16.54 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 146.61, 134.36, 132.74,124.16 (Ar-C), 52.96 (CH_2 of cation), 49.85 (cage C), 7.62 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_9H_{15}B_{11}NO_2]^-$: 288.2199. Found: 288.2220.



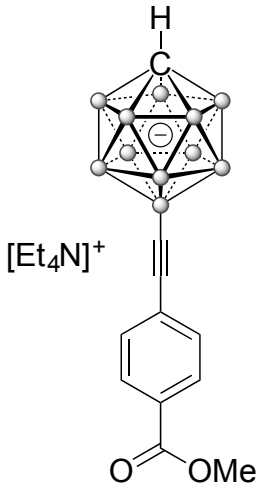
5i (80% yield)

^{1}H{^{11}B} NMR (500 MHz, acetone-d_6, 23 °C): 7.85 (d, J = 8.1 Hz, 2H, Ar-H), 7.34 (d, J = 8.1 Hz, 2H, Ar-H), 3.50 (q, J = 7.1 Hz, 8H, CH_2 of cation), 2.54 (s, 3H, CH_3 of ketone), 2.24 (broad signal, 1H, cage CH), 1.81 (broad signal, 5H, BH), 1.69 (broad signal, 5H, BH), 1.40 (t, J = 7.1 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (160 MHz, acetone-d_6, 23 °C): -7.26 (1B, B12), -12.28 (5B, B7-11), -16.59 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 197.19 (C=O), 135.71, 132.05, 131.89, 128.85 (Ar-C), 93.17 (alkynyl C), 52.96 (CH_2 of cation), 49.46 (cage C), 26.60 (ketone CH_3), 7.63 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{11}H_{18}B_{11}O]^-$: 285.2454. Found: 285.2459.



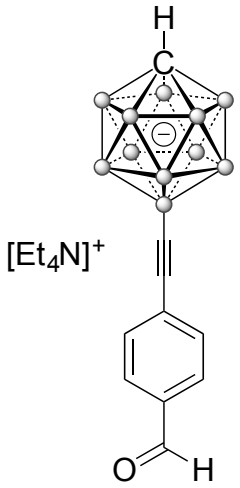
5j (77% yield)

^{1}H{^{11}B} NMR (500 MHz, acetone-d_6, 23 °C): 7.87 (d, J = 8.3 Hz, 2H, Ar-H), 7.35 (d, J = 8.3 Hz, 2H, Ar-H), 3.85 (s, 3H, CH_3 of ester), 3.51 (q, J = 7.1 Hz, 8H, CH_2 of cation), 2.24 (broad signal, 1H, cage CH), 1.80 (broad signal, 5H, BH), 1.69 (broad signal, 5H, BH), 1.3 (tt, J = 7.1 Hz, 1.9 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (160 MHz, acetone-d_6, 23 °C): -7.21 (1B, B12), -12.25 (5B, B7-11), -16.60 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 166.83 (C=O), 131.89, 129.95 129.90, 128.59 (Ar-C), 93.21 (alkynyl C), 52.95 (CH_3 of ester), 52.24 (CH_2 of cation), 49.46 (cage C), 7.64 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{11}H_{18}B_{11}O_2]^-$: 301.2403. Found: 301.2401.



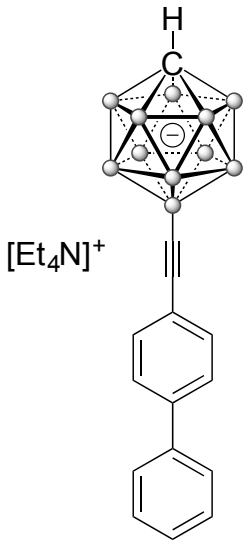
5k (82% yield)

^{1}H{^{11}B} NMR (500 MHz, acetone-d_6, 23 °C): 9.97 (s, 1H, CHO-H), 7.78 (d, *J* = 8.2Hz, 2H, Ar-H), 7.42 (d, *J* = 8.2Hz, 2H, Ar-H), 3.50 (q, *J* = 7.2 Hz, 8H, CH_2 of cation), 2.25 (broad signal, 1H, cage CH), 1.81 (broad signal, 5H, BH), 1.69 (broad signal, 5H, BH), 1.40 (tt, *J* = 7.2 Hz, 1.8 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (160 MHz, acetone-d_6, 23 °C): -7.30 (1B, B12), -12.24 (5B, B7-11), -16.56 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 192.19 (CHO), 135.23, 133.53, 132.41, 130.03 (Ar-C), 52.92 (CH_2 of cation), 49.55 (cage C), 7.61 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{10}H_{16}B_{11}]^-$: 271.2303. Found: 271.2303.



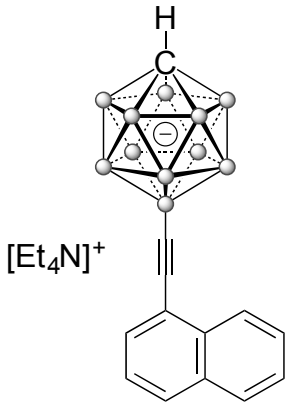
5l (79% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 7.66-7.61 (m, 2H, Ar-H), 7.56-7.53 (m, 2H, Ar-H), 7.47-7.40 (m, 2H, Ar-H), 7.36-7.31 (m, 3H, Ar-H), 3.45 (q, *J* = 7.1 Hz, 8H, CH_2 of cation), 2.23 (broad signal, 1H, cage CH), 1.81 (broad signal, 5H, BH), 1.69 (broad signal, 5H, BH), 1.37 (tt, *J* = 7.1 Hz, 1.7 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -6.89 (1B, B12), -12.23 (5B, B7-11), -16.66 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 141.27, 139.54, 132.51,129.74, 128.17, 127.47, 127.31, 126.69 (biphenyl-C), 53.03 (CH_2 of cation), 49.11 (cage C), 7.69 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{15}H_{20}B_{11}]^-$: 319.2661. Found: 319.2653.



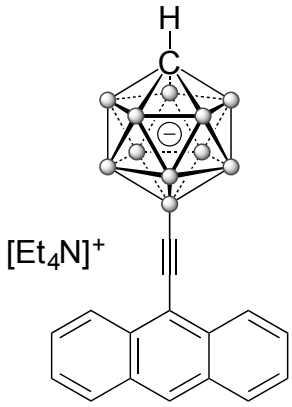
5m (84% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 8.46-8.31 (m, 1H, Ar-H), 7.88-7.81 (m, 1H, Ar-H), 7.77-7.71 (m, 1H, Ar-H), 7.57-7.33 (overlapping m, 4H, Ar-H), 3.39 (q, J = 7.1 Hz, 8H, CH_2 of cation), 2.26 (broad signal, 1H, cage CH), 1.89 (broad signal, 5H, BH), 1.73 (broad signal, 5H, BH), 1.32 (tt, J = 7.1 Hz, 1.7 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -6.84 (1B, B12), -12.14 (5B, B7-11), -16.56 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 134.61, 134.24, 129.39,128.84, 127.69, 127.45, 126.91, 126.20 (Ar-C), 52.96 (CH_2 of cation), 49.16 (cage C), 7.16 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{13}H_{18}B_{11}]^-$: 293.2505. Found: 293.2506.



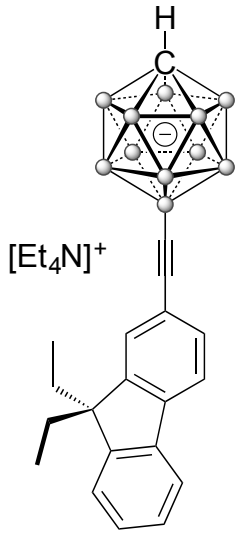
5n (75% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 8.61 (d, *J* = 8.3 Hz, 2H, Ar-H), 8.38 (s, 1H, Ar-H) 8.01 (d, *J* = 8.3 Hz, 2H, Ar-H), 7.53-7.48 (overlapping m, 4H, Ar-H), 3.36 (q, *J* = 7.2 Hz, 8H, CH_2 of cation), 2.31 (broad signal, 1H, cage CH), 1.99 (broad signal, 5H, BH), 1.78 (broad signal, 5H, BH), 1.28 (tt, *J* = 7.2 Hz, 1.7 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -6.68 (1B, B12), -12.02 (5B, B7-11), -16.49 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 133.04, 132.29, 129.23, 128.34, 126.54, 126.39, 125.91, 121.90 (Ar-C), 52.93 (CH_2 of cation), 49.32 (cage C), 7.58 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{17}H_{20}B_{11}]^-$: 343.2661. Found: 343.2662.



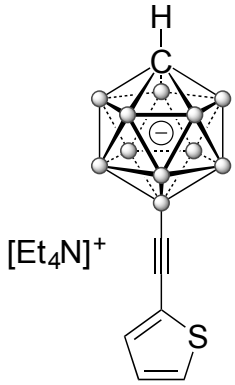
5o (42% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 7.76-7.70 (m, 1H, Ar-H), 7.64 (d, *J* =7.8 Hz, 1H, Ar-H), 7.41-7.20 (overlapping m, 5H, fluorene-H), 3.49 (q, *J* = 7.1 Hz, 8H, CH_2 of cation), 2.22 (broad signal, 1H, cage CH), 1.83 (broad signal, 5H, BH), 1.69 (broad signal, 5H, BH), 1.39 (tt, *J* = 7.2 Hz, 1.7 Hz, 12H, CH_3 of cation), 1.29 (broad signal, 4H, CH_2 of fluorene ethyl), 0.22 (t, *J* = 7.1 Hz, 6H, CH_3 of fluorene ethyl).

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -6.86 (1B, B12), -12.22 (5B, B7-11), -16.64 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 150.63, 150.27, 142.23, 140.70, 130.99, 127.82, 127.75, 126.43, 126.31, 123.64, 120.43, 120.09 (Ar-C), 56.77 (fluorene-CH_3), 53.04 (CH_2 of cation), 48.97 (cage C), 32.20 (fluorene CH_2), 8.71 (fluorene CH_3), 7.66 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{20}H_{28}B_{11}]^-$: 387.3287. Found: 387.3323.



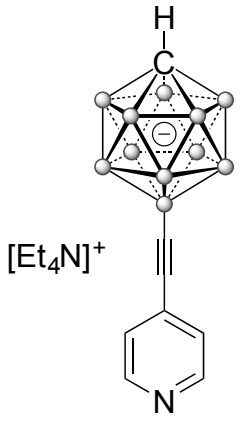
5p (66% yield)

^{1}H{^{11}B} NMR (500 MHz, acetone-d_6, 23 °C): 7.19-7.17 (m, 1H, Ar-H), 6.93-6.88 (overlapping m, 2H, Ar-H), 3.49 (q, J = 7.1 Hz, 8H, CH_2 of cation), 2.23 (broad signal, 1H, cage CH), 1.79 (broad signal, 5H, BH), 1.68 (broad signal, 5H, BH), 1.39 (tt, J = 7.2 Hz, 1.7 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (160 MHz, acetone-d_6, 23 °C): -7.20 (1B, B12), -12.30 (5B, B7-11), -16.62 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 130.15, 127.55, 127.49, 125.43 (Ar-C), 52.99 (CH_2 of cation), 49.33 (cage C), 7.76 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_7H_{14}B_{11}S]^-$: 249.1918. Found: 249.1932.



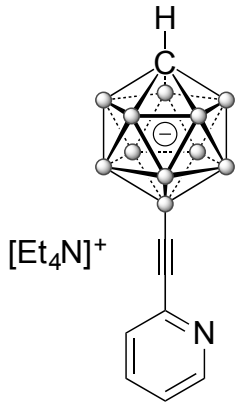
5q (90% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 8.43-8.38 (m, 2H, py-H), 7.16-7.11 (m, 2H, py-H), 3.47 (q, J = 7.1 Hz, 8H, CH_2 of cation), 2.26 (broad signal, 1H, cage CH), 1.78 (broad signal, 5H, BH), 1.68 (broad signal, 5H, BH), 1.38 (tt, J = 7.1 Hz, 1.8 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -7.53 (1B, B12), -12.28 (5B, B7-11), -16.54 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 150.30, 134.85, 126.17 (py-C), 109.15, 91.42 (alkynyl-C), 52.30 (CH_2 of cation), 49.74 (cage C), 7.65 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_8H_{15}B_{11}N]^-$: 244.2301. Found: 244.2306.



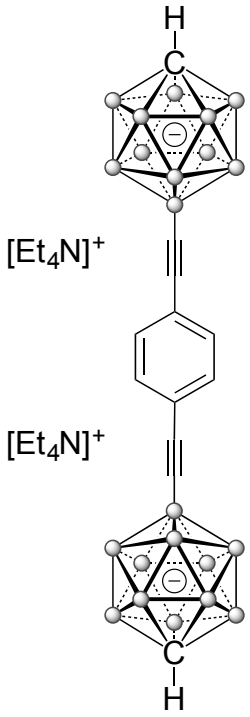
5r (80% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 8.43 (broad signal, 1H, Ar-H), 7.66-7.59 (m, 1H, Ar-H),7.30-7.1 (overlapping m, 2H, Ar-H), 3.48 (q, J = 7.1 Hz, 8H, CH_2 of cation), 2.26 (broad signal, 1H, cage CH), 1.80 (broad signal, 5H, BH), 1.68 (broad signal, 5H, BH), 1.37 (tt, J = 7.1 Hz, 1.8 Hz, 12H, CH_3 of cation).

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -8.12 (1B, B12), -12.35 (5B, B7-11), -16.38 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 150.14, 146.56, 136.52, 127.42, 122.14 (Ar-C), 52.98 (CH_2 of cation), 49.52 (cage C), 7.71 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_8H_{15}B_{11}N]^-$: 244.2306. Found: 244.2305.



5s (95% yield)

^{1}H{^{11}B} NMR (500 MHz, acetone-d_6, 23 °C): 7.11 (4H, Ar-H), 3.44 (q, J = 7.1 Hz, 16H, CH_2 of cation), 2.21 (broad signal, 2H, cage CH), 1.76 (broad signal, 10H, BH), 1.66 (broad signal, 10H, BH), 1.39 (tt, J = 7.1 Hz, 1.7 Hz, 24H, CH_3 of cation).

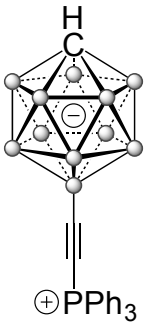
^{11}B{^{1}H} NMR (160 MHz, acetone-d_6, 23 °C): -7.05 (2B, B12), -12.41 (10B, B7-11), -16.82 (10B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 131.65, 125.39 (Ar-C), 53.00 (CH_2 of cation), 49.05 (cage C), 7.67 (CH_3 of cation).

High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{12}H_{26}B_{22}]^{2-}$: 204.2119. Found: 204.2124.

Procedure for the synthesis of 7

A dry 15 mL Schlenk flask, equipped with a magnetic stir bar, was charged with [Cs][$CB_{11}H_{11}$-12-C≡CH] (90 mg, 0.3 mmol, 1 equiv), $Pd(PPh_3)_4$ (18 mg, 0.016 mmol, 0.05 equiv), and CuI (10 mg, 0.052 mmol, 0.018 equiv) in anhydrous THF/Et_3N (7.5ml/1.5ml) under N_2. The mixture was stirred at 60 °C for 24 h. Water (5 mL) was added, and the organic volatiles were removed using a rotary evaporator. The resulting orange solid was dissolved in CH_2Cl_2 and filtered through a fritted glass funnel (F pore size) to remove the metal catalyst. The filtrate was concentrated, and the crude product was purified by preparative TLC (20x20 cm plate, 1 mm silica gel layer, eluent CH_2Cl_2/EtOAc = 5:1). The top band of the plate was scratched off, ground into a powder and suspended in CH_2Cl_2. The suspension was filtered, and the filtrate was evaporated to dryness using a rotary evaporator and further dried in a vacuum at 60 °C overnight. Compound **7** was obtained as a slightly orange solid (75.6 mg, 58.4%).



7 (58% yield)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): 7.98-7.76 (overlapping m 15H, Ar-H), 2.49 (broad signal, 1H, cage CH), 1.86 (broad signal, 5H, BH), 1.78 (broad signal, 5H, BH),

^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): -10.48 (1B, B12), -12.22 (5B, B7-11), -15.90 (5B, B2-6).

^{13}C{^{1}H} NMR (101 MHz, acetone-d_6, 23 °C): 136.22 (d, J = 2.9 Hz), 133.96 (d, J = 12.3 Hz), 131.30 (d, J = 14.0 Hz), 121.07 (d, J = 99.9 Hz), 53.25 (cage C).

ESI-MS (positive mode, MeOH): *m/z* calcd for $[C_{21}H_{26}B_{11}P + Na]^+$: 451.2761. Found: 451.2774.

III X-ray Crystallography

Crystal structure of 5b

Compound [Et_4N]**5b** (15 mg) was dissolved in acetone (0.5 mL) in a 1 mL glass vial. The resulting colorless solution was filtered into a 18 cm long 5 mm NMR tube and layered with hexane (1 mL). Colorless crystals of the composition [Et_4N][$C_{10}H_{18}B_{11}$] suitable for X-ray diffraction grew within 5 days at 25 °C.

```
Bond precision:  C-C = 0.0018 A          Wavelength=0.71073

Cell:            a=8.8067(2)    b=24.6376(8)        c=11.8907(4)
                 alpha=90       beta=106.705(1)     gamma=90
Temperature:     296 K

                 Calculated                 Reported
Volume           2471.11(13)                2471.11(13)
Space group      P 21/n                     P 1 21/n 1
Hall group       -P 2yn                     -P 2yn
Moiety formula   C10 H18 B11, C8 H20 N      C8 H20 N, C10 H18 B11
Sum formula      C18 H38 B11 N              C18 H38 B11 N
Mr               387.40                     387.40
Dx,g cm-3        1.041                      1.041
Z                4                          4
Mu (mm-1)        0.052                      0.052
F000             832.0                      832.0
F000'            832.17
h,k,lmax         11,32,15                   11,32,15
Nref             6145                       6132
Tmin,Tmax        0.978,0.989                0.654,0.746
Tmin'            0.966

Correction method= # Reported T Limits: Tmin=0.654 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 28.299

R(reflections)= 0.0485( 4987)     wR2(reflections)= 0.1477( 6132)

S = 1.057                 Npar= 276
```

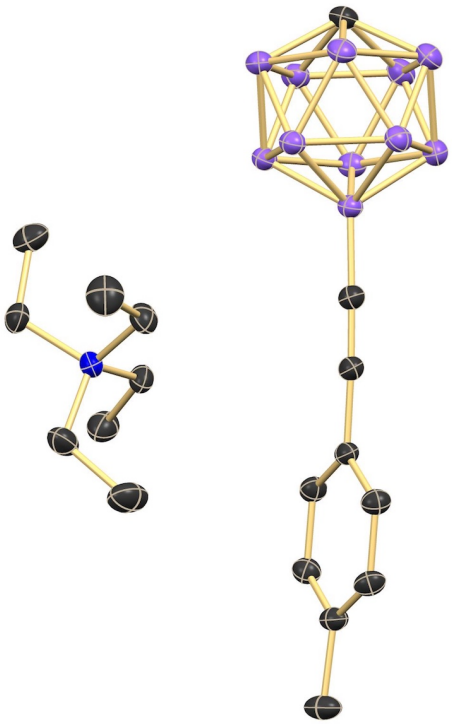


Figure S8. ORTEP representation of [Et_4N]**5b**. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

Crystal structure of 5k

Compound $[Et_4N]$**5k** (20 mg) was dissolved in THF (1 mL) in a 4 mL glass vial. The resulting colorless solution was layered with hexane (2 mL). Colorless crystals of the composition $[Et_4N][C_{10}H_{16}B_{11}O]$ suitable for X-ray diffraction grew within 4 days at 12 °C.

```
Bond precision:  C-C = 0.0025 A          Wavelength=0.71073

Cell:          a=9.4648(10)      b=11.1951(12)    c=12.0223(13)
               alpha=94.711(4)   beta=92.228(4)   gamma=107.742(4)
Temperature:   170 K

                Calculated                Reported
Volume          1206.5(2)                 1206.4(2)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C10 H16 B11 O, C8 H20 N   C10 H16 B11 O, C8 H20 N
Sum formula     C18 H36 B11 N O           C18 H36 B11 N O
Mr              401.39                    401.39
Dx,g cm-3       1.105                     1.105
Z               2                         2
Mu (mm-1)       0.059                     0.059
F000            428.0                     428.0
F000'           428.11
h,k,lmax        12,14,15                  12,14,15
Nref            5353                      5260
Tmin,Tmax       0.987,0.995               0.647,0.746
Tmin'           0.976

Correction method= # Reported T Limits: Tmin=0.647 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.983          Theta(max)= 27.159

R(reflections)= 0.0532( 3873)     wR2(reflections)= 0.1532( 5260)

S = 1.018                 Npar= 284
```

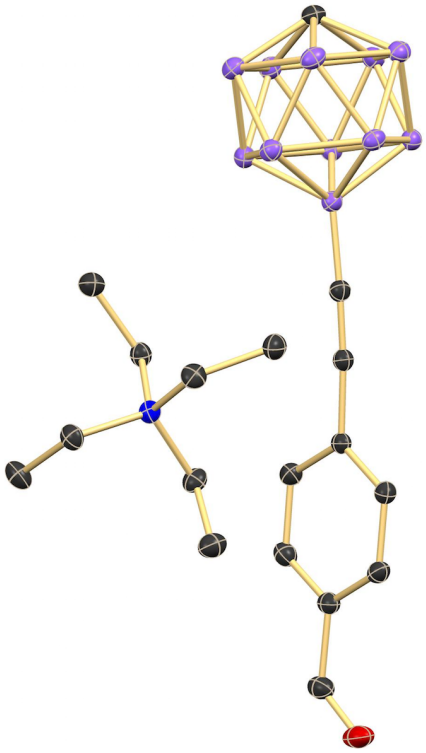


Figure S9. ORTEP representation of [Et_4N]**5k**. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

Crystal structure of 5q

Compound $[Et_4N]$**5q** (20 mg) was dissolved in THF (1 mL) in a 4 mL glass vial. The resulting colorless solution was layered with hexane (2 mL). Colorless crystals of the composition $[Et_4N]_2[C_8H_{15}B_{11}N]_2$ suitable for X-ray diffraction grew within 4 days at 12 °C.

```
Bond precision:  C-C = 0.0031 A          Wavelength=0.71073

Cell:            a=17.8925(10)     b=22.8056(10)      c=11.5812(6)
                 alpha=90          beta=95.226(2)     gamma=90
Temperature:     170 K

                 Calculated                Reported
Volume           4706.1(4)                 4706.1(4)
Space group      P 21/c                    P 1 21/c 1
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C8 H15 B11 N, C8 H20 N    C8 H15 B11 N, C8 H20 N
Sum formula      C16 H35 B11 N2            C16 H35 B11 N2
Mr               374.37                    374.37
Dx,g cm-3        1.057                     1.057
Z                8                         8
Mu (mm-1)        0.054                     0.054
F000             1600.0                    1600.0
F000'            1600.31
h,k,lmax         22,28,14                  22,28,14
Nref             10041                     10014
Tmin,Tmax        0.976,0.997               0.690,0.745
Tmin'            0.976

Correction method= # Reported T Limits: Tmin=0.690 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 26.768

R(reflections)= 0.0613( 6664)     wR2(reflections)= 0.1835( 10014)

S = 1.016                 Npar= 531
```

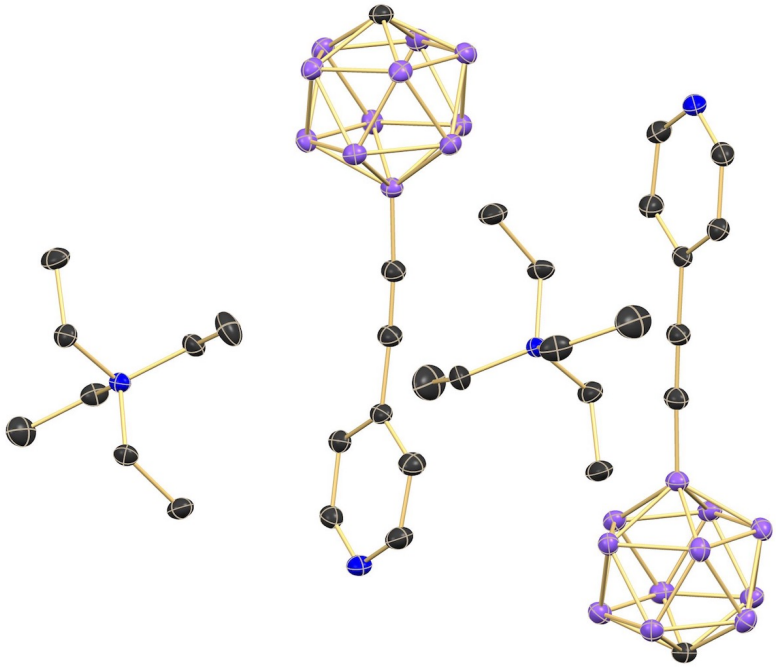


Figure S10. ORTEP representation of $[Et_4N]_2$[**5q**]$_2$. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

Crystal structure of 7

Compound **7** (15 mg) was dissolved in acetone (0.5 mL) in a 1 mL glass vial. The resulting slightly yellow solution was filtered into a 18 cm long 5 mm NMR tube and layered with hexane (1 mL). Colorless crystals of the composition $[C_{21}H_{26}B_{11}P]_2$•acetone suitable for X-ray diffraction grew within 7 days at 25 °C.

Bond precision:	C-C = 0.0024 A	Wavelength=0.71073	
Cell:	a=32.0811(11)	b=12.8344(4)	c=13.7547(5)
	alpha=90	beta=108.944(2)	gamma=90
Temperature:	170 K		

	Calculated	Reported
Volume	5356.6(3)	5356.6(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C21 H26 B11 P), C3 H6 O	2(C21 H26 B11 P), C3 H6 O
Sum formula	C45 H58 B22 O P2	C45 H58 B22 O P2
Mr	914.67	914.67
Dx,g cm-3	1.134	1.134
Z	4	4
Mu (mm-1)	0.116	0.116
F000	1904.0	1904.0
F000'	1905.28	
h,k,lmax	41,16,17	41,16,17
Nref	5918	5903
Tmin,Tmax	0.954,0.968	0.692,0.746
Tmin'	0.946	

Correction method= # Reported T Limits: Tmin=0.692 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 27.108

R(reflections)= 0.0441(4934) wR2(reflections)= 0.1180(5903)

S = 1.038 Npar= 336

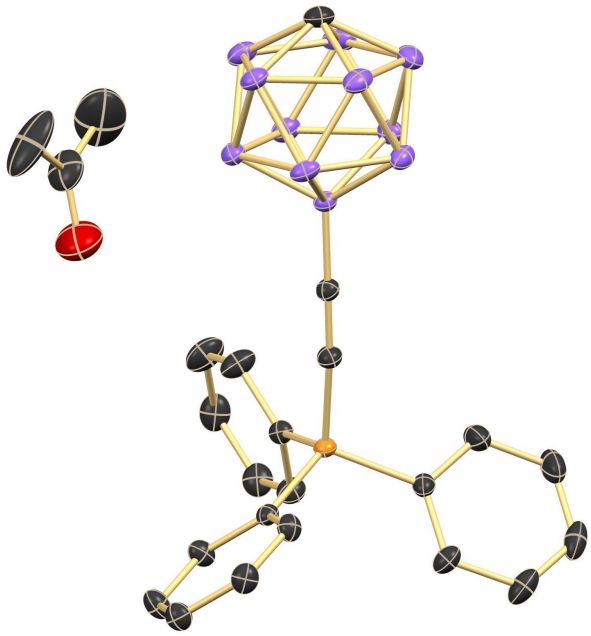


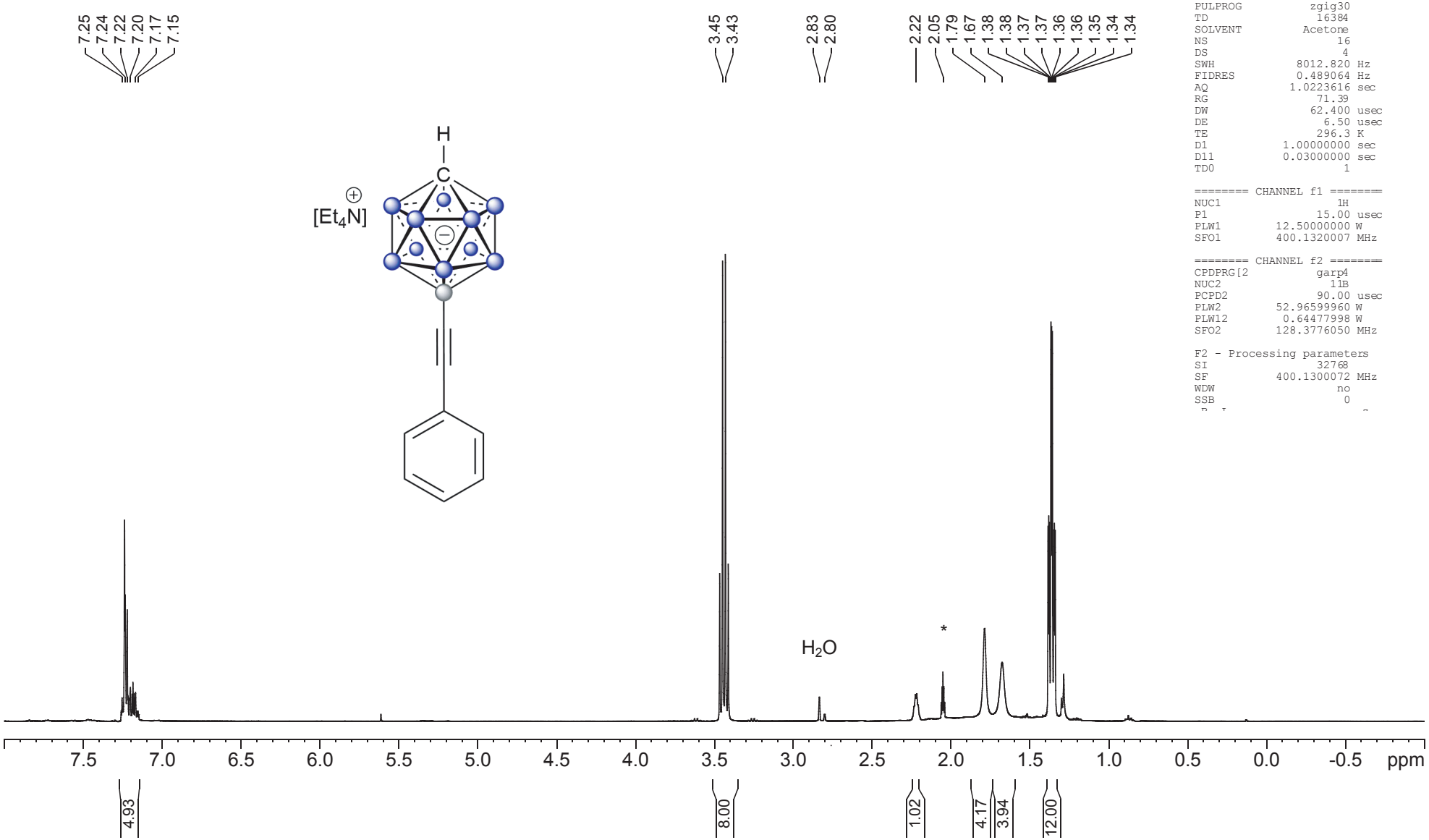
Figure S11. ORTEP representation of **7**•acetone. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

V References

[1] C. A. Reed, *Acc. Chem. Res.* **2010**, *43*, 121–128; A. Himmelspach, G. J. Reiss, M. Finze, *Inorg. Chem.* **2012**, *51*, 2679–2688.

[2] J. R. Holmes D. Kivelson, W. C. Drinkard, *J. Chem. Phys.* **1962**, *37*, 150–152;
a more recent summary is available online from the Sigma-Aldrich company:
https://www.sigmaaldrich.com/content/dam/sigma-aldrich/docs/Aldrich/General_Information/double_water_peaks.pdf

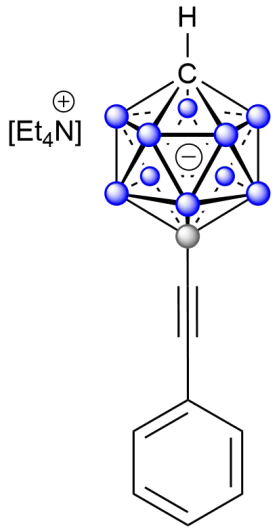
$[Et_4N][CB_{11}H_{11}\text{-CC-Ph}]$, in acetone - d_6*
$^1H\{^{11}B\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20190128-JT-3-CB11-CC-Ph
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_           20190129
Time              22.28
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT        Acetone
NS                  16
DS                   4
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG               71.39
DW               62.400 usec
DE                6.50 usec
TE               296.3 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2               11B
PCPD2             90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                32768
SF          400.1300072 MHz
WDW                  no
SSB                   0
```

$[Et_4N][CB_{11}H_{11}\text{-CC-Ph}]$, in acetone - d_6

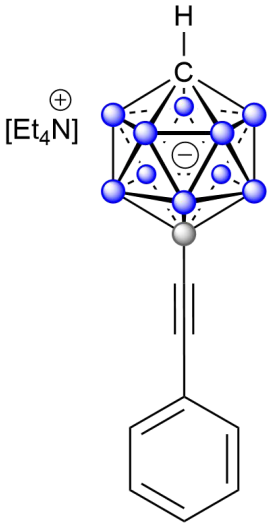
^{11}B, 128 MHz, T = 22 C




```
Current Data Parameters
NAME      20190128-JT-3-CB11-CC-Ph
EXPNO                4
PROCNO               1

F2 - Acquisition Parameters
Date_          20190129
Time              22.41
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE                295.8 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI                32768
SF         128.3776050 MHz
WDW                  EM
SSB                   0
LB                10.00 Hz
GB                    0
PC                 1.40
```

$[Et_4N][CB_{11}H_{11}\text{-CC-Ph}]$, in acetone - d_6

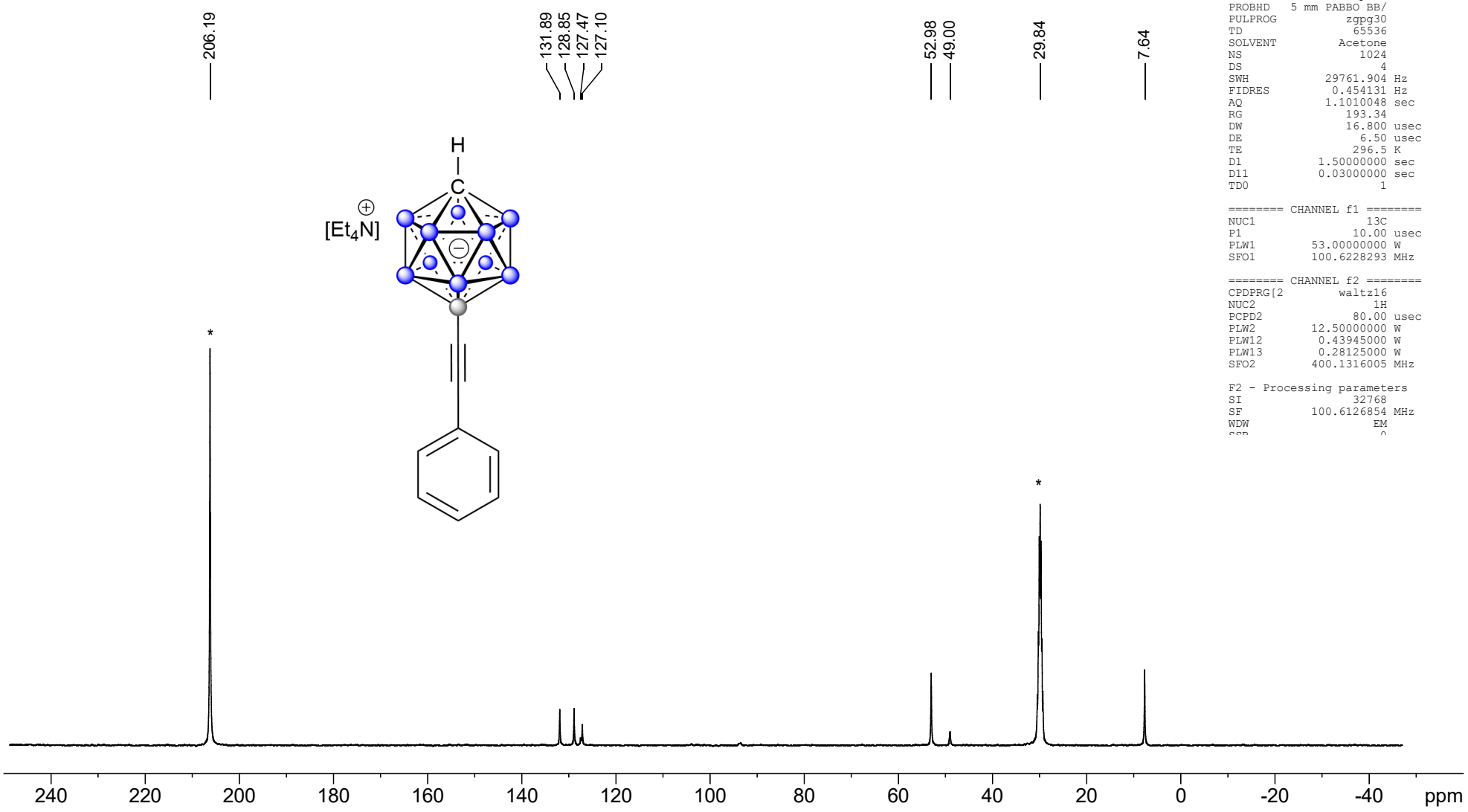
$^{11}B\{^1H\}$, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20190128-JT-3-CB11-CC-Ph
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20190129
Time              22.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              296.7 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                32768
SF           128.3776050 MHz
WDW                  EM
SSB                   0
```

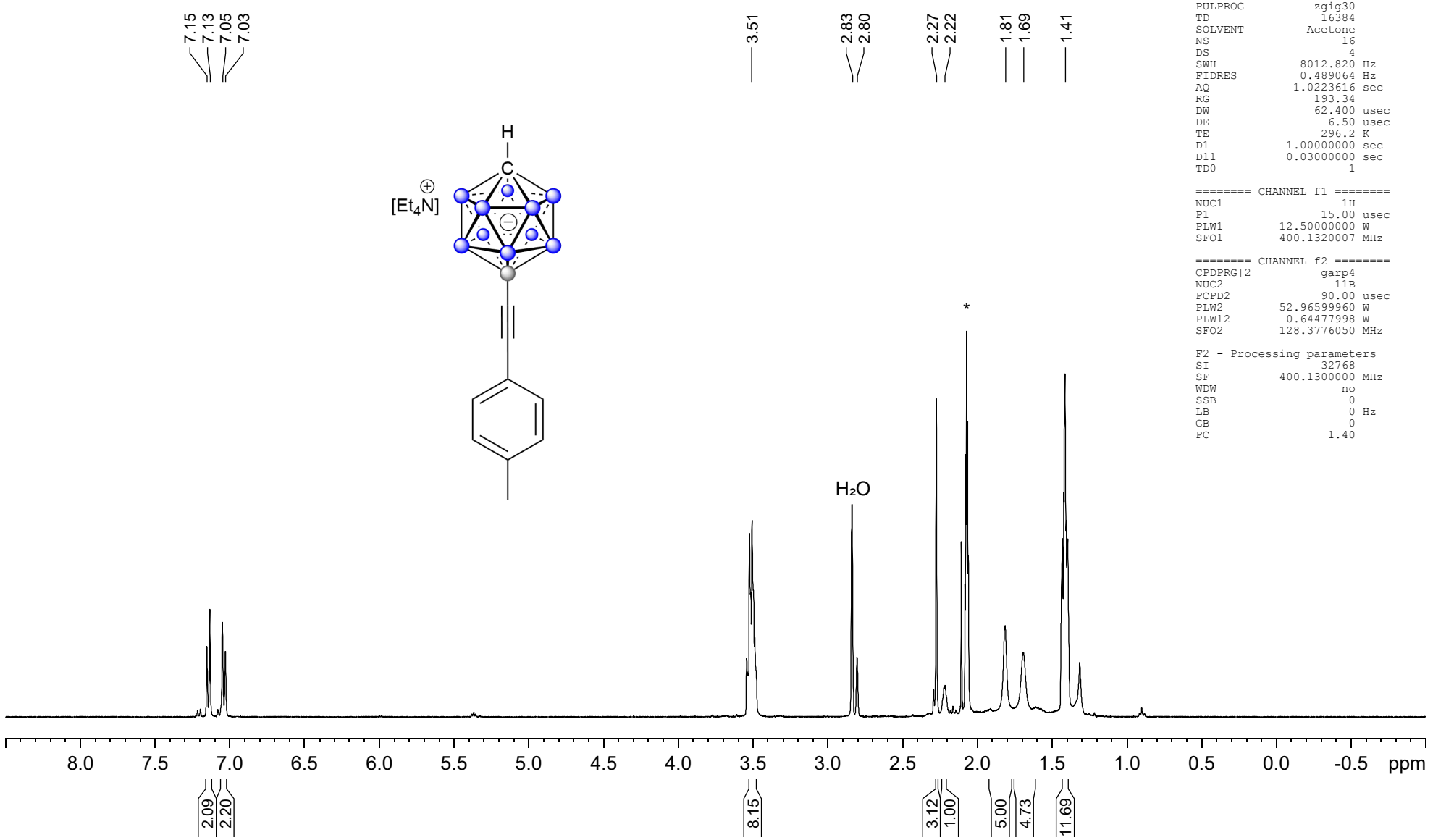
$[Et_4N][CB_{11}H_{11}\text{-}CC\text{-}Ph]$, in acetone - d_6 *

$^{13}C\{^1H\}$, 101 MHz, T = 23 C




```
Current Data Parameters
NAME      20190128-JT-3-CB11-CC-Ph
EXPNO                5
PROCNO               1

F2 - Acquisition Parameters
Date_          20190129
Time              23.28
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                1024
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG              193.34
DW              16.800 usec
DE               6.50 usec
TE              296.5 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1       100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126854 MHz
WDW                EM
```

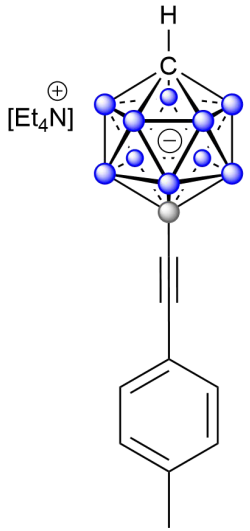
$[Et_4N][CB_{11}H_{11}$-CC-Ph-4-Me], in acetone - d_6*
$^1H\{^{11}B\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20181202-JT-CB11-CC-Ph-4-Me
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20181203
Time             20.01
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT        Acetone
NS                  16
DS                   4
SWH           8012.820 Hz
FIDRES        0.489064 Hz
AQ           1.0223616 sec
RG              193.34
DW              62.400 usec
DE               6.50 usec
TE              296.2 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               15.00 usec
PLW1        12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2               11B
PCPD2            90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2       128.3776050 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  no
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-4-Me], in acetone - d_6

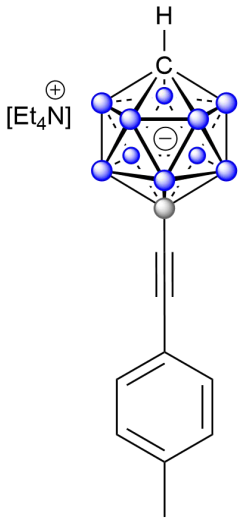
^{11}B, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20190117-JT-CB11-CC-Ph-4-Me
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_           20190118
Time              18.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.4 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB                   0
LB                10.00 Hz
GB                    0
PC                 1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-4-Me], in acetone -d_6

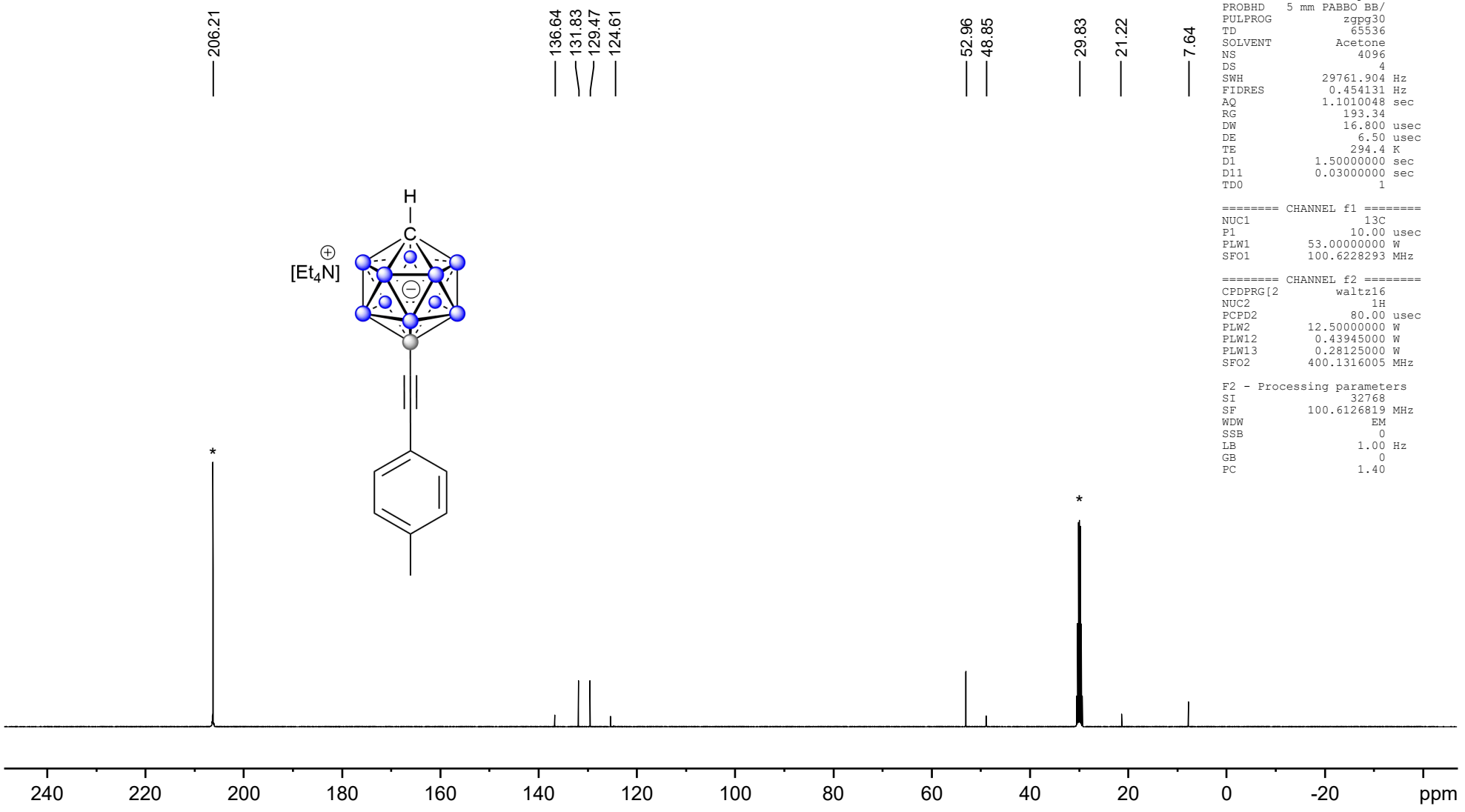
$^{11}B\{^1H\}$, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20190117-JT-CB11-CC-Ph-4-Me
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20190118
Time              18.04
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ            1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              298.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF          128.3776050 MHz
WDW                EM
SSB                 0
```

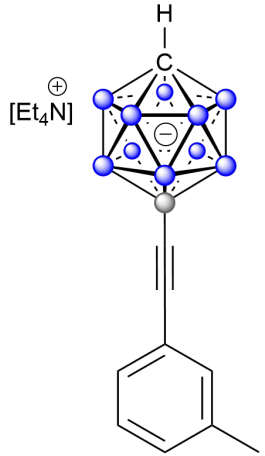
[Et4N][CB11H11-CC-Ph-4-Me], in acetone -d6*

$^{13}C\{^{1}H\}$, 101 MHz, T = 23 C



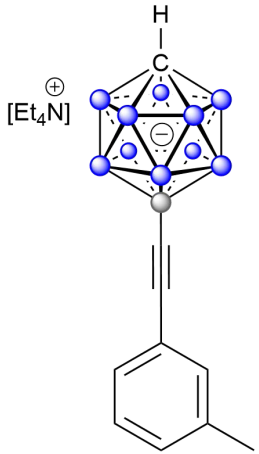

```
Current Data Parameters
NAME      20190117-JT-CB11-CC-Ph-4-Me
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20210615
Time               6.27
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 4096
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               294.4 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126819 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-3-Me], in acetone - d_6*
$^1H\{^{11}B\}$, 500 MHz, T = 23 C




```
Current Data Parameters
NAME      20220506-CC-Ph-3-Me
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_           20220507
Time       3.52
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgig30
TD         65536
SOLVENT            Acetone
NS            16
DS             0
SWH              12500.000 Hz
FIDRES             0.190735 Hz
AQ               2.6214399 sec
RG            114
DW           40.000 usec
DE            6.50 usec
TE           295.8 K
D1              5.00000000 sec
D11             0.03000000 sec

======== CHANNEL f1 ========
NUC1           1H
P1           11.70 usec
PLW1           19.00000000 W
SFO1           500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2              garp
NUC2          11B
PCPD2               100.00 usec
PLW2           95.00000000 W
PLW12           1.63030005 W
SFO2           160.4615690 MHz

F2 - Processing parameters
SI          65536
SF             500.1300102 MHz
WDW             no
SSB            0
LB             0 Hz
GB             0
PC                     1.00
```

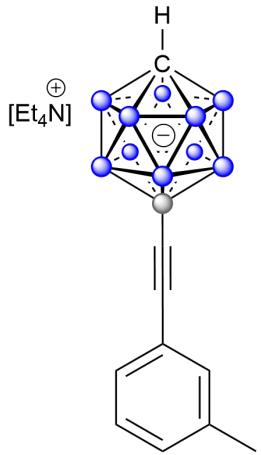
[Et$_4$N][CB$_{11}$H$_{11}$-CC-Ph-3-Me], in acetone - d$_6$
^{11}B, 160 MHz, T = 23 C




```
Current Data Parameters
NAME      20220429-LF-234-mTol-
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_            20220430
Time        7.17
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD          64098
SOLVENT           Acetone
NS             64
DS              0
SWH            32051.281 Hz
FIDRES          0.500036 Hz
AQ             0.9999288 sec
RG            203
DW           15.600 usec
DE            6.50 usec
TE           296.4 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1          11B
P1           13.10 usec
PLW1            95.00000000 W
SFO1           160.4615792 MHz

F2 - Processing parameters
SI           32768
SF              160.4615790 MHz
WDW              EM
SSB              0
LB           10.00 Hz
GB              0
PC           1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-3-Me], in acetone - d_6

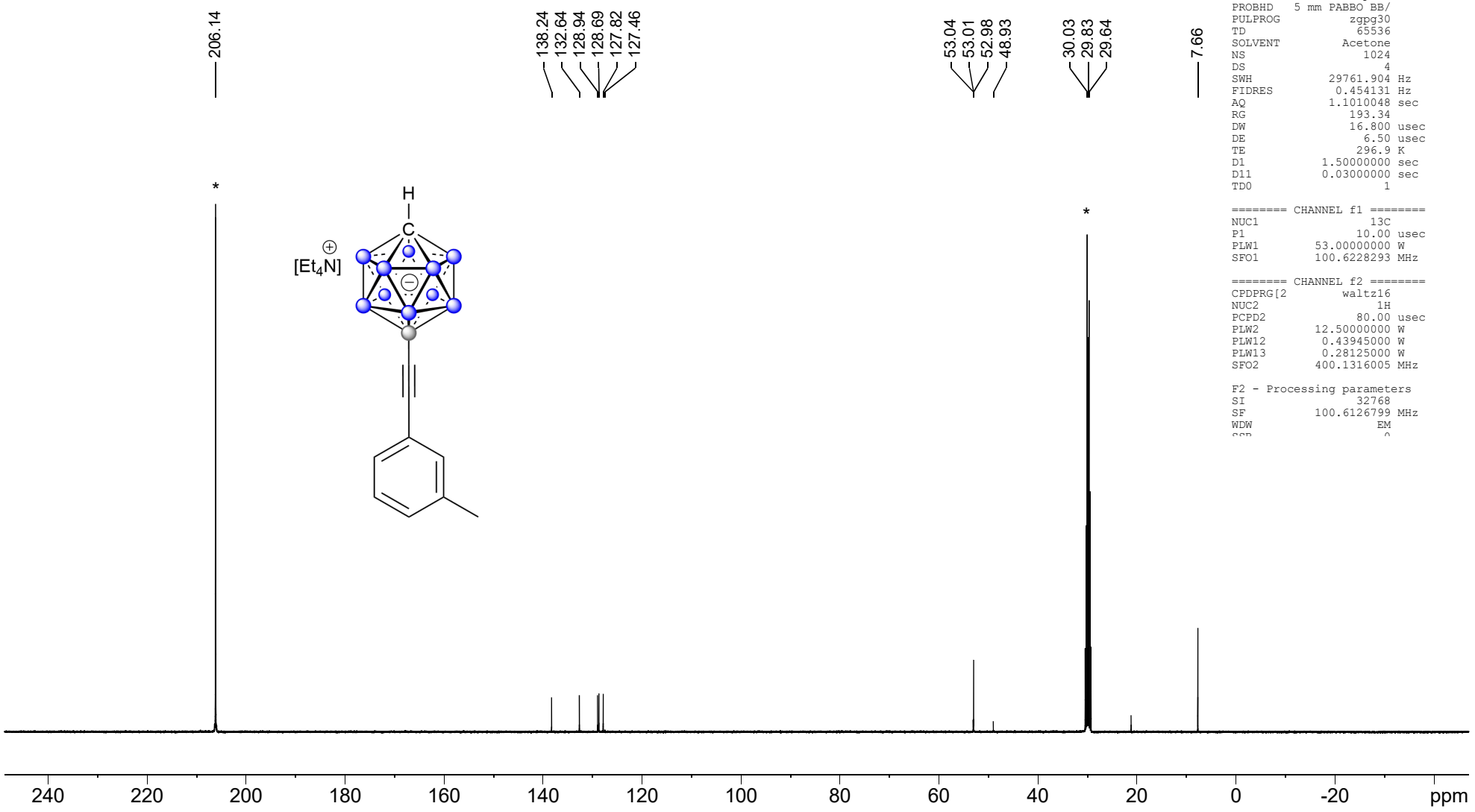
$^{11}B\{^1H\}$, 160 MHz, T = 23 C




```
Current Data Parameters
NAME      20220429-LF-234-mTol
EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
Date_            20220430
Time          7.20
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD           65536
SOLVENT            Acetone
NS             64
DS              0
SWH              32051.281 Hz
FIDRES            0.489064 Hz
AQ               1.0223616 sec
RG            203
DW           15.600 usec
DE            6.50 usec
TE           296.9 K
D1               1.00000000 sec
D11              0.03000000 sec

======== CHANNEL f1 ========
NUC1           11B
P1          13.10 usec
PLW1           95.00000000 W
SFO1           160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2            1H
PCPD2          80.00 usec
PLW2           19.00000000 W
PLW12           0.42394000 W
PLW13           0.27131999 W
SFO2           500.1325007 MHz

F2 - Processing parameters
SI           32768
SF              160.4615790 MHz
WDW              EM
SSB              0
LB           10.00 Hz
GB                        0
PC                     1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-3-Me], in acetone - d_6*

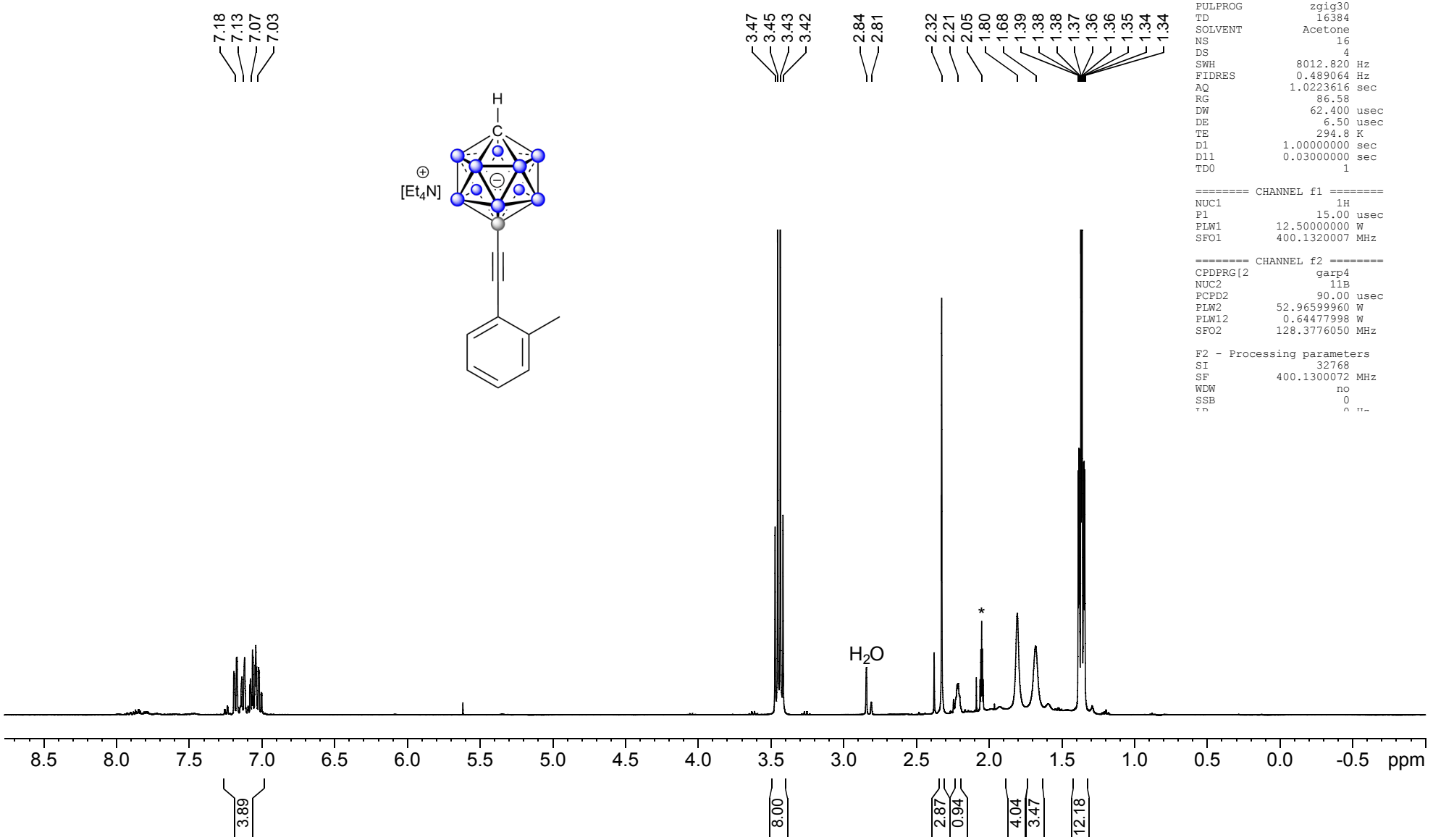
$^{13}C\{^1H\}$, 101 MHz, T = 23 C




```
Current Data Parameters
NAME      20190126-JT-1-CB11-CC-Ph-3-
EXPNO                 6
PROCNO                1

F2 - Acquisition Parameters
Date_           20190127
Time              14.46
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               296.9 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126799 MHz
WDW                  EM
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-2-Me], in acetone - d_6*

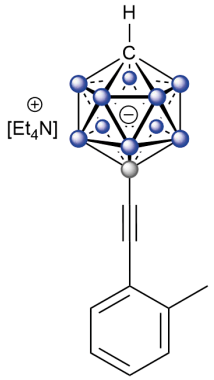
$^1H\{^{11}B\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20190219-JT-CB11-CC-Ph-2-Me
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20190221
Time              20.20
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT        Acetone
NS                  16
DS                   4
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ           1.0223616 sec
RG                86.58
DW              62.400 usec
DE               6.50 usec
TE              294.8 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1       400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2               11B
PCPD2             90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2       128.3776050 MHz

F2 - Processing parameters
SI                32768
SF           400.1300072 MHz
WDW                  no
SSB                   0
```

[Et4N][CB11H11-CC-Ph-2-Me], in acetone - d6

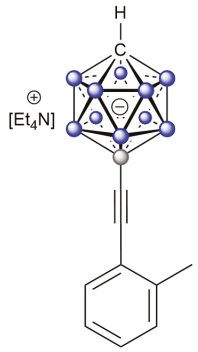
11B, 160 MHz, T = 23 C




```
Current Data Parameters
NAME      20211112-LF-217-Ph-2Me-11B-500-11455
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20211113
Time                1.15
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 64098
SOLVENT          Acetone
NS                    44
DS                     0
SWH            32051.281 Hz
FIDRES          0.500036 Hz
AQ             0.9999288 sec
RG                   203
DW                15.600 usec
DE                 6.50 usec
TE                296.9 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                 11B
P1                 13.10 usec
PLW1         95.00000000 W
SFO1         160.4615792 MHz

F2 - Processing parameters
SI                 32768
SF          160.4615790 MHz
WDW                   EM
SSB                    0
LB                 10.00 Hz
GB                     0
PC                  1.40
```

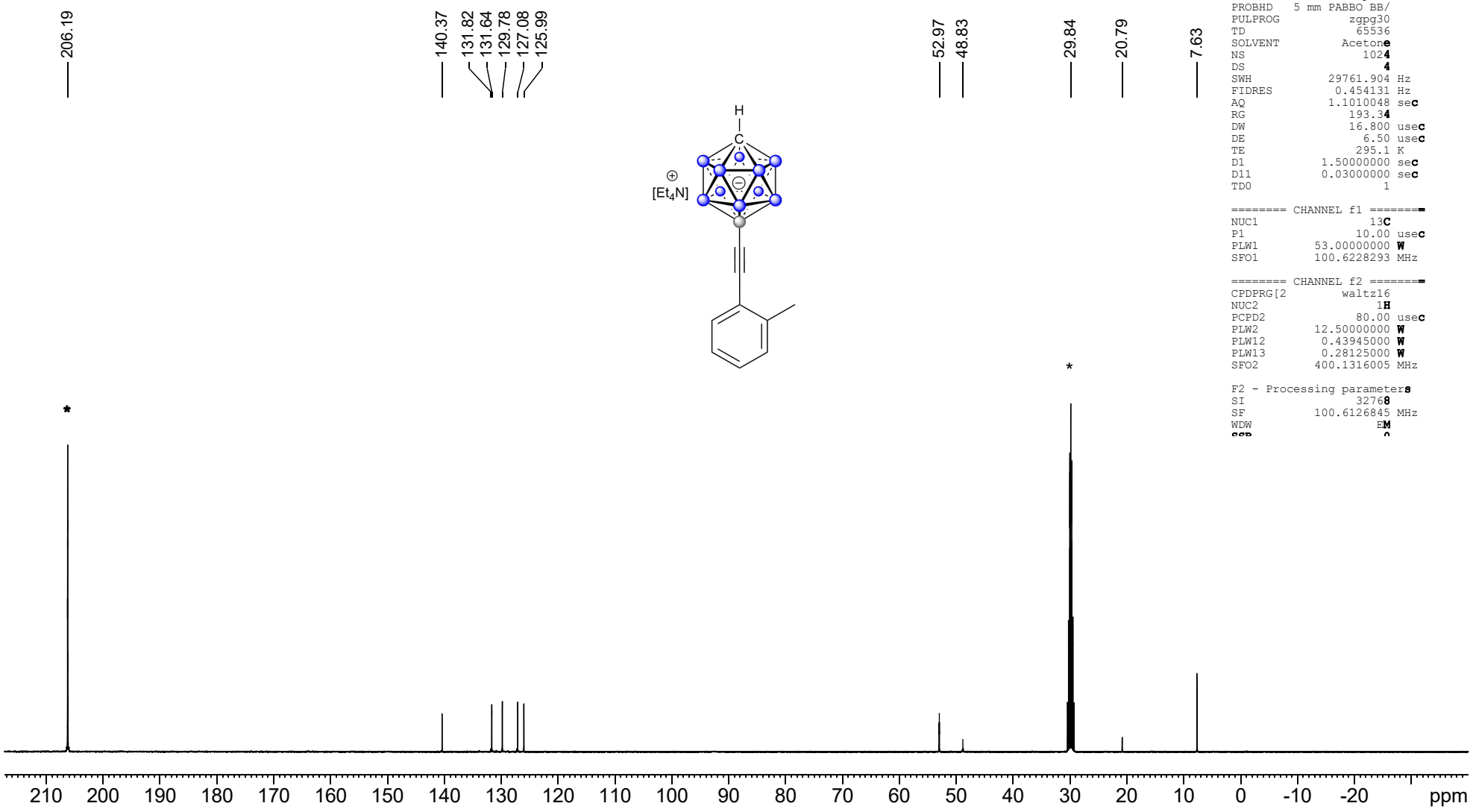
$[Et_4N][CB_{11}H_{11}\text{-}CC\text{-}Ph\text{-}2\text{-}Me]$, in acetone - d_6

$^{11}B\{^1H\}$, 160 MHz, T = 23 C




```
Current Data Parameters
NAME      20211112-LF-217-Ph-2-Me-500-11340
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20211112
Time              1.10
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                   44
DS                    0
SWH           32051.281 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                  203
DW               15.600 usec
DE                6.50 usec
TE                296.9 K
D1           1.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1                13.10 usec
PLW1        95.00000000 W
SFO1       160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2        19.00000000 W
PLW12        0.42394000 W
PLW13        0.27131999 W
SFO2       500.1325007 MHz

F2 - Processing parameters
SI                 32768
SF          160.4615790 MHz
WDW                   EM
SSB                    0
LB                15.00 Hz
GB                     0
PC                  1.40
```

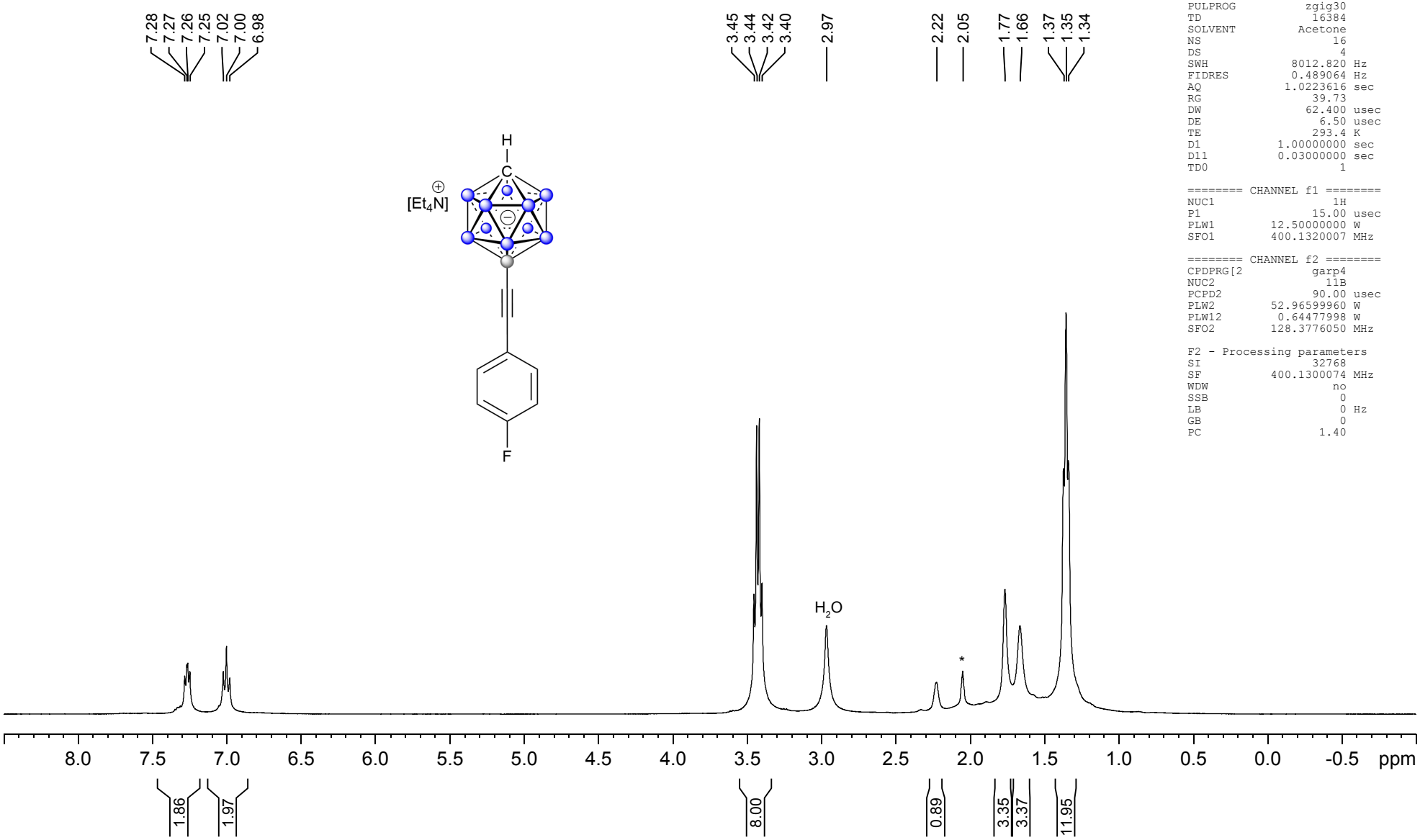
[Et_4N][$CB_{11}H_{11}$-CC-Ph-2-Me], in acetone - d_6*
$^{13}C\{^1H\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20190219-JT-CB11-CC-Ph-2-Me
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20190221
Time              21.19
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG                193.34
DW               16.800 usec
DE                6.50 usec
TE                295.1 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6126845 MHz
WDW                   EM
SSB                    0
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-4-F], in acetone - d_6^*

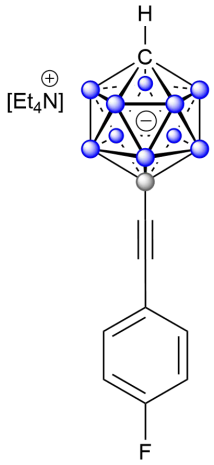
$^1H\{^{11}B\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20190127-JT-3-CC-Ph-4-F
EXPNO                           2
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20210526
Time                         4.02
INSTRUM                     spect
PROBHD    5 mm PABBO BB/
PULPROG                   zgig30
TD                         16384
SOLVENT                  Acetone
NS                            16
DS                             4
SWH                     8012.820 Hz
FIDRES                  0.489064 Hz
AQ                     1.0223616 sec
RG                         39.73
DW                        62.400 usec
DE                         6.50 usec
TE                        293.4 K
D1                   1.00000000 sec
D11                  0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        15.00 usec
PLW1                 12.50000000 W
SFO1                400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2                  garp4
NUC2                         11B
PCPD2                     90.00 usec
PLW2                 52.96599960 W
PLW12                 0.64477998 W
SFO2                128.3776050 MHz

F2 - Processing parameters
SI                         32768
SF                  400.1300074 MHz
WDW                           no
SSB                            0
LB                             0 Hz
GB                             0
PC                          1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-4-F], in acetone - d_6

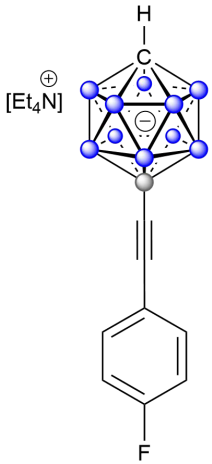
^{11}B, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20190127-JT-3-CC-Ph-4-F
EXPNO                           4
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20210526
Time                         4.15
INSTRUM                     spect
PROBHD   5 mm PABBO BB/
PULPROG                        zg
TD                          65536
SOLVENT                   Acetone
NS                              128
DS                                4
SWH                       25510.203 Hz
FIDRES                     0.389255 Hz
AQ                        1.2845056 sec
RG                           193.34
DW                           19.600 usec
DE                            6.50 usec
TE                           292.9 K
D1                     1.00000000 sec
TD0                               1

======== CHANNEL f1 ========
NUC1                           11B
P1                            9.93 usec
PLW1                  52.96599960 W
SFO1                 128.3776052 MHz

F2 - Processing parameters
SI                            32768
SF                   128.3776050 MHz
WDW                            EM
SSB                             0
LB                           10.00 Hz
GB                              0
PC                            1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-4-F], in acetone - d_6

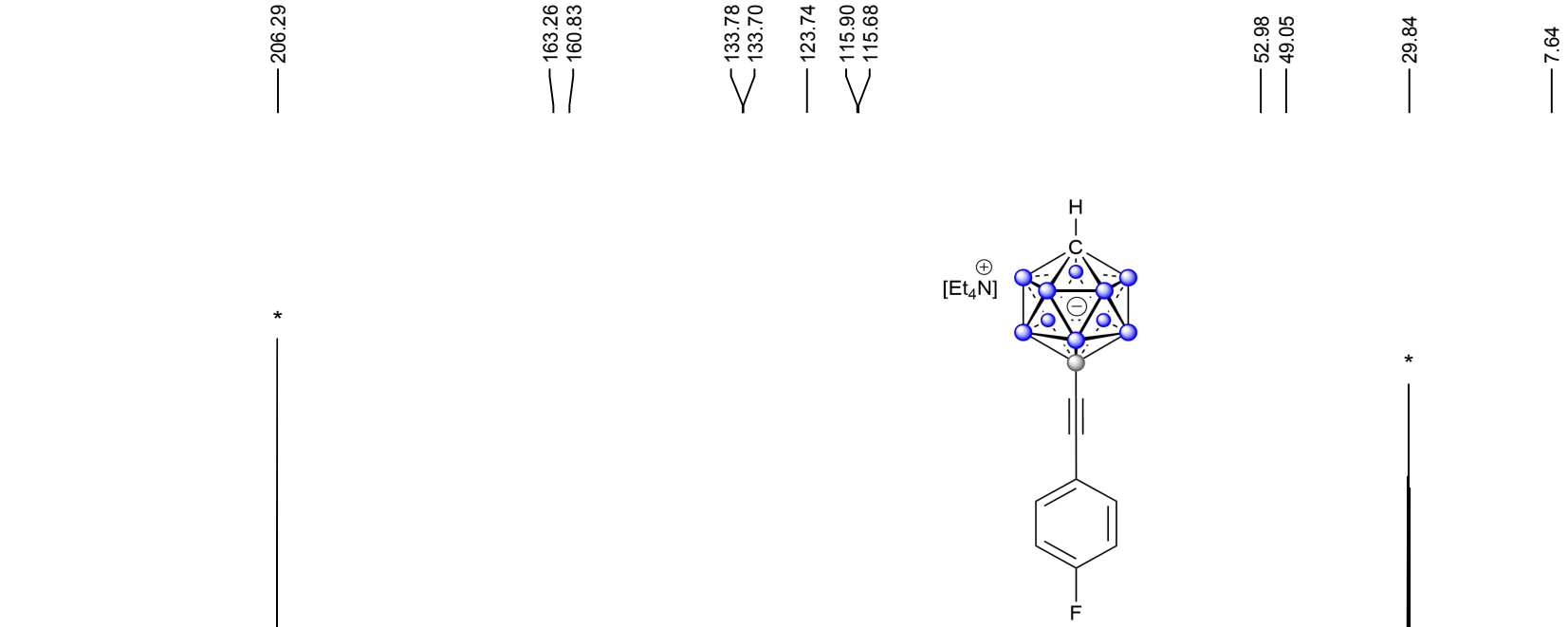
^{11}B {^1H}, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20190127-JT-3-CC-Ph-4-F
EXPNO                           3
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20210526
Time                         4.08
INSTRUM                     spect
PROBHD    5 mm PABBO BB/
PULPROG                   zgpg30
TD                         65536
SOLVENT                  Acetone
NS                             128
DS                               4
SWH                    25510.203 Hz
FIDRES                  0.389255 Hz
AQ                     1.2845056 sec
RG                        193.34
DW                        19.600 usec
DE                         6.50 usec
TE                        294.0 K
D1                    1.00000000 sec
D11                   0.03000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         11B
P1                          9.93 usec
PLW1                52.96599960 W
SFO1               128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                     80.00 usec
PLW2                12.50000000 W
PLW12                0.43945000 W
PLW13                0.28125000 W
SFO2               400.1320007 MHz

F2 - Processing parameters
SI                           32768
SF                 128.3776050 MHz
WDW                             EM
SSB                              0
LB                           10.00 Hz
GB                               0
PC                            1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-4-F], in acetone - d_6*

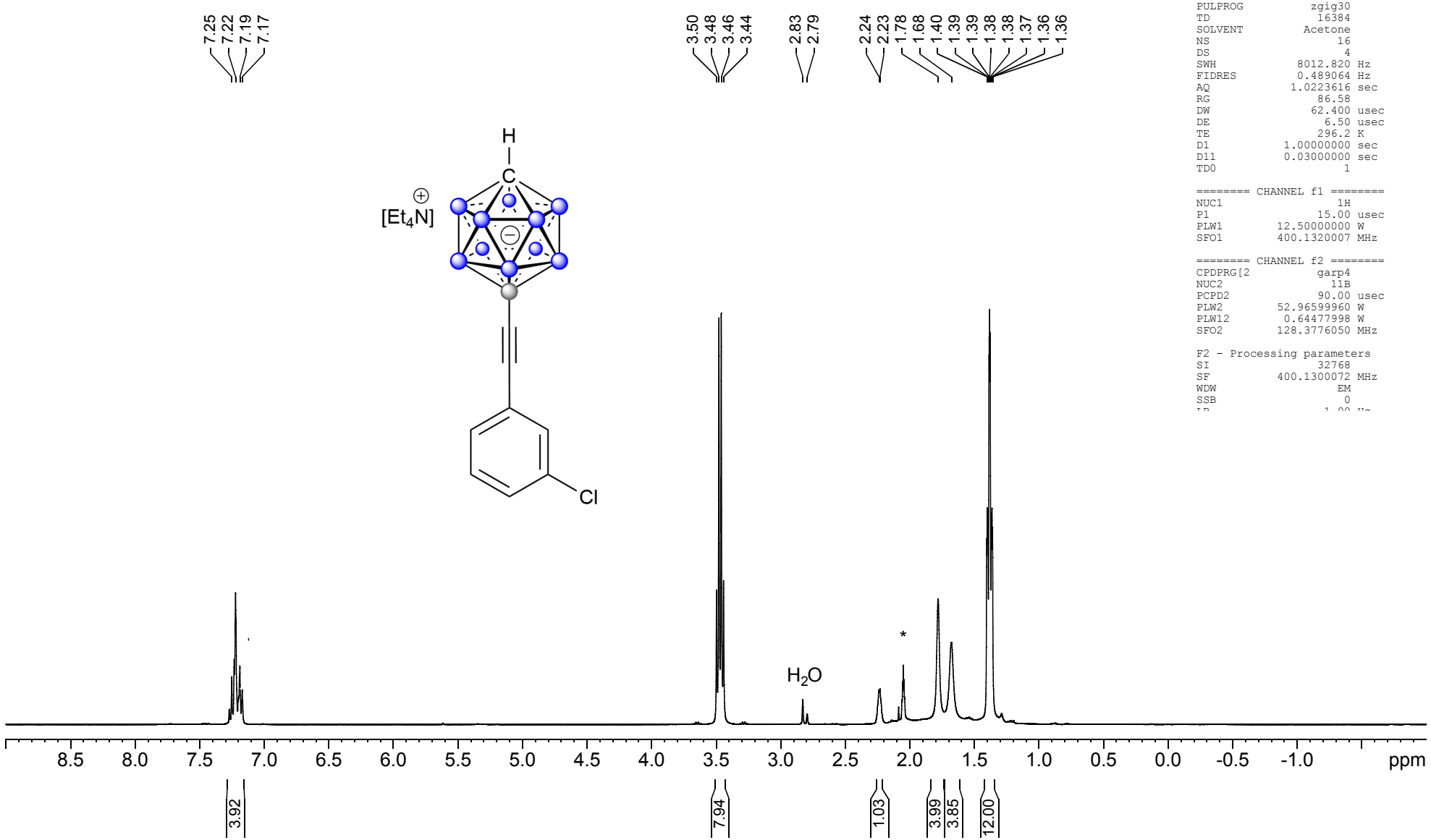
$^{13}C\{^1H\}$, 101 MHz, T = 23 C




```
Current Data Parameters
NAME      20190127-JT-3-CB11-CC-Ph-4-F
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20190128
Time              21.46
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                1024
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG              193.34
DW              16.800 usec
DE               6.50 usec
TE              296.8 K
D1          1.50000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1       53.00000000 W
SFO1      100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2       12.50000000 W
PLW12       0.43945000 W
PLW13       0.28125000 W
SFO2      400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126872 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-3-Cl], in acetone - d_6 *

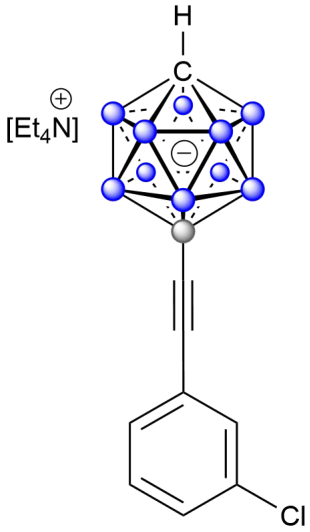
$^1H\{^{11}B\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20190121-JT-CB11-CC-Ph-3-Cl
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20190122
Time              23.30
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT         Acetone
NS                  16
DS                   4
SWH            8012.820 Hz
FIDRES            0.489064 Hz
AQ             1.0223616 sec
RG                86.58
DW                62.400 usec
DE                 6.50 usec
TE                296.2 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2             90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2         128.3776050 MHz

F2 - Processing parameters
SI                32768
SF           400.1300072 MHz
WDW                  EM
SSB                   0
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-3-Cl], in acetone - d_6

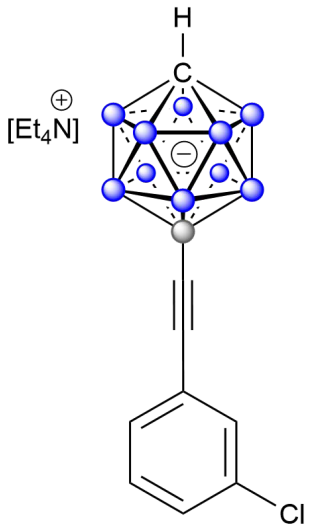
^{11}B, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20190121-JT-CB11-CC-Ph-3-Cl
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_           20190122
Time              23.41
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               297.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB                   0
LB                10.00 Hz
GB                    0
PC                 1.40
```

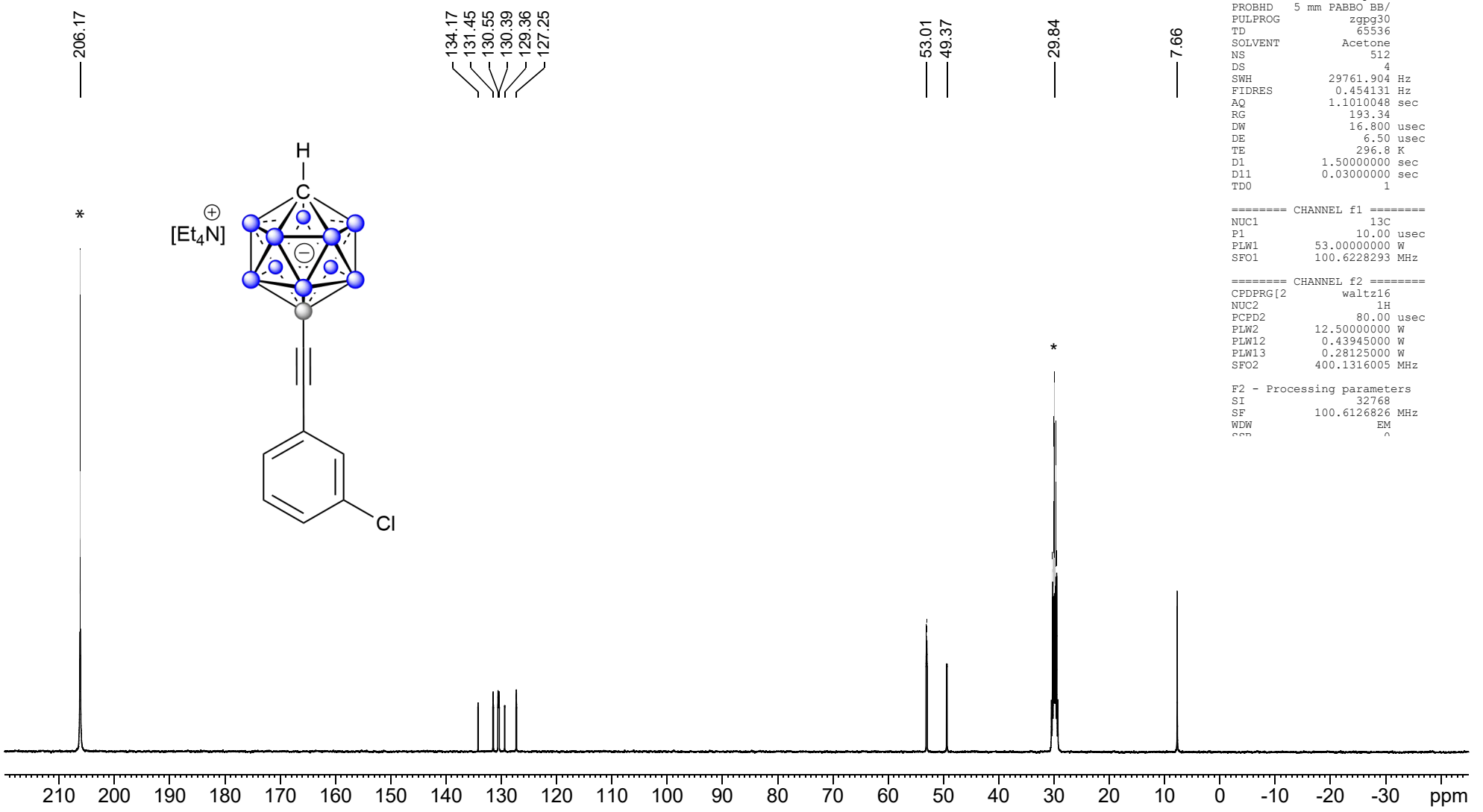
$[Et_4N][CB_{11}H_{11}$-CC-Ph-3-Cl], in acetone - d_6

$^{11}B\{^1H\}$, 128 MHz, T = 23 C



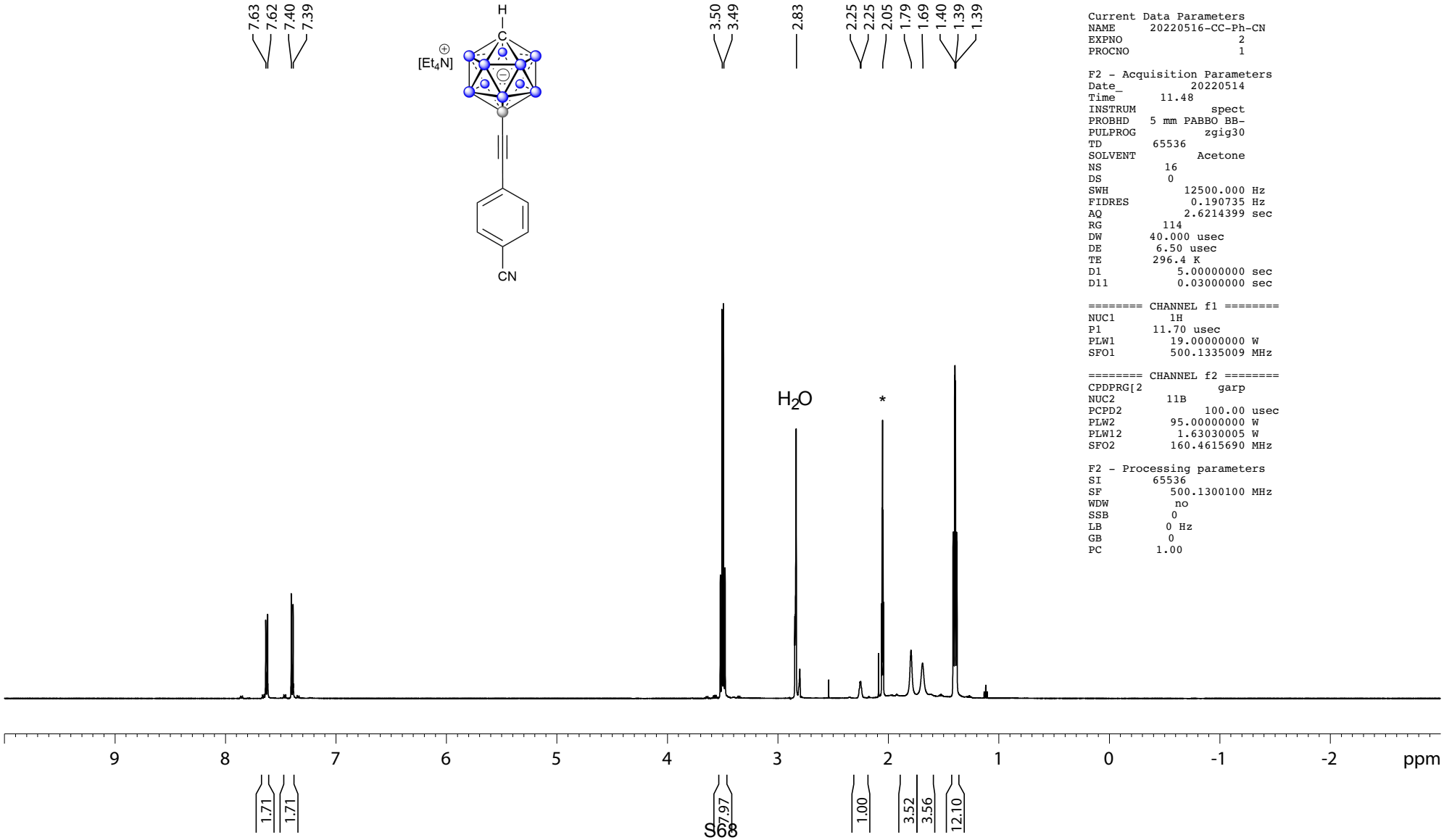

```
Current Data Parameters
NAME      20190121-JT-CB11-CC-Ph-3-Cl
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20190122
Time              23.36
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.6 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB                   0
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-3-Cl], in acetone - d_6*
$^{13}C\{^1H\}$, 101 MHz, T = 23 C



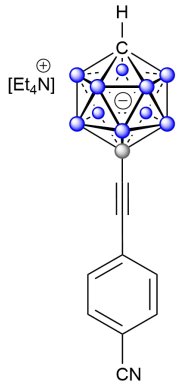

```
Current Data Parameters
NAME      20190121-JT-CB11-CC-Ph-3-Cl
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_           20190123
Time                0.06
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               296.8 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PLW1        53.00000000 W
SFO1       100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126826 MHz
WDW                  EM
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-CN], in acetone - d_6*
$^1H\{^{11}B\}$, 500 MHz, T = 23 C



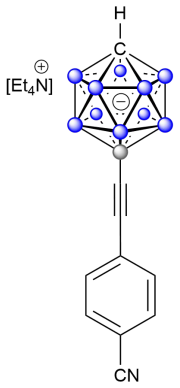

```
Current Data Parameters
NAME      20220516-CC-Ph-CN
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220514
Time       11.48
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgig30
TD         65536
SOLVENT          Acetone
NS            16
DS             0
SWH           12500.000 Hz
FIDRES          0.190735 Hz
AQ             2.6214399 sec
RG           114
DW          40.000 usec
DE           6.50 usec
TE          296.4 K
D1             5.00000000 sec
D11            0.03000000 sec

======== CHANNEL f1 ========
NUC1          1H
P1         11.70 usec
PLW1         19.00000000 W
SFO1         500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2              garp
NUC2         11B
PCPD2              100.00 usec
PLW2          95.00000000 W
PLW12          1.63030005 W
SFO2          160.4615690 MHz

F2 - Processing parameters
SI          65536
SF             500.1300100 MHz
WDW             no
SSB             0
LB            0 Hz
GB              0
PC           1.00
```

[Et$_4$N][CB $_{11}$H$_{11}$-CC-Ph-CN], in acetone - d $_6$
^{11}B, 160 MHz, T = 23 C



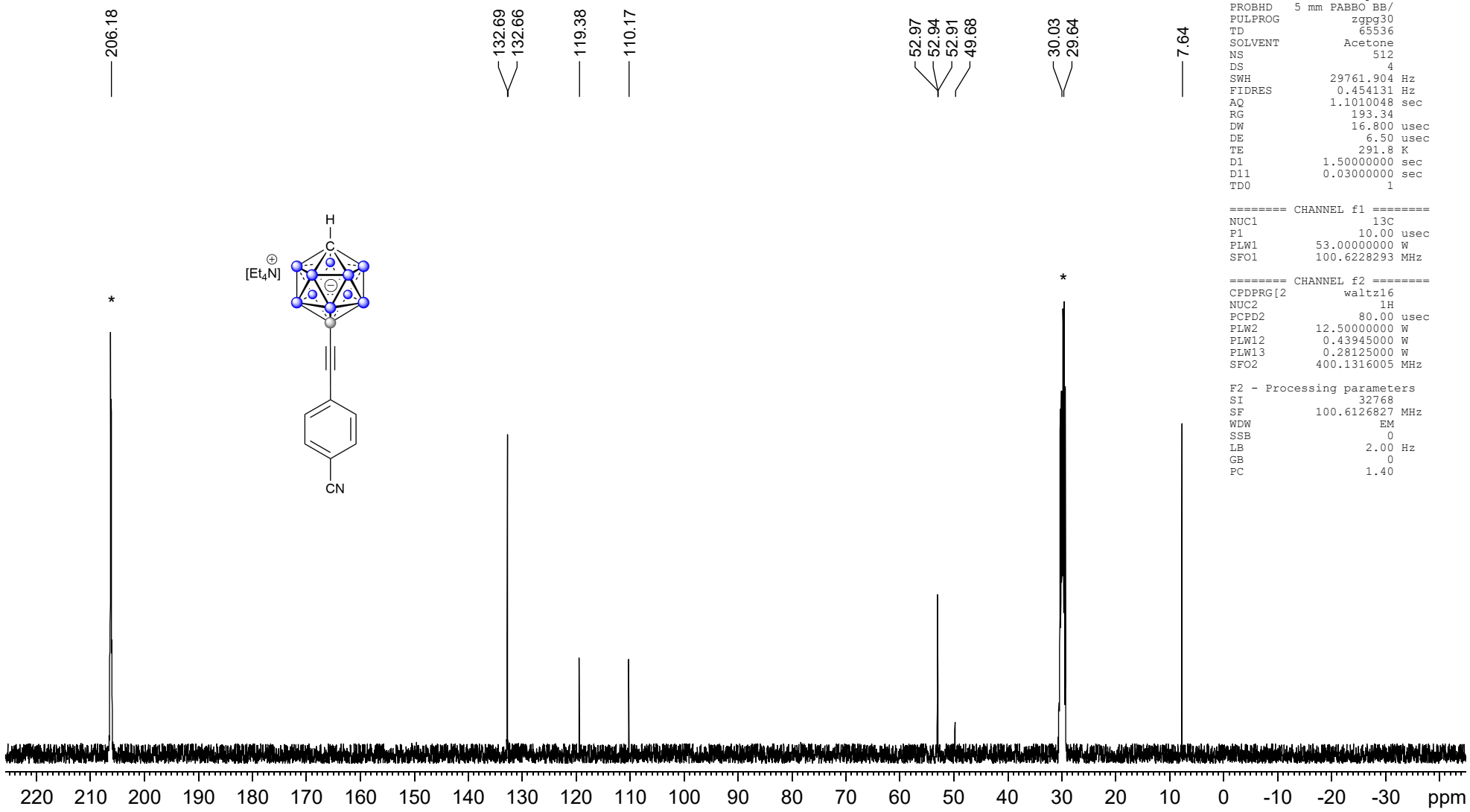

```
Current Data Parameters
NAME      20220516-CC-Ph-CN
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_          20220514
Time       11.51
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD         64098
SOLVENT            Acetone
NS           64
DS           0
SWH             32051.281 Hz
FIDRES           0.500036 Hz
AQ              0.9999288 sec
RG           203
DW          15.600 usec
DE           6.50 usec
TE          296.1 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1          11B
P1          13.10 usec
PLW1          95.00000000 W
SFO1          160.4615792 MHz

F2 - Processing parameters
SI          32768
SF             160.4615790 MHz
WDW            EM
SSB            0
LB          10.00 Hz
GB             0
PC          1.40
```

$[Et_4N][CB_{11}H_{11}\text{-}CC\text{-}Ph\text{-}CN]$, in acetone - d_6
$^{11}B\{^1H\}$, 160 MHz, T = 23 C



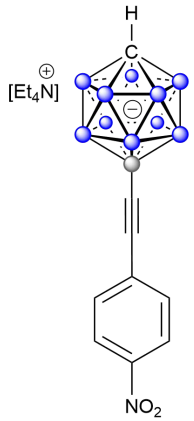

```
Current Data Parameters
NAME      20220516-CC-Ph-CN
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220514
Time       11.54
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD         65536
SOLVENT            Acetone
NS           64
DS            0
SWH             32051.281 Hz
FIDRES           0.489064 Hz
AQ               1.0223616 sec
RG           203
DW          15.600 usec
DE           6.50 usec
TE          296.6 K
D1              1.00000000 sec
D11             0.03000000 sec

======== CHANNEL f1 ========
NUC1          11B
P1          13.10 usec
PLW1          95.00000000 W
SFO1          160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2          1H
PCPD2       80.00 usec
PLW2          19.00000000 W
PLW12          0.42394000 W
PLW13          0.27131999 W
SFO2          500.1325007 MHz

F2 - Processing parameters
SI          32768
SF            160.4615790 MHz
WDW            EM
SSB           0
LB          10.00 Hz
GB                       0
PC                    1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-CN], in acetone - d_6*
$^{13}C\{^1H\}$, 101 MHz, T = 23 C



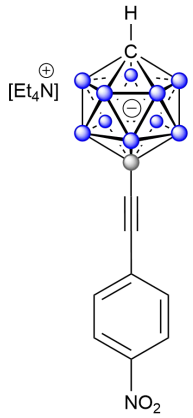

```
Current Data Parameters
NAME      20181209-JT-2-CB11-CC-Ph-CN
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_           20181210
Time              15.00
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               291.8 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126827 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-NO_2], in acetone - d_6*
$^1H\{^{11}B\}$, 500 MHz, T = 23 C



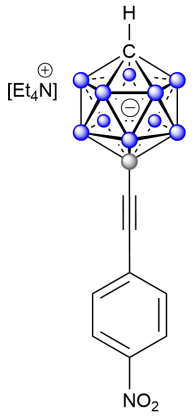

```
Current Data Parameters
NAME      20220516-CC-Ph-NO2
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_           20220514
Time       11.35
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG           zgig30
TD         65536
SOLVENT          Acetone
NS            16
DS             0
SWH              12500.000 Hz
FIDRES            0.190735 Hz
AQ               2.6214399 sec
RG             114
DW            40.000 usec
DE             6.50 usec
TE            296.2 K
D1               5.00000000 sec
D11              0.03000000 sec

======== CHANNEL f1 ========
NUC1          1H
P1           11.70 usec
PLW1           19.00000000 W
SFO1           500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2               garp
NUC2          11B
PCPD2                100.00 usec
PLW2           95.00000000 W
PLW12           1.63030005 W
SFO2           160.4615690 MHz

F2 - Processing parameters
SI          65536
SF             500.1300100 MHz
WDW             no
SSB             0
LB              0 Hz
GB              0
PC           1.00
```

[Et$_4$N][CB $_{11}$H$_{11}$-CC-Ph-NO2], in acetone - d $_6$
^{11}B, 160 MHz, T = 23 C




```
Current Data Parameters
NAME     20220516-CC-Ph-NO2
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220514
Time      11.37
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD        64098
SOLVENT          Acetone
NS          64
DS          0
SWH           32051.281 Hz
FIDRES         0.500036 Hz
AQ            0.9999288 sec
RG          203
DW        15.600 usec
DE         6.50 usec
TE        296.0 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1        11B
P1        13.10 usec
PLW1        95.00000000 W
SFO1        160.4615792 MHz

F2 - Processing parameters
SI        32768
SF          160.4615790 MHz
WDW          EM
SSB          0
LB        15.00 Hz
GB          0
PC         1.40
```

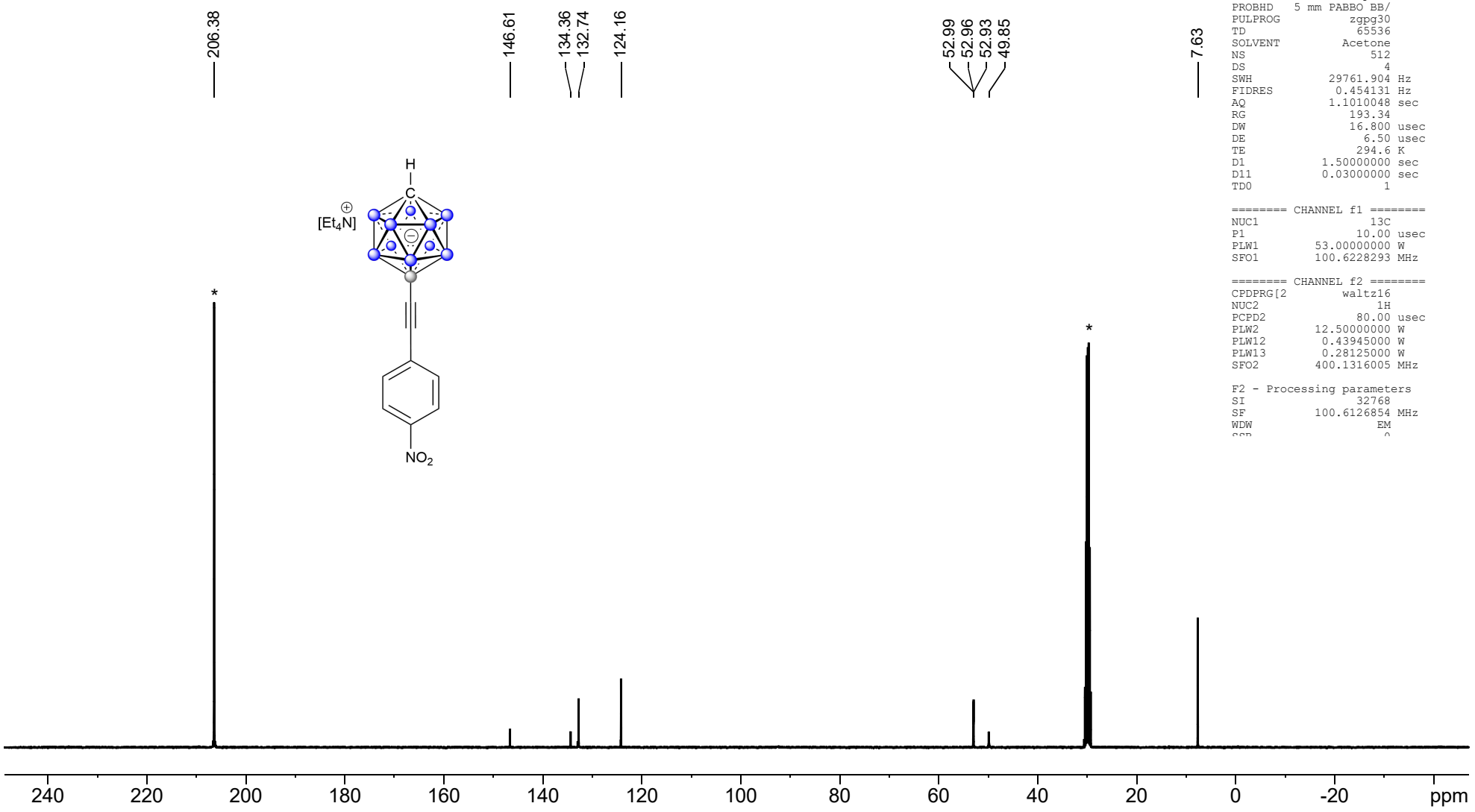
$[Et_4N][CB_{11}H_{11}$-CC-Ph-$NO_2]$, in acetone - d_6
$^{11}B\{^1H\}$, 160 MHz, T = 23 C




```
Current Data Parameters
NAME      20220516-CC-Ph-NO2
EXPNO                     4
PROCNO                    1

F2 - Acquisition Parameters
Date_           20220514
Time       11.41
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD            65536
SOLVENT          Acetone
NS              64
DS               0
SWH            32051.281 Hz
FIDRES           0.489064 Hz
AQ             1.0223616 sec
RG              203
DW            15.600 usec
DE             6.50 usec
TE             296.5 K
D1               1.00000000 sec
D11              0.03000000 sec

======== CHANNEL f1 ========
NUC1         11B
P1          13.10 usec
PLW1           95.00000000 W
SFO1           160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2          1H
PCPD2        80.00 usec
PLW2          19.00000000 W
PLW12          0.42394000 W
PLW13          0.27131999 W
SFO2          500.1325007 MHz

F2 - Processing parameters
SI          32768
SF             160.4615790 MHz
WDW             EM
SSB             0
LB          15.00 Hz
GB               0
PC           1.40
```

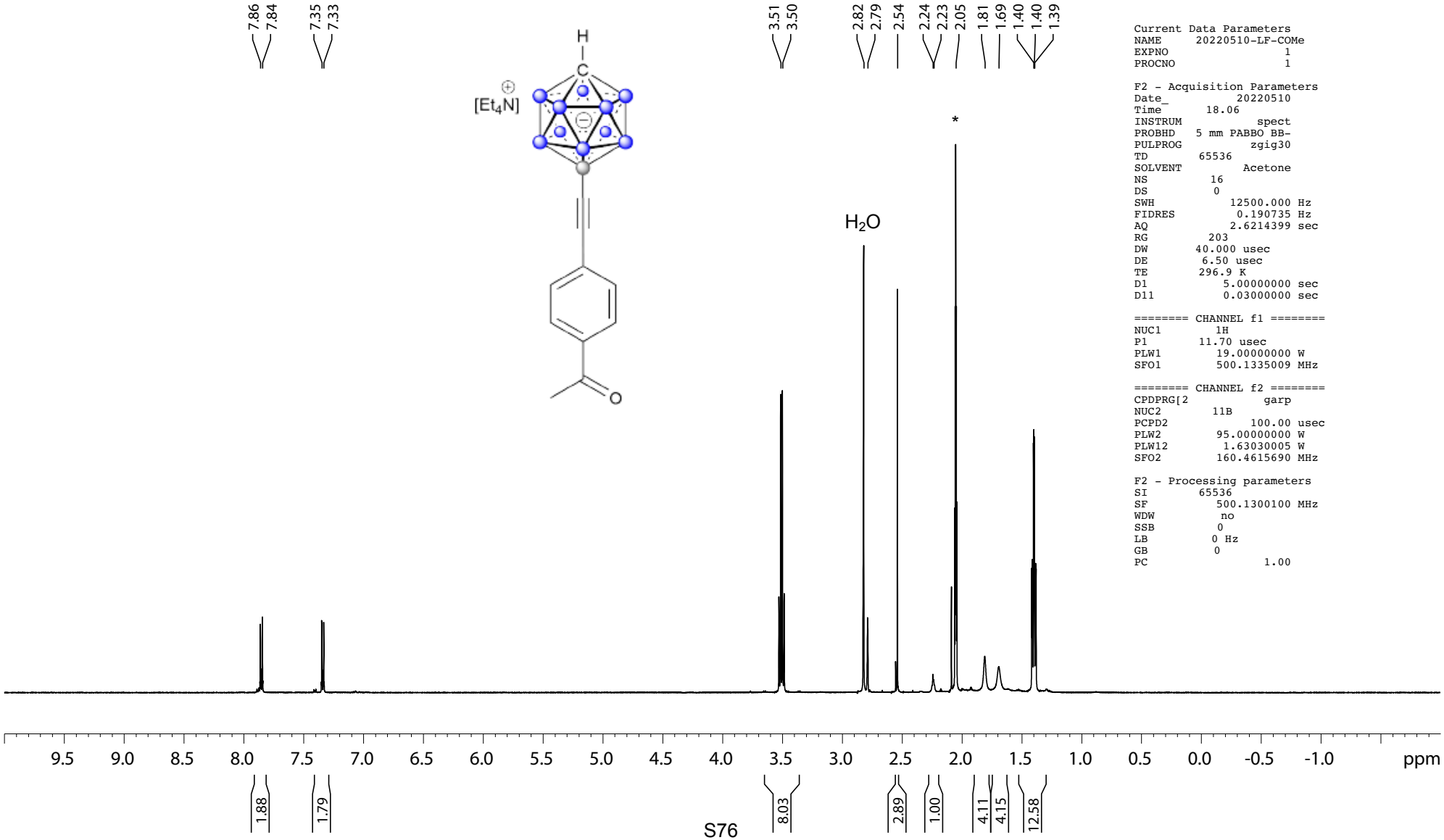
$[Et_4N][CB_{11}H_{11}$-CC-Ph-$NO_2]$, in acetone - d_6*

$^{13}C\{^1H\}$, 101 MHz, T = 23 C




```
Current Data Parameters
NAME      20190221-JT-2-CB11-CC-Ph-NO
EXPNO                8
PROCNO               1

F2 - Acquisition Parameters
Date_          20190222
Time             21.14
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT       Acetone
NS                512
DS                  4
SWH         29761.904 Hz
FIDRES       0.454131 Hz
AQ          1.1010048 sec
RG             193.34
DW             16.800 usec
DE              6.50 usec
TE             294.6 K
D1          1.50000000 sec
D11         0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
NUC1               13C
P1               10.00 usec
PLW1        53.00000000 W
SFO1       100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2       waltz16
NUC2               1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI               32768
SF          100.6126854 MHz
WDW                 EM
SSB                 0
```

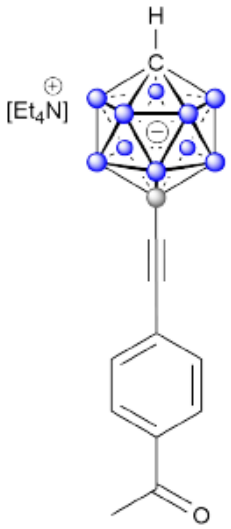
$[Et_4N][CB_{11}H_{11}$-CC-Ph-4-COMe], in acetone - d_6*
$^1H\{^{11}B\}$, 500 MHz, T = 23 C




```
Current Data Parameters
NAME      20220510-LF-COMe
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220510
Time       18.06
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zgig30
TD          65536
SOLVENT           Acetone
NS            16
DS             0
SWH            12500.000 Hz
FIDRES           0.190735 Hz
AQ             2.6214399 sec
RG           203
DW          40.000 usec
DE           6.50 usec
TE          296.9 K
D1              5.00000000 sec
D11             0.03000000 sec

======== CHANNEL f1 ========
NUC1          1H
P1           11.70 usec
PLW1           19.00000000 W
SFO1           500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2               garp
NUC2          11B
PCPD2               100.00 usec
PLW2           95.00000000 W
PLW12           1.63030005 W
SFO2           160.4615690 MHz

F2 - Processing parameters
SI          65536
SF             500.1300100 MHz
WDW             no
SSB            0
LB            0 Hz
GB             0
PC                     1.00
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-4-COMe], in acetone - d_6

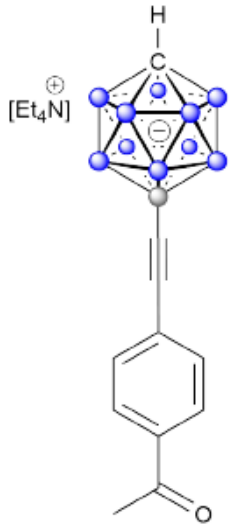
^{11}B, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20220425-CT-CC-COMe
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_           20220425
Time       0.05
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD         64098
SOLVENT             Acetone
NS           64
DS           0
SWH             32051.281 Hz
FIDRES           0.500036 Hz
AQ              0.9999288 sec
RG           203
DW          15.600 usec
DE          6.50 usec
TE          296.9 K
D1             1.00000000 sec

======== CHANNEL f1 ========
NUC1         11B
P1          13.10 usec
PLW1           95.00000000 W
SFO1           160.4615792 MHz

F2 - Processing parameters
SI          32768
SF            160.4615790 MHz
WDW            EM
SSB           0
LB          10.00 Hz
GB            0
PC          1.40
```

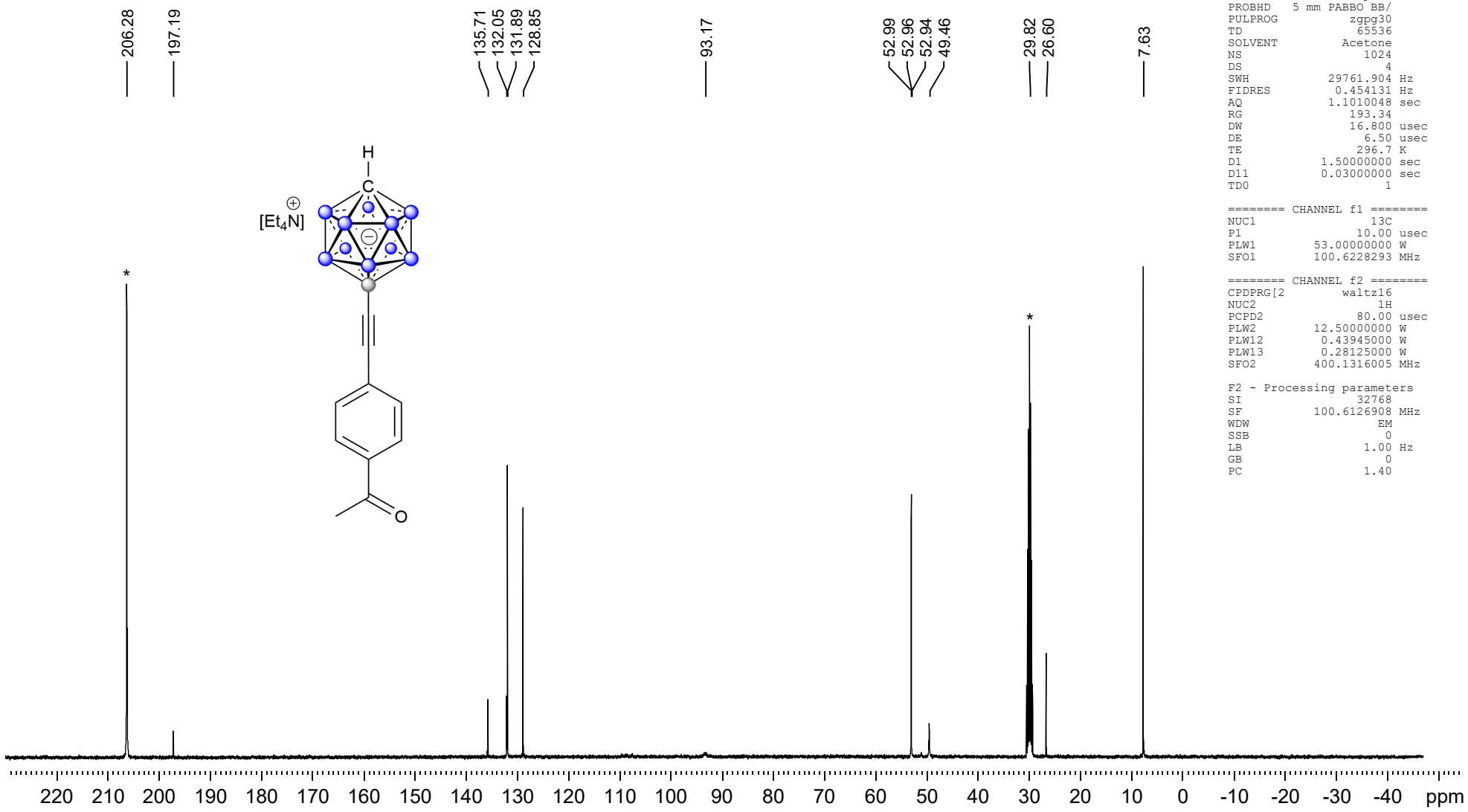
$[Et_4N][CB_{11}H_{11}$-CC-Ph-4-COMe], in acetone - d_6

$^{11}B\{^1H\}$, 128 MHz, T = 23 C



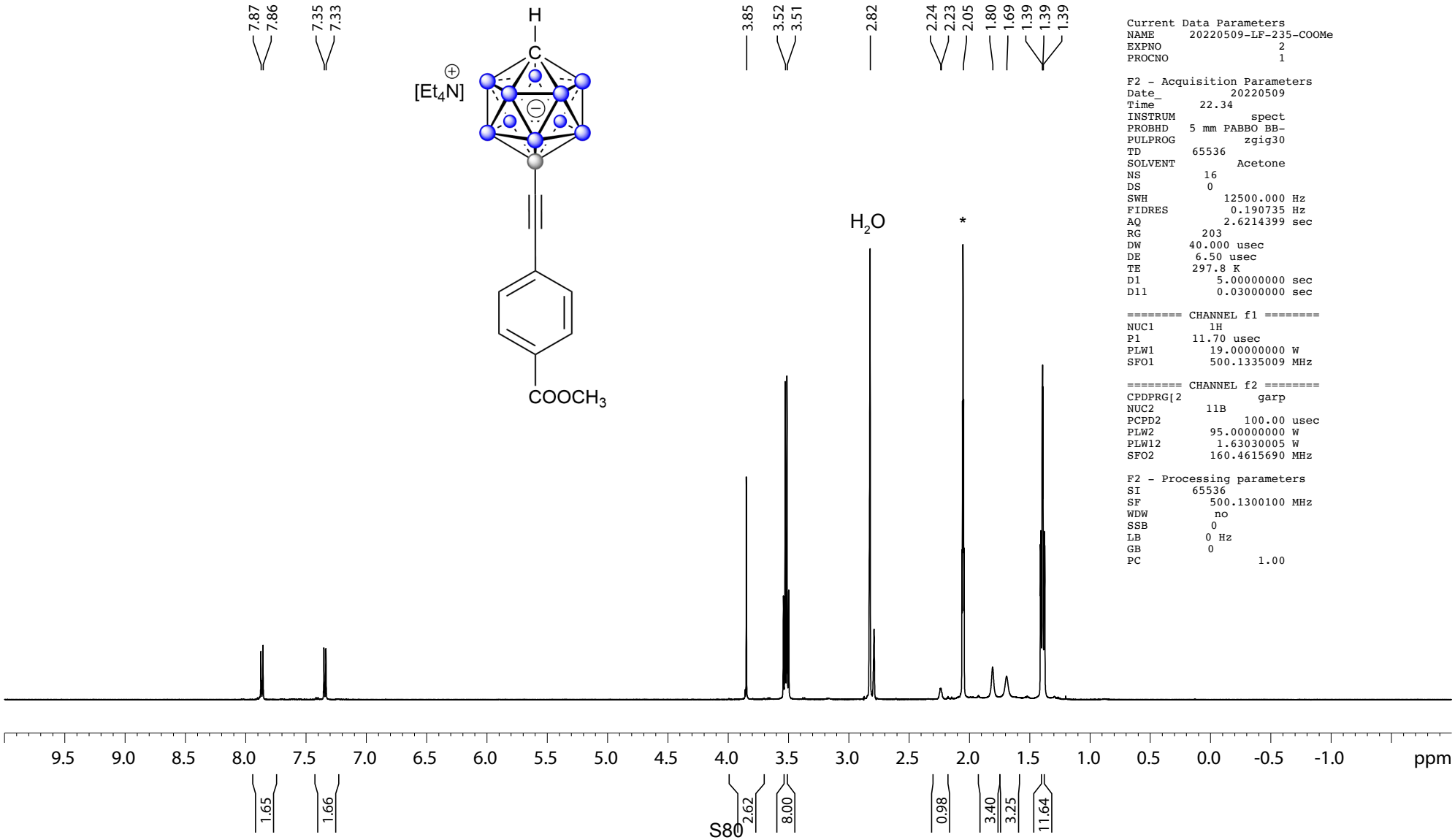

```
Current Data Parameters
NAME      20220425-CT-CC-COMe
EXPNO                      4
PROCNO                     1

F2 - Acquisition Parameters
Date_              20220425
Time          0.08
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD           65536
SOLVENT            Acetone
NS             64
DS              0
SWH               32051.281 Hz
FIDRES             0.489064 Hz
AQ                1.0223616 sec
RG              203
DW             15.600 usec
DE              6.50 usec
TE             296.9 K
D1                1.00000000 sec
D11               0.03000000 sec

======== CHANNEL f1 ========
NUC1            11B
P1             13.10 usec
PLW1              95.00000000 W
SFO1              160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2            1H
PCPD2          80.00 usec
PLW2              19.00000000 W
PLW12              0.42394000 W
PLW13              0.27131999 W
SFO2              500.1325007 MHz

F2 - Processing parameters
SI             32768
SF                160.4615790 MHz
WDW                EM
SSB                0
LB             10.00 Hz
GB                        0
PC                     1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-4-COMe], in acetone - d_6*
$^{13}C\{^1H\}$, 101 MHz, T = 23 C




```
Current Data Parameters
NAME      20190127-JT-4-CB11-CC-Ph-CO-Me
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20190128
Time              22.37
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               296.7 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126908 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

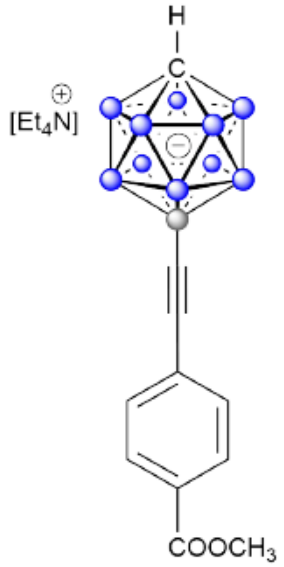
[Et4N] [CB11H11-CC-Ph-4-COOMe], in acetone - d6*
$^1H\{^{11}B\}$, 500 MHz, T = 23 C




```
Current Data Parameters
NAME      20220509-LF-235-COOMe
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_           20220509
Time       22.34
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG          zgig30
TD         65536
SOLVENT          Acetone
NS            16
DS             0
SWH            12500.000 Hz
FIDRES           0.190735 Hz
AQ             2.6214399 sec
RG           203
DW         40.000 usec
DE          6.50 usec
TE         297.8 K
D1             5.00000000 sec
D11            0.03000000 sec

======== CHANNEL f1 ========
NUC1          1H
P1         11.70 usec
PLW1         19.00000000 W
SFO1         500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2              garp
NUC2         11B
PCPD2              100.00 usec
PLW2          95.00000000 W
PLW12          1.63030005 W
SFO2          160.4615690 MHz

F2 - Processing parameters
SI         65536
SF            500.1300100 MHz
WDW            no
SSB            0
LB             0 Hz
GB             0
PC                    1.00
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-4-COOMe], in acetone - d_6

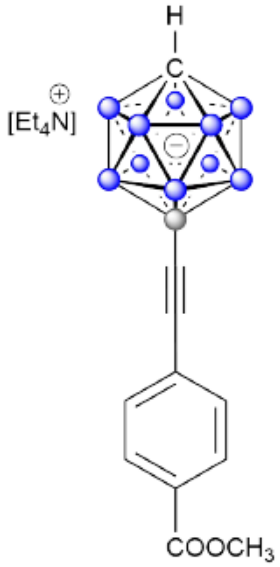
^{11}B, 160 MHz, T = 23 C




```
Current Data Parameters
NAME      20220509-LF-235-COOMe
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20220509
Time       22.37
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD        64098
SOLVENT           Acetone
NS           64
DS           0
SWH             32051.281 Hz
FIDRES           0.500036 Hz
AQ              0.9999288 sec
RG           203
DW          15.600 usec
DE           6.50 usec
TE          297.5 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1         11B
P1          13.10 usec
PLW1           95.00000000 W
SFO1           160.4615792 MHz

F2 - Processing parameters
SI          32768
SF             160.4615790 MHz
WDW            EM
SSB            0
LB          20.00 Hz
GB             0
PC          1.40
```

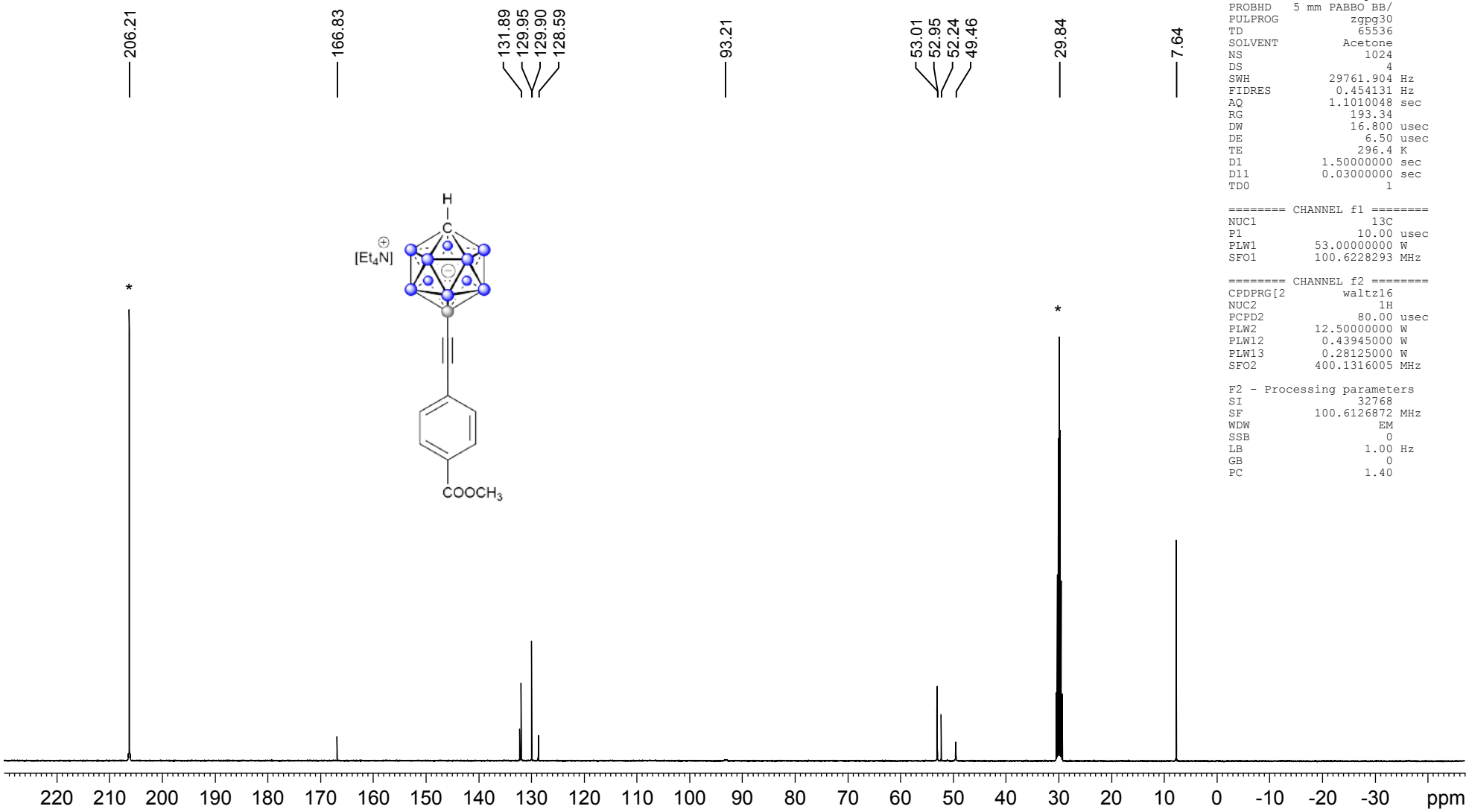
$[Et_4N][CB_{11}H_{11}$-CC-Ph-4-COOMe], in acetone - d_6

$^{11}B\{^1H\}$, 160 MHz, T = 23 C



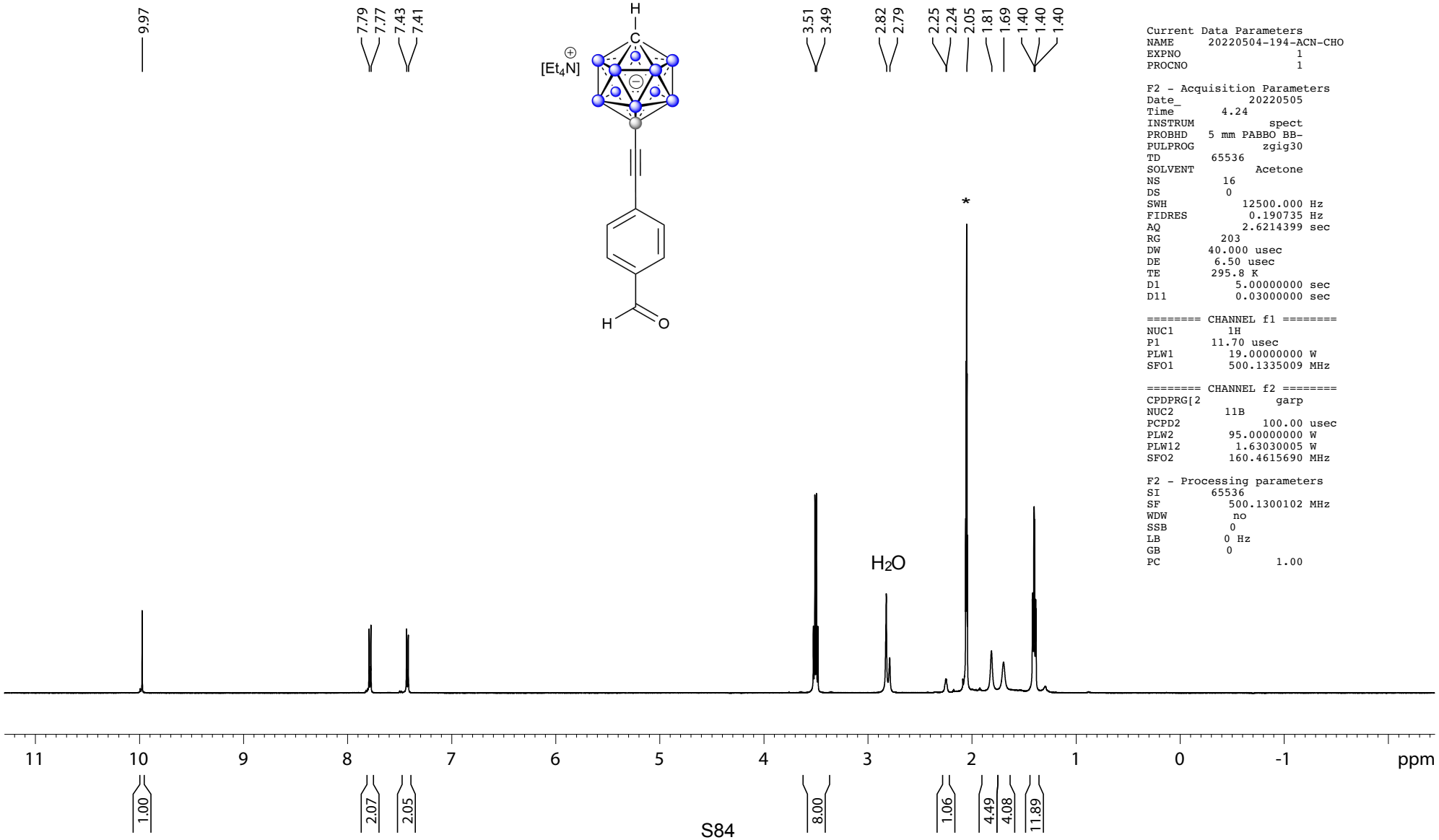

```
Current Data Parameters
NAME      20220509-LF-235-COOMe
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220509
Time       22.40
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD         65536
SOLVENT           Acetone
NS           64
DS           0
SWH             32051.281 Hz
FIDRES           0.489064 Hz
AQ              1.0223616 sec
RG           203
DW          15.600 usec
DE           6.50 usec
TE          298.0 K
D1             1.00000000 sec
D11            0.03000000 sec

======== CHANNEL f1 ========
NUC1         11B
P1          13.10 usec
PLW1           95.00000000 W
SFO1           160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2          1H
PCPD2       80.00 usec
PLW2          19.00000000 W
PLW12          0.42394000 W
PLW13          0.27131999 W
SFO2          500.1325007 MHz

F2 - Processing parameters
SI          32768
SF             160.4615790 MHz
WDW            EM
SSB            0
LB          10.00 Hz
GB                      0
PC                   1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-4-COOMe], in acetone - d_6*
$^{13}C\{^1H\}$, 128 MHz, T = 23 C



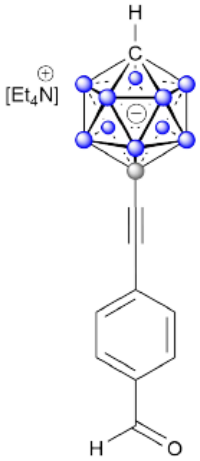

```
Current Data Parameters
NAME      20190128-JT-2-CB11-CC-Ph-4-COOMe
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20190129
Time              11.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                1024
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG              193.34
DW              16.800 usec
DE               6.50 usec
TE              296.4 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6126872 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-CHO], in acetone - d_6*
$^1H\{^{11}B\}$, 500 MHz, T = 23 C



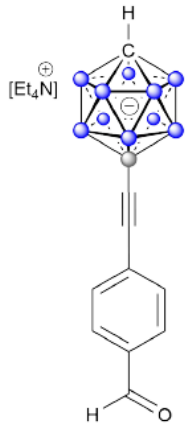

```
Current Data Parameters
NAME      20220504-194-ACN-CHO
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_           20220505
Time       4.24
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgig30
TD             65536
SOLVENT           Acetone
NS               16
DS                0
SWH            12500.000 Hz
FIDRES           0.190735 Hz
AQ             2.6214399 sec
RG              203
DW             40.000 usec
DE              6.50 usec
TE             295.8 K
D1                5.00000000 sec
D11               0.03000000 sec

======== CHANNEL f1 ========
NUC1         1H
P1          11.70 usec
PLW1          19.00000000 W
SFO1          500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2                garp
NUC2         11B
PCPD2                100.00 usec
PLW2          95.00000000 W
PLW12          1.63030005 W
SFO2          160.4615690 MHz

F2 - Processing parameters
SI          65536
SF            500.1300102 MHz
WDW            no
SSB            0
LB             0 Hz
GB             0
PC                    1.00
```

$[Et_4N][CB_{11}H_{11}$-CC-Ph-CHO], in acetone - d_6
^{11}B, 160 MHz, T = 23 C




```
Current Data Parameters
NAME      20220504-194-ACN-CHO
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_           20220505
Time       4.26
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD        64098
SOLVENT          Acetone
NS           64
DS            0
SWH          32051.281 Hz
FIDRES         0.500036 Hz
AQ           0.9999288 sec
RG          203
DW         15.600 usec
DE          6.50 usec
TE         295.1 K
D1            1.00000000 sec

======== CHANNEL f1 ========
NUC1         11B
P1         13.10 usec
PLW1          95.00000000 W
SFO1          160.4615792 MHz

F2 - Processing parameters
SI         32768
SF            160.4615790 MHz
WDW            EM
SSB            0
LB         20.00 Hz
GB            0
PC         1.40
```

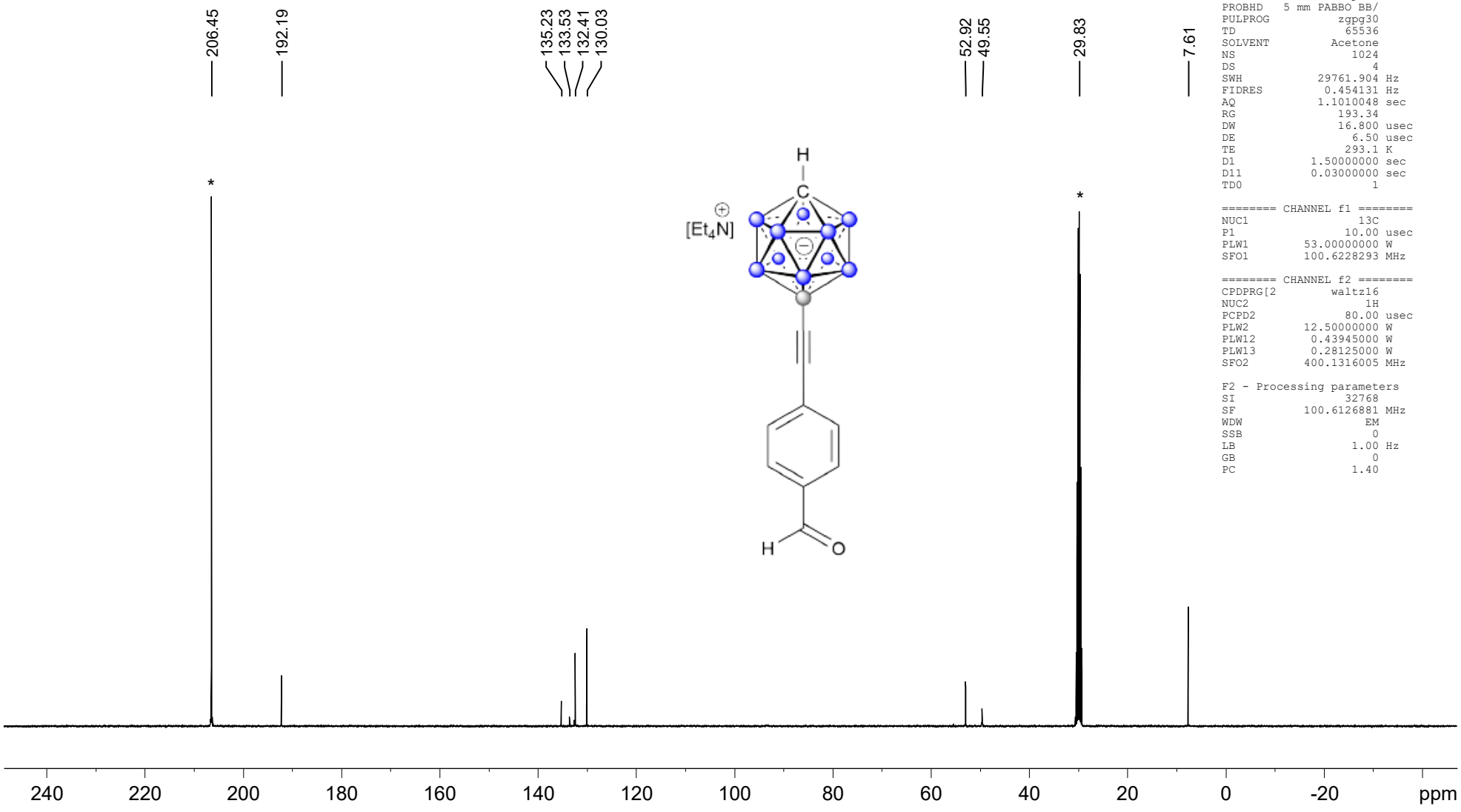
$[Et_4N][CB_{11}H_{11}$-CC-Ph-CHO], in acetone - d_6
$^{11}B\{^1H\}$, 160 MHz, T = 23 C




```
Current Data Parameters
NAME      20220504-194-ACN-CHO
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_            20220505
Time       4.30
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD         65536
SOLVENT            Acetone
NS           64
DS            0
SWH              32051.281 Hz
FIDRES            0.489064 Hz
AQ               1.0223616 sec
RG             203
DW            15.600 usec
DE             6.50 usec
TE            295.4 K
D1               1.00000000 sec
D11              0.03000000 sec

======== CHANNEL f1 ========
NUC1           11B
P1            13.10 usec
PLW1             95.00000000 W
SFO1             160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2           1H
PCPD2         80.00 usec
PLW2           19.00000000 W
PLW12           0.42394000 W
PLW13           0.27131999 W
SFO2           500.1325007 MHz

F2 - Processing parameters
SI          32768
SF             160.4615790 MHz
WDW             EM
SSB             0
LB          20.00 Hz
GB                       0
PC                    1.40
```

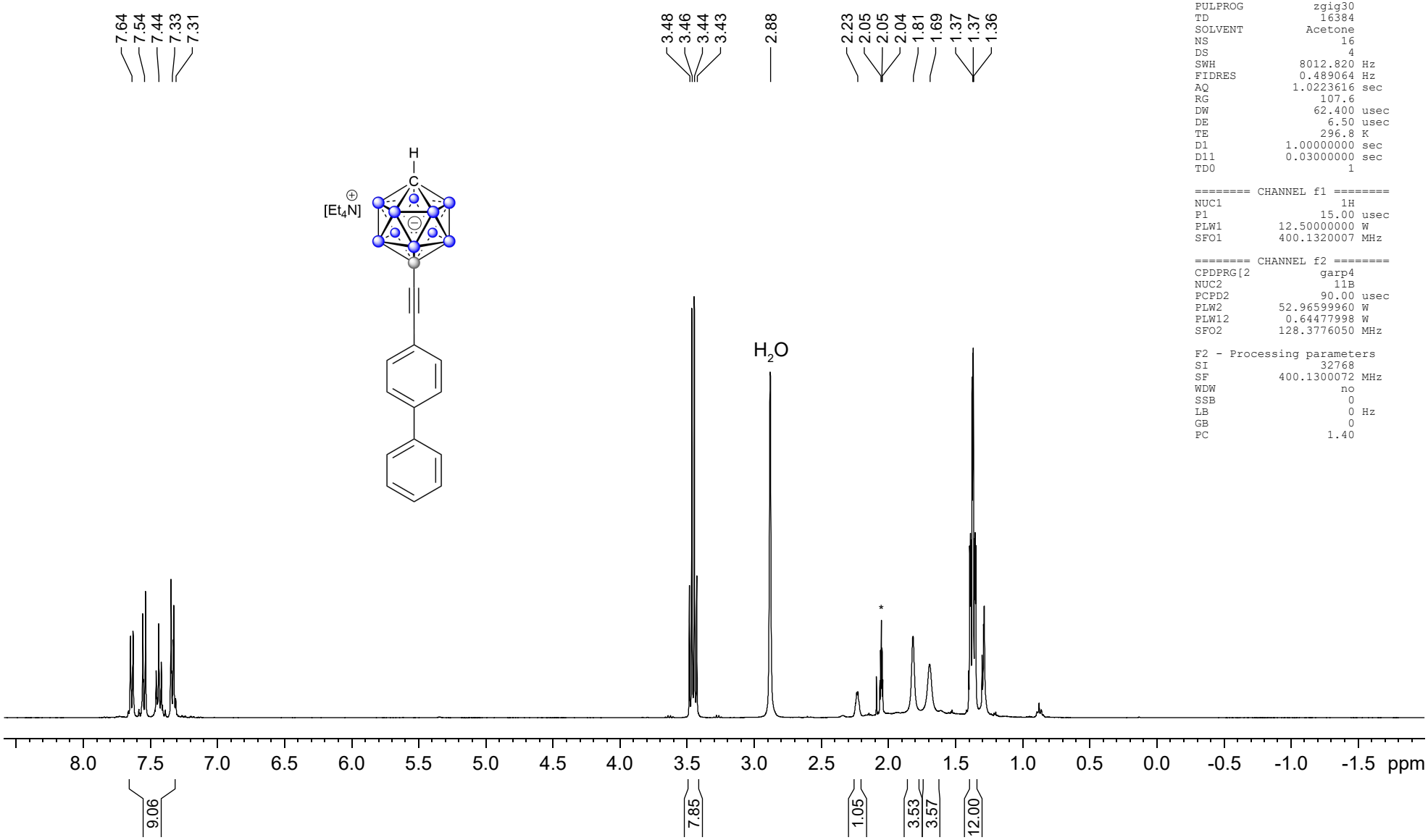
$[Et_4N][CB_{11}H_{11}$-CC-Ph-CHO], in acetone - d_6*

$^{13}C\{^1H\}$, 101 MHz, T = 23 C




```
Current Data Parameters
NAME      20210623-LF-194-CHO
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20210624
Time                 11.55
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                    1024
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                  16.800 usec
DE                   6.50 usec
TE                  293.1 K
D1               1.50000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PLW1          53.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PLW2          12.50000000 W
PLW12          0.43945000 W
PLW13          0.28125000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6126881 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

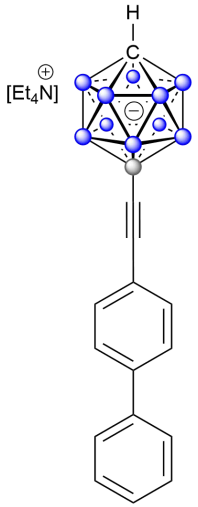
$[Et_4N][CB_{11}H_{11}$-CC-diphenyl], in acetone - d_6*
$^1H\{^{11}B\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20190128-JT-1-CB11-CC-D-Ph
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_           20190129
Time               6.21
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES        0.489064 Hz
AQ           1.0223616 sec
RG                107.6
DW               62.400 usec
DE                6.50 usec
TE               296.8 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2                11B
PCPD2             90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2         128.3776050 MHz

F2 - Processing parameters
SI                32768
SF           400.1300072 MHz
WDW                  no
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-diphenyl], in acetone - d_6

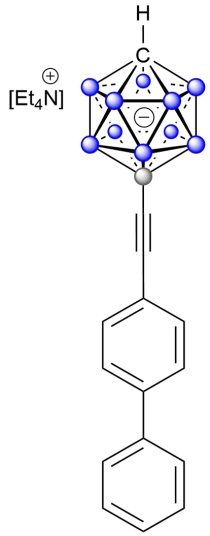
^{11}B, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20190128-JT-1-CB11-CC-D-Ph
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20190129
Time               6.33
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               295.8 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB                   0
LB                10.00 Hz
GB                    0
PC                 1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-diphenyl], in acetone - d_6

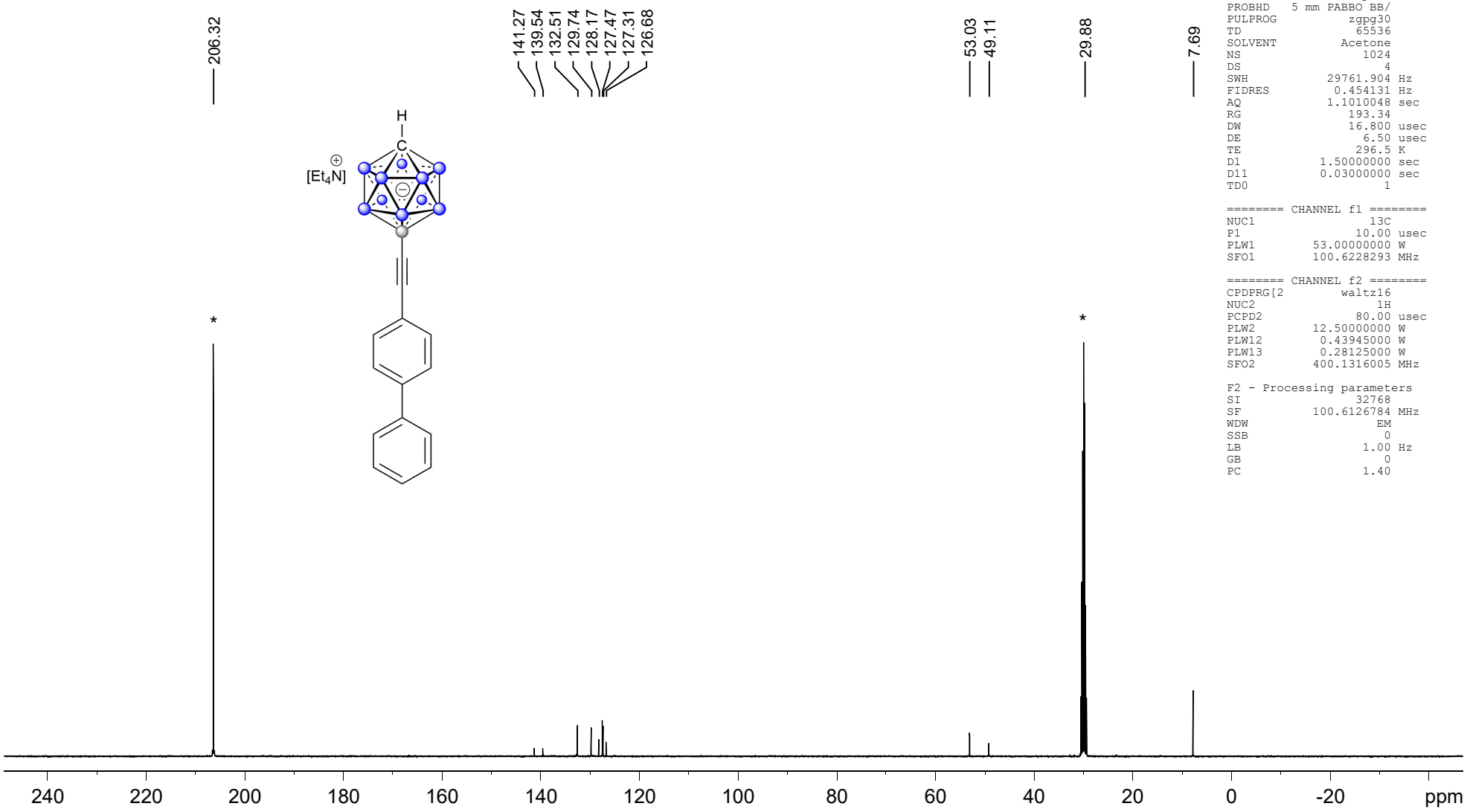
$^{11}B\{^1H\}$, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20190128-JT-1-CB11-CC-D-Ph
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20190129
Time               6.28
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.8 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1        128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF          128.3776050 MHz
WDW                   EM
SSB                   0
LB                10.00 Hz
GB                    0
PC                 1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-diphenyl], in acetone - d_6*

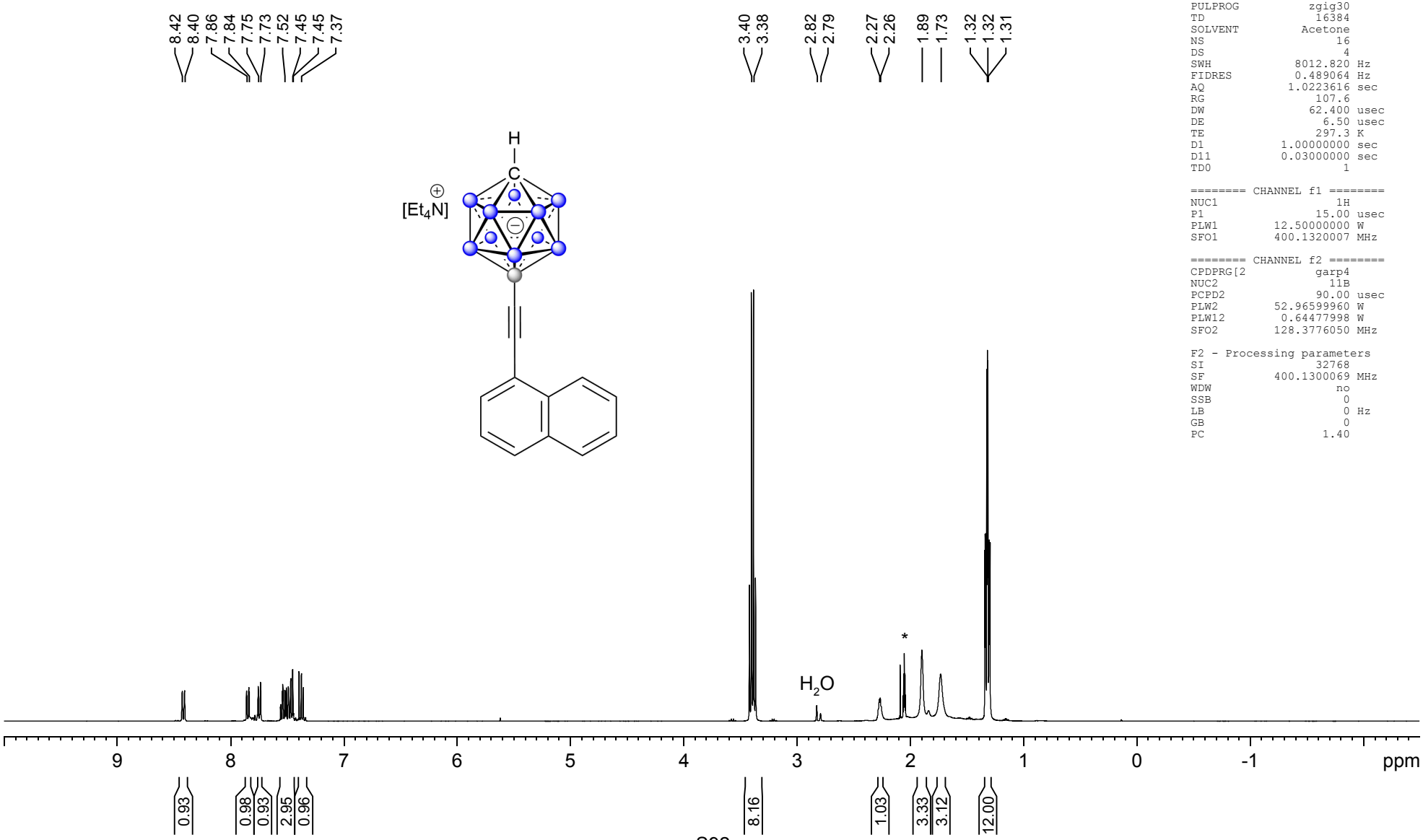
$^{13}C\{^1H\}$, 101 MHz, T = 23 C




```
Current Data Parameters
NAME      20190128-JT-1-CB11-CC-D-Ph
EXPNO                5
PROCNO               1

F2 - Acquisition Parameters
Date_           20190129
Time                7.20
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG                193.34
DW              16.800 usec
DE               6.50 usec
TE              296.5 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6126784 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-naphthalene], in acetone - d_6 *

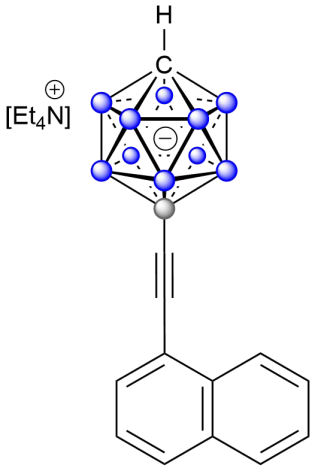
$^1H\{^{11}B\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20190127-JT-1-CB11-CC-Np
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20190128
Time              15.53
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT        Acetone
NS                  16
DS                   4
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                107.6
DW               62.400 usec
DE                6.50 usec
TE               297.3 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2                11B
PCPD2             90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                32768
SF          400.1300069 MHz
WDW                  no
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-naphthalene], in acetone - d_6

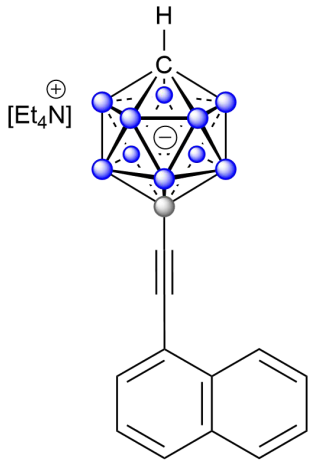
^{11}B, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20190127-JT-1-CB11-CC-Np
EXPNO                4
PROCNO               1

F2 - Acquisition Parameters
Date_          20190128
Time             16.05
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              296.1 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                 32768
SF          128.3776050 MHz
WDW                EM
SSB                 0
LB                10.00 Hz
GB                  0
PC                1.40
```

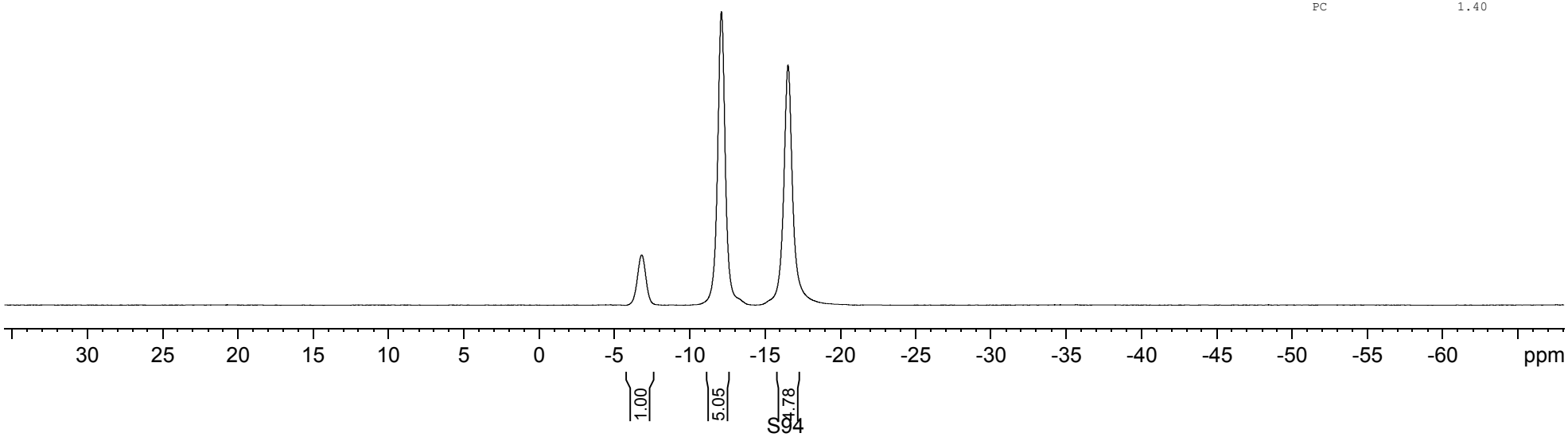
$[Et_4N][CB_{11}H_{11}$-CC-naphthalene], in acetone - d_6

$^{11}B\{^1H\}$, 128 MHz, T = 23 C



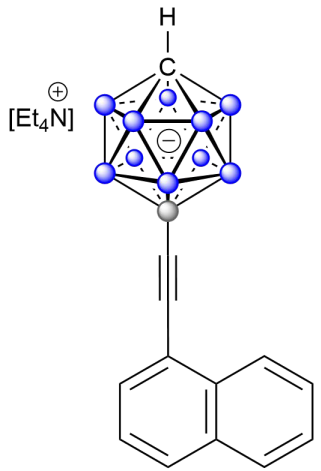
-6.84 -12.14 -16.56

```
Current Data Parameters
NAME      20190127-JT-1-CB11-CC-Np
EXPNO                3
PROCNO               1

F2 - Acquisition Parameters
Date_          20190128
Time              15.59
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ            1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              297.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               11B
P1                9.93 usec
PLW1        52.96599960 W
SFO1        128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2               1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1320007 MHz

F2 - Processing parameters
SI               32768
SF          128.3776050 MHz
WDW                EM
SSB                 0
LB              10.00 Hz
GB                  0
PC               1.40
```



$[Et_4N][CB_{11}H_{11}$-CC-naphthalene], in acetone - d_6*

$^{13}C\{^1H\}$, 101 MHz, T = 23 C

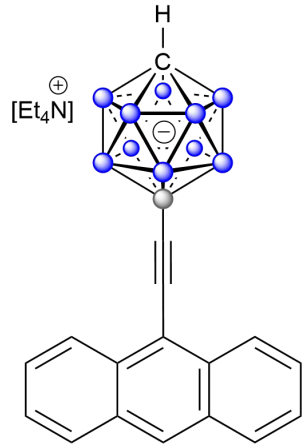


206.17 | 134.61 | 134.24 | 129.39 | 128.84 | 127.69 | 127.45 | 126.91 | 126.20 | 52.96 | 49.16 | 30.03 | 29.84 | 29.65 | 7.61

```
Current Data Parameters
NAME      20190127-JT-1-CB11-CC-Np
EXPNO                5
PROCNO               1

F2 - Acquisition Parameters
Date_          20190128
Time             16.52
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT       Acetone
NS               1024
DS                  4
SWH          29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG               193.34
DW              16.800 usec
DE               6.50 usec
TE              298.0 K
D1          1.50000000 sec
D11         0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
NUC1               13C
P1               10.00 usec
PLW1        53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2               1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI              32768
SF          100.6126827 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

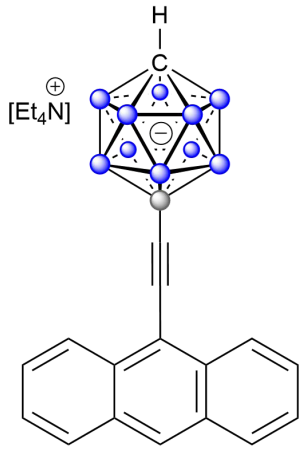
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 ppm

[Et_4N][$CB_{11}H_{11}$-CC-anthracene], in acetone - d_6*
^1H {^{11}B}, 128 MHz, T = 23 C



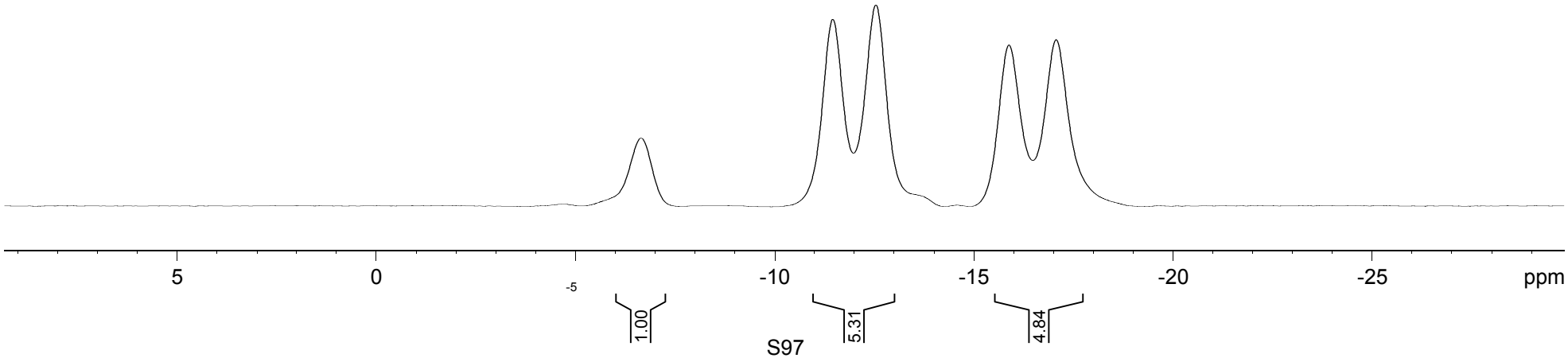

```
Current Data Parameters
NAME      20190128-JT-4-CB11-CC-En
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_           20190129
Time              23.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             1.0223616 sec
RG                107.6
DW               62.400 usec
DE                6.50 usec
TE               297.1 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2             90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2         128.3776050 MHz

F2 - Processing parameters
SI                32768
SF           400.1300072 MHz
WDW                  no
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-anthracene], in acetone - d_6
^{11}B, 128 MHz, T = 23 C

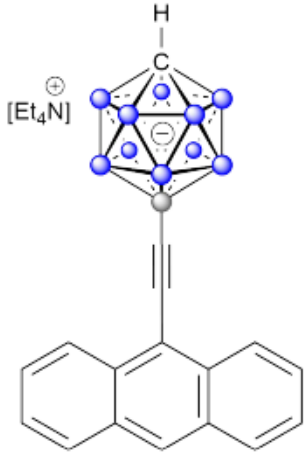


-6.66
-11.47
-12.56
-15.90
-17.08

```
Current Data Parameters
NAME      20190128-JT-4-CB11-CC-En
EXPNO                4
PROCNO               1

F2 - Acquisition Parameters
Date_          20190129
Time              23.46
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              296.0 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               11B
P1                9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI                32768
SF         128.3776050 MHz
WDW                EM
SSB                 0
LB                10.00 Hz
GB                  0
PC                1.40
```

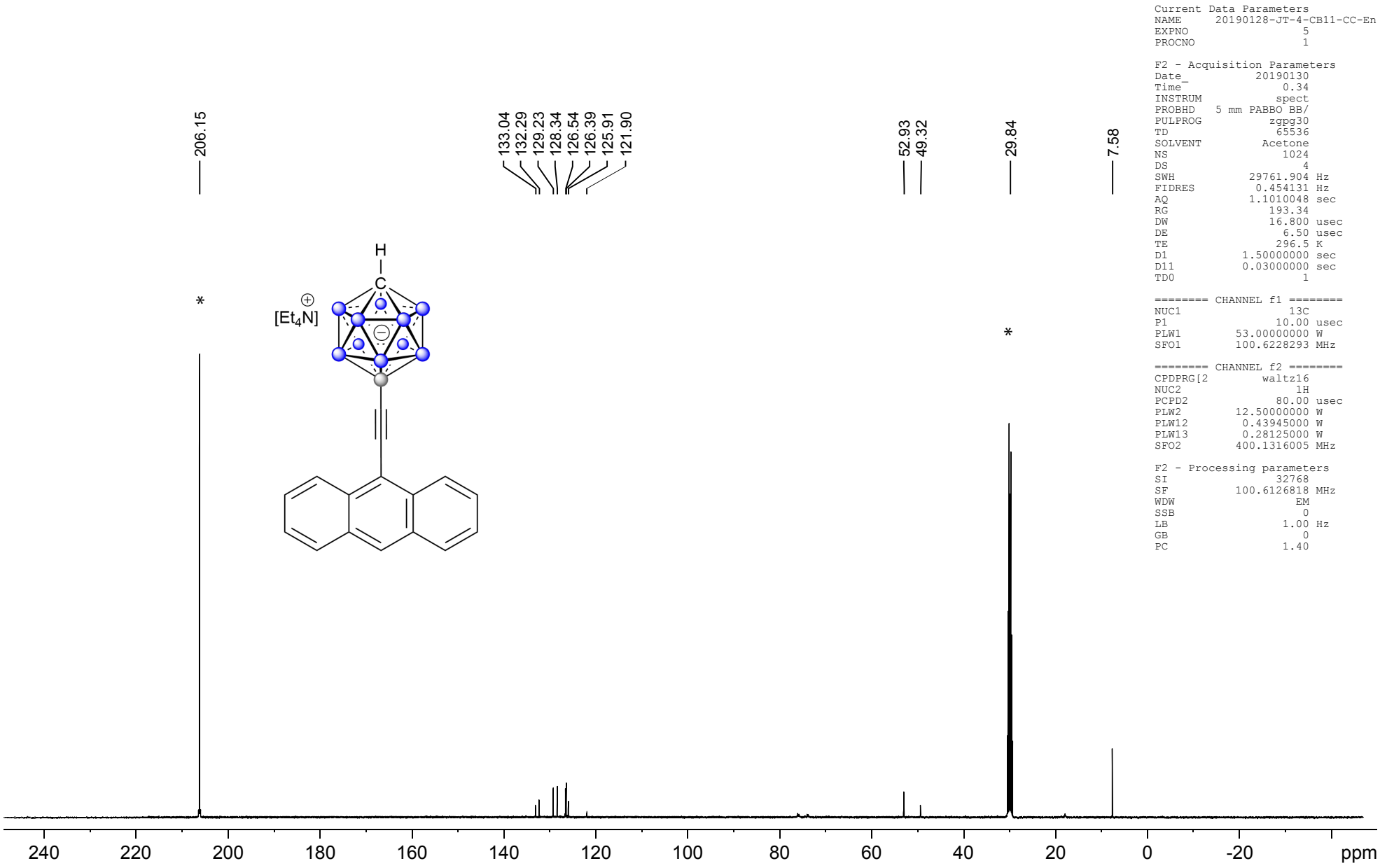


$[Et_4N][CB_{11}H_{11}$-CC-anthracene], in acetone - d_6
^{11}B {^1H}, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20190128-JT-4-CB11-CC-En
EXPNO                3
PROCNO               1

F2 - Acquisition Parameters
Date_          20190129
Time              23.41
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW              19.600 usec
DE                6.50 usec
TE               297.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF          128.3776050 MHz
WDW                 EM
SSB                  0
LB                10.00 Hz
GB                   0
PC                1.40
```

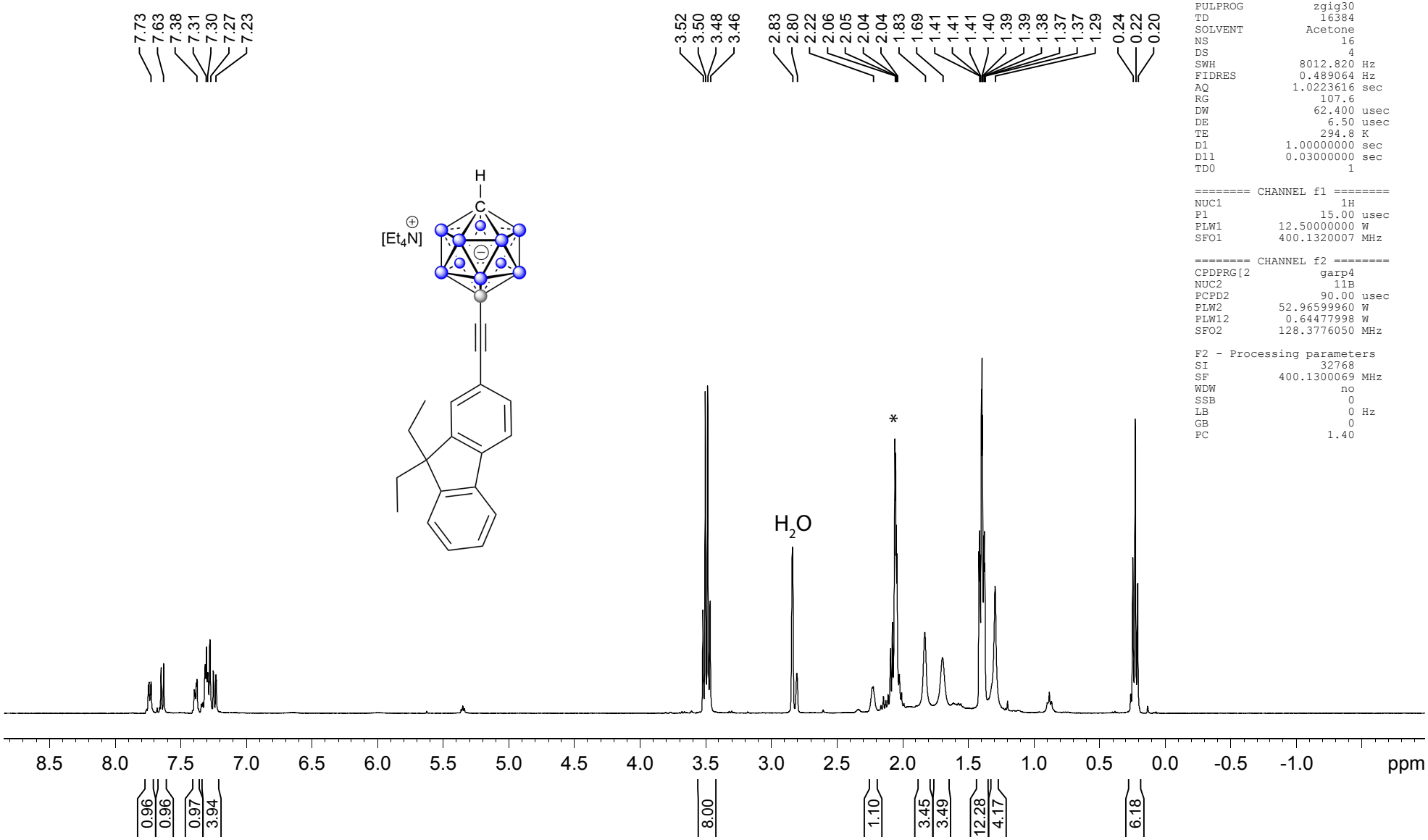
$[Et_4N][CB_{11}H_{11}$-CC-anthracene], in acetone - d_6*
$^{13}C\{^1H\}$, 101 MHz, T = 23 C




```
Current Data Parameters
NAME      20190128-JT-4-CB11-CC-En
EXPNO                5
PROCNO               1

F2 - Acquisition Parameters
Date_          20190130
Time               0.34
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                1024
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG              193.34
DW              16.800 usec
DE               6.50 usec
TE              296.5 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126818 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-Fl], in acetone - d_6*

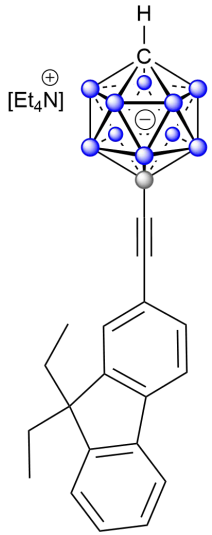
$^1H\{^{11}B\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20190221-JT-3-CB11-CC-Fl
EXPNO                6
PROCNO               1

F2 - Acquisition Parameters
Date_           20190222
Time              21.21
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES            0.489064 Hz
AQ             1.0223616 sec
RG                107.6
DW                62.400 usec
DE                 6.50 usec
TE                294.8 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2             90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                32768
SF           400.1300069 MHz
WDW                  no
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.40
```

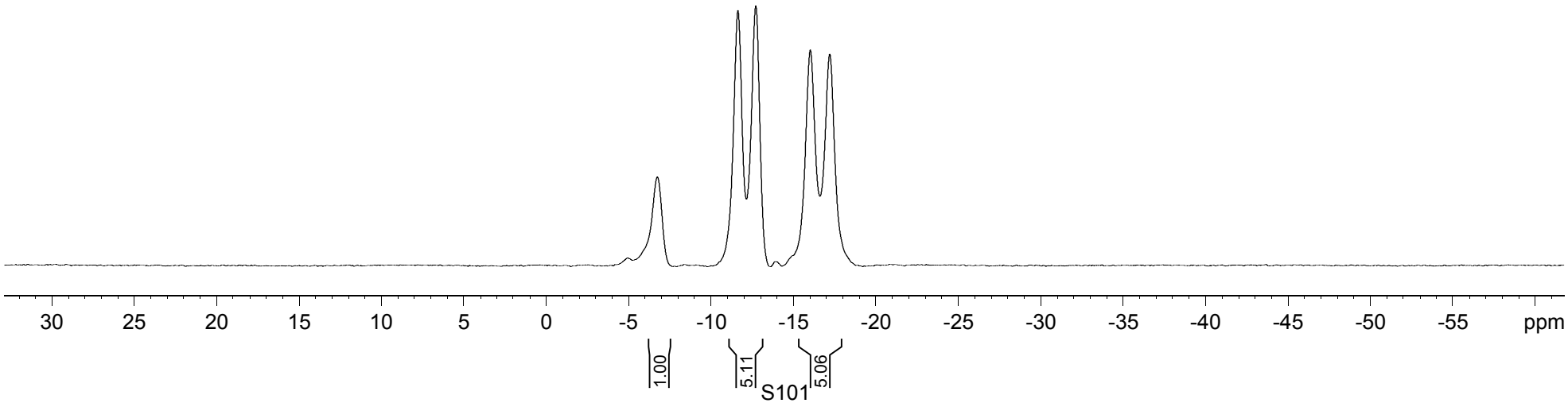
$[Et_4N][CB_{11}H_{11}$-CC-Fl], in acetone - d_6

^{11}B, 128 MHz, T = 23 C



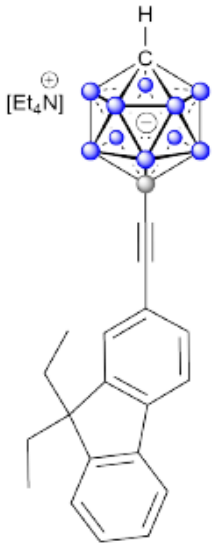
-6.77
-11.66
-12.74
-16.05
-17.23

```
Current Data Parameters
NAME      20190221-JT-3-CB11-CC-Fl
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20190222
Time              21.32
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW             19.600 usec
DE              6.50 usec
TE              294.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                 EM
SSB                  0
LB               10.00 Hz
GB                   0
PC                1.40
```



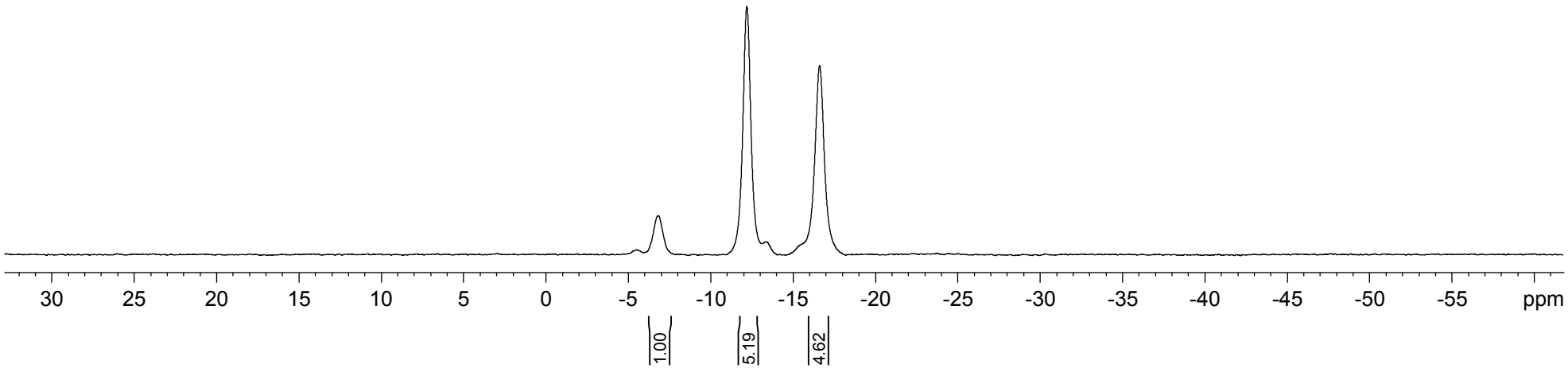
$[Et_4N][CB_{11}H_{11}$-CC-Fl], in acetone - d_6

$^{11}B\{^1H\}$, 128 MHz, T = 23 C



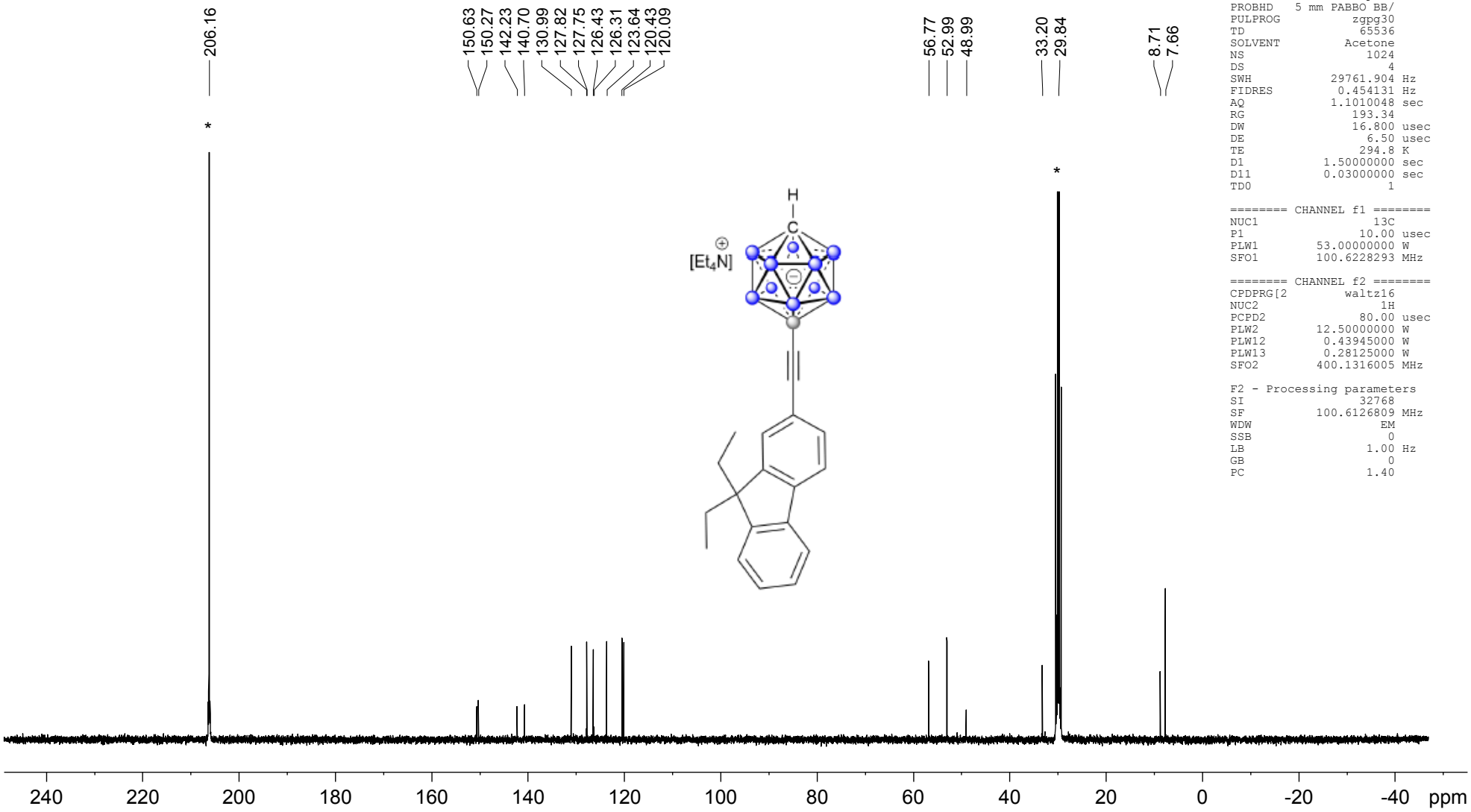
-6.86 -12.22 -16.64

```
Current Data Parameters
NAME      20190221-JT-3-CB11-CC-Fl
EXPNO                7
PROCNO               1

F2 - Acquisition Parameters
Date_          20190222
Time             21.27
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT         Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW            19.600 usec
DE             6.50 usec
TE             295.1 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                11B
P1                9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF          128.3776050 MHz
WDW                  EM
SSB                  0
LB               10.00 Hz
GB                   0
PC                1.40
```



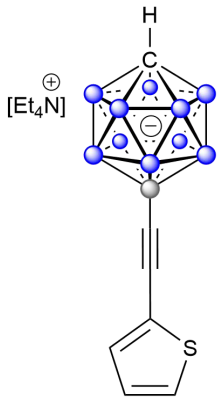
$[Et_4N][CB_{11}H_{11}$-CC-Fl], in acetone - d_6*

$^{13}C\{^1H\}$, 101 MHz, T = 23 C




```
Current Data Parameters
NAME      20190221-JT-3-CB11-CC-Fl
EXPNO                9
PROCNO               1

F2 - Acquisition Parameters
Date_          20190222
Time              22.20
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                1024
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG              193.34
DW              16.800 usec
DE               6.50 usec
TE              294.8 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126809 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-2-Thiophene], in acetone - d_6*
$^1H\{^{11}B\}$, 500 MHz, T = 23 C



7.19 7.19 7.18 7.18 6.93 6.93 6.93 6.92 6.90 6.89 6.88 6.88

3.49 3.48 2.85 2.82 2.23 2.22 2.05 1.79 1.68 1.39 1.39 1.39

H_2O

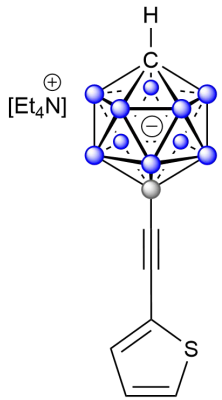
*

```
Current Data Parameters
NAME      20220506-CC-2-Thio
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20220507
Time       3.45
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgig30
TD         65536
SOLVENT           Acetone
NS           16
DS            0
SWH             12500.000 Hz
FIDRES            0.190735 Hz
AQ              2.6214399 sec
RG            114
DW          40.000 usec
DE           6.50 usec
TE          295.9 K
D1             5.00000000 sec
D11            0.03000000 sec

======== CHANNEL f1 ========
NUC1          1H
P1         11.70 usec
PLW1         19.00000000 W
SFO1         500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2               garp
NUC2         11B
PCPD2              100.00 usec
PLW2          95.00000000 W
PLW12          1.63030005 W
SFO2          160.4615690 MHz

F2 - Processing parameters
SI         65536
SF            500.1300100 MHz
WDW            no
SSB            0
LB           0 Hz
GB             0
PC          1.00
```

12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 ppm

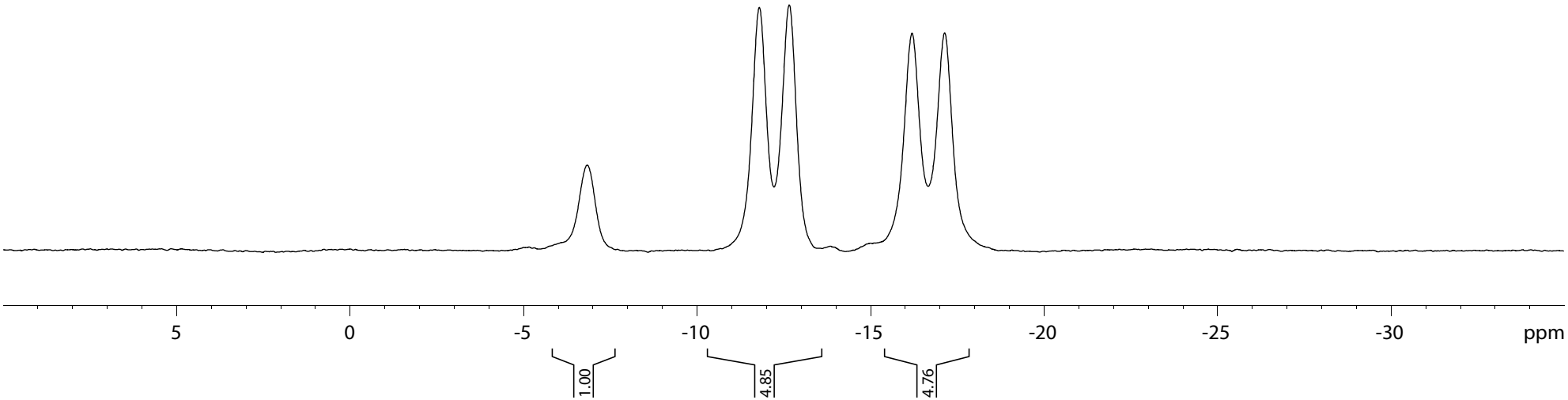
1.08 2.21 8.00 1.11 4.84 4.55 12.29

$[Et_4N][CB_{11}H_{11}$-CC-Th], in acetone - d_6
^{11}B, 160 MHz, T = 23 C



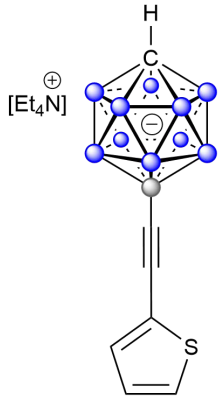
-6.84
-11.81
-12.67
-16.21
-17.15

```
Current Data Parameters
NAME      20220424-LF-231-Thio
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_           20220424
Time       19.34
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD         64098
SOLVENT           Acetone
NS           64
DS           0
SWH             32051.281 Hz
FIDRES           0.500036 Hz
AQ              0.9999288 sec
RG          203
DW         15.600 usec
DE          6.50 usec
TE         295.8 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1         11B
P1          13.10 usec
PLW1          95.00000000 W
SFO1          160.4615792 MHz

F2 - Processing parameters
SI         32768
SF            160.4615790 MHz
WDW            EM
SSB           0
LB          10.00 Hz
GB            0
PC          1.40
```



$[Et_4N][CB_{11}H_{11}\text{-CC-Th}]$, in acetone - d_6

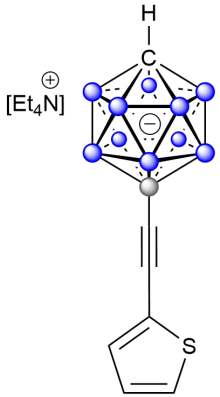
$^{11}B\{^1H\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20220424-LF-231-thio
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220424
Time       19.24
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD         65536
SOLVENT           Acetone
NS           64
DS           0
SWH             32051.281 Hz
FIDRES           0.489064 Hz
AQ              1.0223616 sec
RG           203
DW          15.600 usec
DE           6.50 usec
TE          296.4 K
D1             1.00000000 sec
D11            0.03000000 sec

======== CHANNEL f1 ========
NUC1          11B
P1          13.10 usec
PLW1          95.00000000 W
SFO1          160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2          1H
PCPD2       80.00 usec
PLW2          19.00000000 W
PLW12          0.42394000 W
PLW13          0.27131999 W
SFO2          500.1325007 MHz

F2 - Processing parameters
SI          32768
SF             160.4615790 MHz
WDW            EM
SSB            0
LB          10.00 Hz
GB             0
PC          1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-Th], in acetone - d_6*

$^{13}C\{^1H\}$, 101 MHz, T = 23 C



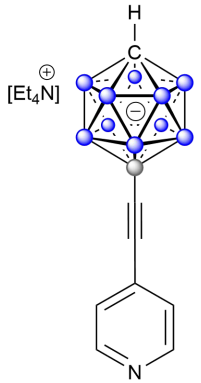
206.19 130.15 127.55 127.49 125.43 53.03 52.99 52.96 49.33 29.84 7.67

```
Current Data Parameters
NAME      20190222-JT-3-CB11-CC-Th
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20190223
Time       20.48
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD        65536
SOLVENT          Acetone
NS          1024
DS             4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG          193.34
DW          16.800 usec
DE           6.50 usec
TE          295.3 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0          1

======== CHANNEL f1 ========
NUC1         13C
P1          10.00 usec
PLW1           53.00000000 W
SFO1           100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2         1H
PCPD2               80.00 usec
PLW2           12.50000000 W
PLW12           0.43945000 W
PLW13           0.28125000 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI          32768
SF             100.6126809 MHz
WDW            EM
SSB            0
LB           1.00 Hz
GB             0
PC           1.40
```

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 ppm

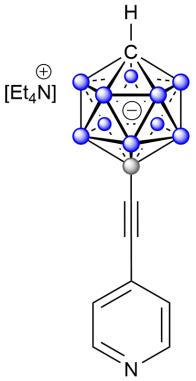
[Et_4N][$CB_{11}H_{11}$-CC-py], in acetone - d_6*
$^1H\{^{11}B\}$, 400 MHz, T = 23 C


```
Current Data Parameters
NAME      20181024-zk-CC-Py-NEt4
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20180523
Time                       16.30
INSTRUM                    spect
PROBHD   5 mm PABBO BB/
PULPROG                  zgig30
TD                        16384
SOLVENT                 Acetone
NS                             16
DS                              4
SWH                     8012.820 Hz
FIDRES                  0.489064 Hz
AQ                    1.0223616 sec
RG                         78.69
DW                        62.400 usec
DE                         6.50 usec
TE                        294.8 K
D1                    1.00000000 sec
D11                   0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        15.00 usec
PLW1                 12.50000000 W
SFO1                400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2                  garp4
NUC2                         11B
PCPD2                     90.00 usec
PLW2                 52.96599960 W
PLW12                 0.64477998 W
SFO2                128.3776050 MHz

F2 - Processing parameters
SI                         32768
SF                  400.1300074 MHz
WDW                           no
SSB                            0
```



$[Et_4N][CB_{11}H_{11}$-CC-py], in acetone - d_6

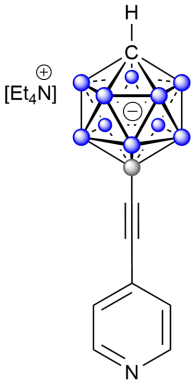
^{11}B, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20181024-zk-CC-Py-NEt4
EXPNO                          3
PROCNO                         1

F2 - Acquisition Parameters
Date_              20180523
Time                  16.42
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg
TD                    65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH                25510.203 Hz
FIDRES             0.389255 Hz
AQ                 1.2845056 sec
RG                    193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   293.9 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     11B
P1                      9.93 usec
PLW1            52.96599960 W
SFO1           128.3776052 MHz

F2 - Processing parameters
SI                       32768
SF              128.3776050 MHz
WDW                         EM
SSB                          0
LB                       10.00 Hz
GB                           0
PC                        1.40
```

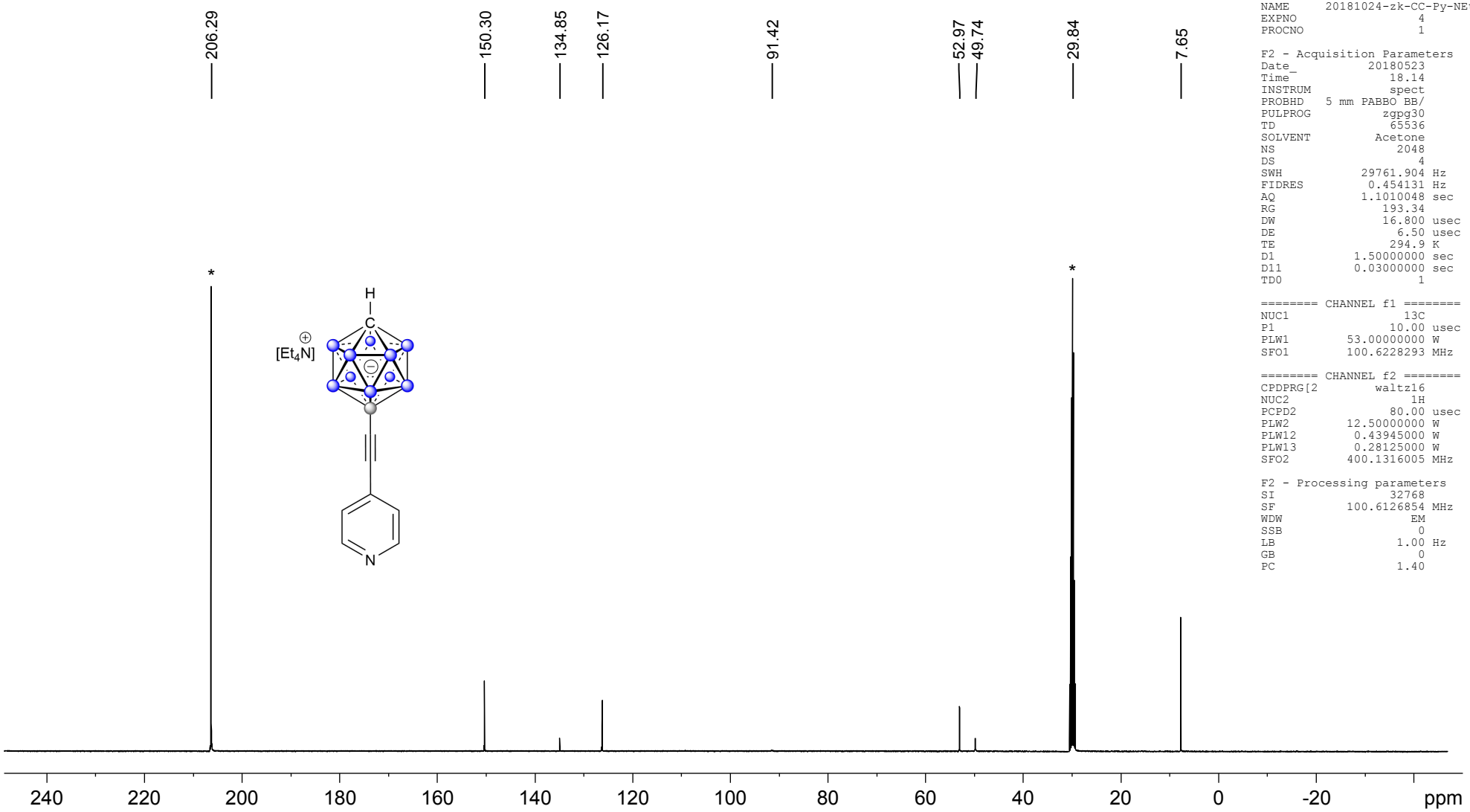
$[Et_4N][CB_{11}H_{11}$-CC-py], in acetone - d_6

$^{11}B\{^1H\}$, 128 MHz, T = 23 C



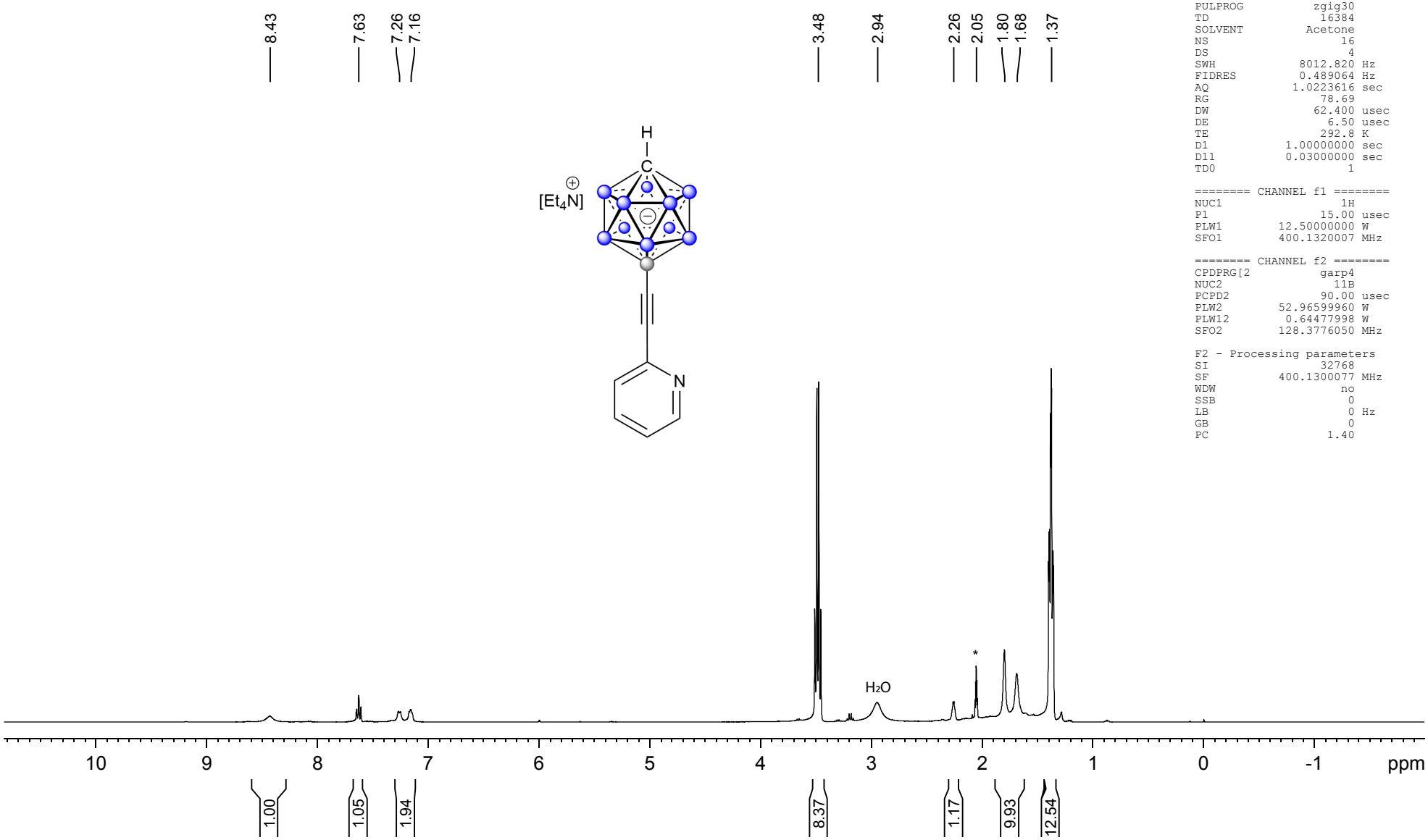

```
Current Data Parameters
NAME      20181024-zk-CC-Py-NEt4
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20180523
Time                       16.36
INSTRUM                    spect
PROBHD   5 mm PABBO BB/
PULPROG                  zgpg30
TD                        65536
SOLVENT                 Acetone
NS                            128
DS                              4
SWH                   25510.203 Hz
FIDRES                 0.389255 Hz
AQ                    1.2845056 sec
RG                       193.34
DW                       19.600 usec
DE                         6.50 usec
TE                        294.5 K
D1                    1.00000000 sec
D11                   0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         11B
P1                          9.93 usec
PLW1                52.96599960 W
SFO1               128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                     80.00 usec
PLW2                12.50000000 W
PLW12                0.43945000 W
PLW13                0.28125000 W
SFO2               400.1320007 MHz

F2 - Processing parameters
SI                           32768
SF                 128.3776050 MHz
WDW                             EM
```

$[Et_4N][CB_{11}H_{11}$-CC-py], in acetone - d_6*
$^{13}C\{^1H\}$, 101 MHz, T = 23 C




```
Current Data Parameters
NAME      20181024-zk-CC-Py-NEt4
EXPNO                          4
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20180523
Time                       18.14
INSTRUM                    spect
PROBHD    5 mm PABBO BB/
PULPROG                   zgpg30
TD                         65536
SOLVENT                  Acetone
NS                          2048
DS                             4
SWH                    29761.904 Hz
FIDRES                  0.454131 Hz
AQ                     1.1010048 sec
RG                        193.34
DW                        16.800 usec
DE                         6.50 usec
TE                        294.9 K
D1                   1.50000000 sec
D11                  0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                        10.00 usec
PLW1                 53.00000000 W
SFO1                100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                     80.00 usec
PLW2                 12.50000000 W
PLW12                 0.43945000 W
PLW13                 0.28125000 W
SFO2                400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                  100.6126854 MHz
WDW                           EM
SSB                            0
LB                         1.00 Hz
GB                             0
PC                         1.40
```

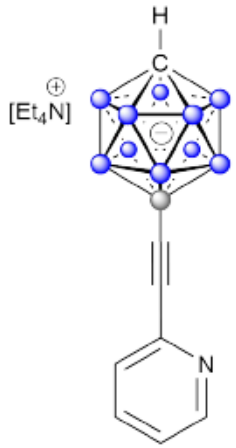
[Et_4N][$CB_{11}H_{11}$-CC-2-py], in acetone - d_6*
$^1H\{^{11}B\}$, 400 MHz, T = 23 C




```
Current Data Parameters
NAME      20210624-LF-180-2-py
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20210625
Time                 15.45
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgig30
TD                  16384
SOLVENT           Acetone
NS                     16
DS                      4
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                 1.0223616 sec
RG                    78.69
DW                    62.400 usec
DE                     6.50 usec
TE                   292.8 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      15.00 usec
PLW1               12.50000000 W
SFO1               400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2                garp4
NUC2                       11B
PCPD2                   90.00 usec
PLW2               52.96599960 W
PLW12               0.64477998 W
SFO2               128.3776050 MHz

F2 - Processing parameters
SI                       32768
SF                 400.1300077 MHz
WDW                         no
SSB                          0
LB                           0 Hz
GB                           0
PC                        1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-2-py], in acetone - d_6

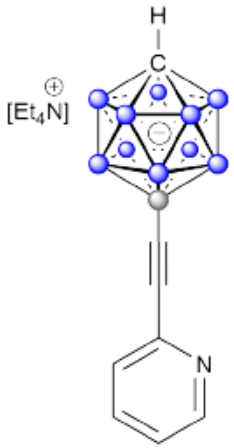
^{11}B, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20210621-ct020-2pycolumn
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_           20210622
Time              12.36
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               291.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB                   0
LB                10.00 Hz
GB                    0
PC                 1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-2-py], in acetone - d_6

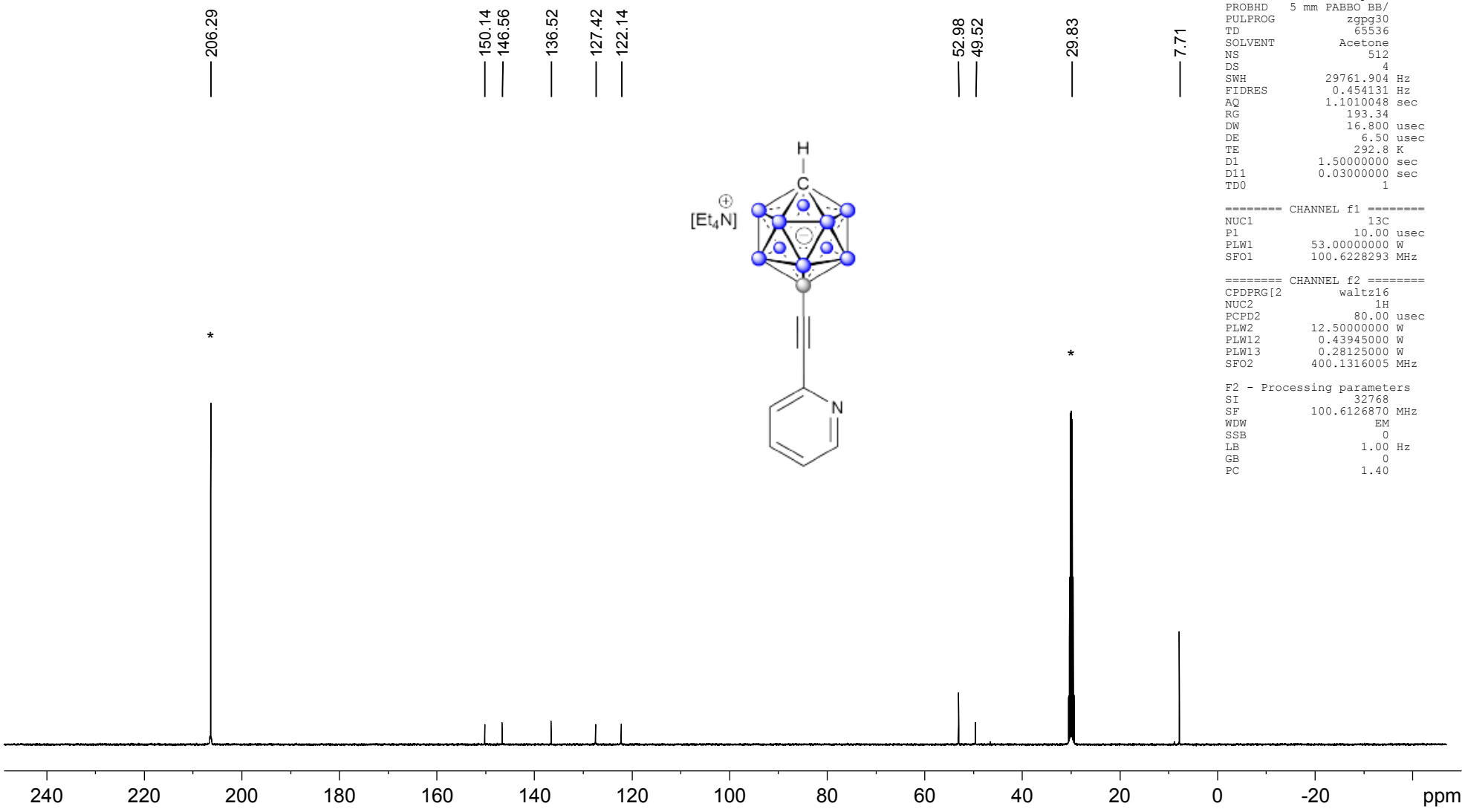
$^{11}B\{^1H\}$, 128 MHz, T = 23 C




```
Current Data Parameters
NAME      20210621-ct020-2pycolumn
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20210622
Time              12.30
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ            1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              292.3 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1        128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF          128.3776050 MHz
WDW                  EM
SSB                   0
LB                10.00 Hz
GB                    0
PC                 1.40
```

$[Et_4N][CB_{11}H_{11}$-CC-2-py], in acetone - d_6*

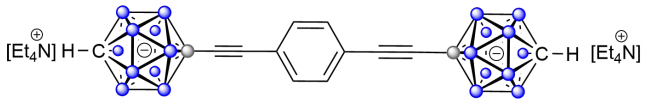
$^{13}C\{^1H\}$, 101 MHz, T = 23 C



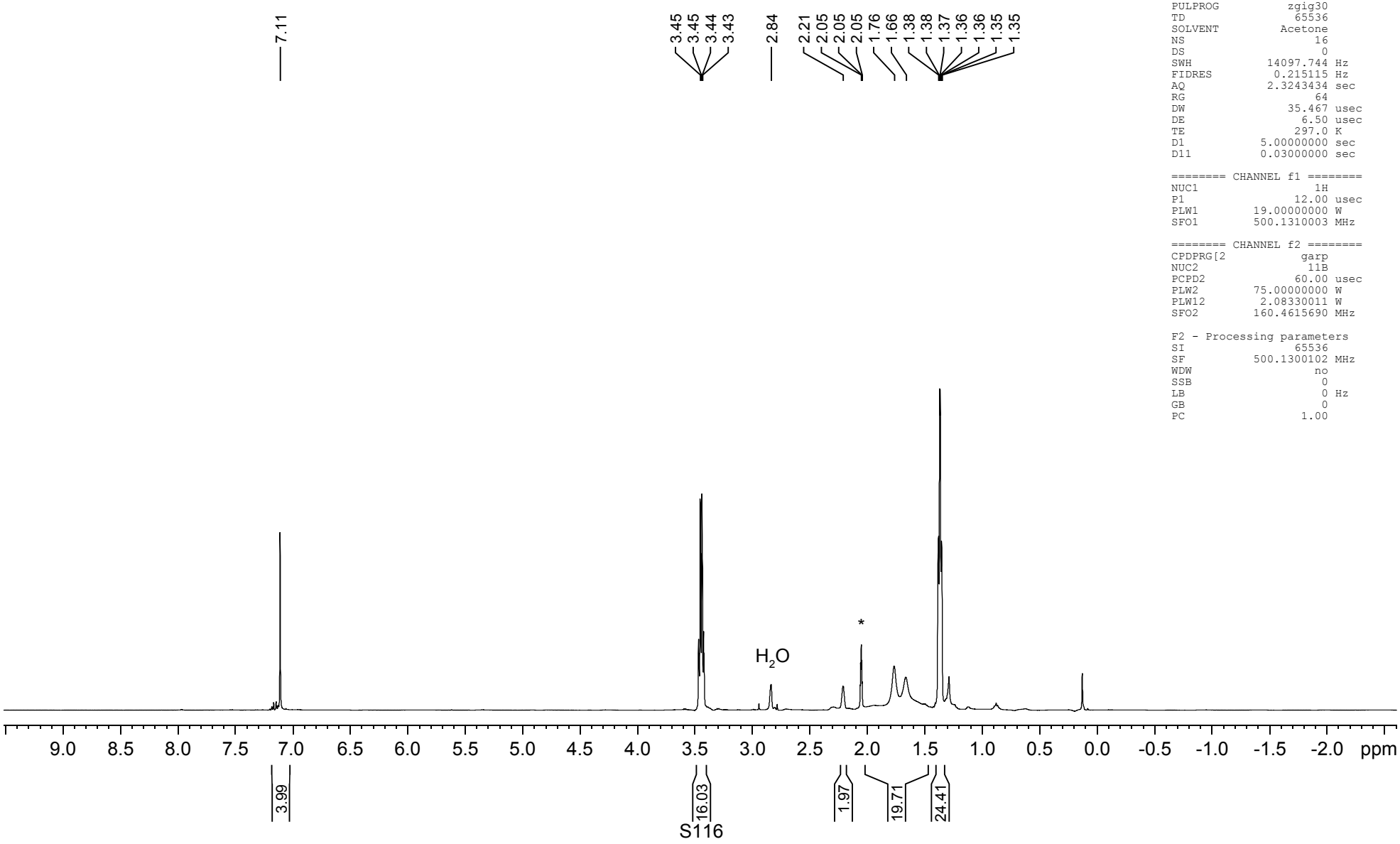

```
Current Data Parameters
NAME      20210624-LF-180-2-py
EXPNO                        5
PROCNO                       1

F2 - Acquisition Parameters
Date_              20210625
Time                 16.22
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT           Acetone
NS                    512
DS                      4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                16.800 usec
DE                 6.50 usec
TE                292.8 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
PLW1           53.00000000 W
SFO1           100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PLW2           12.50000000 W
PLW12           0.43945000 W
PLW13           0.28125000 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6126870 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

[Et_4N][$CB_{11}H_{11}$-CC-Ph-CC-$CB_{11}H_{11}$], in acetone - d_6*

$^1H\{^{11}B\}$, 500 MHz, T = 23 C

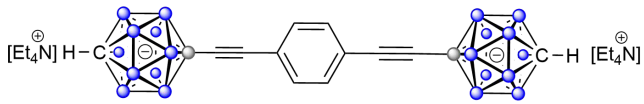



```
Current Data Parameters
NAME      20181025-zk-[NEt4][C2-Ben-C2]
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20160525
Time              16.25
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgig30
TD               65536
SOLVENT         Acetone
NS                  16
DS                   0
SWH           14097.744 Hz
FIDRES        0.215115 Hz
AQ            2.3243434 sec
RG                  64
DW               35.467 usec
DE                6.50 usec
TE               297.0 K
D1            5.00000000 sec
D11           0.03000000 sec

======== CHANNEL f1 ========
NUC1                1H
P1                12.00 usec
PLW1        19.00000000 W
SFO1        500.1310003 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                11B
PCPD2             60.00 usec
PLW2        75.00000000 W
PLW12        2.08330011 W
SFO2        160.4615690 MHz

F2 - Processing parameters
SI               65536
SF          500.1300102 MHz
WDW                 no
SSB                  0
LB                   0 Hz
GB                   0
PC                1.00
```



$[Et_4N][CB_{11}H_{11}$-CC-Ph-CC-$CB_{11}H_{11}]$, in acetone - d_6

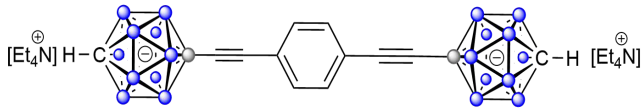
^{11}B, 160 MHz, T = 23 C




```
Current Data Parameters
NAME      20181025-zk-[NEt4][C2-Ben-C2]
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20160428
Time              15.53
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zg
TD                64098
SOLVENT         Acetone
NS                   32
DS                    0
SWH           32051.281 Hz
FIDRES         0.500036 Hz
AQ            0.9999288 sec
RG                  203
DW               15.600 usec
DE               16.00 usec
TE               295.6 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1               10.00 usec
PLW1        75.00000000 W
SFO1       160.4615792 MHz

F2 - Processing parameters
SI                 32768
SF          160.4615993 MHz
WDW                  EM
SSB                   0
LB               10.00 Hz
GB                    0
PC                 1.40
```

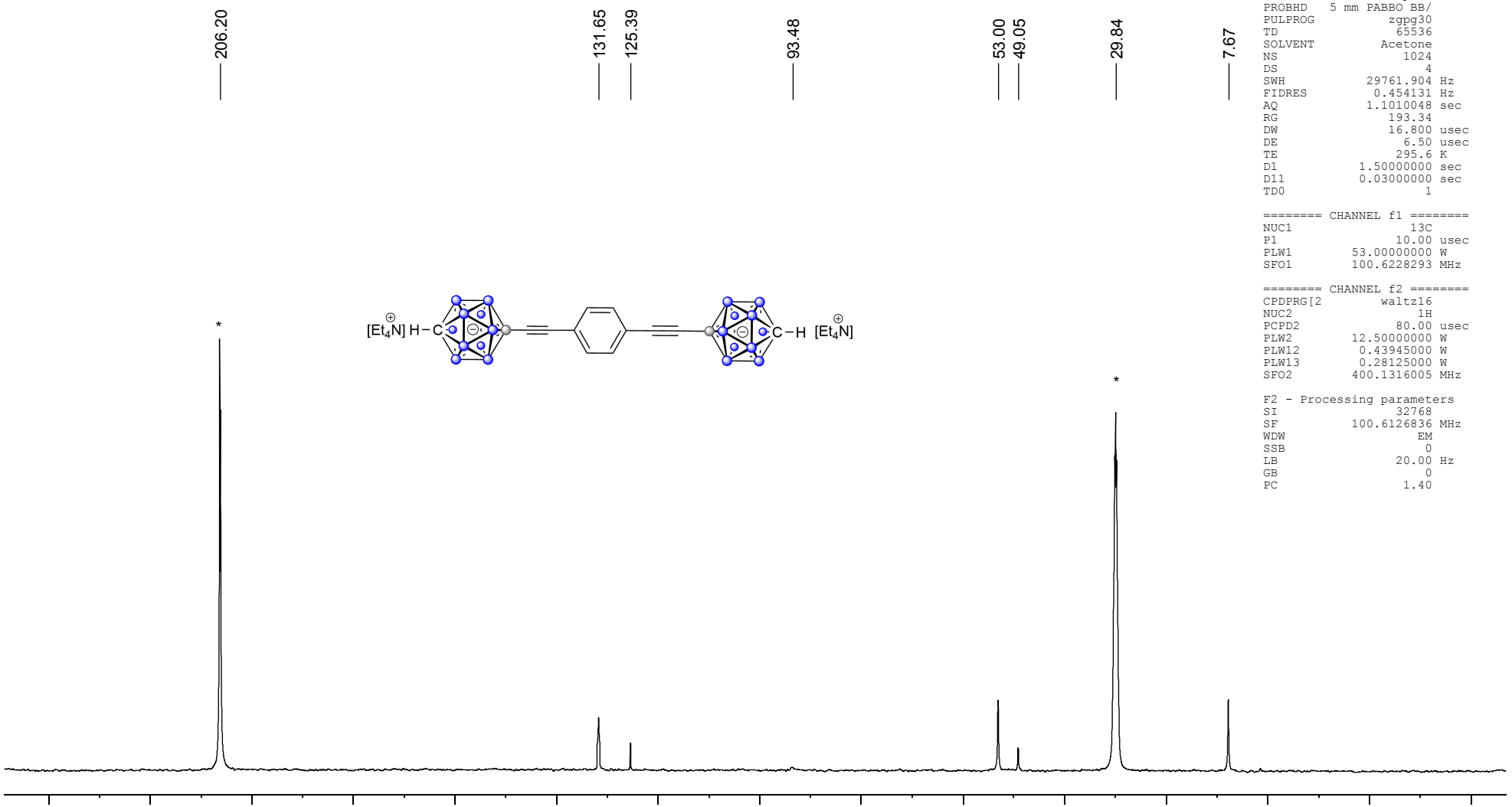
$[Et_4N][CB_{11}H_{11}\text{-CC-Ph-CC-}CB_{11}H_{11}]$, in acetone - d_6

$^{11}B\{^1H\}$, 160 MHz, T = 23 C



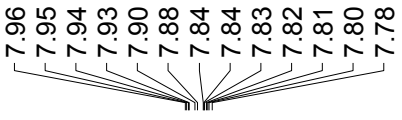

```
Current Data Parameters
NAME      20181025-zk-[NEt4][C2-Ben-C2]
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20160428
Time              15.55
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                   32
DS                    0
SWH           32051.281 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                  203
DW               15.600 usec
DE                6.50 usec
TE               296.0 K
D1            1.00000000 sec
D11           0.03000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1                10.00 usec
PLW1        75.00000000 W
SFO1       160.4615792 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2        19.00000000 W
PLW12        0.42750001 W
PLW13        0.27360001 W
SFO2       500.1330885 MHz

F2 - Processing parameters
SI                32768
SF          160.4615993 MHz
WDW                  EM
SSB                   0
LB                10.00 Hz
GB                    0
PC                 1.40
```

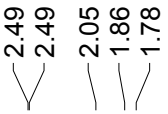
$[Et_4N][CB_{11}H_{11}\text{-CC-Ph-CC-}CB_{11}H_{11}]$, in acetone - d_6*
$^{13}C\{^1H\}$, 101 MHz, T = 23 C

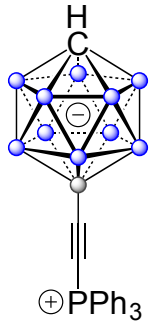



```
Current Data Parameters
NAME      20181025-zk-[NEt4][C2-Ben-C2]
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20160526
Time               7.37
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                1024
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW             16.800 usec
DE              6.50 usec
TE             295.6 K
D1          1.50000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126836 MHz
WDW                EM
SSB                 0
LB              20.00 Hz
GB                  0
PC               1.40
```

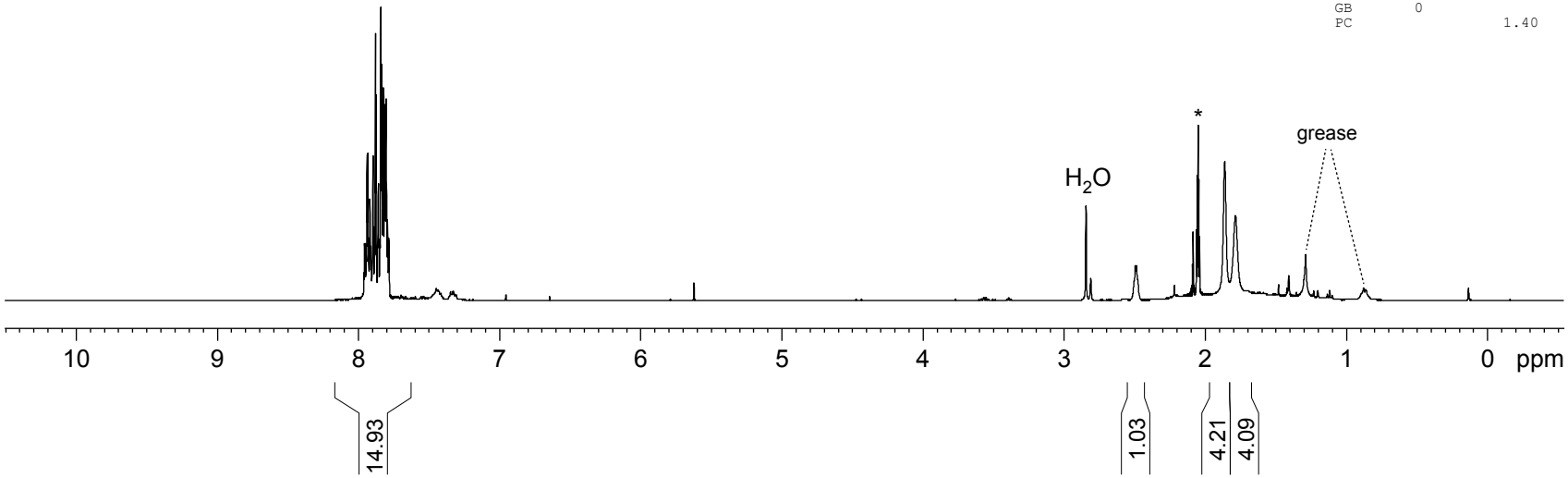
PPh3 coupling product, acetone-d6*
1H{11B} NMR, 400 MHz, T = 24 C



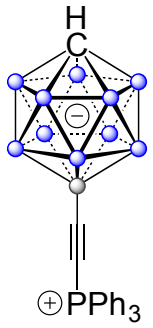





```
Current Data Parameters
NAME      20211124-ct-pph3_coupling-C
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20211125
Time              4.31
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                107.6
DW               62.400 usec
DE                6.50 usec
TE               294.4 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2             90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2         128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF           400.1300072 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.40
```

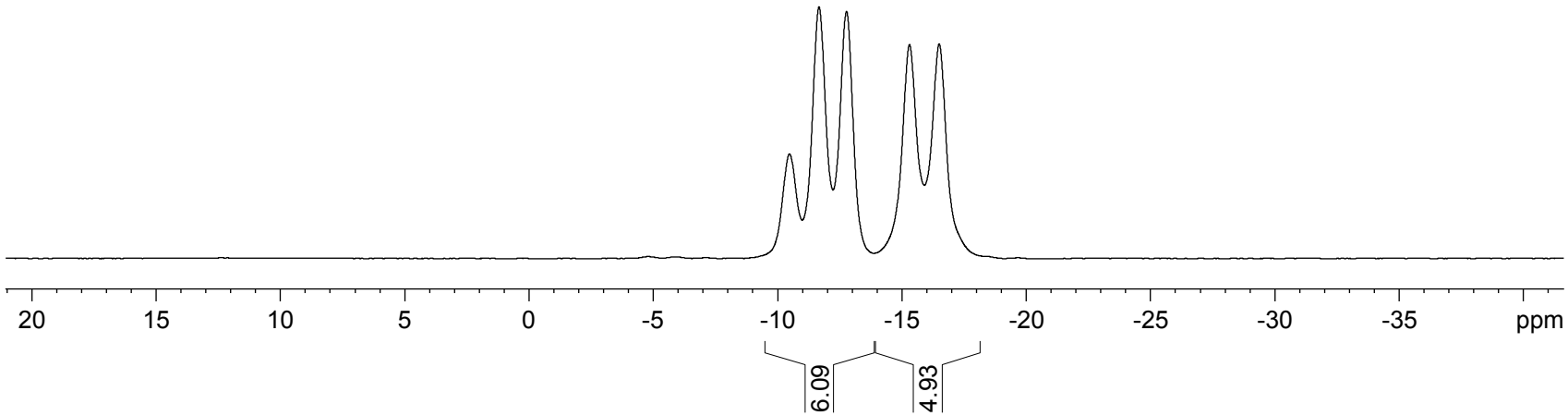


PPh3 coupling product, acetone-d6
11B NMR, 128 MHz, T = 24 C

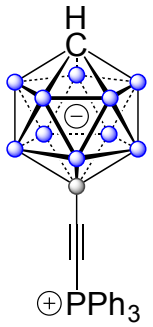


-10.47
-11.66
-12.77
-15.30
-16.49

```
Current Data Parameters
NAME      20211124-ct-pph3_coupling-C
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_              20211125
Time                  4.43
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG                zg
TD                  65536
SOLVENT           Acetone
NS                    128
DS                      4
SWH             25510.203 Hz
FIDRES           0.389255 Hz
AQ               1.2845056 sec
RG                 193.34
DW                 19.600 usec
DE                  6.50 usec
TE                 294.3 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  11B
P1                   9.93 usec
PLW1          52.96599960 W
SFO1         128.3776052 MHz

F2 - Processing parameters
SI                    32768
SF           128.3776050 MHz
WDW                     EM
SSB       0
LB                  10.00 Hz
GB        0
PC                   1.40
```

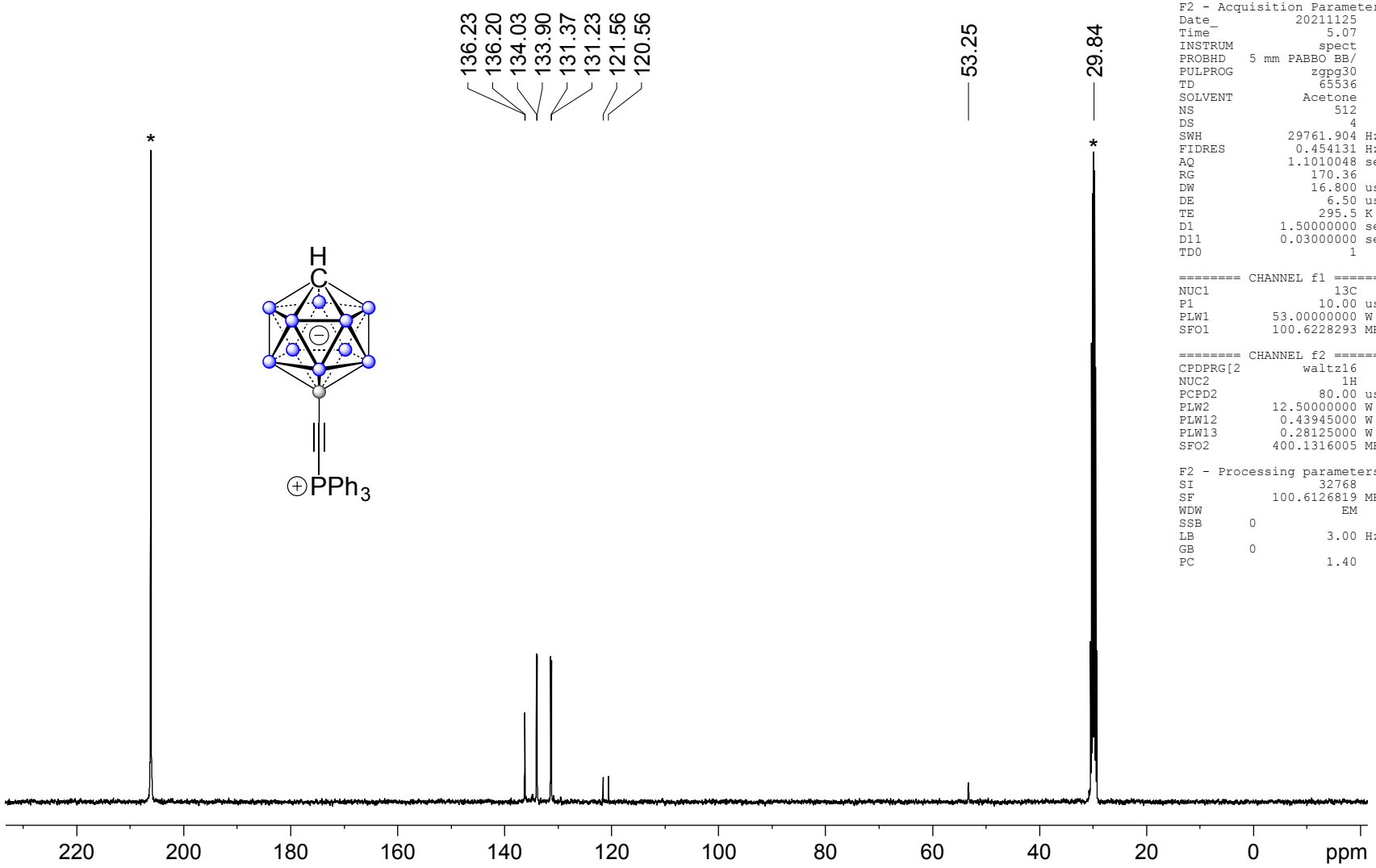


PPh3 coupling product, acetone-d6
11B{1H} NMR, 128 MHz, T = 24 C



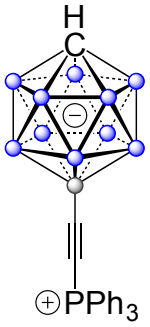

```
Current Data Parameters
NAME      20211124-ct-pph3_coupling-C
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20211125
Time               4.37
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               295.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1        128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2              80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF          128.3776050 MHz
WDW                 EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

PPh3 coupling product, acetone-d6*
13C{1H} NMR, 100 MHz, T = 24 C

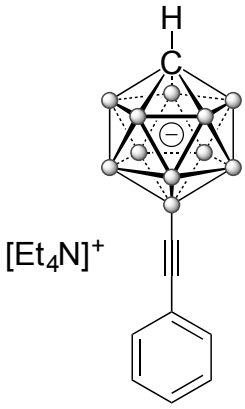



```
Current Data Parameters
NAME      20211124-ct-pph3_coupling-C
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20211125
Time               5.07
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                170.36
DW                16.800 usec
DE                 6.50 usec
TE                295.5 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126819 MHz
WDW                  EM
SSB       0
LB                3.00 Hz
GB        0
PC                1.40
```

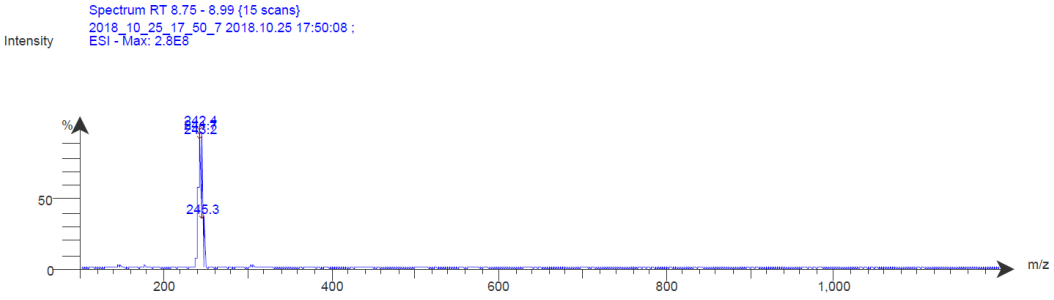
PPh3 coupling product, acetone-d6
31P{1H} NMR, 162 MHz, T = 24 C



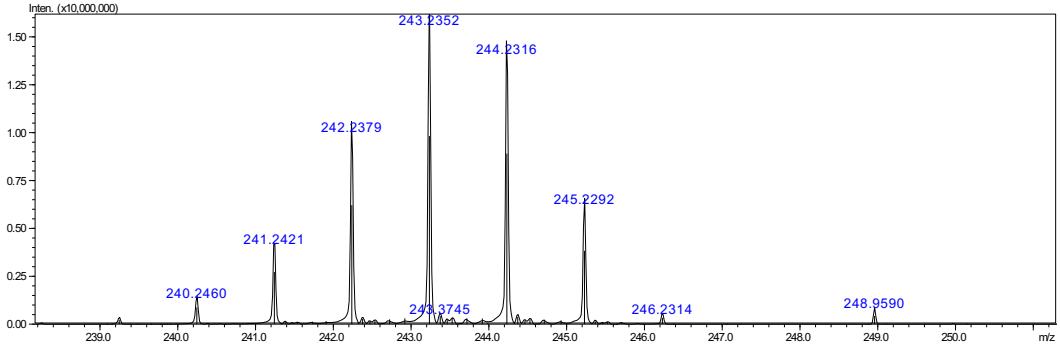

```
Current Data Parameters
NAME      20210811_CHEN_Tao_20210722-ct022
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210723
Time               19.37
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    4
SWH           64102.562 Hz
FIDRES         0.978127 Hz
AQ            0.5111808 sec
RG               193.34
DW                7.800 usec
DE                6.50 usec
TE                296.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 31P
P1                15.00 usec
PLW1        15.00000000 W
SFO1        161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          161.9755930 MHz
WDW                  EM
SSB       0
LB                5.00 Hz
GB        0
PC                1.40
```

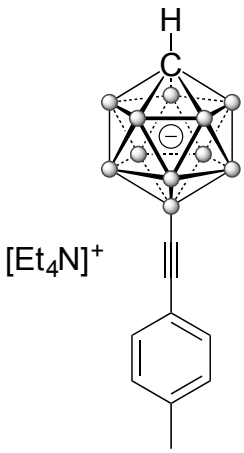


Advion MS

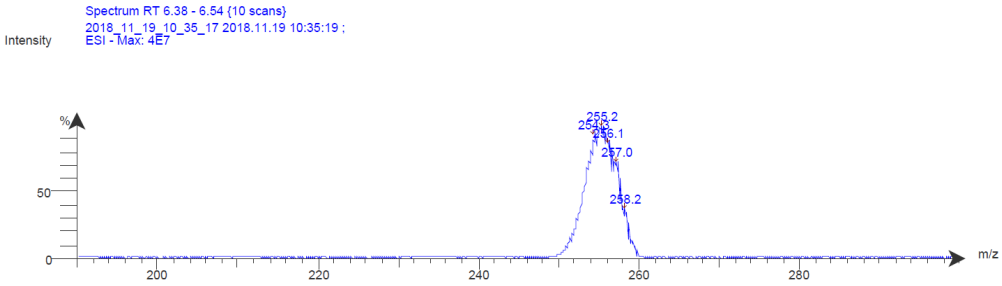


Agilent MS

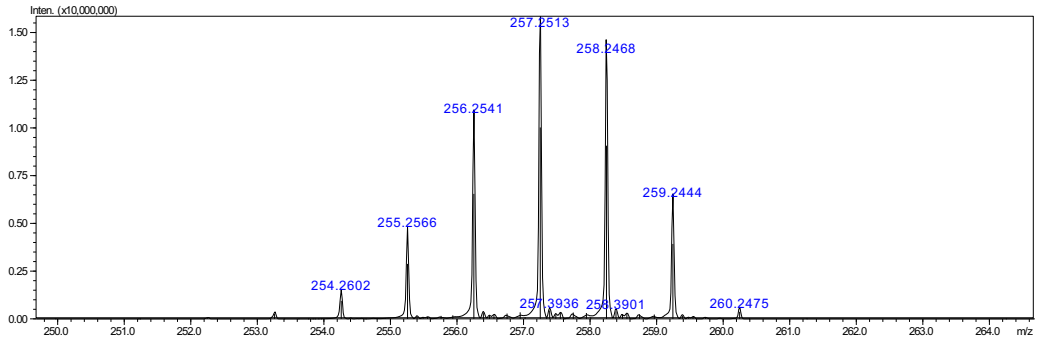


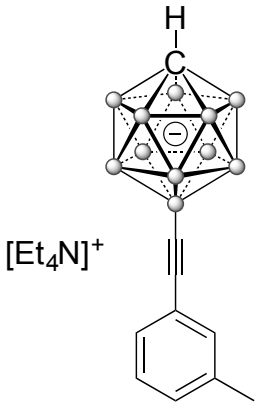


Advion MS

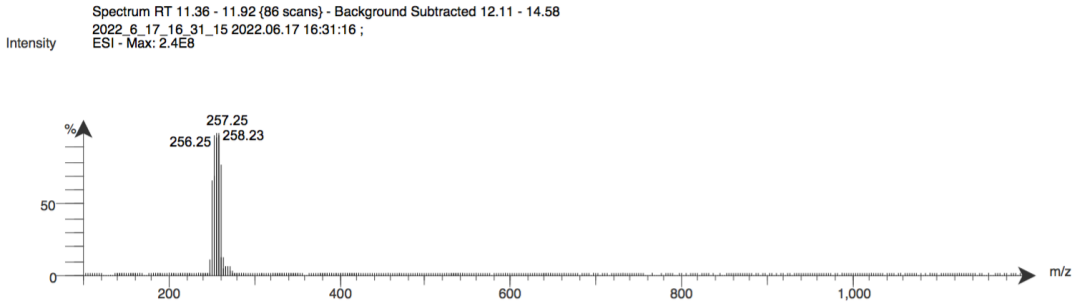


Agilent MS

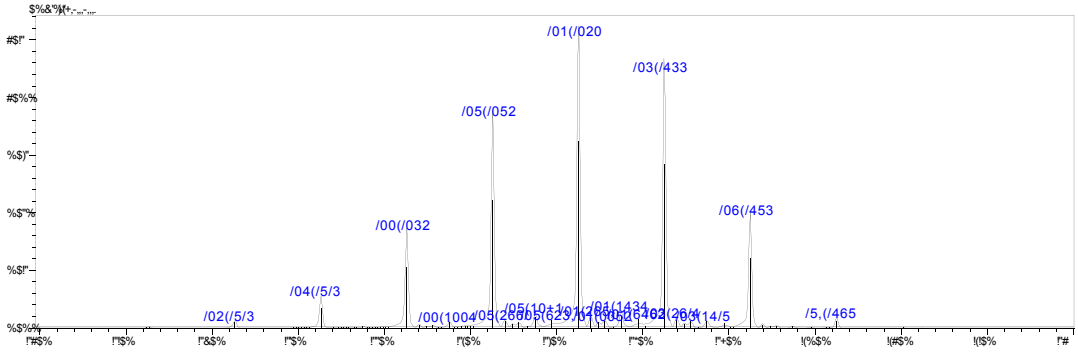


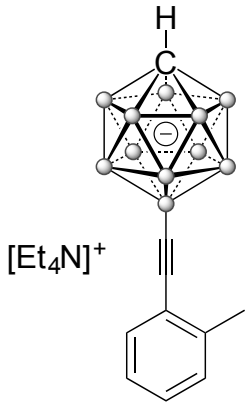


Advion MS

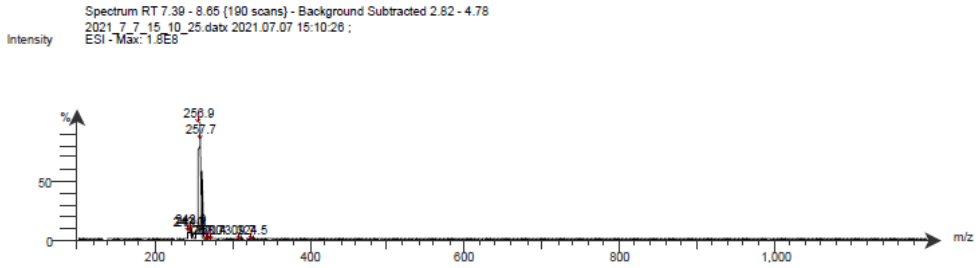


Agilent MS

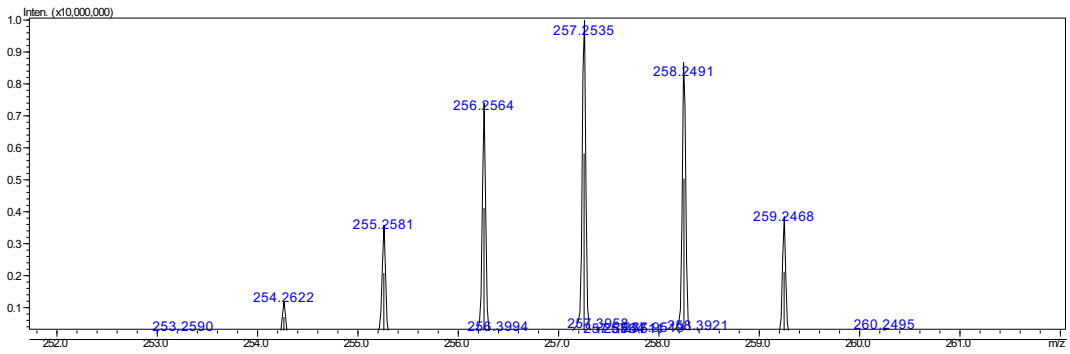


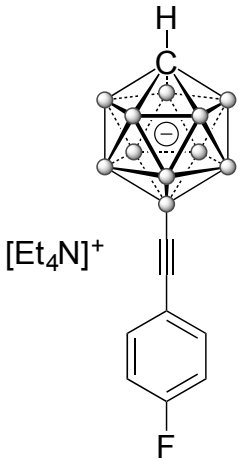


Advion MS

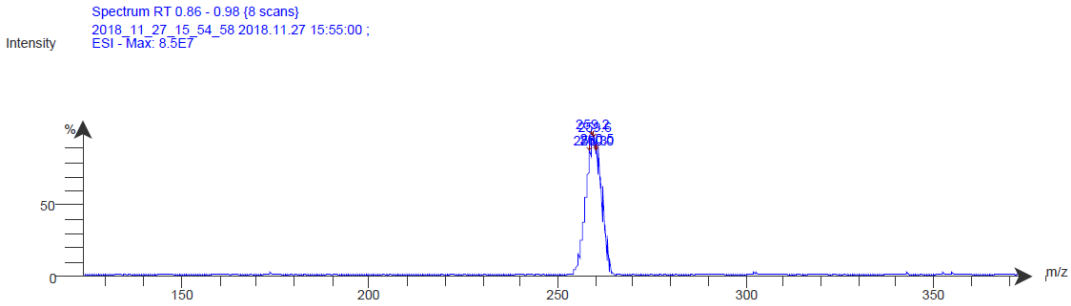


Agilent MS





Advion MS



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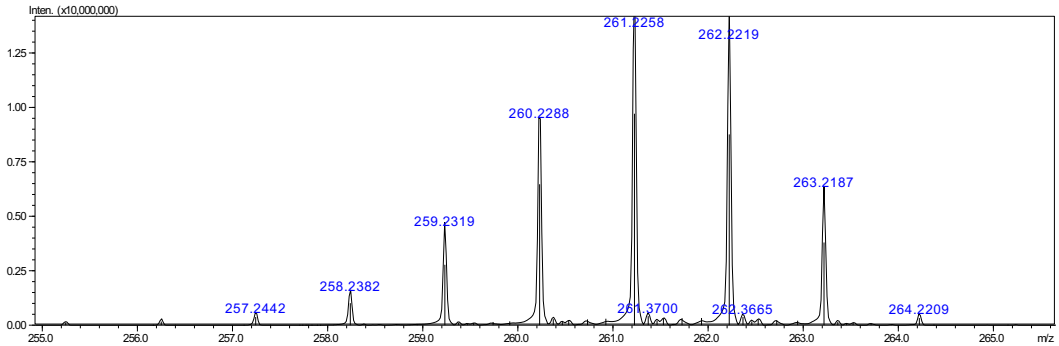

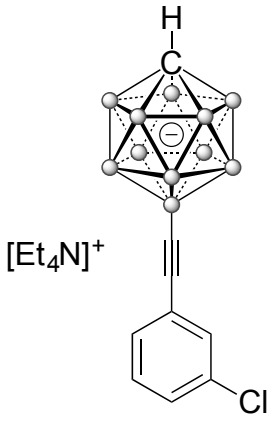

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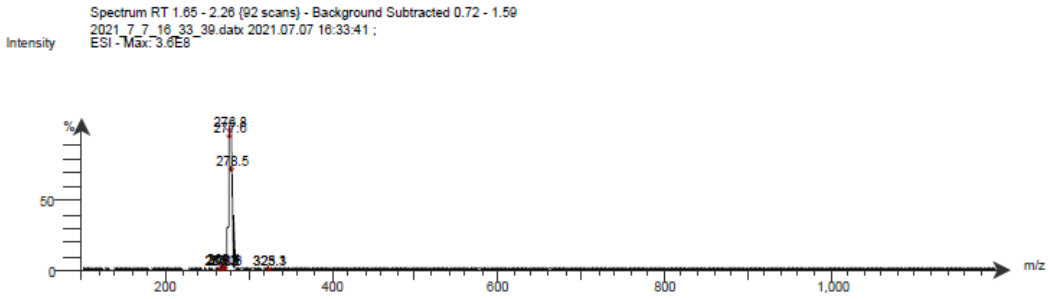

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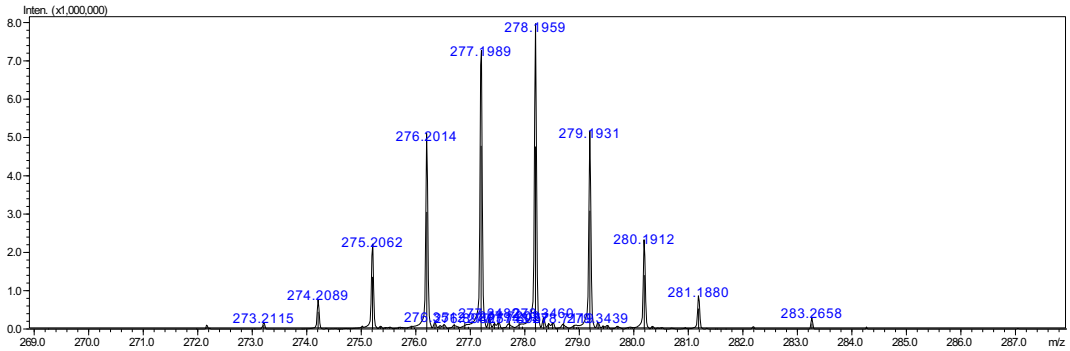

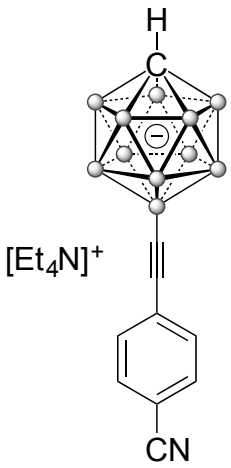

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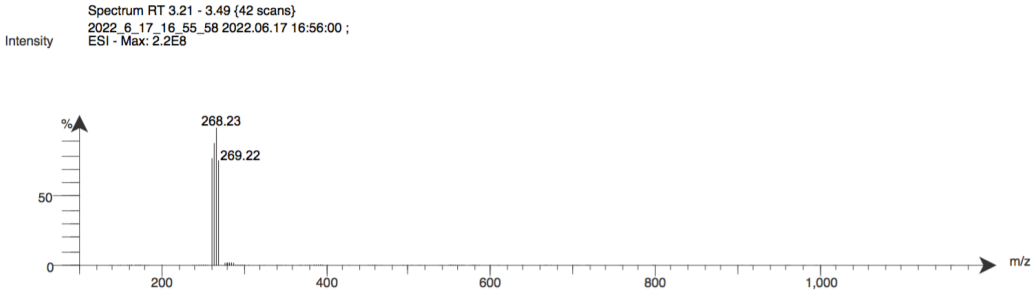

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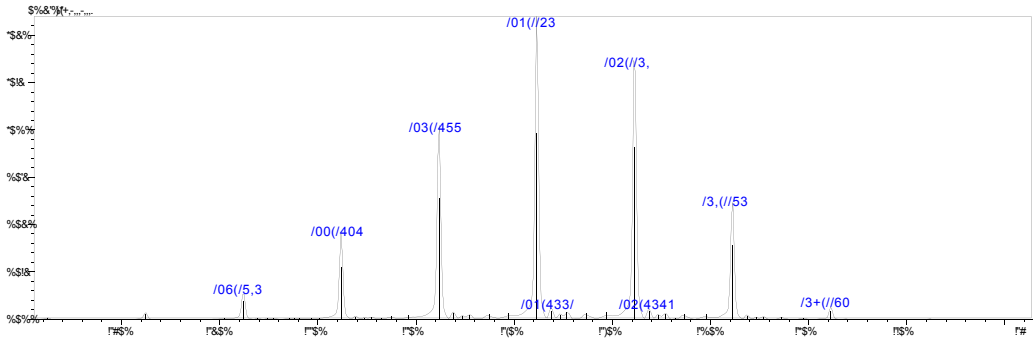

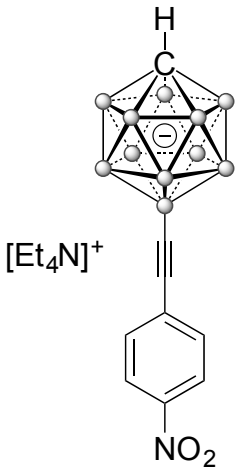

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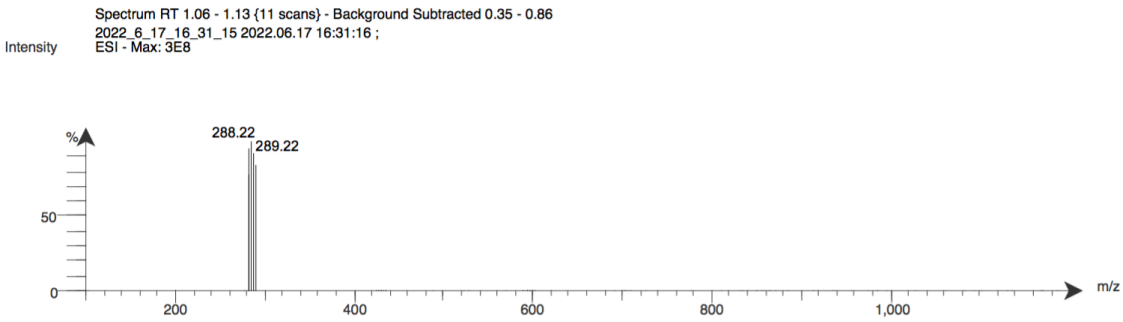

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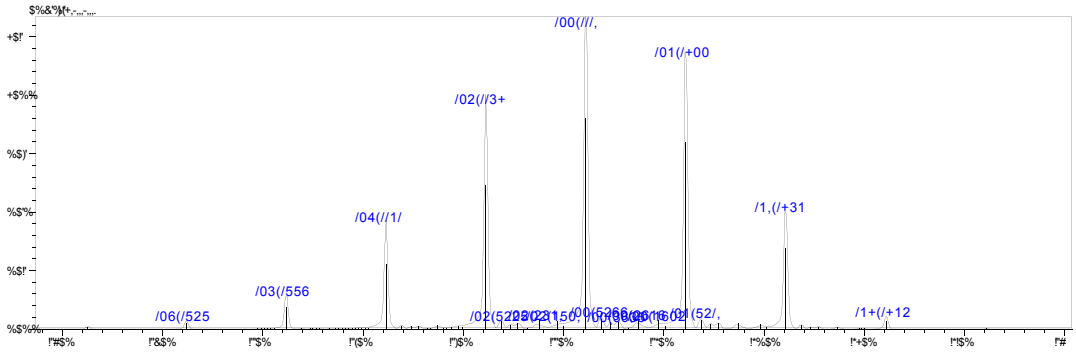

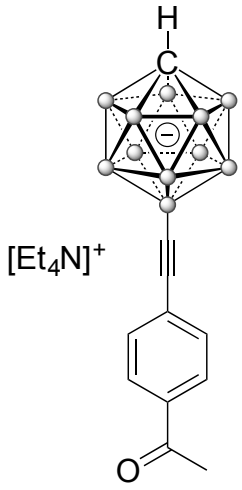

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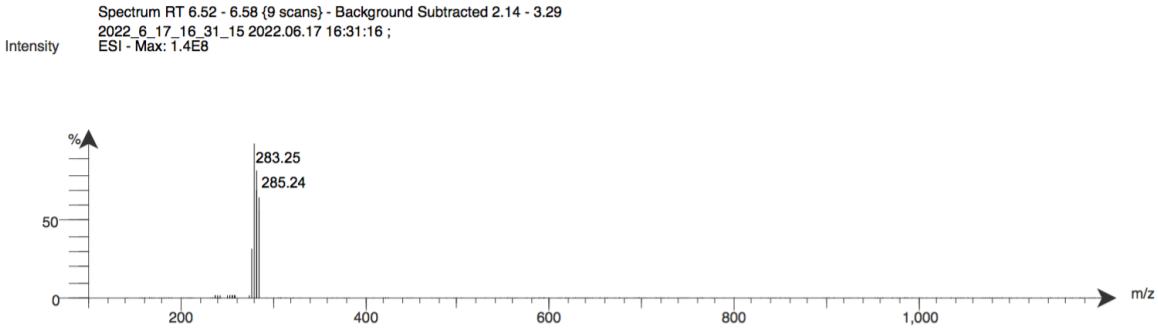

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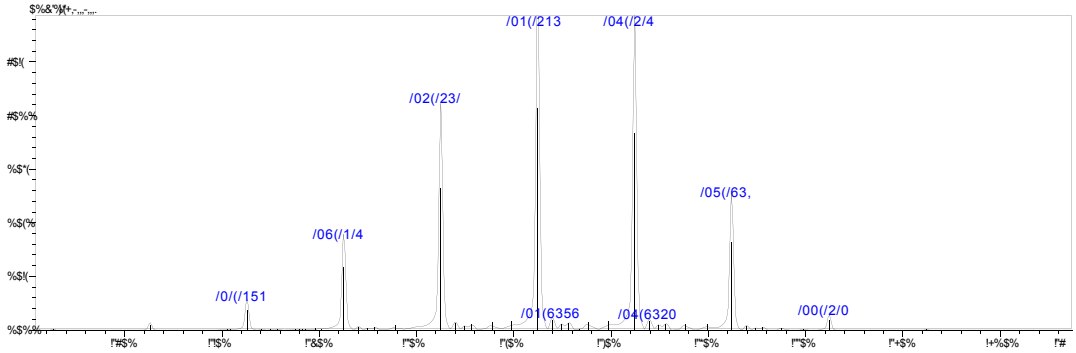

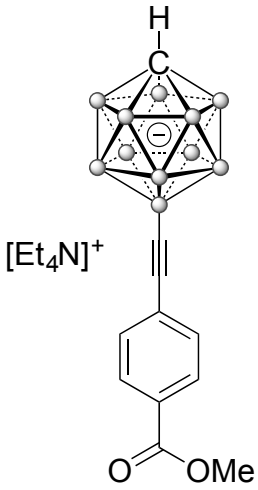

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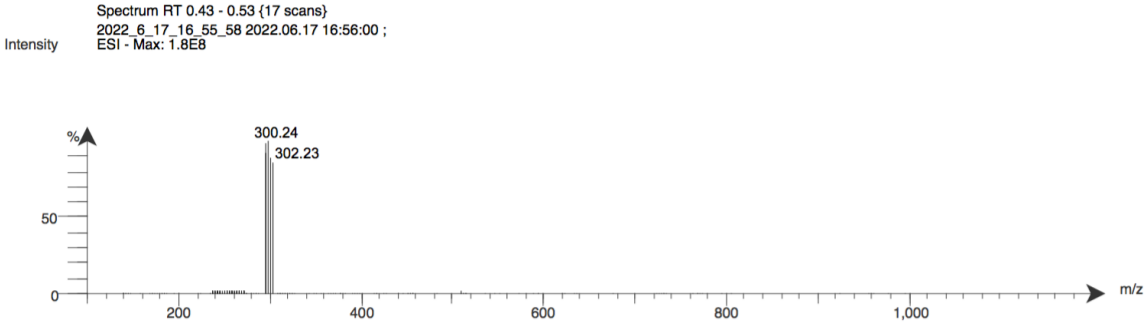

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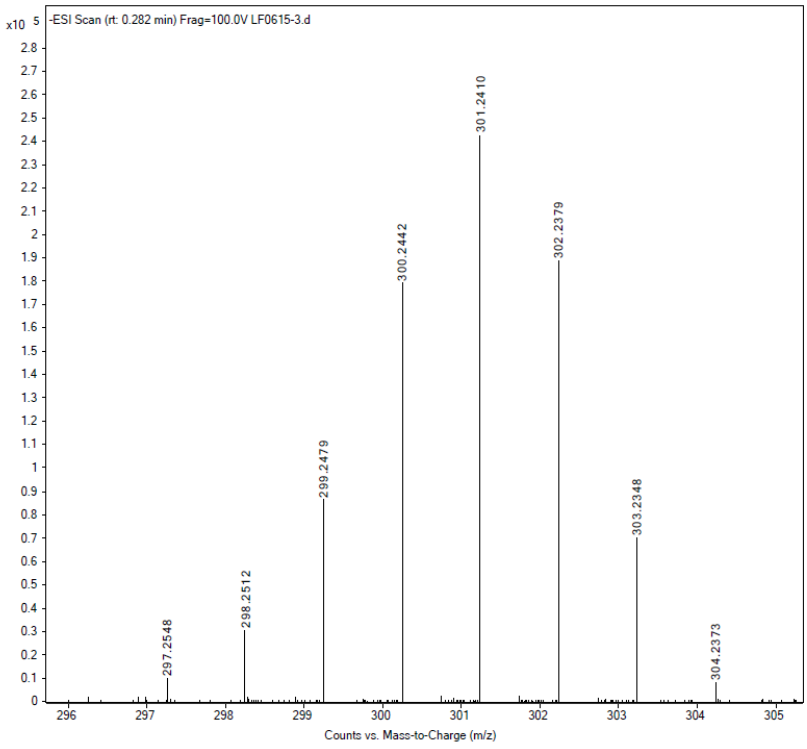

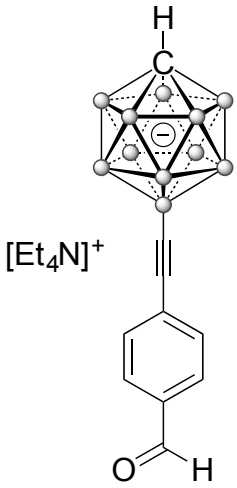

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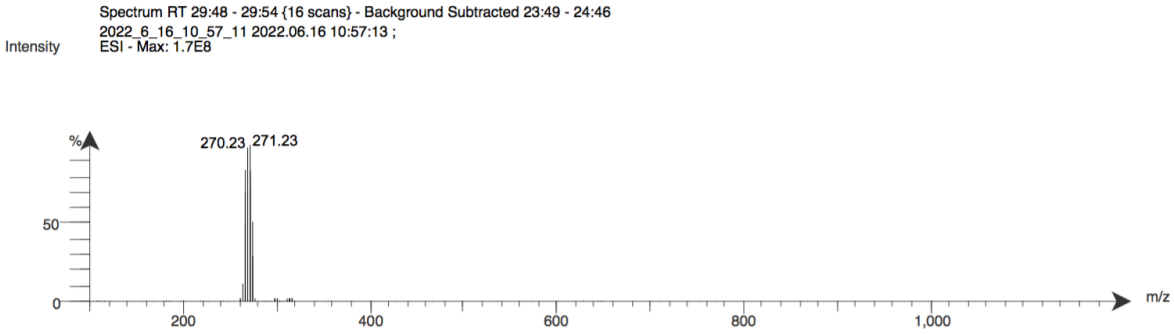

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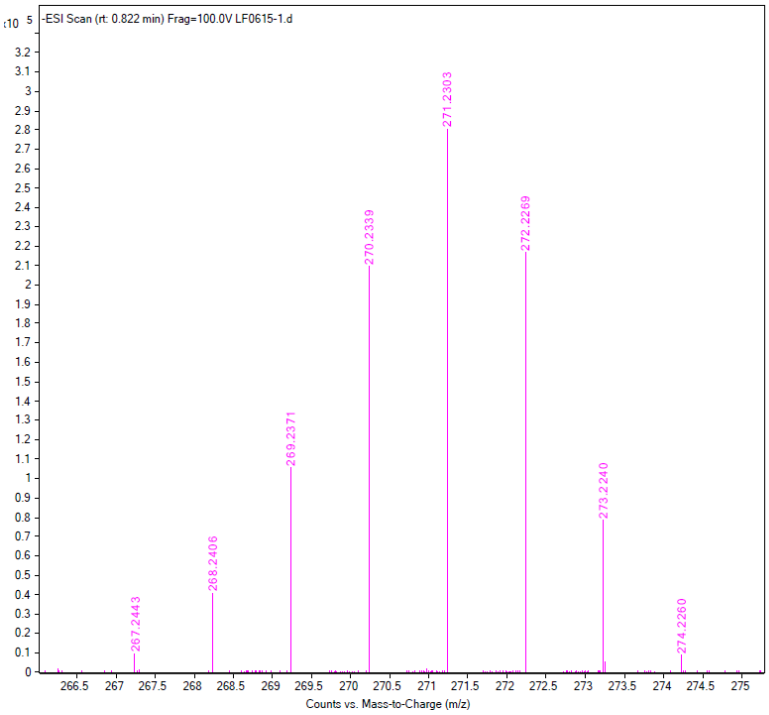

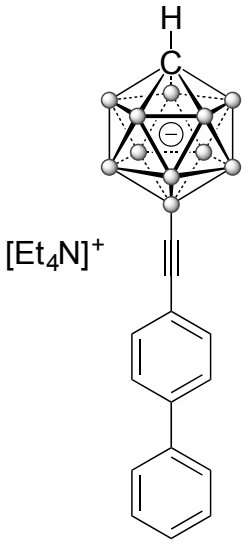

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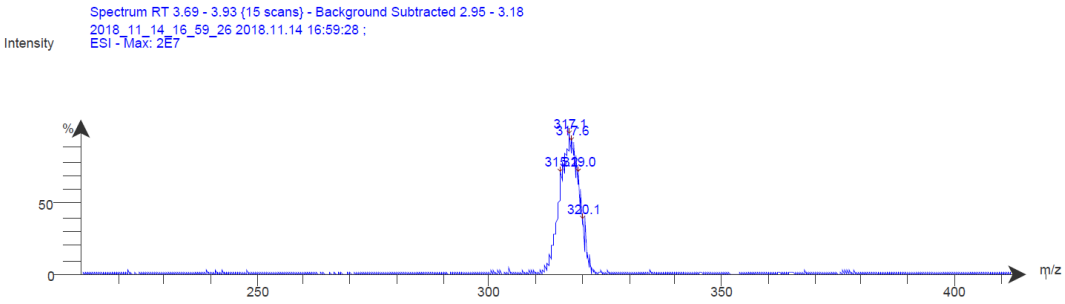

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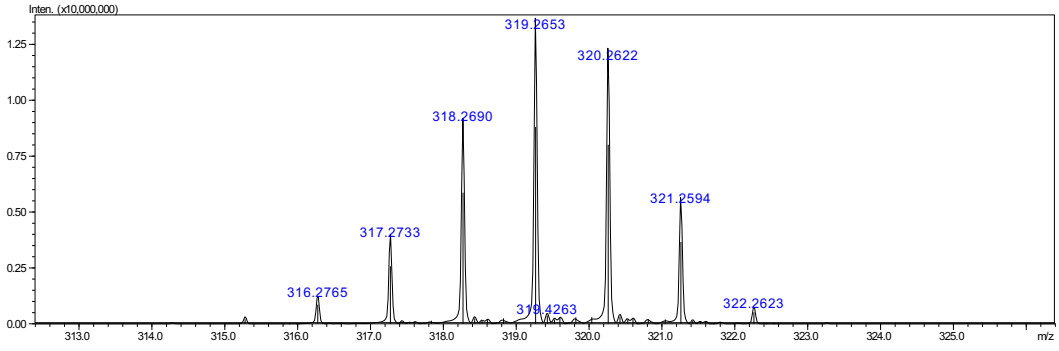

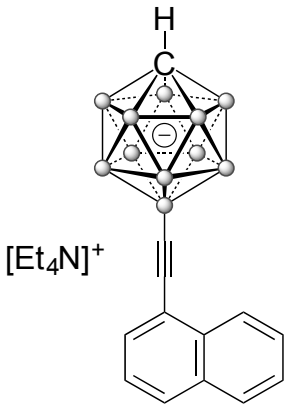

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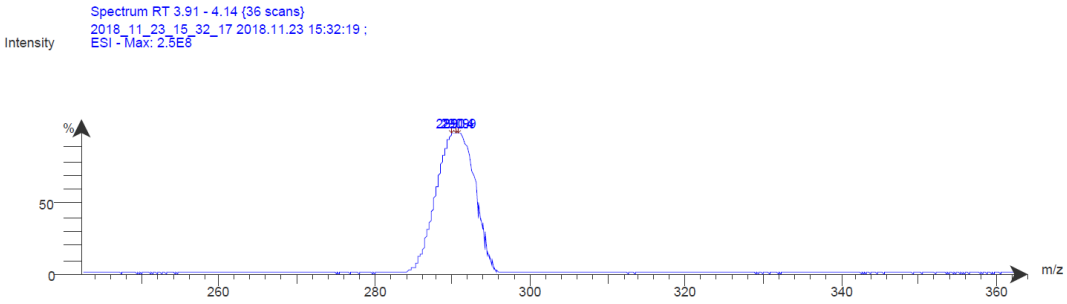

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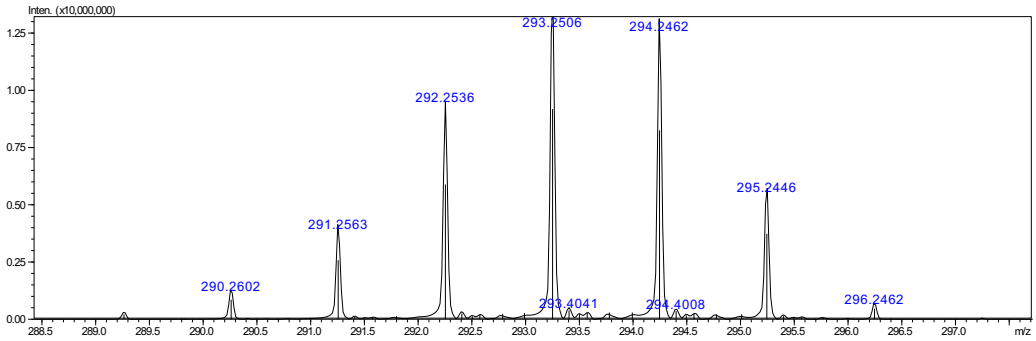

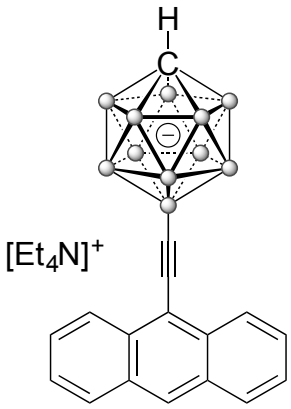

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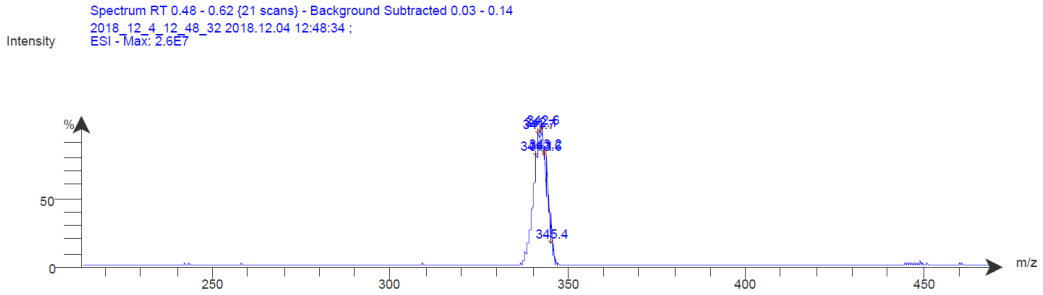

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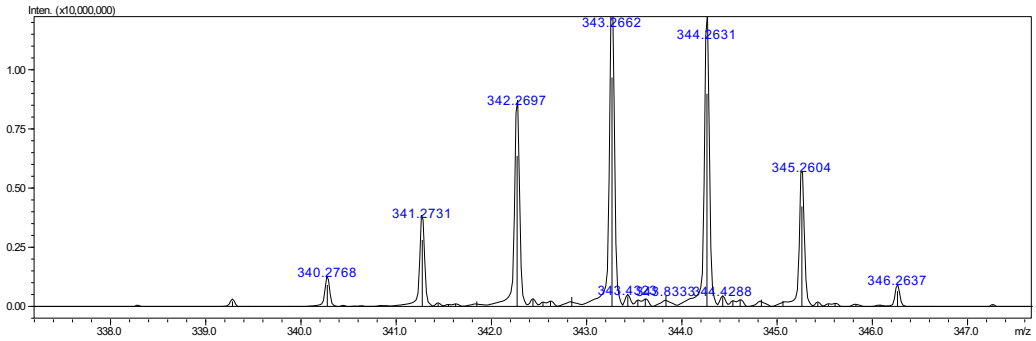

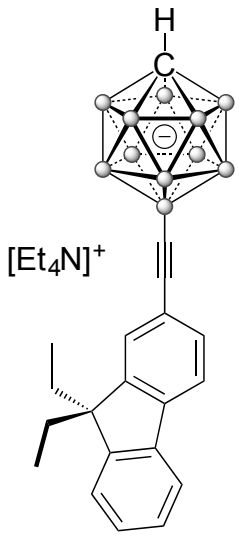

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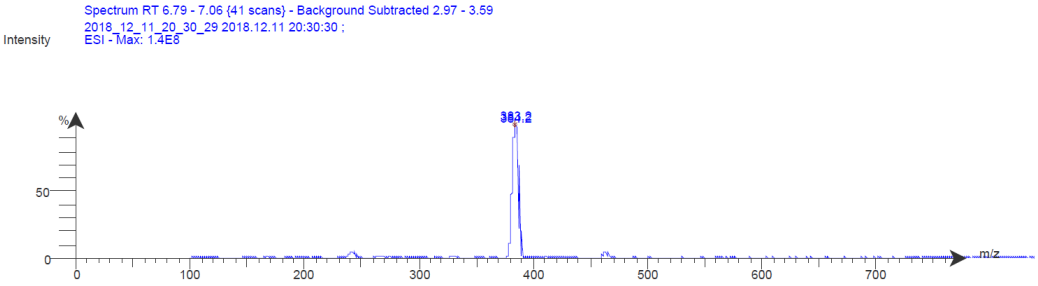

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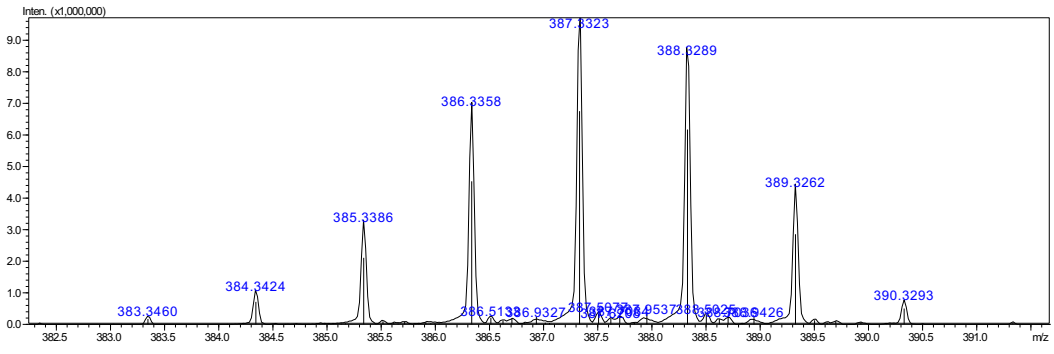

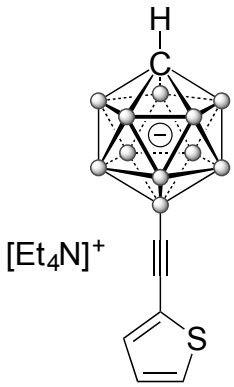

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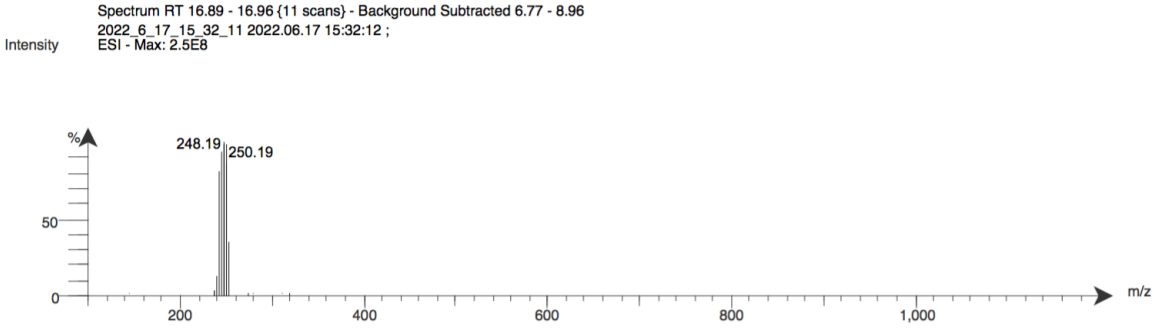

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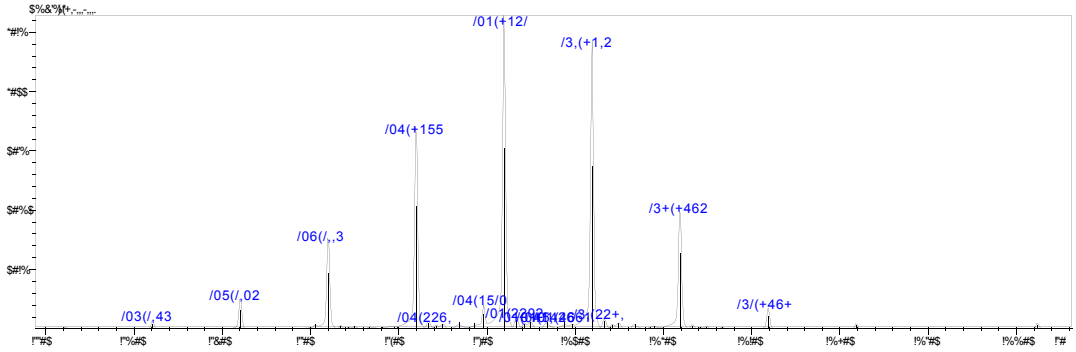

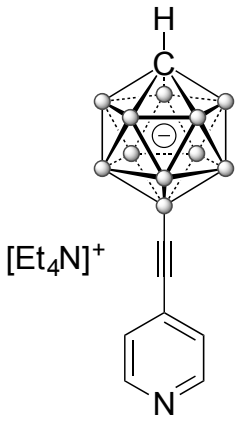

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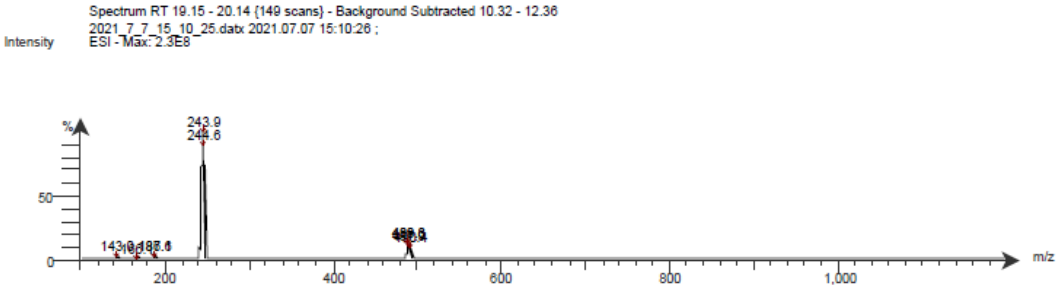
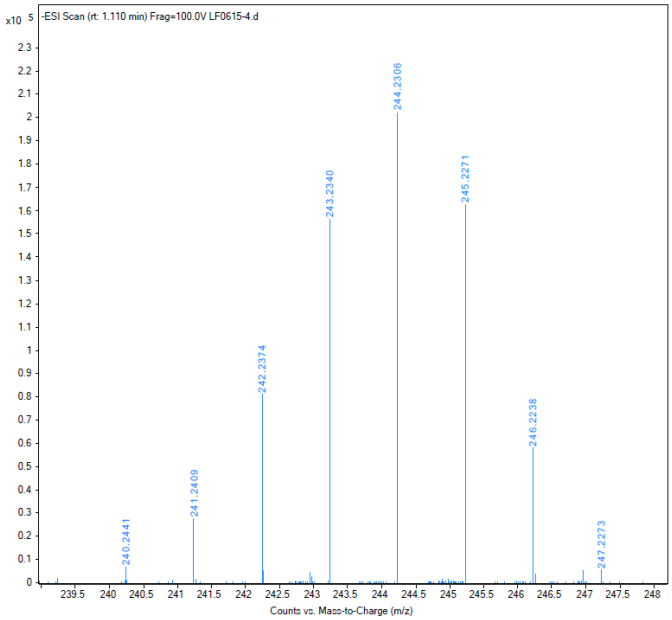
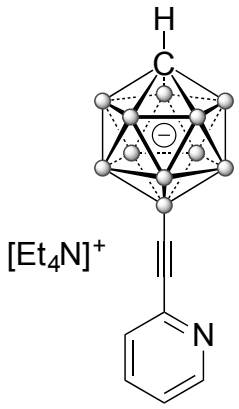


The small signal at *m/z* 489 corresponds to $[2M+H]^-$

Agilent MS





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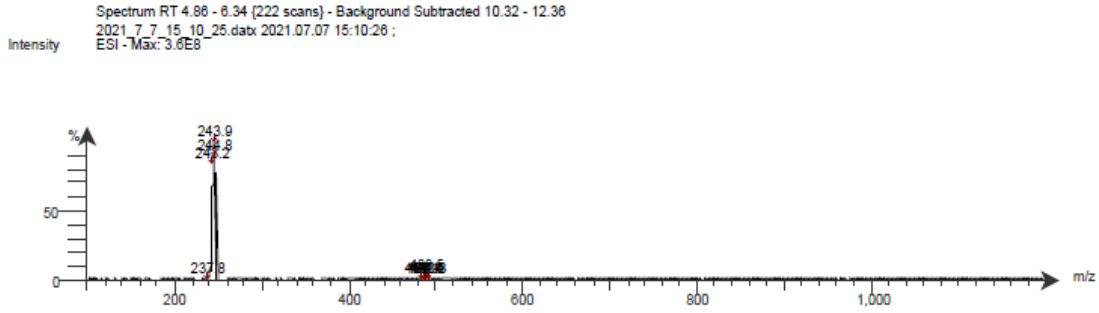
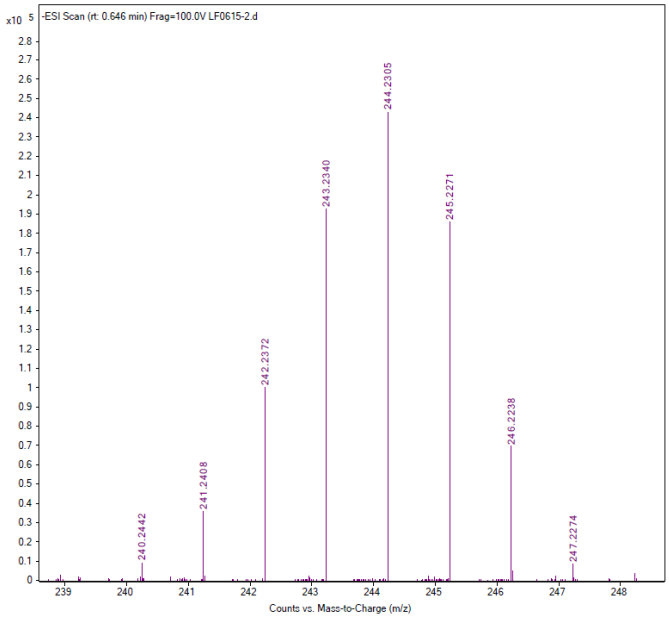
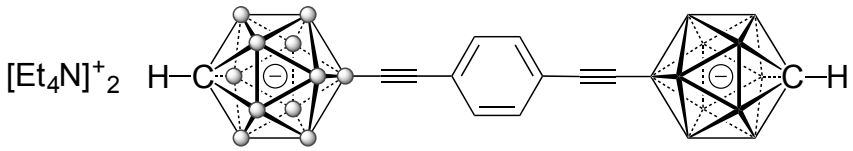


The small signal at *m/z* 489 corresponds to $[2M+H]^-$

Agilent MS





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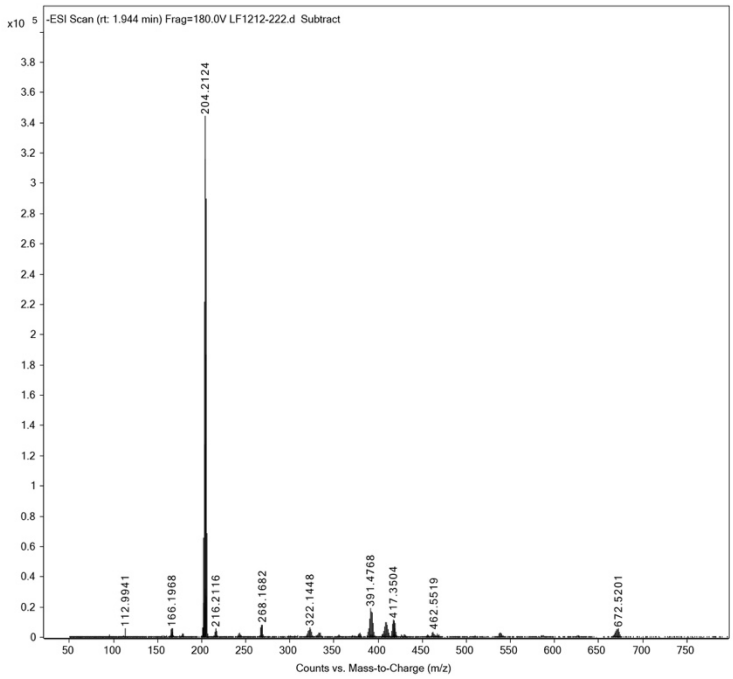

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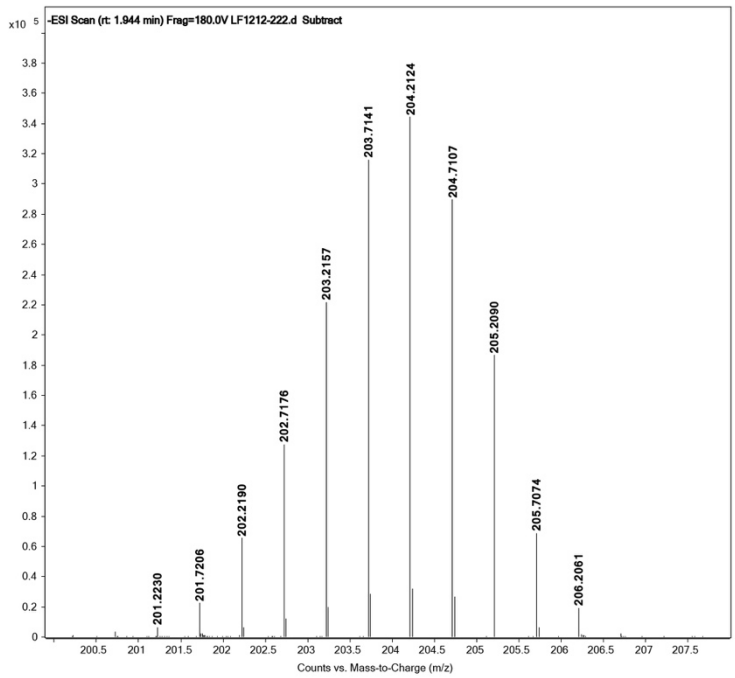

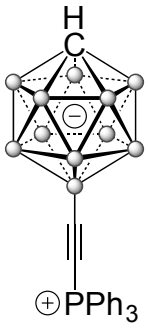

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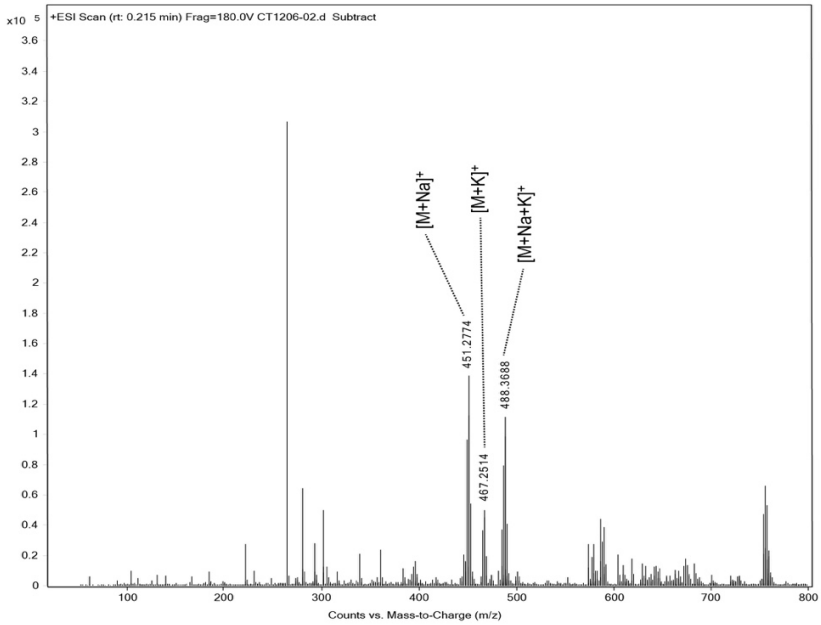

Agilent MS