

Supplementary Information for

**Palladium-Catalyzed Penta-Functionalization of Monocarboranes
with Alkenes *via* Regioselective B–H/C–H Bond Coupling**

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I General Information

Chemicals

If not otherwise specified, reagents and organic solvents were commercially available and used without further purification. Acetone-*d*₆ and acetonitrile-*d*₃ were purchased from Cambridge Isotope Laboratories and filtered through Al₂O₃ prior to use. Anhydrous solvents were prepared by passage through activated Al₂O₃ and stored over 3 Å molecular sieves. Previously reported carborane anions [CB₁₁H₁₂]⁻, [1-(CO₂H)-CB₁₁H₁₁]⁻, [1-(CO₂H)-CB₁₁H₁₀-12-Br]⁻, [CB₁₁H₁₁-12-Cl]⁻, [CB₁₁H₁₁-12-CH₃]⁻, [CB₁₁H₁₁-12-Ph]⁻, [1-(CO₂H)-CB₁₁H₁₀-12-CN]⁻ and **2u/v** were prepared according to the literature.[1-8]

Reaction Conditions

Glassware for air-sensitive reactions was dried at 150 °C for 12 h and allowed to cool in a vacuum.

Characterization

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

NMR spectra were recorded on a Bruker AVANCE III 500 spectrometer (¹H NMR 500.13 MHz, ¹³C NMR 125.77 MHz, ¹¹B NMR 160.46 MHz) or a Bruker AVANCE III 400 spectrometer (¹H NMR 400.13 MHz, ¹³C NMR 100.62 MHz, ¹¹B NMR 128.38 MHz) at 23 °C. Chemical shifts are given in ppm. ¹H NMR and ¹³C NMR spectra were referenced using the solvent signals (¹H: residual CHD₂C(O)CD₃ = 2.05 ppm, residual CHD₂CN = 1.94 ppm, ¹³C{¹H}: CD₃C(O)CD₃ = 29.84 ppm, CD₃CN = 1.32 ppm). ¹¹B and ¹¹B{¹H} NMR spectra were calibrated against external BF₃*Et₂O = 0 ppm (BF₃*Et₂O capillary in C₆D₆). 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.

General notes:

- The CH₃ group of the [Et₄N]⁺ cation showed $^3J_{1H,14N}$ coupling to the central nitrogen atom, and therefore the signal appeared as a triplet of triplets ($^3J_{1H,1H}$ and $^3J_{1H,14N}$). Generally speaking, coupling to ¹⁴N is sometimes observed in highly symmetrically coordinated nitrogen compounds; the coupling constant is not uniformly related to the distance to the nitrogen atom.
- In certain ¹H and ¹H{¹¹B} NMR spectra measured in acetone-*d*₆, double water peaks were observed. This is a result of different resonances from H₂O and HOD and has been described in the literature.[9]

Low-resolution ESI-MS data were recorded on Advion Expression CMS instrument. High-resolution MS data were recorded using IT-TOF detection (Shimadzu, Japan) equipped with an electrospray ionization source (ESI). Accurate mass determination was corrected by calibration using sodium trifluoroacetate clusters as a reference.

Single-crystal X-ray diffraction studies were performed on an Oxford Diffraction Gemini A Ultra diffractometer equipped with 135 mm Atlas CCD detector and using Mo or Cu X-ray sources or on a Bruker D8 Venture instrument with Ga wavelength.

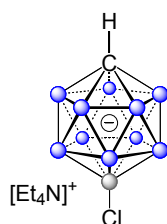
Elemental analysis was carried out by the analytical facilities of the Department of Chemistry at Zhejiang University. Three representative samples were measured in order to confirm that bulk purity by spectroscopic methods corresponded to bulk purity by elemental analysis:

3o: Analysis calculated for [Et₄N][C₄₂H₄₁B₁₁ClO₂]: C, 69.64; H, 7.13; N, 1.62; found: C, 69.44; H, 7.19; N, 1.53.

3r: Analysis calculated for [Et₄N][C₄₈H₄₆B₁₁O₂]: C, 74.40; H, 7.36; N, 1.55; found: C, 74.10; H, 7.46; N, 1.47.

4r: Analysis calculated for [Et₄N][C₄₇H₄₆B₁₁]: C, 76.81; H, 7.73; N, 1.63; found: C, 76.22; H, 7.92; N, 1.55.

II Experimental Section



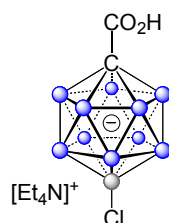
[Et₄N][CB₁₁H₁₁-12-Cl]: This carborane anion has been reported before.[5] A modified procedure is given below. The spectroscopic data match with those reported.

To a stirred solution of [Cs][CB₁₁H₁₂] (200 mg, 0.72 mmol) in CH₃OH (12 mL) was added *N*-chlorosuccinimide (105 mg, 0.79 mmol). The reaction mixture was then stirred at 40 °C for 24 h while being monitored by (–)-ESI mass spectrometry. Na₂SO₃ (19 mg, 0.15 mmol) was added to the mixture, followed by 1 M HCl (30 mL). Methanol was removed under reduced pressure. The aqueous solution was extracted with Et₂O (3 x 35 mL). Water (15 ml) was added to the combined extracts, and Et₂O was removed under reduced pressure. The aqueous solution was filtered, and [Et₄N]Br (227 mg, 1.08 mmol) was added to the filtrate. The precipitate that formed was collected by vacuum filtration, washed with water and dried under vacuum to give a colorless solid (157 mg, 71%).

¹H{¹¹B} NMR (400 MHz, acetone-*d*₆, 23 °C): δ 3.48 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.19-2.07 (m, 1H, CH), 2.02-1.70 (broad signal, 5H, BH), 1.69-1.47 (broad signal, 5H, BH), 1.39 (tt, *J* = 7.3 Hz, 1.8 Hz, 12H, CH₃ of cation).

¹¹B{¹H} NMR (128 MHz, acetone-*d*₆, 23 °C): δ 3.78 (1B), -12.75 (5B), -17.55 (5B).

¹³C{¹H} NMR (101 MHz, acetone-*d*₆, 23 °C): δ 52.99 (CH₂ of cation), 42.63 (cage C), 7.66 (CH₃ of cation).



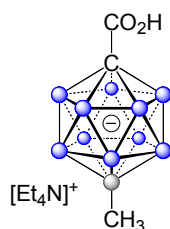
1b: A dry 100 mL round bottom flask equipped with magnetic stir bar was charged with [Et₄N][CB₁₁H₁₁-12-Cl] (600 mg, 1.95 mmol) and capped with a rubber septum. Anhydrous THF (25 mL) was then added to the flask, and the resulting solution was cooled to 0 °C in an ice bath. A solution of *n*-BuLi (2.5 M in hexane, 2.4 mL, 6 mmol) was slowly added. After 1 h of stirring at 0 °C, a slightly turbid, yellowish solution was obtained. Dry CO₂ gas was then bubbled through the mixture at 0 °C (2-3 bubbles/s) for 5 h. Water (2 mL) was slowly added, and the solution was concentrated on a rotary evaporator. The residue was dissolved in water and washed with diethyl ether (under these basic conditions the dianionic product was in the water layer). The aqueous phase was acidified with 1 M HCl (pH = 2) and extracted with diethyl ether (3 x 40 mL). The combined organic extracts were evaporated under reduced pressure, and the crude product was dissolved in water (10 mL) and filtered through a glass frit. [Et₄N]Br (630 mg, 3 mmol) was added to the filtrate, and the resulting white precipitate was collected in a glass frit and dried in a vacuum to give **1b** (556 mg, 81% yield).

¹H{¹¹B} NMR (500 MHz, acetone-*d*₆, 23 °C): δ 3.48 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 1.94 (broad signal, 5H, BH), 1.86 (broad signal, 5H, BH), 1.40 (tt, *J* = 7.3 Hz, 1.9 Hz, 12H, CH₃ of cation).

¹¹B{¹H} NMR (160 MHz, acetone-*d*₆, 23 °C): δ 5.12 (1B), -12.63 (5B), -15.11 (5B).

¹³C{¹H} NMR (125 MHz, acetone-*d*₆, 23 °C): δ 168.57 (CO), 60.77 (cage C), 53.02 (CH₂ of cation), 7.66 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₂H₁₁B₁₁ClO₂]⁻, 221.1544; found, 221.1542.



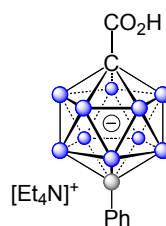
1d: Following a similar procedure as for the preparation of **1b**, using [Et₄N][CB₁₁H₁₁-12-Me] (500 mg, 1.74 mmol) as starting material, **1d** was obtained as a colorless solid (438 mg, 76%).

¹H{¹¹B} NMR (500 MHz, acetone-*d*₆, 23 °C): δ 3.48 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 1.94 (broad signal, 5H, BH), 1.62 (broad signal, 5H, BH), 1.40 (tt, *J* = 7.3 Hz, 1.9 Hz, 12H, CH₃ of cation), 0.00 (s, 3H, CH₃).

¹¹B{¹H} NMR (160 MHz, acetone-*d*₆, 23 °C): δ 2.45 (s, 1B), -11.83 (s, 5B), -14.26 (s, 5B).

¹³C{¹H} NMR (125 MHz, acetone-*d*₆, 23 °C): δ 168.95 (CO), 62.32 (cage C), 53.00 (CH₂ of cation), 7.67 (CH₃ of cation). The CH₃ group appeared as a broad and weak signal at 5.5 ppm.

HRMS (ESI): *m/z* Calcd. for [C₃H₁₄B₁₁O₂]⁻, 201.2090; found, 201.2093.



1e: Following a similar procedure as for the preparation of **1b**, using $[\text{Et}_4\text{N}][\text{CB}_{11}\text{H}_{11}\text{-12-Ph}]$ (500 mg, 1.43 mmol) as starting material, **1e** was obtained as a colorless solid (388 mg, 69%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 7.42-7.32 (m, 2H, ArH), 7.05-6.90 (overlapping m, 3H, ArH), 3.43 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.04 (broad signal overlapping with solvent residual signal, 5H, BH), 1.85 (broad signal, 5H, BH), 1.35 (tt, $J = 7.3\text{Hz}, 1.9$ Hz, 12H, CH_3 of cation).

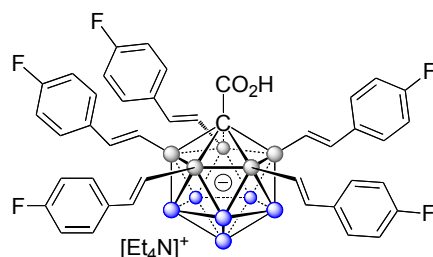
$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6 , 23 °C): δ 3.20 (s, 1B), -12.39 (s, , 5B), -14.20 (s, 5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6 , 23 °C): δ 168.75 (CO), 133.56, 126.89, 125.41 (aryl C), 64.64 (cage C), 52.96 (CH_2 of cation), 7.64 (CH_3 of cation). The B-C(*ipso*) signal could not be detected unambiguously.

HRMS (ESI): m/z Calcd. for $[\text{C}_8\text{H}_{16}\text{B}_{11}\text{O}_2]^-$, 263.2247; found, 263.2244.

General Procedure A for the palladium-catalyzed penta-alkenylation

To a 10 mL glass vial equipped with a magnetic stir bar, carborane carboxylic acid **1** (0.150 mmol), Pd(OAc)₂ (0.015 mmol), AgOAc (1.5 mmol) and dry acetonitrile (4 mL) were added. To the stirring mixture the required alkene **2** (0.81 mmol) was added, and the resulting mixture was stirred for 24 h at 25 °C. The mixture was filtered through celite, and the filtrate was treated with [Et₄N]Br (5 equiv). The white precipitate that formed was removed by filtration, and the filtrate was then evaporated to dryness under reduced pressure. Purification was done by chromatography on silica gel by eluting with CH₂Cl₂ to afford the desired product **3**.



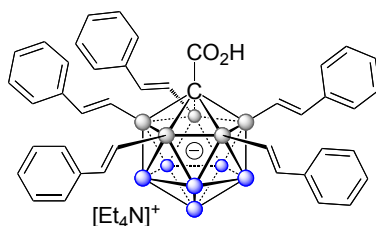
3a: Prepared following the general procedure A, using **1a** and 4-fluorostyrene, **3a** was obtained as a colorless solid (118 mg, 86%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 7.46-7.31 (m, 10H, ArH), 7.12-6.98 (m, 10H, ArH), 6.94 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 6.66 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 3.32 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.48-1.56 (overlapping broad signals, 6H, BH), 1.29 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6 , 23 °C): δ ca. -2.02 to -9.83 (overlapping signals, 6B), -12.90 (overlapping signals, 5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6 , 23 °C): δ 165.75 (CO), 162.40 (d, $J = 243$ Hz, C-F), 138.27 (BCHCH), 137.55 (d, $J = 3.0$ Hz, C(*ipso*)), 131.66 (broad signal, BCH), 128.03 (d, $J = 7.7$ Hz, C(*ortho*)), 115.75 (d, $J = 22.0$ Hz, C(*meta*)), 68.38 (cage C), 52.88 (CH_2 of cation), 7.56 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{42}\text{H}_{37}\text{B}_{11}\text{F}_5\text{O}_2]^-$, 787.3810; found, 787.3833.



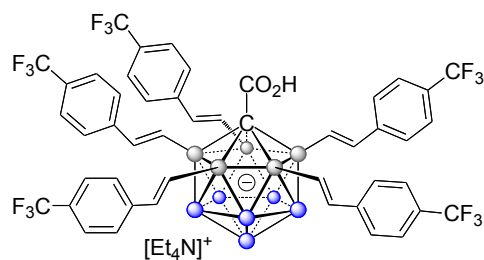
3b: Prepared following the general procedure A, using **1a** and styrene, **3b** was obtained as a colorless solid (93 mg, 75%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6 , 23 °C): δ 7.41-7.28 (m, 10H, ArH), 7.27-7.16 (m, 10H, ArH), 7.15-7.05 (m, 5H, ArH), 6.96 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 6.73 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 3.37 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.15-1.35 (m, 6H, BH), 1.31 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6 , 23 °C): δ ca. -3.51 to -10.11 (overlapping signals, 6B), ca. -12.95 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6 , 23 °C): δ 165.83 (CO), 141.29 (aryl C), 139.58 (BCHCH), 132.26 (broad signal, BCH), 129.10 (aryl CH), 127.08 (aryl CH), 126.57 (aryl CH), 68.53 (cage C), 52.96 (CH_2 of cation), 7.63 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{42}\text{H}_{42}\text{B}_{11}\text{O}_2]^-$, 697.4281; found, 697.4326.



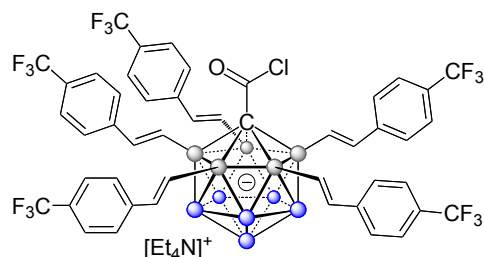
3c: Prepared following the general procedure A, using **1a** and 4-trifluoromethylstyrene, **3c** was obtained as a colorless solid (122 mg, 70%).

¹H{¹¹B} NMR (500 MHz, acetone-*d*₆, 23 °C): δ 7.69-7.47 (overlapping m, 20H, ArH), 7.04 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 6.90 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 3.41 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.47-1.76 (overlapping broad signals, 6H, BH), 1.34 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation).

¹¹B{¹H} NMR (160 MHz, acetone-*d*₆, 23 °C): δ ca. -2.46 to -9.26 (overlapping signals, 6B), -12.52 (5B).

¹³C{¹H} NMR (125 MHz, acetone-*d*₆, 23 °C): δ 165.67 (CO), 144.67 (C(*ipso*)), 138.57 (BCHCH), 135.13 (broad signal, BCHCH), 128.50 (q, *J* = 32 Hz, C(*para*)), 126.97 (C(*ortho*)), 126.19 (C(*meta*)), 125.55 (q, *J* = 271 Hz, CF₃), 68.51 (cage C), 52.98 (CH₂ of cation), 7.61 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₄₇H₃₇B₁₁F₁₅O₂]⁻, 1037.3650; found, 1037.3671.



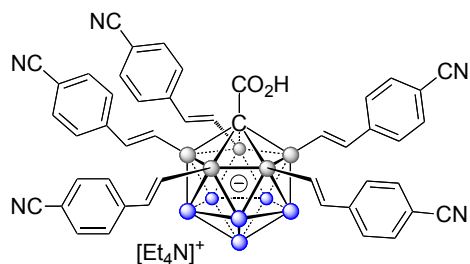
3c-Cl: To a stirred solution of **3c** (105 mg, 0.090 mmol) in dry CH_2Cl_2 (5 mL) were added dimethylformamide (4 drops) and oxalyl chloride (0.015 mL, 0.18 mmol) under nitrogen atmosphere. The reaction mixture was allowed to stir for 15 min at room temperature. All the volatiles were removed carefully under vacuum with nitrogen-cooled solvent traps. The residue was then stirred with hexane (5 mL) at 25 °C for 10 min and collected by filtration through a glass frit. After drying in a vacuum, a colorless solid was obtained and identified as acid chloride **3c-Cl** in >95% purity as evidenced by NMR spectroscopy and mass spectrometry (99 mg, 93% yield).

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetonitrile- d_3 , 23 °C): δ 7.65-7.48 (overlapping m, 20H, ArH), 7.04 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 6.69 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 3.12 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.58-1.58 (overlapping broad signals, 6H, BH), 1.18 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetonitrile- d_3 , 23 °C): δ ca. -0.80 to -9.40 (overlapping signals, 6B), -12.52 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetonitrile- d_3 , 23 °C): δ 166.26 (CO), 143.96 (C(*ipso*)), 140.06 (BCHCH), 132.47 (broad signal, BCHCH), 128.98 (q, $J = 32$ Hz, C(*para*)), 127.20 (C(*ortho*)), 126.38 (C(*meta*)), 125.55 (q, $J = 270$ Hz, CF_3), 74.90 (cage C), 52.99 (CH_2 of cation), 7.60 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{47}\text{H}_{36}\text{B}_{11}\text{ClF}_{15}\text{O}]^-$, 1055.3311; found, 1055.3348.



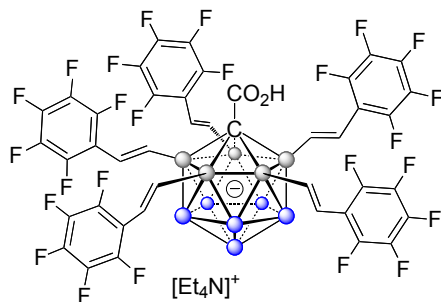
3d: Prepared following the general procedure A, using **1a** and 4-cyanostyrene, **3d** was obtained as a colorless solid (90 mg, 63%).

¹H{¹¹B} NMR (400 MHz, acetone-*d*₆, 23 °C): δ 7.70-7.57 (m, 10H, ArH), 7.56-7.45(m, 10H, ArH), 6.97 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 6.87 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 3.48 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.29-1.84 (overlapping broad signals, 6H, BH), 1.39 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation).

¹¹B{¹H} NMR (128 MHz, acetone-*d*₆, 23 °C): δ ca. -3.11 to -9.13 (overlapping signals, 6B), -12.50 (5B).

¹³C{¹H} NMR (100 MHz, acetone-*d*₆, 23 °C): δ 165.55 (CO), 145.07 (aryl C), 138.59 (BCHCH), 136.13 (broad signal, BCHCH), 133.17, 127.23 (aryl C), 119.67 (CN), 110.37 (aryl C), 68.45 (cage C), 52.96 (CH₂ of cation), 7.63 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₄₇H₃₇B₁₁N₅O₂]⁻, 822.4043; found, 822.4064.



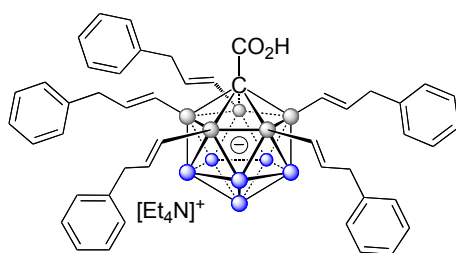
3e: Prepared following the general procedure A, using **1a** and pentafluorostyrene, **3e** was obtained as a colorless solid (102 mg, 53%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6 , 23 °C): δ 6.98 (d, $J = 18.6$ Hz, 5H, alkenyl CH), 6.83 (d, $J = 18.6$ Hz, 5H, alkenyl CH), 3.51 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.49-2.05 (overlapping broad signals, 6H, BH), 1.41 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6 , 23 °C): δ ca. -3.90 to -9.30 (overlapping signals, 6B), -12.41 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6 , 23 °C): δ 164.97 (CO), 145.51 (m with $^1J_{\text{C-F}} = 248$ Hz, aryl C), 142.42 (broad signal, BCHCH), 140.08 (m with $^1J_{\text{C-F}} = 250$ Hz, C(*para*)), 138.57 (m with $^1J_{\text{C-F}} = 246$ Hz, aryl C), 123.55 (BCHCH), 115.40 (t, $J = 13$ Hz, C(*ipso*)), 68.36 (cage C), 53.05 (CH_2 of cation), 7.66 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{42}\text{H}_{17}\text{B}_{11}\text{F}_{25}\text{O}_2]^-$, 1147.1926; found, 1147.1946.



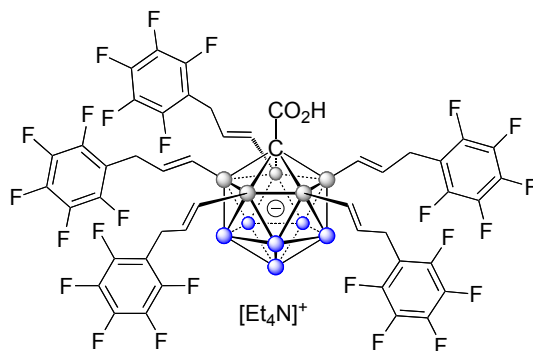
3f: Prepared following the general procedure A, using **1a** and allylbenzene, **3f** was obtained as a colorless solid (97 mg, 72%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 7.35-7.17 (overlapping m, 20H, ArH), 7.16-7.07 (m, 5H, ArH), 6.18-5.97 (m, 5H, alkenyl CH), 5.96-5.78 (m, 5H, alkenyl CH), 3.57-3.17 (overlapping signals, 18H, CH_2 of cation and PhCH_2), 2.00-1.61 (broad overlapping signals, 6H, BH), 1.30 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6 , 23 °C): δ ca. -1.41 to -10.05 (overlapping signals, 6B), -13.51 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6 , 23 °C): δ 165.46 (CO), 142.74 (aryl C), 138.97 (BCHCH), 133.33 (broad signal, BCH), 129.43 (aryl CH), 128.86 (aryl CH), 126.22 (aryl CH), 68.30 (cage C), 52.96 (CH_2 of cation), 43.36 (PhCH_2), 7.64 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{47}\text{H}_{52}\text{B}_{11}\text{O}_2]^-$, 767.5064; found, 767.5081.



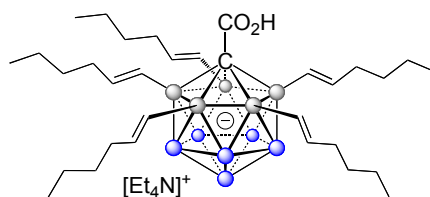
3g: Prepared following the general procedure A, using **1a** and allylpentafluorobenzene, **3g** was obtained as a colorless solid (119 mg, 59%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 5.88-5.64 (m, 5H, alkenyl CH), 5.48 (d, $J = 17.3$ Hz, 5H, alkenyl CH), 3.49 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 3.31 (d, $J = 5.4$ Hz, 10H, CH_2), 2.02-1.45 (overlapping broad signals, 6H, BH), 1.39 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6 , 23 °C): δ ca. -3.82 to -10.32 (overlapping signals, 6B), ca. -13.71 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6 , 23 °C): δ 164.92 (CO), 145.79 (m with $^1J_{\text{C-F}} = 244$ Hz, aryl C), 140.18 (m with $^1J_{\text{C-F}} = 248$ Hz, C(*para*)), 138.18 (m with $^1J_{\text{C-F}} = 248$ Hz, aryl C), 133.81 (one sharp and one broad signal, overlapping, BCHCH and BCHCH), 115.71 (t, $J = 19$ Hz, C(*ipso*)), 67.93 (cage C), 53.01 (CH_2 of cation), 28.63 (CH_2), 7.64 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{47}\text{H}_{27}\text{B}_{11}\text{F}_{25}\text{O}_2]^-$, 1217.2708; found, 1217.2728.



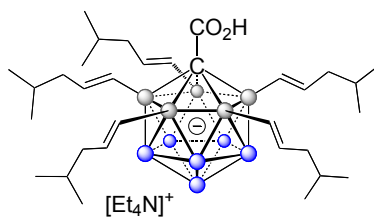
3h: Prepared following the general procedure A, using **1a** and 1-hexene, **3h** was obtained as a colorless solid (88 mg, 81%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6 , 23 °C): δ 6.00-5.79 (m, 5H, alkenyl CH), 5.60 (d, $J = 17.40$ Hz, 5H, alkenyl CH), 3.47 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.05-1.89 (m, 10H, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$) 1.84-1.53 (overlapping broad signals, 6H, BH), 1.39 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation), 1.36-1.22 (overlapping m, 20H, $\text{CH}_3\text{CH}_2\text{CH}_2$), 1.00-0.75 (m, 15H, CH_3CH_2).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6 , 23 °C): δ ca. -3.63 to -10.17 (overlapping signals, 6B), -13.68 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6 , 23 °C): δ 164.42 (CO), 141.48 (BCHCH), 130.94 (broad signal, BCHCH), 68.77 (cage C), 53.02 (CH_2 of cation), 36.49 ($\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$), 32.57 ($\text{CH}_3\text{CH}_2\text{CH}_2$), 22.76 (CH_3CH_2), 14.34 (CH_3CH_2), 7.70 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{32}\text{H}_{62}\text{B}_{11}\text{O}_2]^-$, 597.5846; found, 597.5843.



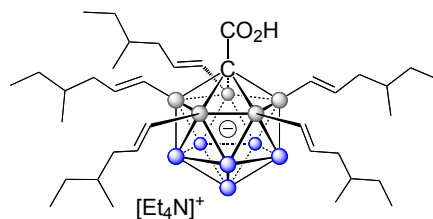
3i: Prepared following the general procedure A, using **1a** and 4-methyl-1-pentene, **3i** was obtained as a colorless solid (92 mg, 84%).

¹H{¹¹B} NMR (500 MHz, acetone-*d*₆, 23 °C): δ 5.95-5.84 (m, 5H, alkenyl CH), 5.62 (d, *J* = 17.40 Hz, 5H, alkenyl CH), 3.48 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 1.95-1.85 (m, 10H, CH₂), 1.84-1.64 (overlapping broad signals, 6H, BH), 1.63-1.52 (m, 5H, (CH₃)₂CH), 1.39 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation), 0.94-0.81 (m, 30H, (CH₃)₂CH).

¹¹B{¹H} NMR (160 MHz, acetone-*d*₆, 23 °C): δ ca. -3.64 to -10.39 (overlapping signals, 6B), -13.56 (5B).

¹³C{¹H} NMR (101 MHz, acetone-*d*₆, 23 °C): δ 164.57 (CO), 140.09 (BCHCH), 132.74 (broad signal, BCHCH), 68.53 (cage C), 53.00 (CH₂ of cation), 46.52 (CH₂), 29.34 (CH₃)₂CH, 22.80 (CH₃)₂CH, 7.68 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₃₂H₆₂B₁₁O₂]⁻, 597.5846; found, 597.5849.



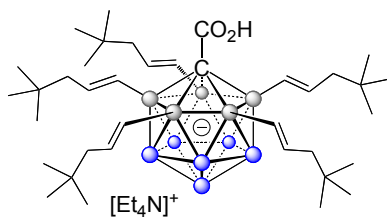
3j: Prepared following the general procedure A, using **1a** and (\pm)-4-methyl-1-hexene, **3j** was obtained as a colorless solid (98 mg, 82%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6 , 23 °C): δ 6.00-5.79 (m, 5H, alkenyl CH), 5.63 (d, $J = 17.40$ Hz, 5H, alkenyl CH), 3.48 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.05-1.96 (m, 5H, BCHCHCH_2), 1.92-1.80 (m, 5H, BCHCHCH_2), 1.79-1.53 (broad overlapping signals, 6H, BH), 1.48-1.33 (overlapping m, 22H, CH_3CH_2 and CH_3 of cation), 1.20-1.05 (m, 5H, CH_3CH), 0.92-0.78 (overlapping m, 30H, CH_3).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6 , 23 °C): δ ca. -3.66 to -10.58 (overlapping signals, 6B), -13.18 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6 , 23 °C): δ 164.52 (CO), 139.96 (BCHCH), 132.62 (broad signal, BCHCH), 68.60 (cage C), 53.03 (CH_2 of cation), 44.21 (BCHCHCH_2), 35.87 (CH_3CH), 19.62 (CH_3CH), 11.88 (CH_3CH_2), 7.69 (CH_3 of cation). One CH_2 signal could not be detected unambiguously because of overlap with the solvent signal.

HRMS (ESI): m/z Calcd. for $[\text{C}_{37}\text{H}_{72}\text{B}_{11}\text{O}_2]^-$, 667.6629; found, 667.6634.



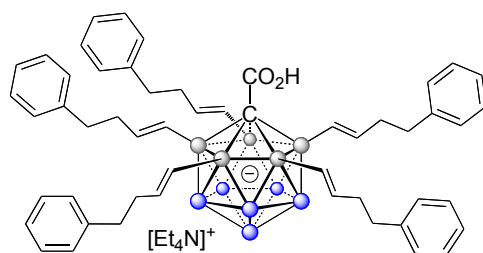
3k: Prepared following the general procedure A, using **1a** and 4,4-dimethyl-1-pentene, was obtained as a colorless solid **3k** (94 mg, 79%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 6.13-5.83 (m, 5H, alkenyl CH), 5.67 (d, $J = 17.40$ Hz, 5H, alkenyl CH), 3.48 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 1.98-1.84 (m, 10H, CH_2), 1.83-1.52 (overlapping broad signals, 6H, BH), 1.39 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation), 0.94-0.82 (s, 45H, $(\text{CH}_3)_3\text{C}$).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6 , 23 °C): δ ca. -3.02 to -10.49 (overlapping signals, 6B), -13.57 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6 , 23 °C): δ 164.64 (CO), 138.29 (BCHCH), 134.09 (broad signal, BCHCH), 68.35 (cage C), 53.00 (CH_2 of cation), 51.65 (CH_2), 31.73 ($(\text{CH}_3)_3\text{C}$), 7.67 (CH_3 of cation). The carborane CH_3 signal could not be detected unambiguously because of overlap with the solvent signal.

HRMS (ESI): m/z Calcd. for $[\text{C}_{37}\text{H}_{72}\text{B}_{11}\text{O}_2]^-$, 667.6629; found, 667.6638.



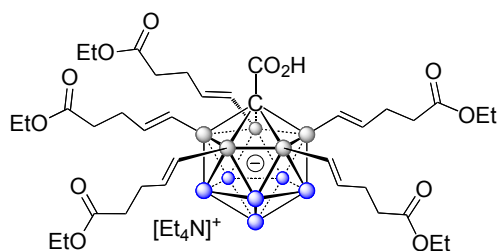
3I: Prepared following the general procedure A, using **1a** and 4-phenyl-1-butene, **3I** was obtained as a colorless solid (110 mg, 76%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 7.38-7.18 (overlapping m, 20H, ArH), 7.17-7.06 (m, 5H, ArH), 6.20-5.88 (m, 5H, alkenyl CH), 5.75 (d, $J = 17.5$ Hz, 5H, alkenyl CH), 3.38 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.79-2.55 (m, 10H, CH_2), 2.46-2.20 (m, 10H, CH_2), 2.01-1.53 (overlapping broad signals, 6H, BH), 1.32 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6 , 23 °C): δ ca. -0.80 to -10.66 (overlapping signals, 6B), -13.47 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6 , 23 °C): δ 164.82 (CO), 143.45 (BCHCH), 140.67 (aryl C), 131.41 (broad signal, BCH), 129.20 (aryl CH), 128.91 (aryl CH), 126.24 (aryl CH), 68.42 (cage C), 52.91 (CH_2 of cation), 38.98 (CH_2), 37.00 (CH_2), 7.63 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{52}\text{H}_{62}\text{B}_{11}\text{O}_2]^-$, 837.5846; found, 837.5870.



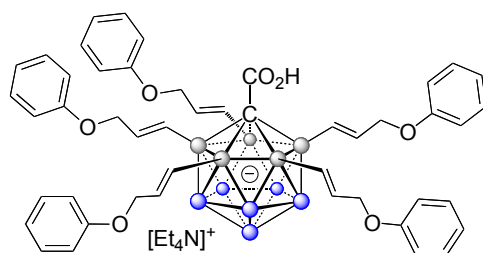
3m: Prepared following the general procedure A, using **1a** and ethyl 4-petenoate, **3m** was obtained as a colorless solid (94 mg, 66%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6 , 23 °C): δ 5.99-5.74 (m, 5H, BCHCH), 5.64 (d, $J = 17.5$ Hz, 5H, BCHCH), 4.07 (q, $J = 7.1$ Hz, 10H, CH_3CH_2), 3.50 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.51-2.16 (m, 20H, $(\text{CH}_2)_2\text{CO}_2\text{Et}$), 1.90-1.51 (broad overlapping signals, 6H, BH), 1.40 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation), 1.21 (t, $J = 7.1$ Hz, 15H, CH_3CH_2).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6 , 23 °C): δ ca. -4.55 to -9.71 (overlapping signals, 6B), -13.56 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6 , 23 °C): δ 173.42 (CO_2Et), 164.82 (COOH), 139.02 (BCHCH), 131.98 (broad signal, BCH), 66.28 (cage C), 60.36 (CH_3CH_2), 53.04 (CH_2 of cation), 35.03 ($\text{CH}_2\text{CH}_2\text{CO}_2\text{Et}$), 32.08 ($\text{CH}_2\text{CH}_2\text{CO}_2\text{Et}$), 14.62 (CH_3CH_2), 7.69 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{37}\text{H}_{62}\text{B}_{11}\text{O}_{12}]^-$, 817.5338; found, 817.5357.

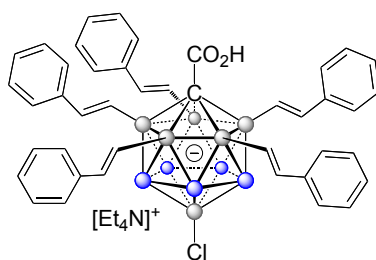


3n: Prepared following the general procedure A, using **1a** and allyl phenyl ether, **3n** was obtained as a colorless solid (108 mg, 74%).

¹H{¹¹B} NMR (500 MHz, acetone-*d*₆, 23 °C): δ 7.30-7.12 (m, 10H, ArH), 7.00-6.87 (m, 10H, ArH), 6.86-6.80 (m, 5H, ArH), 6.19-5.87 (m, 10H, alkenyl CH), 4.38 (d, *J* = 4.7 Hz, 10H), 3.42 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.04-1.44 (broad overlapping signals, 6H, BH), 1.35 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation).

¹¹B{¹H} NMR (160 MHz, acetone-*d*₆, 23 °C): δ ca. -4.49 to -11.40 (overlapping signals, 6B), -13.36 (5B).

¹³C{¹H} NMR (126 MHz, acetone-*d*₆, 23 °C): δ 165.48 (CO), 160.03 (aryl C), 135.98 (BCHCH), 135.05 (broad signal, BCH), 130.01 (aryl CH), 120.79 (aryl CH), 115.77 (aryl CH), 71.99 (CH₂), 67.73 (cage C), 52.99 (CH₂ of cation), 7.66 (CH₃ of cation).
HRMS (ESI): *m/z* Calcd. for [C₄₇H₅₂B₁₁O₇]⁻, 847.4809; found, 847.4828.



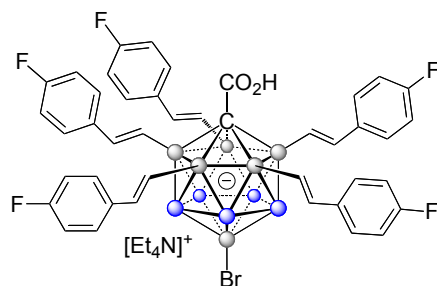
3o: Prepared following the general procedure A, using **1b** and styrene, **3o** was obtained as a colorless solid (92 mg, 71%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6 , 23 °C): δ 7.45-7.31 (m, 10H, ArH), 7.29-7.18 (m, 10H, ArH), 7.17-7.08 (m, 5H, ArH), 6.99 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 6.68 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 3.28 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.61-2.05 (broad signal, 5H, BH), 1.26 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6 , 23 °C): δ 3.72 (s, 1B), -7.07 (5B), -12.73 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6 , 23 °C): δ 166.52 (CO), 140.93 (aryl C), 140.19 (BCHCH), 130.71 (broad signal, BCH), 129.15 (aryl CH), 127.33 (aryl CH), 126.59 (aryl CH), 60.55 (cage C), 52.92 (CH_2 of cation), 7.62 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{42}\text{H}_{41}\text{B}_{11}\text{ClO}_2]^-$, 731.3891; found, 731.3910.



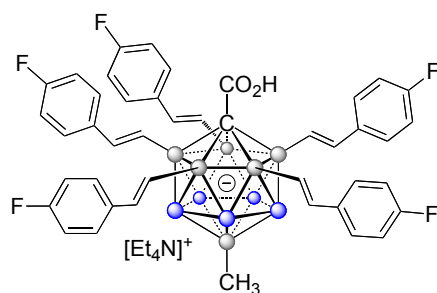
3p: Prepared following the general procedure A, using **1c** and 4-fluorostyrene, **3p** was obtained as a colorless solid (116 mg, 78%).

¹H{¹¹B} NMR (500 MHz, acetone-*d*₆, 23 °C): δ 7.48-7.30 (m, 10H, ArH), 7.09-6.97 (m, 10H, ArH), 6.94 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 6.56 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 3.41 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.65-2.05 (broad signal, 5H, BH), 1.34 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation).

¹¹B{¹H} NMR (128 MHz, acetone-*d*₆, 23 °C): δ -3.01 (s, 1B), -6.72 (5B), -12.66 (5B).

¹³C{¹H} NMR (100 MHz, acetone-*d*₆, 23 °C): δ 166.53 (CO), 162.57 (d, *J* = 243 Hz, C-F), 138.97 (BCHCH), 137.36 (aryl C, C(*ipso*)), 130.36 (broad signal, BCH), 128.19 (d, *J* = 6.1 Hz, C(*ortho*)), 115.82 (d, *J* = 21.5 Hz, C(*meta*)), 62.44 (cage C), 52.97 (CH₂ of cation), 7.64 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₄₂H₃₆B₁₁BrF₅O₂]⁻, 865.2915; found, 865.2956.

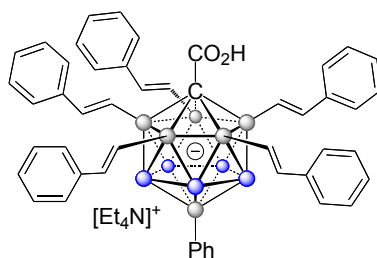


3q: Prepared following the general procedure A, using **1d** and 4-fluorostyrene, **3q** was obtained as a colorless solid (114 mg, 82%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 7.45-7.30 (m, 10H, ArH), 7.09-6.96 (m, 10H, ArH), 6.92 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 6.63 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 3.35 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.65-2.02 (broad signal, 5H, BH), 1.30 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation), 0.23 (s, 3H, CH_3).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6 , 23 °C): δ 1.39 (s, 1B), -6.15 (5B), -11.6 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, acetone- d_6 , 23 °C): δ 166.47 (CO), 163.58 (aryl C), 162.38 (d, $J = 243$ Hz, C-F), 138.11 (BCHCH), 137.68 (aryl C, C(*ipso*)), 131.95 (broad signal, BCH), 128.01 (d, $J = 7.6$ Hz, C(*ortho*)), 115.73 (d, $J = 21.4$ Hz, C(*meta*)), 62.27 (cage C), 52.89 (CH_2 of cation), 7.57 (CH_3 of cation), 4.83 (broad signal, CH_3).
HRMS (ESI): m/z Calcd. for $[\text{C}_{43}\text{H}_{39}\text{B}_{11}\text{F}_5\text{O}_2]^-$, 801.3966; found, 801.3983.



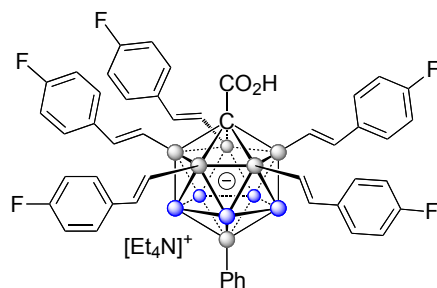
3r: Prepared following the general procedure A, using **1e** and styrene, **3r** was obtained as a colorless solid (84 mg, 62%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 7.65-7.52 (m, 2H, ArH), 7.44-7.31 (m, 10H, ArH), 7.29-7.17 (m, 10H, ArH), 7.16-7.08 (overlapping m, 7H, ArH), 7.07-6.95 (overlapping m, 6H, ArH, alkenyl CH), 6.77 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 3.20 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.61-2.07 (broad signal, 5H, BH), 1.20 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6 , 23 °C): δ 1.87 (s, 1B), -6.18 (5B), -12.35 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, acetone- d_6 , 23 °C): δ 166.48 (CO), 141.17 (aryl C), 139.72 (BCHCH), 133.77(aryl C), 131.74 (broad signal, BCH), 129.12 (aryl CH), 127.15 (aryl CH), 127.04 (aryl C), 126.56 (aryl C), 125.60 (aryl C), 64.48 (cage C), 52.83 (CH_2 of cation), 7.57 (CH_3 of cation). The B12-C signal could not be detected unambiguously.

HRMS (ESI): m/z Calcd. for $[\text{C}_{48}\text{H}_{46}\text{B}_{11}\text{O}_2]^-$, 773.4594; found, 773.4615.



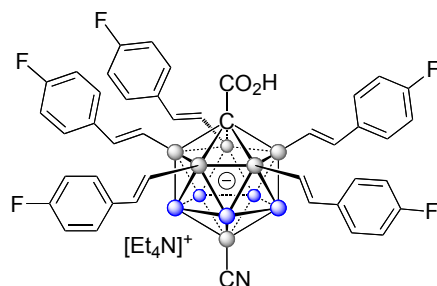
3s: Prepared following the general procedure A, using **1e** and 4-fluorostyrene, **3s** was obtained as a colorless solid (103 mg, 69%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 7.64-7.54 (m, 2H, ArH), 7.47-7.32 (m, 10H, ArH), 7.17-7.09 (m, 2H, ArH), 7.08-6.90 (overlapping m, 16H, ArH, alkenyl CH), 6.67 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 3.28 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.60-2.05 (broad signal, 5H, BH), 1.26 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6 , 23 °C): δ 1.95 (s, 1B), -6.16 (5B), -12.31 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6 , 23 °C): δ 166.44 (CO), 162.46 (d, $J = 243$ Hz, C-F), 138.43 (BCHCH), 137.59 (aryl C, C(*ipso*)), 133.74 (aryl C) 131.58 (broad signal, BCH), 128.10 (d, $J = 7.6$ Hz, C(*ortho*)), 127.07 (aryl C), 125.68 (aryl C), 115.78 (d, $J = 21.4$ Hz, C(*meta*)), 64.37 (cage C), 52.85 (CH_2 of cation), 7.56 (CH_3 of cation). The B12-C signal could not be detected unambiguously.

HRMS (ESI): m/z Calcd. for $[\text{C}_{48}\text{H}_{41}\text{B}_{11}\text{F}_5\text{O}_2]^-$, 863.4123; found, 863.4145.



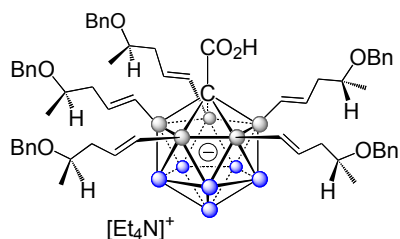
3t: Prepared following the general procedure A, using **1f** and 4-fluorostyrene, **3t** was obtained as a colorless solid (102 mg, 72%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 7.49-7.28 (m, 10H, ArH), 7.12-6.97 (m, 10H, ArH), 6.93 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 6.55 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 3.43 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.58-2.05 (broad signal, 5H, BH), 1.35 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6 , 23 °C): δ -6.31 (5B), ca. -10.55 to -16.60 (overlapping signals, 6B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6 , 23 °C): δ 165.44 (CO), 162.44 (d, $J = 244$ Hz, C-F), 139.28 (BCHCH), 137.22 (aryl C, C(*ipso*)), 129.82 (broad signal, BCH), 128.26 (d, $J = 7.9$ Hz, C(*ortho*)), 115.86 (d, $J = 21.6$ Hz, C(*meta*)), 69.05 (cage C), 52.94 (CH_2 of cation), 7.63 (CH_3 of cation). The B-CN signal could not be detected unambiguously.

HRMS (ESI): m/z Calcd. for $[\text{C}_{43}\text{H}_{36}\text{B}_{11}\text{F}_5\text{NO}_2]^-$, 812.3762; found, 812.3785.



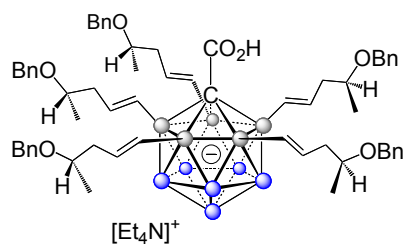
3u: Prepared following the general procedure, using **1a** and {[(2*R*)-pent-4-en-2-yloxy]methyl}benzene, **3u** was obtained as a colorless solid (130 mg, 73%). The eluent for column chromatography was EtOAc.

¹H{¹¹B} NMR (400 MHz, acetone-*d*₆, 23 °C): δ 7.43-7.26 (overlapping m, 20H, ArH), 7.25-7.17 (m, 5H, ArH), 6.02-5.87 (m, 5H, alkenyl CH), 5.76 (d, *J* = 17.4 Hz, 5H, alkenyl CH), 4.57-4.42 (m, 10H, OCH₂), 3.60-3.44 (m, 5H, OCH), 3.36 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.50-2.32 (m, 5H, CHCH₂), 2.18-2.04 (m, 5H, CHCH₂) 1.96-1.54 (overlapping broad signals, 6H, BH), 1.32 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation), 1.14 (d, *J* = 6.0 Hz, 15H, CH₃CH).

¹¹B{¹H} NMR (128 MHz, acetone-*d*₆, 23 °C): δ ca. -1.60 to -10.54 (overlapping signals, 6B), -13.52 (5B).

¹³C{¹H} NMR (101 MHz, acetone-*d*₆, 23 °C): δ 165.05 (CO), 140.73 (BCHCH), 137.22 (aryl C), 134.13 (broad signal, BCH), 128.87 (aryl CH), 128.14 (aryl CH), 127.73 (aryl CH), 76.19 (OCH), 70.66 (OCH₂), 68.12 (cage C), 52.91 (CH₂ of cation), 44.18 (CHCH₂), 20.07 (CH₃CH), 7.64 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₆₂H₈₂B₁₁O₇]⁻, 1057.7157; found, 1057.7194.



3v: Prepared following the general procedure, using **1a** and {[(2*S*)-pent-4-en-2-yloxy]methyl}benzene, **3v** was obtained as a colorless solid (126 mg, 71%). The eluent for column chromatography was EtOAc.

¹H{¹¹B} NMR (500 MHz, acetone-*d*₆, 23 °C): δ 7.43-7.26 (overlapping m, 20H, ArH), 7.25-7.17 (m, 5H, ArH), 6.02-5.87 (m, 5H, alkenyl CH), 5.76 (d, *J* = 17.4 Hz, 5H, alkenyl CH), 4.57-4.42 (m, 10H, OCH₂), 3.56-3.48 (m, 5H, OCH), 3.45 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.49-2.35 (m, 5H, CHCH₂), 2.12-2.06 (m, 5H, CHCH₂) 1.92-1.60 (broad overlapping signals, 6H, BH), 1.37 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation), 1.14 (d, *J* = 6.0 Hz, 15H, CH₃CH).

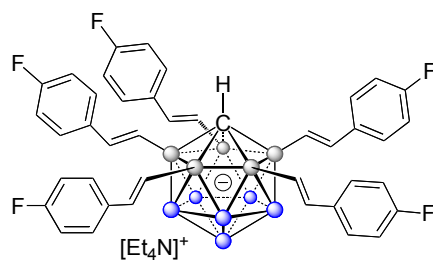
¹¹B{¹H} NMR (128 MHz, acetone-*d*₆, 23 °C): δ ca. -1.60 to -10.54 (overlapping signals, 6B), -13.54 (5B).

¹³C{¹H} NMR (126 MHz, acetone-*d*₆, 23 °C): δ 165.03 (CO), 140.84 (aryl C), 137.33 (BCHCH), 134.07 (broad signal, BCH), 128.90 (aryl CH), 128.19 (aryl CH), 127.74 (aryl CH), 76.28 (OCH), 70.72 (OCH₂), 68.23 (cage C), 53.01 (CH₂ of cation), 44.26 (CHCH₂), 20.13 (CH₃CH), 7.68 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₆₂H₈₂B₁₁O₇]⁻, 1057.7157; found, 1057.7190.

General Procedure B for the decarboxylation of the penta-alkenylation products

A 10 mL microwave vial was charged with carborane acid **1** (0.060 mmol), NaOAc (0.60 mmol) and capped under nitrogen. DMA (4 mL) was added via a syringe, and the resulting mixture was heated to 150 °C in a microwave reactor. The progress of the reaction was monitored by (-)-ESI-MS analysis. After the completion of the reaction, all the volatiles were removed in vacuo, and the residue was dissolved in EtOAc and washed with an aqueous solution of [Et₄N]Br (3 x 10 mL). The organic layer was dried over MgSO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography (silica gel, eluent: dichloromethane) to afford **4** as a colorless solid.



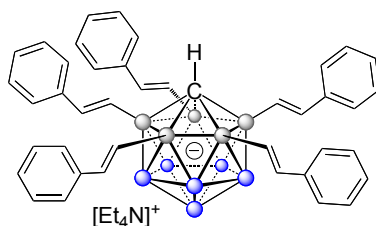
4a: Prepared following the general procedure, starting from **3a** , **4a** was obtained as a colorless solid (45 mg, 86%).

¹H{¹¹B} NMR (400 MHz, acetone-*d*₆, 23 °C): δ 7.41-7.27 (m, 10H, ArH), 7.06-6.86 (m, 10H, ArH), 6.78 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 6.43 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 3.45 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.81 (s, 1H, cage CH), 2.05-1.75 (broad overlapping signals, 6H, BH), 1.37 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation).

¹¹B{¹H} NMR (128 MHz, acetone-*d*₆, 23 °C): δ ca. -4.70 to -11.20 (overlapping signals with peaks at -7.70 and -9.67, 6B), -13.03 (5B).

¹³C{¹H} NMR (100 MHz, Acetone-*d*₆, 23 °C): δ 162.43 (d, *J* = 243 Hz, C-F), 137.97 (BCHCH), 137.47 (d, *J* = 2.8 Hz, C(*ipso*)), 132.40 (broad signal, BCH), 128.00 (d, *J* = 8.0 Hz, C(*ortho*)), 115.74 (d, *J* = 21.5 Hz, C(*meta*)), 57.27 (cage C), 52.97 (CH₂ of cation), 7.64 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₄₁H₃₇B₁₁F₅]⁻, 743.3912; found, 743.3928.



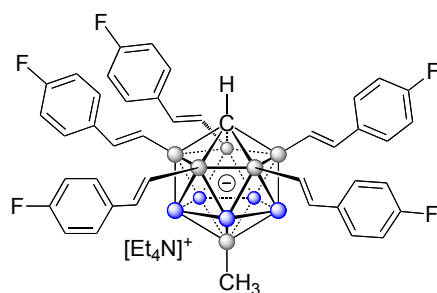
4b: Prepared following the general procedure, starting from **3b**, **4b** was obtained as a colorless solid (37 mg, 79%).

¹H{¹¹B} NMR (400 MHz, acetone-*d*₆, 23 °C): δ 7.40-7.28 (m, 10H, ArH), 7.27-7.14 (m, 10H, ArH), 7.13-6.98 (m, 5H, ArH), 6.84 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 6.54 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 3.36 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.06-1.74 (broad overlapping signals, 6H, BH), 1.31 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation). The ¹H/¹³C HSQC spectrum shows that the cage CH signal is overlapping with the double water peak.

¹¹B{¹H} NMR (128 MHz, acetone-*d*₆, 23 °C): δ ca. -4.98 to -11.30 (overlapping signals with peaks at -7.63 and -9.71, 6B), -13.02 (5B).

¹³C{¹H} NMR (101 MHz, acetone-*d*₆, 23 °C): δ 141.00 (aryl C), 139.26 (BCHCH), 132.78 (broad signal, BCH), 129.08 (aryl CH), 127.07 (aryl CH), 126.46 (aryl CH), 57.42 (cage C), 52.93 (CH₂ of cation), 7.61 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₄₁H₄₂B₁₁]⁻, 653.4383; found, 653.4398.



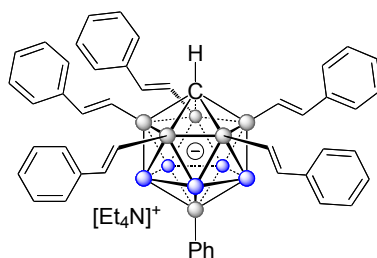
4q: Prepared following the general procedure, starting from **3q**, **4q** was obtained as a colorless solid (46 mg, 87%).

¹H{¹¹B} NMR (400 MHz, acetone-*d*₆, 23 °C): δ 7.42-7.26 (m, 10H, ArH), 7.05-6.89 (m, 10H, ArH), 6.77 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 6.43 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 3.45 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.57 (s, 1H, cage CH), 2.05-1.76 (broad signal, 5H, BH), 1.36 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation), 0.16 (s, 3H, CH₃).

¹¹B{¹H} NMR (128 MHz, acetone-*d*₆, 23 °C): δ -0.98 (s, 1B), -8.03 (5B), -11.68 (5B).

¹³C{¹H} NMR (101 MHz, acetone-*d*₆, 23 °C): δ 162.38 (d, *J* = 243 Hz, C-F), 137.82 (BCHCH), 137.53 (aryl C, C(*ipso*)), 132.55 (broad signal, BCH), 127.97 (d, *J* = 7.7 Hz, C(*ortho*)), 115.73 (d, *J* = 21.5 Hz, C(*meta*)), 52.96 (CH₂ of cation), 51.00 (cage C), 7.63 (CH₃ of cation). The B-CH₃ signal could not be detected unambiguously.

HRMS (ESI): *m/z* Calcd. for [C₄₂H₃₉B₁₁F₅]⁻, 757.4068; found, 757.4084.



4r: Prepared following the general procedure, starting from **3r**, **4r** was obtained as a colorless solid (39 mg, 76%).

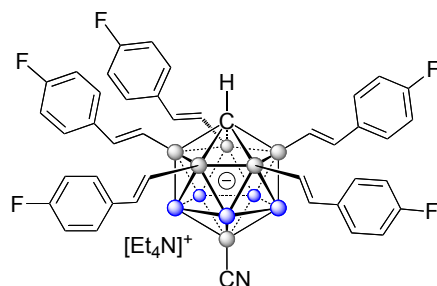
¹H{¹¹B} NMR (500 MHz, acetone-*d*₆, 23 °C): δ 7.63-7.52 (m, 2H, ArH), 7.39-7.29 (m, 10H, ArH), 7.25-7.15 (m, 10H, ArH), 7.13-7.04 (overlapping m, 7H, ArH), 7.03-6.97 (m, 1H, ArH), 6.89 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 6.58 (d, *J* = 18.0 Hz, 5H, alkenyl CH), 3.34 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.79 (s, 1H, cage CH), 2.54-2.06 (broad signal, 5H, BH), 1.29 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation).

The cage CH signal is overlapping with the double water peak.

¹¹B{¹H} NMR (160 MHz, acetone-*d*₆, 23 °C): δ -0.23 (s, 1B), -7.85 (5B), -12.36 (5B).

¹³C{¹H} NMR (126 MHz, acetone-*d*₆, 23 °C): δ 141.03 (aryl C), 139.45 (BCHCH), 133.94 (aryl C), 132.67 (broad signal, BCH), 129.10 (aryl CH), 127.10 (aryl CH), 126.93 (aryl CH), 126.51 (aryl CH), 125.32 (aryl CH), 53.38 (cage C), 52.94 (CH₂ of cation), 7.62 (CH₃ of cation). The B-C(Ph) signal could not be detected unambiguously.

HRMS (ESI): *m/z* Calcd. for [C₄₇H₄₆B₁₁]⁻, 729.4696; found, 729.4721.



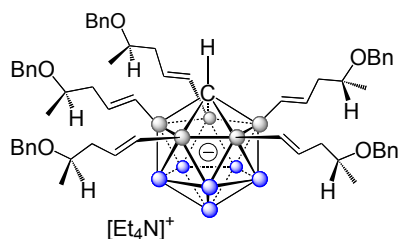
4t: Prepared following the general procedure, starting from **3t**, **4t** was obtained as a colorless solid (43 mg, 80%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 7.43-7.30 (m, 10H, ArH), 7.05-6.93 (m, 10H, ArH), 6.81 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 6.38 (d, $J = 18.0$ Hz, 5H, alkenyl CH), 3.46 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.96 (s, 1H, cage CH), 2.44-2.05 (broad signal, 5H, BH), 1.38 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6 , 23 °C): δ -7.75 (5B), -13.38 (5B), -15.53 (1B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, acetone- d_6 , 23 °C): δ 163.82 (d, $J = 243$ Hz, C-F), 138.98 (BCHCH), 137.05 (d, $J = 2.2$ Hz, C(*ipso*)), 130.59 (broad signal, BCH), 128.19 (d, $J = 7.8$ Hz, C(*ortho*)), 115.83 (d, $J = 21.6$ Hz, C(*meta*)), 57.87 (cage C), 52.96 (CH_2 of cation), 7.64 (CH_3 of cation). The B-CN signal could not be detected unambiguously.

HRMS (ESI): m/z Calcd. for $[\text{C}_{42}\text{H}_{36}\text{B}_{11}\text{F}_5\text{N}]^-$, 768.3864; found, 768.3879.



4u: Prepared following the general procedure, starting from **3u**, **4u** was obtained as a colorless solid (58 mg, 84%).

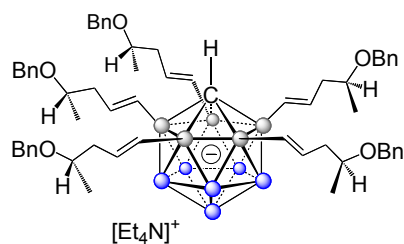
¹H{¹¹B} NMR (500 MHz, acetone-*d*₆, 23 °C): δ 7.40-7.33 (m, 10H, ArH), 7.33-7.27 (m, 10H, ArH), 7.25-7.18 (m, 5H, ArH), 5.79-5.63 (m, 5H, alkenyl CH), 5.55 (d, *J* = 17.4 Hz, 5H, alkenyl CH), 4.62-4.39 (m, 10H, OCH₂), 3.58-3.40 (overlapping signals, 13H, OCH and CH₂ of cation), 2.50-2.28 (m, 5H, CHCH₂), 2.14-2.02 (m, 5H, CHCH₂) 1.89-1.47 (broad overlapping signals, 6H, BH), 1.38 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation), 1.14 (d, *J* = 6.0 Hz, 15H, CH₃CH).

The ¹H/¹³C HSQC spectrum shows that the cage CH signal is overlapping with the solvent residual signal and the multiplet at 2.14-2.02 ppm.

¹¹B{¹H} NMR (160 MHz, acetone-*d*₆, 23 °C): δ ca. -5.86 to -12.58 (overlapping signals with peaks at -8.53 and -10.36, 6B), -13.89 (5B).

¹³C{¹H} NMR (126 MHz, acetone-*d*₆, 23 °C): δ 140.81 (BCHCH), 135.74 (aryl C), 135.20 (broad signal, BCH), 128.90 (aryl CH), 128.16 (aryl CH), 127.77 (aryl CH), 76.27(OCH), 70.66 (OCH₂), 56.96 (cage C), 53.00 (CH₂ of cation), 44.13 (CHCH₂), 20.09 (CH₃CH), 7.67 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₆₁H₈₂B₁₁O₅]⁻, 1013.7258; found, 1013.7244.



4v: Prepared following the general procedure, starting from **3v**, **4v** was obtained as a colorless solid (55 mg, 80%).

¹H{¹¹B} NMR (500 MHz, acetone-*d*₆, 23 °C): δ 7.41-7.33 (m, 10H, ArH), 7.33-7.27 (m, 10H, ArH), 7.26-7.18 (m, 5H, ArH), 5.78-5.64 (m, 5H, alkenyl CH), 5.55 (d, *J* = 17.4 Hz, 5H, alkenyl CH), 4.60-4.40 (m, 10H, OCH₂), 3.56-3.38 (overlapping signals, 13H, OCH and CH₂ of cation), 2.47-2.30 (m, 5H, CHCH₂), 2.11-2.04 (m, 5H, CHCH₂), 1.80-1.50 (broad overlapping signals, 6H, BH), 1.38 (tt, *J* = 7.3 Hz, 1.6 Hz, 12H, CH₃ of cation), 1.14 (d, *J* = 6.0 Hz, 15H, CH₃CH).

The cage CH signal is overlapping with the solvent residual signal and the multiplet at 2.11-2.04 ppm.

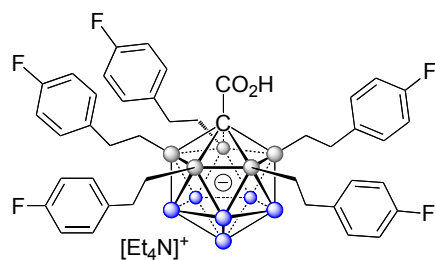
¹¹B{¹H} NMR (160 MHz, acetone-*d*₆, 23 °C): δ ca. -5.46 to -12.18 (overlapping signals with peaks at -8.47 and -10.39, 6B), -13.86 (5B).

¹³C{¹H} NMR (126 MHz, acetone-*d*₆, 23 °C): δ 140.82 (BCHCH), 135.34 (aryl C, BCH), 128.90 (aryl CH), 128.16 (aryl CH), 127.77 (aryl CH), 76.28 (OCH), 70.67 (OCH₂), 56.97 (cage C), 53.01 (CH₂ of cation), 44.13 (CHCH₂), 20.09 (CH₃CH), 7.67 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₆₁H₈₂B₁₁O₅]⁻, 1013.7258; found, 1013.7291.

General Procedure C for the reduction of the penta-alkenylation products

To a solution of **3** (0.10 mmol) in THF (8 mL) in a 25 mL round-bottom flask was added 10% Pd on carbon (20 mg). The mixture was stirred under H₂ (balloon pressure) for 2 h. The catalyst was filtered off, and the solvent was removed under reduced pressure. The crude product was purified by column chromatography (silica gel, eluent: dichloromethane) to afford **5** as a colorless solid.



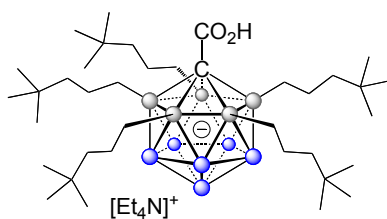
5a: Prepared following the general procedure, starting from **3a**, **5a** was obtained as a colorless solid (83 mg, 90%).

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6 , 23 °C): δ 7.32-7.17 (m, 10H, ArH), 7.10-6.90 (m, 10H, ArH), 3.45 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.92-2.78 (m, 10H, BCH_2CH_2), 2.06-1.56 (broad overlapping signals, 6H, BH), 1.37 (tt, $J = 7.3$ Hz, 1.6 Hz, 12H, CH_3 of cation), 1.22-1.07 (m, 10H, BCH_2CH_2).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6 , 23 °C): δ ca. 0.52 to -9.42 (overlapping signals with peaks at -4.52 and -5.81, 6B), -15.59 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6 , 23 °C): δ 166.26 (CO), 161.60 (d, $J = 240$ Hz, C-F), 144.10 (aryl C, $C(\textit{ipso})$), 130.17 (d, $J = 7.6$ Hz, $C(\textit{ortho})$), 115.40 (d, $J = 20.8$ Hz, $C(\textit{meta})$), 70.98 (cage C), 52.97 (CH_2 of cation), 36.12 (BCH_2CH_2), 19.98 (broad signal, BCH_2CH_2), 7.64 (CH_3 of cation).

HRMS (ESI): m/z Calcd. for $[\text{C}_{42}\text{H}_{47}\text{B}_{11}\text{F}_5\text{O}_2]^-$, 797.4592; found, 797.4633.



5k: Prepared following the general procedure, starting from **3k**, **5k** was obtained as a colorless solid (70 mg, 87%).

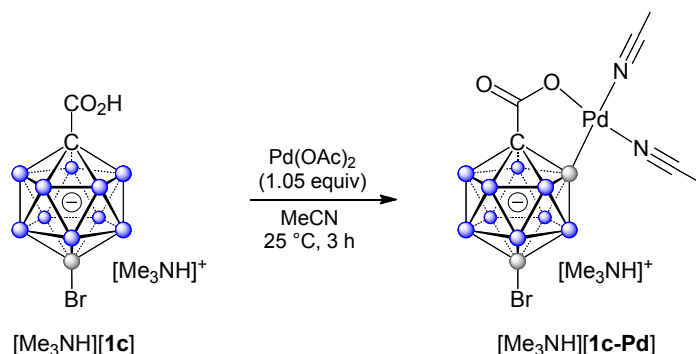
¹H{¹¹B} NMR (400 MHz, acetone-*d*₆, 23 °C): δ 3.50 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.00-1.50 (broad overlapping signals, 6H, BH), 1.49-1.33 (m, 22H, CH₂ of cation and BCH₂CH₂), 1.30-1.18 (m, 10H, (CH₃)₃CCH₂), 0.87 (s, 45H, (CH₃)₃C), 0.75-0.62 (m, 10H, BCH₂CH₂).

¹¹B{¹H} NMR (128 MHz, acetone-*d*₆, 23 °C): δ ca. -0.05 to -9.03 (overlapping signals with peaks at -4.49 and -6.59, 6B), -15.78 (5B).

¹³C{¹H} NMR (101 MHz, acetone-*d*₆, 23 °C): δ 166.75 (CO), 71.34 (cage C), 53.00 (CH₂ of cation), 49.54, 31.15, 30.07, 25.14, 18.15 (broad signal, BCH₂CH₂), 7.69 (CH₃ of cation).

HRMS (ESI): *m/z* Calcd. for [C₃₇H₈₂B₁₁O₂]⁻, 677.7411; found, 677.7452.

Preparation of palladium complex **1c-Pd**



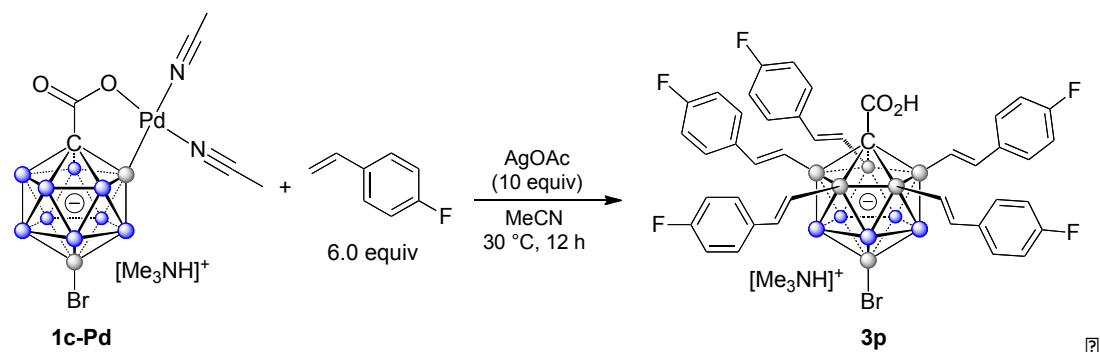
In a glovebox, Pd(OAc)₂ (103 mg, 0.458 mmol) was added to a stirred solution of [Me₃NH][1-COOH-CB₁₁H₁₀-12-Br] (142 mg, 0.437 mmol) in dry acetonitrile (0.50 mL) in a 2 mL glass vial. The resulting mixture was stirred at 25 °C for 5 h. The pale precipitate that formed was collected by vacuum filtration through a fine glass frit, washed with hexane and dried in a vacuum. The filtrate was left to evaporate slowly at room temperature (evaporation of *ca.* 60% of the solvent) to yield colorless crystals, which were collected by filtration. The combined solids were dried at 25 °C in a vacuum to give palladium complex **1c-Pd** (182 mg, 82%).

¹H{¹¹B} NMR (500 MHz, acetonitrile-*d*₃, 23 °C): δ 2.73 (s, 9H, CH₃ of cation), 1.96 (s, 6H, CH₃CN), 1.90-1.25 (broad overlapping signals, 9H, BH). MeCN ligand exchange with the solvent leads to the signal at 1.96 ppm, which corresponds to free MeCN.

¹¹B{¹H} NMR (160 MHz, acetonitrile-*d*₃, 23 °C): δ -3.46 (s, 1B, B-Br), *ca.* -10.50 to -17.50 (overlapping signals with peaks at -12.64, -13.39 and 14.91, 9B), -21.92 (s, 1B, B-Pd).

¹³C{¹H} NMR (126 MHz, acetonitrile-*d*₃, 23 °C): δ 179.51 (CO), 67.71 (cage C), 45.55 (CH₃ of cation).

Reaction of **1c-Pd** with fluorostyrene in the presence of AgOAc



□

Under nitrogen protection, **1c-Pd** (10 mg, 19 μmol), 4-fluorostyrene (6.0 equiv) and AgOAc (10 equiv) were combined in dry MeCN (0.6 mL) in a 4 mL glass vial. The vial was heated to 30 $^\circ\text{C}$, and the reaction was monitored by ESI mass spectrometry. During the transformation, mono-, di-, tri-, tetra- and penta-substituted products were observed, but no other intermediates. The mass spectrum of the reaction mixture after 12 h is displayed in Figure S1. It shows clean formation of the penta-alkenylated product **3p**.

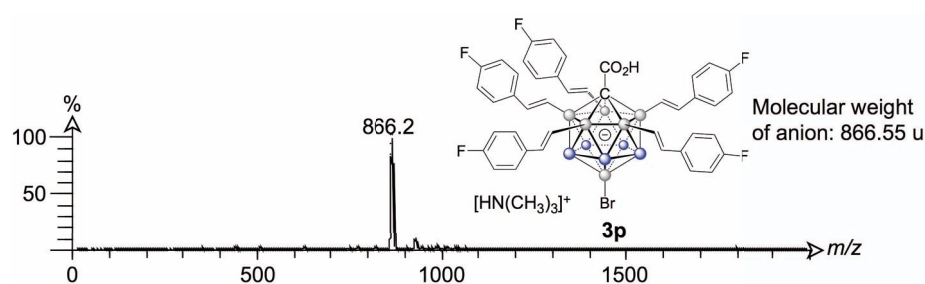
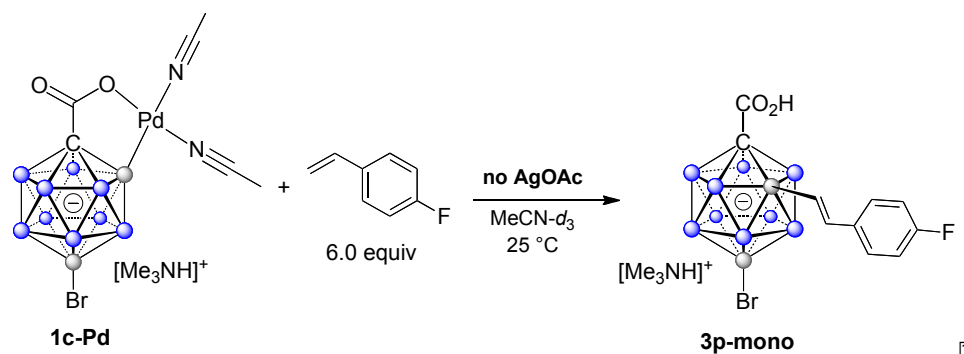


Figure S1. Full-range (-)ESI mass spectrum of the reaction mixture **1c-Pd** + 4-fluorostyrene (6.0 equiv) + AgOAc (10 equiv) in MeCN after 12 h at 30 $^\circ\text{C}$.

Reaction of **1c-Pd** with fluorostyrene in the absence of AgOAc



□

Under nitrogen protection, **1c-Pd** (10 mg, 19 μmol) and 4-fluorostyrene (6.0 equiv) were combined in dry $\text{MeCN-}d_3$ (0.6 mL) in a 4 mL glass vial. The mixture was stirred at 25 $^\circ\text{C}$, and the reaction was monitored by ESI mass spectrometry and NMR spectroscopy. After 1 h, 3 h, 5 h and 12 h, clean formation of the mono-alkenylated product **3p-mono** was observed, and no other intermediates were detected. The $^1\text{H}\{^{11}\text{B}\}$ and $^{11}\text{B}\{^1\text{H}\}$ NMR spectra of the reaction mixture after 3 h are displayed in Figures S2 and S3; the mass spectrum after 3 h is displayed in Figure S4.

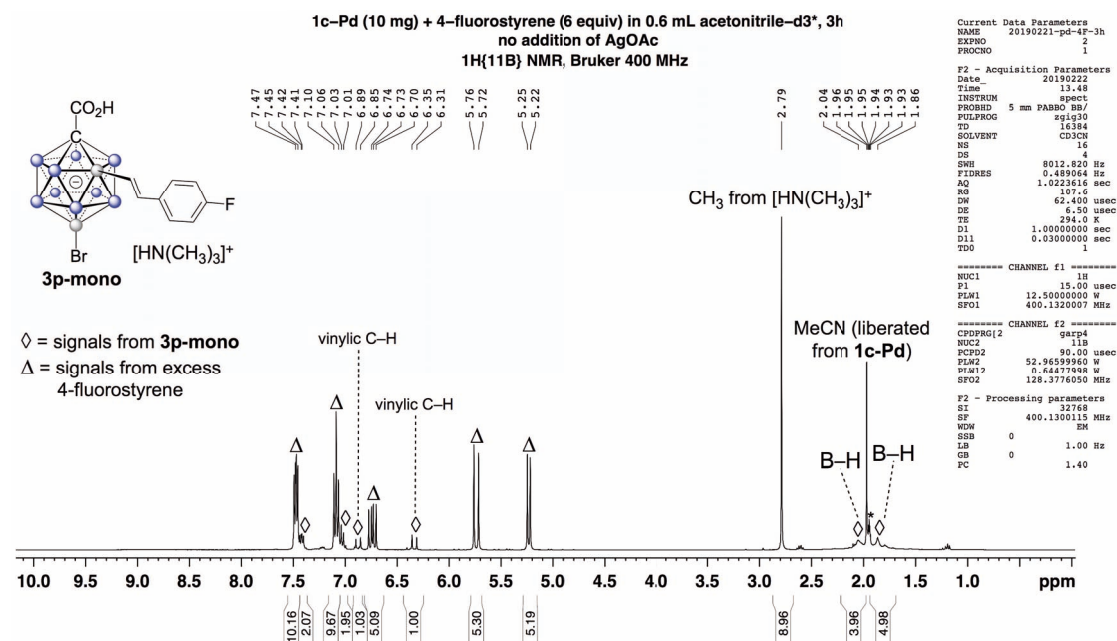


Figure S2. $^1\text{H}\{^{11}\text{B}\}$ NMR spectrum of the reaction mixture **1c-Pd** + 4-fluorostyrene (6.0 equiv) in $\text{MeCN-}d_3$ after 3 h at 25 $^\circ\text{C}$ (400 MHz, 23 $^\circ\text{C}$).

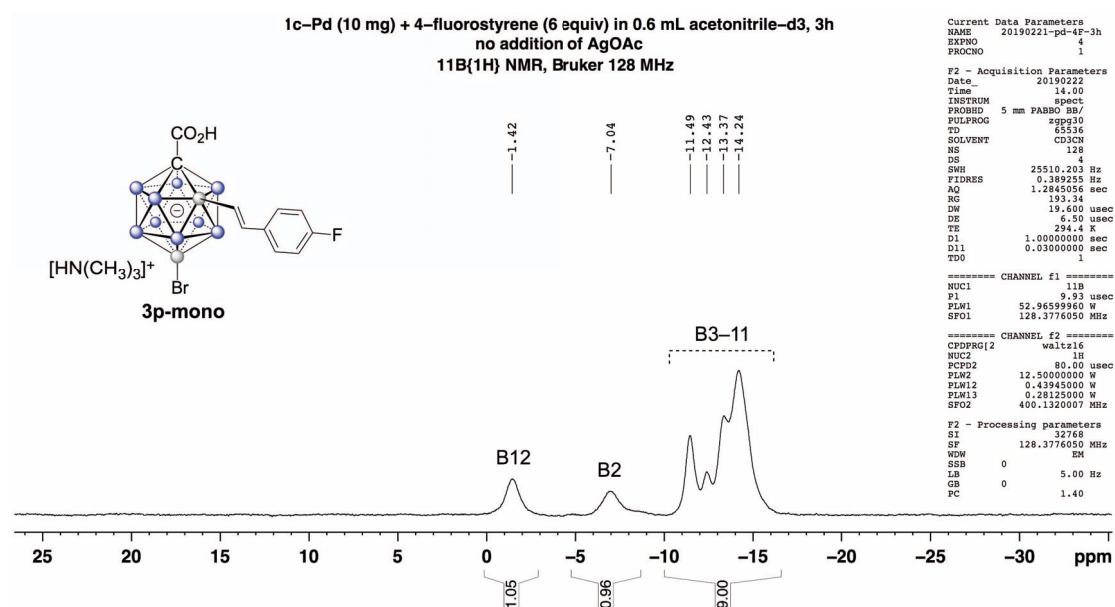


Figure S3. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of the reaction mixture **1c-Pd** + 4-fluorostyrene (6.0 equiv) in $\text{MeCN-}d_3$ after 3 h at 25 °C (128 MHz for ^{11}B , 23 °C).

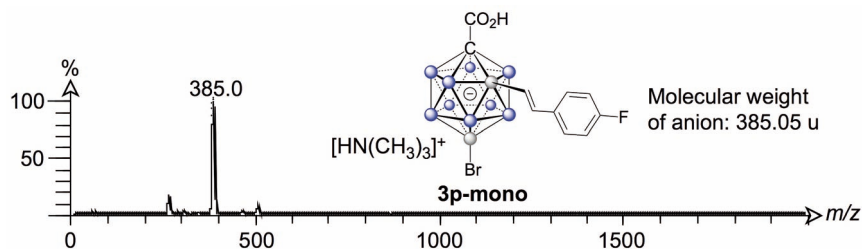
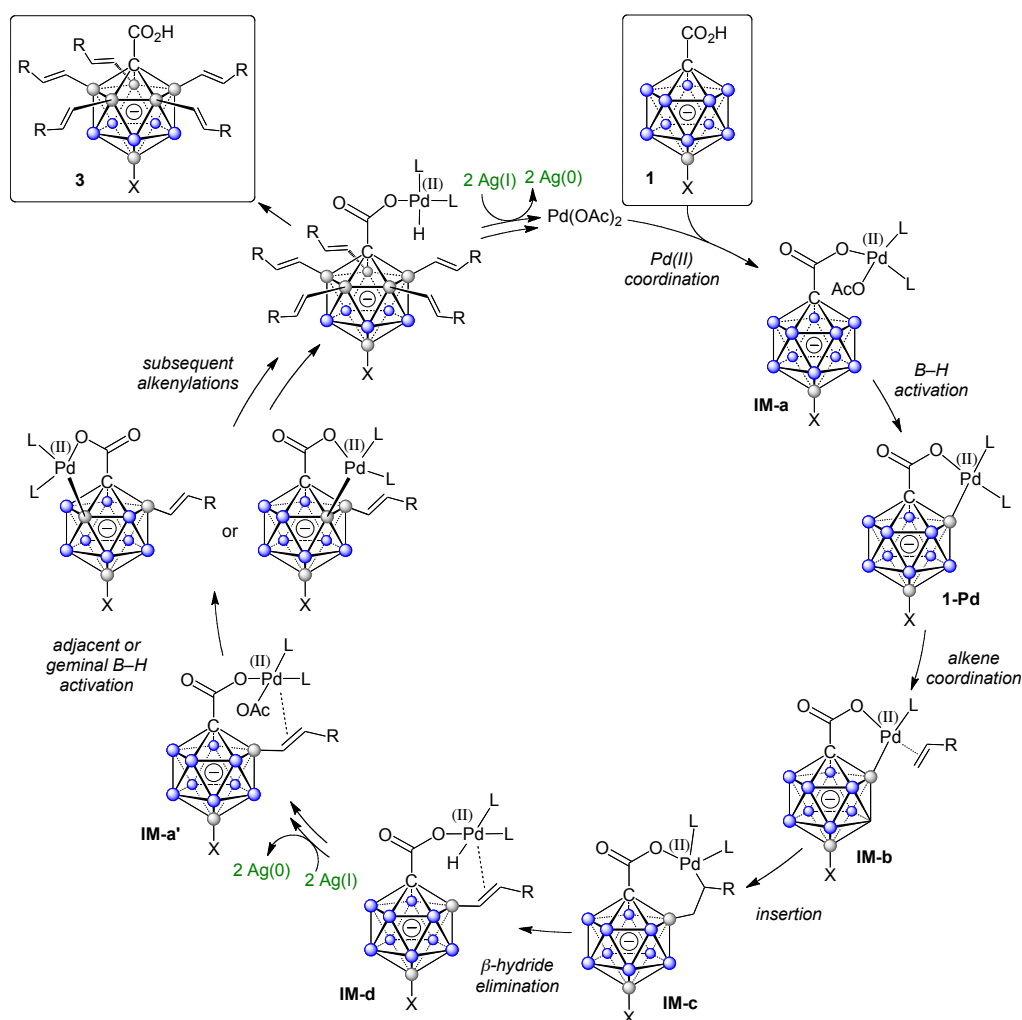


Figure S4. Full-range (-)ESI mass spectrum of the reaction mixture **1c-Pd** + 4-fluorostyrene (6.0 equiv) in $\text{MeCN-}d_3$ after 3 h at 25 °C.

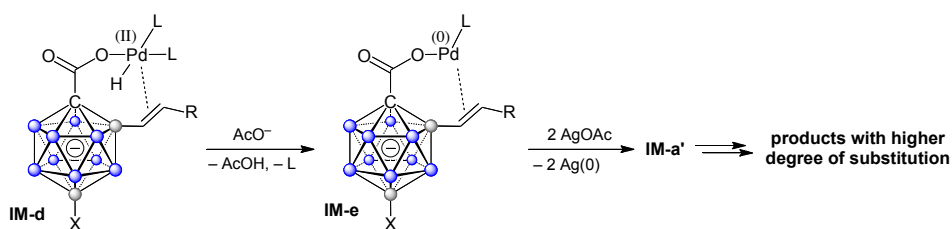
Proposed mechanism for the penta-alkenylation

A plausible mechanism for the penta-alkenylation is displayed in Scheme S1. Binding of the carboxylate group of **1** to Pd(II) affords the initial intermediate **IM-a**. Cyclometalation–deprotonation then gives palladacycle **1-Pd** with a direct B–Pd bond. Intermediates **IM-b/IM-c** are formed by alkene coordination/insertion, which is followed by β -hydride elimination to furnish Pd–H complex **IM-d**. Subsequent reaction with AgOAc leads to **IM-a'**, which contains one alkenyl substituent. Based on the above control experiment starting from **1c-Pd** and excess 4-fluorostyrene in the absence of AgOAc, it seems likely that the steps until formation of **IM-d** occur fast



Scheme S1. Proposed mechanism for the five-fold B–H activation/B–C coupling cascade; L = solvent molecule or AcO[−].

and that AgOAc is necessary to promote subsequent coupling steps. Currently we believe that base-assisted elimination of H^+/L ($L = AcO^-$ or solvent) from **IM-d** affords **IM-e** with a formal Pd(0) center (Scheme S2); formation of H_2 was not observed in any of the experiments of this study. Oxidation of **IM-e** by two equivalents of Ag(I) re-establishes the Pd(II) oxidation state, thereby enabling the system to undergo further B–H activation/alkenylation processes. They are assumed to occur in a similar manner until the final product **3** and Pd(II) are liberated.



Scheme S2. Putative Pd(0) intermediate **IM-e** formed by deprotonation/ligand dissociation from **IM-d**, followed by reoxidation of the Pd center; $L =$ solvent molecule or AcO^- .

III X-ray Crystallography

Crystal structure of **3b** (CCDC 1886700)

Compound **3b** (15 mg, 0.018 mmol) was dissolved in acetone (0.5 mL) in a 1 mL glass vial. The resulting colorless solution was filtered into a 18 cm long NMR tube and layered with hexanes (1 mL). Colorless crystals of the composition [Et₄N][**3b**]-acetone suitable for X-ray diffraction grew within 3 d at room temperature.

Bond precision:	C-C = 0.0073 Å	Wavelength=1.34139	
Cell:	a=11.9981(3)	b=20.7041(4)	c=21.3976(4)
	alpha=90	beta=92.910(1)	gamma=90
Temperature:	170 K		
	Calculated	Reported	
Volume	5308.5(2)	5308.52(19)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C42 H42 B11 O2, C8 H20 N, C3 H6 O	C42 H42 B11 O2, C3 H6 O, C8 H20 N	
Sum formula	C53 H68 B11 N O3	C53 H68 B11 N O3	
Mr	885.99	885.99	
Dx, g cm ⁻³	1.109	1.109	
Z	4	4	
Mu (mm ⁻¹)	0.305	0.308	
F000	1888.0	1888.0	
F000'	1891.50		
h,k,lmax	14,25,26	14,25,26	
Nref	10119	10024	
Tmin,Tmax	0.982,0.991	0.638,0.751	
Tmin'	0.976		
Correction method= # Reported T Limits: Tmin=0.638 Tmax=0.751			
AbsCorr = MULTI-SCAN			
Data completeness=	0.991	Theta(max)= 54.945	
R(reflections)=	0.0991(5609)	wR2(reflections)= 0.3133(10024)	
S =	1.030	Npar= 662	

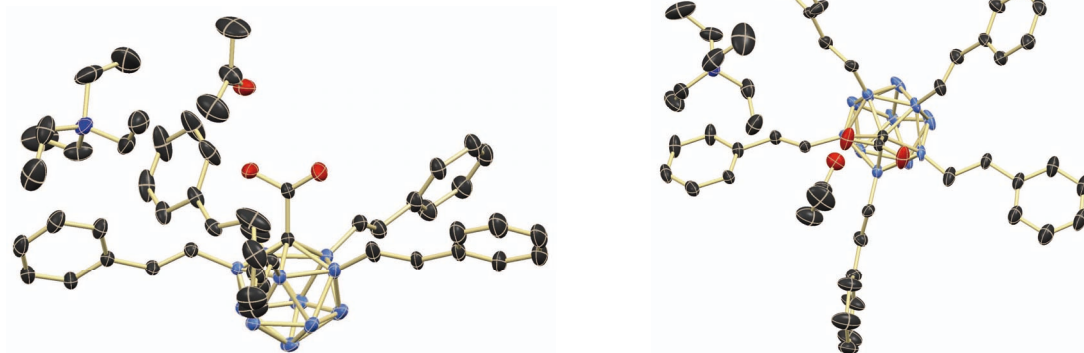


Figure S5. Crystal structure of $[\text{Et}_4\text{N}][\mathbf{3b}] \cdot \text{acetone}$ (left: side view; right: view along C(cage)–B12 axis); hydrogen atoms are omitted for clarity; 30% displacement ellipsoids; one of the styrene substituents is disordered, and only one set of the disordered atoms is shown.

Crystal structure of 4b (CCDC 1886699)

Compound **4b** (10 mg, 0.013 mmol) was dissolved in acetone (0.4 mL) in a 1 mL glass vial. The resulting colorless solution was filtered into a 18 cm long NMR tube and layered with hexanes (1 mL). Colorless crystals of the composition [Et₄N][**4b**] suitable for X-ray diffraction grew within 3 d at room temperature.

Bond precision:	C-C = 0.0066 Å	Wavelength=1.34139	
Cell:	a=23.5746(11) alpha=90	b=18.8529(6) beta=90	c=22.1333(6) gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	9837.1(6)	9837.1(6)	
Space group	I b a m	I b a m	
Hall group	-I 2 2c	-I 2 2c	
Moiety formula	C41 H42 B11, C8 H20 N [+ solvent]	C8 H20 N, C41 H42 B11	
Sum formula	C49 H62 B11 N [+ solvent]	C49 H62 B11 N	
Mr	783.91	783.90	
Dx, g cm ⁻³	1.059	1.059	
Z	8	8	
Mu (mm ⁻¹)	0.263	0.267	
F000	3344.0	3344.0	
F000'	3349.68		
h,k,lmax	28,23,27	28,23,27	
Nref	4844	4797	
Tmin,Tmax	0.962,0.987	0.563,0.751	
Tmin'	0.948		
Correction method= # Reported T Limits: Tmin=0.563 Tmax=0.751			
AbsCorr = MULTI-SCAN			
Data completeness=	0.990	Theta(max)=	55.098
R(reflections)=	0.0839(3107)	wR2(reflections)=	0.2591(4797)
S =	1.037	Npar=	337



Figure S6. Crystal structure of [Et₄N][**4b**] (left: side view; right: view along C(cage)–B12 axis); hydrogen atoms and disordered parts are omitted for clarity; 30% displacement ellipsoids.

The Alert level B message for this structure indicates a short H···H contact and is the result of some disorder in this structure. While the disorder concerning one of the vinyl groups (C18/19) could be resolved successfully, the related disorder of the neighbouring phenyl group (C12–17) could not. The short contact is a consequence of that.

Crystal structure of 1c-Pd (CCDC 1886701)

Compound **1c-Pd** (15 mg, 0.029 mmol) was dissolved in acetonitrile (0.5 mL) in a 2 mL glass vial. The resulting clear solution was left to evaporate slowly at room temperature. Colorless crystals of the composition $[\text{Me}_3\text{NH}][\mathbf{1c-Pd}]$ suitable for X-ray diffraction grew within 4 d.

Bond precision:	C-C = 0.0173 Å	Wavelength=0.71073	
Cell:	a=8.7468(9)	b=10.0535(7)	c=26.411(3)
	alpha=90	beta=95.913(8)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	2310.1(4)	2310.1(4)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C6 H15 B11 Br N2 O2 Pd, C3 H10 N	C3 C6 H15 B11 Br N2 O2 Pd, C3 H10 N	
Sum formula	C9 H25 B11 Br N3 O2 Pd	C9 H25 B11 Br N3 O2 Pd	
Mr	512.53	512.54	
Dx, g cm ⁻³	1.474	1.474	
Z	4	4	
Mu (mm ⁻¹)	2.541	2.541	
F000	1008.0	1008.0	
F000'	1003.09		
h, k, lmax	10, 12, 31	10, 12, 31	
Nref	4224	4195	
Tmin, Tmax	0.430, 0.776	0.442, 1.000	
Tmin'	0.341		
Correction method= # Reported T Limits: Tmin=0.442 Tmax=1.000			
AbsCorr = MULTI-SCAN			
Data completeness=	0.993	Theta(max)= 25.350	
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S =	1.054	Npar= 249	

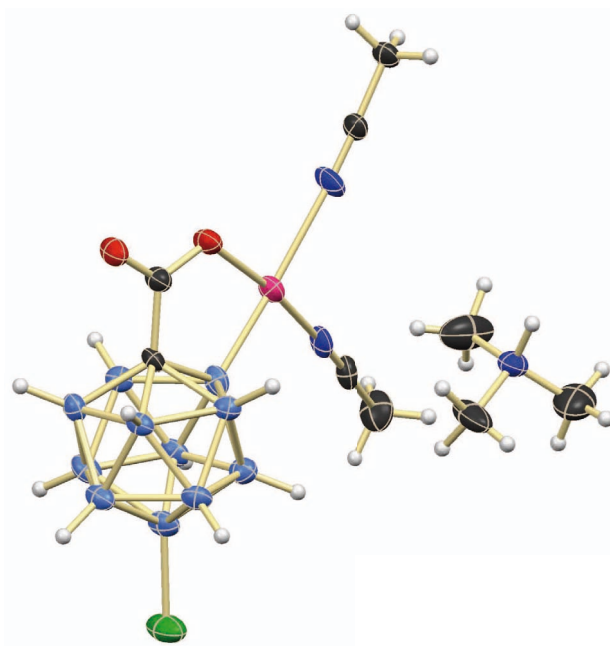


Figure S7. Crystal structure of [Me₃NH][1c-Pd]; 30% displacement ellipsoids.

IV References

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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

V NMR Spectra

Following on pp. S56–S201

VI Mass Spectra

Following on pp. S202–S236

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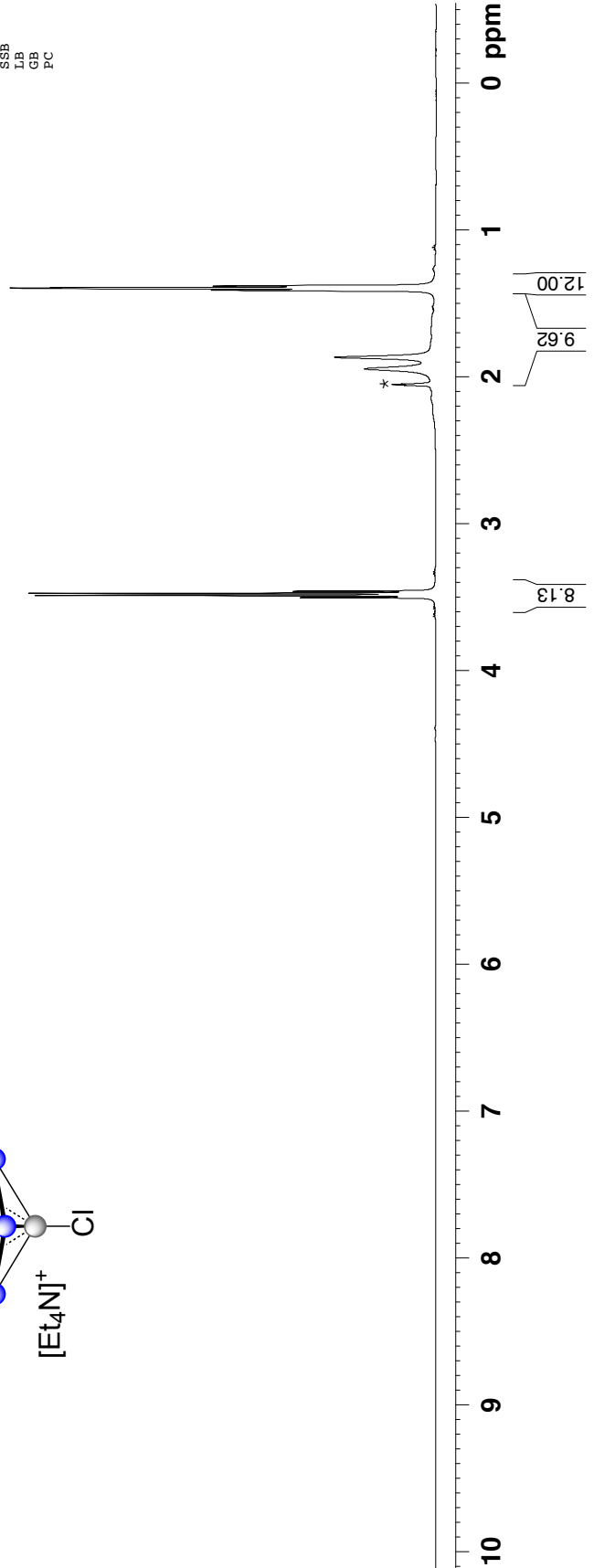
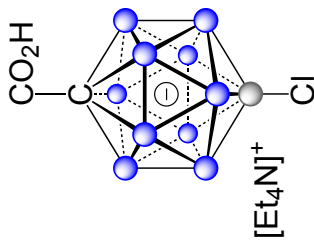
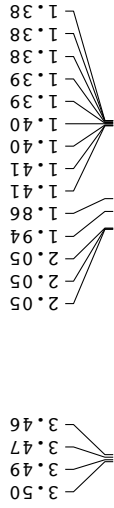
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**1-COOH-12-Cl-CB11 product 30 mg in 0.6 ml acetone-d6
 11B NMR, 160 MHz, 23 C**

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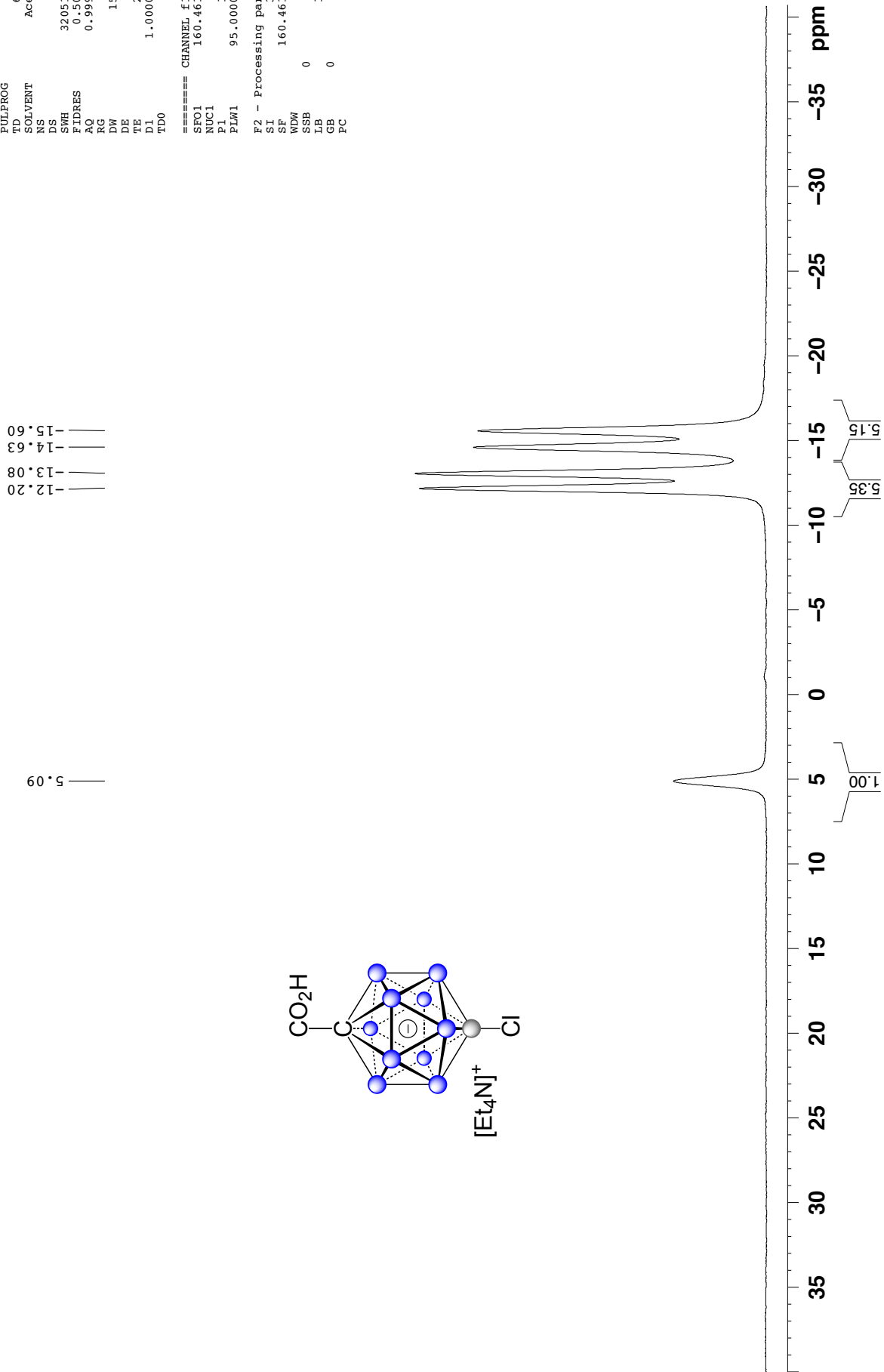
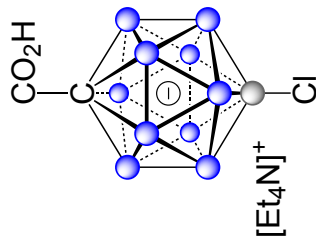
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1-COOH-12-Cl-CB11 product 30 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 160 MHz, 23 C

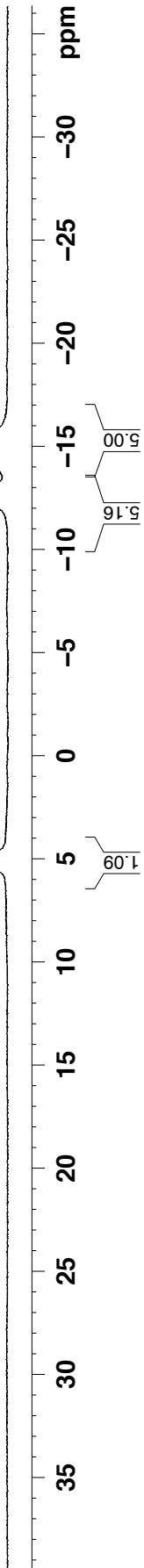
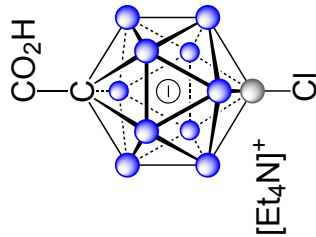
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12-Br-1-COOH-Pd product 30 mg in 0.6 ml acetonitrile-d3*
¹H{¹B} NMR, 500 MHz, 23 C

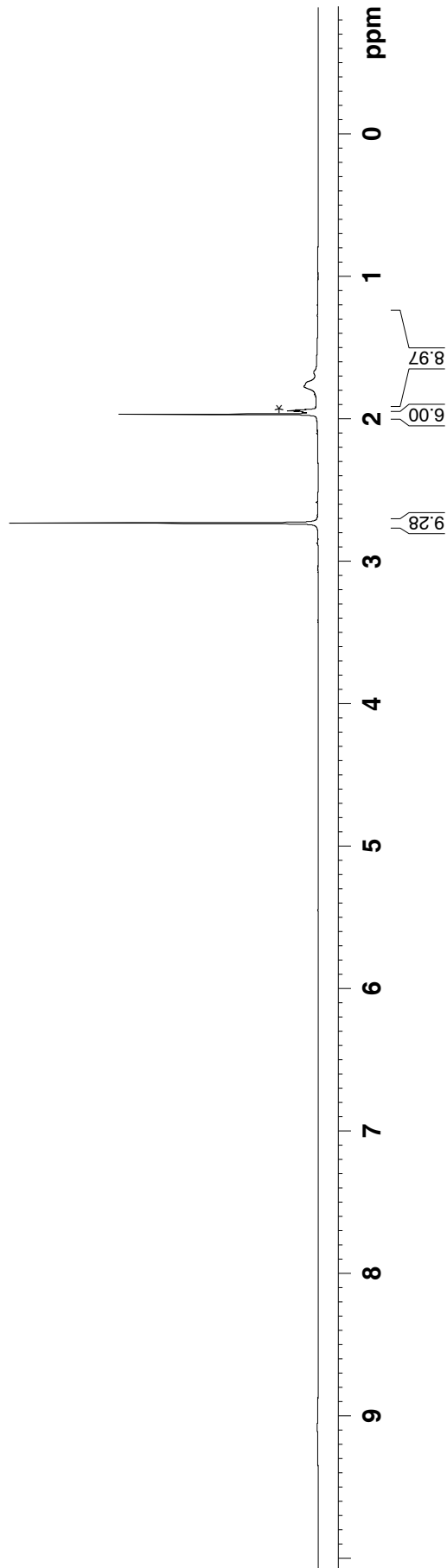
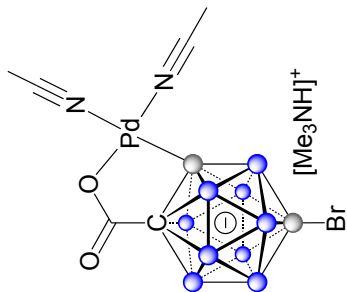
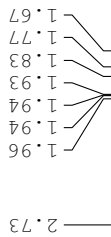
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**12-Br-1-COOH-Pd product 30 mg in 0.6 ml acetonitrile-d3
11B NMR, 160 MHz, 23 C**

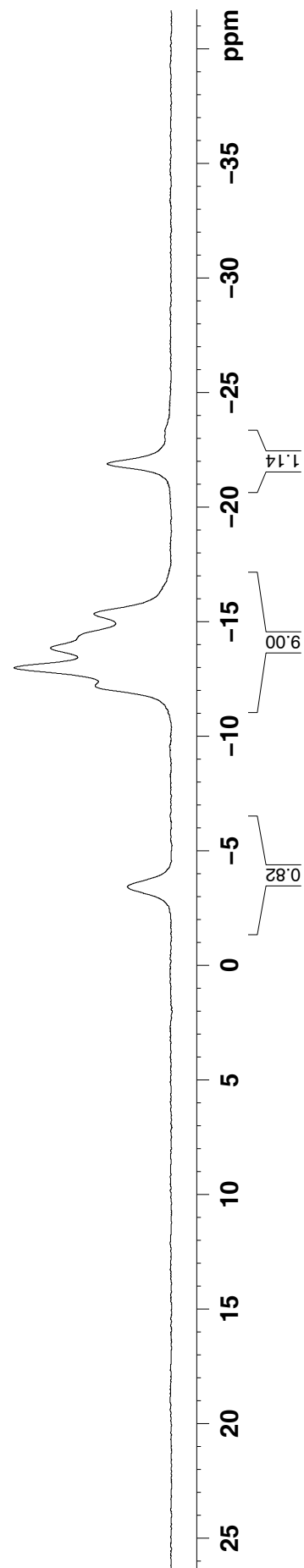
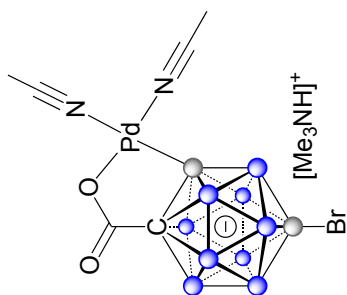
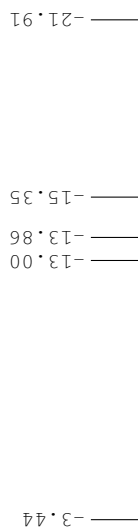
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**12-Br-1-COOH-Pd product 30 mg in 0.6 ml acetonitrile-d3
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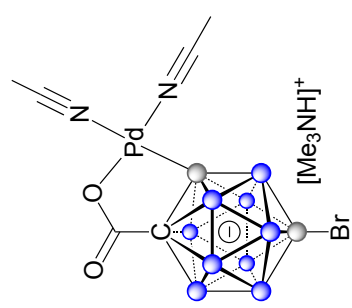
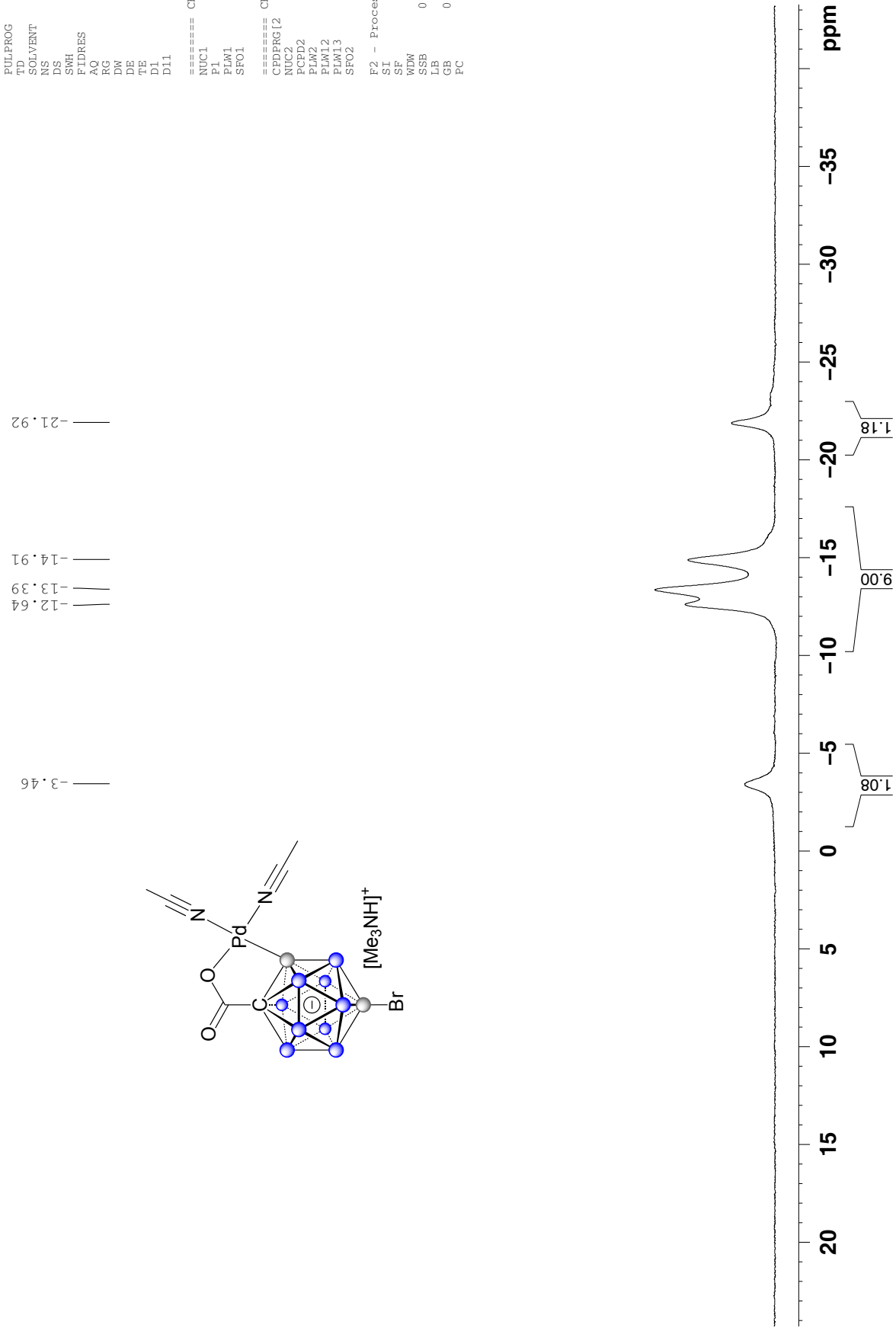
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**12-Br-1-COOH-Pd product 30 mg in 0.6 ml acetonitrile-d3*
¹³C{¹H} NMR, 126 MHz, 23 C**

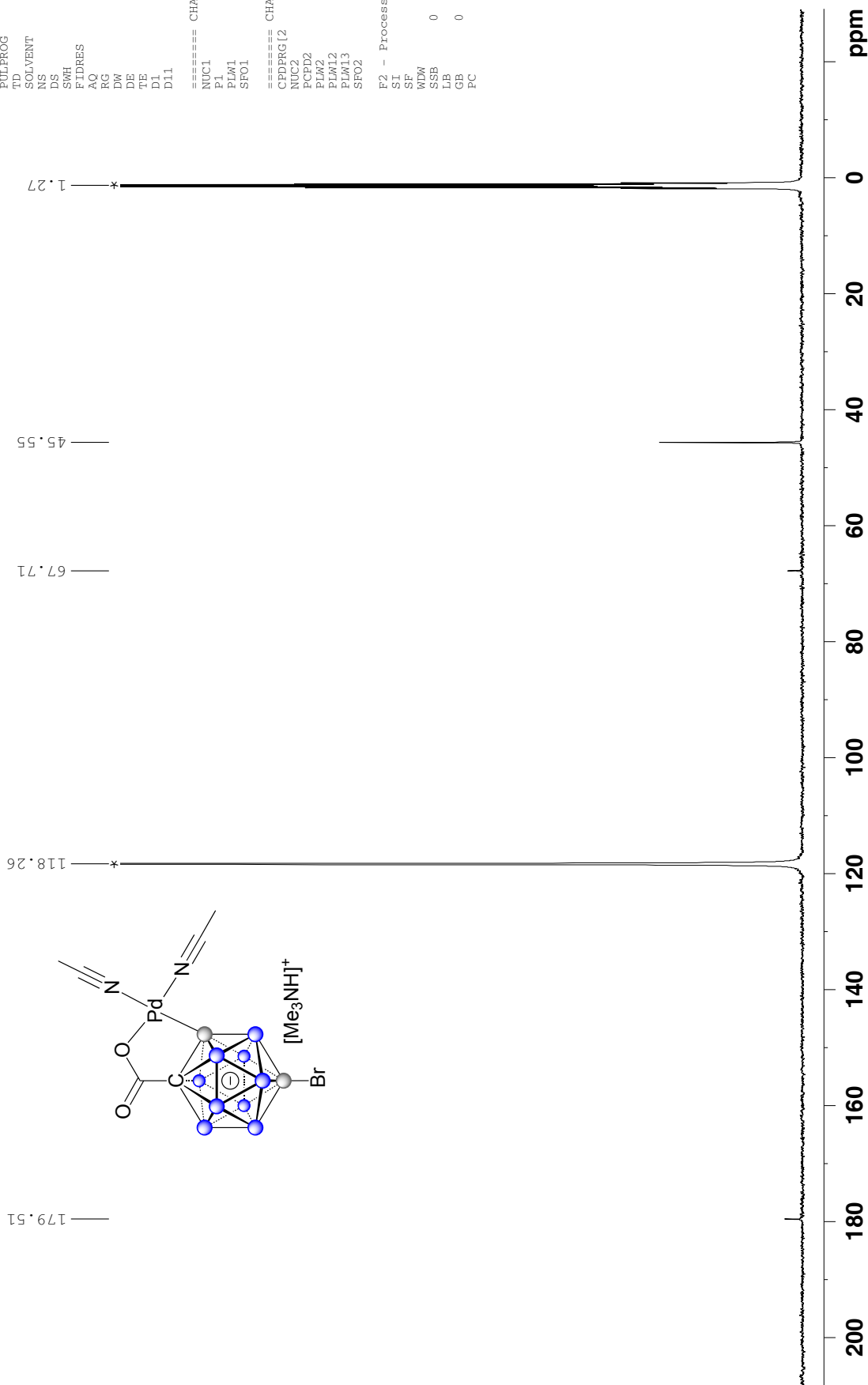
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 D1 1.50000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.50 usec
 PLW1 95.00000000 W
 SFO1 125.7716224 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 P2 80.00 usec
 PLW2 19.00000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7576724 MHz
 EM
 WDW 0
 SSB 0
 LB 6.00 Hz
 GB 0
 PC 1.40



1-COOH-12-Me-CB11 product 30 mg in 0.6 ml acetone-d6 *
¹H{¹¹B}NMR, 500 MHz, 23 C

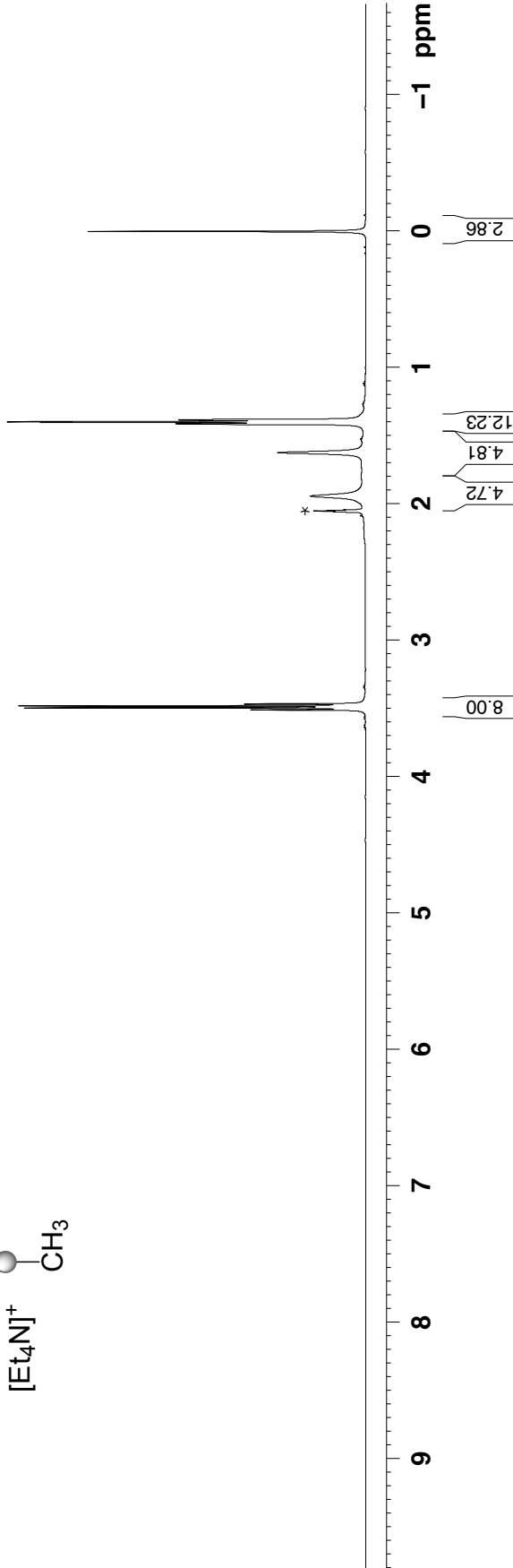
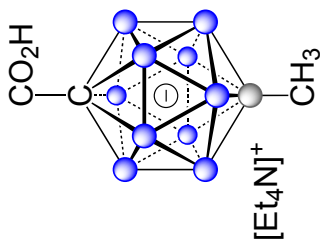
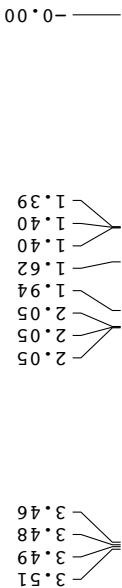
Current Data Parameters
 NAME 12-Me-acid
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180824
 Time_ 6.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg1930
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 0
 SWH 12500.000 Hz
 FIDRES 0.190735 Hz
 AQ 2.6214399 sec
 RG 64
 DW 40.000 usec
 DE 6.50 usec
 TE 296.0 K
 D1 5.00000000 sec
 D11 0.03000000 sec
 TDO 1

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

=====
 CHANNEL f2 =====
 SFO2 160.4615690 MHz
 NUC2 ¹¹B
 CPDPRG[2] garp
 FCPD2 100.00 usec
 PLW2 95.00000000 W
 PLW12 1.63030005 W

F2 - Processing parameters
 SI 65536
 SF 500.1300087 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



**1-COOH-12-Me-CB11 product 30 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

```

Current Data Parameters
NAME      12-Me-acid
EXPNO    2
PROCNO    1

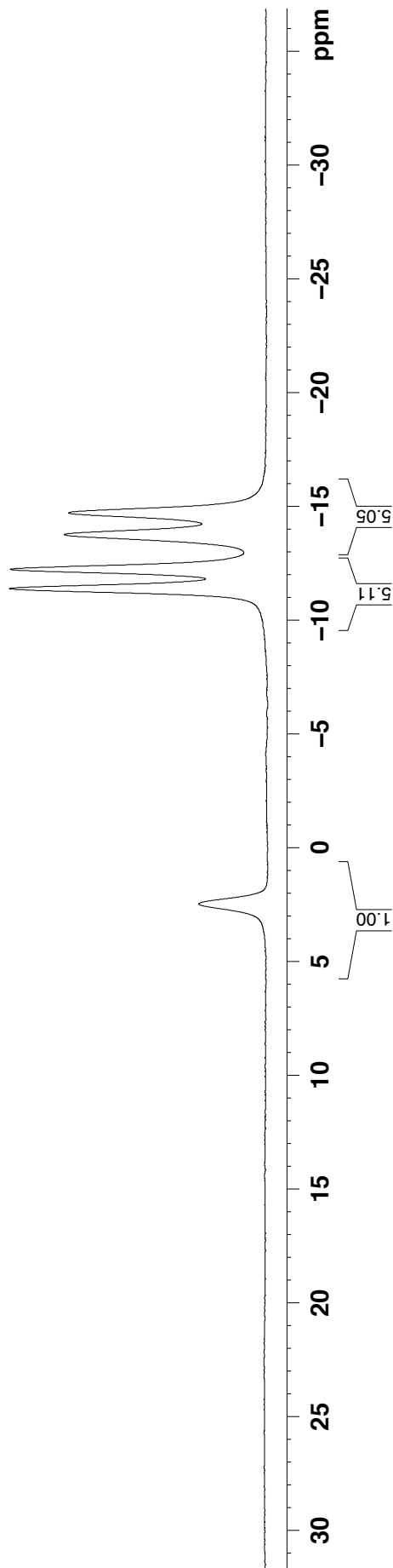
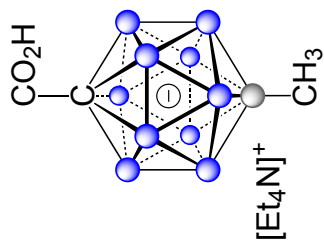
F2 - Acquisition Parameters
Date_     20180824
Time      6.24
INSTRUM   spect
PROBHD    5 mm PABBO BB
PULPROG   zgpg30
TD        64098
SOLVENT   Acetone
NS        30
DS        3
SWH       32051.281 Hz
FIDRES    0.500036 Hz
AQ         0.9999288 sec
RG         203
DW         15.600 usec
DE         6.50 usec
TE         295.9 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
SF01      160.4615792 MHz
NUC1      11B
P1         13.10 usec
PLW1      95.00000000 W

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

— 11.40
— 12.25
— 13.77
— 14.73

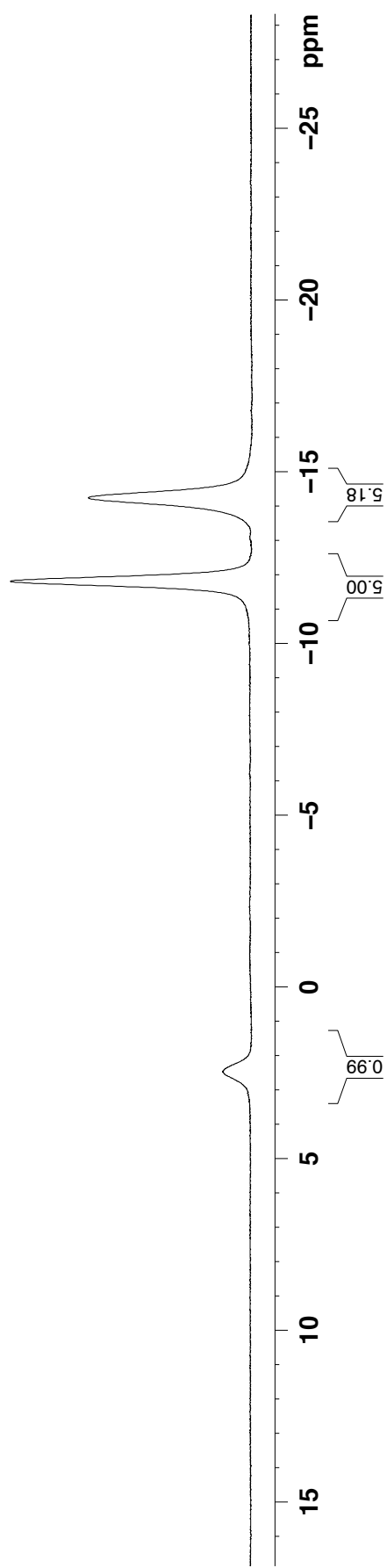
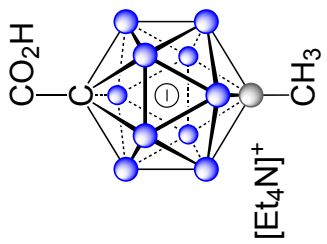
— 2.46



1-COOH-12-Me-CB11 product 30 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 160 MHz, 23 C

Current Data Parameters
 NAME 12-Me-acid
 EXPNO 3
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20180824
 Time_ 6:24
 INSTRUM spect
 PROBHD 5 mm PABBO1BBL
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 30
 DS 30
 SWH 32051.281 Hz
 FIDRES 0.7489064 Hz
 AQ 1.0223616 sec
 RG 203
 DW 15.600 usec
 DE 6.50 usec
 TE 296.3 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 SF01 160.4615790 MHz
 NUC1 11B
 P1 13.10 usec
 PLW1 95.0000000 W
 ===== CHANNEL f2 =====
 SF02 500.1325007 MHz
 NUC2 1H
 P2 19.0000000 usec
 PLW2 0.0639001 W
 PLW12 0.26008999 W
 PLW13 0.26008999 W
 F2 - Processing parameters
 SI 32768
 SF 160.4615790 MHz
 VDWM 0 EM
 SSB 0
 LB 0
 GB 0
 PC 1.40



1-COOH-12-Me-CB11 product 30 mg in 0.6 ml acetone-d6 *
¹³C{¹H} NMR, 125 MHz, 23 C

```

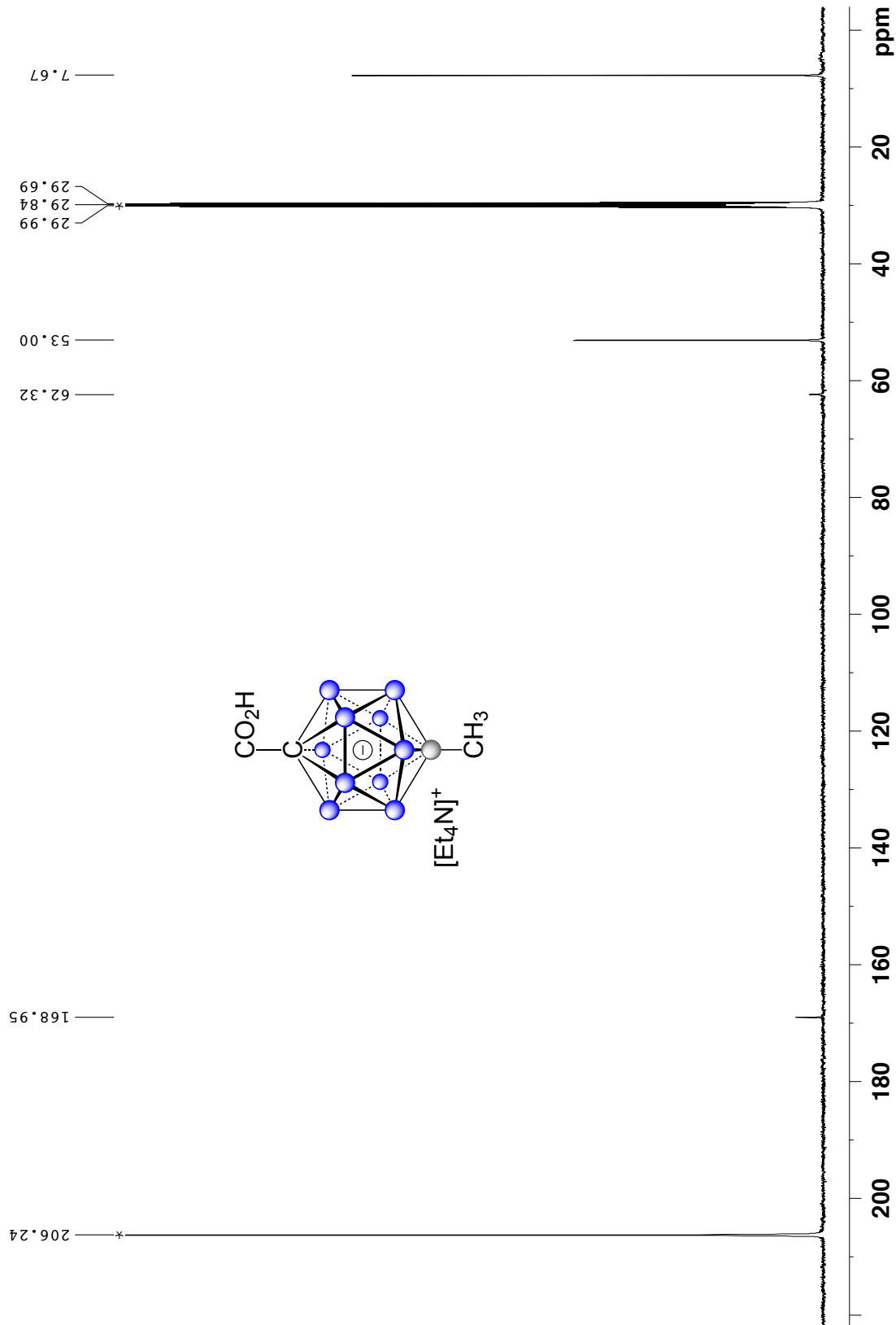
Current Data Parameters
NAME      12-Me-acid
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20180824
Time      7.08
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         1024
DS         4
SWH        37878.789 Hz
FIDRES     0.577984 Hz
AQ         0.8650752 sec
RG         203
DM         13.200 usec
DE         6.50 usec
TE         296.1 K
D1         1.5000000 sec
D11        0.0500000 sec
TD0        1

==== CHANNEL f1 ====
SFO1      125.7716224 MHz
NUC1      13C
FLW1      95.0000000 W

==== CHANNEL f2 ====
SFO2      500.1320005 MHz
NUC2      1H
waltz16
CPDPRG2[ waltz16
PCPD2     80.00 usec
FLM2      19.0000000 W
FLW2      0.40639001 W
FLW13     0.26008999 W

F2 - Processing parameters
SI         32768
SF         125.7576811 MHz
WDW        EM
SSB        0
GB         0
PC         1.40
  
```



1-COOH-12-Ph-CB11 product 30 mg in 0.6 ml acetone-d6 *
¹H{¹B}NMR, 400 MHz, 23 C

```

Current Data Parameters
NAME      12-Ph-acid
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20180801
Time     14.05
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       295.3 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 =====
CPDPRG2  garp4
NUC2     11B
P2       90.00 usec
PLW2     52.96599960 W
SFO2     128.3776050 MHz

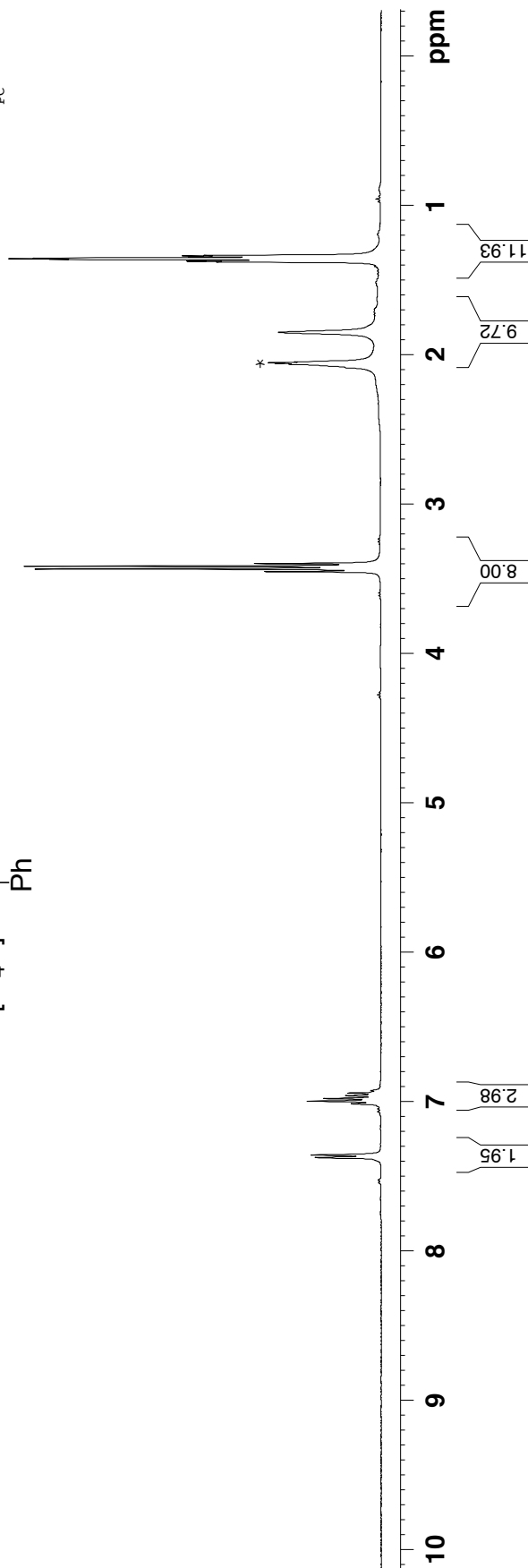
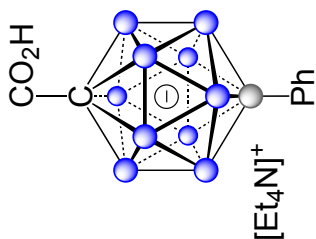
F2 - Processing parameters
SI       32768
SF       400.1300073 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

3.45
3.43
3.40

2.06
2.06
2.05
2.04
1.85

1.36
1.35
1.35

7.37
7.36
7.01
6.98
6.96
6.94



1-COOH-12-Ph-CB11 product 30 mg in 0.6 ml acetone-d6
 11B NMR, 128 MHz, 23 C

```

Current Data Parameters
NAME      12-Ph-acid
EXPNO     2
PROCNO    1

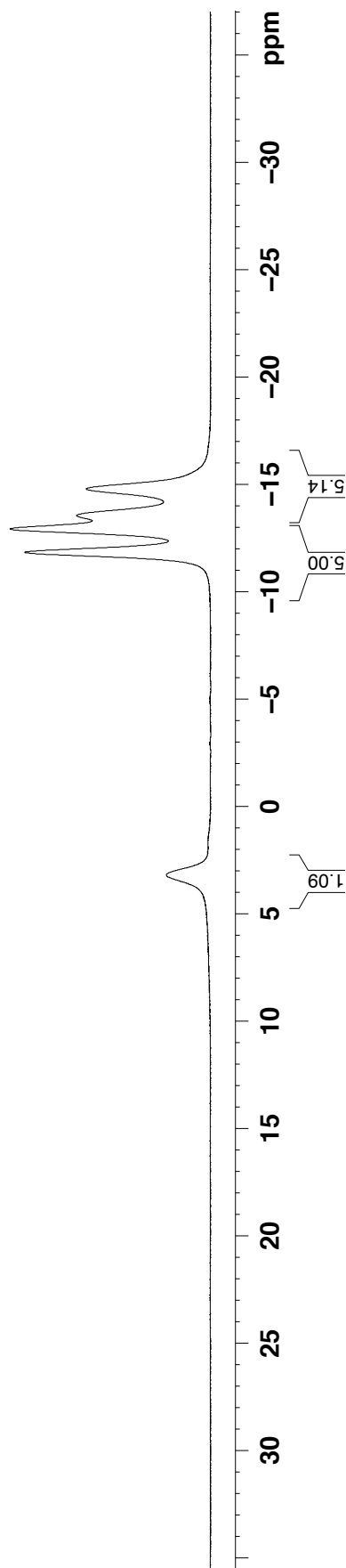
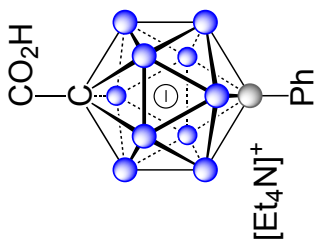
F2 - Acquisition Parameters
Date_     20180801
Time      14.11
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg
TD         65536
SOLVENT   Acetone
NS         128
DS         4
SWH        25510.203 Hz
FIDRES     0.389235 Hz
AQ         1.2845056 sec
RG         193.34
DW         19.600 usec
DE         6.50 usec
TE         294.9 K
D1         1.0000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       11B
P1         9.93 usec
PL1        52.9659960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI         32768
SF         128.3776050 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

11.86
 12.95
 13.58
 14.81

3.17



1-COOH-12-Ph-CB11 product 30 mg in 0.6 ml acetone-d6
 11B{1H} NMR, 128 MHz, 23 C

```

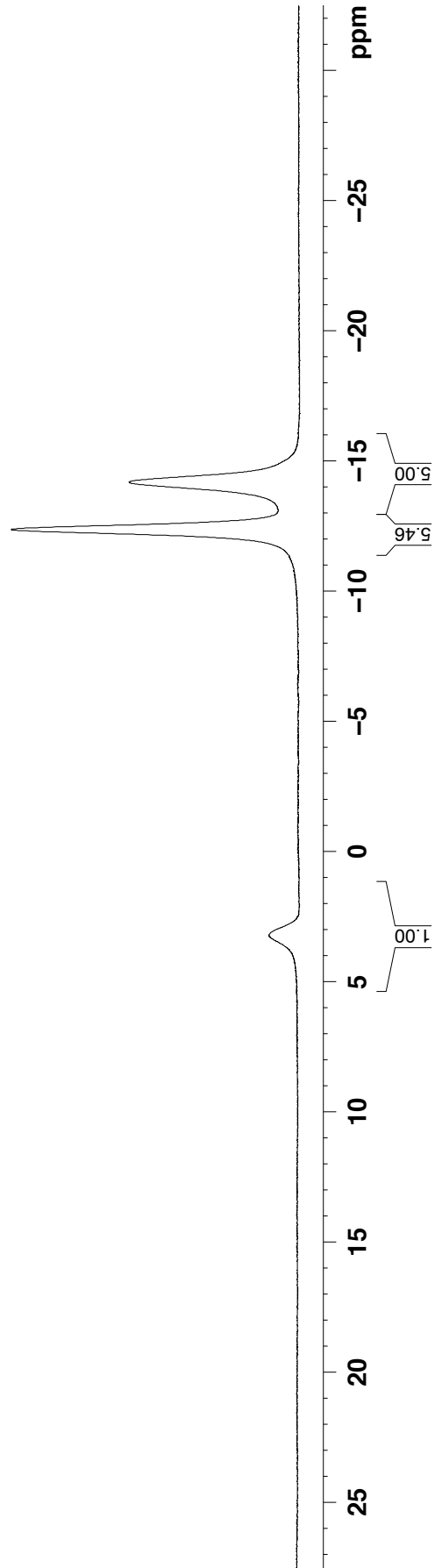
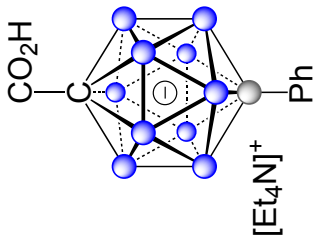
Current Data Parameters
NAME      12-Ph-acid
EXPNO    3
PROCNO   1

F2 - Acquisition Parameters
Date_    20180801
Time     14.17
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  Acetone
NS       128
DS       4
SWH      25510.203 Hz
FIDRES   0.389235 Hz
AQ       1.2845056 sec
RG       193.34
DW       19.600 usec
DE       6.50 usec
TE       295.5 K
D1       1.0000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1      11B
P1        9.93 usec
PLW1     52.9659960 W
SFO1     128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PLW2     12.5000000 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        1.00 Hz
GB        0
PC        1.40
  
```



1-COOH-12-Ph-CB11 product 30 mg in 0.6 ml acetone-d6 *
¹³C{¹H} NMR, 101 MHz, 23 C

```

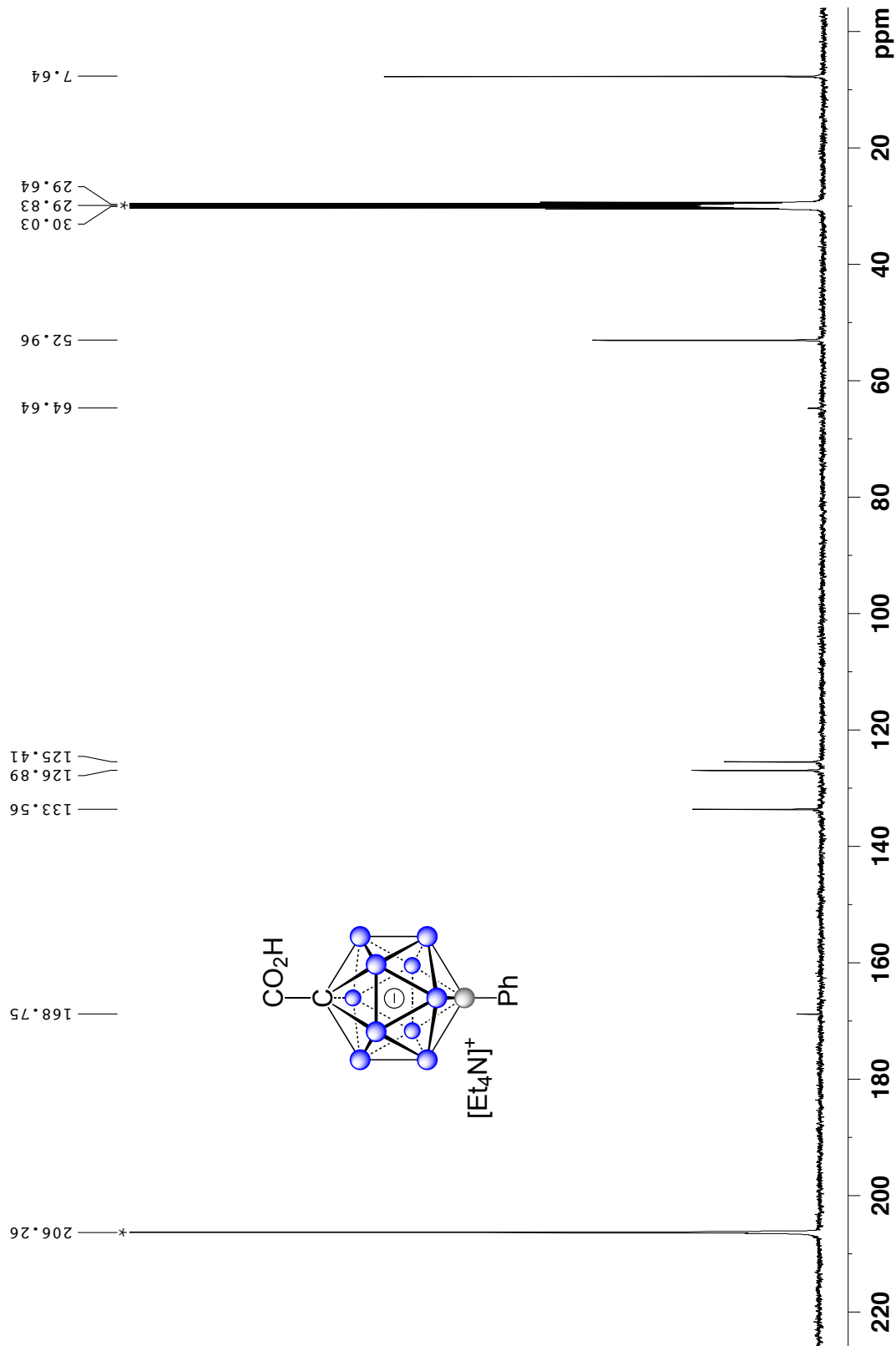
Current Data Parameters
NAME      12-Ph-acid-13C
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20180802
Time     13.43
INSTRUM spect
PROBHD   5 mm PABRO/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       285.5 K
D1       1.50000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1      13C
P1        10.00 usec
PLW1     53.00000000 W
SF01     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
SF02     400.1316005 MHz

F2 - Processing parameters
SI        32768
SF        100.6126835 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40
  
```



Penta-4-F-styrene product 80 mg in 0.6 ml acetone-d6 *
¹H{¹¹B} NMR, 400 MHz, 23 C

Current Data Parameters
 NAME penta-4-F-styrene
 EXPNO 1
 PROCNO 1

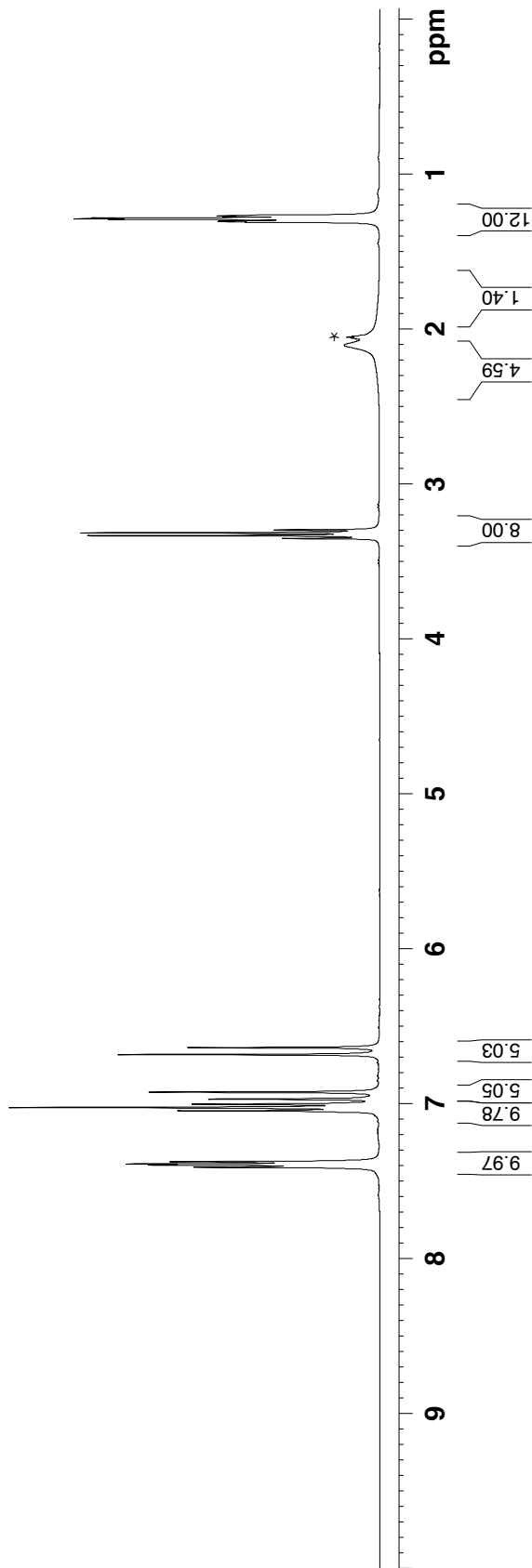
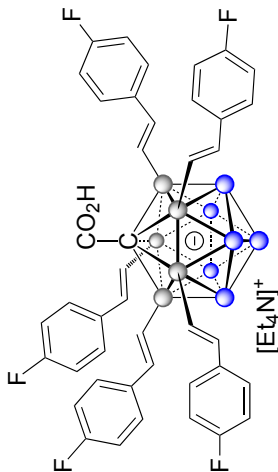
F2 - Acquisition Parameters
 Date_ 20180529
 Time_ 18.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 23.04
 DW 62.400 usec
 DE 6.50 usec
 TE 294.3 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PLW1 12.5000000 W
 SFO1 400.1320007 MHz
 ===== CHANNEL f2 =====
 CPDPRG12 garp4
 NUC2 ¹¹B
 P2 90.00 usec
 PLW2 52.9659960 W
 PLW12 0.6447798 W
 SFO2 128.3776050 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300073 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

2.10
 2.05
 1.31
 1.30
 1.30
 1.29
 1.29
 1.29
 1.28
 1.27
 1.27
 1.27
 1.26

3.35
 3.33
 3.31
 3.29

7.41
 7.39
 7.39
 7.37
 7.04
 7.02
 7.00
 6.97
 6.92
 6.68
 6.64



**Penta-4-F-styrene product 80 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

```

Current Data Parameters
NAME      Penta-4-F-styrene
EXPNO    2
PROCNO   1

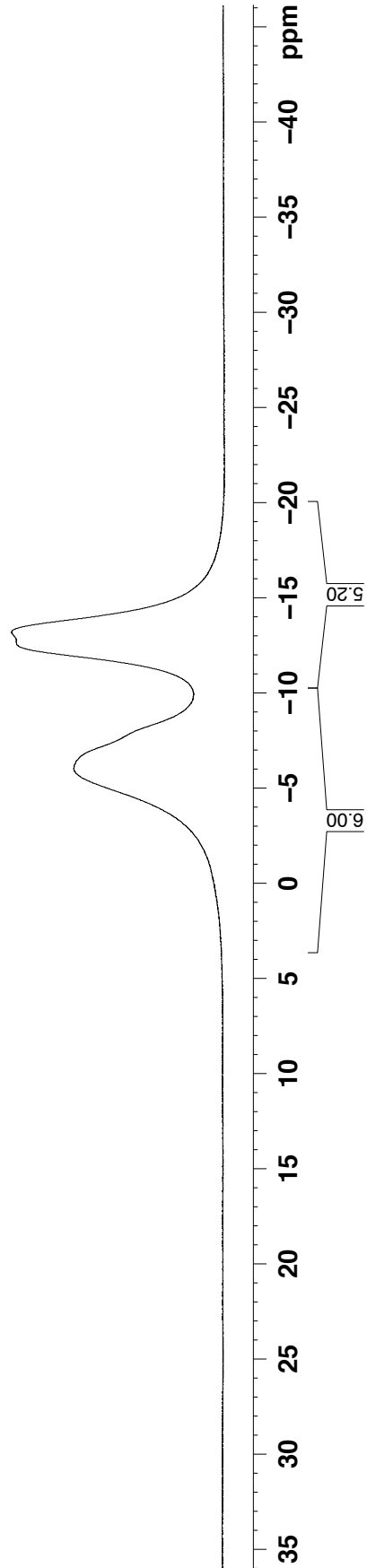
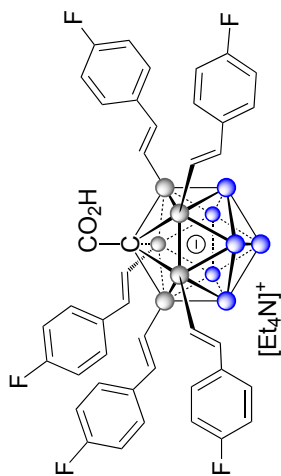
F2 - Acquisition Parameters
Date_    20180529
Time     18:22
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  Acetone
NS       128
DS       4
SWH      25510.203 Hz
FIDRES   0.389255 Hz
AQ       1.2845056 sec
RG       193.34
RW       19.600 usec
DE       1.000 usec
TE       294.2 K
D1       1.00000000 sec
TD0      1
  
```

```

===== CHANNEL f1 =====
NUC1     11B
P1       9.93 usec
PL1      52.9659960 W
SFO1     128.3776052 MHz

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

6.05
-12.55
-13.23



Penta-4-F-styryne product 80 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 128 MHz, 23 C

```

Current Data Parameters
NAME      Penta-4-F-styrene
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20180529
Time      18.28
INSTRUM   spect
PROBHD    5 mm PABBO1B1/
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         124
DS         4
SWH        25510.203 Hz
FIDRES     0.389255 Hz
AQ         1.2845056 sec
RG         193.34
DE         19.604 usec
TE         293.2 K
D1         1.0000000 sec
D11        0.0300000 sec
TDO       1
  
```

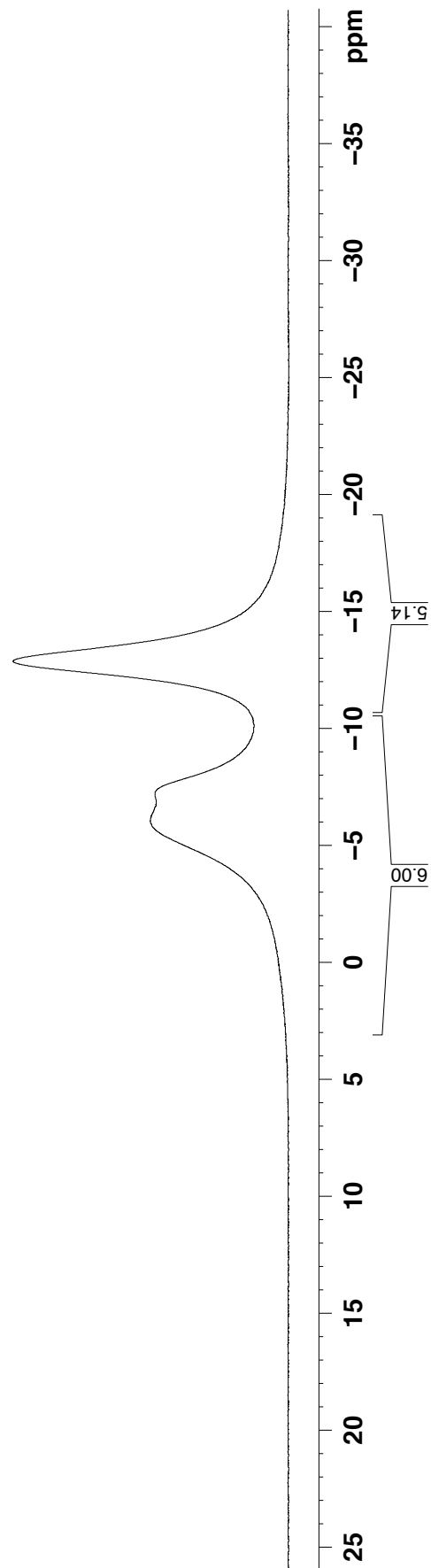
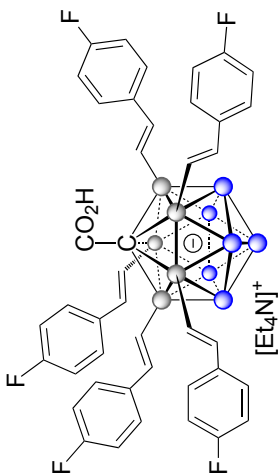
```

===== CHANNEL f1 =====
NUC1      11B
P1         9.93 usec
P1M1      52.9659960 W
SFO1      128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG[2] waitz16
NUC2       1H
P2         80.01 usec
P2M2      12.5000000 W
SFO2      400.1320007 MHz

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

— 12.90
 — 7.24
 — 6.07



Penta-4-F-styrene product 80 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 101 MHz, 23 C

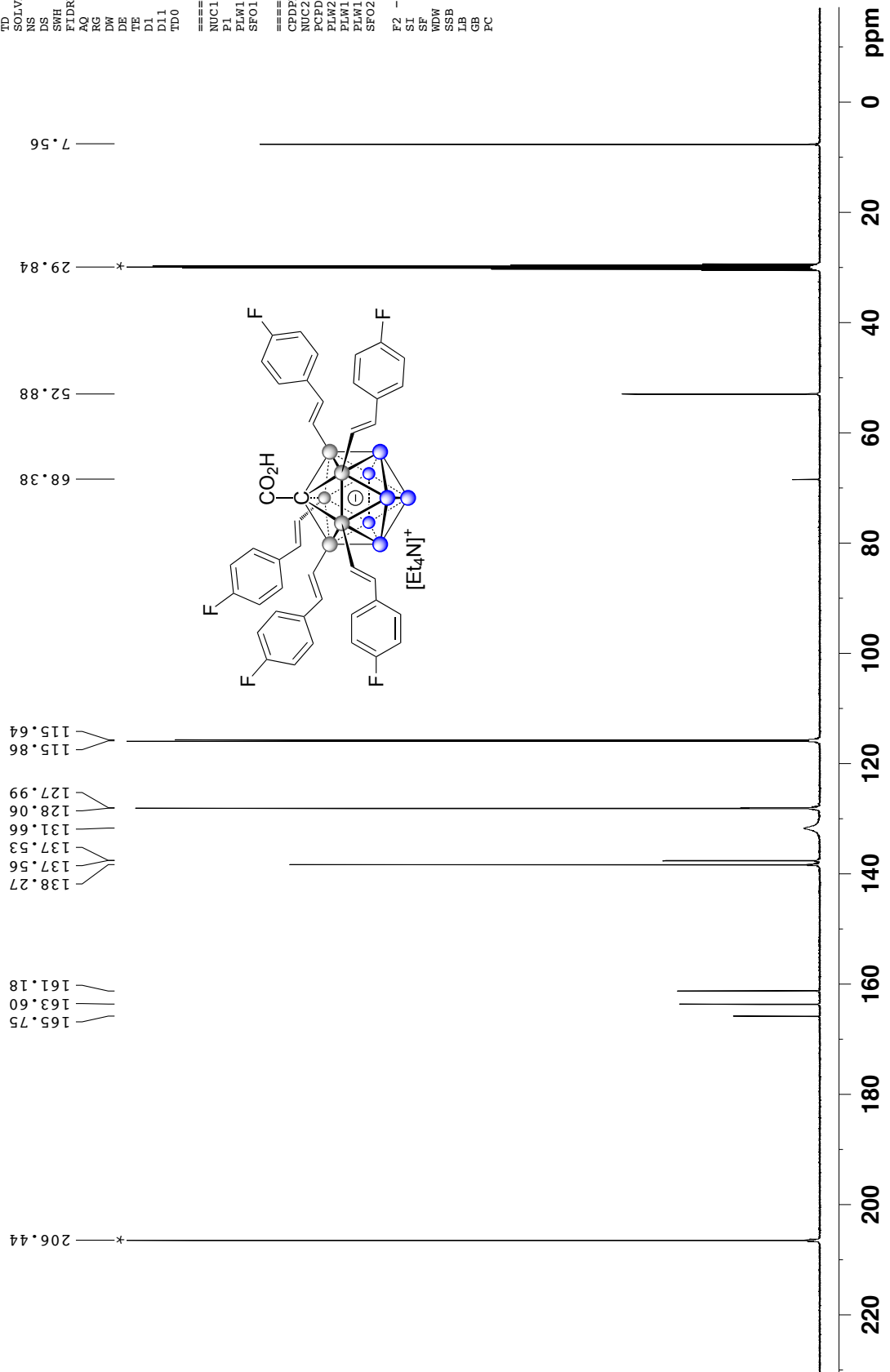
Current Data Parameters
 NAME penta-4-F-styrene
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180529
 Time_ 20.01
 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 294.2 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 100.6126935 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Penta-styrene product 50 mg in 0.6 ml acetone-d6
¹H{¹H} NMR, 500 MHz, 23 C

```

Current Data Parameters
NAME      penta-styrene
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20180509
Time      2.08
INSTRUM   spect
PROBHD    5 mm FAPBEO B3
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         16
DS         4
SWH        12500.000 Hz
FIDRES     0.190735 Hz
AQ         2.621499 sec
RG         71.8
DE         40.000 usec
TE         296.3 K
D1         5.0000000 sec
D11        0.03000000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         11.70 usec
PL1        19.0000000 W
SFO1       500.1330009 MHz

===== CHANNEL f2 =====
CPDPRG2   garp
NUC2       13C
P2         100.000 usec
PL2        95.0000000 W
SFO2       125.7603505 MHz

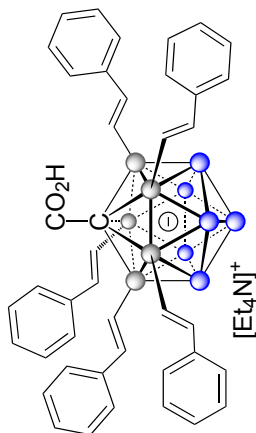
F2 - Processing parameters
SI         65536
SF         500.1300101 MHz
WDW        EM
SSB        0
LB         0
GB         0
PC         1.00
  
```

1.30
1.30
1.31
1.31
1.32
1.32
1.33
1.33

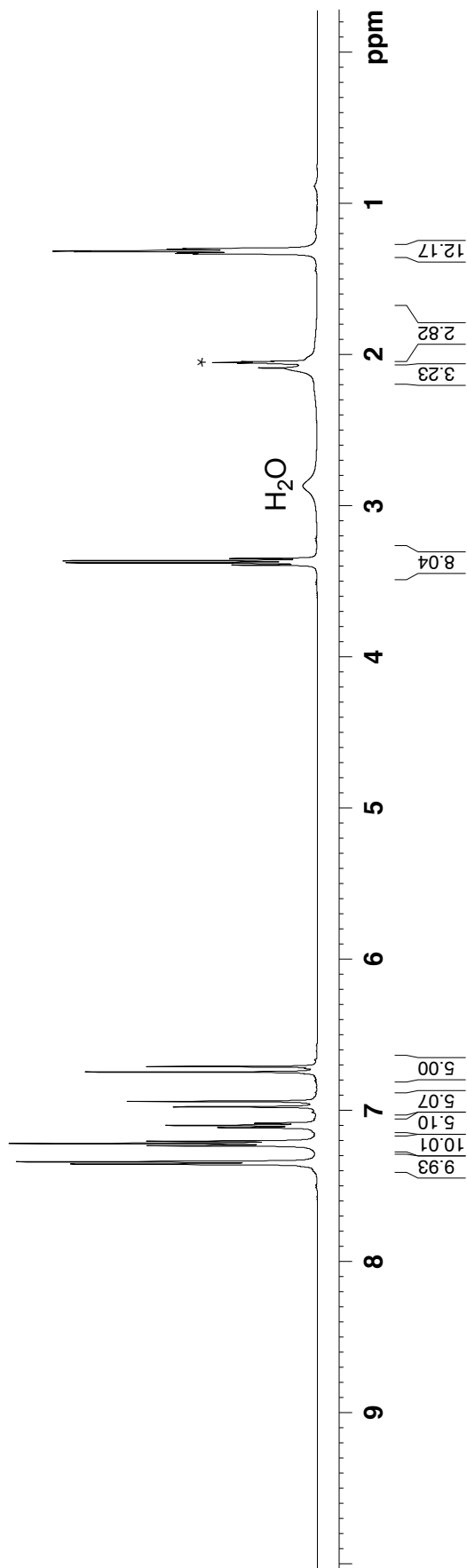
2.05
2.09

2.87

3.35
3.36
3.38
3.39



6.71
6.74
6.94
6.97
7.08
7.10
7.11
7.20
7.22
7.23
7.34
7.35



**Penta-styrene product 50 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

```

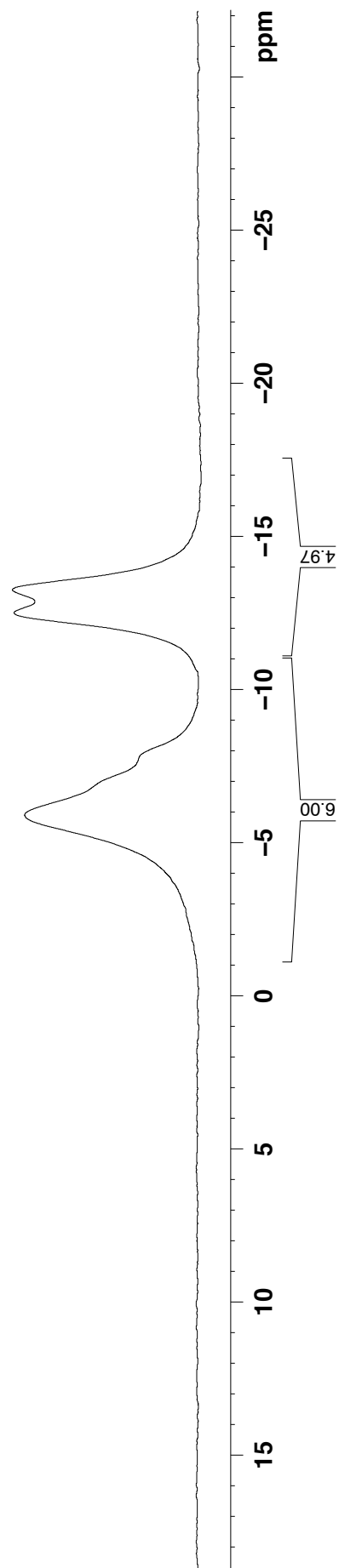
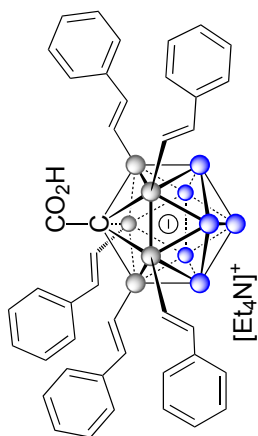
Current Data Parameters
NAME      penta-styrene
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_     20180509
Time      2.10
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        95.0000000 W
SF01        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
  
```

6.03
12.59
13.35



**Penta-styrene product 50 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 160 MHz, 23 C**

```

Current Data Parameters
NAME      Penta-styrene
EXPNO     3
PROCNO    1

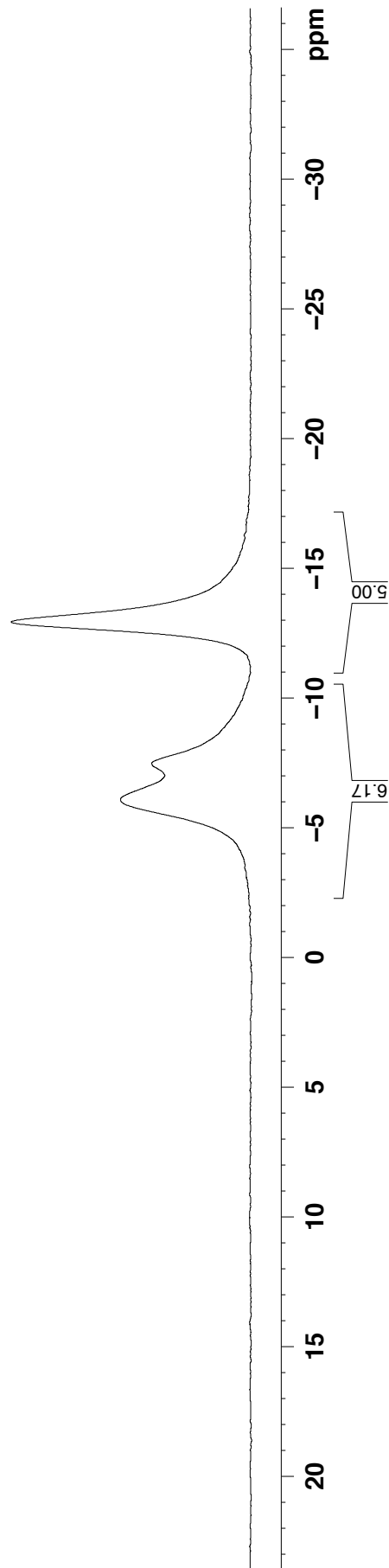
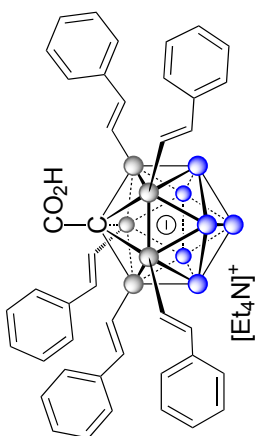
F2 - Acquisition Parameters
Date_     20180509
Time      2.14
INSTRUM   spect
PROBHD    5 mm PABBO1BBL
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         64
DS         4
SWH        32051.281 Hz
FIDRES     0.7489064 Hz
AQ          1.0223616 sec
RG          303
PC          15.600 usec
DE          6.50 usec
TE          295.8 K
D1          1.00000000 sec
D11         0.03000000 sec

===== CHANNEL f1 =====
NUC1       11B
P1         13.10 usec
PL1        95.00000000 W
SFO1       160.4615790 MHz

===== CHANNEL f2 =====
CPDPRG2    waitz16
NUC2        1H
PCPD2       80.00 usec
PL2         19.00000000 W
PL12        0.0639001 W
PL13        0.26008999 W
SFO2       500.1325007 MHz

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

12.95
 7.50
 6.09



**Penta-styrene product 50 mg in 0.6 ml acetone-d6
¹³C{¹H} NMR, 126 MHz, 23 C**

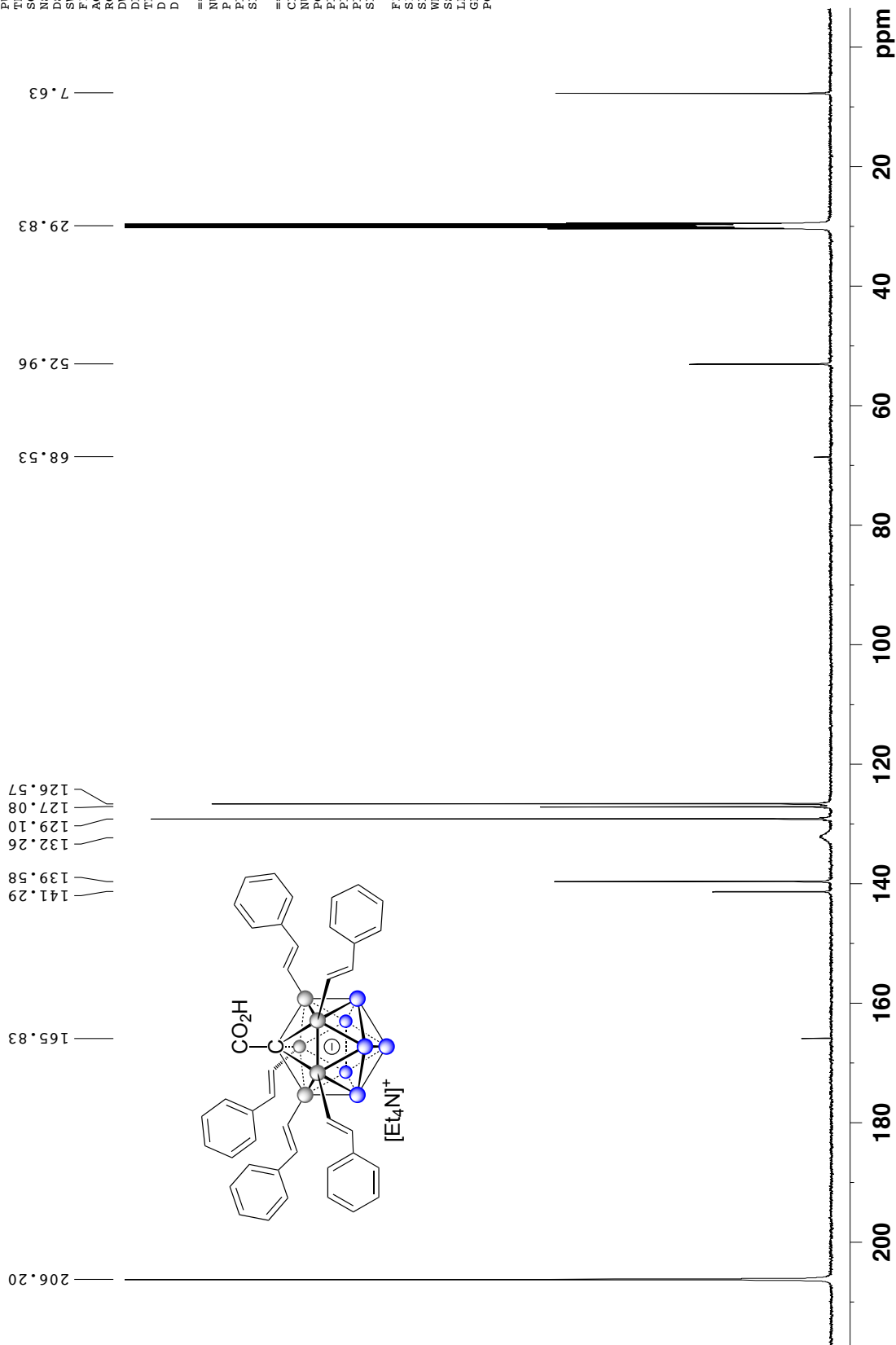
Current Data Parameters
 NAME penta-styrene
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180509
 Time 4.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 3100
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.1 K
 D1 1.5000000 sec
 D11 0.0300000 sec

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.50 usec
 PLW1 95.0000000 W
 SFO1 125.7716224 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waitz16
 NUC2 ¹H
 PCD2 80.00 usec
 PLW2 19.0000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7576810 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



**Penta-CF₃-styrene-acid chloride product 30 mg in 0.6 ml acetonitrile-d₃*
¹H{¹¹B} NMR, 500 MHz, 23 C**

Current Data Parameters
 NAME Penta-CF₃-styrene-acid chl
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181219
 Time 23.32
 INSTRUM spect
 PROHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CD₃CN
 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 296.9 K
 D1 5.0000000 sec
 D11 0.0300000 sec

=====
 CHANNEL f1 =====
 NUC1 ¹H
 P1 11.70 usec
 PLW1 19.0000000 W
 SFO1 500.1335009 MHz

=====
 CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 ¹¹B
 P2 100.00 usec
 PLW2 95.0000000 W
 PLM12 1.6303005 W
 SFO2 160.4615690 MHz

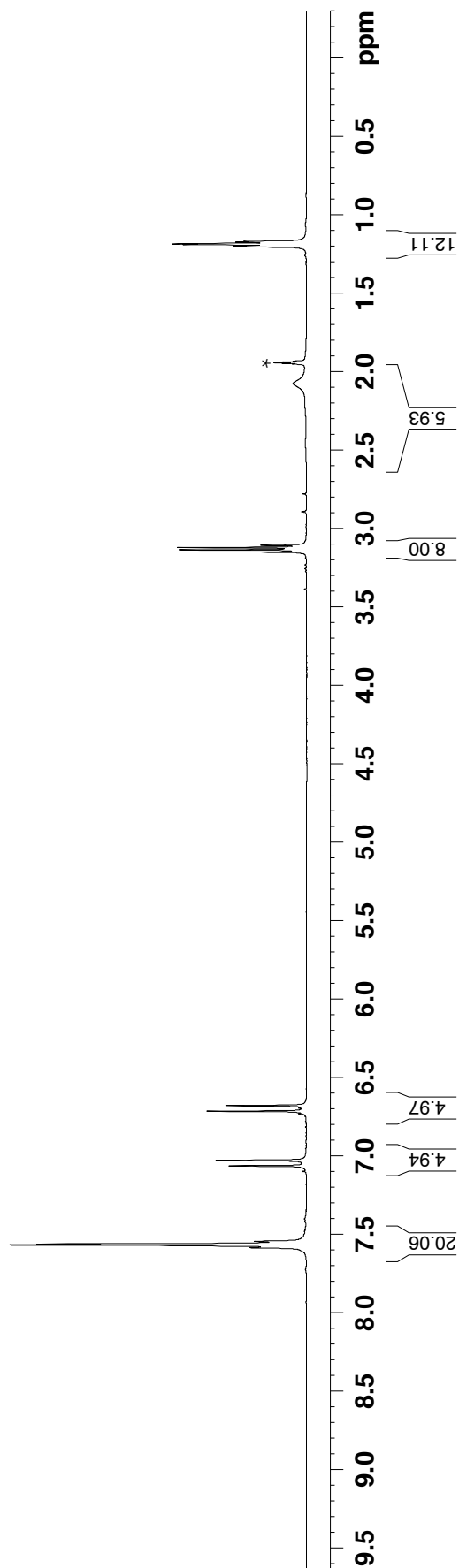
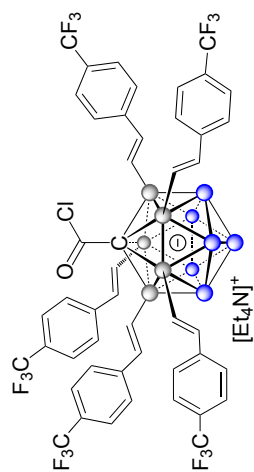
F2 - Processing parameters
 SI 65536
 SF 500.1300156 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1.20
1.19
1.17
1.17
1.17
1.17
1.17

2.07
1.94

3.15
3.13
3.12
3.10

7.57
7.56
7.06
7.03
6.71
6.68



**Penta-CF3-styrene-acid chloride product 30 mg in 0.6 ml acetonitrile-d3
11B NMR, 160 MHz, 23 C**

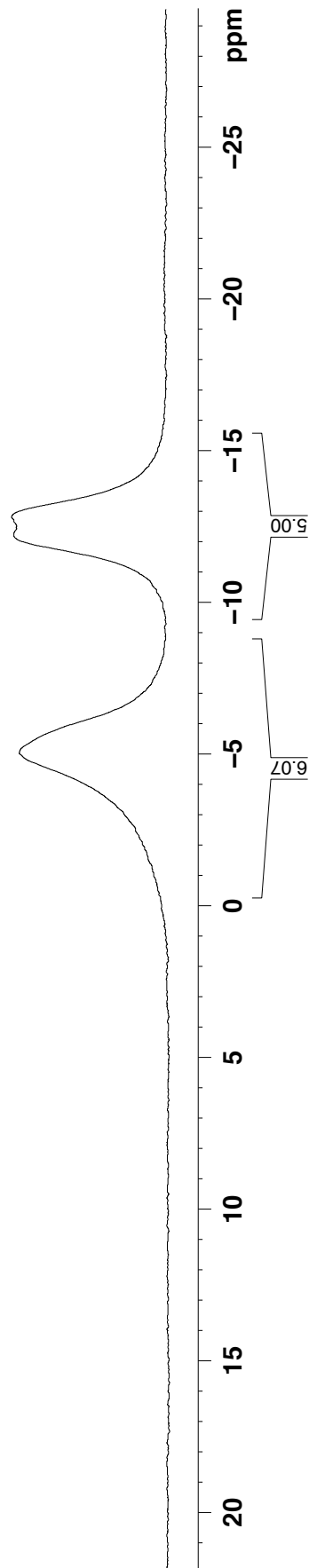
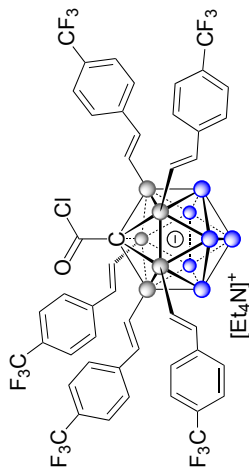
Current Data Parameters
 NAME Penta-CF3-styrene-acid chl
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181208
 Time 2.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 64098
 SOLVENT CD3CN
 NS 128
 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 1.0000000 sec

==== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 usec
 PLW1 95.0000000 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

5.05
 12.17
 12.83



**Penta-CF3-styrene-acid chloride product 30 mg in 0.6 ml acetonitrile-d₃
11B{1H} NMR, 160 MHz, 23 C**

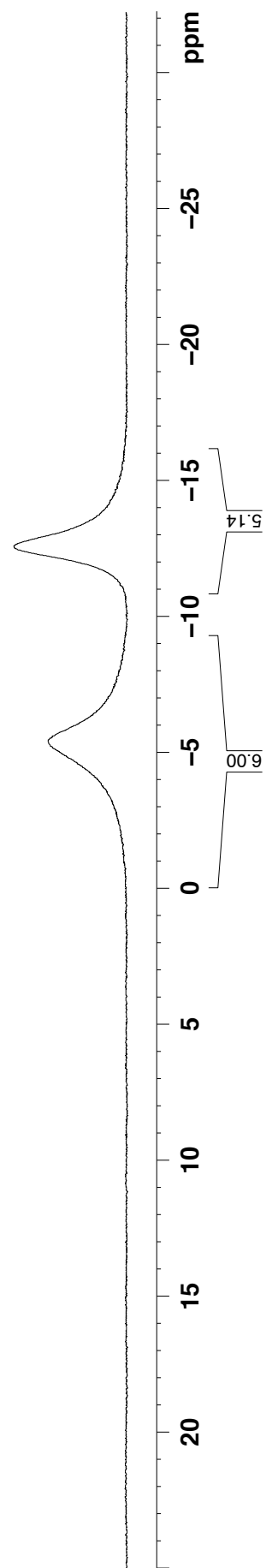
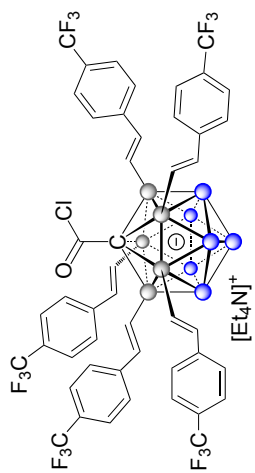
Current Data Parameters
 NAME Penta-CF3-styrene-acid chl
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181208
 Time 2.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CD3CN
 NS 128
 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 1.0000000 sec
 D11 0.0300000 sec

==== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 usec
 PLW1 95.0000000 W
 SFO1 160.4615790 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 FCPD2 80.00 usec
 PLW2 19.0000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SFO2 500.1325007 MHz

F2 - Processing parameters
 SI 32768
 SF 160.4615790 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



Penta-CF3-styrene-acid chloride product 30 mg in 0.6 ml acetonitrile-d3*
¹³C{¹H} NMR, 126 MHz, 23 C

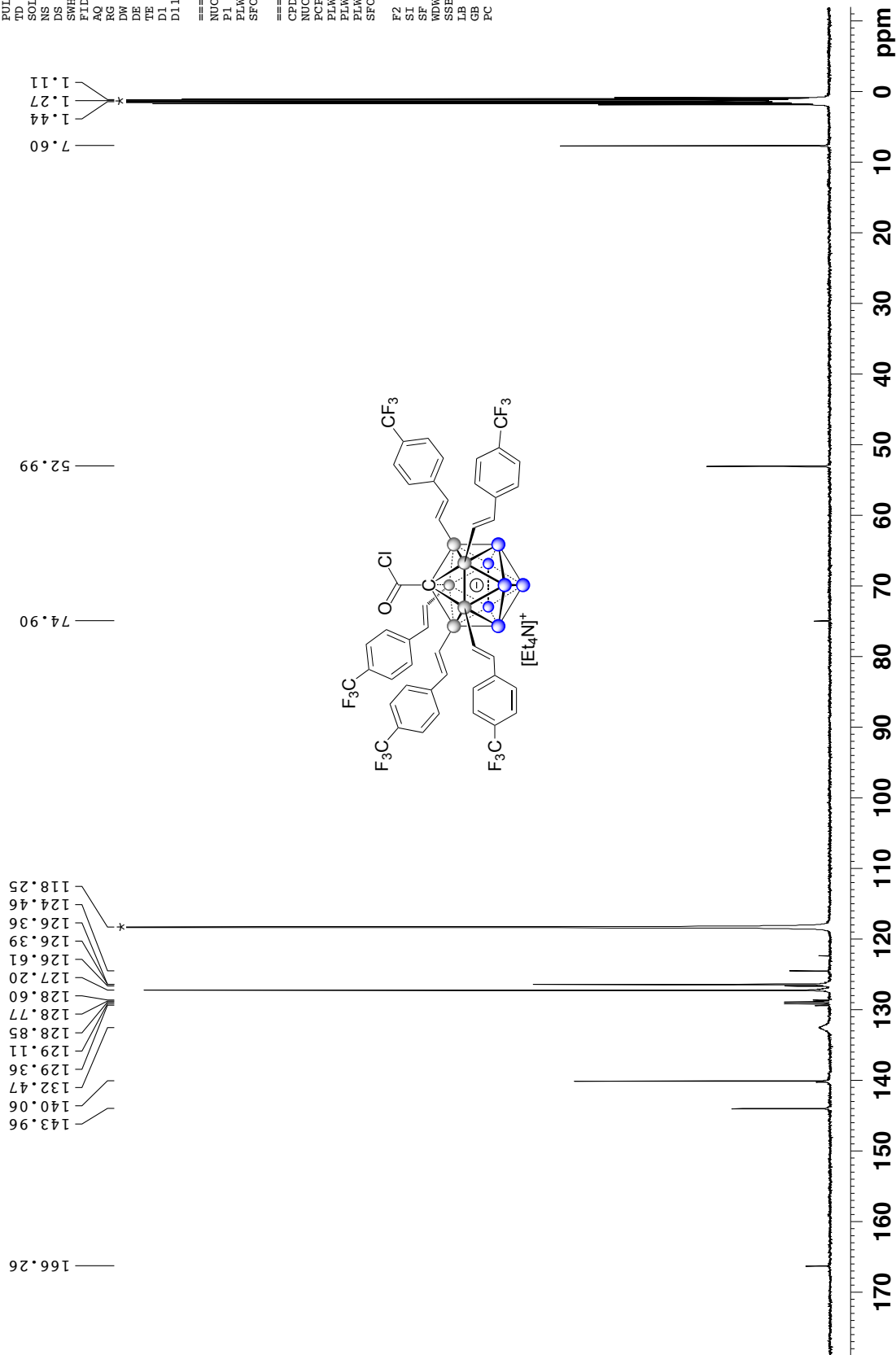
Current Data Parameters
 NAME Penta-CF3-styrene-acid chl
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181208
 Time 4.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 CD3CN
 SOLVENT 3100
 NS 4
 DS 37878.789 Hz
 SWH 0.577984 Hz
 FIDRES 0.8650752 sec
 AQ 203
 RG 13.200 usec
 DE 6.50 usec
 TE 295.4 K
 D1 1.5000000 sec
 D11 0.0300000 sec

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.50 usec
 PLW1 95.0000000 W
 SFO1 125.7716224 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 19.0000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7576712 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40



Penta-4-CF3-styrene product 50 mg in 0.6 ml acetone-d6 *
¹H{¹¹B} NMR, 500 MHz, 23 C

```

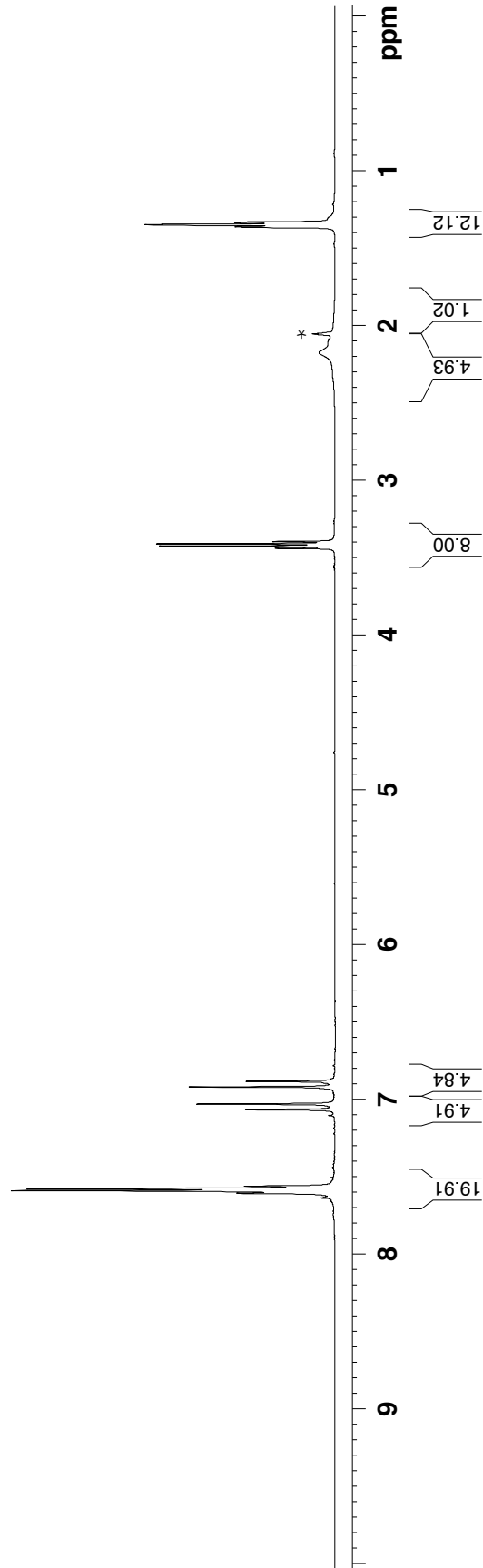
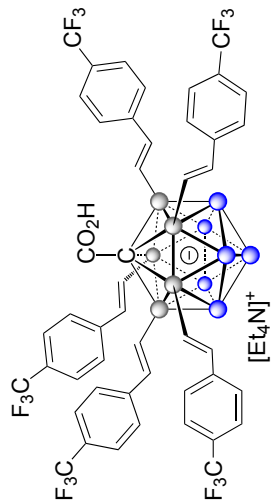
Current Data Parameters
NAME      penta-4-CF3-styrene
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20180529
Time     22.50
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  Acetone
NS       16
DS       0
SWH      12500.000 Hz
FIDRES   0.190735 Hz
AQ       2.6214399 sec
RG       22.6
DW       40.000 usec
DE       6.50 usec
TE       296.4 K
D1       5.0000000 sec
D11      0.0300000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       11.70 usec
PLW1     19.0000000 W
SFO1     500.1335009 MHz

===== CHANNEL f2 =====
CPDPRG2  garp
NUC2     11B
PCPD2    100.00 usec
PLW2     95.0000000 W
PLW12    1.6303005 W
SFO2     160.4615690 MHz

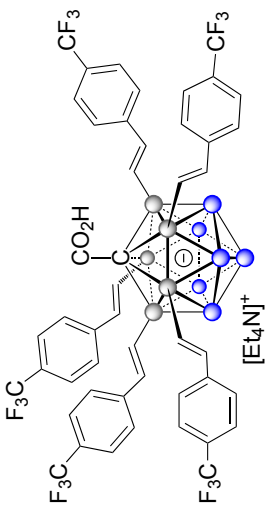
F2 - Processing parameters
SI       65536
SF       500.1300100 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.00
  
```



**Penta-CF3-styrene product 50 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

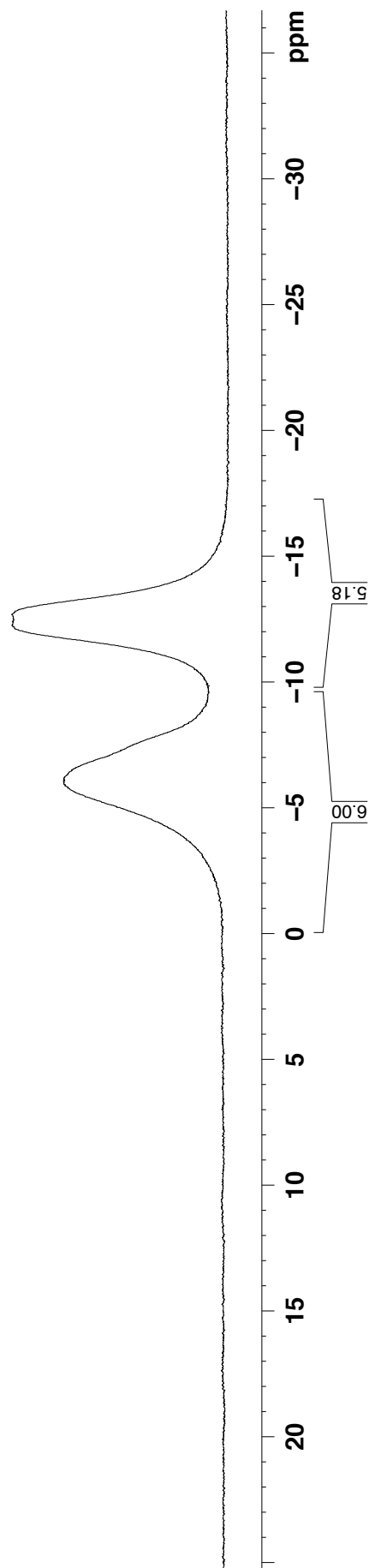
Current Data Parameters
 NAME penta-4-CF3-styrene
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180529
 Time_ 22.53
 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 295.9 K
 D1 1.00000000 sec



6.11
 -12.24
 -12.69

==== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 usec
 PLW1 95.0000000 W
 SF01 160.4615792 MHz
 F2 - Processing parameters
 SI 32768
 SF 160.4615790 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



**Penta-4-CF₃-styrene product 50 mg in 0.6 ml acetone-d₆
11B{1H} NMR, 160 MHz, 23 C**

Current Data Parameters
 NAME penta-4-CF₃-styrene
 EXPNO 3
 PROCNO 1

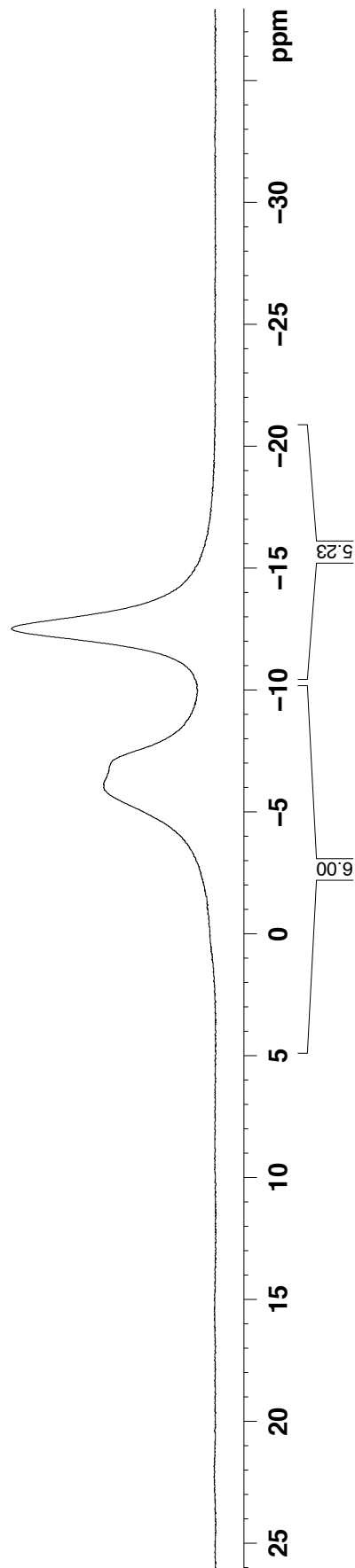
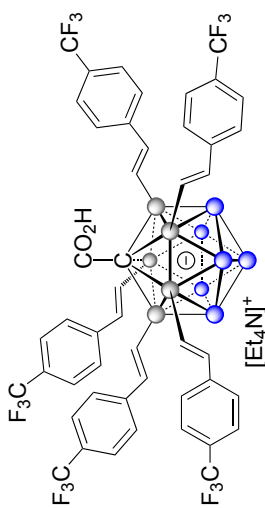
F2 - Acquisition Parameters
 Date_ 20180529
 Time_ 22.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 64
 DS 0
 SWH 32051.281 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 203
 DW 15.600 usec
 DE 6.50 usec
 TE 296.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 usec
 PLW1 95.0000000 W
 SF01 160.4615790 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 19.0000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SF02 500.1325007 MHz

F2 - Processing parameters
 SI 32768
 SF 160.4615790 MHz
 WDW EM
 SSB 0
 LB 4.00 Hz
 GB 0
 PC 1.40

— -6.17
 — -12.52



Penta-4-CF₃-styrene product 50 mg in 0.6 ml acetone-d₆ *
¹³C{¹H} NMR, 125 MHz, 23 C

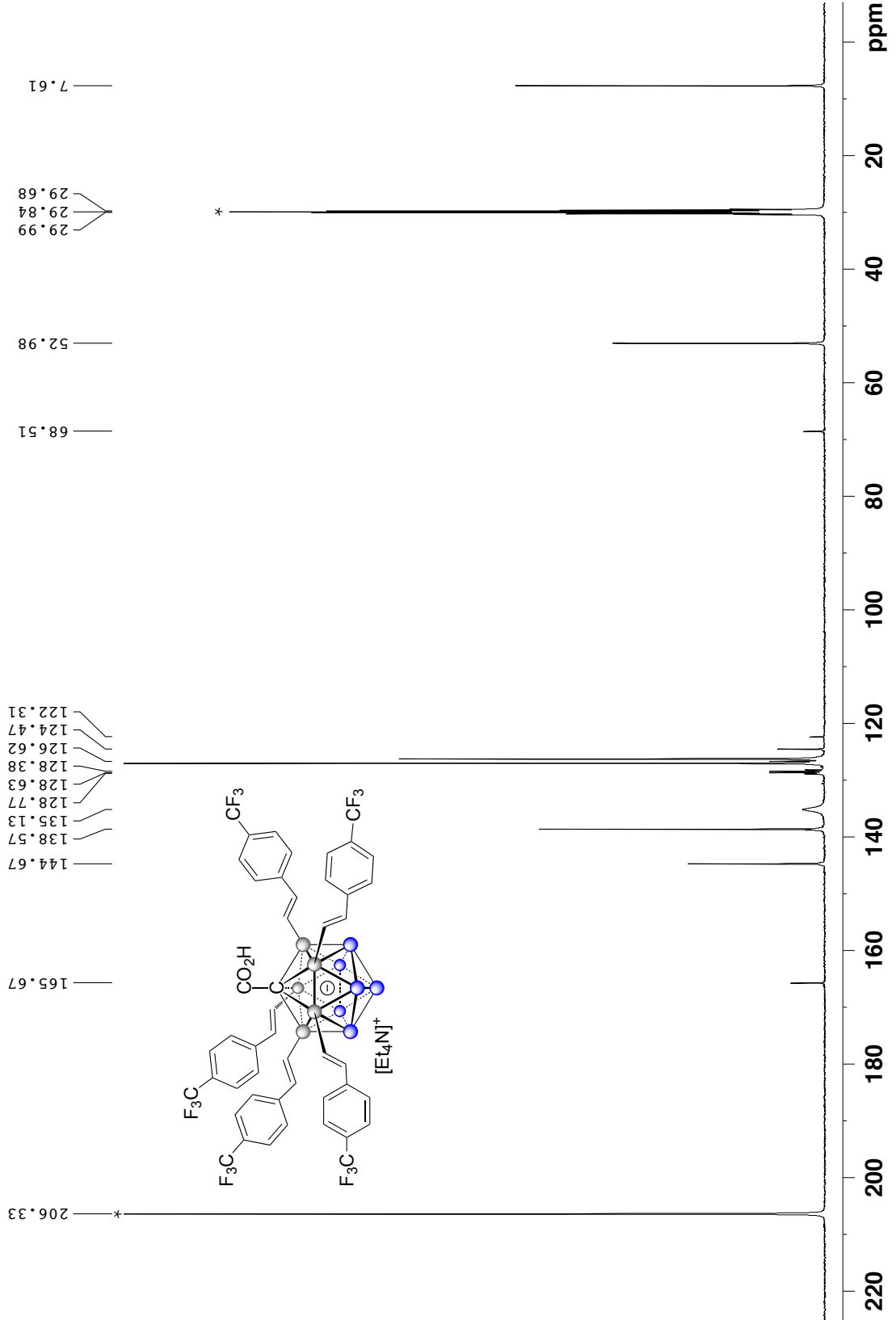
Current Data Parameters
 NAME penta-4-CF₃-styrene
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180530
 Time_ 0.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 2050
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.6 K
 D1 1.50000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.50 usec
 PLW1 95.00000000 W
 SFO1 125.7716224 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 19.00000000 W
 PLW1 0.40639001 W
 PLW3 0.26008999 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7576822 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40



Penta-4-CN-styrene product 40 mg in 0.6 ml acetone-d6*
¹H{¹¹B} NMR, 400 MHz, 23 C

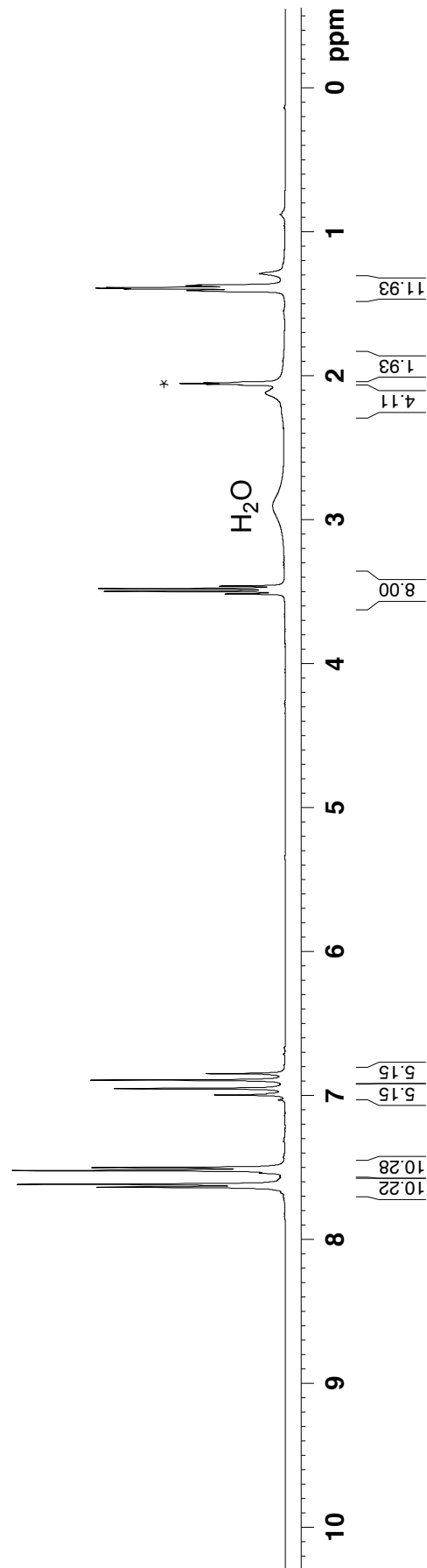
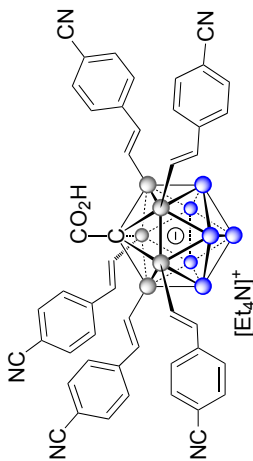
Current Data Parameters
 NAME penta-4-cn-styrene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180702
 Time 0.55
 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 410.1 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PLW1 12.5000000 W
 SFO1 400.1320007 MHz

==== CHANNEL f2 =====
 CPDPRG[2] garp4
 NUC2 ¹¹B
 P2 90.00 usec
 PLW2 52.9659960 W
 PLW12 0.64477998 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300073 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



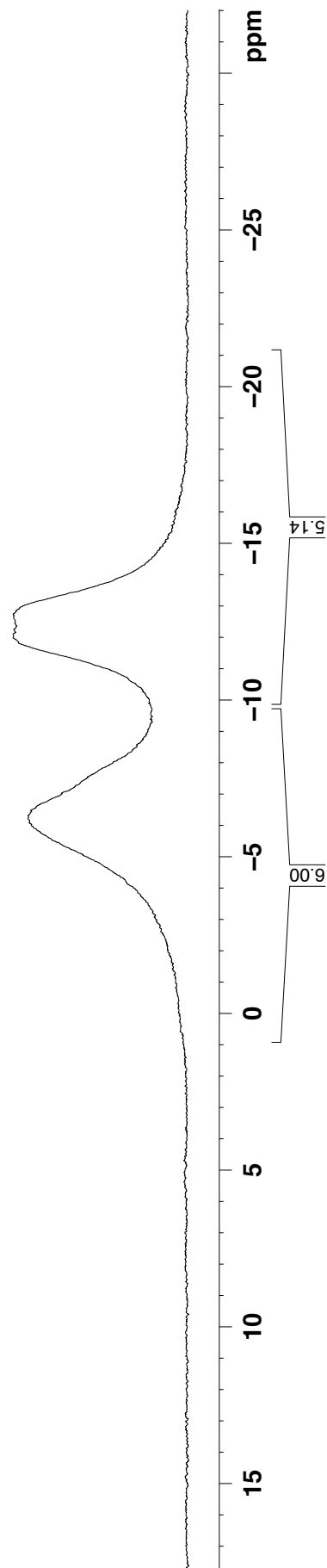
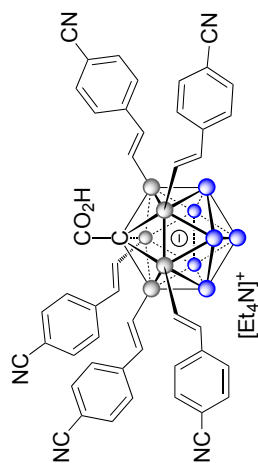
**Penta-CN-styrene product 40 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME penta-4-cn-styrene
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180702
 Time_ 1.00
 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 410.1 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SF01 128.3776052 MHz
 F2 - Processing Parameters
 SI 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

6.50
 -12.01
 -12.77



**Penta-4-CN-styrene product 40 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 128 MHz, 23 C**

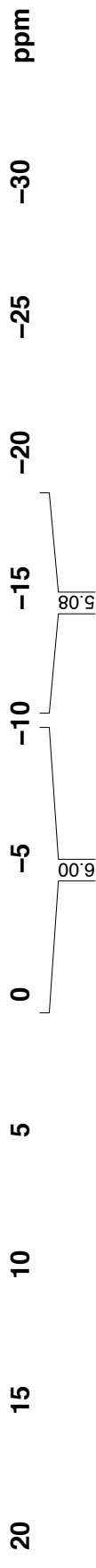
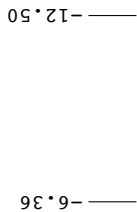
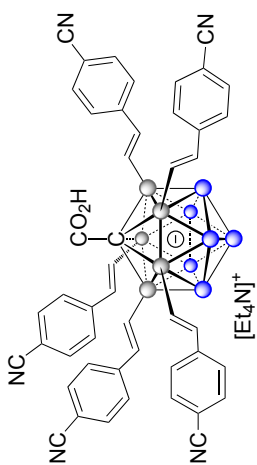
Current Data Parameters
 NAME penta-4-cn-styrene
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180702
 Time 1.07
 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 417.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 ¹¹B
 P1 9.93 usec
 PLW1 52.9659960 W
 SFO1 128.3776050 MHz

==== CHANNEL f2 =====
 CPDPRG2 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
 EM
 WDW 0
 SSB 0
 LB 4.00 Hz
 GB 0
 PC 1.40



Penta-4-CN-styrene product 40 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 128 MHz, 23 C

Current Data Parameters
 NAME penta-4-cn-styrene-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20180702
 Time_ 10.00
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG zgpg30
 ZF50 85.536
 SOLVENT Acetone
 NS 3072
 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 415.0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====

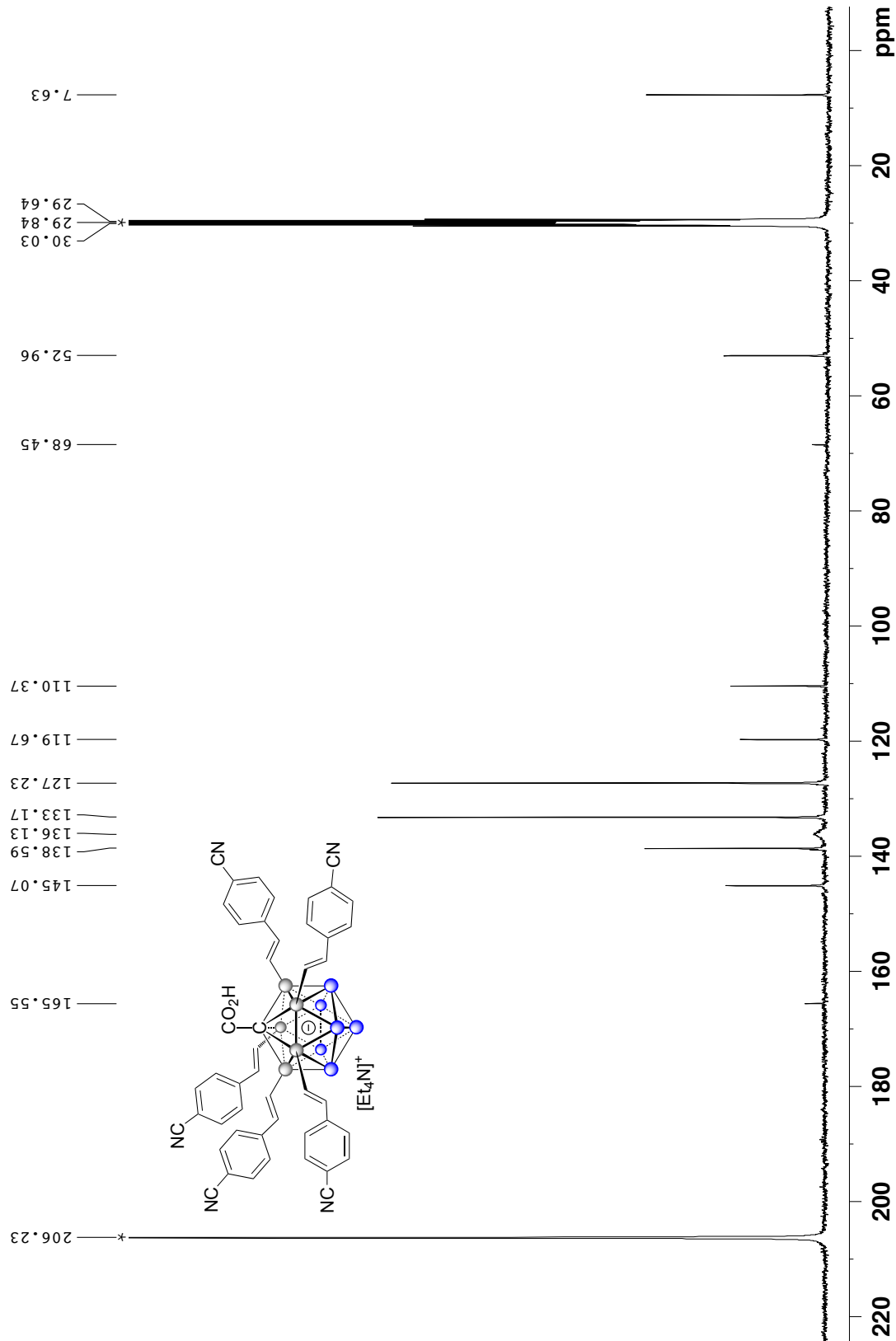
NUC1 ¹³C
 P1 10.00 usec
 PLW1 53.00000000 W
 SFO1 100.6228293 MHz

==== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 ¹H
 P2 80.00 usec
 PCPD2 12.50000000 W
 PLW2 0.43945000 W
 PLW3 0.28125000 W
 SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
 SF 100.6126819 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40



Penta-C6F5 product 40 mg in 0.6 ml acetone-d6 *
¹H{¹¹B} NMR, 500 MHz, 23 C

Current Data Parameters
 NAME penta-C6F5
 EXPNO 1
 PROCNO 1

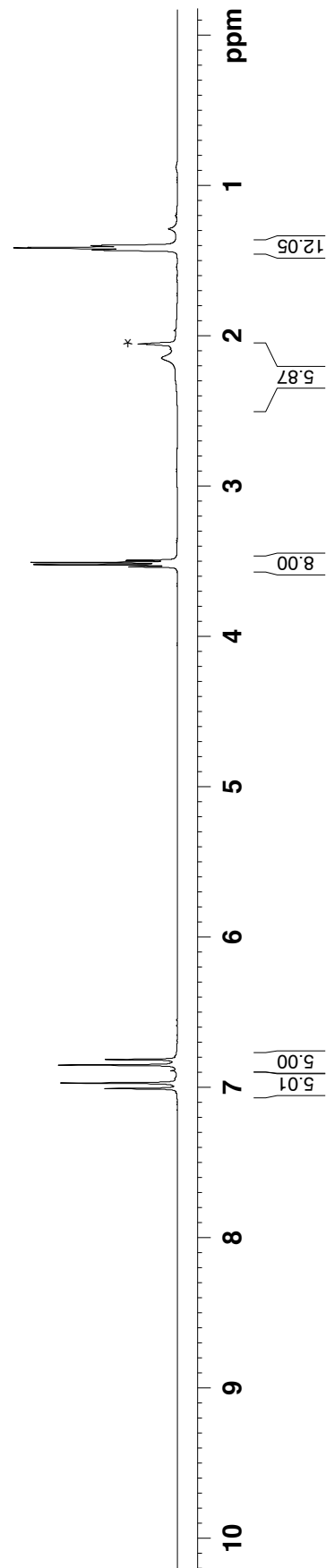
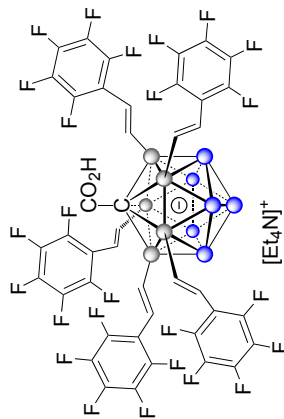
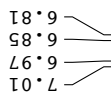
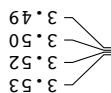
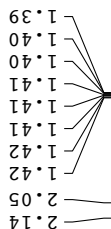
F2 - Acquisition Parameters
 Date_ 20181001
 Time 5.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 0

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 5.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1335009 MHz
 NUC1 ¹H
 P1 12.00 usec
 PLW1 19.0000000 W

==== CHANNEL f2 =====
 SFO2 160.4615690 MHz
 NUC2 ¹¹B
 CPDPRG[2] garp
 FCPD2 100.00 usec
 PLW2 95.0000000 W
 PLW12 1.63030005 W

F2 - Processing parameters
 SI 65536
 SF 500.1300088 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



**Penta-C6F5 product 40 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

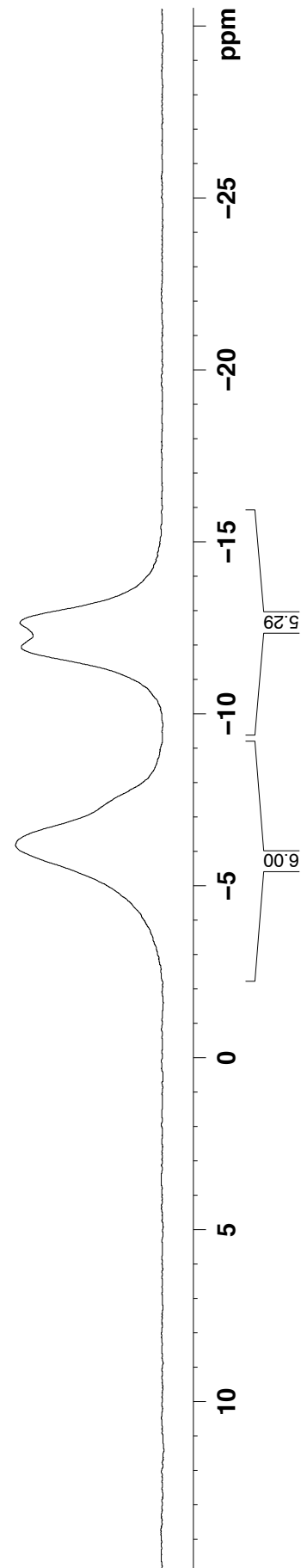
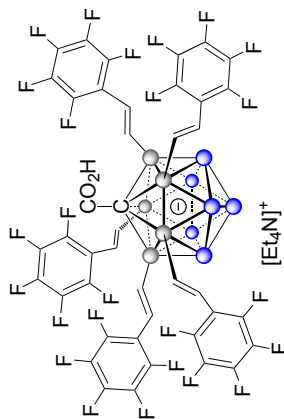
Current Data Parameters
 NAME penta-C6F5
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181001
 Time_ 5.50
 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 296.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SF01 160.4615792 MHz
 NUC1 11B
 P1 13.10 usec
 PLW1 95.00000000 W

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

6.19
 -7.59
 -11.95
 -12.66



Penta-C6F5 product 40 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 160 MHz, 23 C

```

Current Data Parameters
NAME      Penta-C6F5
EXPNO     3
PROCNO    1

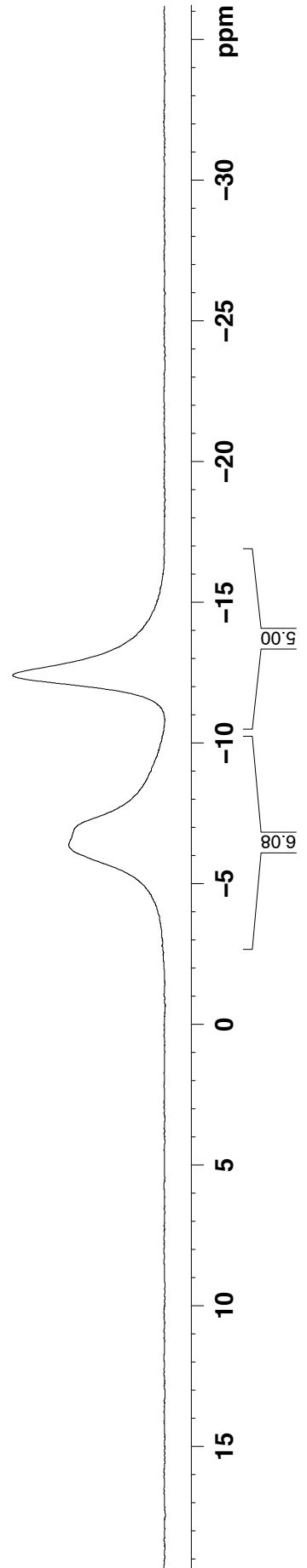
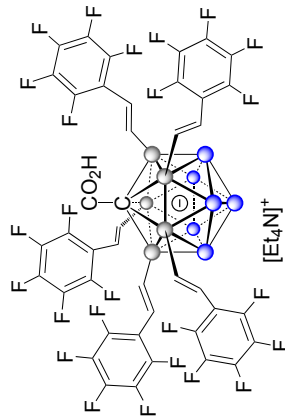
F2 - Acquisition Parameters
Date_     20181001
Time      5.51
INSTRUM   spect
PROBHD    5 mm PABBOBBL
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         64
DS         4
SWH        32051.281 Hz
FIDRES     0.489064 Hz
AQ          1.0223616 sec
RG          303
RW          15.600 usec
DE          6.50 usec
TE          296.3 K
D1          1.0000000 sec
D11         0.0300000 sec
TDO        1

===== CHANNEL f1 =====
SF01       160.4615790 MHz
NUC1        11B
P1          13.10 usec
PLW1       95.0000000 W

===== CHANNEL f2 =====
SF02       500.1325007 MHz
NUC2         1H
PCPDPRG[2] waltz16
PCPD2       80.00 usec
PLM2        0.0639001 W
PLM12       0.26008999 W
PLM13       0.26008999 W

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

-12.41
 -7.07
 -6.38



Penta-C6F5 product 40 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 126 MHz, 23 C

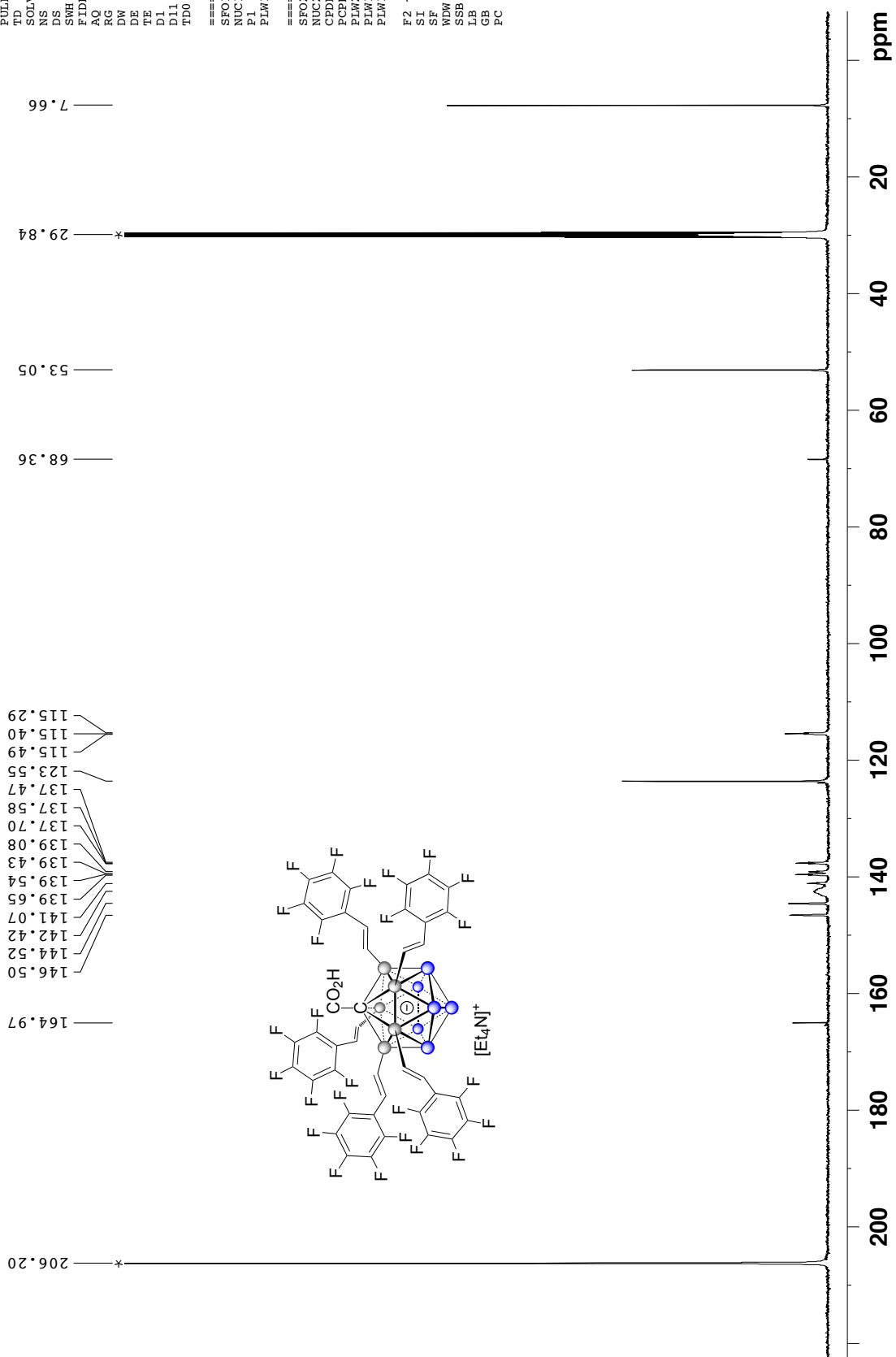
Current Data Parameters
 NAME penta-C6F5
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181001
 Time 8.00
 INSTRUM spect
 PROBHD 5 mm PABBO BE-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 3100
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.3 K
 D1 1.5000000 sec
 D11 0.0300000 sec
 TLD0 1

==== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 ¹³C
 P1 10.70 usec
 PLW1 95.0000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPDZ 80.00 usec
 PLW2 19.0000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W

F2 - Processing parameters
 SI 32768
 SF 125.7576741 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



penta-CH2Ph product 40 mg in 0.6 ml acetone-d6*
¹H{¹B} NMR, 400 MHz, 23 C

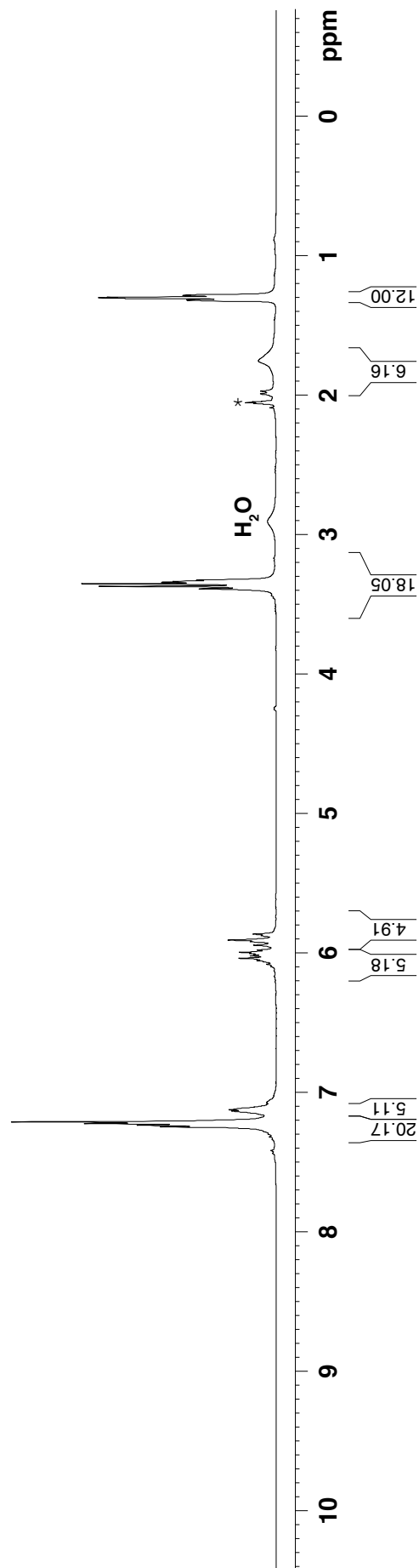
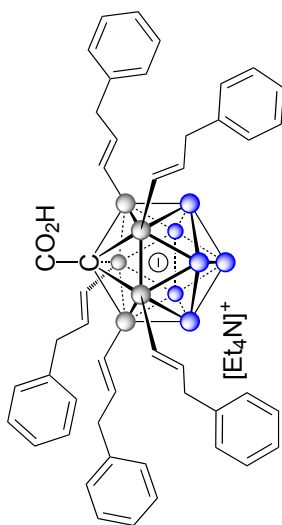
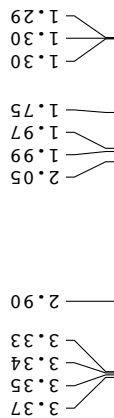
Current Data Parameters
 NAME penta-CH2Ph-1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180611
 Time_ 15:46
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 16384
 SOLVENT acetone
 NS 4
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 64.43
 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 12.5000000 W
 SFO1 400.1320007 MHz

==== CHANNEL f2 =====
 CPDPRG[2] garrp4
 NUC2 ¹¹B
 PCDP2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.6447998 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300073 MHz
 MDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40



**penta-CH2Ph product 40 mg in 0.6 ml acetone-d6
1B NMR, 160 MHz, 23 C**

```

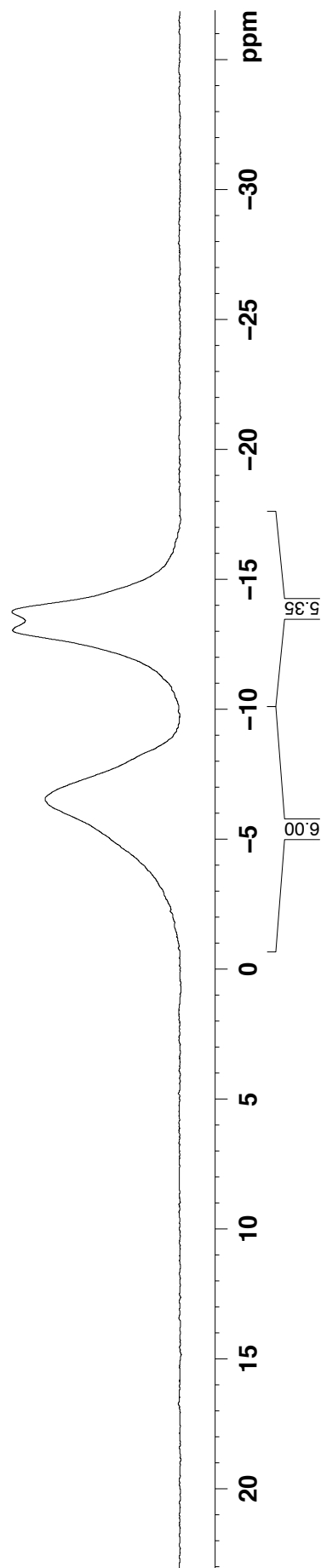
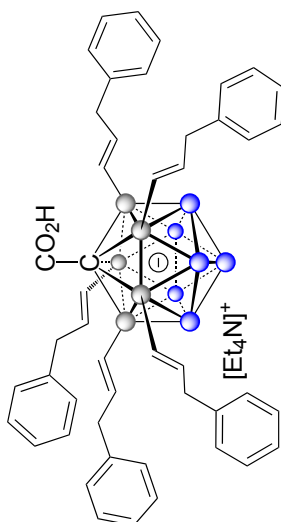
Current Data Parameters
NAME      penta-CH2Ph
EXPNO    3
PROCNO   1

F2 - Acquisition Parameters
Date_     20180824
Time      6.13
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         1.0000000 sec
TD0        1

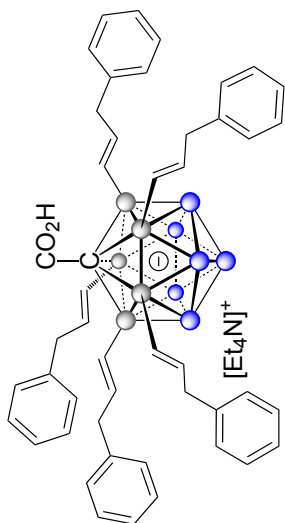
===== CHANNEL f1 =====
SF01      160.4615792 MHz
NUC1       13C
P1         13.10 usec
PLW1       95.0000000 W

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

-6.56
 -13.06
 -13.77



**penta-CH2Ph product 40 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 160 MHz, 23 C**



— 6.66
 — 13.51

```

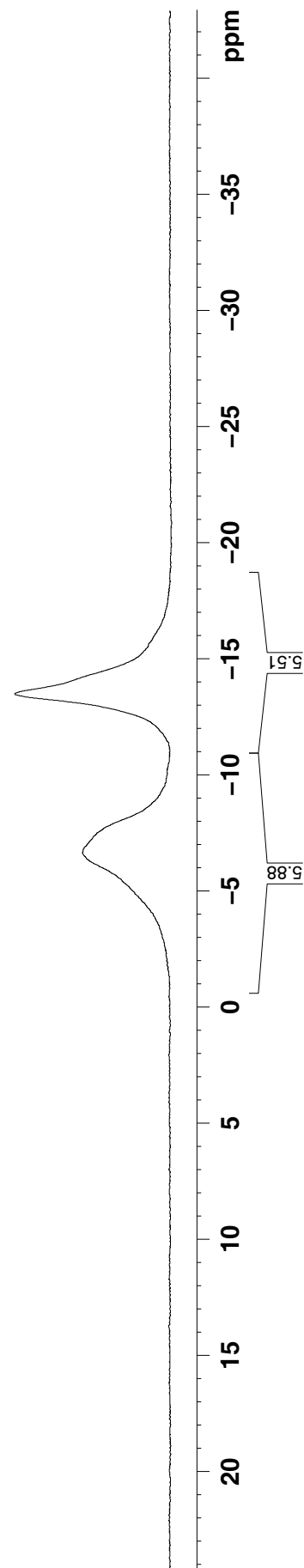
Current Data Parameters
NAME      penta-CH2Ph
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20180824
Time      6.16
INSTRUM   spect
PROBHD    5 mm PABBO BB
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         64
DS         4
SWH        32051.281 Hz
FIDRES     0.789064 Hz
AQ         1.0223616 sec
RG         1.0223616 sec
RC         15.600 usec
DE         5.650 usec
TE         296.5 K
D1         1.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
SF01      160.4615790 MHz
NUC1       11B
P1         13.110 usec
PLW1       95.00000000 W

===== CHANNEL f2 =====
SF02      500.1325007 MHz
NUC2       1H
P2         80.000 usec
PLW2       19.00000000 W
=====
CPDPRG2   waltz16
PLM12     0.0639001 W
PLM13     0.26008999 W

F2 - Processing parameters
SI         32768
SF         160.4615790 MHz
WDW        EM
SSB        0
LB         7.00 Hz
GB         0
PC         1.40
  
```



**penta-CH₂Ph product 40 mg in 0.6 ml acetone-d₆^{*}
¹³C{¹H} NMR, 126 MHz, 23 C**

```

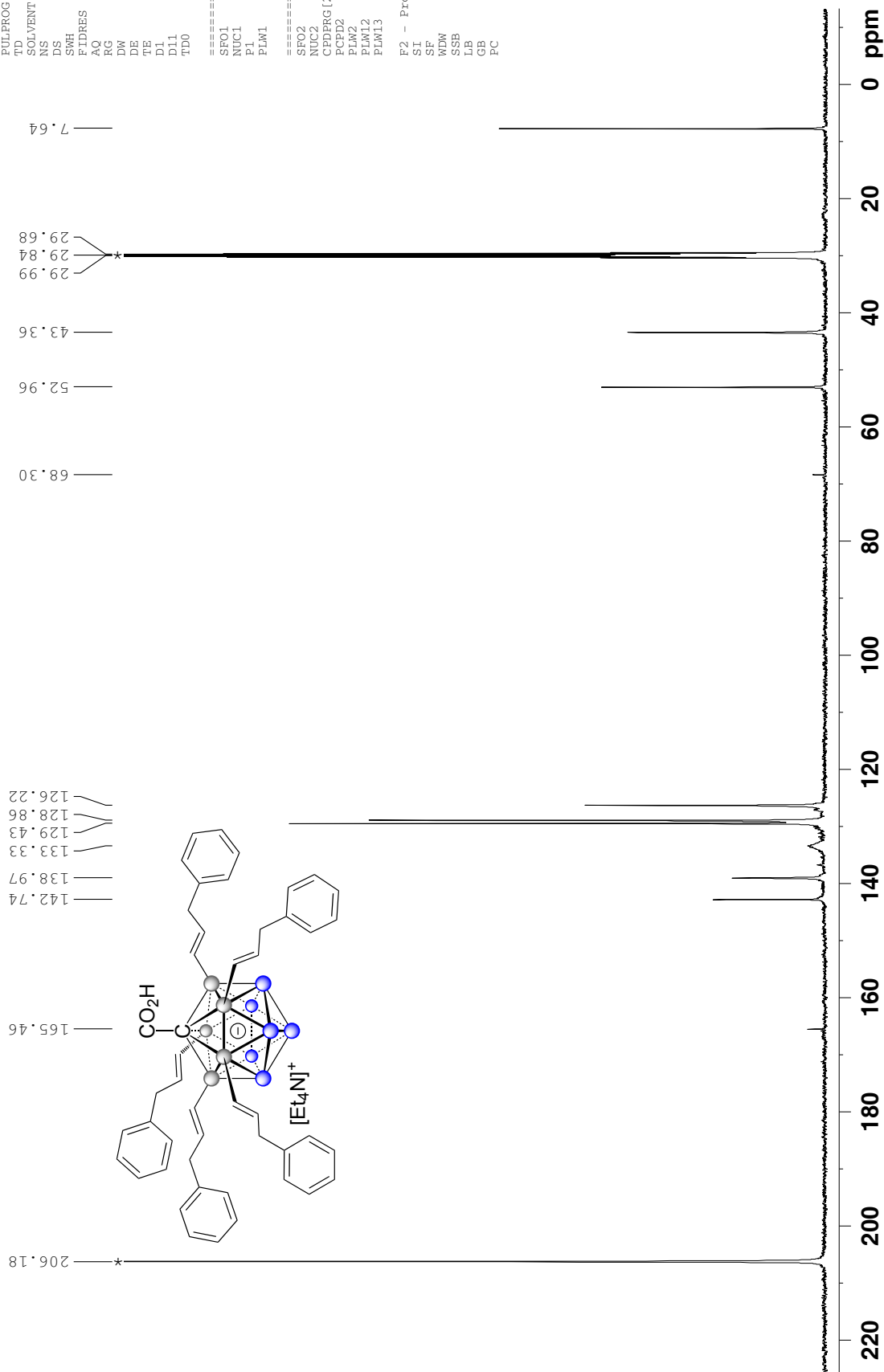
Current Data Parameters
NAME      penta-CH2Ph
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20180823
Time     17.23
INSTRUM  spect
PROBHD   5 mm FAPBEO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  Acetone
NS       1024
DS       4
SWH      37878.789 Hz
FIDRES   0.577984 Hz
AQ       0.8650753 sec
RG       203
DW       13.200 usec
DE       6.50 usec
TE       297.3 K
D1       1.50000000 sec
D11      0.03000000 sec
TDO      1

===== CHANNEL f1 =====
SFO1    125.7716224 MHz
NUC1     13C
P1       10.50 usec
PLW1    95.0000000 W

===== CHANNEL f2 =====
SFO2    500.1320005 MHz
NUC2     1H
PCPD2   waltz16
PCPD2   80.00 usec
PLW2    19.0000000 W
PLW12   0.40639001 W
PLW13   0.26008999 W

F2 - Processing parameters
SI       32768
SF       125.7576835 MHz
WDW      EM
SSB      0
LB       5.00 Hz
GB       0
PC       1.40
  
```



Penta-CH2-C6F5 product 50 mg in 0.6 ml acetone-d6 *
¹H{¹B} NMR, 400 MHz, 23 C

Current Data Parameters
 NAME penta-CH2C6F5
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180527
 Time_ 21:31
 INSTRUM spect
 PROBHD 5 mm FAPBO 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
 DE 62.400 usec
 TE 294.3 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TD0 1

=====
 CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PLW1 12.5000000 W
 SFO1 400.1320007 MHz

=====
 CHANNEL f2 =====
 CPDPRG2 gerp4
 NUC2 ¹¹B
 P1 90.00 usec
 PLW2 52.9659960 W
 PLW12 0.6447798 W
 SFO2 128.3776050 MHz

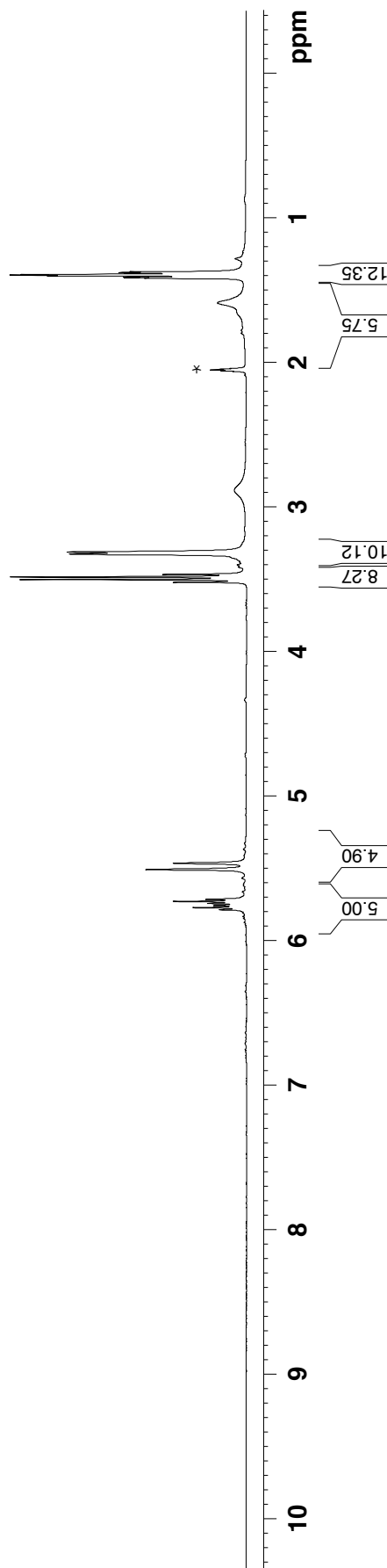
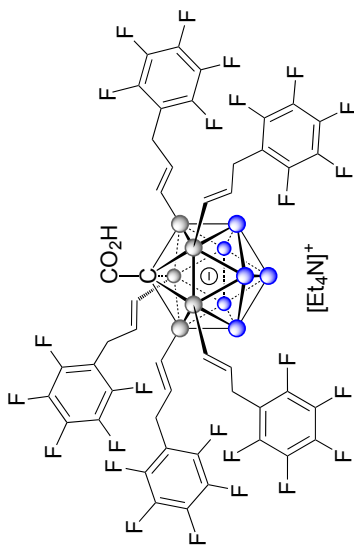
F2 - Processing parameters
 SI 32768
 SF 400.1300072 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

5.77
5.73
5.51
5.46

3.52
3.50
3.48
3.46
3.32
3.31
2.88

2.06
2.05
2.04

1.59
1.40
1.39
1.39



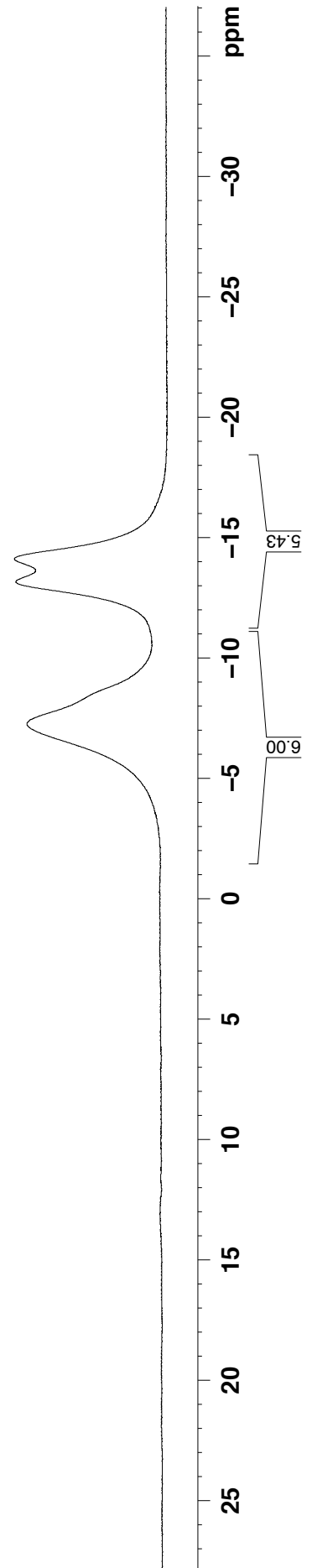
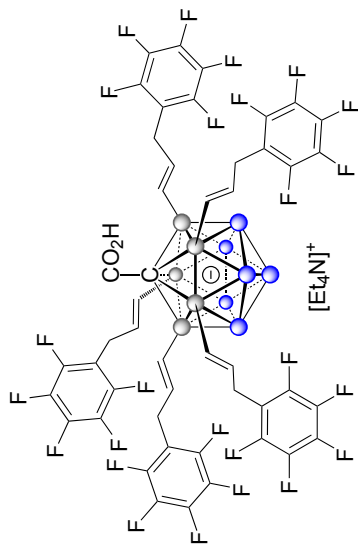
**Penta-CH2-C6F5 product 50 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME Penta-CH2C6F5
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20180527
 Time 21.37
 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 52.9659960 W
 SFO1 128.3776052 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

— 7.29
 — 13.18
 — 14.14

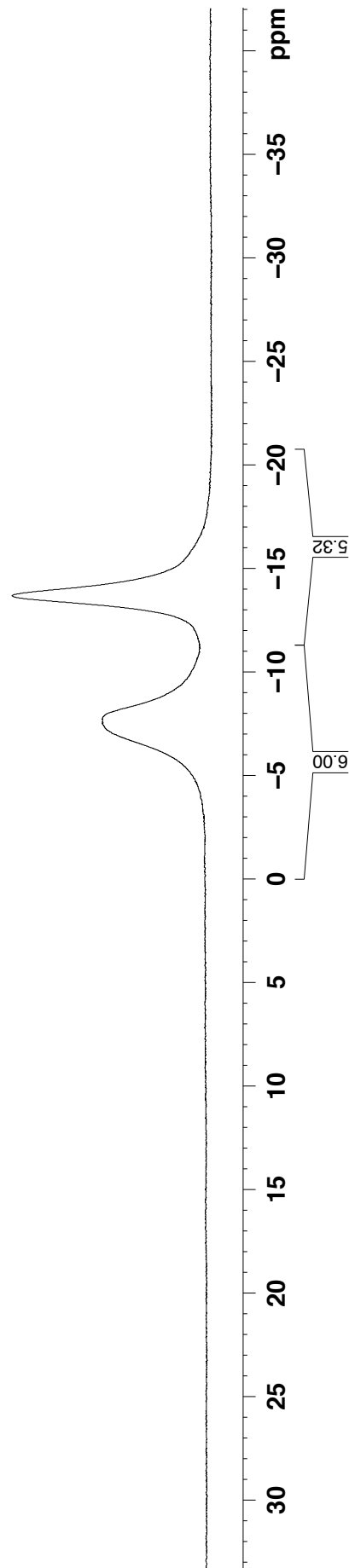
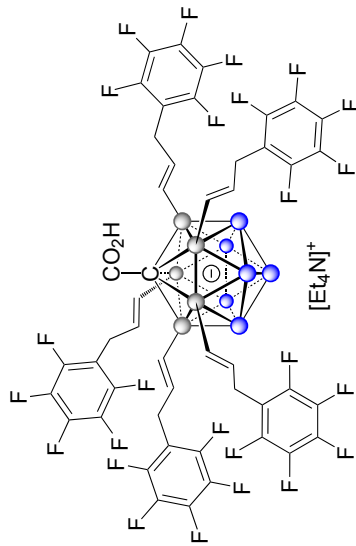


Penta-CH2-C6F5 product 50 mg in 0.6 ml acetone-d6
 11B{1H} NMR, 128 MHz, 23 C

Current Data Parameters
 NAME Penta-CH2C6F5
 EXPNO 3
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20180527
 Time 21.43
 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 294.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SFO1 128.3776050 MHz
 ===== CHANNEL f2 =====
 CPDPRG[2] waitz16
 NUC2 1H
 P2 80.00 usec
 PLW2 12.5000000 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 3.00 Hz
 GB 0
 PC 1.40

13.71
 7.77



Penta-CH2-C6F5 product 50 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 101 MHz, 23 C

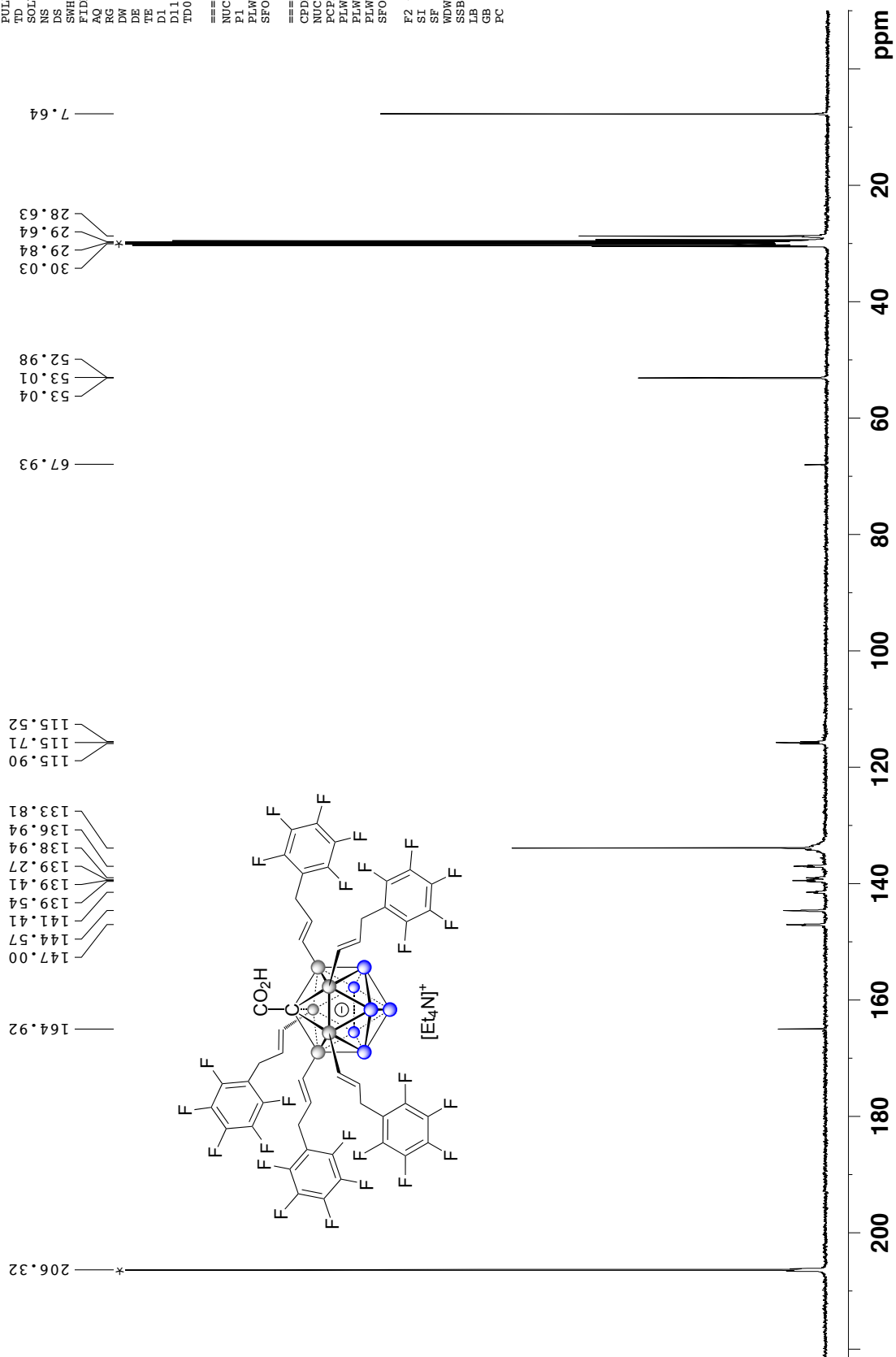
Current Data Parameters
 NAME penta-CH2C6F5
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180527
 Time 23.15
 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 294.5 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] waitz16
 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 100.6126791 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40



Penta-hexene product 40 mg in 0.6 ml acetone-d6 *
¹H{¹H} NMR, 500 MHz, 23 C

```

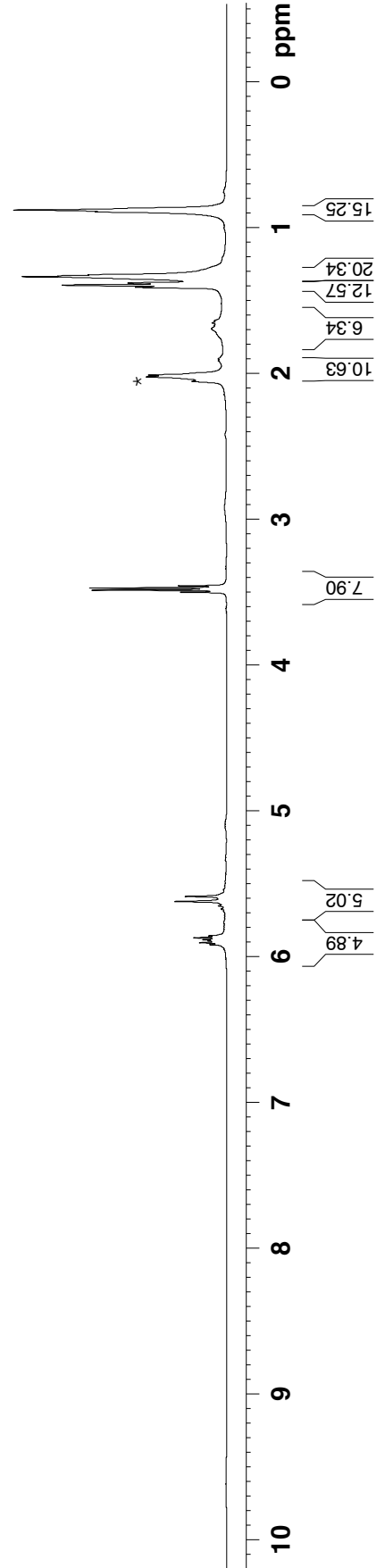
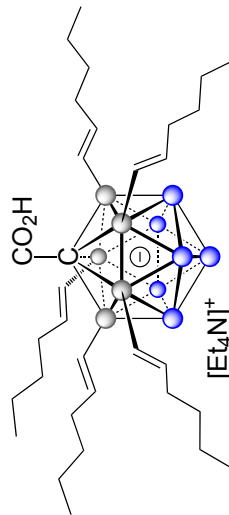
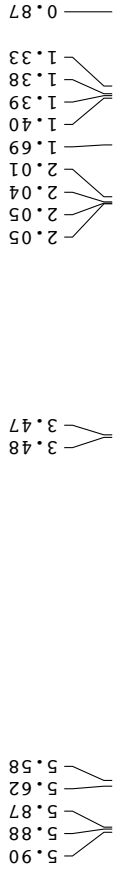
Current Data Parameters
NAME      penta-hexene
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20170509
Time     0.55
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg1930
TD       65536
SOLVENT  Acetone
NS       16
DS       0
SWH      12500.000 Hz
FIDRES   0.190735 Hz
AQ       2.6214399 sec
RG       18
DW       40.000 usec
DE       6.50 usec
TE       295.9 K
D1       5.00000000 sec
D11      0.03000000 sec

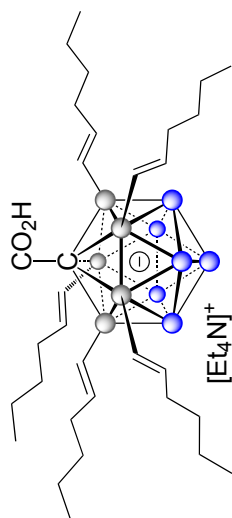
===== CHANNEL f1 =====
NUC1     1H
P1       11.70 usec
PLW1    19.00000000 W
SFO1    500.1335009 MHz

===== CHANNEL f2 =====
CPDPRG2  9arp
NUC2     11B
PCPD2    100.00 usec
PLW2    95.00000000 W
PLM12   1.63030005 W
SFO2    160.4615690 MHz

F2 - Processing parameters
SI       65536
SF       500.1300101 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.00
  
```



**Penta-hexene product 40 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**



— 6.87
— 13.21
— 13.98

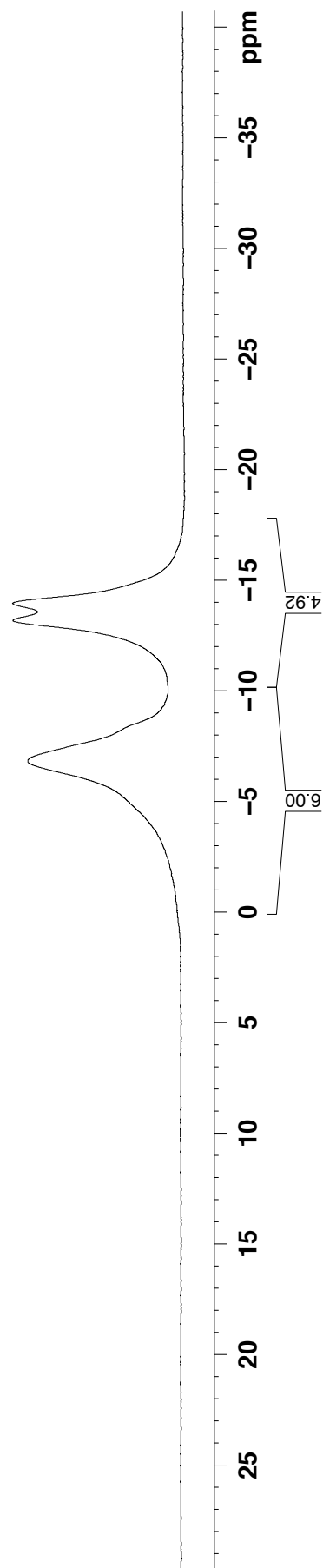
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Current Data Parameters
NAME      penta-hexene
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20170509
Time     0.58
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       295.7 K
D1       1.00000000 sec

===== CHANNEL f1 =====
NUC1     11B
P1       13.10 usec
PLWL     95.0000000 W
SF01     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
    
```



**Penta-hexene product 40 mg in 0.6 ml acetone-d6
¹¹B{¹H} 160 MHz, 23 C**

Current Data Parameters
 NAME Penta-hexene
 EXPNO 3
 PROCNO 1

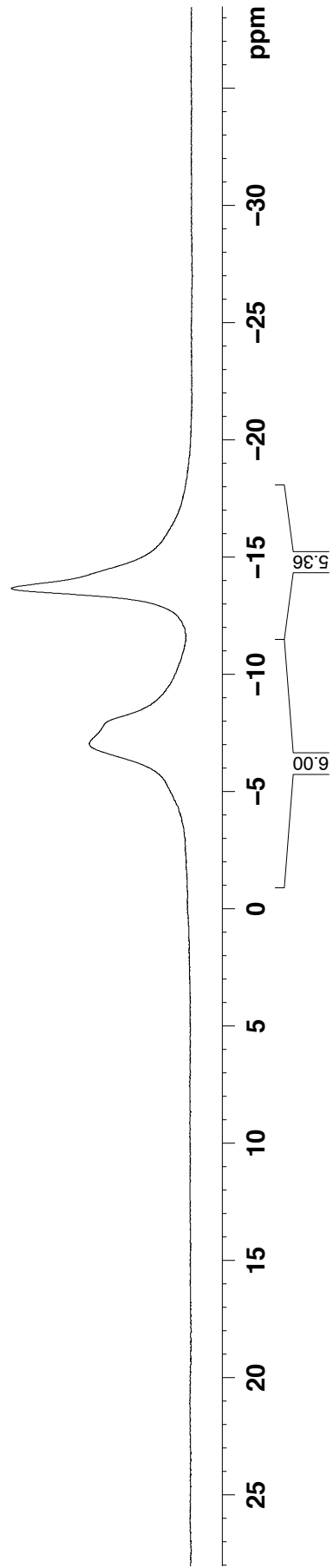
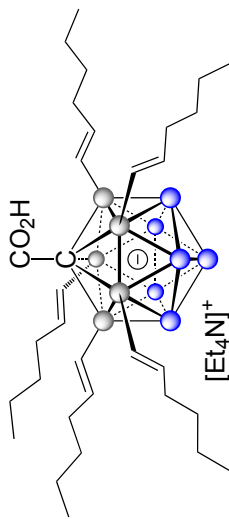
F2 - Acquisition Parameters
 Date_ 20170509
 Time_ 1.0
 INSTRUM spect
 PROBHD 5 mm PABBOEBL
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 64
 DS 4
 SWH 32051.281 Hz
 FIDRES 0.7489664 Hz
 AQ 1.0223616 sec
 RG 320
 DW 15.600 usec
 DE 6.50 usec
 TE 296.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 ¹¹B
 P1 13.10 usec
 PL1 95.0000000 W
 SFO1 160.4615790 MHz

==== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 ¹H
 P2 80.00 usec
 PL2 19.0000000 W
 PL12 0.0639001 W
 PL13 0.26008999 W
 SFO2 500.1325007 MHz

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

— 7.93
 — 7.05
 — 13.68



Penta-hexene product 40 mg in 0.6 ml acetone-d6 *
¹³C{¹H} NMR, 126 MHz, 23 C

```

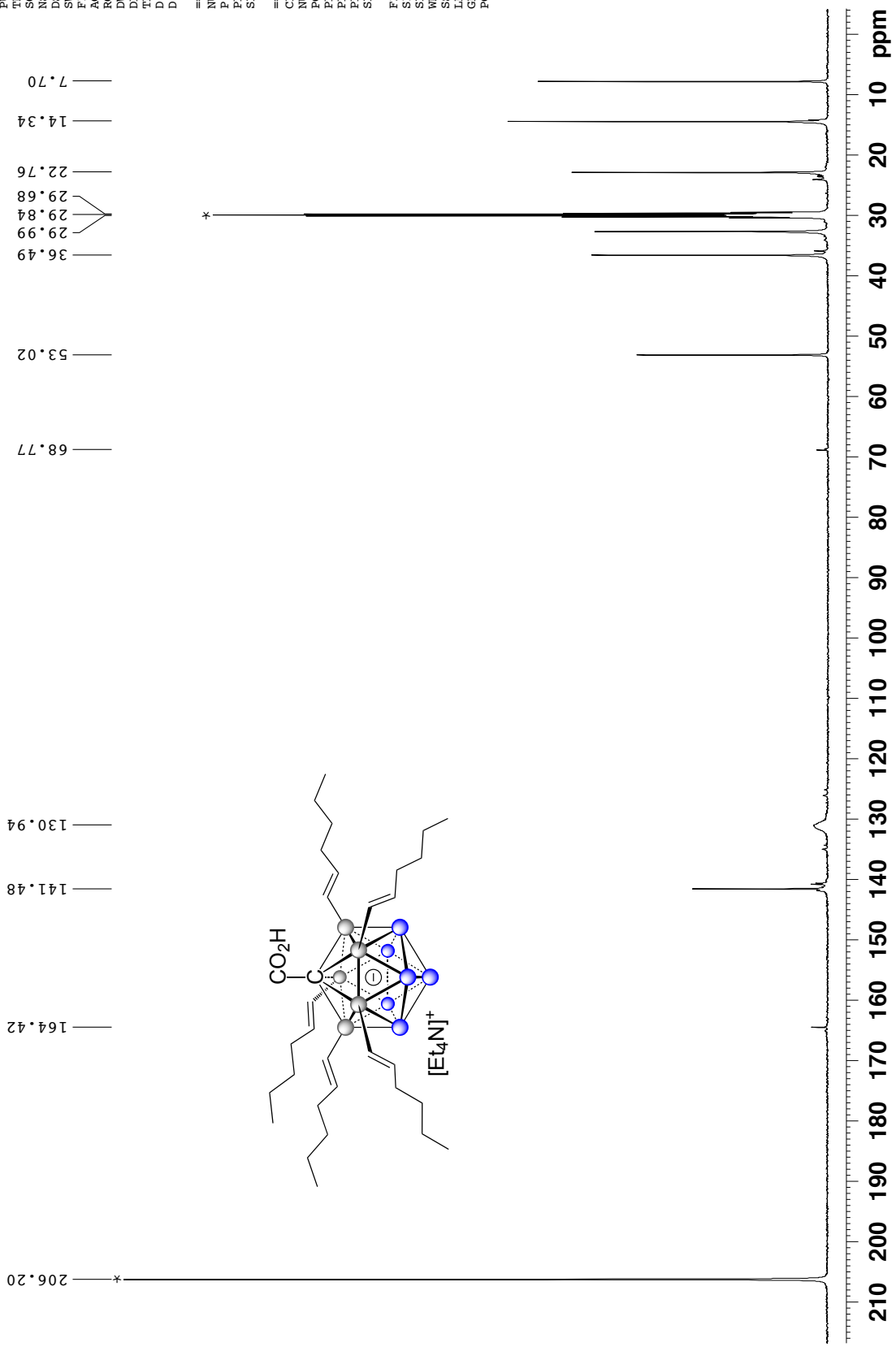
Current Data Parameters
NAME      penta-hexene
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20170509
Time      2.25
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         2048
DS         4
SWH        37878.789 Hz
FIDRES     0.577984 Hz
AQ         0.8650752 sec
RG         203
DW         13.200 usec
DE         6.50 usec
TE         296.4 K
D1         1.50000000 sec
D11        0.03000000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         10.50 usec
PLW1       95.00000000 W
SFO1       125.7716224 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2       1H
PCPDZ      80.00 usec
PLW2       19.00000000 W
PLW12      0.40639001 W
PLW13      0.26008999 W
SFO2       500.1320005 MHz

F2 - Processing parameters
SI         32768
SF         125.7576657 MHz
WDW        EM
SSB        0
LB         5.00 Hz
GB         0
PC         1.40
  
```



penta-4-methyl-1-pentene product 40 mg in 0.6 ml acetone-d6 *
¹H{¹¹B} NMR, 500 MHz, 23 C

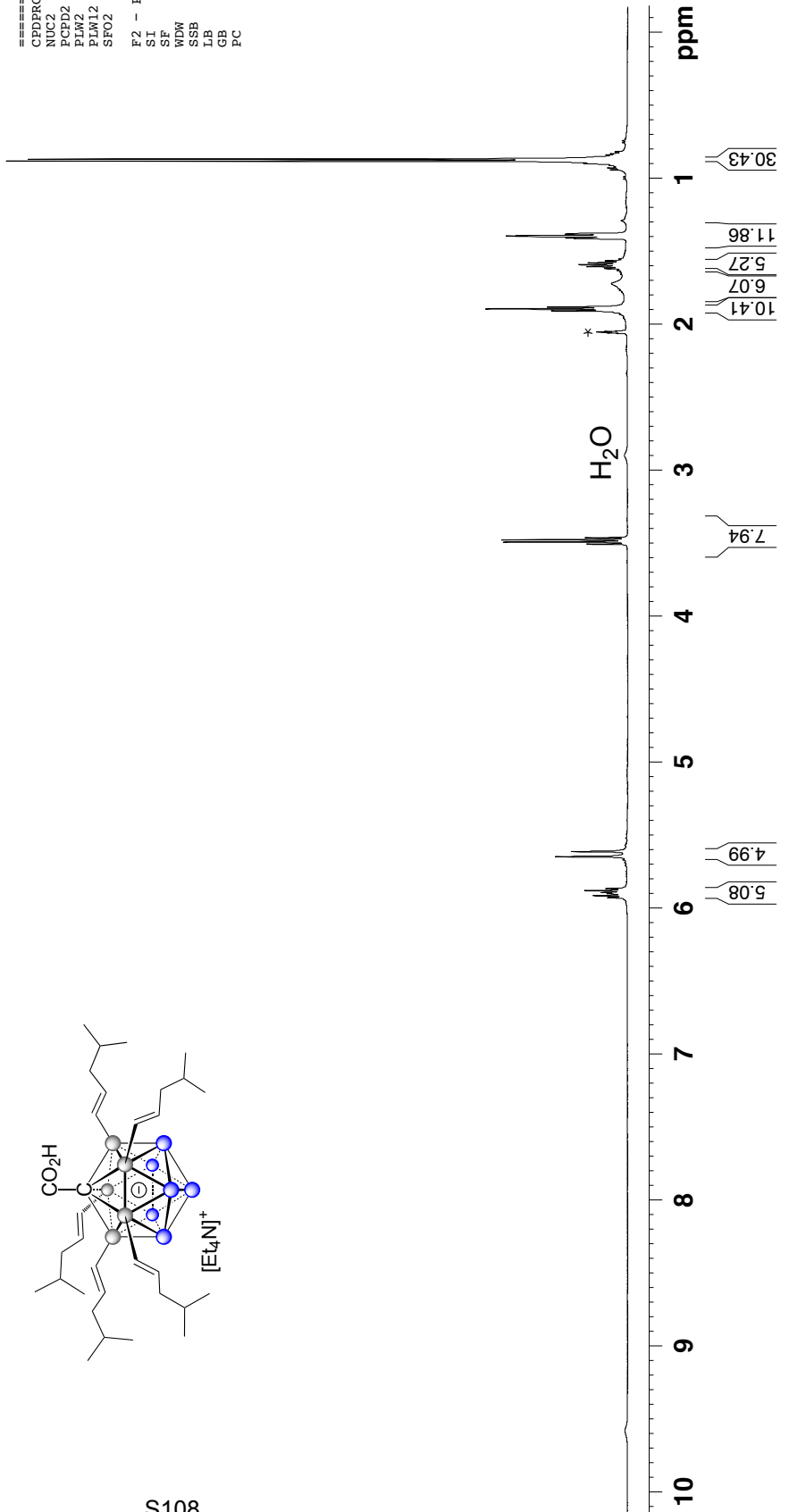
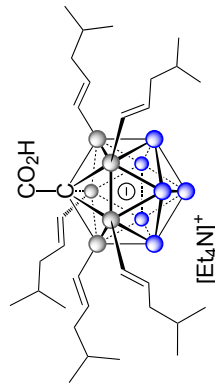
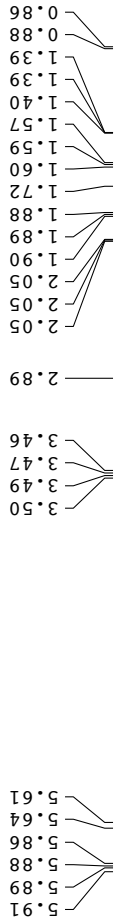
Current Data Parameters
 NAME penta-4-methyl-1-pentene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170414
 Time 16.04
 INSTRUM spect
 PROBHD 5 mm PABEO BB-
 PULPROG zgig30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 0
 SWH 12500.000 Hz
 FIDRES 0.190735 Hz
 AQ 2.6214399 sec
 RG 36
 DW 40.000 usec
 DE 6.50 usec
 TE 296.0 K
 D1 5.0000000 sec
 D11 0.0300000 sec

=====
 CHANNEL f1
 NUC1 ¹H
 P1 11.50 usec
 PLW1 19.0000000 W
 SFO1 500.1335009 MHz

=====
 CHANNEL f2
 CPDPRG[2] garp
 NUC2 ¹¹B
 P2 100.00 usec
 PLW2 95.0000000 W
 PLW12 1.63030005 W
 SFO2 160.4615690 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300103 MHz
 WDW no
 SSB 0 Hz
 LB 0
 GB 0
 PC 1.00



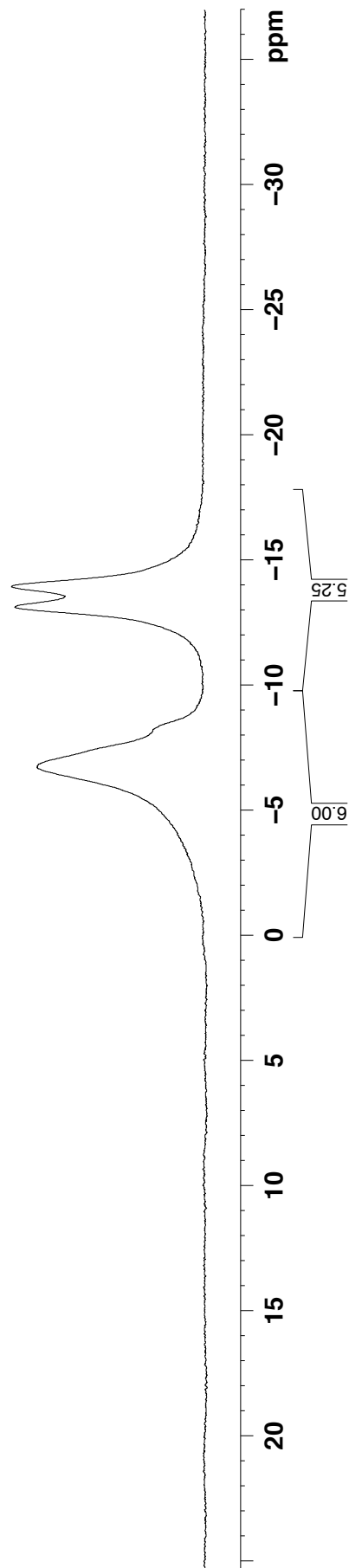
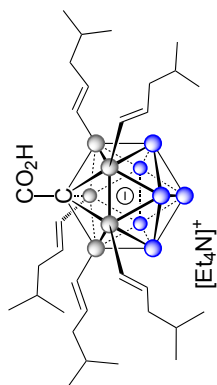
**penta-4-methyl-1-pentene product 40 mg in 0.6 ml acetone-d6
11B NMR, 500 MHz, 23 C**

Current Data Parameters
 NAME penta-4-methyl-1-pentene
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170414
 Time_ 16.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT Acetone
 NS 32
 DS 2
 SWH 32051.281 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 203
 DW 15.600 usec
 DE 6.50 usec
 TE 295.5 K
 D1 2.00000000 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 0
 GB 0
 PC 1.40

6.77
 8.28
 13.12
 13.95



**penta-4-methyl-1-pentene product 40 mg in 0.6 ml acetone-d6
¹H{¹H} NMR, 160 MHz, 23 C**

Current Data Parameters
 NAME penta-4-methyl-1-pentene
 EXPNO 2
 PROCNO 1

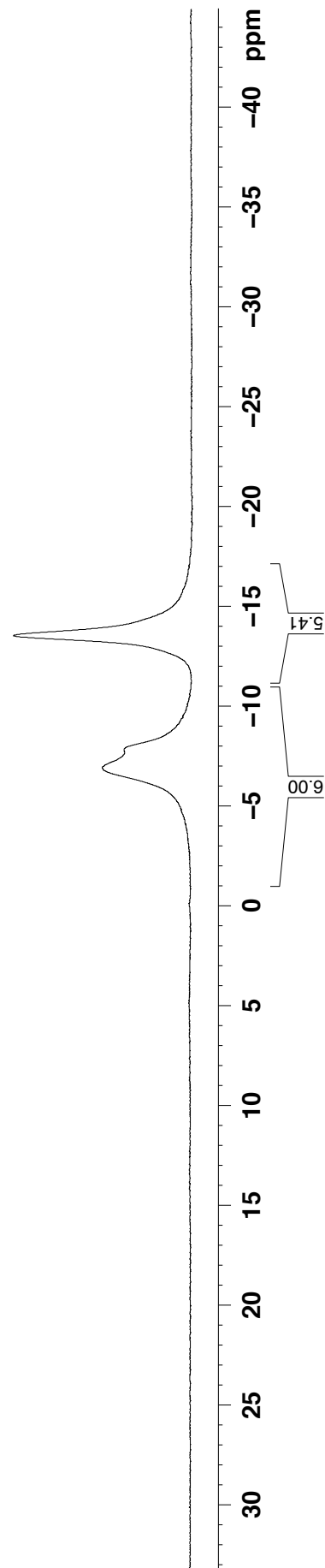
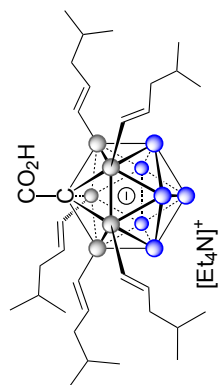
F2 - Acquisition Parameters
 Date_ 20170414
 Time_ 16.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 32
 DS 2
 SFO1 32051.281 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 203
 DW 15.600 usec
 DE 6.50 usec
 TE 295.7 K
 D1 1.0000000 sec
 D11 0.0300000 sec

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 13.10 usec
 PLW1 95.0000000 W
 SFO1 160.4615790 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹³C
 PCPD2 80.00 usec
 PLW2 19.0000000 W
 PLW12 0.3926200 W
 PLW13 0.2512700 W
 SFO2 500.1325007 MHz

F2 - Processing Parameters
 SI 32768
 SF 160.4615790 MHz
 MDW EM
 SSB 0
 LB 0
 GB 0
 PC 5.00 Hz
 1.40

6.93
 7.87
 13.56



penta-4-methyl-1-pentene product 40 mg in 0.6 ml acetone-d6*
¹³C{1H} NMR, 101 MHz, 23 C

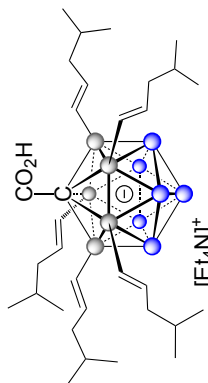
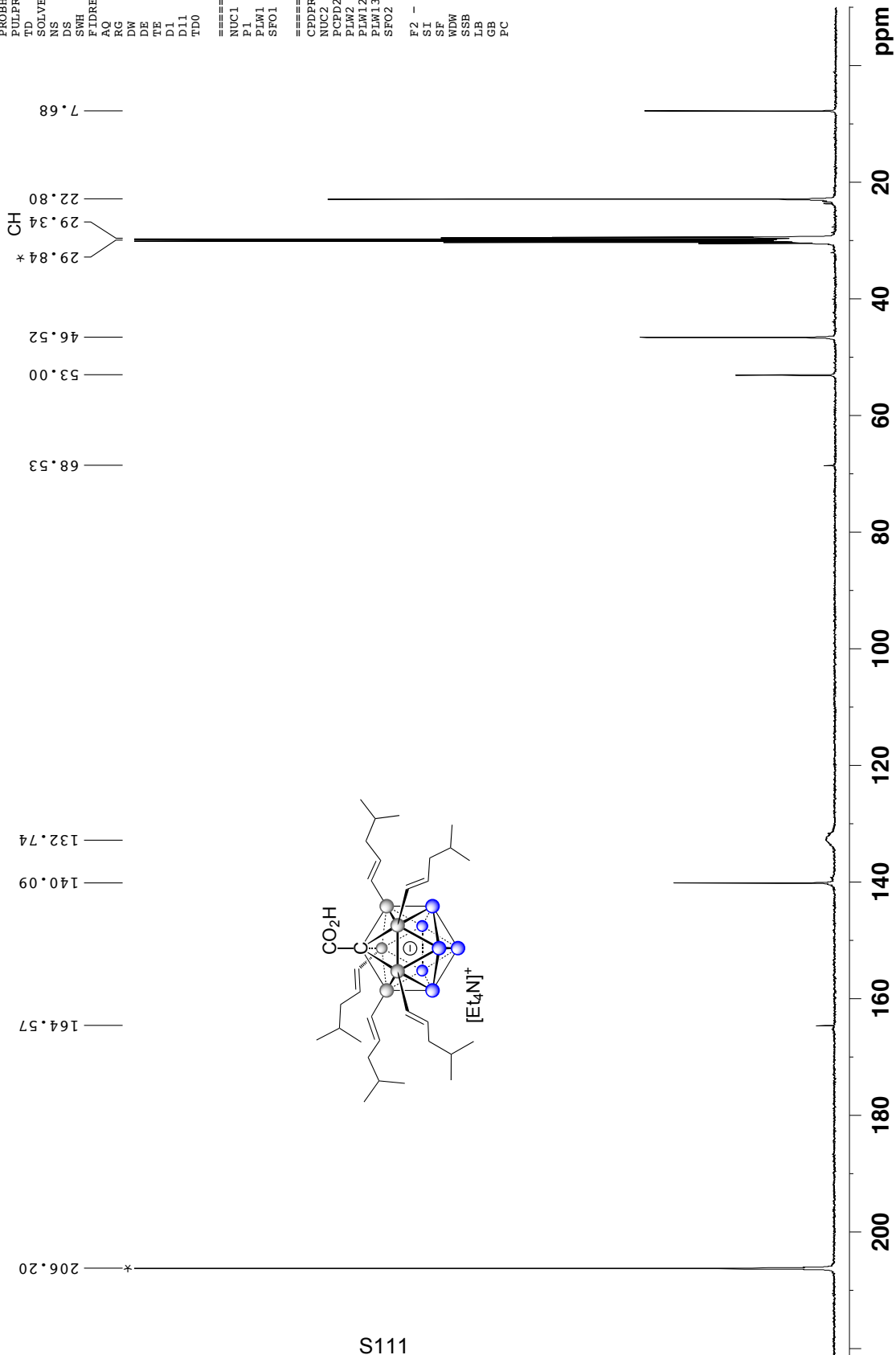
Current Data Parameters
 NAME penta-4-methyl-1-pentene-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170415
 Time 17.42
 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 295.4 K
 D1 1.5000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PLW1 53.0000000 W
 SFO1 100.6228293 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 12.5000000 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 3.00 Hz
 GB 0
 PC 1.40



penta-4-methyl-1-hexene product 40 mg in 0.6 ml acetone-d6 *
¹H{¹³C} NMR, 500 MHz, 23 C

Current Data Parameters
 NAME penta-4-methyl-1-hexene
 EXPNO 1
 PROCNO 1

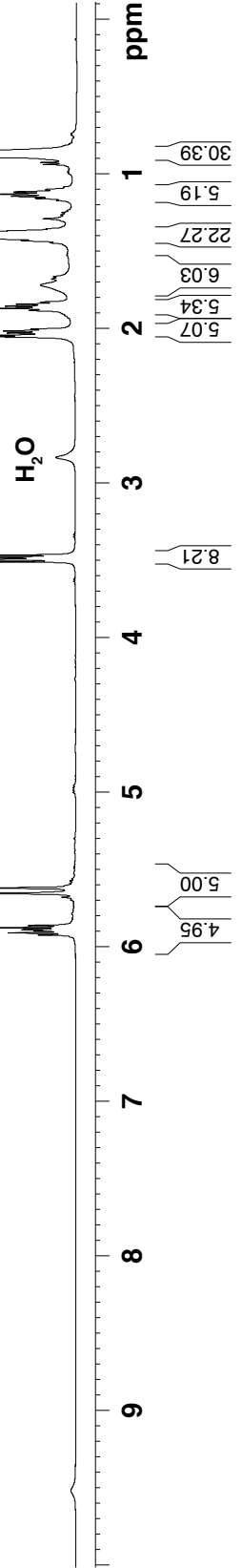
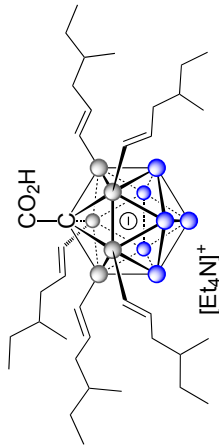
F2 - Acquisition Parameters
 Date_ 20180403
 Time_ 6.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 12500.000 Hz
 FIDRES 0.190735 Hz
 AQ 2.6214399 sec
 RG 22.6
 DW 40.000 usec
 DE 6.50 usec
 TE 296.4 K
 D1 5.00000000 sec
 D11 0.03000000 sec

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

==== CHANNEL f2 =====
 CPDPRG1 2 gatp
 NUC2 ¹³C
 P2 11.16
 PLW2 100.00 usec
 PLW1 95.00000000 W
 SFO2 160.4615690 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1302351 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

5.91
5.89
5.87
5.65
5.62
3.51
3.49
3.48
3.46
2.83
2.05
2.01
1.87
1.85
1.72
1.68
1.66
1.40
1.39
1.39
1.14
1.13
1.11
0.87
0.86
0.86



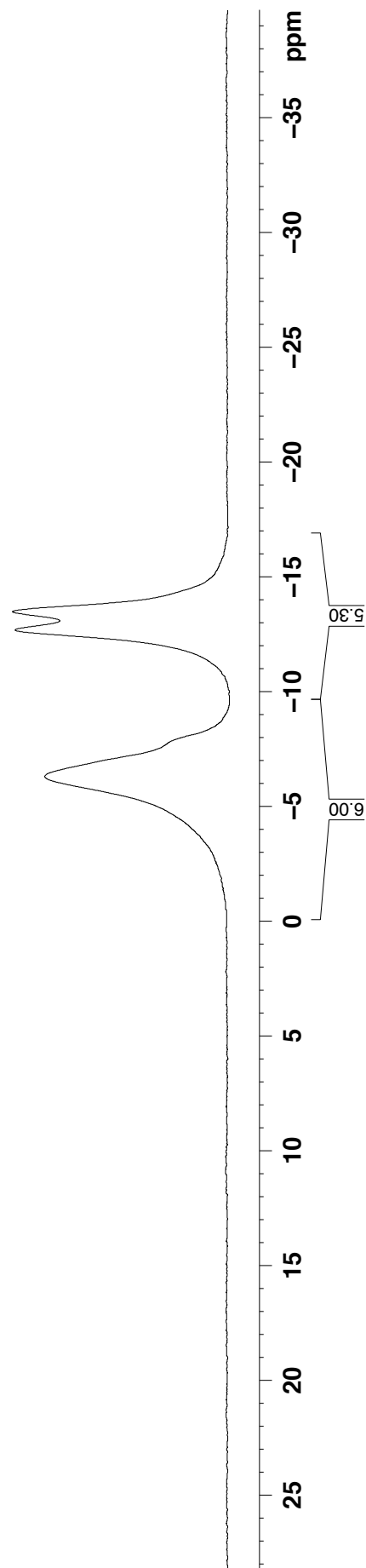
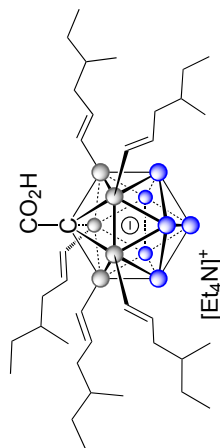
**penta-4-methyl-1-hexene product 40 mg in 0.6 ml acetone-d6
11B NMR, 500 MHz, 23 C**

Current Data Parameters
 NAME penta-4-methyl-1-hexene
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180403
 Time_ 6.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 64098
 SOLVENT DMSO
 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
 SF01 160.4615792 MHz
 F2 - Processing parameters
 SI 32768
 SF 160.4615790 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

6.32
7.89
12.70
13.50



**penta-4--methyl-1-1-hexene product 40 mg in 0.6 ml acetone-d6
11B{1H} NMR, 160 MHz, 23 C**

Current Data Parameters
 NAME penta-4-methyl-1-hexene
 EXPNO 3
 PROCNO 1

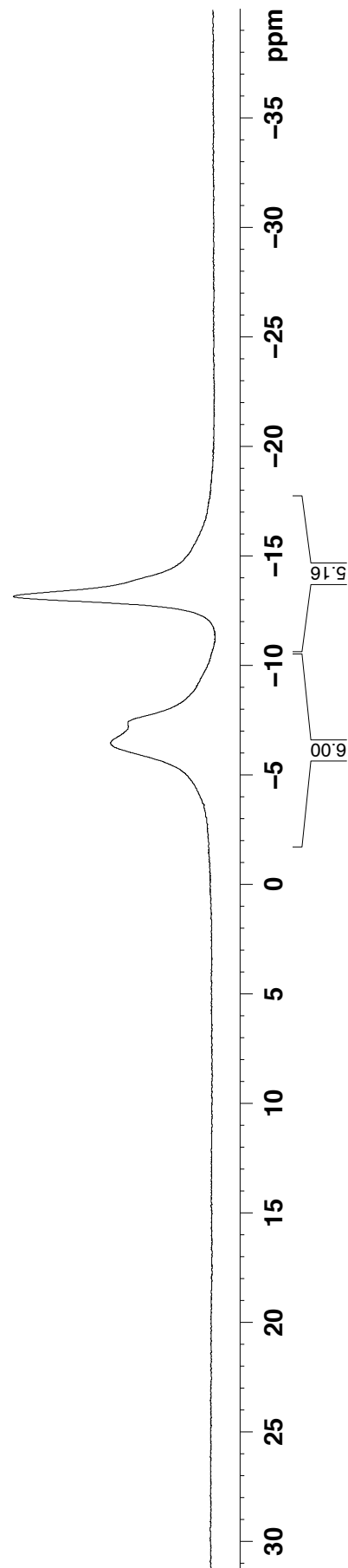
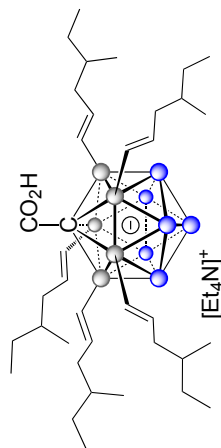
F2 - Acquisition Parameters
 Date_ 20180403
 Time_ 6:27
 INSTRUM spect
 PROBD 5 mm PABBO-EBL
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 4
 SWH 32051.281 Hz
 FIDRES 0.489664 Hz
 AQ 1.0223614 sec
 RG 203
 DW 15.600 usec
 DE 6.50 usec
 TE 296.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 usec
 PL1 95.00000000 W
 SF01 160.4615790 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waitz16
 NUC2 1H
 P2 80.00 usec
 PL2 19.00000000 W
 PL12 0.40839001 W
 PL13 0.26008999 W
 SF02 500.1325007 MHz

F2 - Processing Parameters
 SI 32768
 SF 160.4615790 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

— 13.18
 — 7.45
 — 6.49



penta-4-methyl-1-hexene product 40 mg in 0.6 ml acetone-d6 *
¹³C{1H} NMR, 126 MHz, 23 C

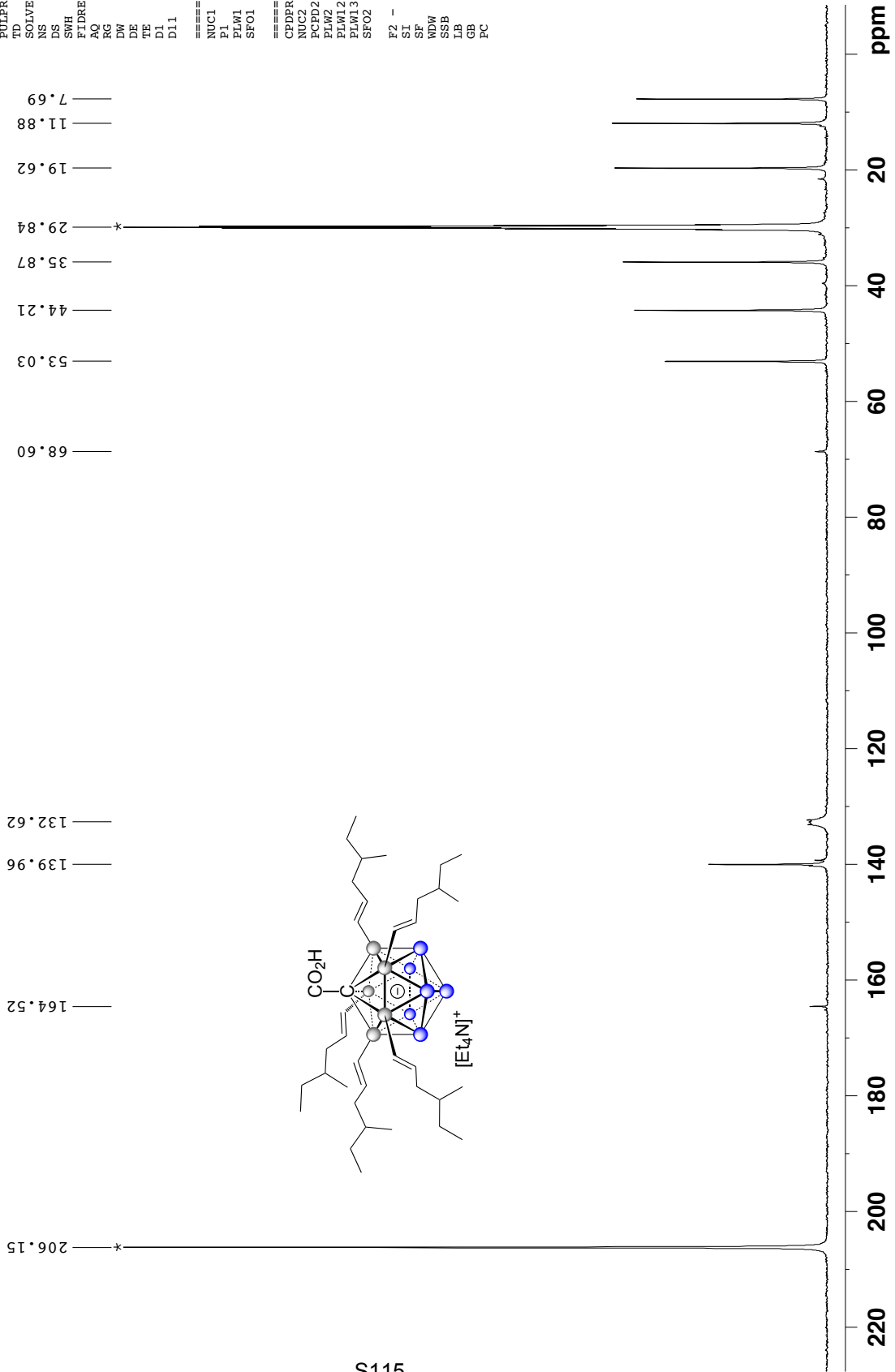
Current Data Parameters
 Name penta-4-methyl-1-hexene
 EXNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180403
 Time_ 7:54
 INSTRUM spect
 PROBHD 5 mm PABBO BBO
 PULPROG zgpg30
 TO SOLVENT DMSO
 NS 2104
 DS 4
 SFH 37878.784 Hz
 FIDRES 0.547084 Hz
 AC 0.8650752 sec
 PC 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.6 K
 D1 1.50000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.150
 PL1 95.0000000 W
 SFO1 125.7716224 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 P2 80.00 usec
 PL2 19.0000000 W
 SFO2 500.1320005 MHz

F2 - Processing Parameters
 SI 32768
 SF 125.7577380 MHz
 WDW EM
 SSB 0
 LB 10.00 Hz
 GB 0
 PC 1.40



**penta-4,4-dimethyl-1-pentene product 50 mg in 0.6 ml acetone-d₆*
¹H{¹H} NMR, 400 MHz, 23 C**

Current Data Parameters
 NAME penta-4,4-dimethyl-1-pentene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date 20180506
 Time 7.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 36.87
 DW 62.400 usec
 DE 6.50 usec
 TE 294.8 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====

NUC1 ¹H
 P1 15.00 usec
 PLW1 12.5000000 W
 SFO1 400.1320007 MHz

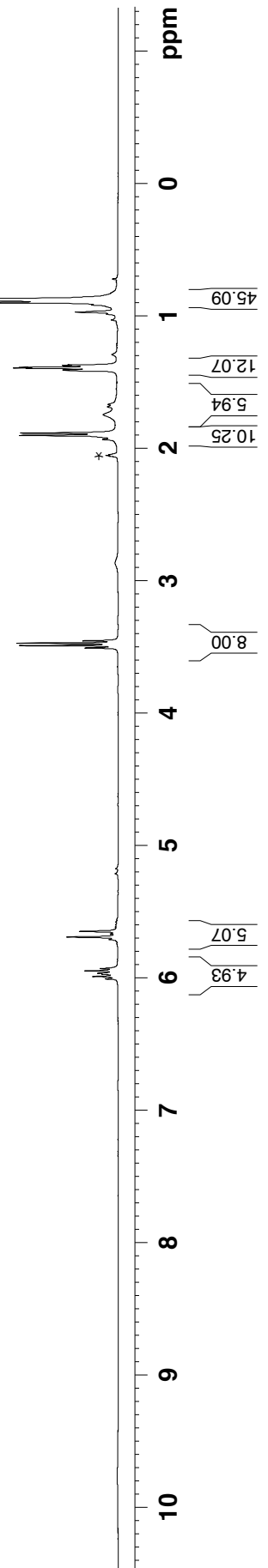
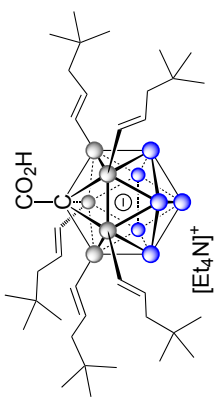
==== CHANNEL f2 =====

CPDPRG2 gatp4
 NUC2 ¹H
 P2 90.00 usec
 PLW2 52.9659960 W
 PLW1 0.6447798 W
 SFO2 128.3776050 MHz

F2 - Processing parameters

SI 32768
 SF 400.1300074 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

5.99
 5.94
 5.69
 5.65
 3.49
 3.47
 2.05
 2.05
 2.04
 1.90
 1.88
 1.74
 1.68
 1.66
 1.39
 1.39
 1.39
 1.38
 0.87



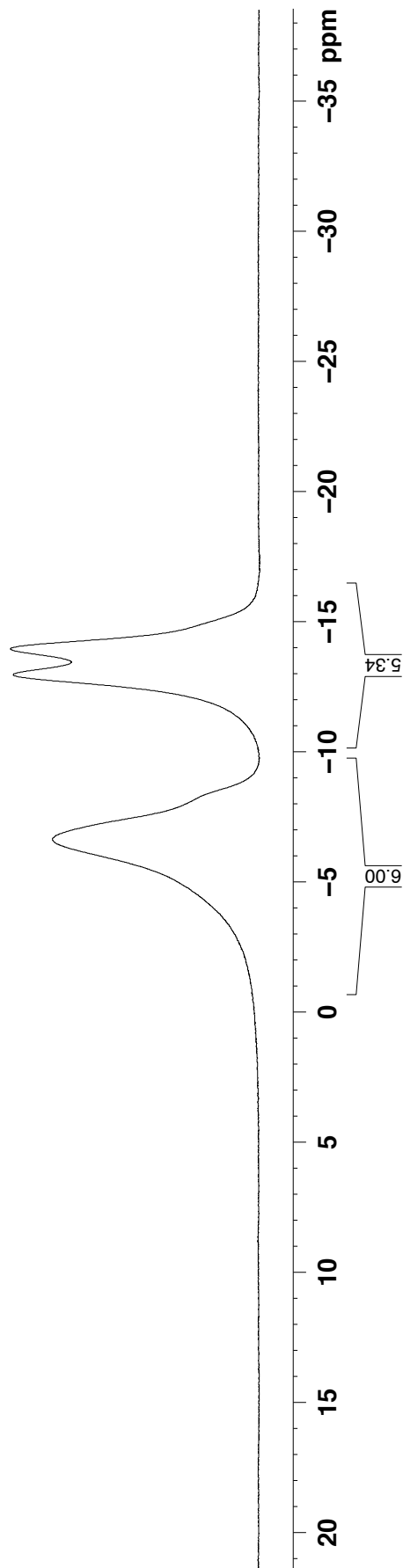
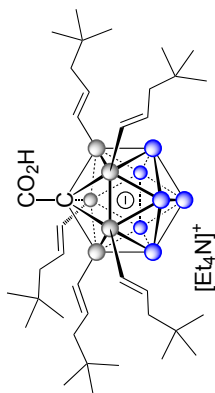
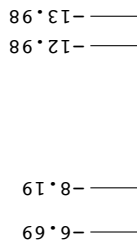
**penta-4,4-dimethyl-1-pentene product 50 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME penta-4,4-dimethyl-1-pentene
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180506
 Time 7.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389235 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 294.7 K
 D1 1.0000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SFO1 128.3776052 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40



**penta-4,4-dimethyl-1-pentene product 50 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME penta-4,4-dimethyl-1-pentene
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

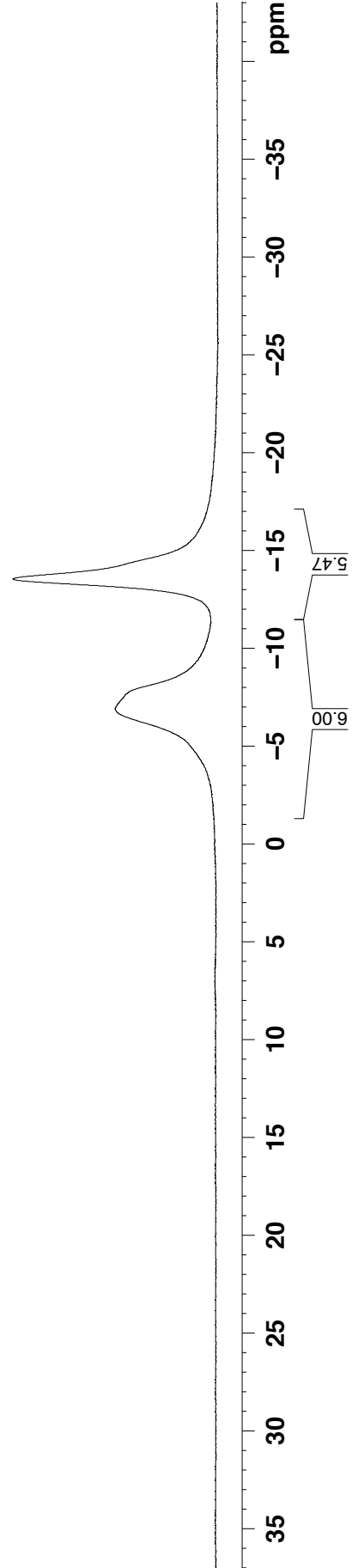
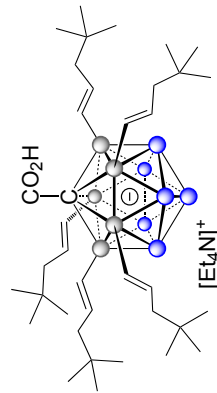
Date_ 20180506
 Time 7.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 295.7 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 ¹¹B
 P1 9.93 usec
 PLW1 52.9659960 W
 SFO1 128.3776050 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 12.5000000 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 3.00 Hz
 GB 0
 FC 1.40

6.91
 13.57



penta-4,4-dimethyl-1-pentene product 50 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 126 MHz, 23 C

Current Data Parameters
 NAME penta-4,4-dimethyl-1-pentene
 EXPNO 4
 PROCNO 1

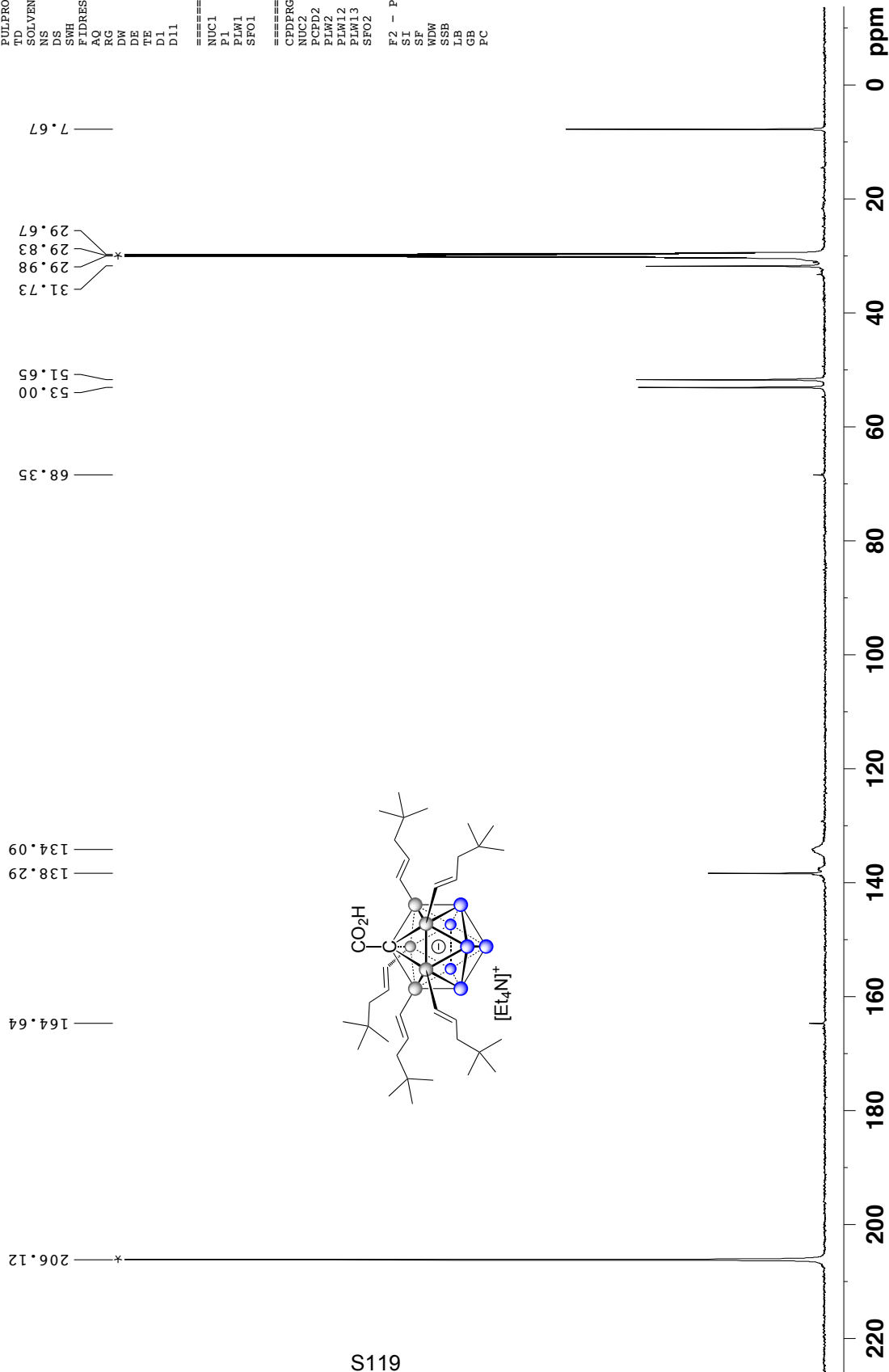
F2 - Acquisition Parameters

Date_ 20180413
 Time 5.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 2048
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.9 K
 D1 1.50000000 sec
 D11 0.03000000 sec

=====
 CHANNEL f1
 NUC1 ¹³C
 P1 10.50 usec
 PLW1 95.0000000 W
 SFO1 125.7716224 MHz

=====
 CHANNEL f2
 CPDPRG2 waltz16
 NUC2 ¹H
 P2 80.00 usec
 PLW2 19.0000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7576846 MHz
 WDW EM
 SSB 0
 LB 6.00 Hz
 GB 0
 PC 1.40



**Penta-CH₂CH₂-Ph product 50 mg in 0.6 ml acetone-d₆ *
¹H{(11B)} NMR, 400 MHz, 23 C**

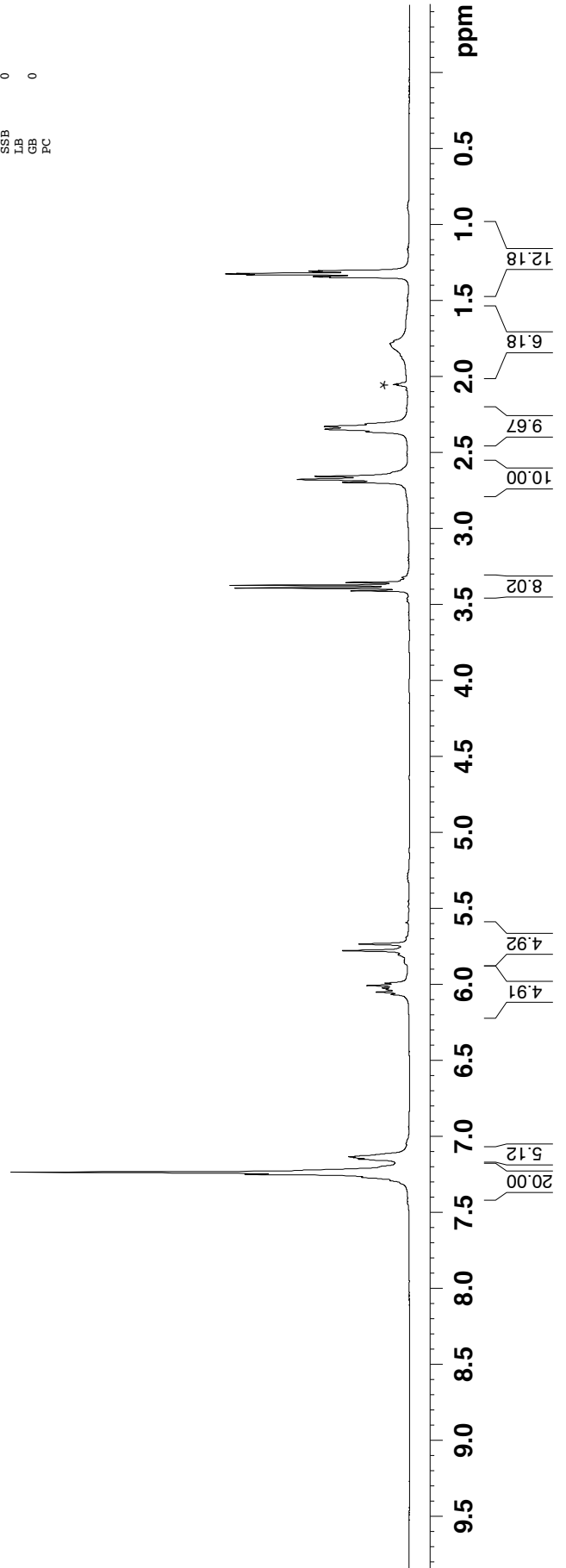
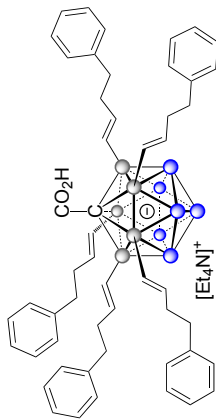
Current Data Parameters
 NAME penta-CH₂CH₂Ph
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180503
 Time_ 16.51
 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 20.46
 DW 62.400 usec
 DE 6.50 usec
 TE 294.7 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 =====
 CPDPRG1(2) gairp4
 NUC2 ¹¹B
 PCPD2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.64477998 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300073 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



**Penta-CH₂CH₂-Ph product 50 mg in 0.6 ml acetone-d₆
11B NMR, 128 MHz, 23 C**

```

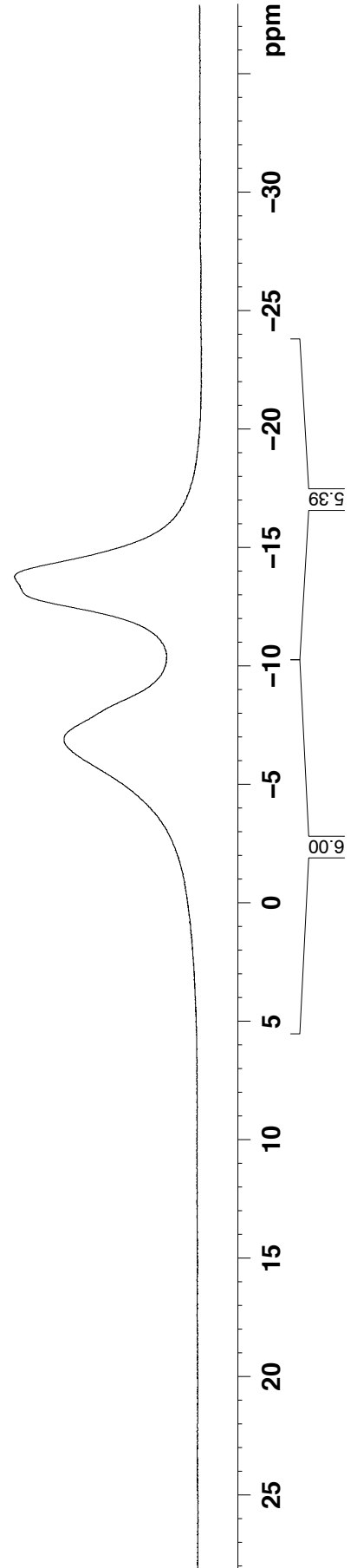
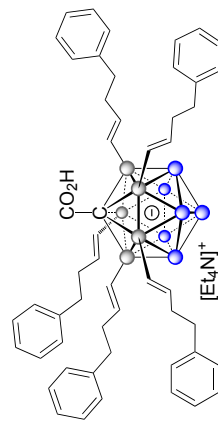
Current Data Parameters
NAME      penta-CH2CH2Ph
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20180503
Time     16.57
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       294.7 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       2.00 Hz
GB       0
PC       1.40
    
```

— 6.92
— 12.91
— 13.79



**Penta-CH₂CH₂-Ph product 50 mg in 0.6 ml acetone-d₆
¹H NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME penta-CH₂CH₂Ph
 EXPNO 3
 PROCNO 1

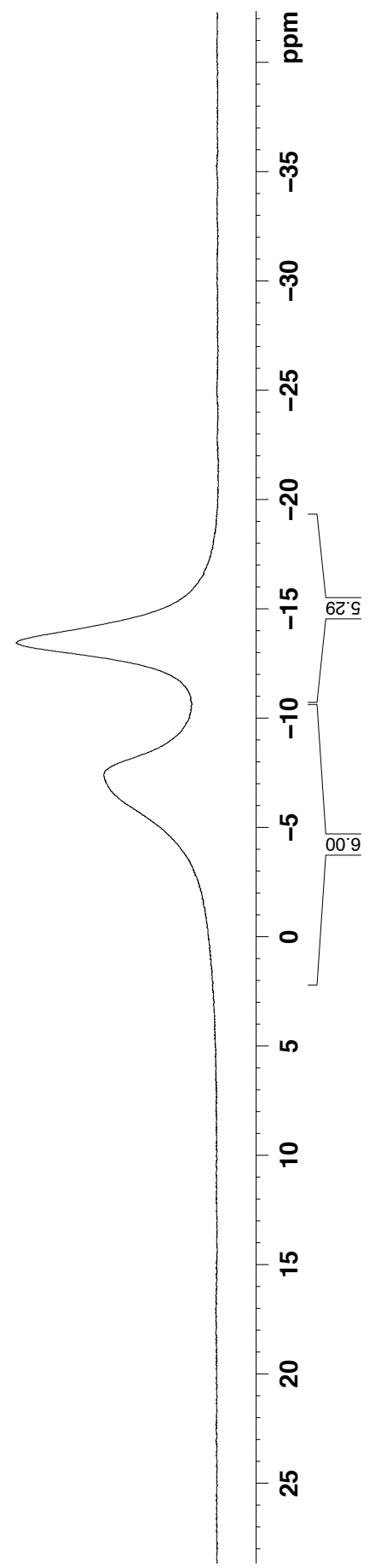
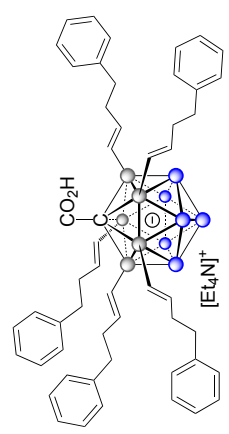
F2 - Acquisition Parameters
 Date_ 20180503
 Time_ 17.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 6536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 295.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 9.93 usec
 PLW1 52.96599960 W
 SFO1 128.3776050 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹³C
 P1 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 0
 GB 0
 PC 1.40

7.43
 13.47



**Penta-CH₂CH₂-Ph product 50 mg in 0.6 ml acetone-d₆ *
¹³C{¹H} NMR, 101 MHz, 23 C**

```

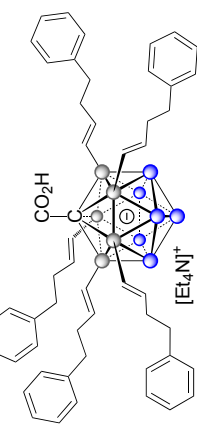
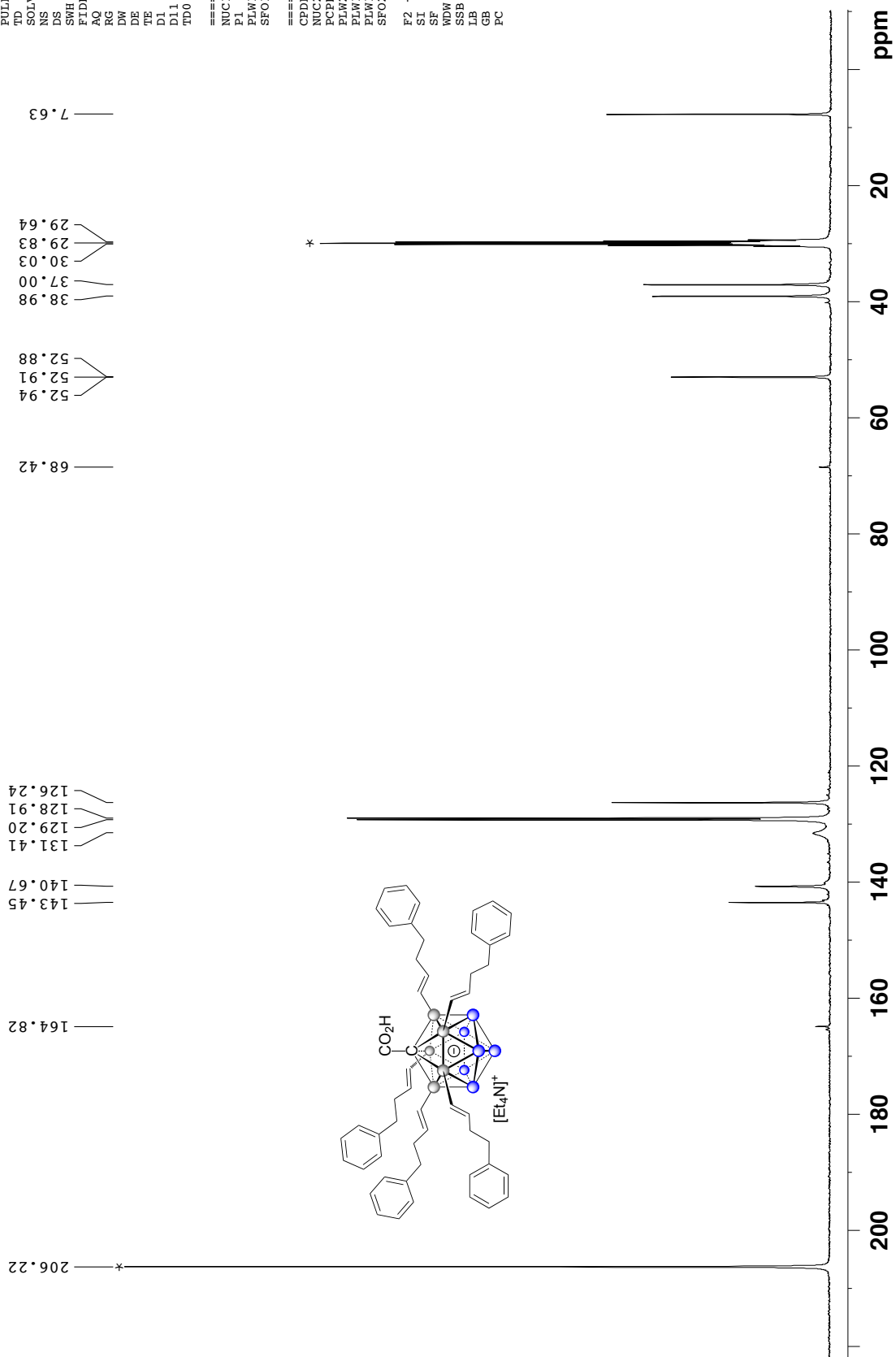
Current Data Parameters
NAME      penta-CH2CH2Ph
EXPNO    4
PROCNO   1

F2 - Acquisition Parameters
Date_    20180503
Time     18.36
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
DE         16.800 usec
TE         296.1 K
D1         1.50000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1      13C
P1         10.00 usec
PLW1      53.0000000 W
SF01      100.6228293 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2      1H
PCPD2     80.00 usec
PLW2      12.5000000 W
PLW12     0.43945000 W
PLW13     0.28125000 W
SF02      400.1316005 MHz

F2 - Processing parameters
SI         32768
SF         100.6126926 MHz
WDW        EM
SSB        0
LB         6.00 Hz
GB         0
PC         1.40
  
```



**penta-CH₂CH₂COOEt product 15 mg in 0.6 ml acetone-d₆ *
¹H{¹B} NMR, 500 MHz, 23 C**

Current Data Parameters
 NAME penta-CH₂CH₂COOEt-1H
 EXPNO 1
 PROCNO 1

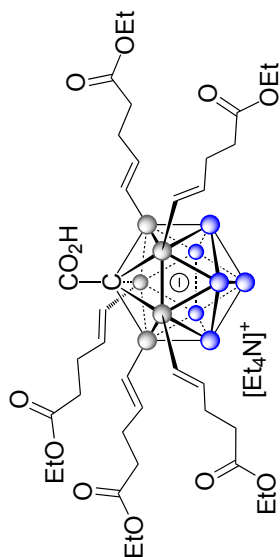
F2 - Acquisition Parameters
 Date_ 20180413
 Time_ 18.44
 INSTRUM spect
 PROBHD 5 mm PABBO-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT acetone
 NS 32
 SH 12500.000 Hz
 FIDRES 0.190735 Hz
 AQ 2.621439 sec
 RG 114
 DW 40.110 usec
 DE 6.59
 TE 29.9 K
 D1 5.000000 sec
 D11 0.0300000 sec

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 11.70 usec
 PL1 19.000000 W
 SFO1 500.1335009 MHz

==== CHANNEL f2 =====
 CPDPRG2 gattp
 NUC2 ¹³C
 PCD2 100.10 usec
 PLD2 95.000000 W
 PLW2 1.6303005 W
 SFO2 160.4615690 MHz

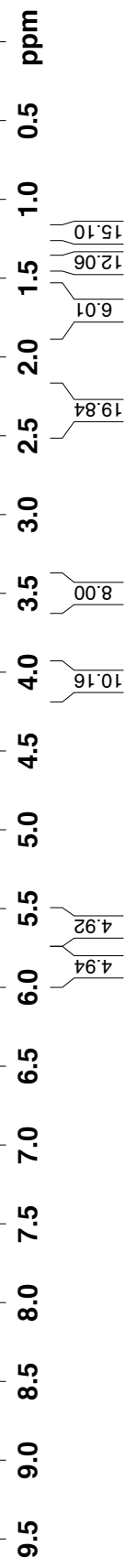
F2 - Processing parameters
 SI 65536
 SF 500.1300191 MHz
 MDW EM
 SSB 0
 LB 0
 GB 0
 FC 1.00

5.89
5.88
5.84
5.79
5.77
5.66
5.62
4.09
4.08
4.06
4.05
3.51
3.50
2.82
2.78
2.34
2.33
2.05
1.75
1.69
1.42
1.41
1.40
1.39
1.22
1.21
1.20



H₂O

*

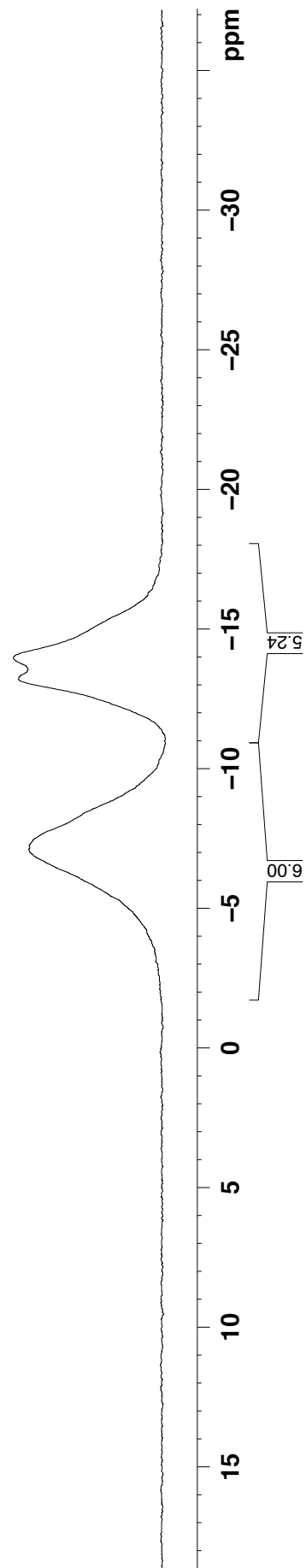
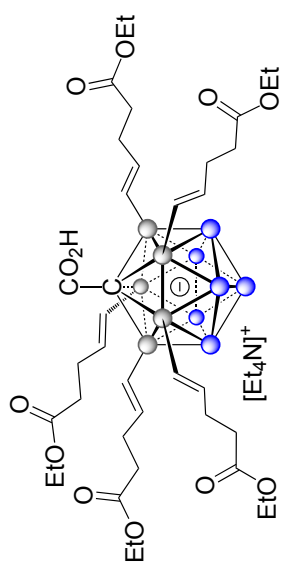


penta-CH₂CH₂COOEt product 40 mg in 0.6 ml acetone-d₆
¹B NMR, 160 MHz, 23 C

Current Data Parameters
 NAME penta-CH₂CH₂COOEt
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180412
 Time_ 7.12
 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 295.5 K
 D1 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 usec
 PLW1 95.0000000 W
 SF01 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

— 7.14
 — 13.24
 — 13.99



**penta-CH₂CH₂COOEt product 40 mg in 0.6 ml acetone-d₆
¹B{¹H} NMR, 160 MHz, 23 C**

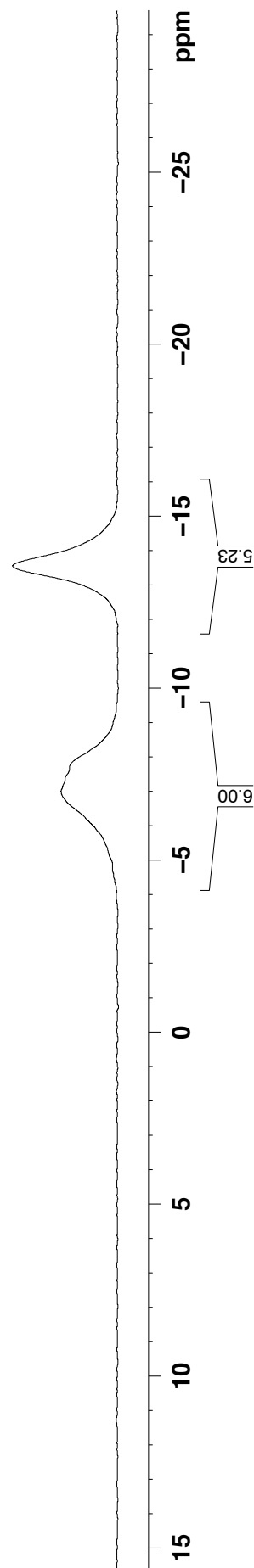
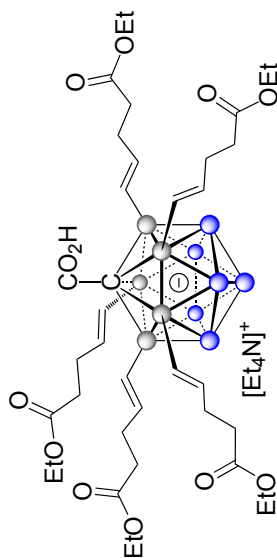
Current Data Parameters
 NAME penta-CH₂CH₂COOEt-13C
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181018
 Time_ 7.06
 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
 TD0 1

=====
 CHANNEL f1 =====
 SFO1 160.4615790 MHz
 NUC1 13C
 P1 13.10 usec
 PLW1 95.00000000 W
 =====
 CHANNEL f2 =====
 SFO2 500.1325007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.00000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W

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

6.94
 7.71
 13.56



penta-CH₂CH₂COOEt product 40 mg in 0.6 ml acetone-d₆
¹³C{¹H} NMR, 126 MHz, 23 C

Current Data Parameters
 NAME penta-CH₂CH₂COOEt-13C
 EXPNO 4
 PROCNO 1

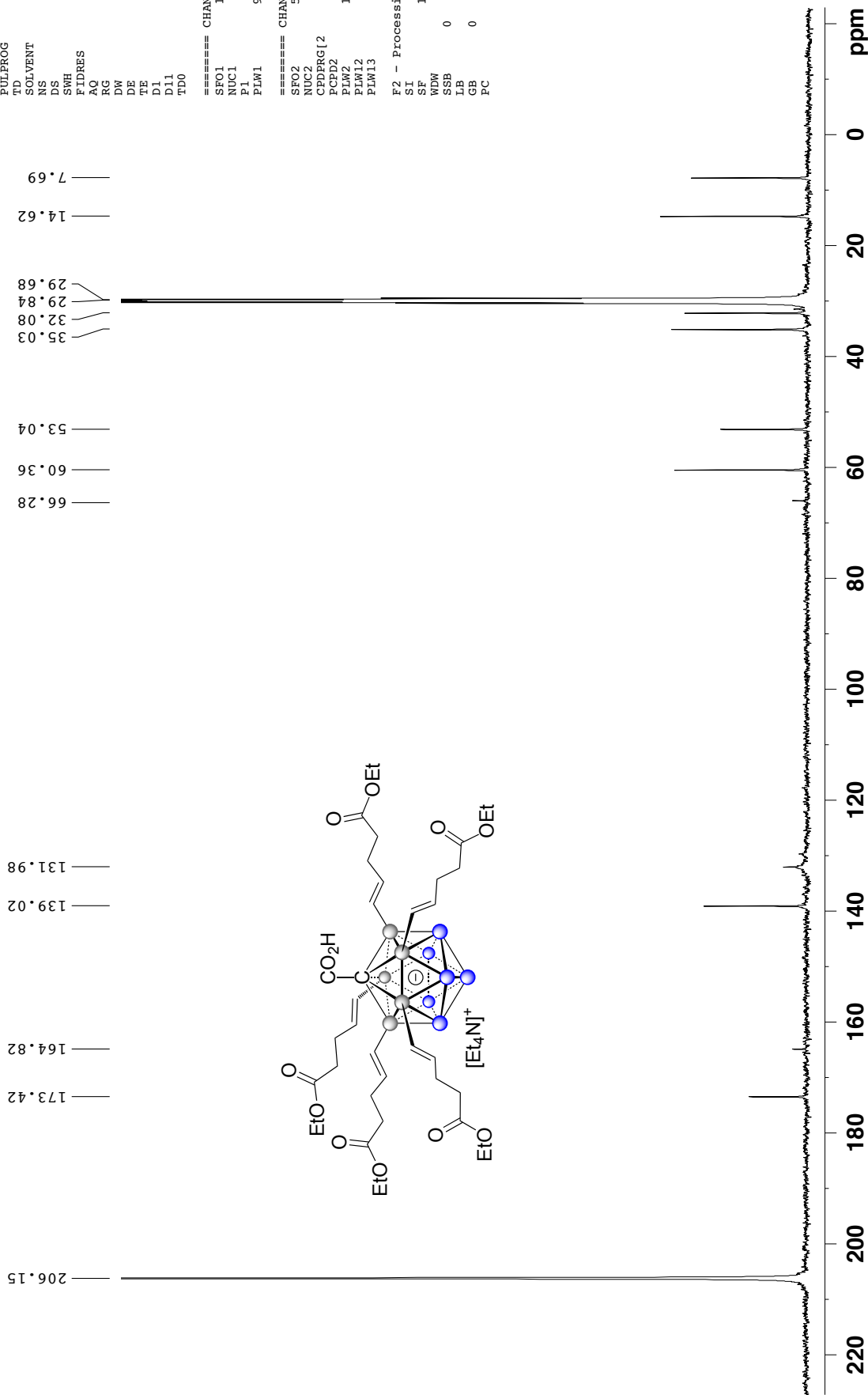
F2 - Acquisition Parameters

Date_ 20181018
 Time_ 8.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 SOLVENT Acetone
 NS 2148
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 10.70 usec
 PLW1 95.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 walz16
 CDEPRG[2] walz16
 PCPD2 80.00 usec
 PLW2 19.00000000 W
 PLW12 0.40630001 W
 PLW13 0.26006999 W

F2 - Processing parameters
 SI 32768
 SF 125.7576763 MHz
 EQ
 WDW 0
 SSB 0
 LB 7.00 Hz
 GB 0
 PC 1.40



Penta-CH2OPh product 40 mg in 0.6 ml acetone-d6 *
¹H{¹B} NMR, 500 MHz, 23 C

```

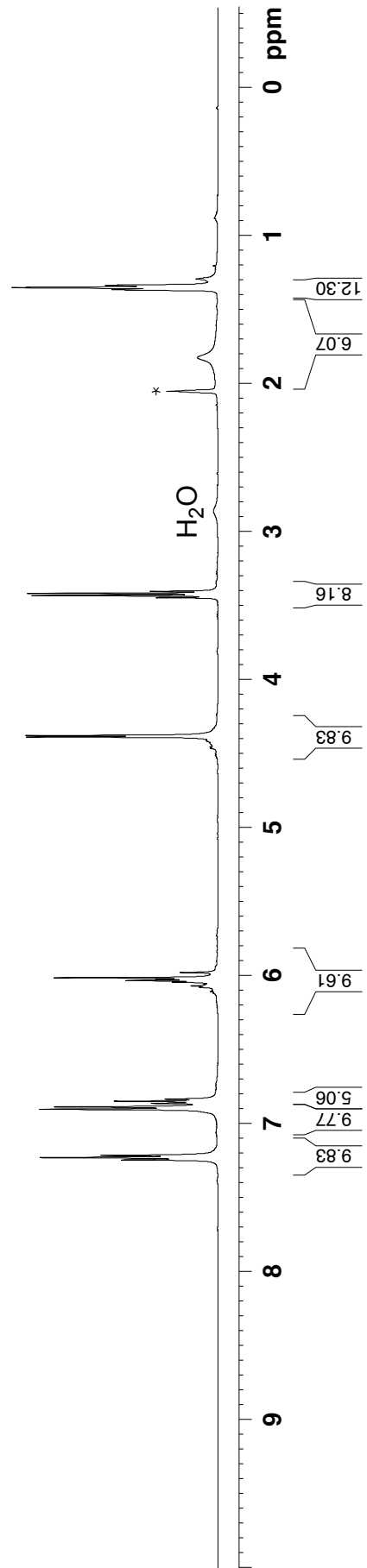
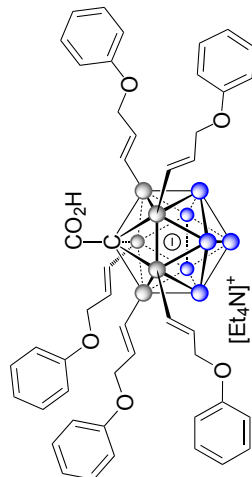
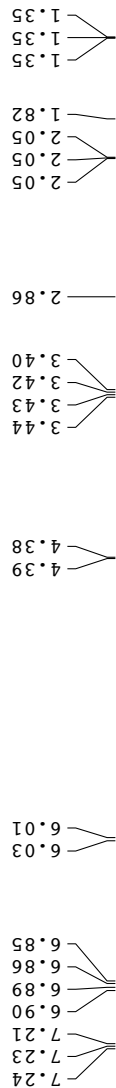
Current Data Parameters
NAME      Penta-CH2OPh
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20180119
Time     4.48
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  Acetone
NS        16
DS        0
SWH       12500.000 Hz
FIDRES   0.190735 Hz
AQ        2.6214399 sec
RG        57
DE        40.000 usec
TE        296.0 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 =====
CPDPRG2   garp
NUC2      13B
P2        100.00 usec
PLW2     95.00000000 W
SFO2     160.4615690 MHz

F2 - Processing parameters
SI        65536
SF        500.1300101 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
    
```



**Penta-CH2OPh product 40 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

```

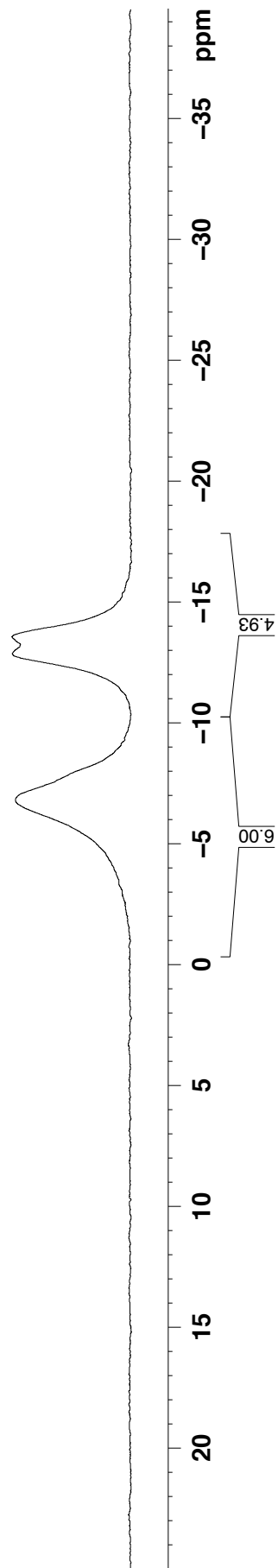
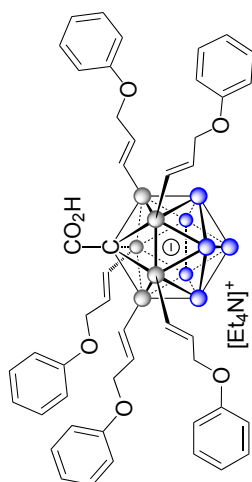
Current Data Parameters
NAME      penta-CH2OPh
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_     20180119
Time      4.51
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          295.7 K
D1          1.00000000 sec

===== CHANNEL f1 =====
NUC1       11B
P1          13.10 usec
PLW1        95.0000000 W
SF01        160.4615792 MHz

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

— 6.82
— 12.81
— 13.59



**Penta-CH₂O^{Ph} product 40 mg in 0.6 ml acetone-d₆
 11B{1H} NMR, 160 MHz, 23 C**

```

Current Data Parameters
NAME      Penta-CH2OPh
EXPNO     3
PROCNO    1

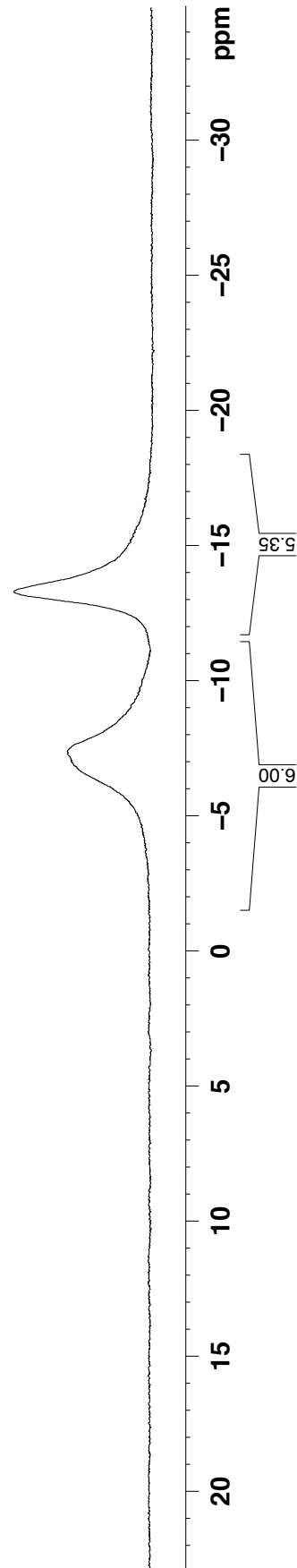
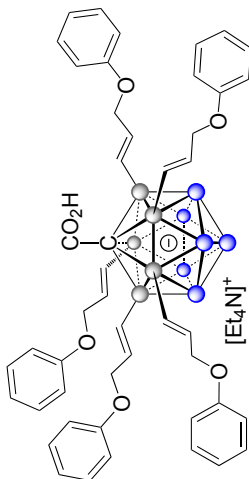
F2 - Acquisition Parameters
Date_     20180119
Time      4.54
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         64
DS         0
SWH        32051.281 Hz
FIDRES     0.489064 Hz
AQ         1.0223616 sec
RG         203
DW         15.600 usec
DE         6.50 usec
TE         296.1 K
D1         1.00000000 sec
D11        0.03000000 sec

===== CHANNEL f1 =====
NUC1       11B
P1         13.10 usec
PLW1       95.0000000 W
SFO1       160.4615790 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2       1H
P2         80.00 usec
PLW2       19.0000000 W
SFO2       406.39001 W

F2 - Processing parameters
SI         32768
SF         160.4615790 MHz
WDW        EM
SSB        0
LB         4.00 Hz
GB         0
PC         1.40
  
```

— 13.36
 — 7.43



**Penta-CH₂Oph product 40 mg in 0.6 ml acetone-d₆ *
¹³C{¹H} NMR, 126 MHz, 23 C**

```

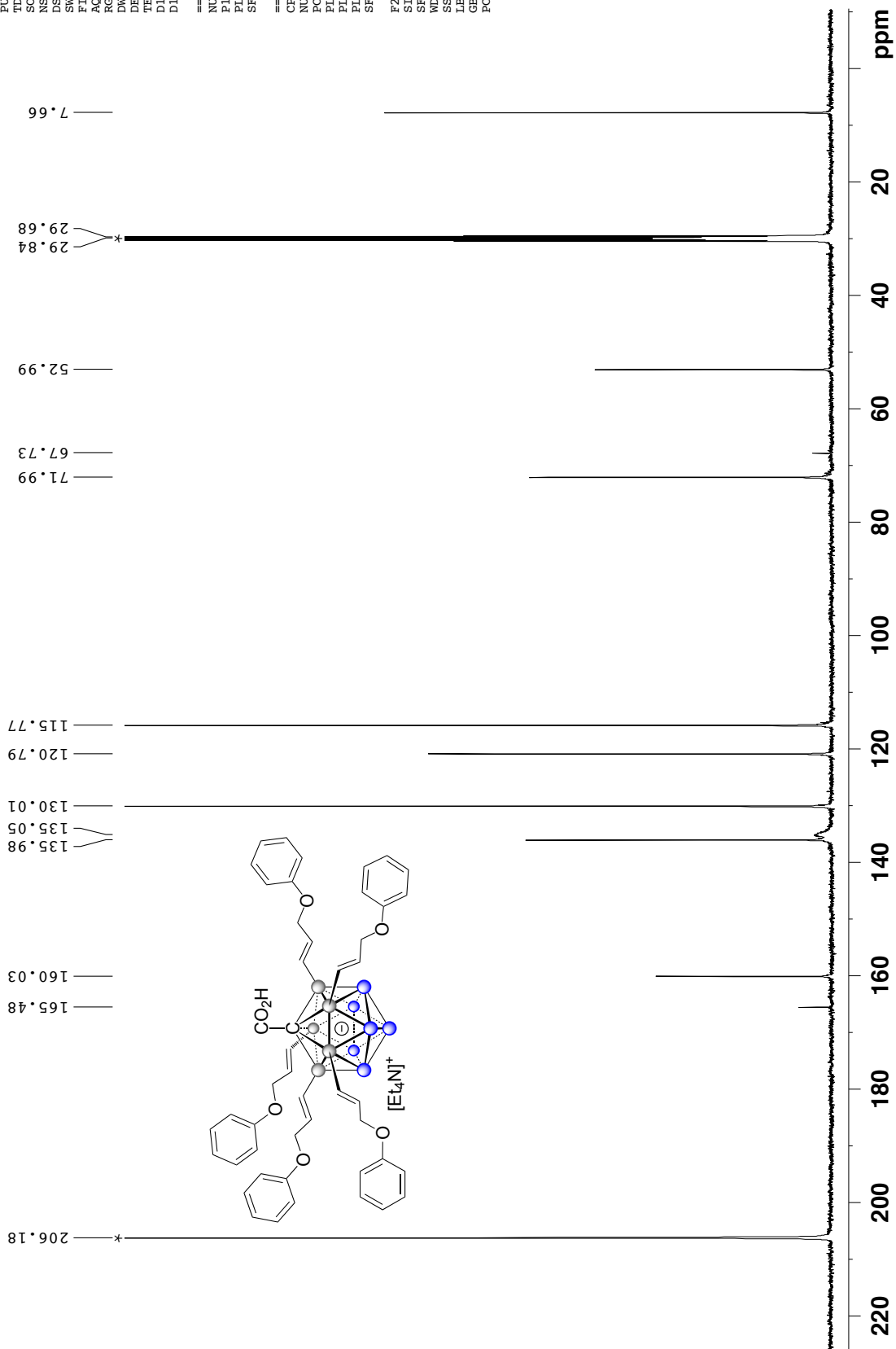
Current Data Parameters
NAME      penta-CH2OPh
EXPNO    4
PROCNO   1

F2 - Acquisition Parameters
Date_    20180119
Time     6.20
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  Acetone
NS       2100
DS       4
SWH      37878.789 Hz
FIDRES   0.577984 Hz
AQ       0.8650752 sec
RG       203
DM       13.200 usec
DE       6.50 usec
TE       296.4 K
D1       1.50000000 sec
D11      0.03000000 sec

===== CHANNEL f1 =====
NUC1     13C
P1       10.50 usec
PLW1     95.00000000 W
SFO1     125.7716224 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2     1H
PCPD2    80.00 usec
PLW2     19.00000000 W
PLW12    0.40639001 W
PLW13    0.26008999 W
SFO2     500.1320005 MHz

F2 - Processing Parameters
SI       32768
SF       125.7576822 MHz
WDW      EM
SSB      0
LB       3.00 Hz
GB       0
PC       1.40
  
```



12-Cl-Penta-styrine product 50 mg in 0.6 ml acetone-d6 *
¹H{¹B} NMR, 500 MHz, 23 C

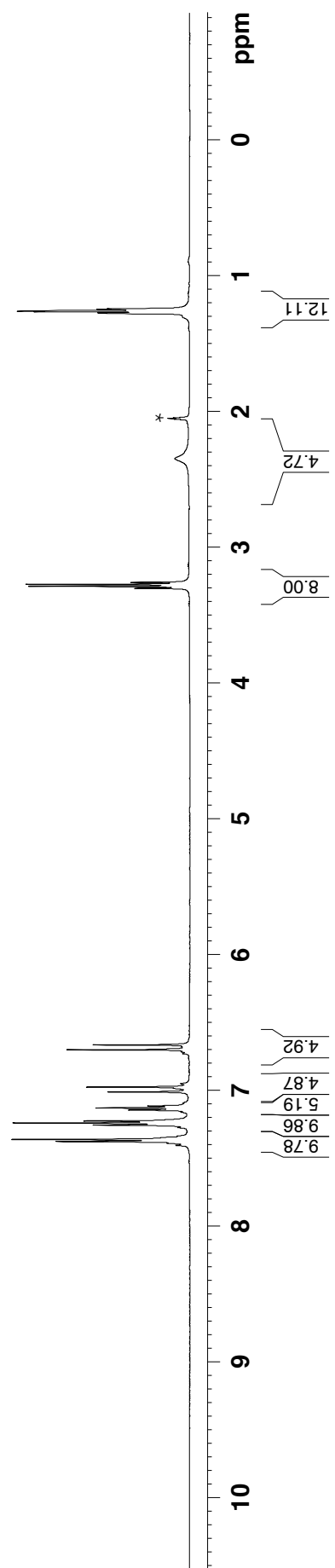
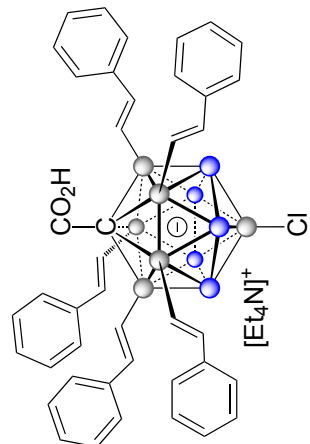
Current Data Parameters
 NAME 12-Cl-penta-styrene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180612
 Time_ 2.31
 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 40.3
 DW 40.000 usec
 DE 6.50 usec
 TE 296.0 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 =====
 CPDPRG2 garp
 NUC2 11B
 PCPD2 100.00 usec
 PLW2 95.00000000 W
 PLW12 1.6303005 W
 SFO2 160.4615690 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.1300100 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

3.30
3.29
3.27
3.26
2.35
2.06
2.05
2.05
2.05
2.05
2.04

7.37
7.36
7.25
7.24
7.22
7.14
7.13
7.11
7.01
6.97
6.70
6.66



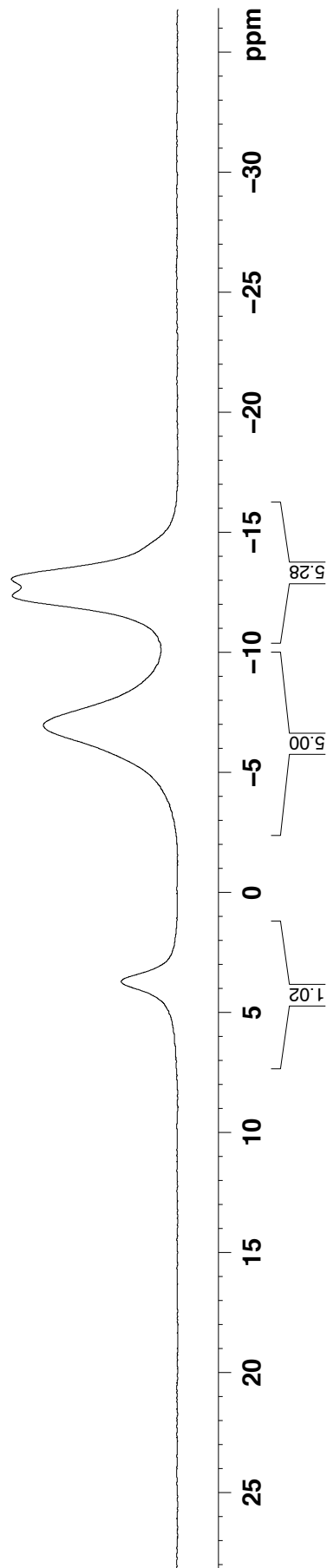
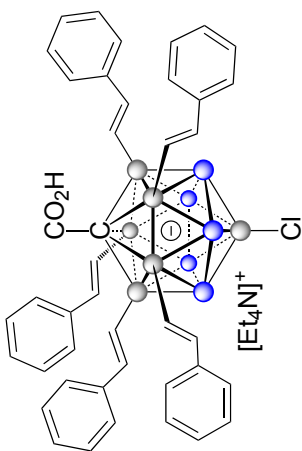
**12-Cl-Penta-styrene product 50 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

Current Data Parameters
 NAME 12-cl-penta-styrene
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180612
 Time_ 2.34
 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 95.0000000 W
 SF01 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

3.70
 -6.97
 -12.40
 -13.07



12-Cl-Penta-styrine product 50 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 160 MHz, 23 C

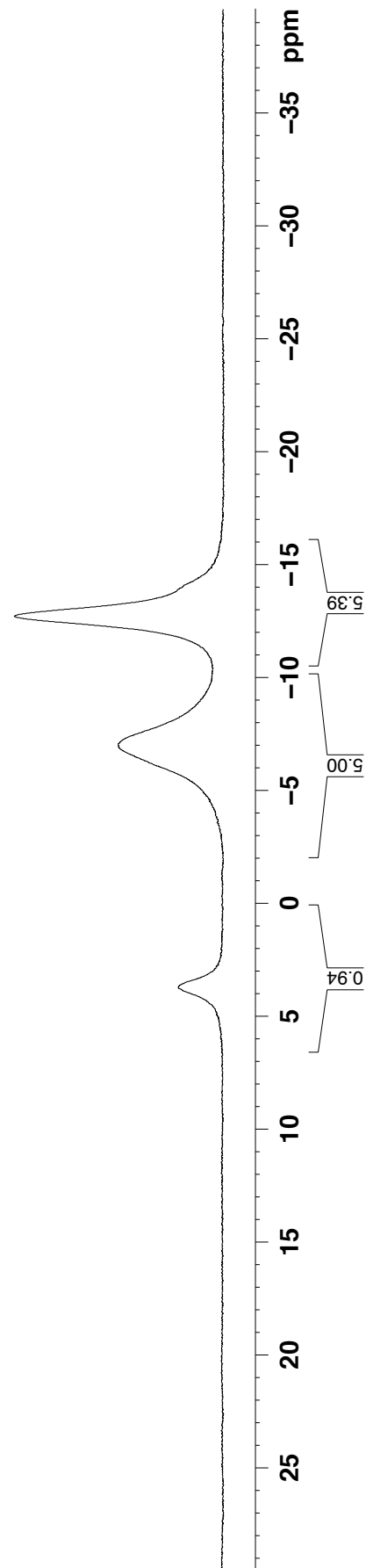
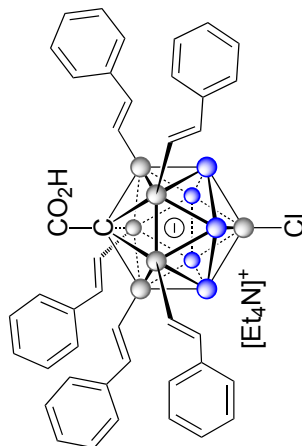
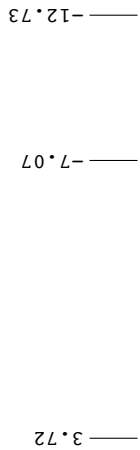
Current Data Parameters
 NAME 12-Cl-penta-styrene
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180612
 Time_ 2.37
 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 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 19.00000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SFO2 500.1325007 MHz

F2 - Processing parameters
 SI 32768
 SF 160.4615790 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



12-Cl-Penta-styrene product 50 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 126 MHz, 23 C

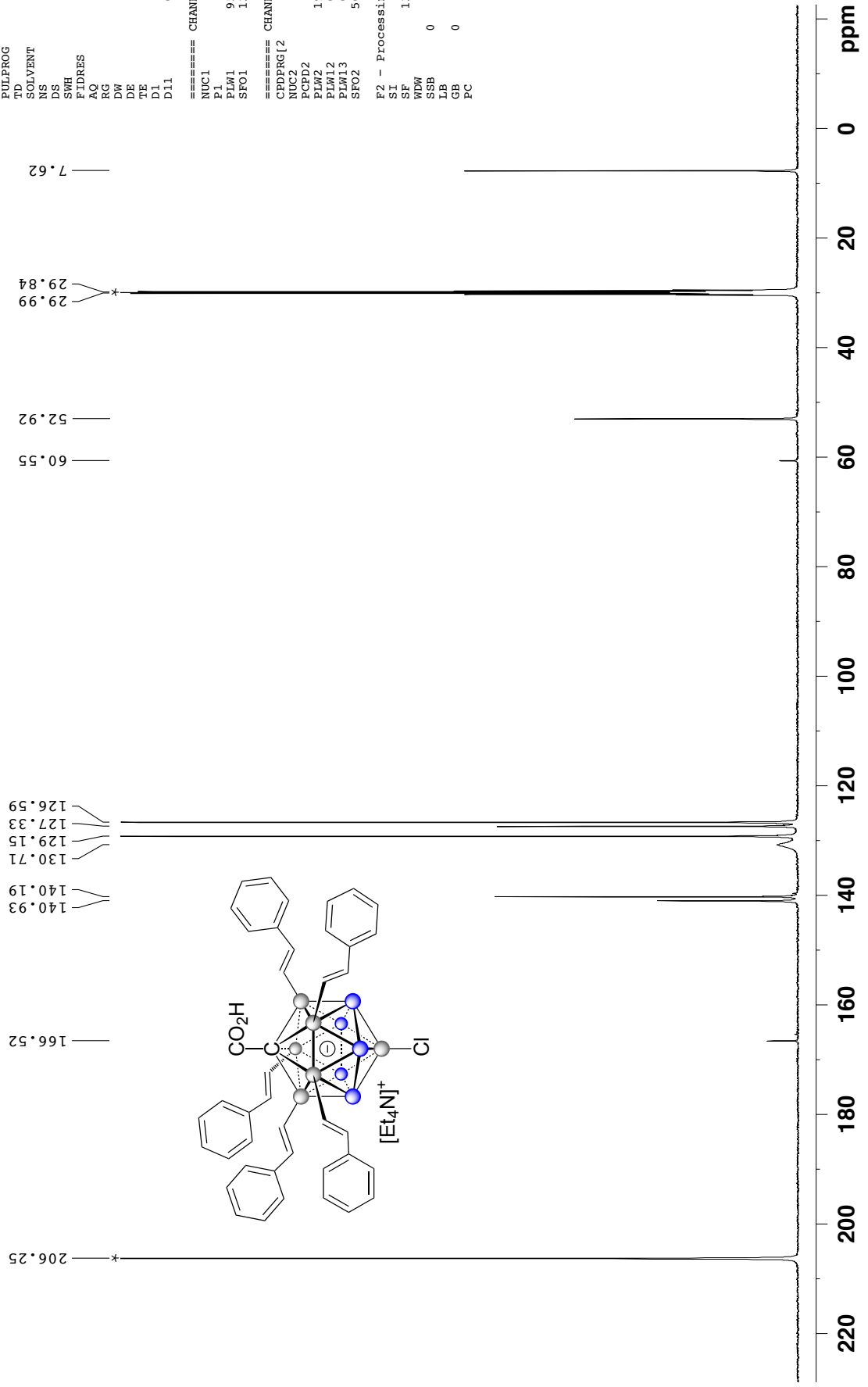
Current Data Parameters
 NAME 12-Cl-penta-styrene
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180612
 Time 4.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 2100
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.6 K
 D1 1.50000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.50 usec
 PLW1 95.0000000 W
 SFO1 125.7716224 MHz

==== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 ¹H
 P2 80.00 usec
 PLW2 19.0000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7576880 MHz
 EM
 WDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



12-Br-Penta-F-styrene product 50 mg in 0.6 ml acetone-d6*
¹H{¹¹B} NMR, 500 MHz, 23 C

Current Data Parameters
 NAME 12-Br-penta-4-F-styrene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180507
 Time 23.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 12500.000 Hz
 FIDRES 0.190735 Hz
 AQ 2.621439 sec
 RG 457.6
 DW 40.000 usec
 DE 6.99 usec
 TE 286.2 K
 D1 5.0000000 sec
 D11 0.0300000 sec

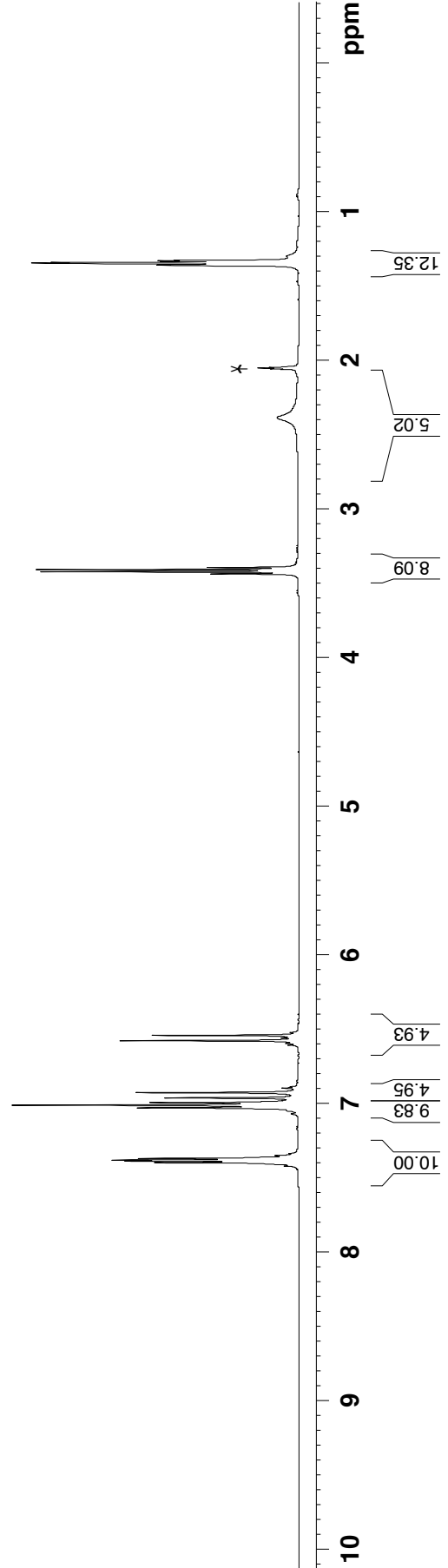
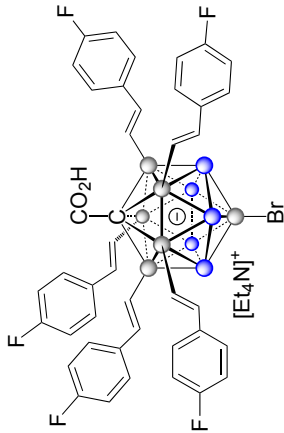
==== CHANNEL f1 =====
 NUC1 ¹H
 P1 11.70 usec
 PL1 19.000000 W
 SFO1 500.1335009 MHz

==== CHANNEL f2 =====
 CPDPRG[2] gtp
 NUC2 ¹¹B
 P2 100.00 usec
 PL2 95.000000 W
 SFO2 160.4615690 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300101 MHz
 WDW EM
 SSB 0 1.00 Hz
 GB 0
 FC 1.00

3.41
3.42
2.38
2.05
2.05
1.34
1.34
1.35

7.40
7.39
7.38
7.37
7.03
7.01
6.99
6.96
6.93
6.58
6.54



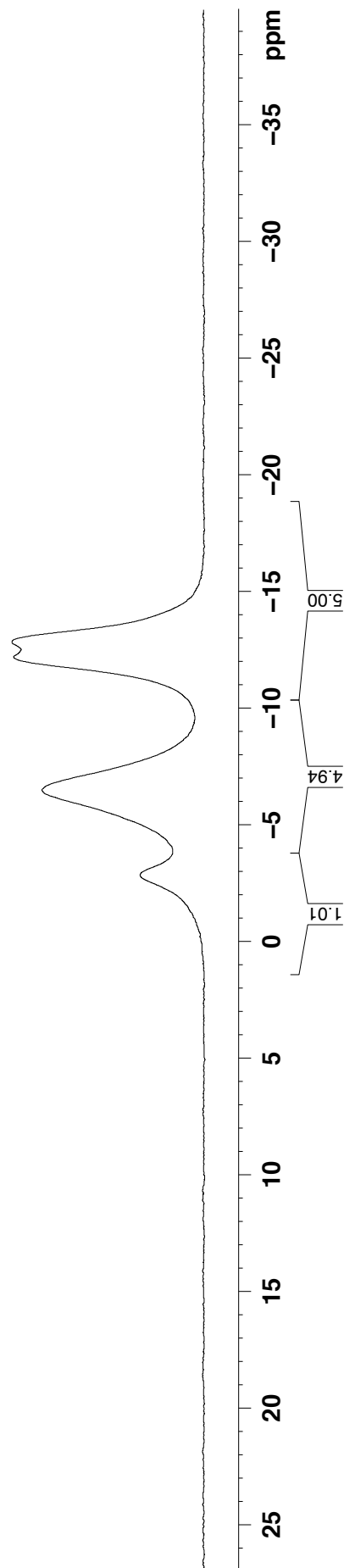
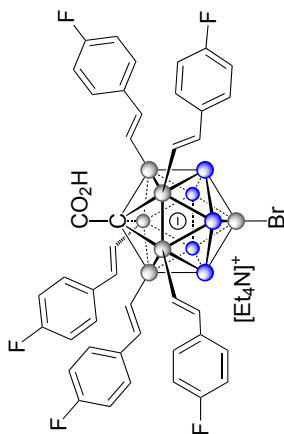
**12-Br-Penta-F-styrene product 50 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

Current Data Parameters
 NAME 12-Br-penta-4-F-styrene
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180507
 Time_ 23.15
 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 295.7 K
 D1 1.0000000 sec

==== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 usec
 PLW1 95.0000000 W
 SF01 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

12.85
 12.20
 6.51
 2.86



**12-Br-Penta-F--styrene product 50 mg in 0.6 ml acetone-d6
11B{1H} NMR, 160 MHz, 23 C**

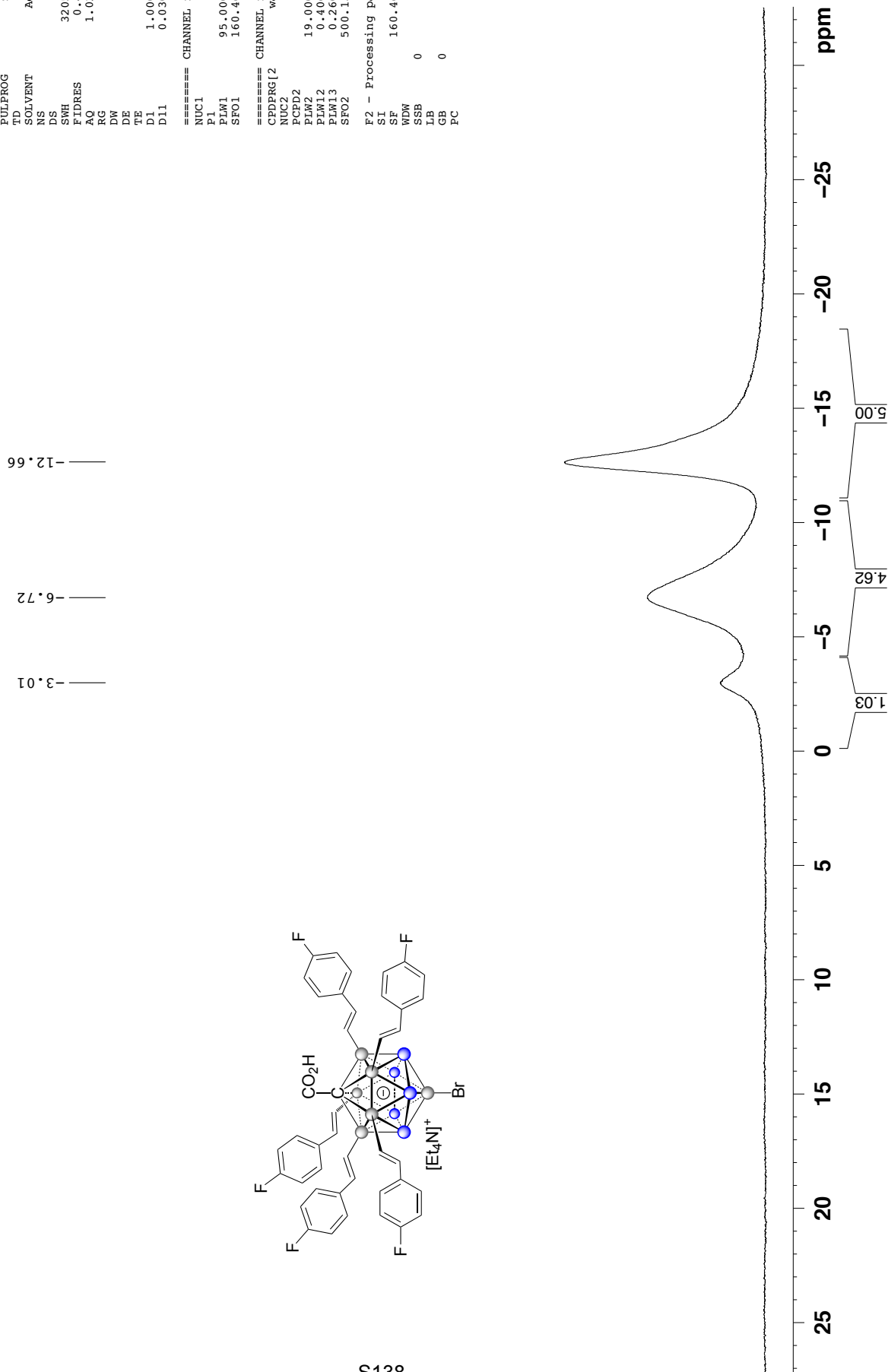
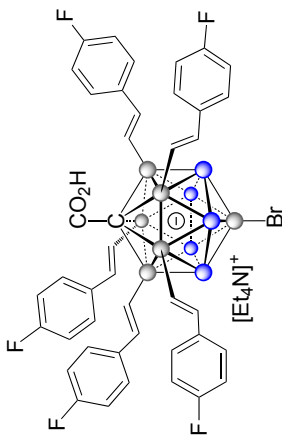
Current Data Parameters
 NAME 12-Br-penta-4-F-styrene
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180507
 Time_ 23.19
 INSTRUM spect
 PROBH 5 mm PABBO-EB
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 64
 DS 4
 SWH 32051.281 Hz
 FIDRES 0.789064 Hz
 AQ 1.0223614 sec
 RG 203
 DW 15.600 usec
 DE 6.50 usec
 TE 295.8 K
 D1 1.00000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 usec
 PL1 95.00000000 W
 SF01 160.4615790 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waitz16
 NUC2 1H
 PCPD2 80.00 usec
 PL12 19.00000000 W
 PL13 0.40839001 W
 PL14 0.26008999 W
 SF02 500.1325007 MHz

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



12-Br-Penta-F-styrene product 50 mg in 0.6 ml acetone-d6*
¹³C{1H} NMR, 126 MHz, 23 C

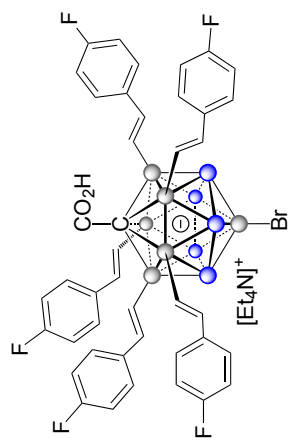
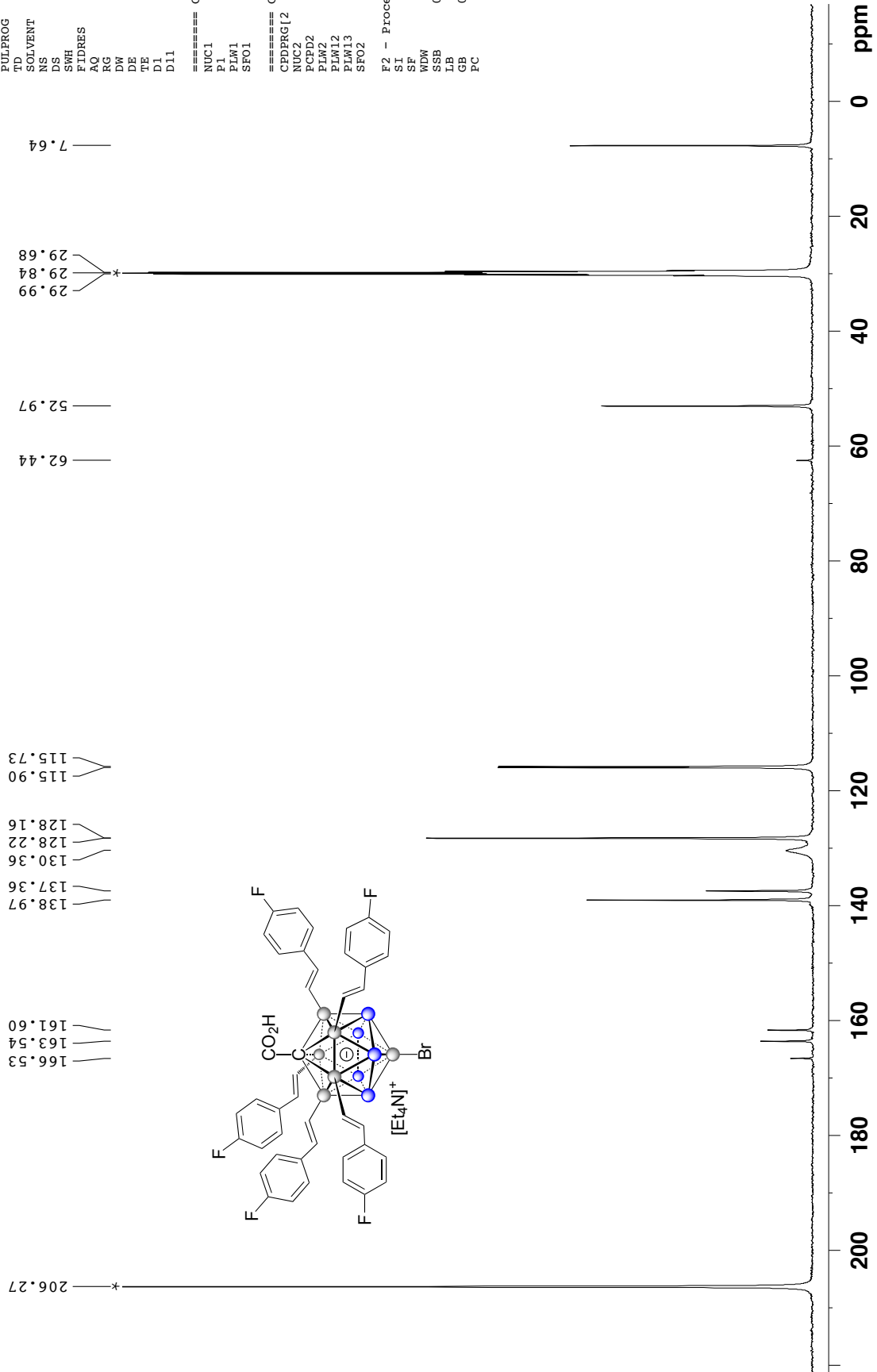
Current Data Parameters
 NAME 12-Br-penta-4-F-styrene
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180508
 Time_ 0.45
 INSTRUM spect
 PROBHD 5 mm FAPBBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 2100
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.5 K
 D1 1.50000000 sec
 D11 0.03000000 sec

=====
 CHANNEL f1
 NUC1 ¹³C
 P1 10.50 usec
 PLW1 95.0000000 W
 SFO1 125.7716224 MHz

=====
 CHANNEL f2
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 19.0000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7576845 MHz
 WDW EM
 SSB 0
 LB 10.00 Hz
 GB 0
 PC 1.40



12-Me-Penta-F-styryne product 50 mg in 0.6 ml acetone-d6 *
¹H{¹H} NMR, 400 MHz, 23 C

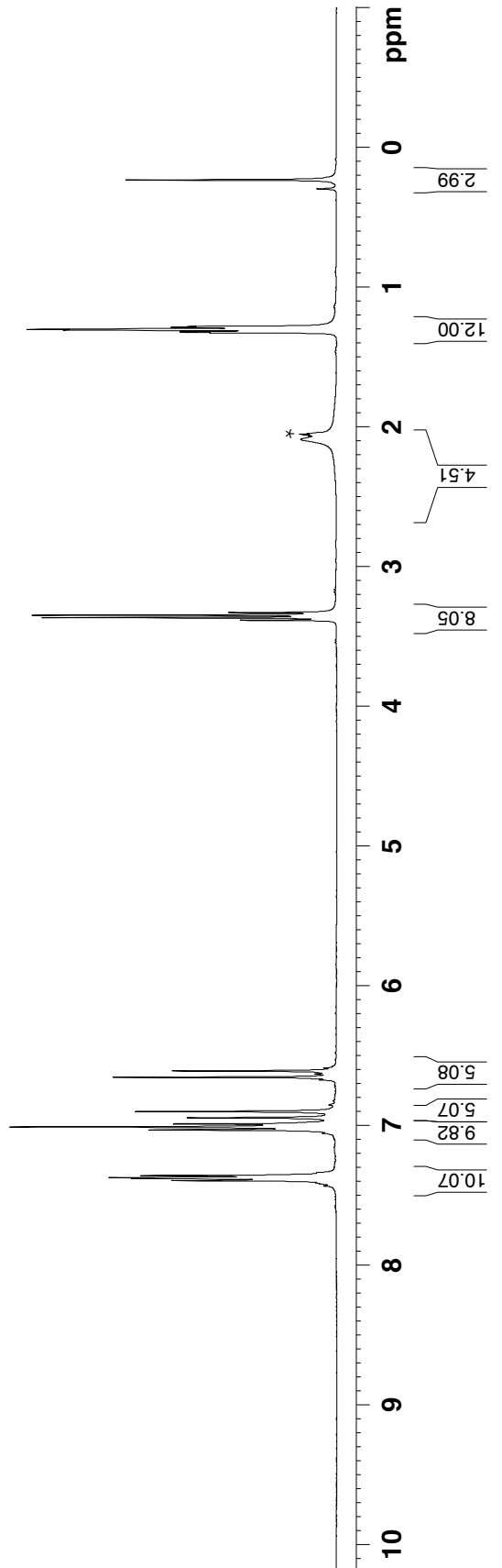
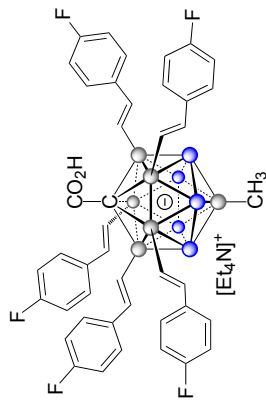
Current Data Parameters
 NAME 12-Me-penta-4-F-styrene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180604
 Time_ 17.03
 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 29.52
 DW 62.400 usec
 DE 6.50 usec
 TE 294.7 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 ¹³C
 P1 11B
 PCPD2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.64477998 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300073 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

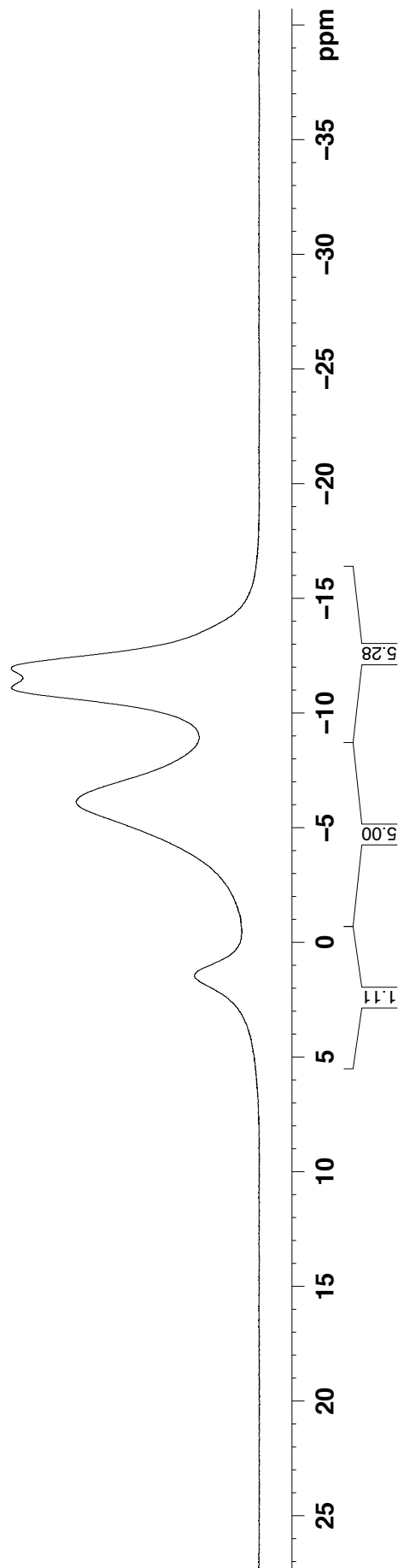
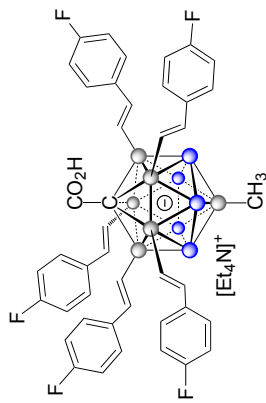
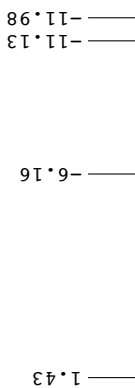


**12-Me-Penta-F-styrine product 50 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME 12-Me-penta-4-F-styrine
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180604
 Time_ 17.09
 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 293.5 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SF01 128.3776052 MHz
 F2 - Processing Parameters
 SI 32768
 SF 128.3776050 MHz
 WDW 0
 SSB 0
 LB 0
 GB 0
 PC 1.40



**12-Me-Penta-F-styryne product 50 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME 12-Me-penta-4-F-styrene
 EXPNO 3
 PROCNO 1

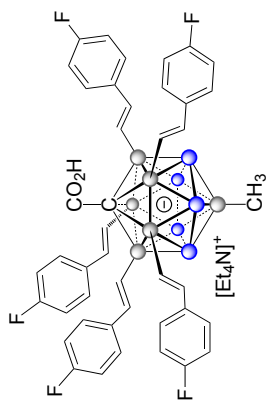
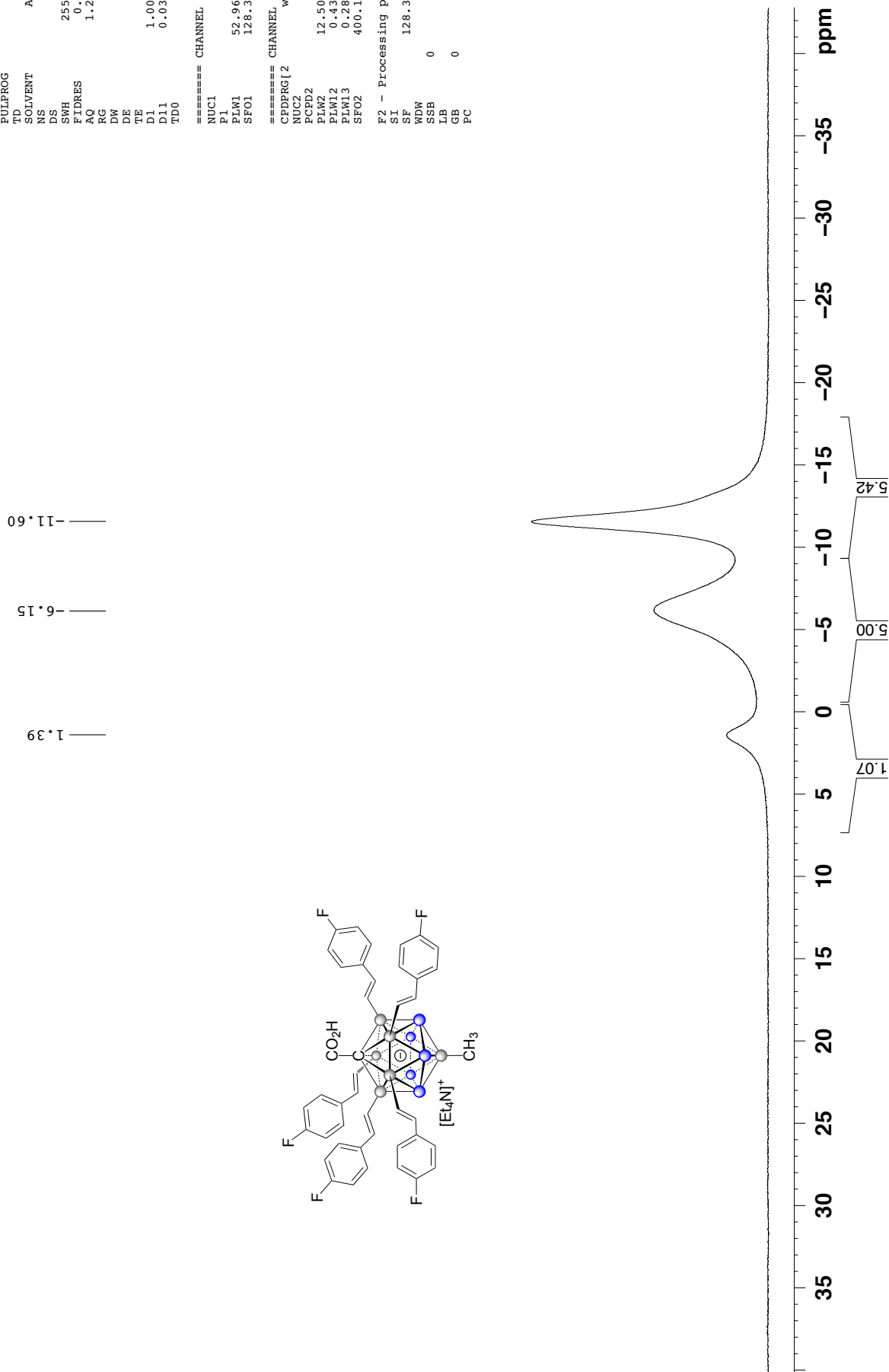
F2 - Acquisition Parameters

Date_ 20180604
 Time_ 17.15
 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 294.6 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 ¹¹B
 P1 9.93 usec
 PLW1 52.9659960 W
 SF01 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
 SF02 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



**12-Me-Penta-F-styryne product 50 mg in 0.6 ml acetone-d6
¹³C{¹H} NMR, 101 MHz, 23 C**

Current Data Parameters
 NAME 12-Me-penta-4-F-styrene
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20180604
 Time_ 18.47
 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
 TDO 1

==== CHANNEL f1 =====

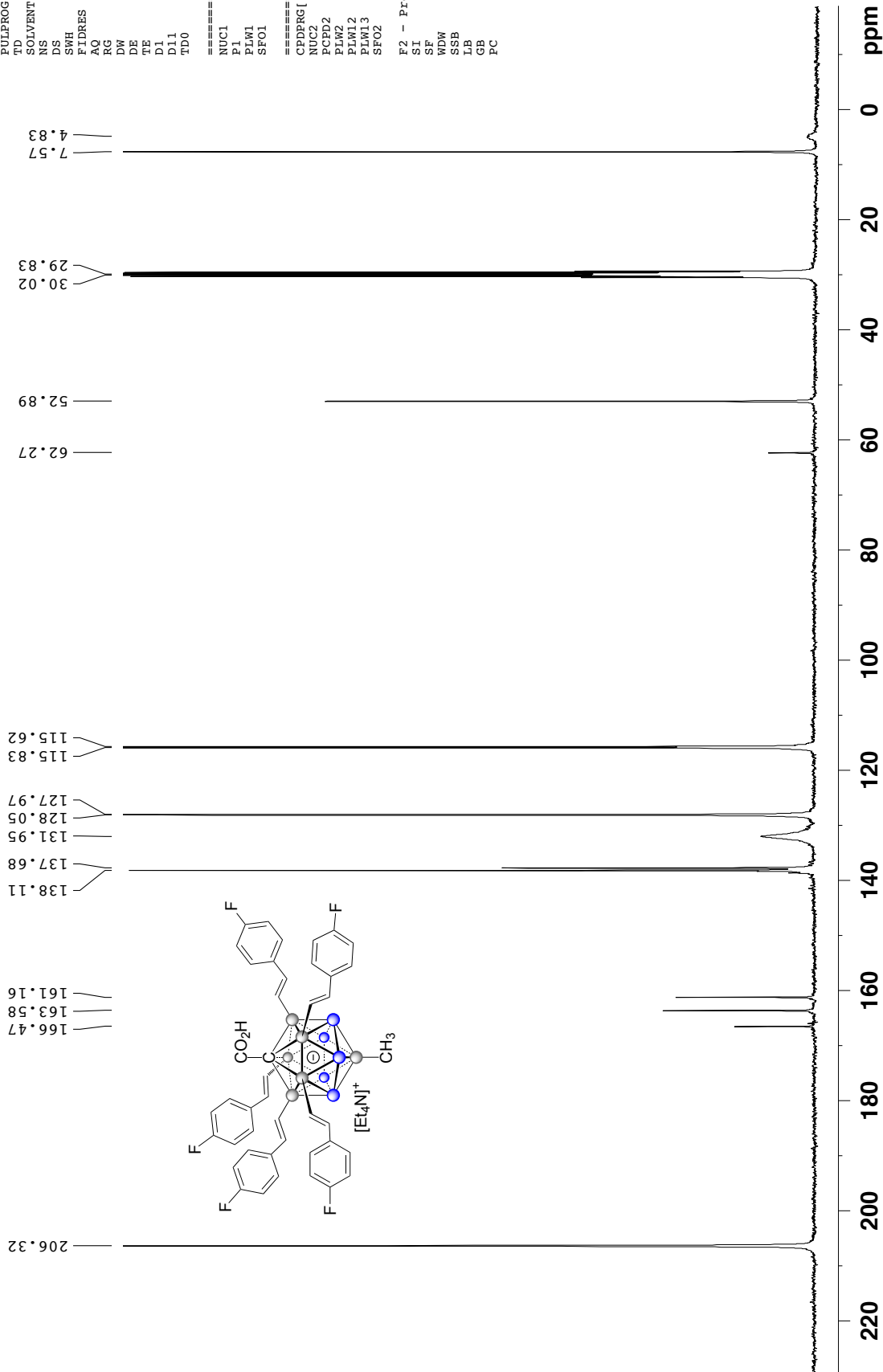
NUC1 13C
 P1 10.00 usec
 PLW1 53.0000000 W
 SF01 100.6228293 MHz

==== CHANNEL f2 =====

CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 12.5000000 W
 PLW12 0.43945000 W
 PLW13 0.28125000 W
 SF02 400.1316005 MHz

F2 - Processing parameters

SI 32768
 SF 100.6126899 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40



12-Ph-Penta-styrene product 50 mg in 0.6 ml acetone-d6*
¹H{¹¹B} NMR, 400 MHz, 23 C

Current Data Parameters
 NAME 12-Ph-penta-styrene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180603
 Time 14.13
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 16384
 SOLVENT acetone
 NS 4
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 53.74
 DW 62.400 usec
 DE 6.50 usec
 TE 293.7 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PL1 12.5000000 W
 SFO1 400.1320007 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 garr4
 NUC2 ¹¹B
 P2 90.00 usec
 PL2 52.9659960 W
 PLW2 0.6447998 W
 SFO2 128.3776050 MHz

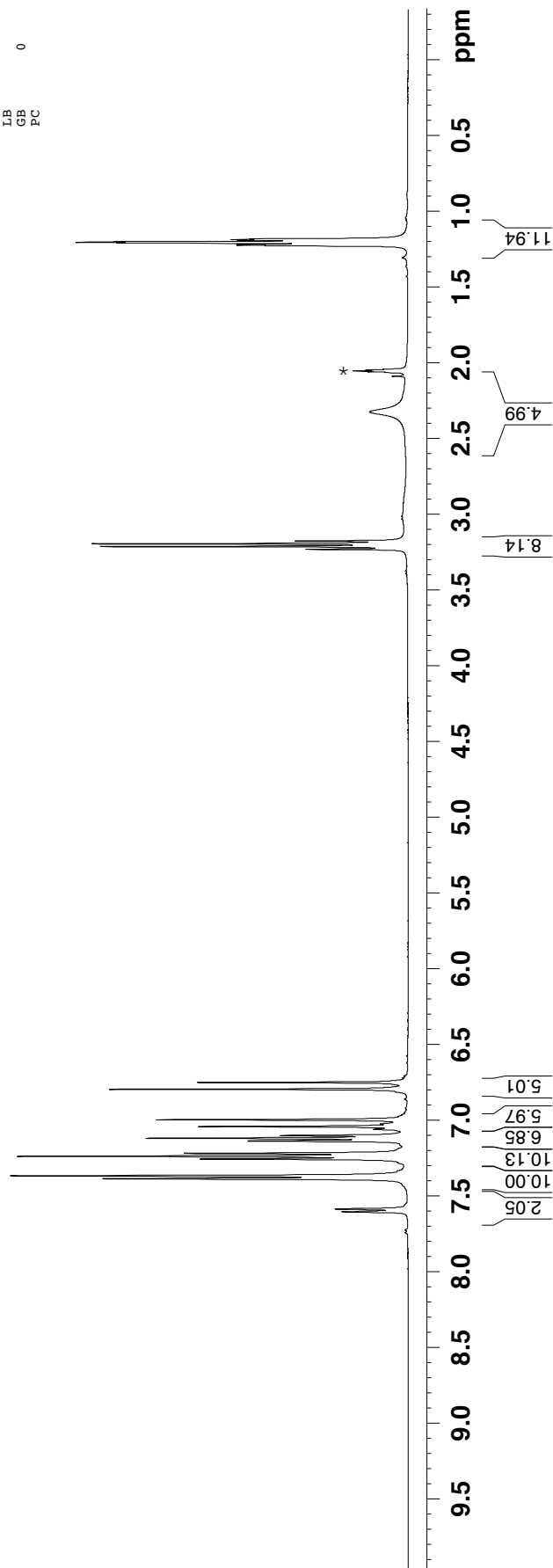
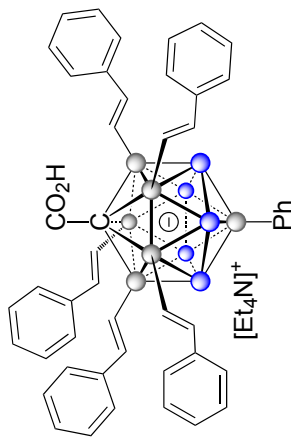
F2 - Processing parameters
 SI 32768
 SF 400.1300072 MHz
 MDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

1.21
1.20
1.20
1.20

2.32
2.06
2.05
2.04

3.21
3.19

7.60
7.58
7.38
7.36
7.25
7.24
7.22
7.14
7.12
7.10
7.04
6.99
6.79
6.75



**12-Ph-Penta-styrene product 50 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

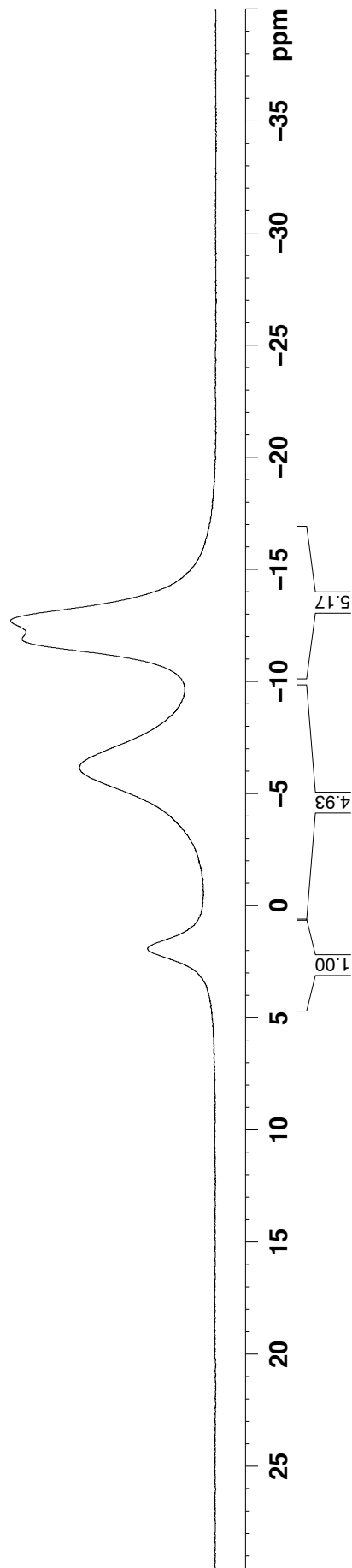
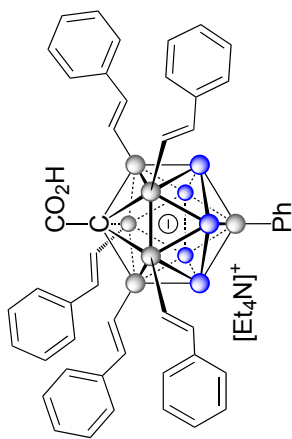
```
Current Data Parameters
NAME      12-Ph-Penta-styrene
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20180605
Time     14.19
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         1.9650 usec
TE         293.6 K
D1         1.00000000 sec
TD0        1
```

```
===== CHANNEL f1 =====
NUC1      11B
P1         9.93 usec
PL1        52.96599660 W
SFO1      128.3776052 MHz

F2 - Processing parameters
SI         32768
SF         128.3776050 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
```

1.91
-6.19
-11.90
-12.74



**12-Ph-Penta-styrene product 50 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 128 MHz, 23 C**

```

Current Data Parameters
NAME      12-Ph-Penta-styrene
EXPNO     3
PROCNO    1

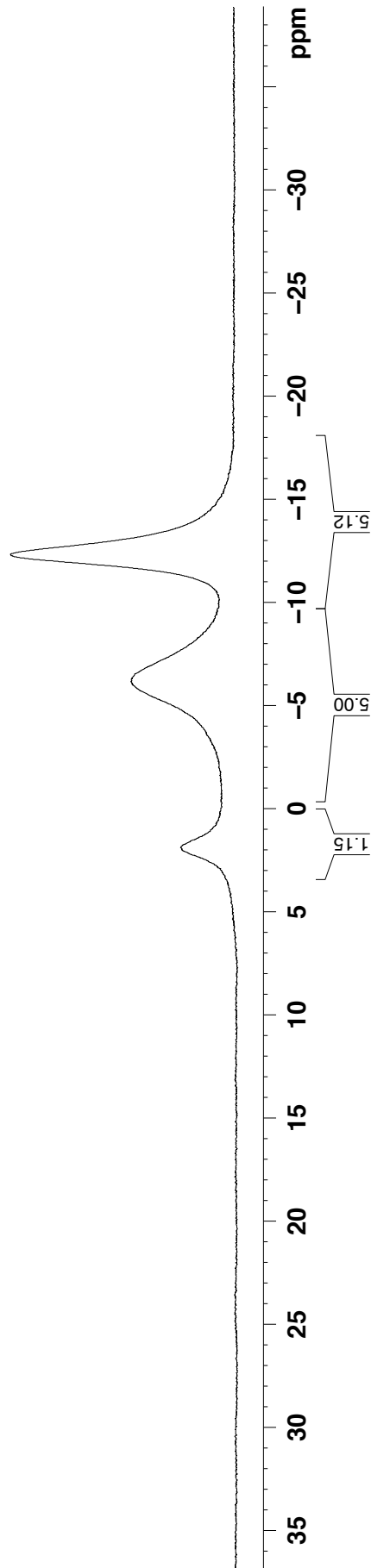
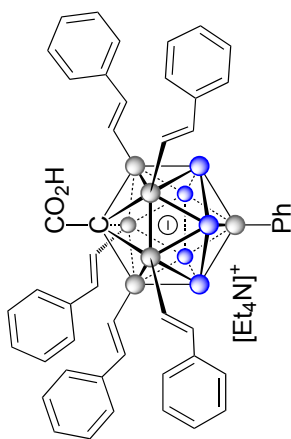
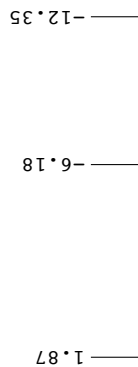
F2 - Acquisition Parameters
Date_     20180605
Time      14.25
INSTRUM   spect
PROBHD    5 mm PABBOBB/
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         124
DS         4
SWH        25510.203 Hz
FIDRES     0.389255 Hz
AQ          1.2845056 sec
RG          193.34
DW          19.600 usec
DE          19.600 usec
TE          294.50 K
D1          1.00000000 sec
D11         0.03000000 sec
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      11B
P1         9.93 usec
PL1        52.9659960 W
SFO1      128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG[2] waitz16
NUC2       1H
PCPD2      80.00 usec
PL2        12.5000000 W
PL12       0.23845000 W
PL13       0.28125000 W
SFO2      400.1320007 MHz

F2 - Processing Parameters
SI         32768
SF         128.3776050 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
  
```



12-Ph-Penta-styrine product 50 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 101 MHz, 23

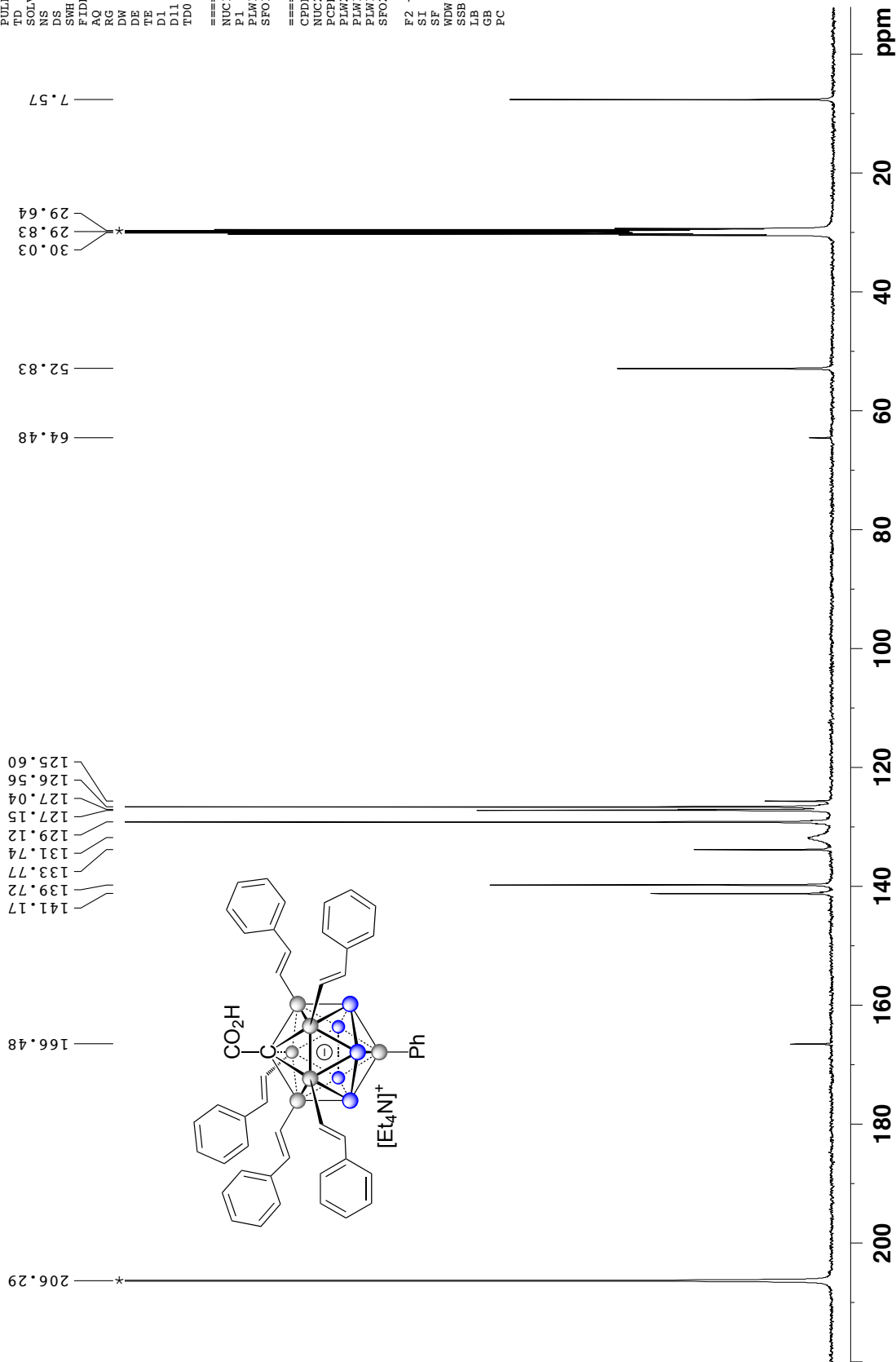
Current Data Parameters
 NAME 12-Ph-penta-styrene
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180603
 Time_ 15.58
 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
 TDO 1

=====
 CHANNEL f1
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 53.0000000 W
 SFO1 100.6228293 MHz

=====
 CHANNEL f2
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 12.5000000 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 5.00 Hz
 GB 0
 PC 1.40



12-Ph-Penta-F-styrene product 50 mg in 0.6 ml acetone-d6*
¹H{¹¹B} NMR, 400 MHz, 23 C

Current Data Parameters
 NAME 12-Ph-penta-4-F-styrene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180610
 Time 5:28

INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 ID 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0723616 sec
 RG 52.99
 DW 62.400 usec
 DE 6.50 usec
 TE 293.7 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TD0 1

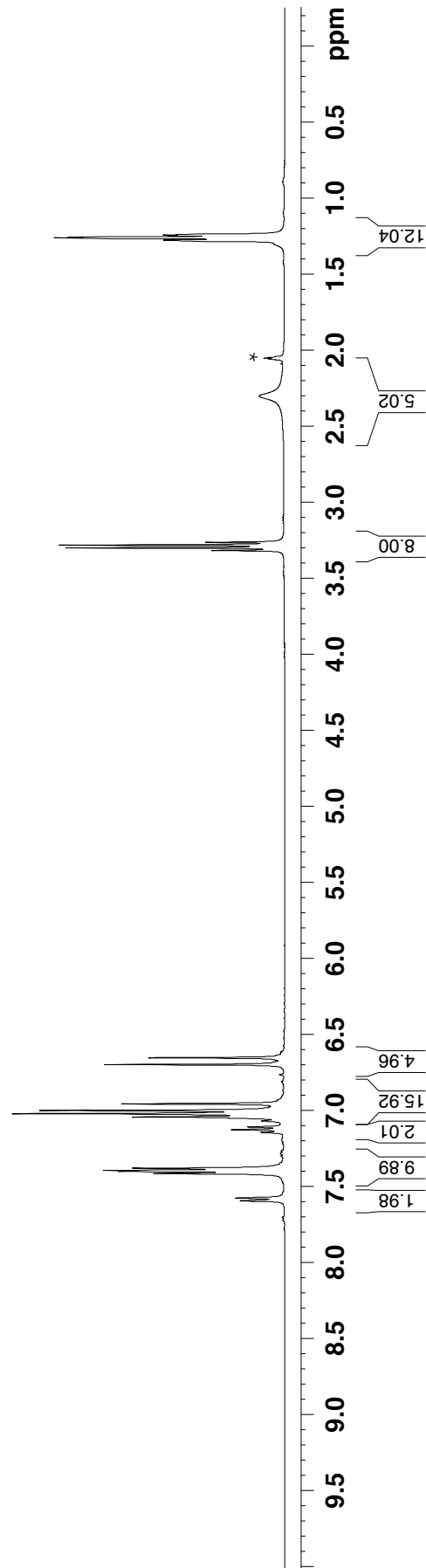
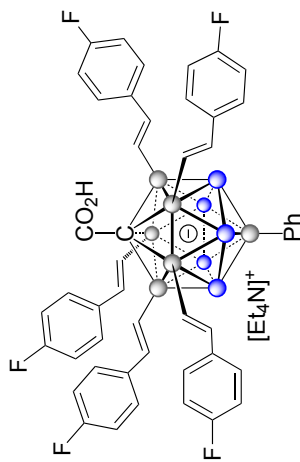
==== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PLW1 12.5000000 W
 SFO1 400.1320007 MHz

==== CHANNEL f2 =====
 CPDPRG[2] garp4
 NUC2 ¹¹B
 P2 90.00 usec
 PLW2 52.9659960 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300071 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

3.26
3.28
3.30
2.04
2.05
2.06
2.30
1.25
1.26
1.26

7.59
7.57
7.41
7.39
7.38
7.14
7.12
7.11
7.04
7.02
7.00
6.95
6.70
6.55



**12-Ph-Penta-F-styrene product 50 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

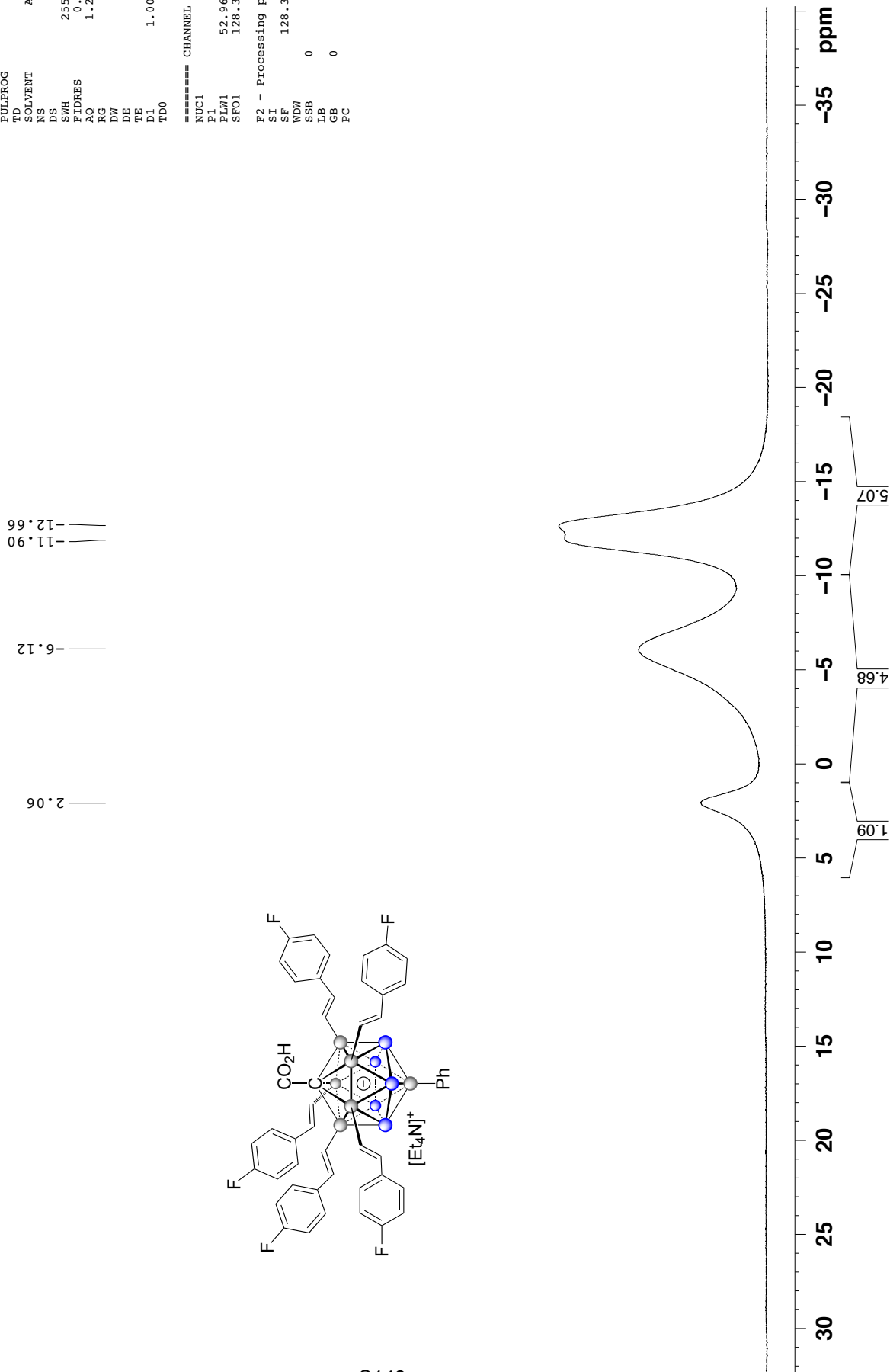
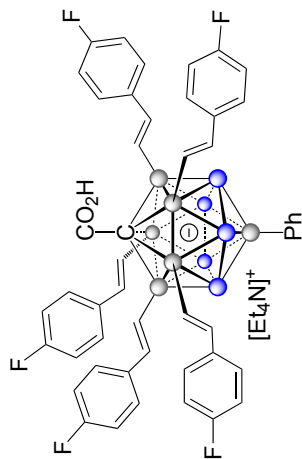
Current Data Parameters
 NAME 12-Ph-penta-4-F-styrene
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180610
 Time 5:34
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FWHZ 0.389255 Hz
 AQ 1.2885056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 293.4 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PL1 52.9650960 W
 SFO1 128.3776052 MHz

F2 - Processing parameters
 S1 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

2.06
 -6.12
 -11.90
 -12.66



**12-Ph-Penta-F-styrene product 50 mg in 0.6 ml acetone-d6
11B{1H} NMR, 128 MHz, 23 C**

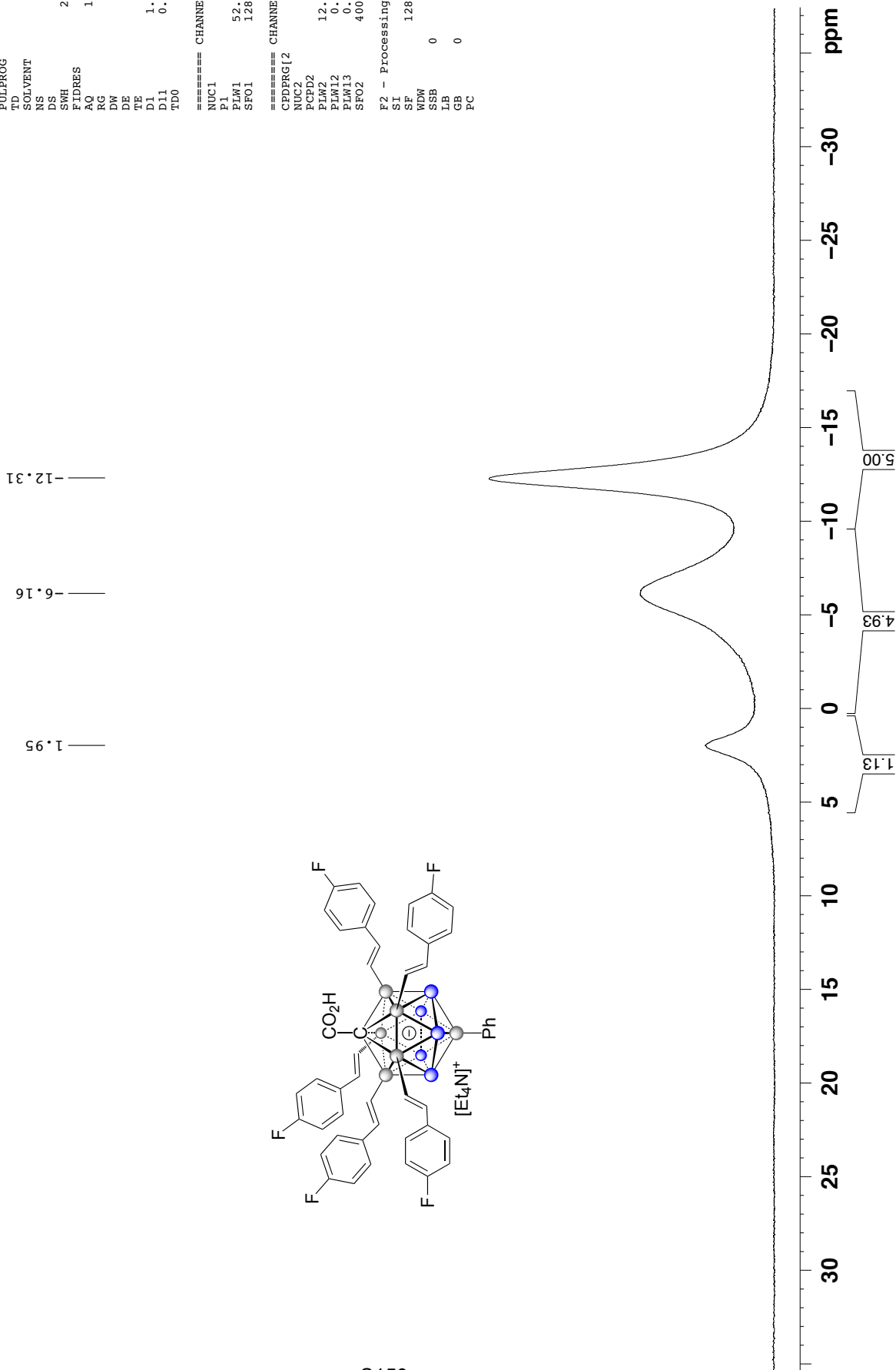
Current Data Parameters
 NAME 12-Ph-penta-4-F-styrene
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180610
 Time 5:40
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG zgpg30
 SOLVENT Acet
 NS 128
 DS 4
 SWH 25510.203 Hz
 FWHZ 0.389255 Hz
 AQ 1.2885056 sec
 RG 193.34
 DW 19.600 usec
 DE 294.6 K
 TE 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PL1 52.9659960 W
 SFO1 128.3776050 MHz

===== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 1H
 PCPD2 80.00 usec
 PLM2 12.50000000 W
 PLM1 0.43945000 W
 PLM3 0.28150000 W
 SFO2 400.1320007 MHz

F2 - Processing parameters
 SZ 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



**12-Ph-Penta-F-styrene product 50 mg in 0.6 ml acetone-d6
13C{1H} NMR, 101 MHz, 23 C**

Current Data Parameters
 NAME 12-Ph-penta-4-F-styrene
 EXPNO 4
 PROCNO 1

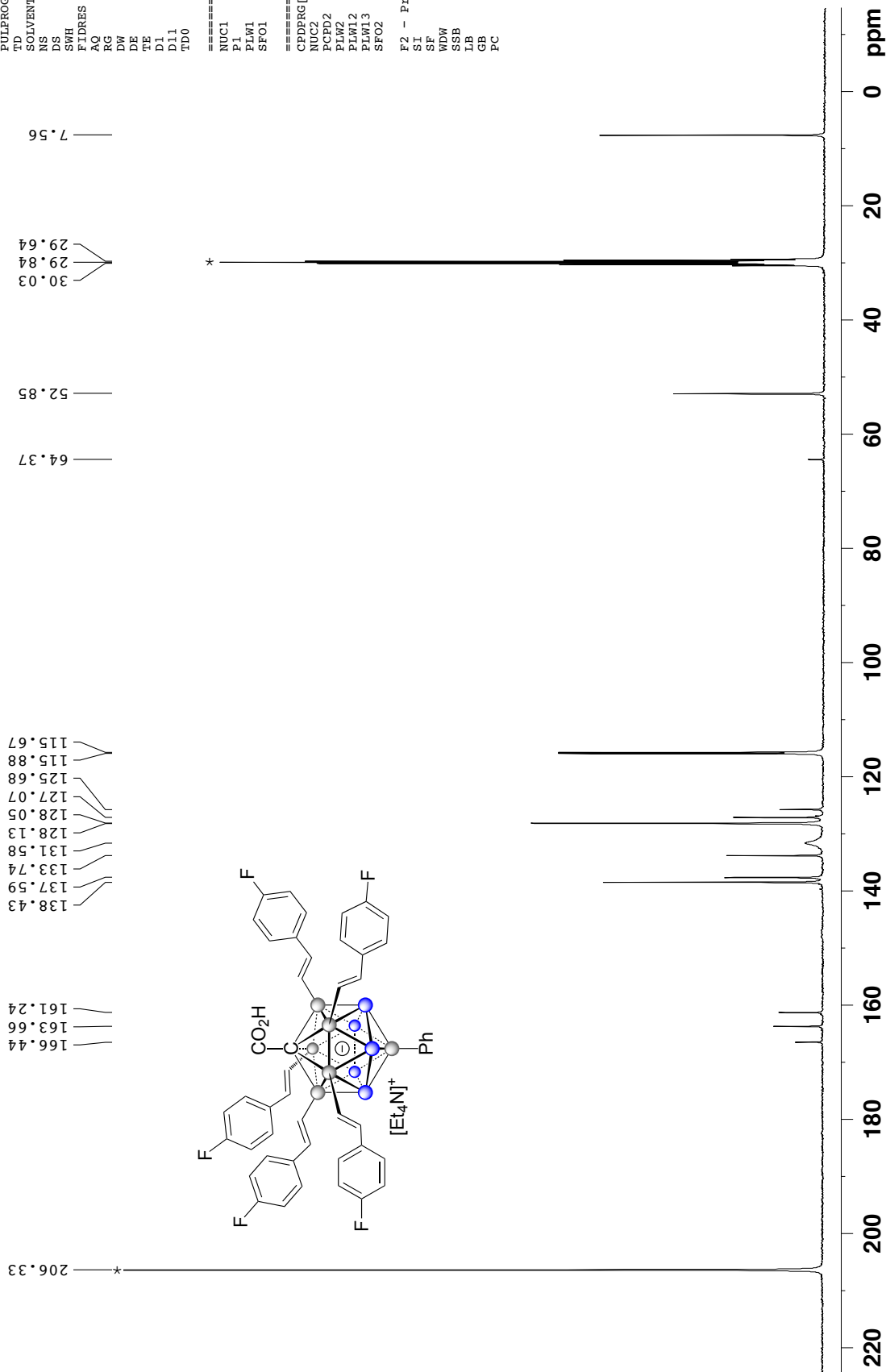
F2 - Acquisition Parameters

Date_ 20180610
 Time_ 7.12
 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 294.1 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PLW1 53.00000000 W
 SF01 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
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126881 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40



12-CN-Penta-F-styrene product 40 mg in 0.6 ml acetone-d6
¹H{¹³C} NMR, 400 MHz, 23 C

Current Data Parameters
 NAME 12-CN-penta-4-F-styrene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20180528
 Time 14.40
 INSTRUM spect
 PROBHD 5 mm PABBO BBO
 PULPROG zgpg30
 D 16384
 SOLVENT acetone
 NS 16
 SH 8012.826 Hz
 FIDRES 0.450064 Hz
 AQ 1.0223616 sec
 RG 78.00
 DE 62.400 usec
 TE 6.79 K
 D1 1.0000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PL1 12.5000000 W
 SFO1 400.1320007 MHz

==== CHANNEL f2 =====
 CPDPRG[2] garr4
 NUC2 ¹³C
 P2 90.10 usec
 PL2 52.96590660 W
 PL12 9.6477998 W
 SFO2 128.3776050 MHz

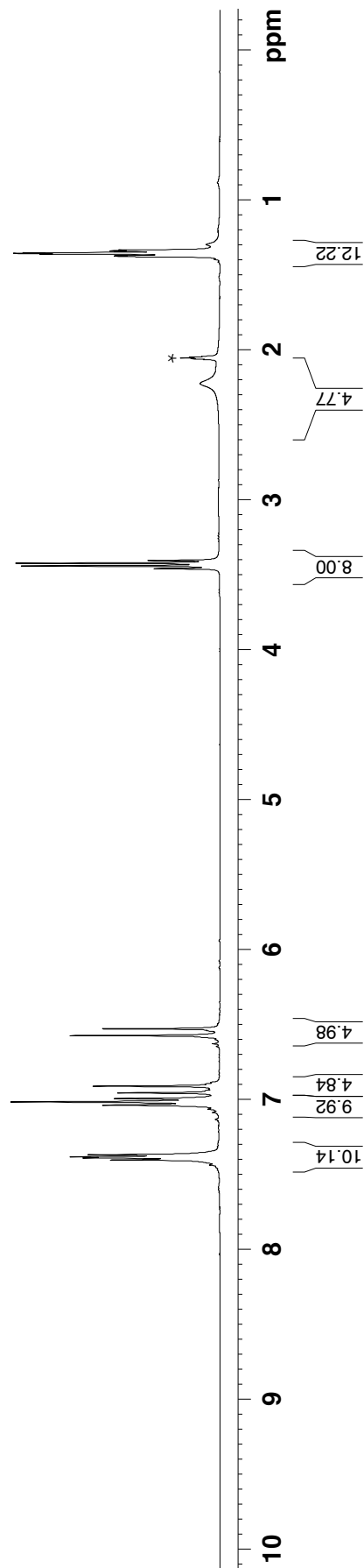
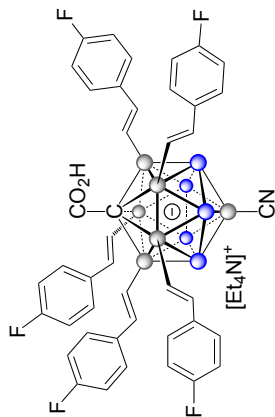
F2 - Processing parameters
 SI 32728
 SF 400.1300072 MHz
 MDW EM
 SSB 0 1.00 Hz
 GB 0 1.40

1.36
1.35
1.35

2.22
2.05
2.04

3.46
3.44
3.42
3.40

7.40
7.39
7.38
7.37
7.04
7.01
6.99
6.95
6.91
6.57
6.53



**12-CN-Penta-F-styrene product 30 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

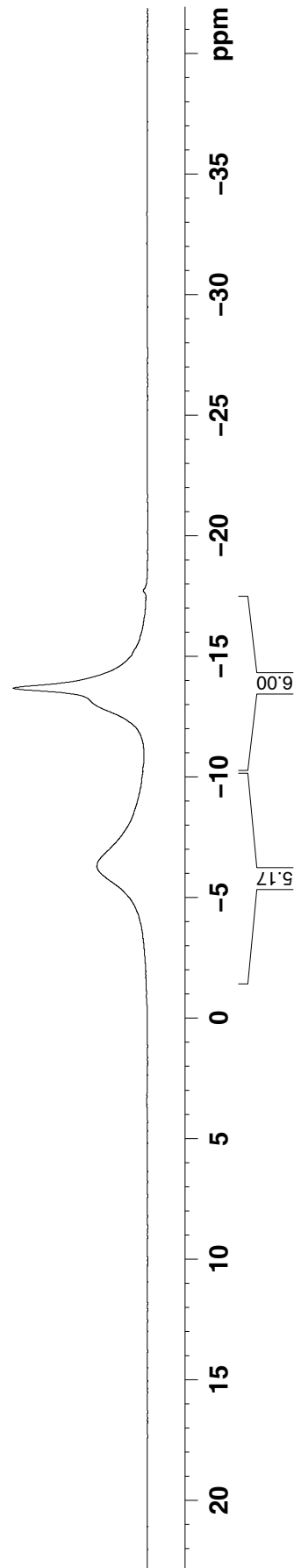
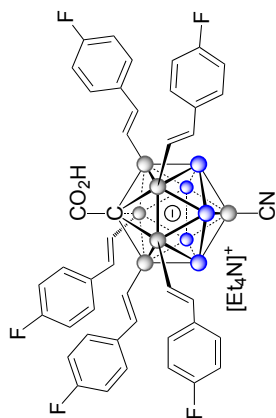
Current Data Parameters
 NAME 12-CN-Penta-F-styrene-new
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181224
 Time 17.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg
 TD 32048
 SOLVENT Acetone
 NS 64
 DS 0
 SWH 32051.281 Hz
 FIDRES 1.000102 Hz
 AC 0.4999488 sec
 RG 203
 DW 15.600 usec
 DE 16.00 usec
 TE 294.9 K
 D1 0.50000000 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
 WTW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

6.32
 12.92
 13.72



**12-CN-Penta-F-styrene product 30 mg in 0.6 ml acetone-d6
11B{1H} NMR, 160 MHz, 23 C**

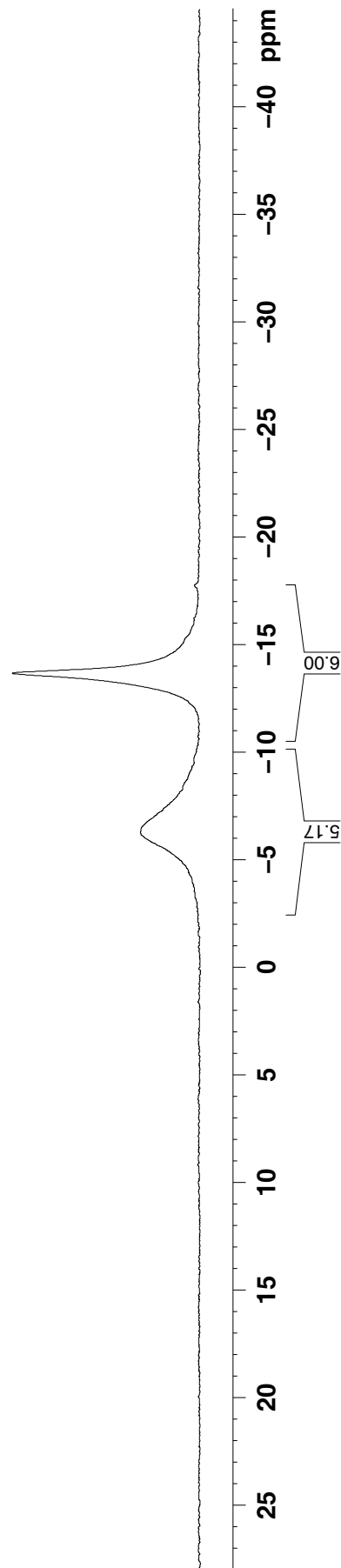
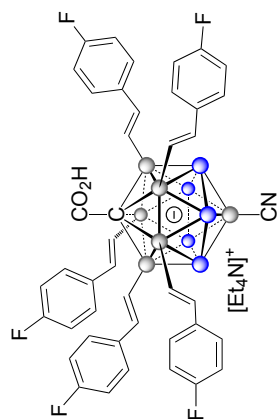
Current Data Parameters
 NAME 12-CN-Penta-F-styrene-new
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181224
 Time 17.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 32048
 SOLVENT Acetone
 NS 64
 DS 0
 SWH 32051.281 Hz
 FIDRES 1.000102 Hz
 AC 0.4999488 sec
 RG 203
 DW 15.600 usec
 DE 6.50 usec
 TE 295.3 K
 D1 0.50000000 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] waitz16
 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
 WDM EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

13.69
 6.31



12-CN-Penta-F-styrene product 40 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 101 MHz, 23 C

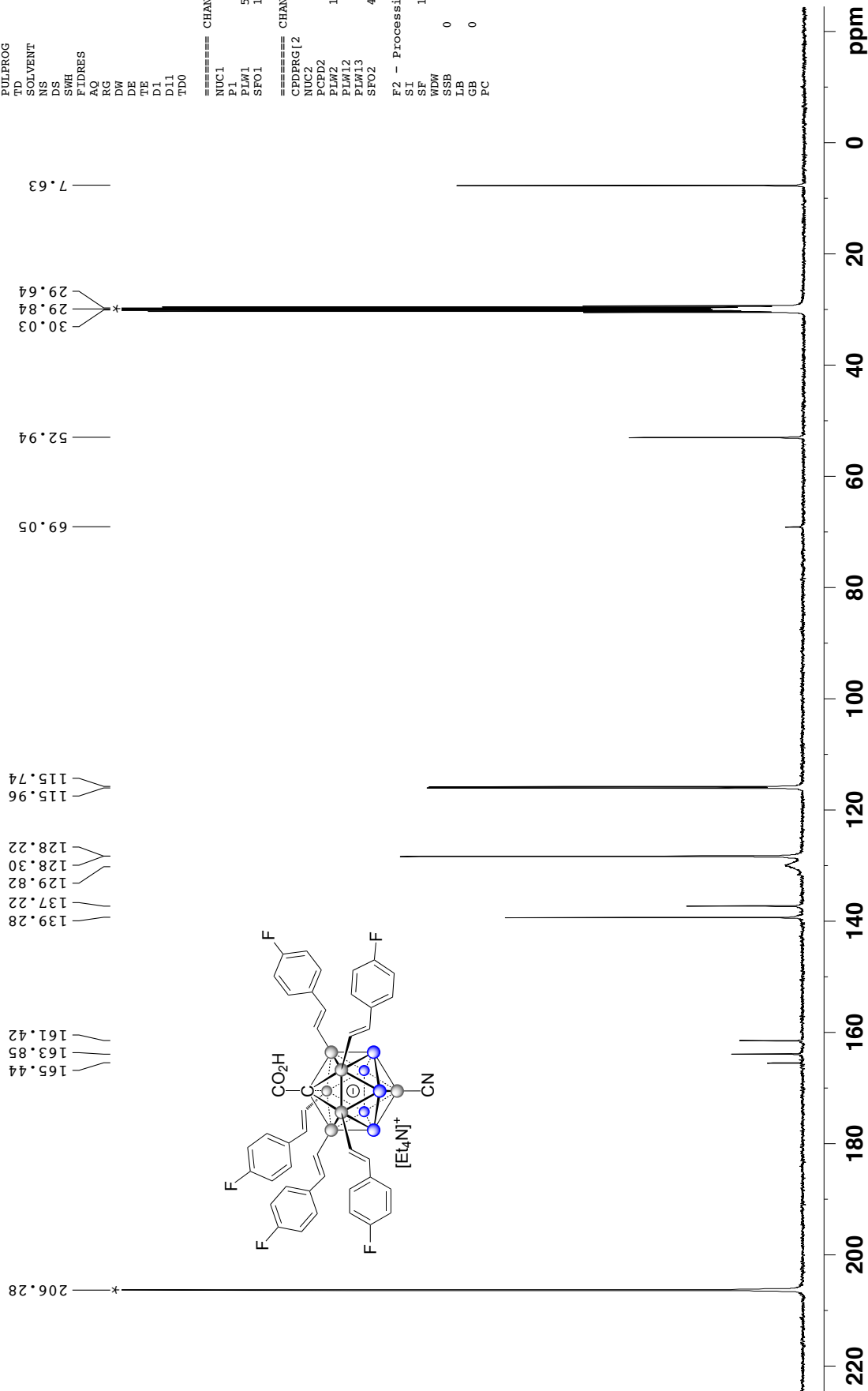
Current Data Parameters
 NAME 12-CN-penta-4-F-styrene
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180528
 Time_ 16.25
 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 294.2 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PLW1 53.0000000 W
 SFO1 100.6228293 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 12.5000000 W
 PLW12 0.43945000 W
 PLW13 0.28125000 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126846 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40



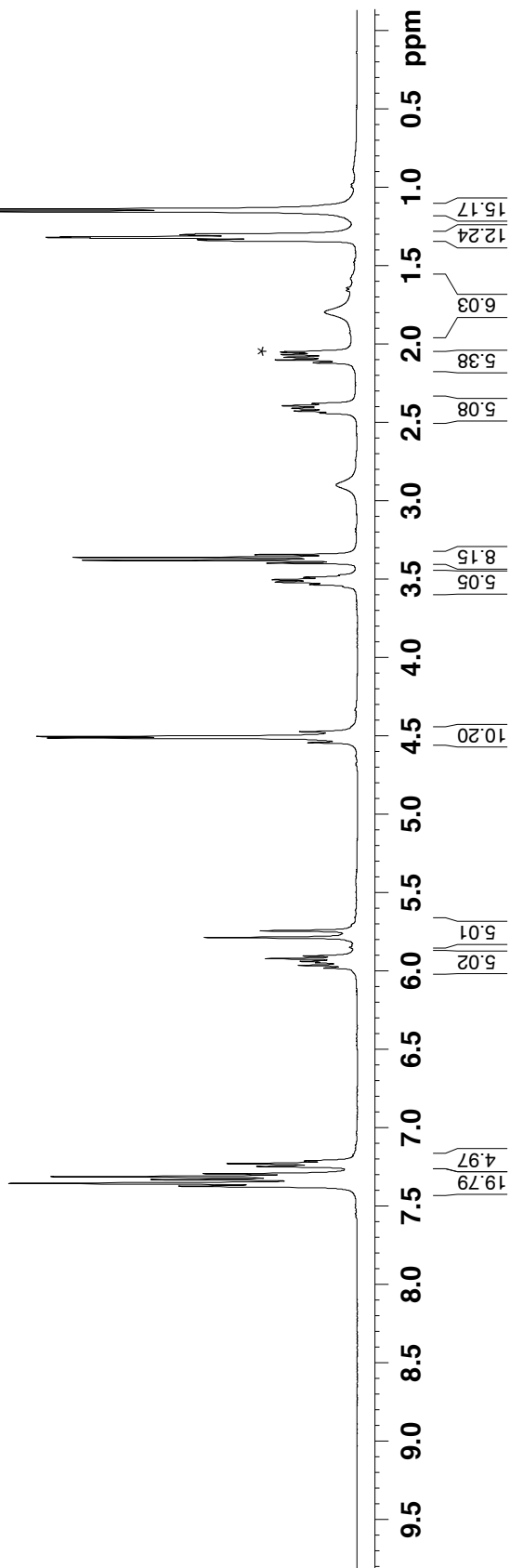
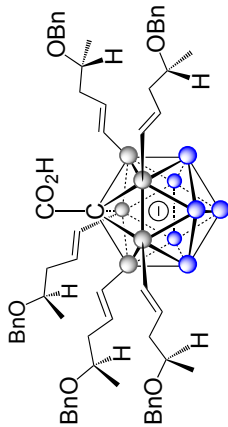
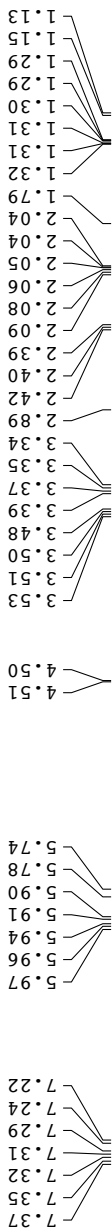
Penta-R-ether product 60 mg in 0.6 ml acetone-d6*
¹H{¹B} NMR, 400 MHz, 23 C

Current Data Parameters
 NAME penta-R-penten-ol
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20180628
 Time 15.53
 INSTRUM spect
 PROBHD 5 mm FAPBBO BB/
 PULPROG zgpg30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 29.52
 DW 62.400 usec
 DE 6.50 usec
 TE 413.7 K
 D1 1.0000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PLW1 12.5000000 W
 SFO1 400.1320007 MHz

==== CHANNEL f2 =====
 CPDPRG[2] garp4
 NUC2 11B
 P2 90.00 usec
 PLW2 52.9659960 W
 PLW12 0.64477998 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300071 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40



**Penta-R-ether product 60 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

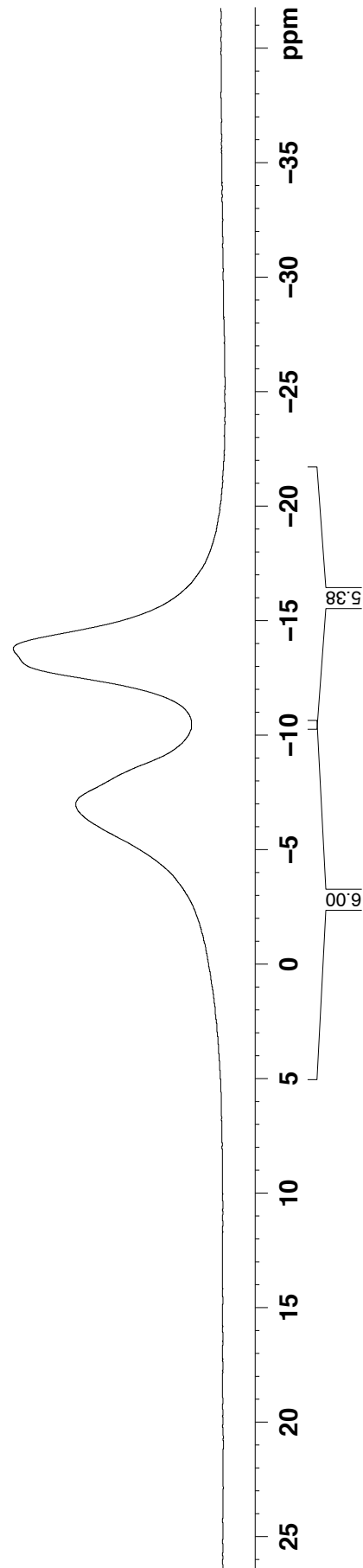
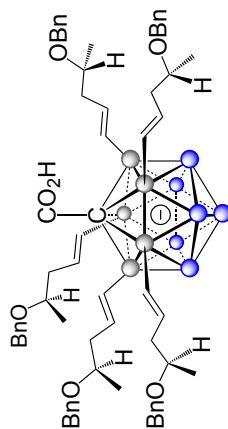
Current Data Parameters
 NAME penta-R-penten-ol
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180628
 Time 15.58
 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 416.6 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SF01 128.3776052 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3776050 MHz
 EM
 WDW 0
 SSB 0 15.00 Hz
 LB 0
 GB 0
 PC 1.40

13.80
 6.94



**Penta-R-ether product 60 mg in 0.6 ml acetone-d6
11B{1H} NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME penta-R-penten-ol
 EXPNO 3
 PROCNO 1

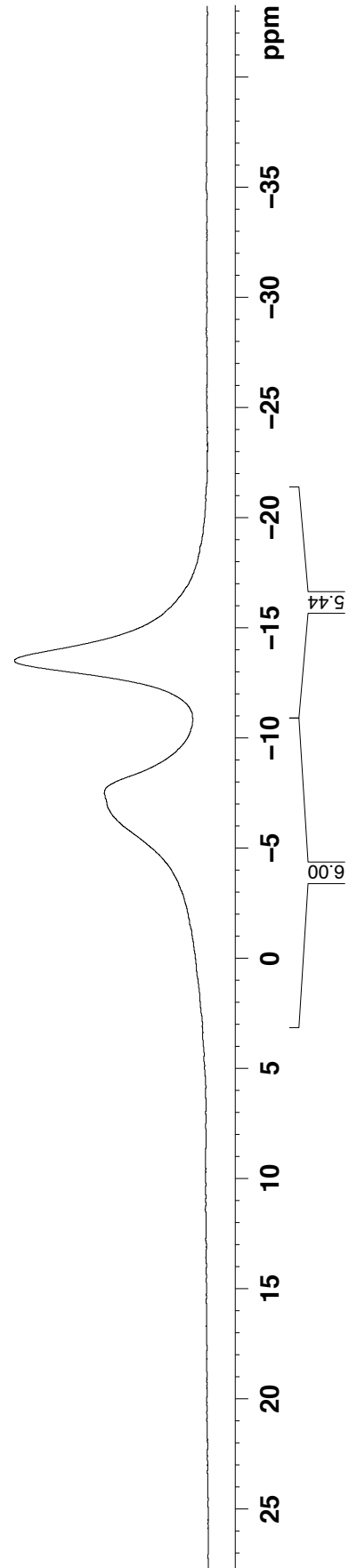
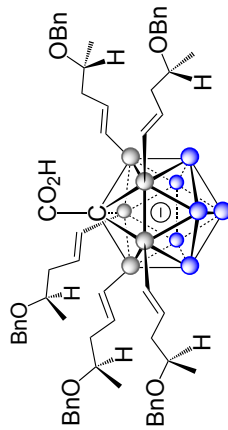
F2 - Acquisition Parameters
 Date_ 20180628
 Time 16.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 417.8 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SF01 128.3776050 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 P2 80.00 usec
 PLW2 12.5000000 W
 PLW12 0.43945000 W
 PLW13 0.28125000 W
 SF02 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3776050 MHz
 EM
 WDW 0
 SSB 0
 LB 15.00 Hz
 GB 0
 PC 1.40

7.52
 13.52



**Penta-R-ether product 60 mg in 0.6 ml acetone-d6*
¹³C{1H} NMR, 101 MHz, 23 C**

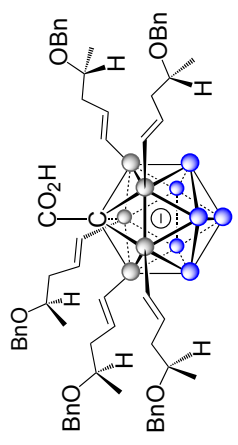
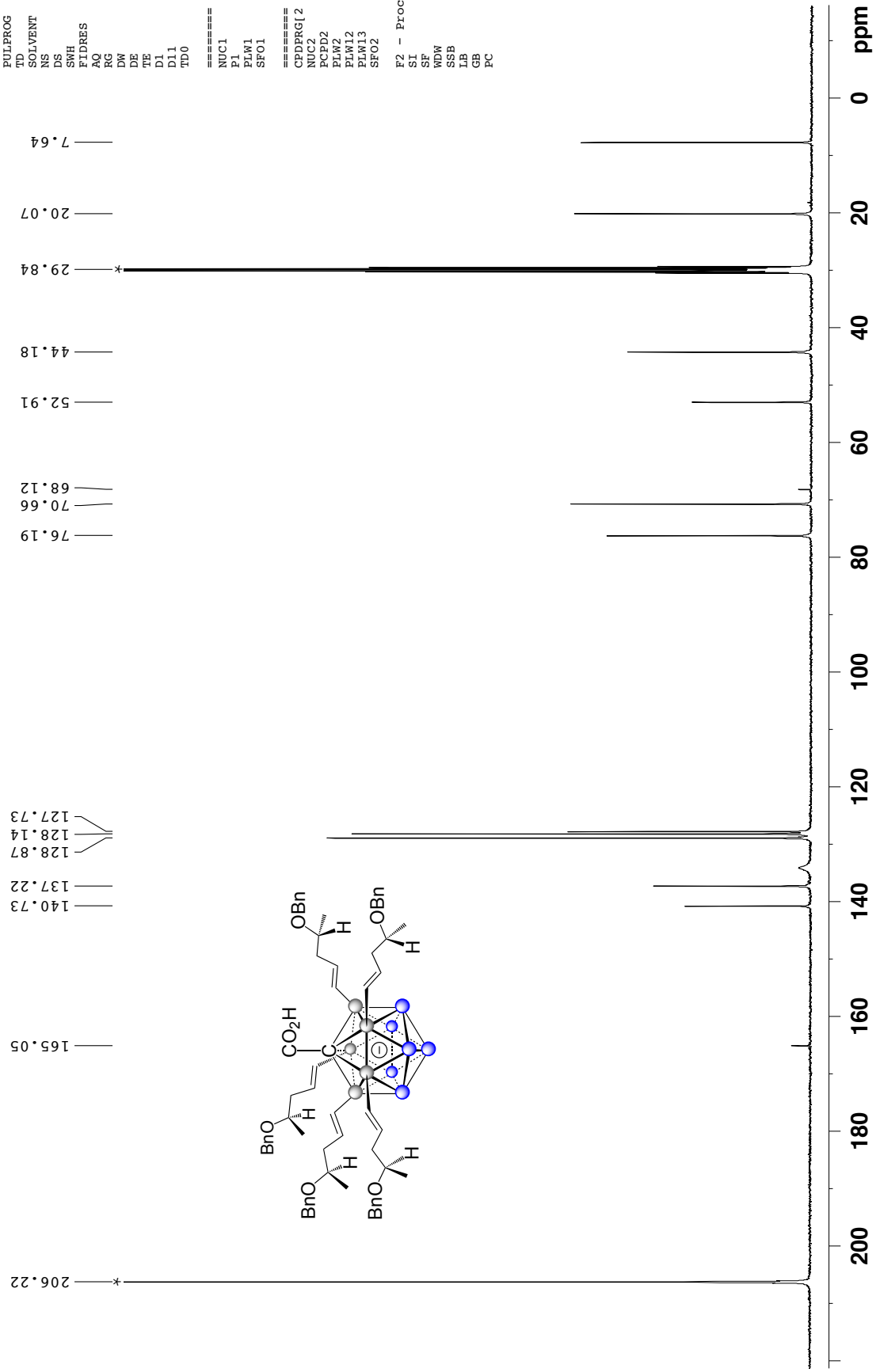
Current Data Parameters
 NAME penta-R-penten-ol
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180628
 Time_ 17.37
 INSTRUM spect
 PROBDH 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
 DM 16.800 usec
 DE 6.50 usec
 TE 416.8 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 53.00000000 W
 SF01 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
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126883 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40



Penta-S-penten-ol product 40 mg in 0.6 ml acetone-d6 *
¹H{¹¹B} NMR, 500 MHz, 23 C

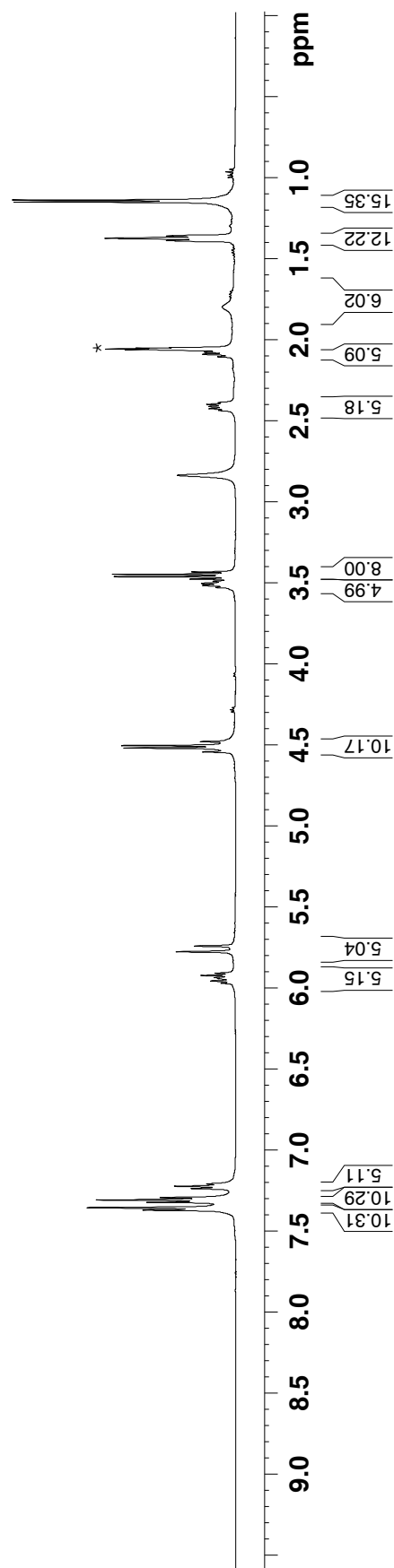
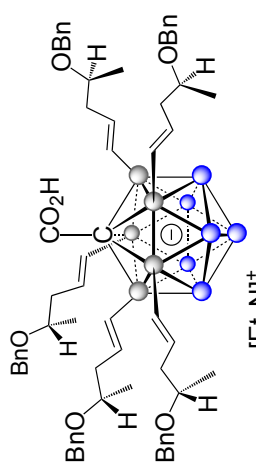
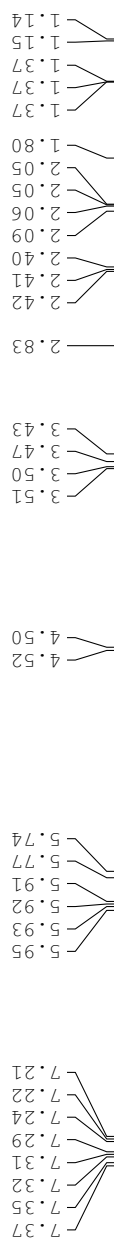
Current Data Parameters
 NAME penta-S-penten-ol
 EXFNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180624
 Time 2.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 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 296.5 K
 D1 5.0000000 sec
 D1.1 0.0300000 sec
 TDO 1

=====
 CHANNEL f1
 SF01 500.1335009 MHz
 NUC1 ¹H
 P1 11.70 usec
 PLW1 19.0000000 W

=====
 CHANNEL f2
 SF02 160.4615690 MHz
 NUC2 ¹¹B
 CPDPRG[2] garp
 PCPD2 100.00 usec
 PLW2 95.0000000 W
 PLW1.2 1.63030005 W

F2 - Processing parameters
 SI 65536
 SF 500.1300065 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.00



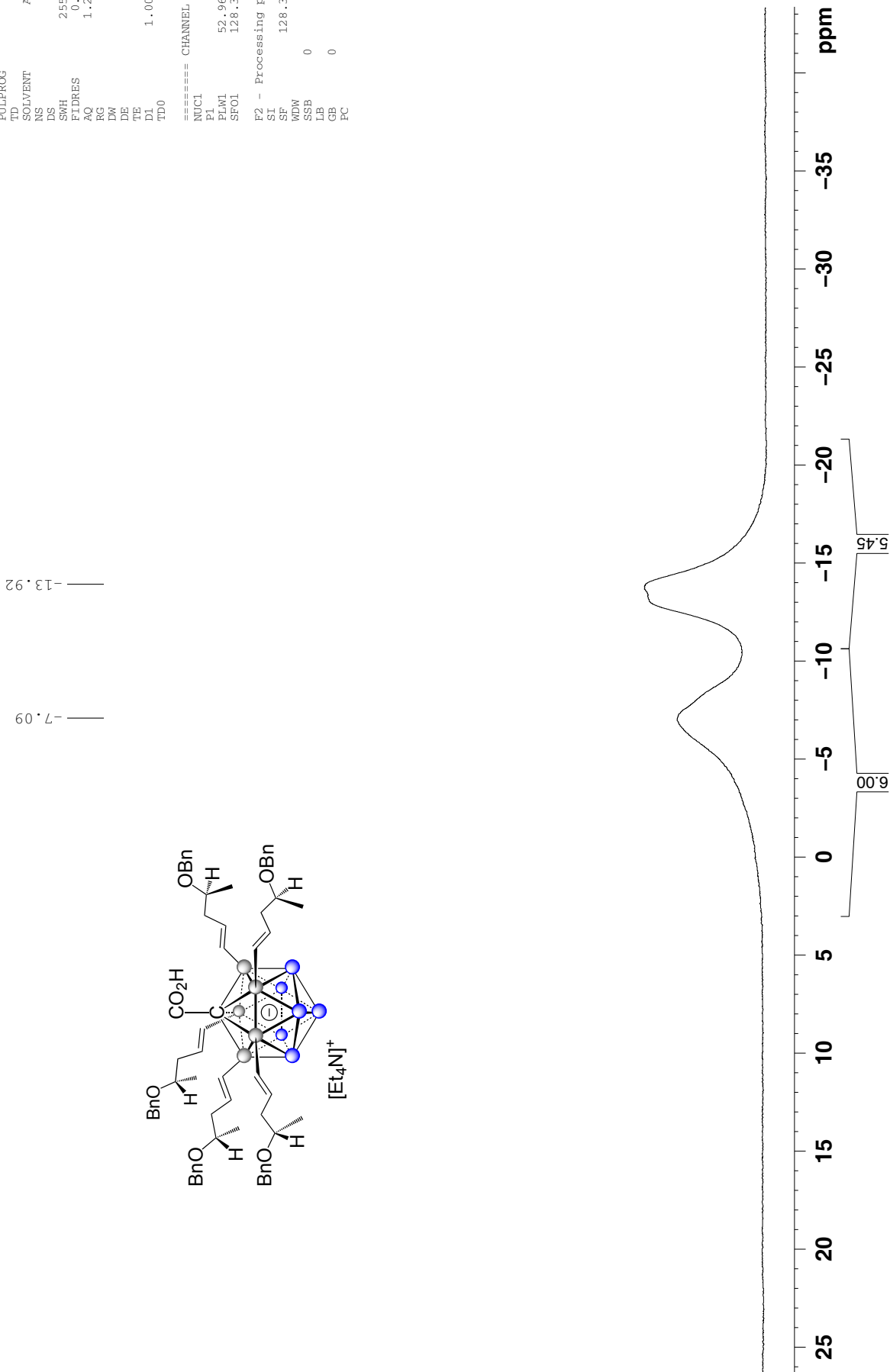
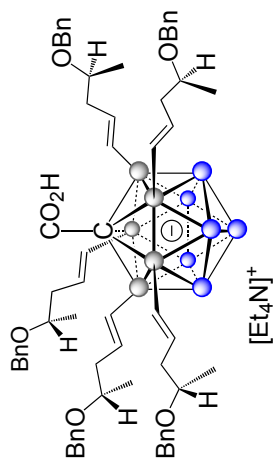
**Penta-S-penten-ol product 40 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME penta-S-penten-ol
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180731
 Time 3.45
 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 295.2 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SF01 128.3776052 MHz
 F2 - Processing Parameters
 SI 32768
 SF 128.3776050 MHz
 WDW 0
 SSB EM
 LB 0
 GB 0
 PC 5.00 Hz
 1.40

13.92
 7.09



**Penta-S-penten-ol product 40 mg in 0.6 ml acetone-d6
 11B{1H} NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME penta-S-penten-ol
 EXPNO 4
 PROCNO 1

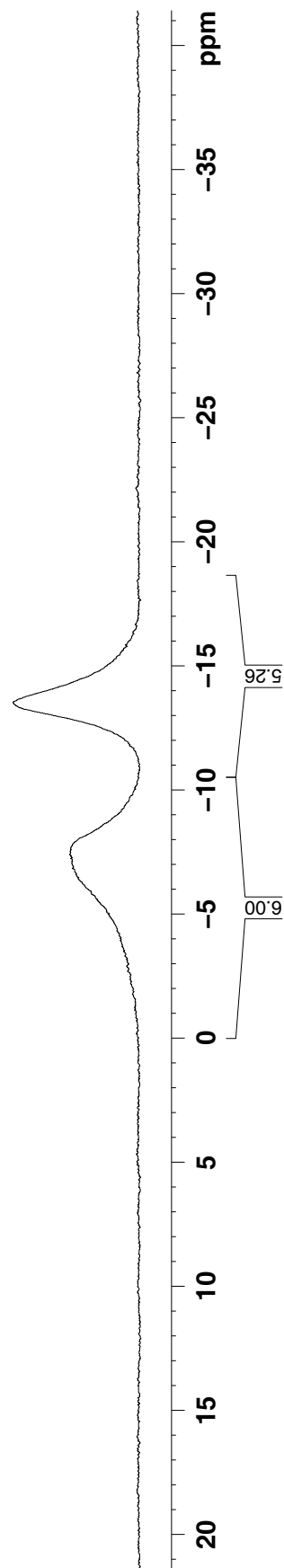
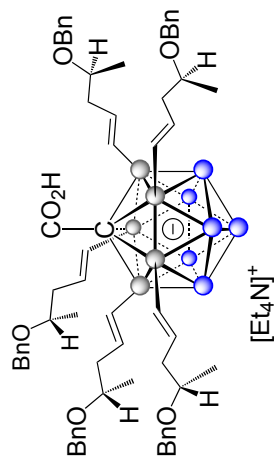
F2 - Acquisition Parameters
 Date_ 20180731
 Time 3.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 6536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 295.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

=====
 CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.96599960 W
 SF01 128.3776050 MHz

=====
 CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 12.50000000 W
 PLW12 0.43945000 W
 PLW13 0.28125000 W
 SF02 400.1320007 MHz

F2 - Processing Parameters
 SI 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

— 13.54
 — 7.42



Penta-S-penten-ol product 40 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 126 MHz, 23 C

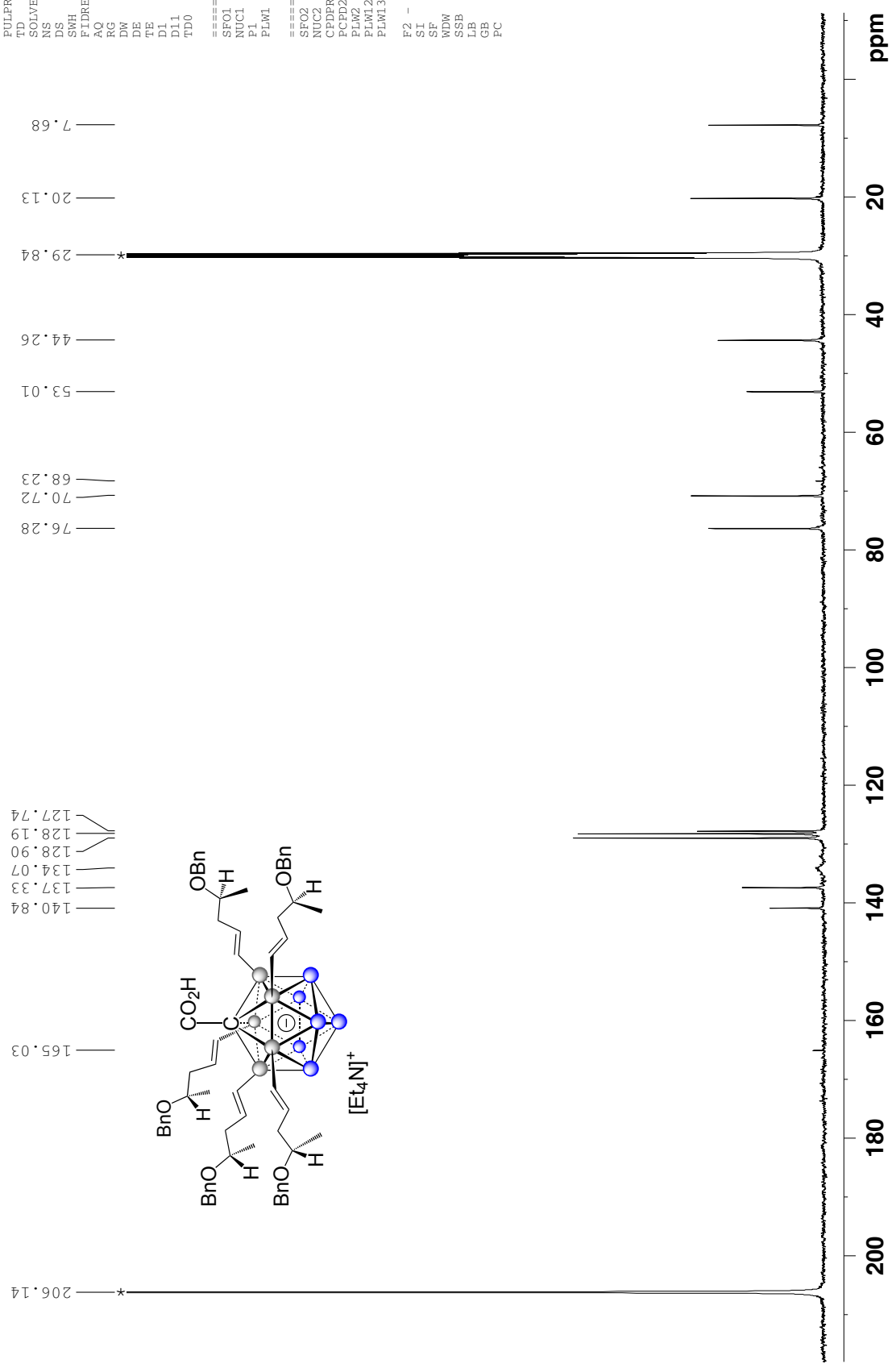
Current Data Parameters
 NAME penta-S-penten-ol
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180824
 Time 4.38
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 3100
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQAQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.5 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 95.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 waltz16
 CPDPRG[2]
 PCPD2 80.00 usec
 PLW2 19.00000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W

F2 - Processing parameters
 SI 32768
 SF 125.7576776 MHz
 MDW EM
 SSB 0
 LB 0
 GB 0
 PC 5.00 Hz
 1.40



**Penta-F-styrene-de product, 40 mg in 0.6 ml acetone-d₆*
¹H{¹¹B} NMR, 400 MHz, 23 C**

Current Data Parameters
 NAME penta-4-F-styrene-de
 EXPNO 1
 PROCNO 1

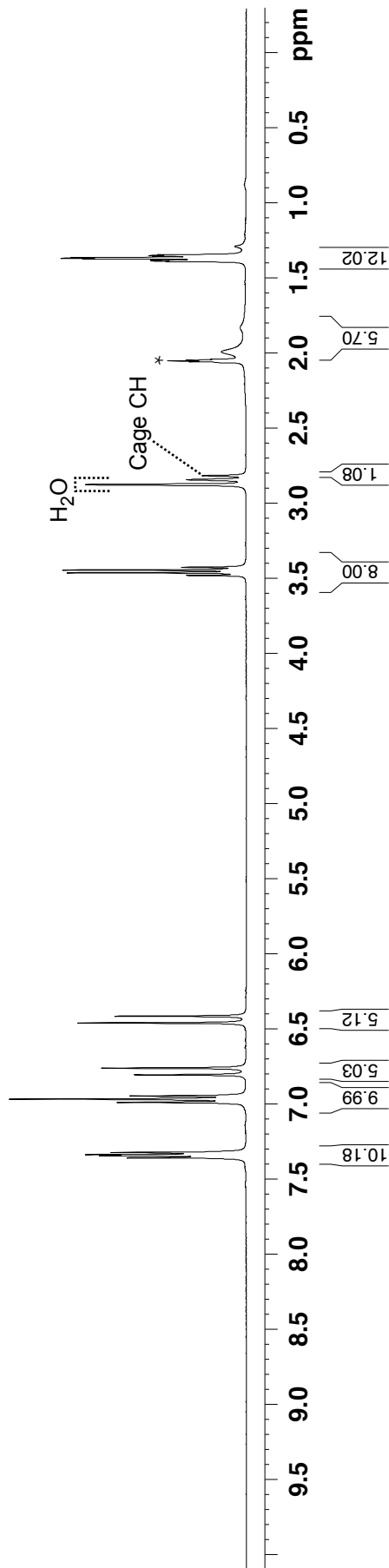
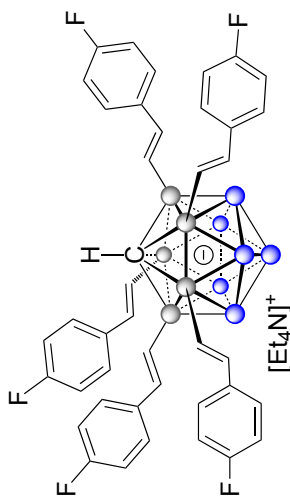
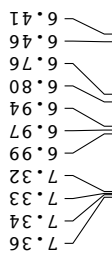
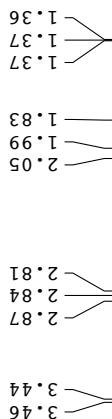
F2 - Acquisition Parameters
 Date_ 20180601
 Time 18.03

INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 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 294.3 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PLW1 12.5000000 W
 SFO1 400.1320007 MHz

==== CHANNEL f2 =====
 CPDPRG[2] garp4
 NUC2 ¹¹B
 P2 90.00 usec
 PLW2 52.9659960 W
 PLW12 0.64477998 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300072 MHz
 EM
 WDW 0
 SSB 0 1.00 Hz
 LB 0
 GB 0
 PC 1.40



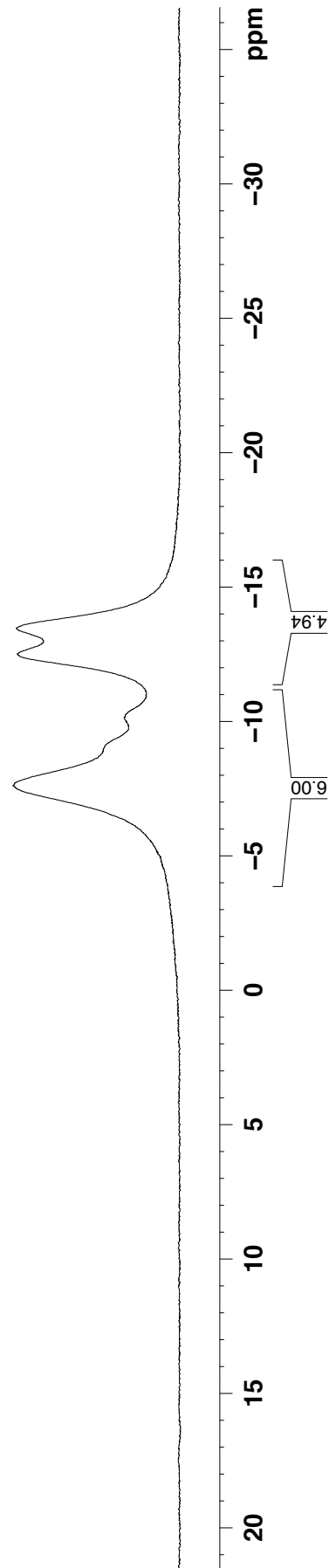
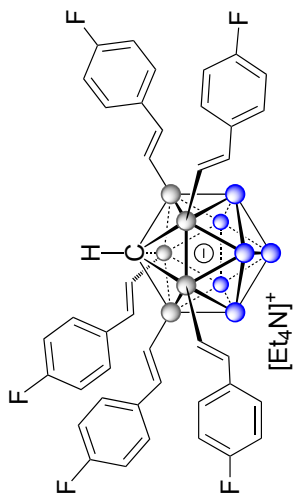
**Penta-F-styrene-de product, 40 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME penta-4-F-styrene-de
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180601
 Time_ 18.08
 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 52.9659960 W
 SFO1 128.3776052 MHz
 F2 - Processing parameters
 SI 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

7.63
9.09
10.12
12.52
13.48



**Penta-F-styrene-de product, 40 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME Penta-4-F-styrene-de
 EXNO 3
 PROCNO 1

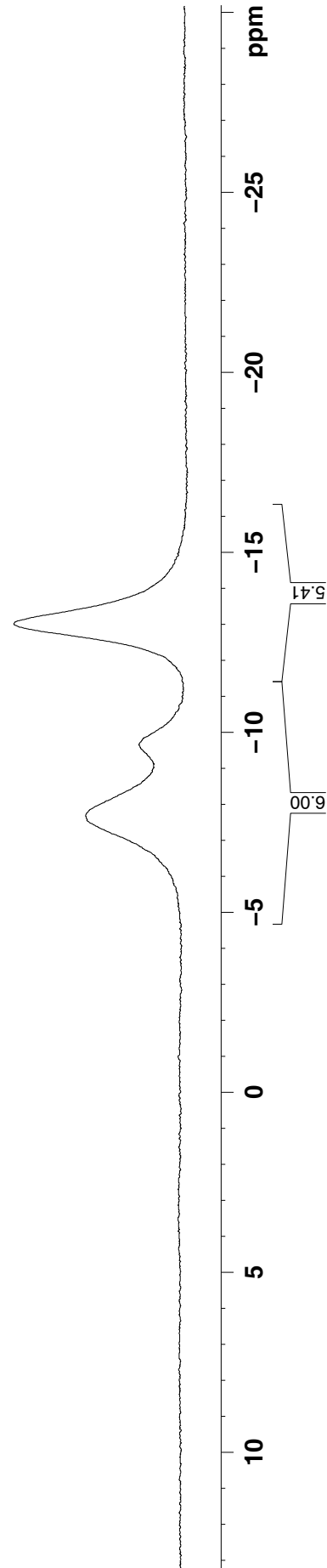
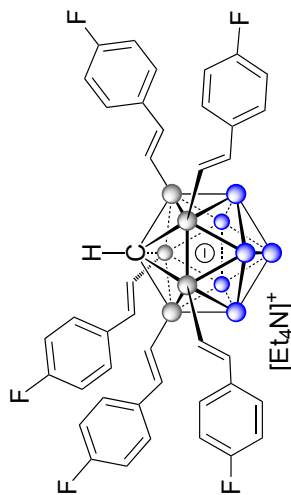
F2 - Acquisition Parameters
 Date_ 20180601
 Time 18.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 124
 DS 2
 SWH 25510.204 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845052 sec
 RG 193.34
 DW 19.600 usec
 DE 6.550 usec
 TE 295.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 ¹¹B
 P1 9.93 usec
 PLM1 52.9659960 W
 SF01 128.3776050 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waitz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLM2 12.5000000 W
 PLM12 0.43945000 W
 PLM13 0.28125000 W
 SF02 400.13200007 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 4.00 Hz
 GB 0
 PC 1.40

13.03
 9.67
 7.70

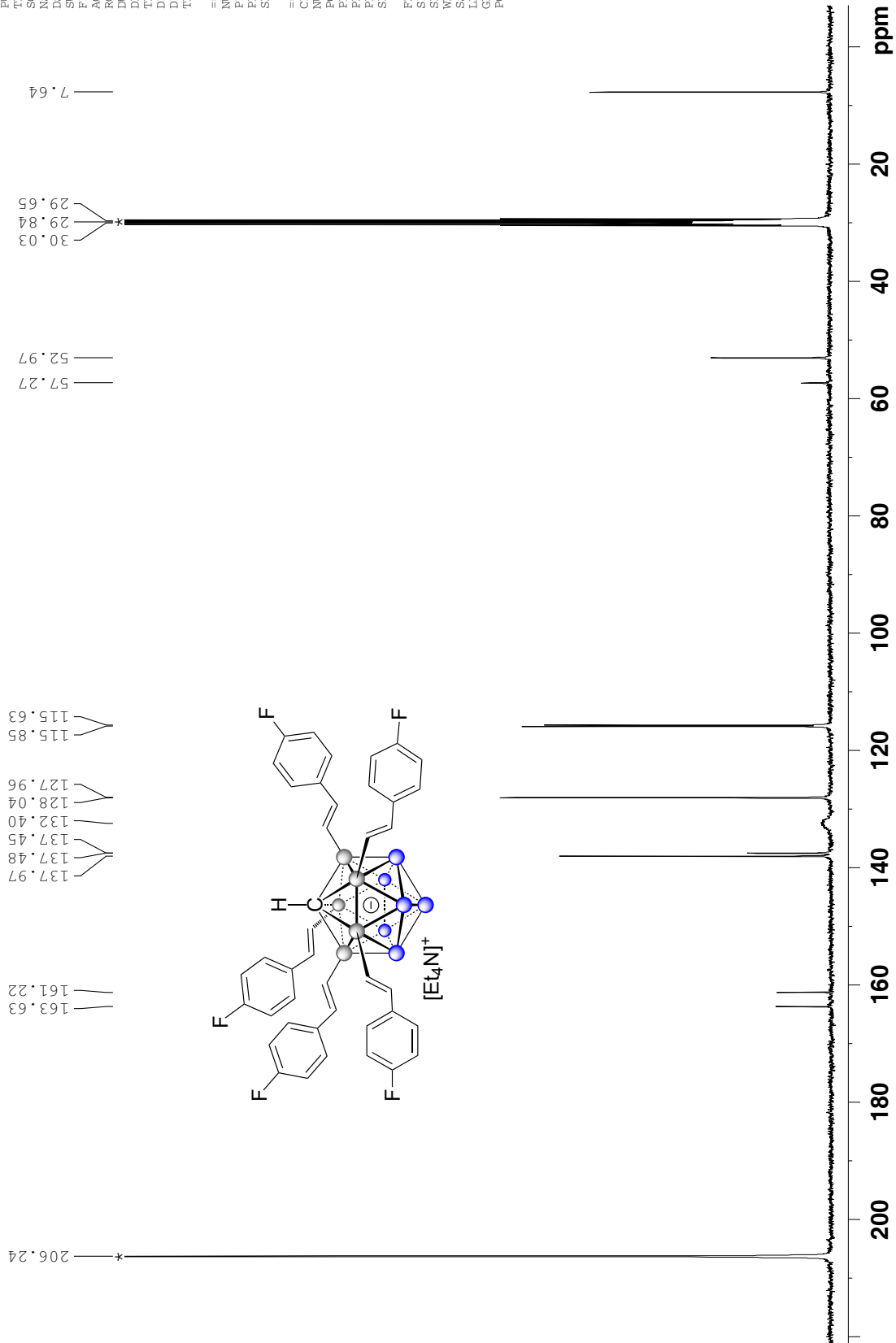


Penta-F-styrene-de product, 40 mg in 0.6 ml acetone-d6 *
¹³C{¹H} NMR, 100 MHz, 23 C

Current Data Parameters
 NAME Penta-4-F-styrene-de
 EXNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180601
 Time 19.47
 INSTRUM spect
 PROBD 5 mm PABBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT ACETONE
 NS 2048
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1101048 sec
 RG 183.34
 DW 16.800 usec
 DE 1.5000000 sec
 TE 297.4 K
 D1 1.5000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.100 usec
 PLM1 53.0000000 W
 SF01 100.6228293 MHz
 ===== CHANNEL f2 =====
 CDPORG[2] waitz[16
 NUC2 ¹H
 P2 80.00 usec
 PLM2 12.5000000 W
 PLM12 0.43945000 W
 PLM13 0.28125000 W
 SF02 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6126618 MHz
 VDM EM
 WDW 0
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



**Penta-styrene-de product, 40 mg in 0.6 ml acetone-d6*
¹H{¹B} NMR, 400 MHz, 23 C**

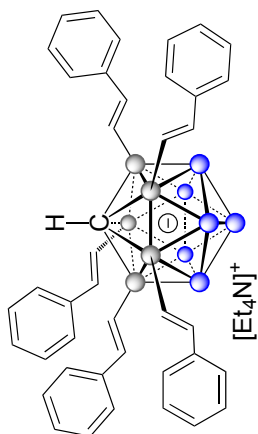
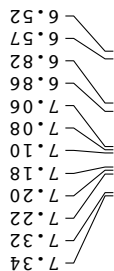
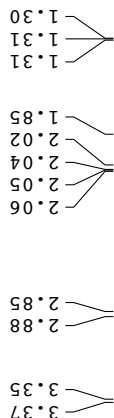
Current Data Parameters
 NAME penta-styrene-de
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180531
 Time_ 17.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 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 294.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

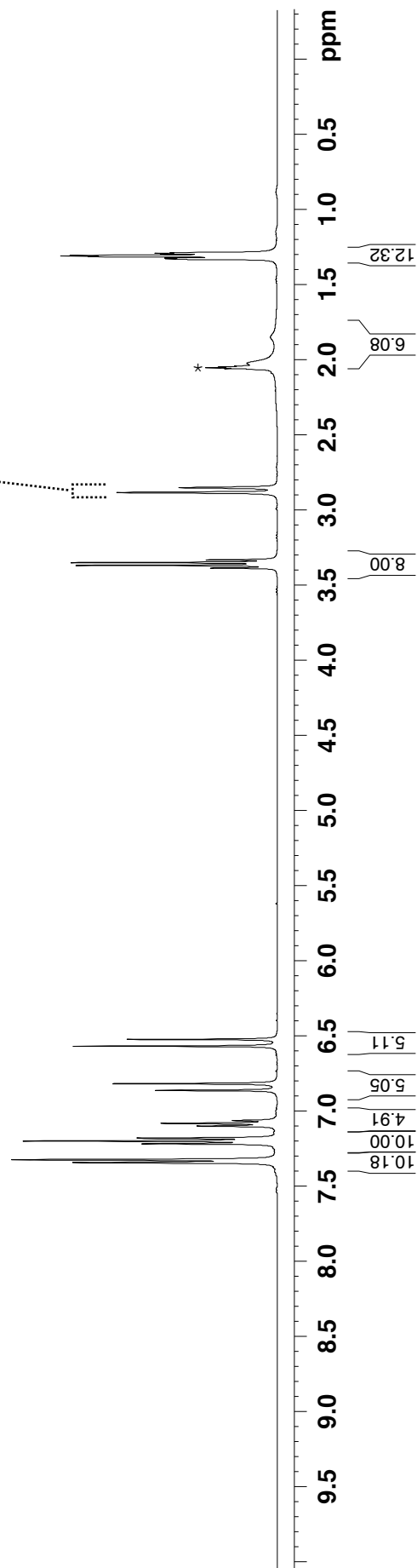
==== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PLW1 12.50000000 W
 SFO1 400.1320007 MHz

==== CHANNEL f2 =====
 CPDPRG1 2 garr4
 NUC2 ¹B
 P2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.64477998 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300072 MHz
 EM
 WDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Cage CH signal overlapping
 with double signal from H₂O
 as confirmed by HSQC spectrum



**Penta-styrene-de product, 40 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

```

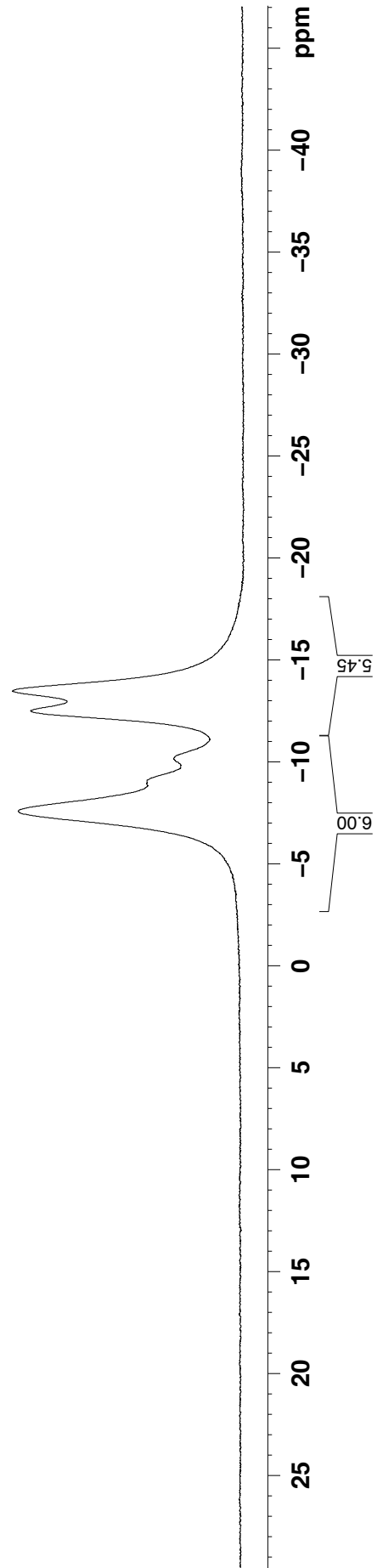
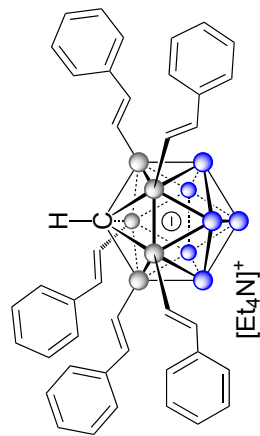
Current Data Parameters
NAME      penta-styrene-de
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20180531
Time     17.40
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       19.604 usec
DE       1.650 usec
TE       293.5 K
D1       1.00000001 sec
TD0      1

===== CHANNEL f1 =====
NUC1     11B
P1       9.193 usec
PL1      52.96599960 W
SFO1     128.3776052 MHz

F2 - Processing parameters
SI       32768
SF       128.3776050 MHz
WDW      EM
SSB      0
LB       3.00 Hz
GB       0
PC       1.40
  
```

-13.49
 -12.51
 -10.18
 -9.19
 -7.61



**Penta-styrene-de product, 40 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 128 MHz, 23 C**

```

Current Data Parameters
NAME      penta-styrene-de
EXPNO    3
PROCNO   1

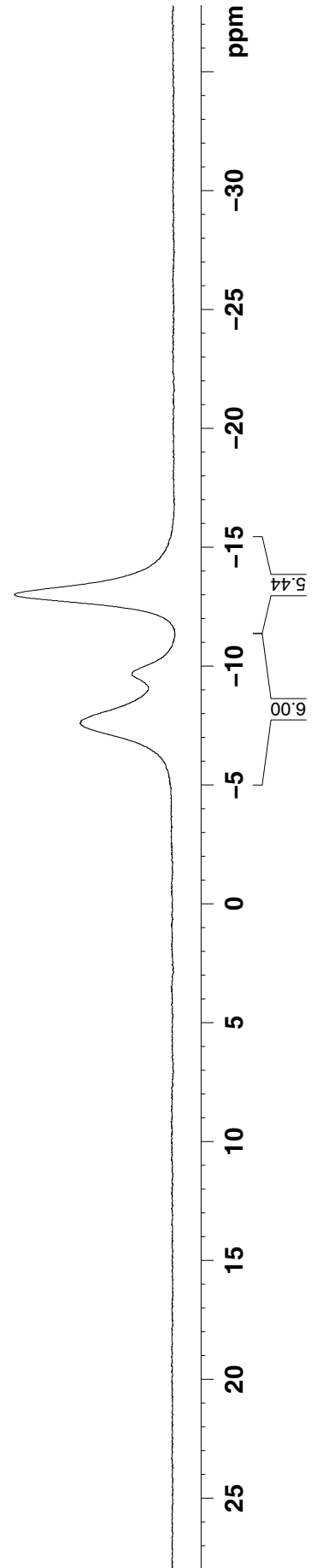
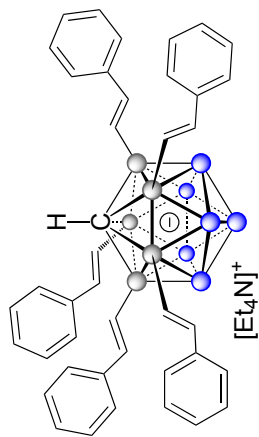
F2 - Acquisition Parameters
Date_    20180531
Time     17.51
INSTRUM  spect
PROBHD   5 mm PABBO BB
PULPROG  zgpg30
TD        65536
SOLVENT  Acetone
NS        124
DS        4
SWH       25510.203 Hz
FIDRES    0.389255 Hz
AQ         1.2845056 sec
RG         193.34
DW         19.604 usec
DE         19.650 usec
TE         294.8 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       11B
P1         9.19 usec
PLM1       52.9659960 W
SFO1       128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2    waitz16
NUC2       1H
P2         80.01 usec
PLM2       12.50000000 W
SFO2       0.23945000 W
PLM12      0.28125000 W
SFO2       400.1320007 MHz

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

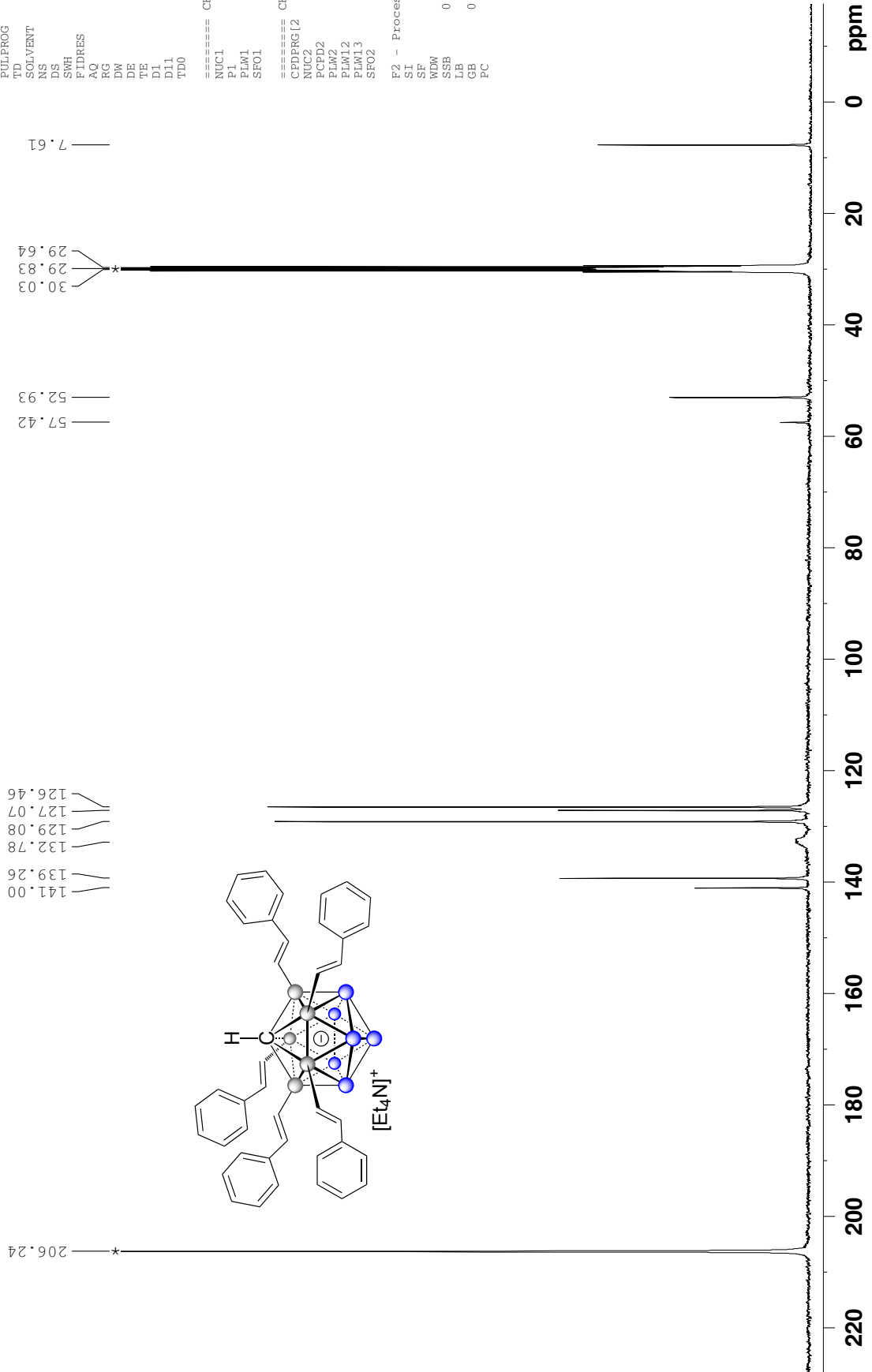
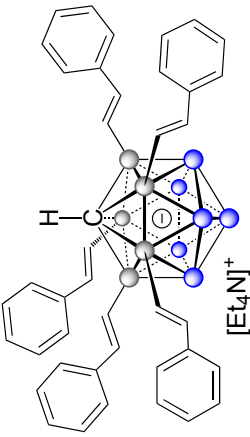
— 13.02
 — 9.71
 — 7.63



Penta-styrene-de product, 40 mg in 0.6 ml acetone-d6 *
¹³C{¹H} NMR, 101 MHz, 23 C

Current Data Parameters
 NAME penta-styrene-de
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180531
 Time 19.28
 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 294.8 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TDO 1

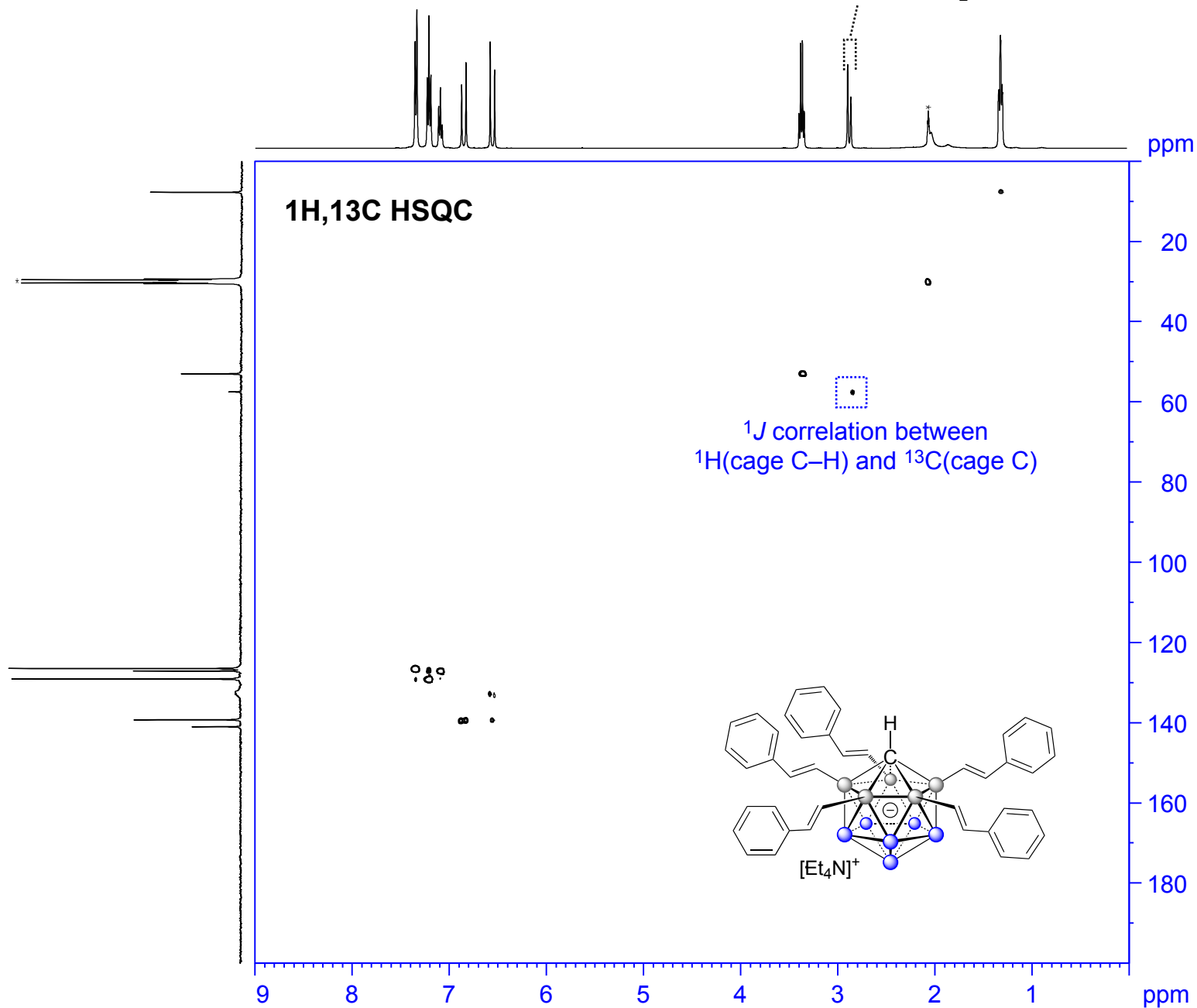


==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 53.0000000 W
 SFO1 100.6228293 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 12.5000000 W
 PLW12 0.43945000 W
 PLW13 0.28125000 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126842 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

¹H cage C-H signal is overlapping with double signal from H₂O



Current Data Parameters
NAME 20180804-phde-hsqc
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180805
Time 20.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgps12
TD 1024
SOLVENT Acetone
NS 2
DS 16
SWH 6009.615 Hz
FIDRES 5.868765 Hz
AQ 0.0851968 sec
RG 193.34
DW 83.200 usec
DE 6.50 usec
TE 295.0 K
CNST2 145.000000
D0 0.0000300 sec
D1 1.5000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
DZ4 0.00086207 sec
IN0 0.00001990 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
P2 30.00 usec
PZ8 1000.00 usec
PLW1 12.50000000 W
SFO1 400.1328009 MHz

===== CHANNEL f2 =====
CPDPRG[2] garp
NUC2 13C
P3 10.00 usec
P4 20.00 usec
PCPD2 70.00 usec
PLW2 53.00000000 W
PLW12 1.08159995 W
SFO2 100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.6238 MHz
FIDRES 196.524048 Hz
SW 249.991 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1299985 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

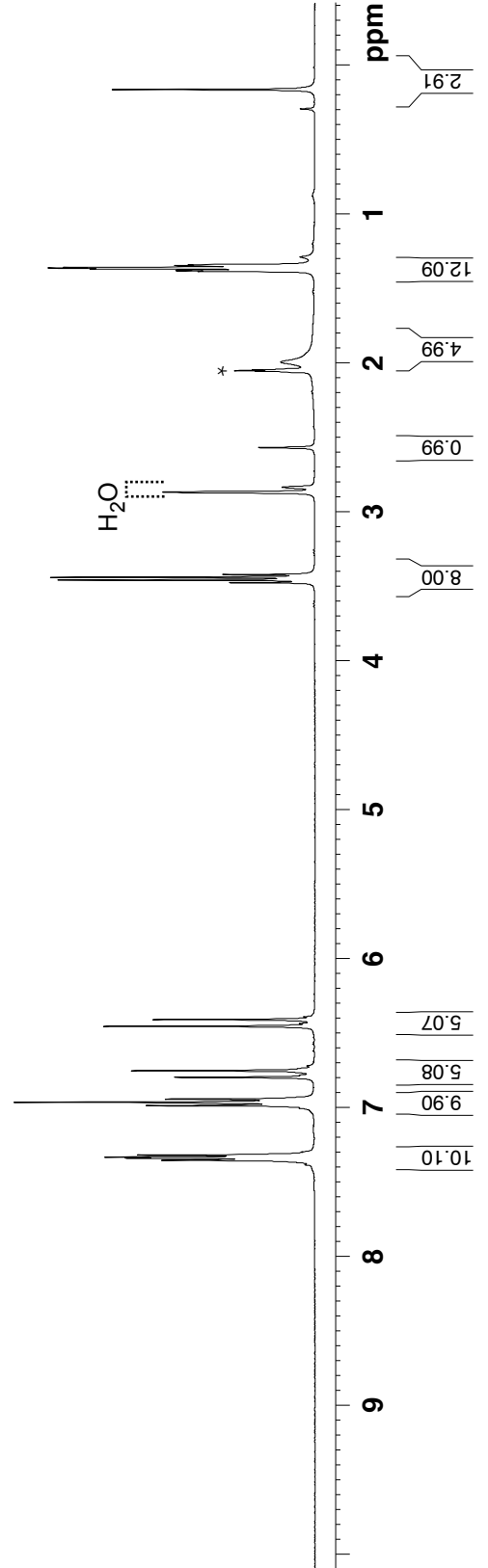
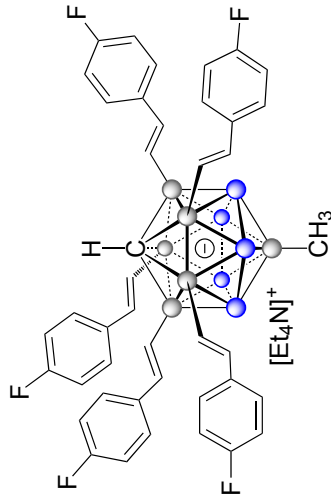
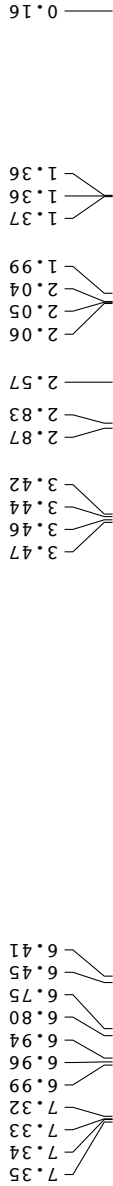
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6126624 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

12-Me-Penta-F-styrene-de product 40 mg in 0.6 ml acetone-d6*
¹H{¹H} NMR, 400 MHz, 23 C

Current Data Parameters
 NAME 12-Me-penta-4-F-styrene-d6
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180610
 Time_ 13:51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 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 293.7 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

=====
 CHANNEL f1
 NUC1 ¹H
 P1 15.00 usec
 PLW1 12.5000000 W
 SF01 400.1320007 MHz
 =====
 CHANNEL f2
 CPDPRG[2] garp4
 NUC2 ¹¹B
 P2 90.00 usec
 PLW2 52.9659960 W
 PLW12 0.6447798 W
 SF02 128.3776050 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300072 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



**12-Me-Penta-F-styryne-de product 40 mg in 0.6 ml acetone-d6
 11B NMR, 128 MHz, 23 C**

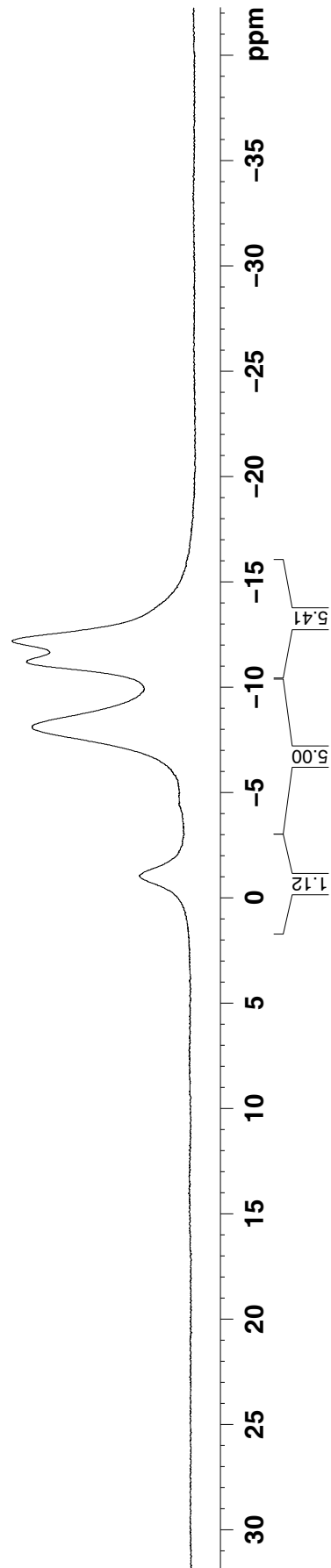
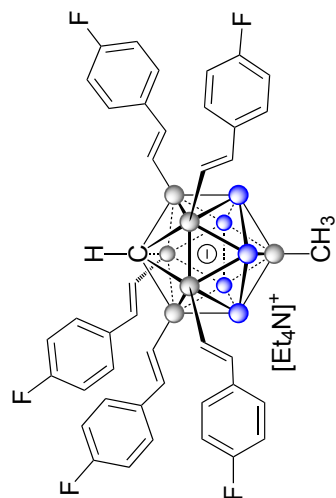
Current Data Parameters
 NAME 12-Me-penta-4-F-styrene-de
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180610
 Time 13.56
 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 293.8 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SFO1 128.3776052 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

1.04
 8.08
 11.21
 12.21



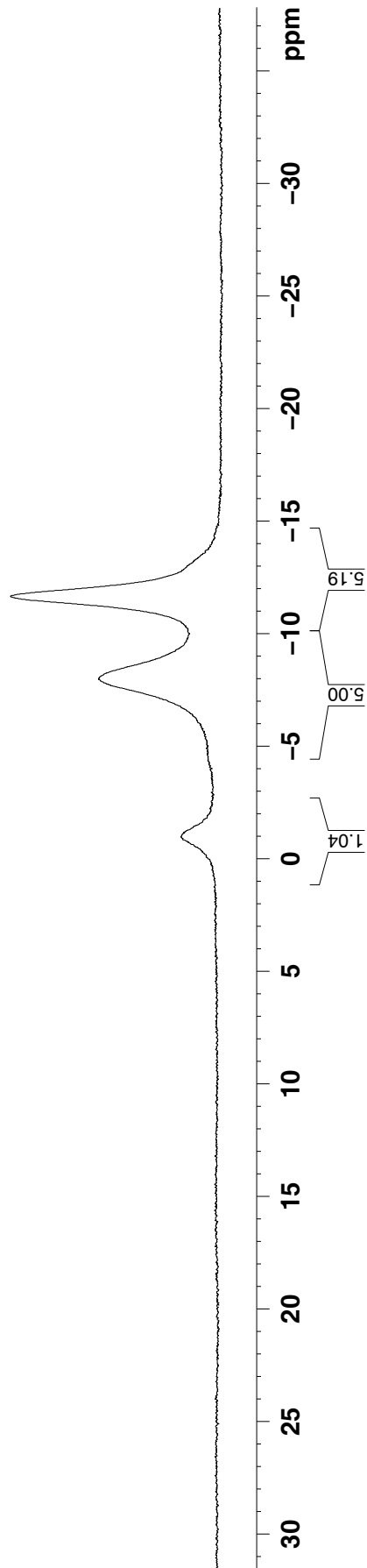
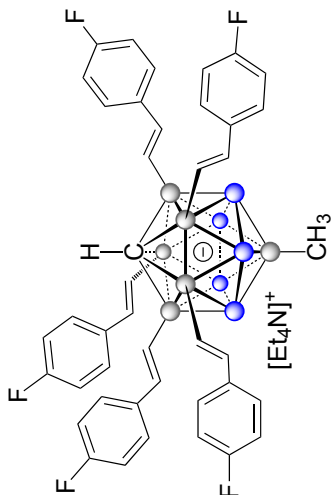
**12-Me-Penta-F-styryne-de product 40 mg in 0.6 ml acetone-d6
11B{1H} NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME 12-Me-penta-4-F-styrene-de
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180610
 Time 14.03
 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 293.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SFO1 128.3776050 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 12.5000000 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 3.00 Hz
 GB 0
 PC 1.40

11.68
8.03
0.98



12-Me-Penta-F-styrine-de product 40 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 101 MHz, 23 C

Current Data Parameters
 NAME 12-Me-penta-4-F-styrine-de
 EXPNO 4
 PROCNO 1

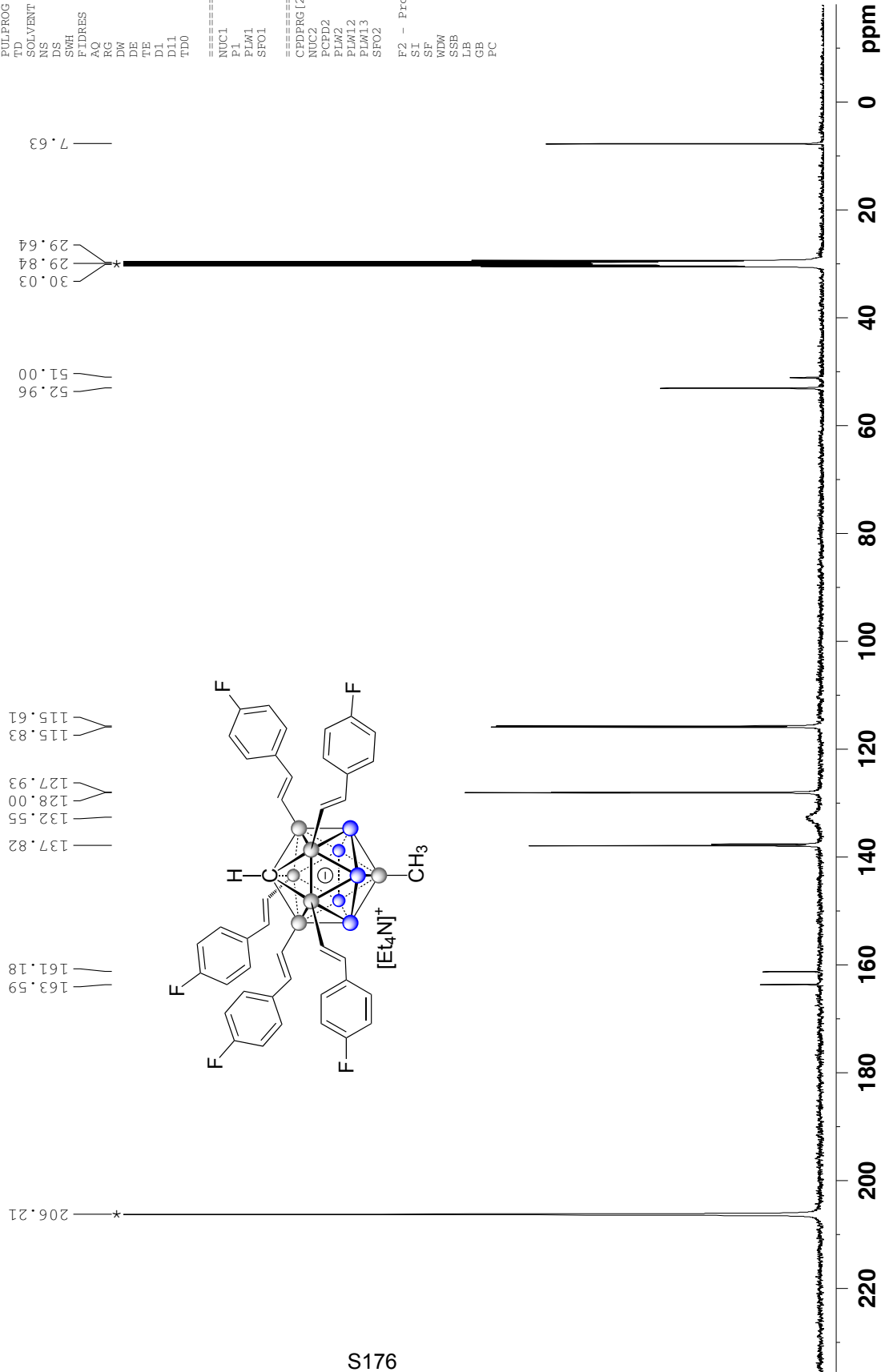
F2 - Acquisition Parameters

Date_ 20180610
 Time 15.35
 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 294.2 K
 D1 1.5000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 53.0000000 W
 SFO1 100.6228293 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 12.5000000 W
 PLW12 0.43945000 W
 PLW13 0.28125000 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126823 MHz
 EM
 WDW 0
 SSB 0
 LB 4.00 Hz
 GB 0
 PC 1.40



12-Ph-Penta-styrene-de product 40 mg in 0.6 ml acetone-d6 *
¹H{¹¹B} NMR, 500 MHz, 23 C

Current Data Parameters
 NAME 12-ph-penta-styrene-de
 EXPNO 1
 PROCNO 1

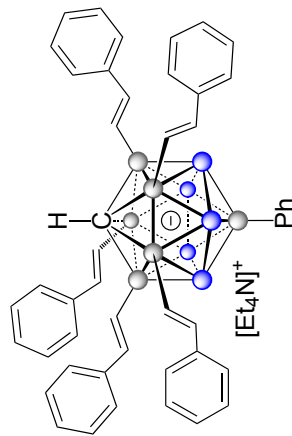
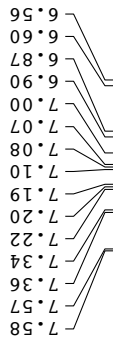
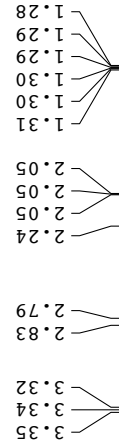
F2 - Acquisition Parameters
 Date_ 20180614
 Time 18.07

INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg1g30
 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 5.0000000 sec
 D11 0.0300000 sec

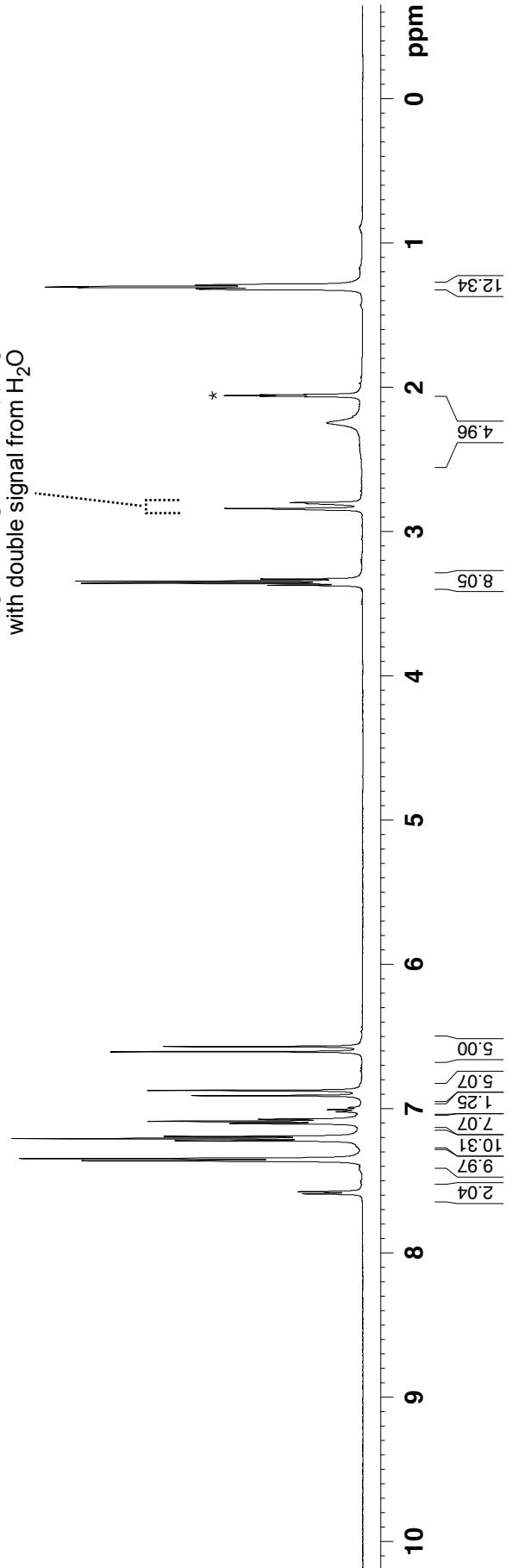
==== CHANNEL f1 =====
 NUC1 ¹H
 P1 11.70 usec
 PL1 19.0000000 W
 SFO1 500.1335009 MHz

==== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 ¹¹B
 P2 100.00 usec
 PL2 95.0000000 W
 SFO2 160.4615690 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300101 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



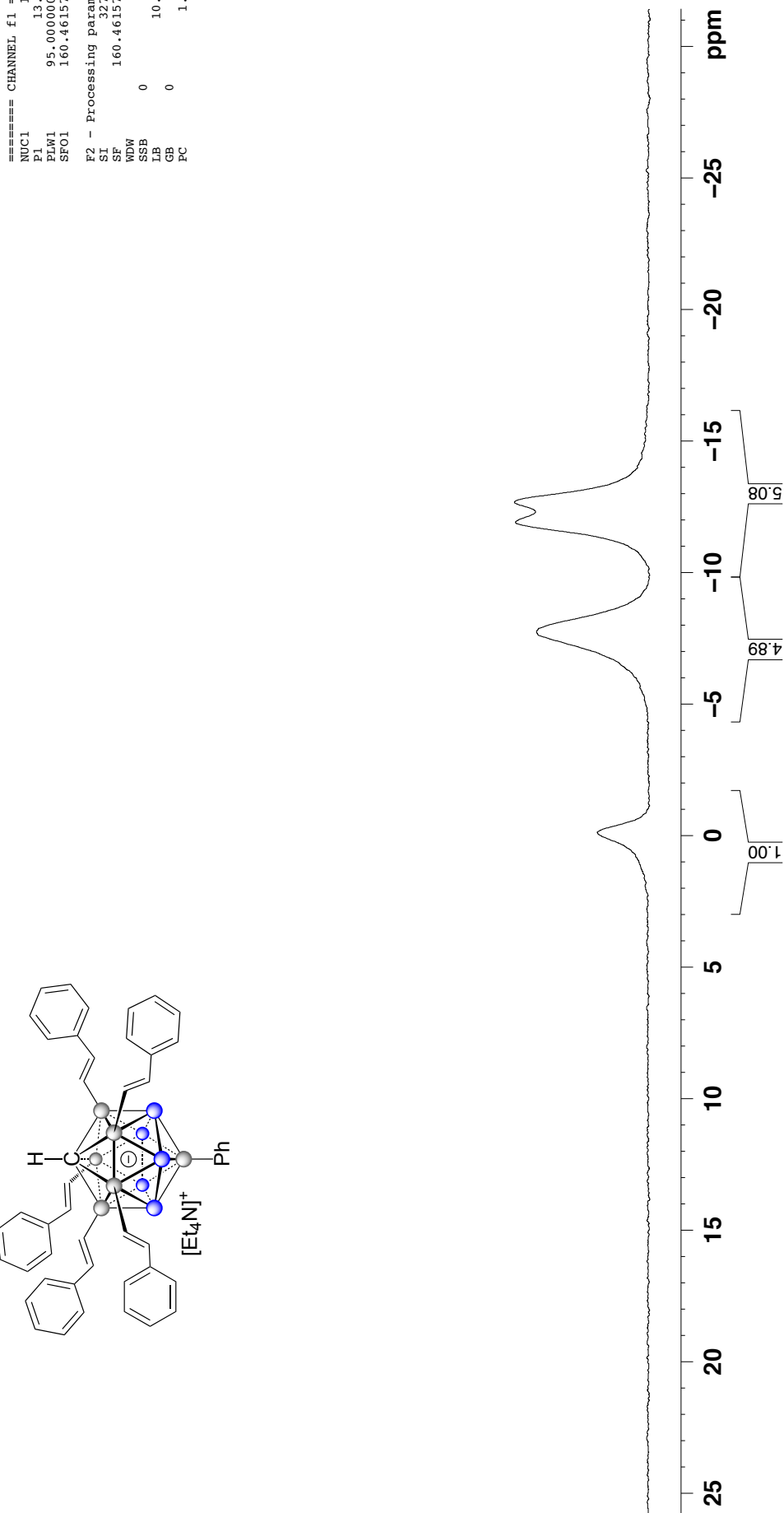
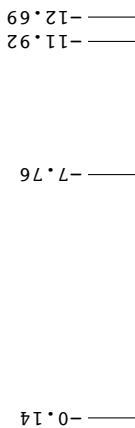
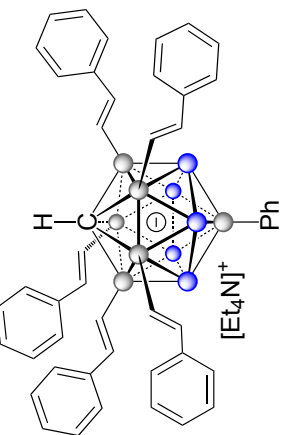
Cage CH signal overlapping
 with double signal from H₂O



**12-Ph-Penta-styrene-de product 40 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

Current Data Parameters
 NAME 12-Ph-penta-styrene-de
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180614
 Time 18.10
 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 295.4 K
 D1 1.00000000 sec



**12-Ph-Penta-styrene-de product 40 mg in 0.6 ml acetone-d6
¹¹B{1H} NMR, 160 MHz, 23 C**

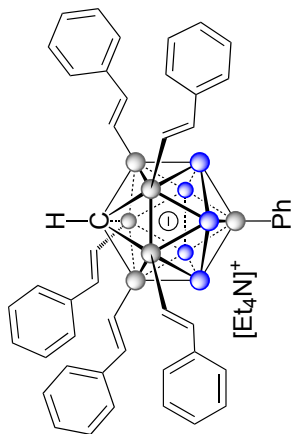
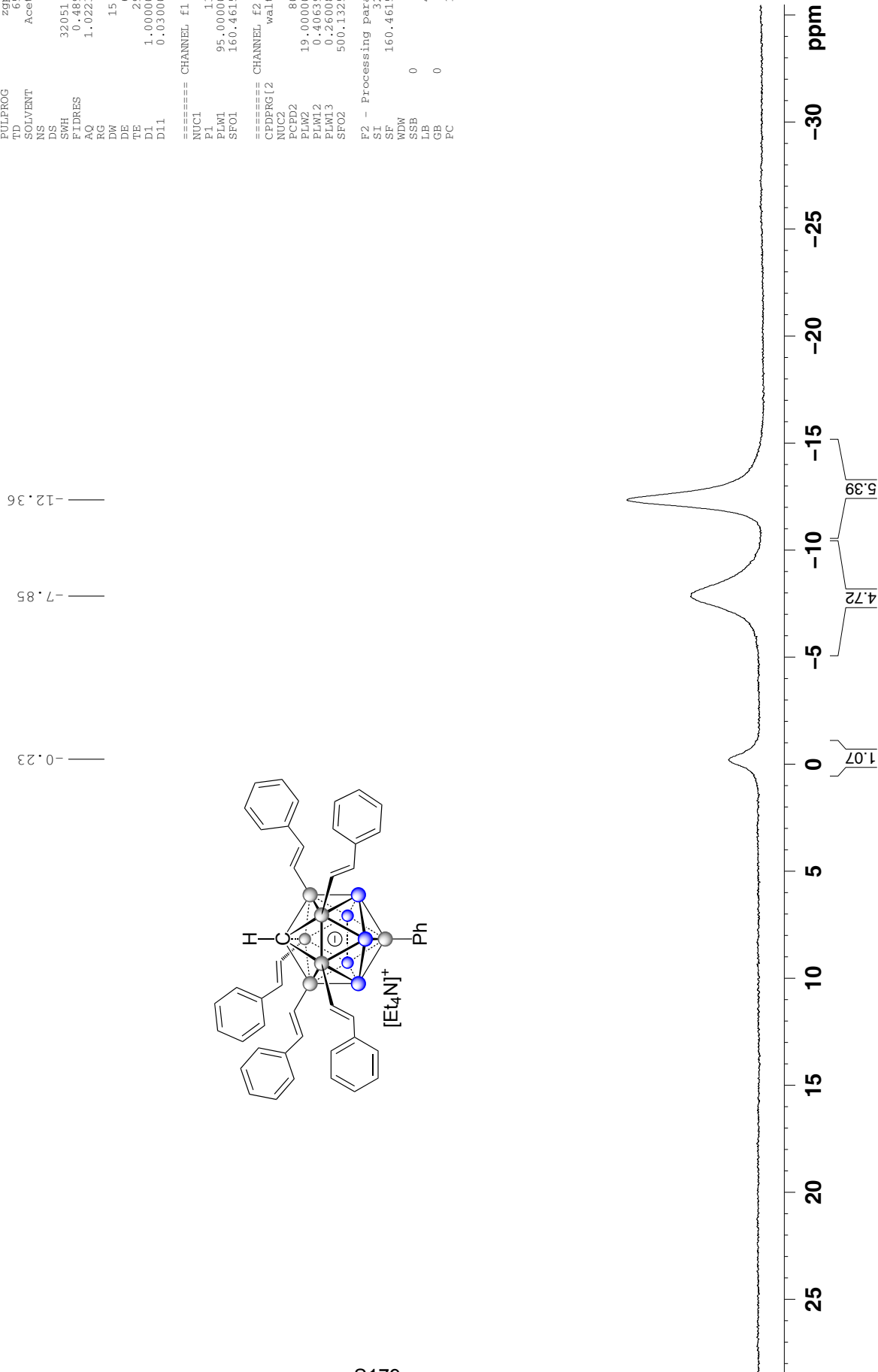
Current Data Parameters
 NAME 12-Ph-penta-styrene-de
 EXNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180611
 Time 18.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB
 PULPROG zgpg30
 ZDELTA 65536
 SOLVENT Acetone
 NS 64
 DS 6
 SWH 32051.281 Hz
 FIDRES 0.489664 Hz
 AQ 1.0223616 sec
 RG 303
 DG 15.600 usec
 DE 6.50
 TE 296.1 K
 D1 1.0000000 sec
 D11 0.0300000 sec

==== CHANNEL f1 =====
 NUC1 ¹¹B
 P1 13.10 usec
 PL1 95.0000000 W
 SFO1 160.4615790 MHz

==== CHANNEL f2 =====
 CPDPRG2 wait16
 NUC2 ¹H
 PCPD2 80.00 usec
 PL12 19.0000000 W
 PL13 0.40639001 W
 PL14 0.36008999 W
 SFO2 500.1325007 MHz

F2 - Processing parameters
 SI 32768
 SF 160.4615790 MHz
 VDWM EM
 SSB 0
 LB 0
 GB 0
 PC 1.40



12-Ph-Penta-styrene-de product 40 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 126 MHz, 23 C

Current Data Parameters
 NAME 12-Ph-penta-styrene-de
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20180614
 Time 19.16
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 2000
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.3 K
 D1 1.50000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====

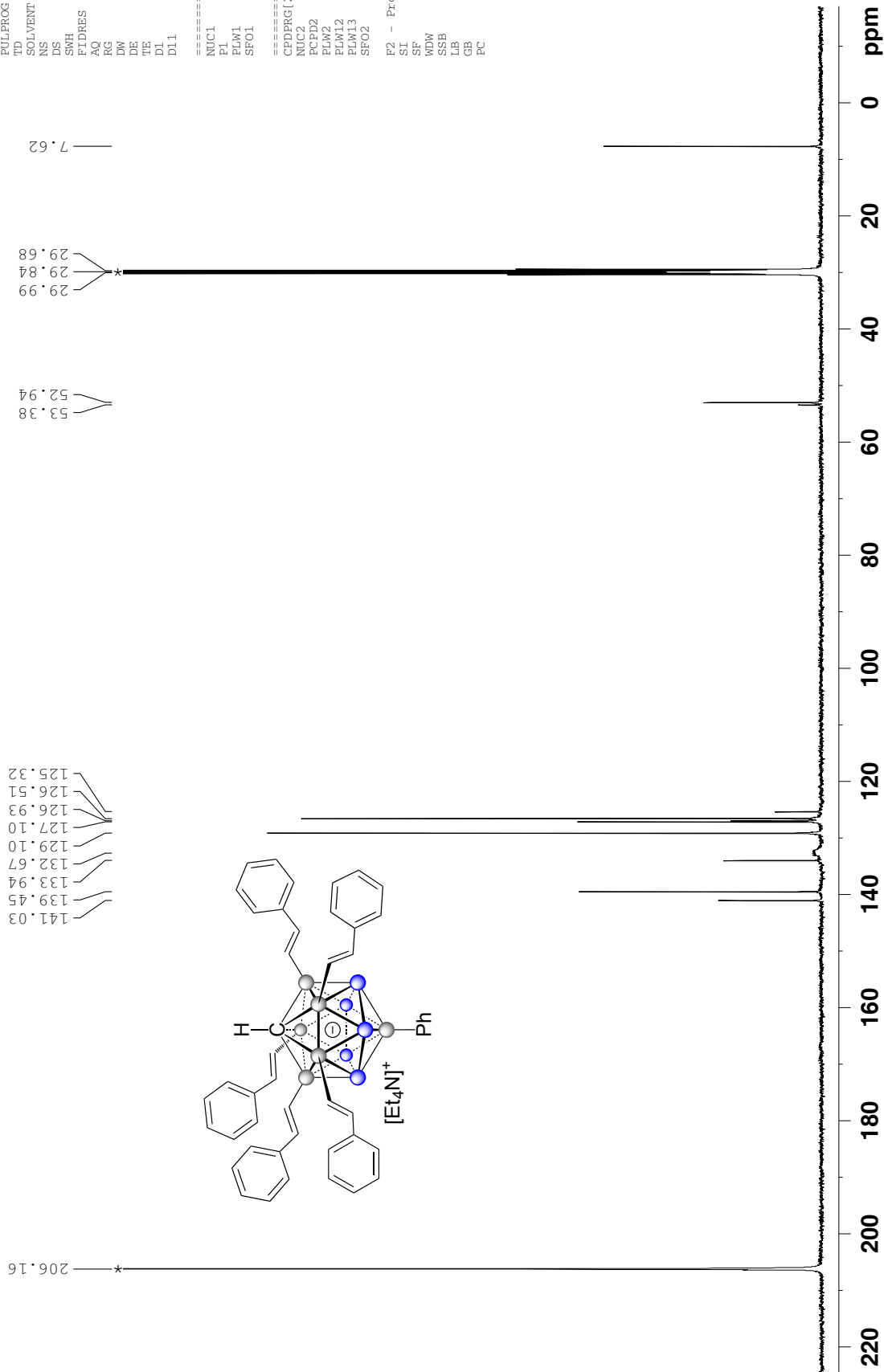
NUC1 13C
 P1 10.50 usec
 PLW1 95.00000000 W
 SF01 125.7716224 MHz

==== CHANNEL f2 =====

CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 19.00000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SF02 500.1320005 MHz

F2 - Processing parameters

SI 32768
 SF 125.7576798 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



12-CN-Penta-F-styryne-de product 40 mg in 0.6 ml acetone-d6
¹H{¹³C} NMR, 400 MHz, 23 C

Current Data Parameters
 NAME 12-CN-penta-4-F-styryne-d6
 EXPNO 1
 PROCNO 1

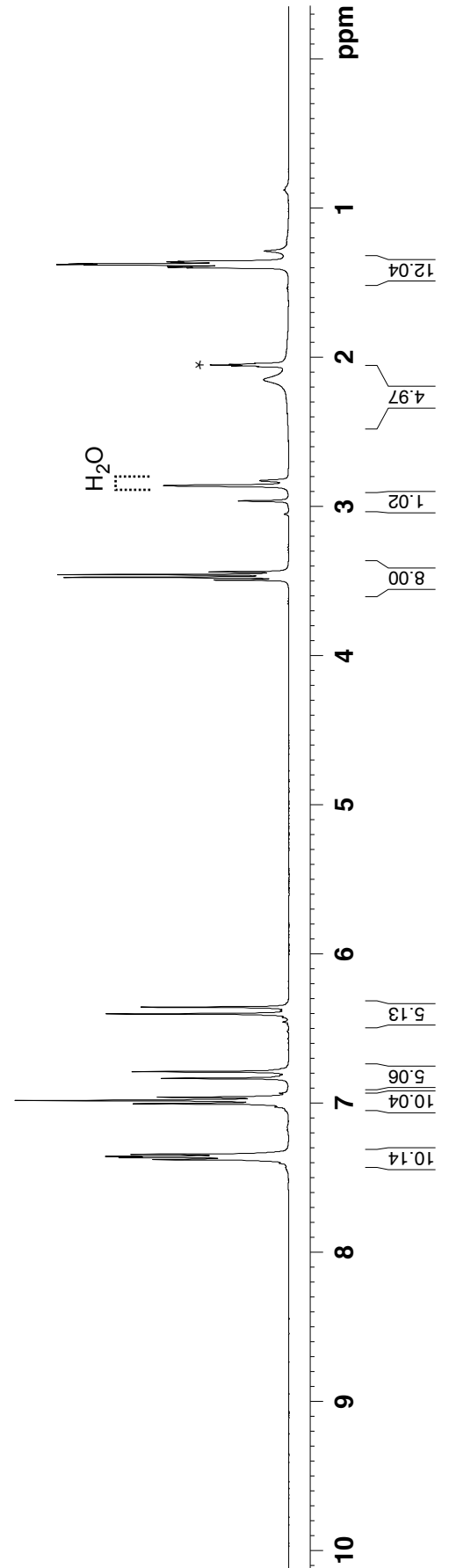
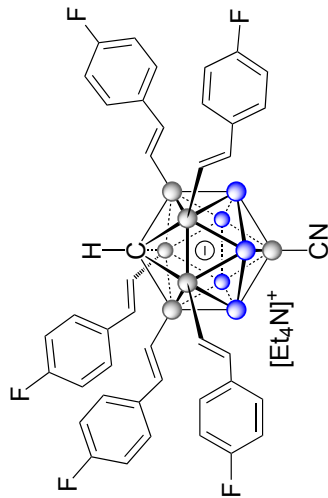
F2 - Acquisition Parameters
 Date_ 20180611
 Time_ 8.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 107.6
 DW 62.400 usec
 DE 6.50 usec
 TE 294.1 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

=====
 CHANNEL f1
 NUC1 ¹H
 P1 15.00 usec
 PLW1 12.5000000 W
 SFO1 400.1320007 MHz
 =====
 CHANNEL f2
 CPDPRG2 garp4
 NUC2 ¹³C
 P1 90.00 usec
 PLW2 52.9659960 W
 PLW12 0.6447798 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300072 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

3.47
3.46
3.44
2.96
2.86
2.83
2.15
2.06
2.06
2.05
2.04
2.04
1.38
1.38
1.37

7.36
7.36
7.34
7.00
6.98
6.96
6.83
6.79
6.40
6.36



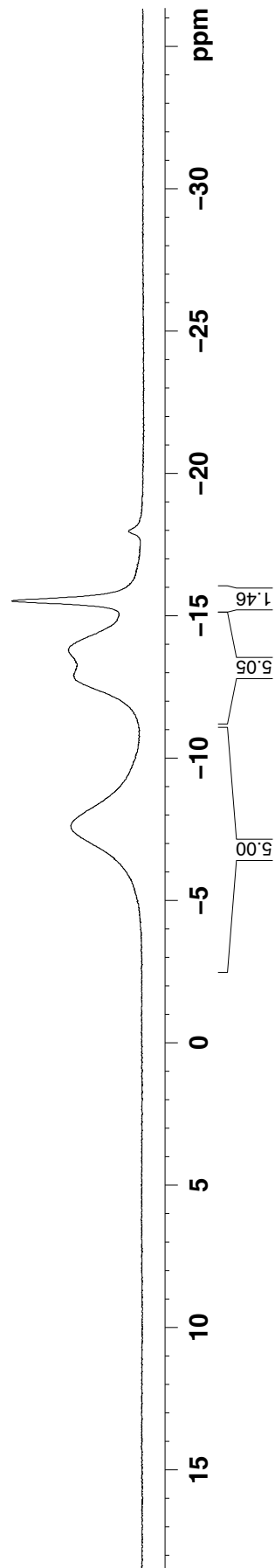
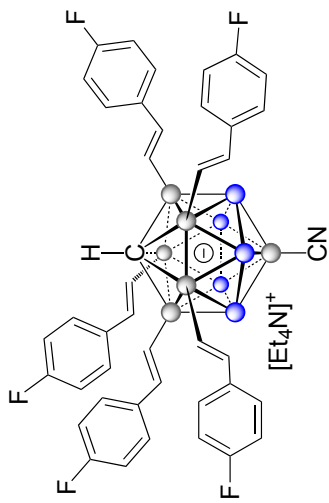
**12-CN-Penta-F-styryne-de product 40 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME 12-CN-penta-4-F-styryne-de
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180611
 Time 8.34
 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 293.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SFO1 128.3776052 MHz
 F2 - Processing parameters
 SI 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

7.64
 12.85
 13.85



**12-CN-Penta-F-styrine-de product 40 mg in 0.6 ml acetone-d6
11B{1H} NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME 12-CN-penta-4-F-styrine-de
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

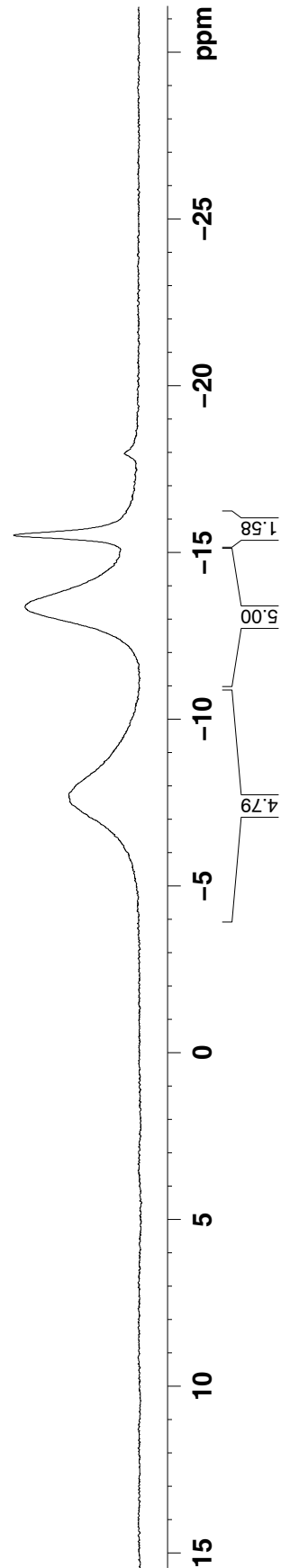
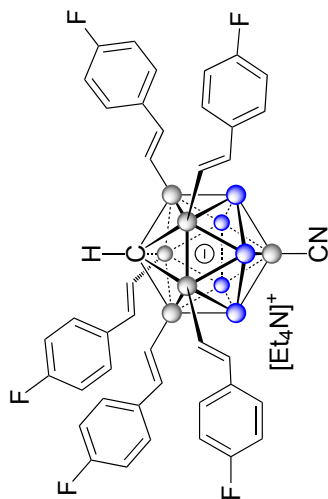
Date_ 20180611
 Time 8.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 294.4 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SFO1 128.3776050 MHz

===== CHANNEL f2 =====
 CPDPRG2 waitz16
 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 3.00 Hz
 GB 0
 PC 1.40

15.53
 13.38
 7.75



12-CN-Penta-F-styryne-de product 40 mg in 0.6 ml acetone-d6 *
¹³C{¹H} NMR, 101 MHz, 23 C

Current Data Parameters
 NAME 12-CN-penta-4-F-styrene-de
 EXPNO 4
 PROCNO 1

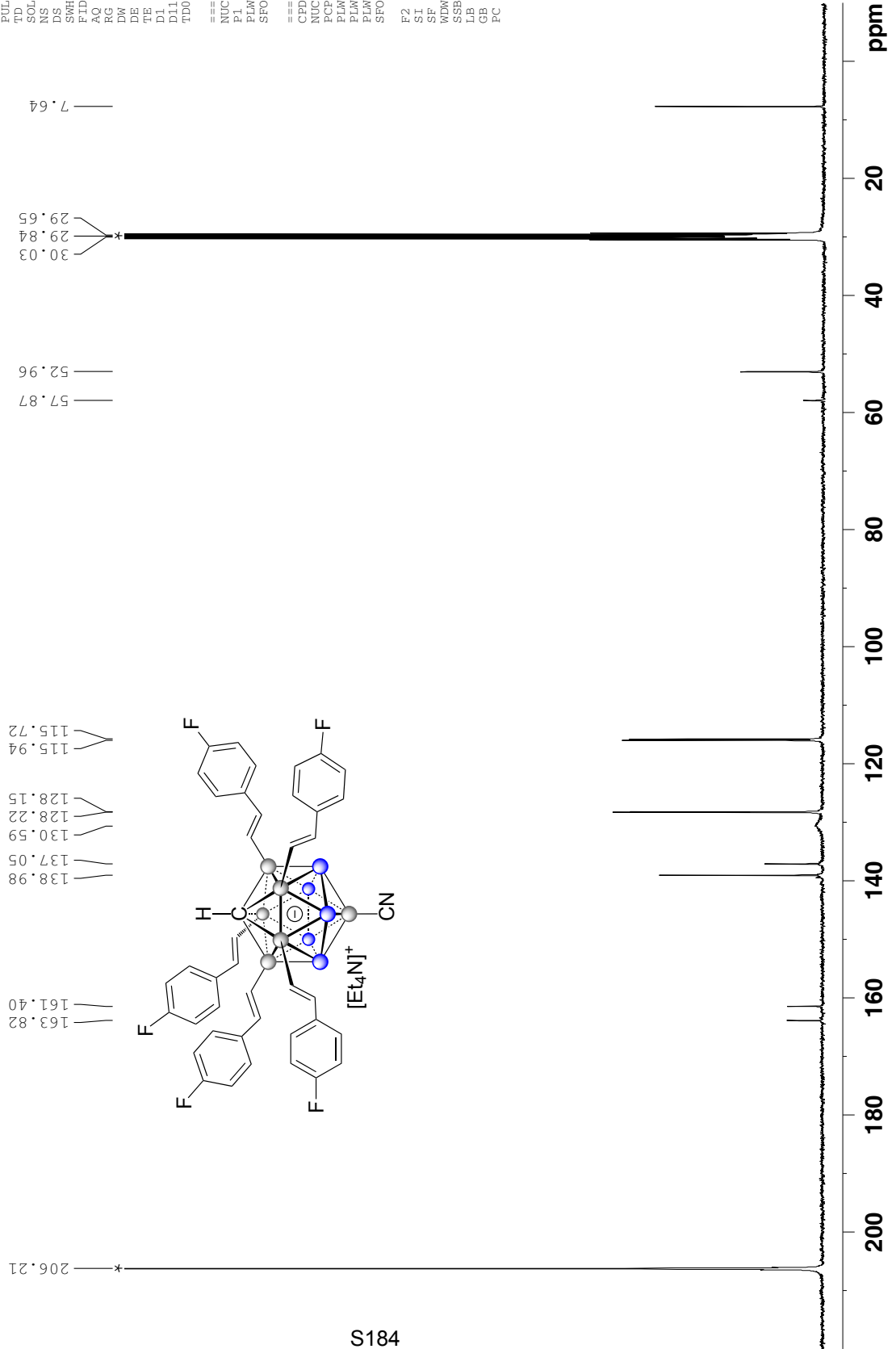
F2 - Acquisition Parameters

Date_ 20180611
 Time 10.12
 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 293.9 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TDO 1

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

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 P2 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



penta-R-penten-ol-de product, 30 mg in 0.6 ml acetone-d6*
¹H{¹³C} NMR, 500 MHz, 23 C

Current Data Parameters
 NAME penta-R-penten-ol-de
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters

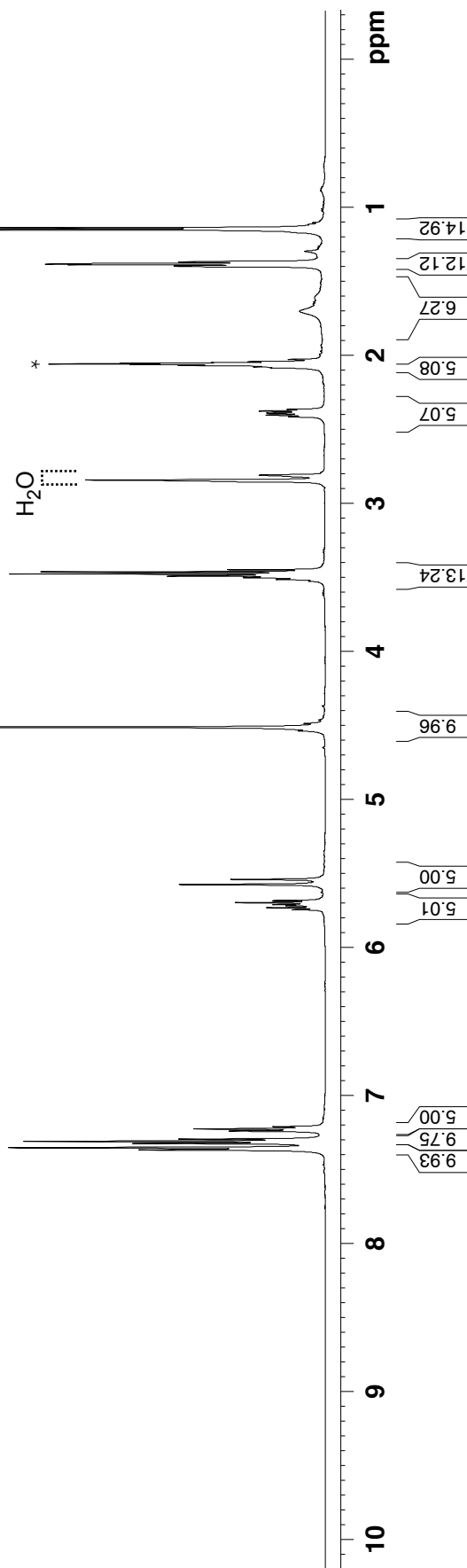
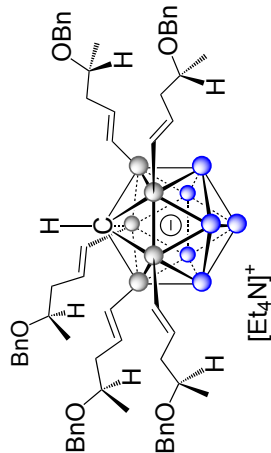
Date_ 20180704
 Time 20.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg1930
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 0
 SWH 12500.000 Hz
 FIDRES 0.190735 Hz
 AQ 2.6214399 sec
 RG 114
 DW 40.000 usec
 DE 6.50 usec
 TE 295.7 K
 D1 5.00000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 11.70 usec
 PLW1 19.0000000 W
 SFO1 500.1335009 MHz

==== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 ¹³C
 P1B 100.00 usec
 PCPD2 95.0000000 W
 PLW2 1.6303005 W
 SFO2 160.4615690 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300080 MHz
 EM
 WDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

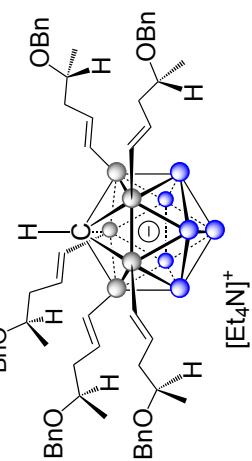
7.21
7.22
7.24
7.29
7.31
7.32
7.35
7.36
5.73
5.71
5.69
5.68
5.57
5.54
4.51
3.47
3.46
2.84
2.81
2.40
2.39
2.37
2.05
1.70
1.38
1.38
1.38
1.15
1.13



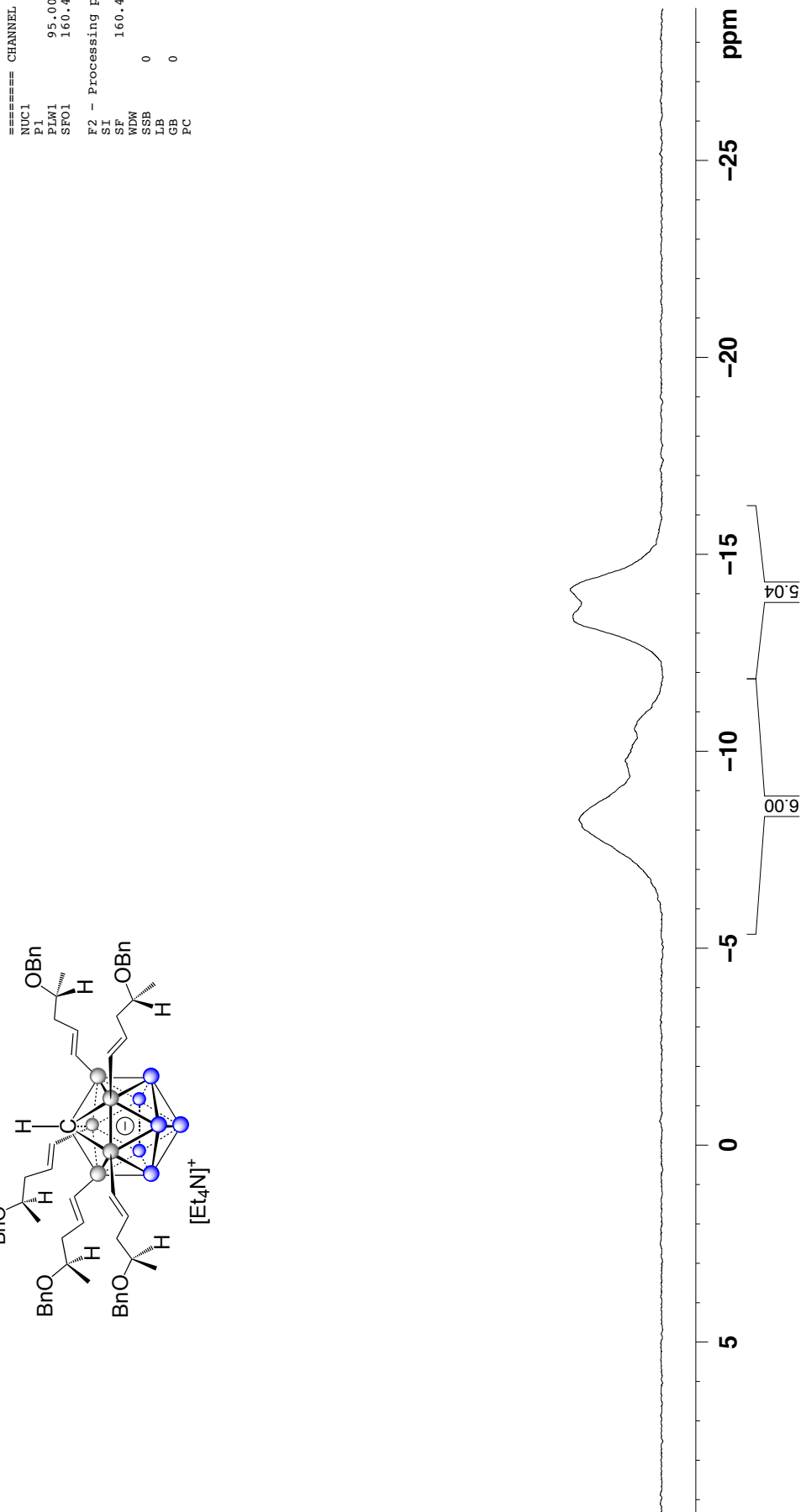
**penta-R-penten-ol-de product, 30 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

Current Data Parameters
 NAME penta-R-penten-ol-de
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180704
 Time_ 13.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 64098
 SOLVENT Acetone
 NS 128
 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 295.5 K
 D1 1.0000000 sec



8.29
 9.85
 10.58
 14.12



**penta-R-penten-ol-de product, 30 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 160 MHz, 23 C**

Current Data Parameters
 NAME penta-R-penten-ol-de
 EXPNO 3
 PROCNO 1

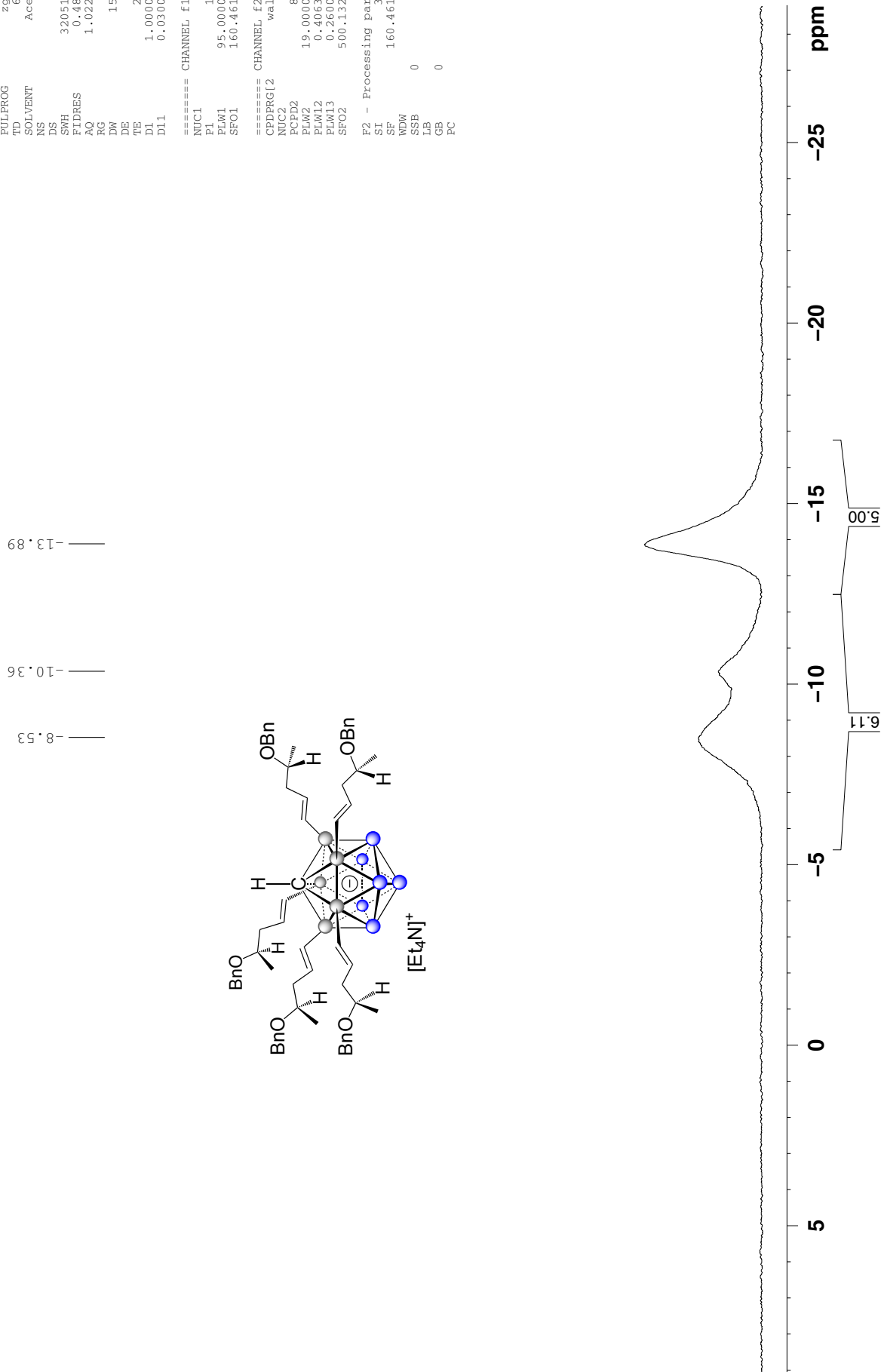
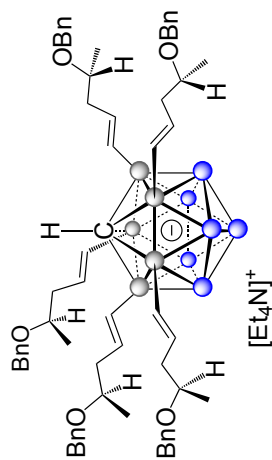
F2 - Acquisition Parameters
 Date_ 20180704
 Time 13.24
 INSTRUM spect
 PROBHD 5 mm PABBO-EB
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 126
 DS 2
 SWH 32051.281 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223614 sec
 RG 203
 DW 15.600 usec
 DE 6.50 usec
 TE 295.8 K
 D1 1.00000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 ¹¹B
 P1 13.10 usec
 PL1 95.0000000 W
 SF01 160.4615790 MHz

==== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PL12 19.0000000 W
 PL13 0.40639001 W
 PL14 0.26008999 W
 SF02 500.1325007 MHz

F2 - Processing parameters
 SI 32768
 SF 160.4615790 MHz
 WDW EM
 SSB 0
 LB 6.00 Hz
 GB 0
 PC 1.40

13.89
 10.36
 8.53



penta-R-penten-ol-de product, 30 mg in 0.6 ml acetone-d6
¹³C{¹H} NMR, 126 MHz, 23 C

Current Data Parameters
 NAME penta-R-penten-ol-de
 EXPNO 4
 PROCNO 1

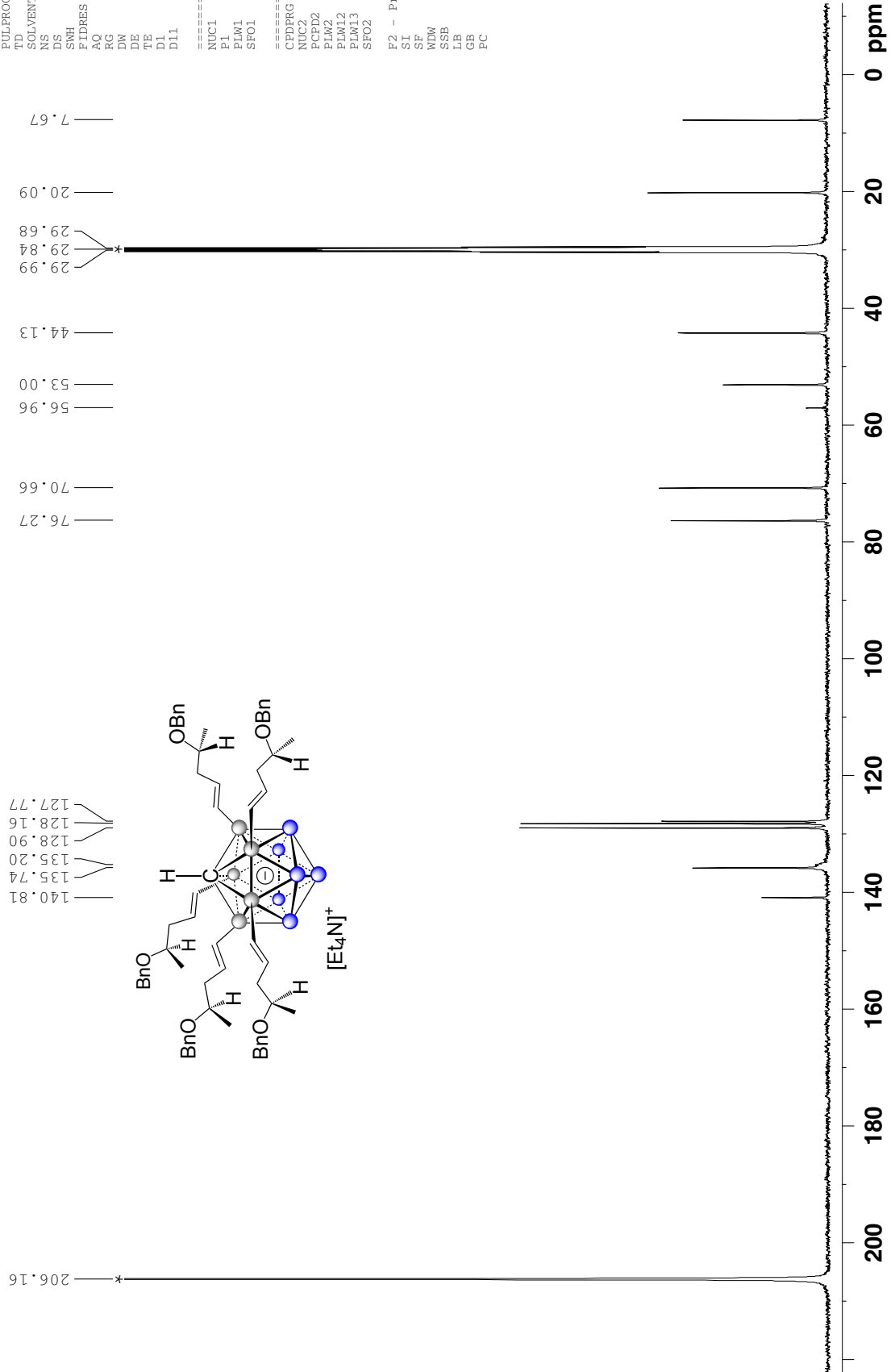
F2 - Acquisition Parameters

Date_ 20180704
 Time 15.22
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 3000
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.5 K
 D1 1.50000000 sec
 D11 0.03000000 sec

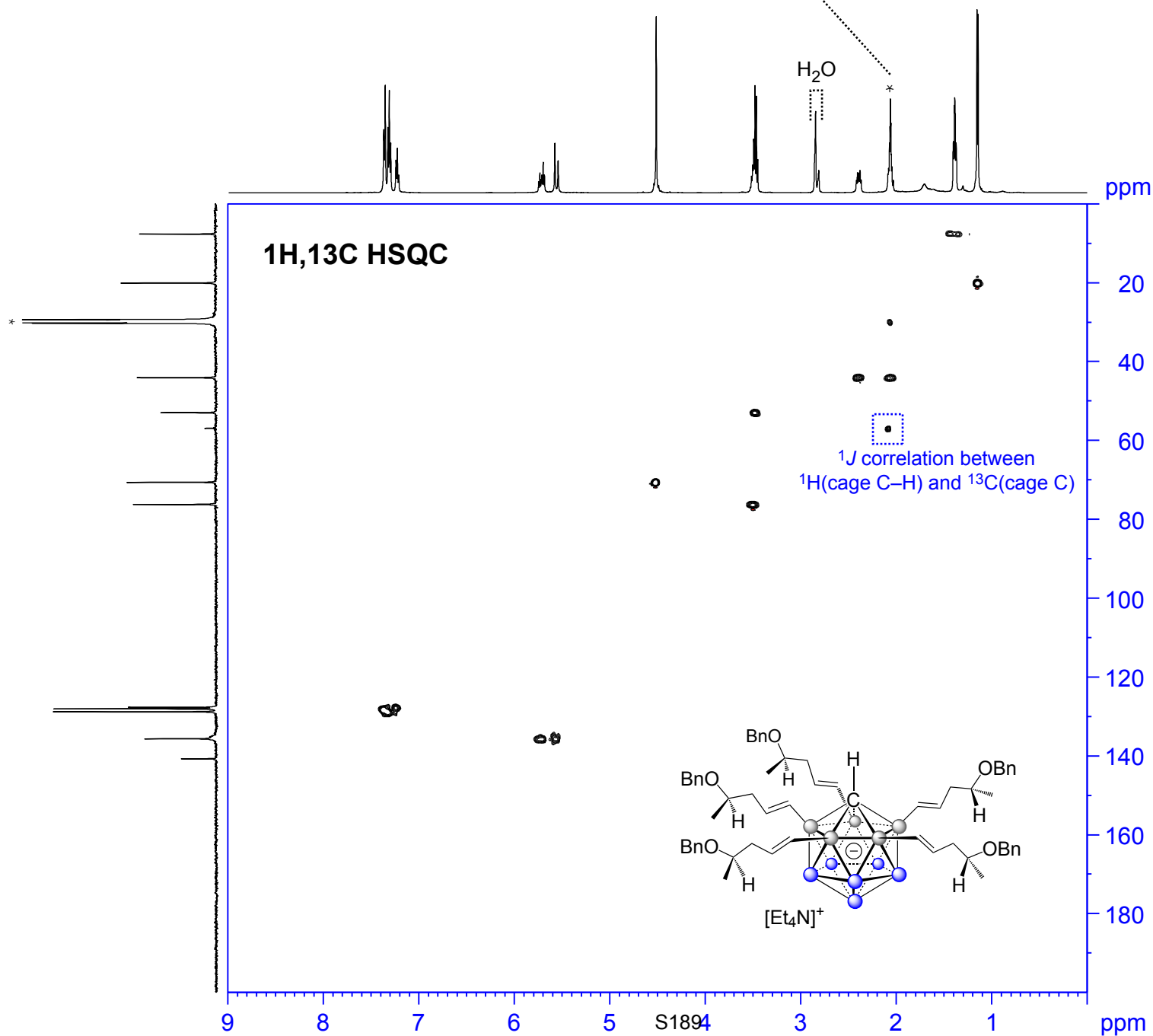
=====
 CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.50 usec
 PLW1 95.0000000 W
 SFO1 125.7716224 MHz

=====
 CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 19.0000000 W
 PLW12 0.40639001 W
 PLW13 0.26008999 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7576794 MHz
 WDW EM
 SSB 0
 LB 6.00 Hz
 GB 0
 PC 1.40



¹H cage C-H signal is overlapping with solvent residual signal and one of the side chain CH₂ signals



Current Data Parameters
NAME 20180730-chide-hsqc
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180731
Time_ 7.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgps12
TD 1024
SOLVENT Acetone
NS 2
DS 16
SWH 6009.615 Hz
FIDRES 5.868765 Hz
AQ 0.0851968 sec
RG 193.34
DW 83.200 usec
DE 6.50 usec
TE 295.1 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
DZ4 0.00086207 sec
IN0 0.00001990 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
P2 30.00 usec
P28 1000.00 usec
PLW1 12.50000000 W
SFO1 400.1328009 MHz

===== CHANNEL f2 =====
CPDPRG[2] garp
NUC2 13C
P3 10.00 usec
P4 20.00 usec
PCPD2 70.00 usec
PLW2 53.00000000 W
PLW12 1.08159995 W
SFO2 100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.6238 MHz
FIDRES 196.524048 Hz
SW 249.991 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

penta-S-penten-ol-de product, 30 mg in 0.6 ml acetone-d6 *
¹H{¹¹B} NMR, 500 MHz, 23 C

Current Data Parameters
 NAME penta-S-penten-ol-de
 EXPNO 1
 PROCNO 1

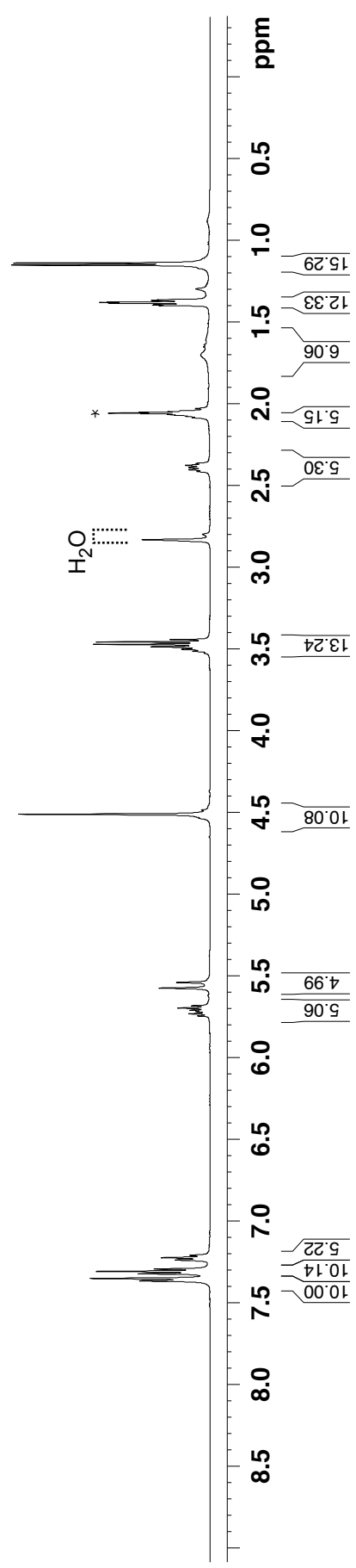
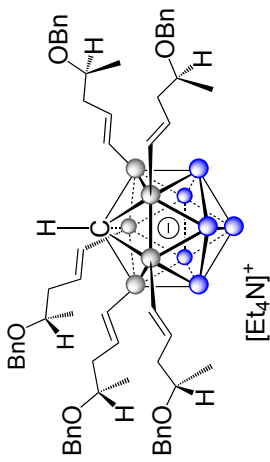
F2 - Acquisition Parameters
 Date_ 20181025
 Time 10.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 0
 SWH 12500.000 Hz
 FIDRES 0.190735 Hz
 AQ 2.6214399 sec
 RG 114
 DW 40.000 usec
 DE 6.50 usec
 TE 296.6 K
 D1 5.0000000 sec
 D11 0.0300000 sec

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 11.70 usec
 PLW1 19.0000000 W
 SF01 500.1335009 MHz

==== CHANNEL f2 =====
 CPDPRG[2] garp
 NUC2 ¹¹B
 P2 100.00 usec
 PLW2 95.0000000 W
 PLW12 1.63030005 W
 SF02 160.4615690 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300079 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

- 7.35
- 7.31
- 7.24
- 7.22
- 5.73
- 5.71
- 5.69
- 5.68
- 5.57
- 5.54
- 4.51
- 3.47
- 3.45
- 2.83
- 2.40
- 2.39
- 2.37
- 2.36
- 2.06
- 2.05
- 2.05
- 1.70
- 1.38
- 1.38
- 1.37
- 1.15
- 1.14



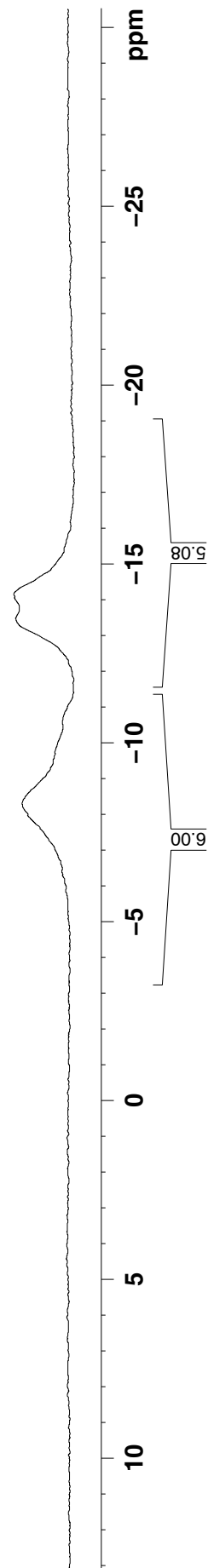
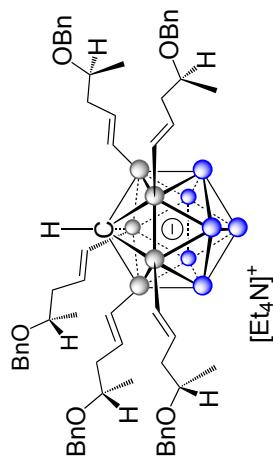
**penta-S-penten-ol-de product, 30 mg in 0.6 ml acetone-d6
11B NMR, 160 MHz, 23 C**

Current Data Parameters
 NAME penta-S-penten-ol-de
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181025
 Time 10.25
 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 296.2 K
 D1 1.00000000 sec

==== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 usec
 PLW1 95.0000000 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

8.32
 9.87
 10.58
 13.43
 14.17



**penta-S-penten-ol-de product, 30 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 160 MHz, 23 C**

Current Data Parameters
 NAME penta-S-penten-ol-de
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

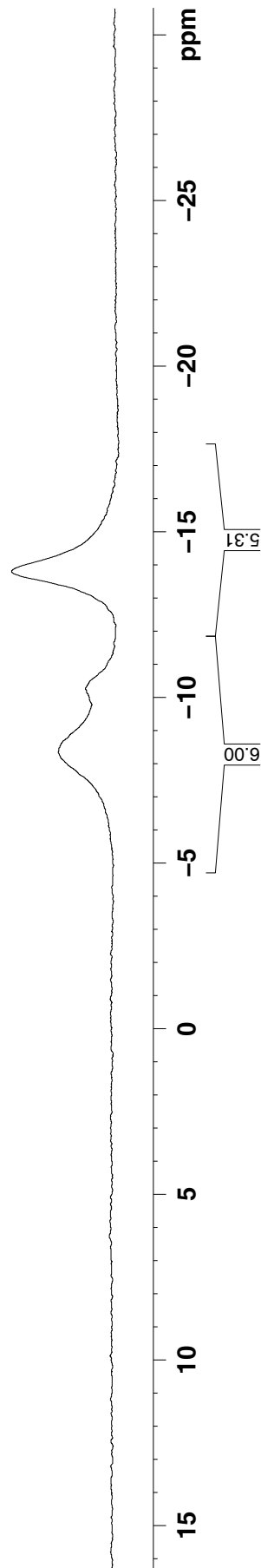
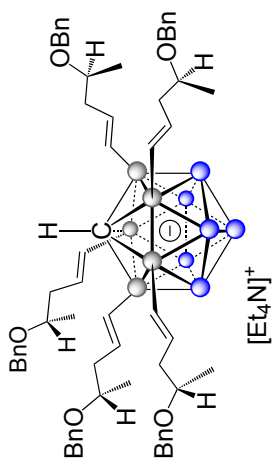
Date_ 20181025
 Time 10.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 64
 DS 0
 SWH 32051.281 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 203
 DW 15.600 usec
 DE 6.50 usec
 TE 296.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec

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

=====
 CHANNEL f2 =====
 CPDPRG [2] waltz16
 NUC2 ¹H
 P2 80.00 usec
 PCPD2 19.00000000 W
 PLW2 0.40639001 W
 PLW12 0.26008999 W
 PLW13 0.26008999 W
 SFO2 500.1325007 MHz

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

13.86
 10.39
 8.47



penta-S-penten-ol-de product, 30 mg in 0.6 ml acetone-d6*
¹³C{¹H} NMR, 126 MHz, 23 C

Current Data Parameters
 NAME Penta-S-penten-ol-de
 EXPNO 4
 PROCNO 1

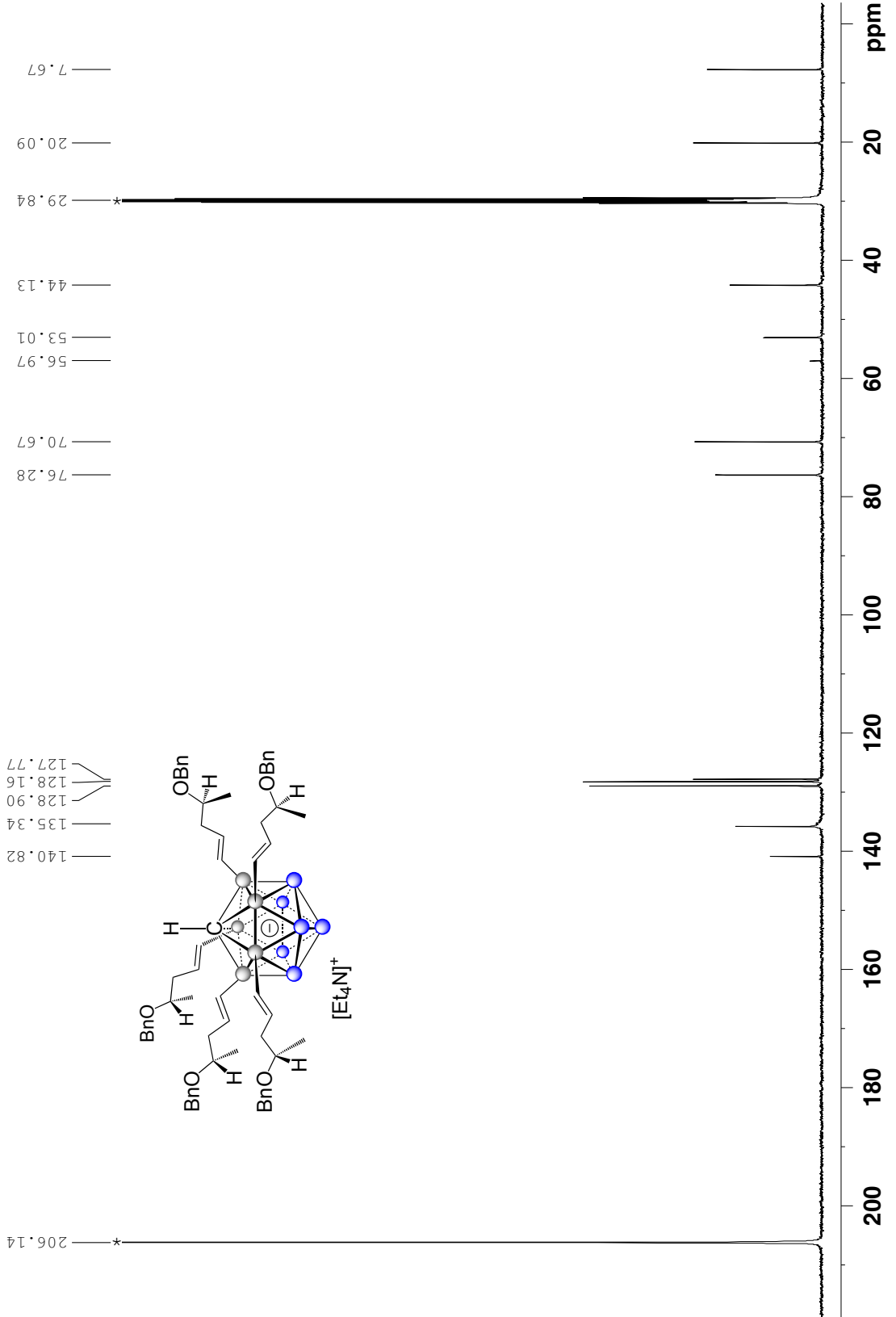
F2 - Acquisition Parameters

Date_ 20181025
 Time 11.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 2048
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.3 K
 DI 1.50000000 sec
 D11 0.03000000 sec

==== CHANNEL f1 =====
 NUC1 13C
 PL 10.50 usec
 PLW1 95.00000000 W
 SFO1 125.7716224 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PL 80.00 usec
 PLW2 19.00000000 W
 PLW3 0.40639001 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7576787 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



penta-4-F-styrene-H product, 50 mg in 0.6 ml acetone-d6*
 $^1\text{H}\{^1\text{B}\}$ NMR, 400 MHz, 23 C

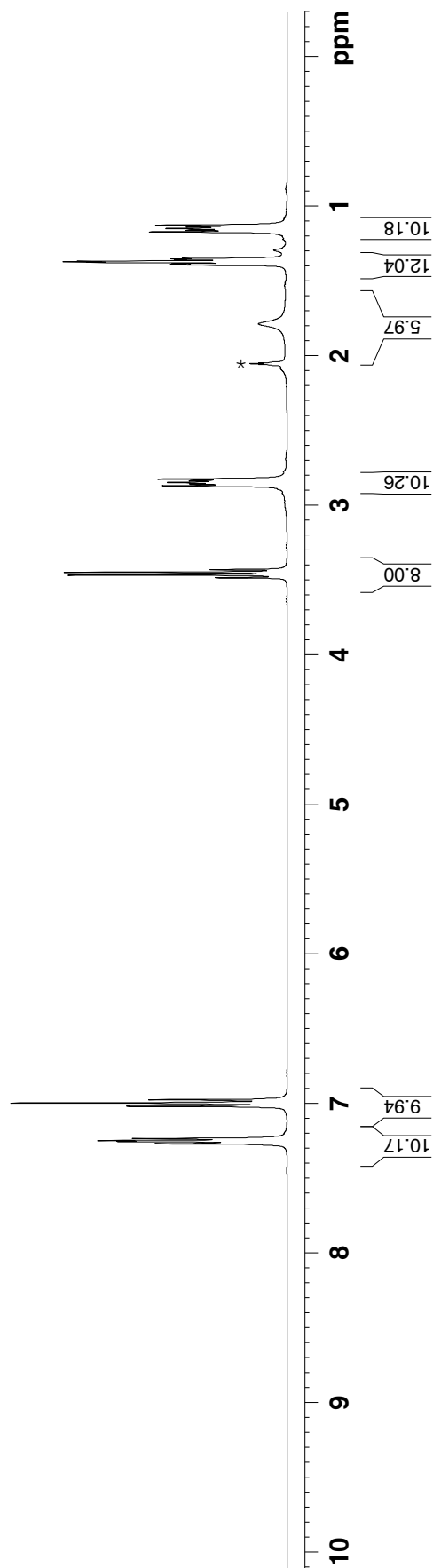
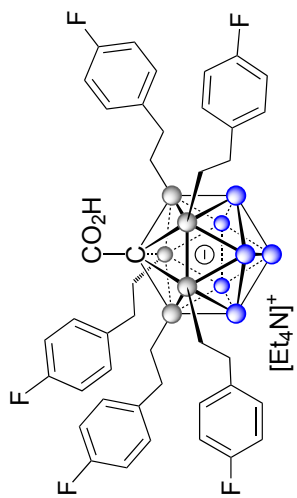
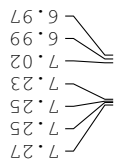
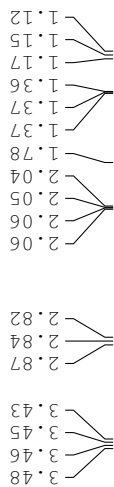
Current Data Parameters
 NAME Pentac-4-F-styrene-H
 EXNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180804
 Time 16:57
 INSTRUM spect
 PROBHID 5 mm FAPBBO BB
 PULPROG zgpg30
 F1 16184
 SOLVENT Acetone
 NS 4
 DS 4
 SWH 8012.826 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 71.39
 DW 62.400 usec
 DE 26.52 usec
 TE 285.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

==== CHANNEL f2 =====
 CPDPRG[2] garr4
 NUC2 ^1H
 PCD2 90.00 usec
 PLW2 52.96599960 MHz
 PLW2 0.64477898 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300072 MHz
 WDW EM
 SSB 0
 GB 0
 CB 0
 PC 1.40



**penta-4-F-styrene-H product, 50 mg in 0.6 ml acetone-d6
11B NMR, 128 MHz, 23 C**

```

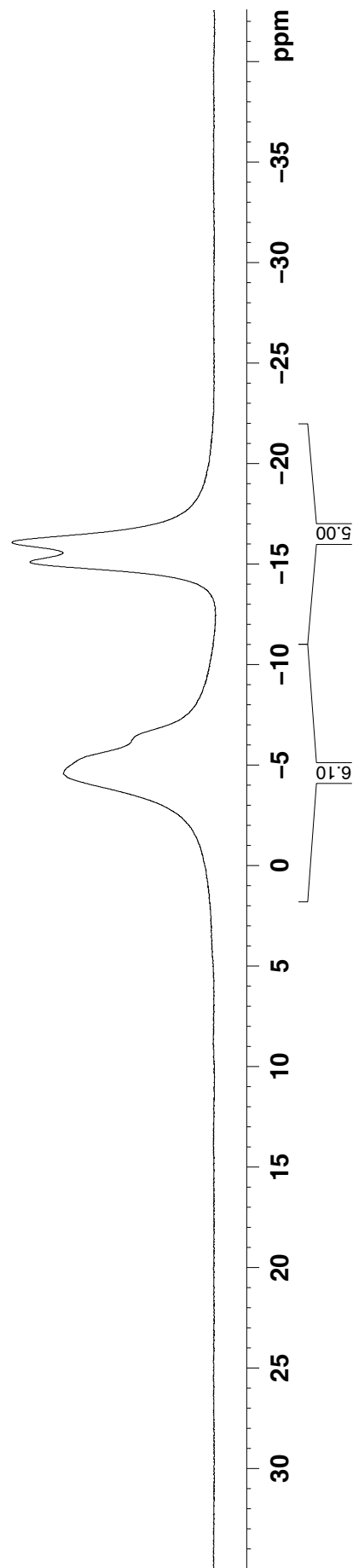
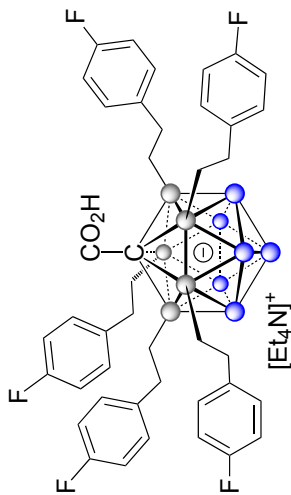
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NAME      penta-4-F-styrene-H
EXPNO    3
PROCNO   1

F2 - Acquisition Parameters
Date_    20180804
Time     17.01
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       1.9650 usec
TE       294.7 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     11B
P1       9.03 usec
PL1      52.9659960 W
SFO1     128.3776052 MHz

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

-4.59
 -6.41
 -15.13
 -16.08



**penta-4-F-styrene-H product, 50 mg in 0.6 ml acetone-d6
¹¹B{¹H} NMR, 128 MHz, 23 C**

```

Current Data Parameters
NAME      penta-4-F-styrene-H
EXPNO    4
PROCNO   1

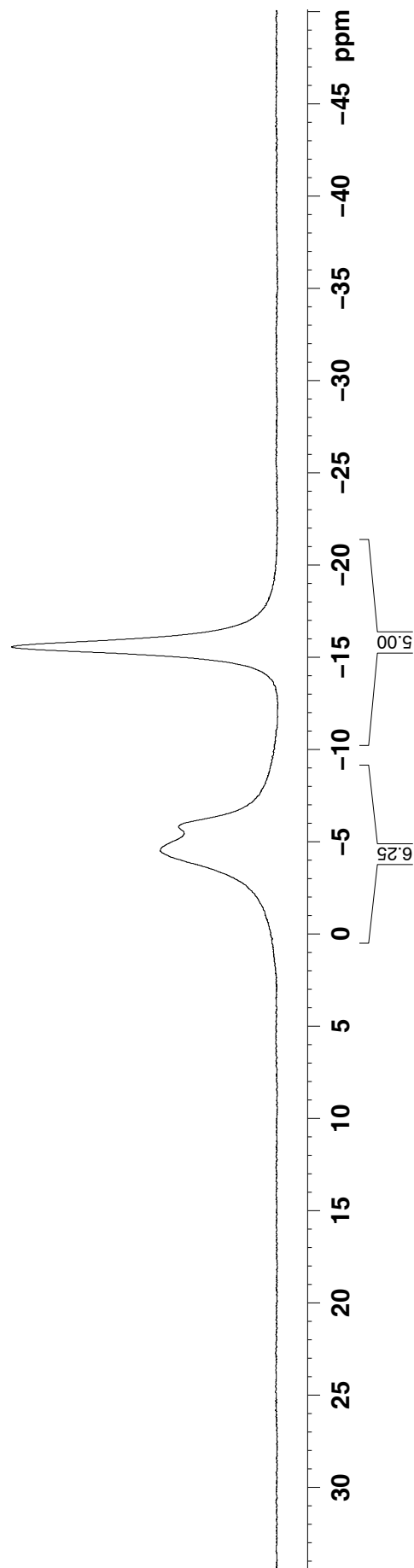
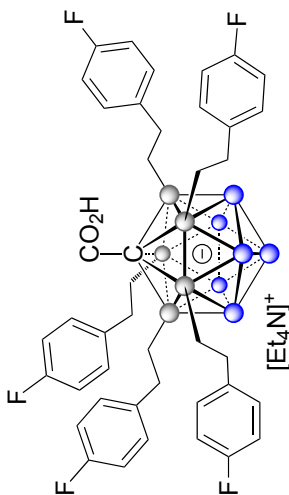
F2 - Acquisition Parameters
Date_    20180804
Time     17.09
INSTRUM  spect
PROBHD   5 mm PABBO BB
PULPROG  zgpg30
TD       65536
SOLVENT  Acetone
NS       124
DS       12
SWH      25510.203 Hz
FIDRES   0.389255 Hz
AQ       1.2845056 sec
RG       193.34
RW       19.600 usec
DE       19.650 usec
TE       298.56 K
D1       1.00000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     11B
P1       9.19 usec
PLM1     52.9659960 W
SFO1     128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2  waitz16
NUC2     1H
P2       80.00 usec
PLM2     12.50000000 W
SFO2     400.1320007 MHz

F2 - Processing parameters
SI       32768
SF       128.3776050 MHz
WDW      EM
SSB      0
LB       4.00 Hz
GB       0
PC       1.40
  
```

15.59
 5.81
 4.52



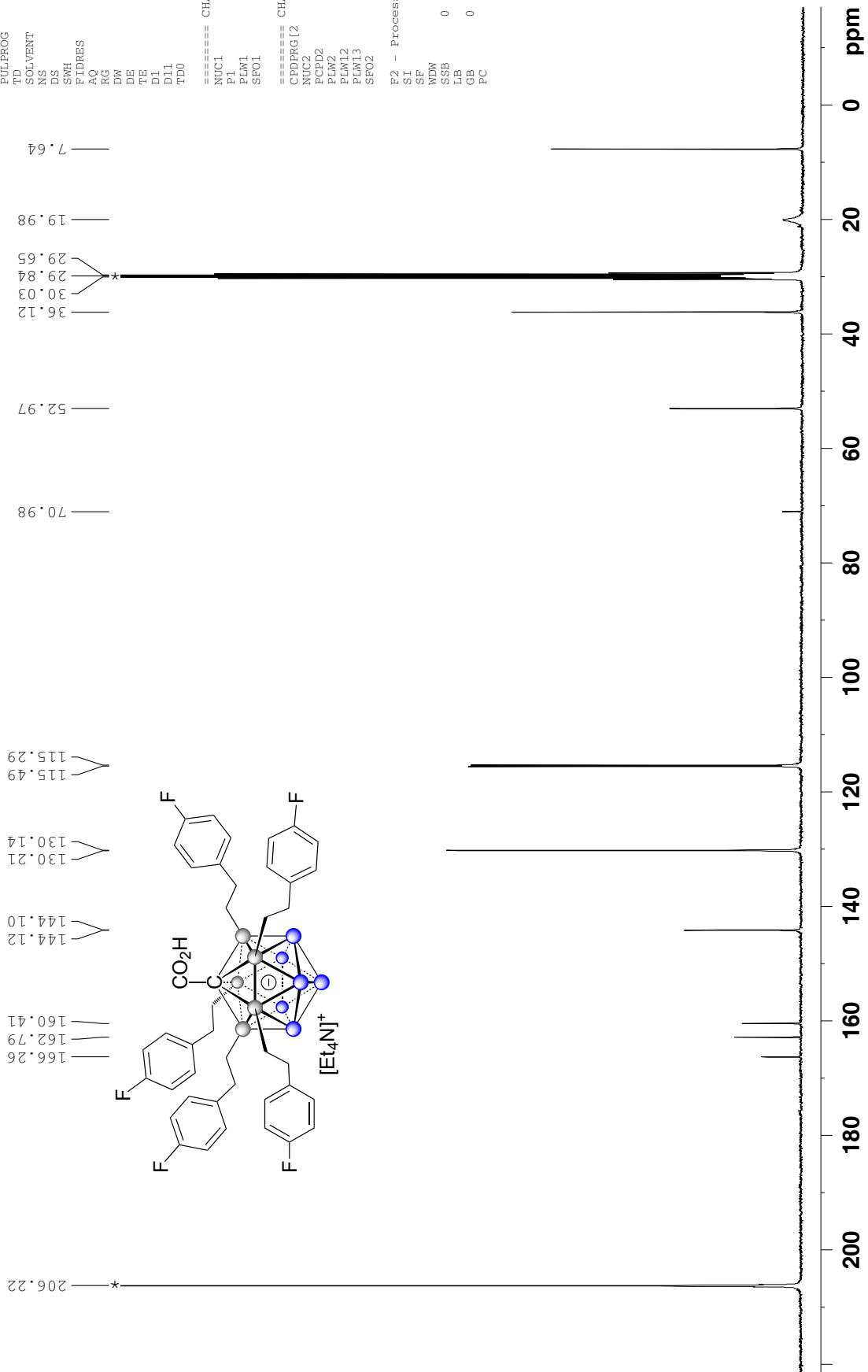
penta-4-F-styrene-H product, 50 mg in 0.6 ml acetone-d6 *
¹³C{¹H} NMR, 101 MHz, 23 C

Current Data Parameters
 NAME penta-4-F-styrene-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180804
 Time_ 18.41
 INSTRUM spect
 PROBDH 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 295.6 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 53.0000000 W
 SFO1 100.6228293 MHz
 ===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 P2 80.00 usec
 PCPD2 12.5000000 W
 PLW2 0.43945000 W
 PLW13 0.28125000 W
 SFO2 400.1316005 MHz

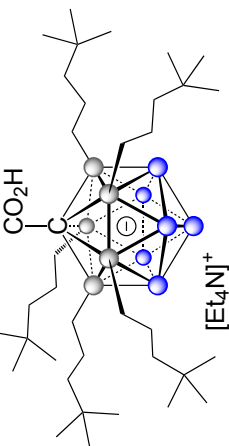
F2 - Processing parameters
 SI 32768
 SF 100.6126829 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40



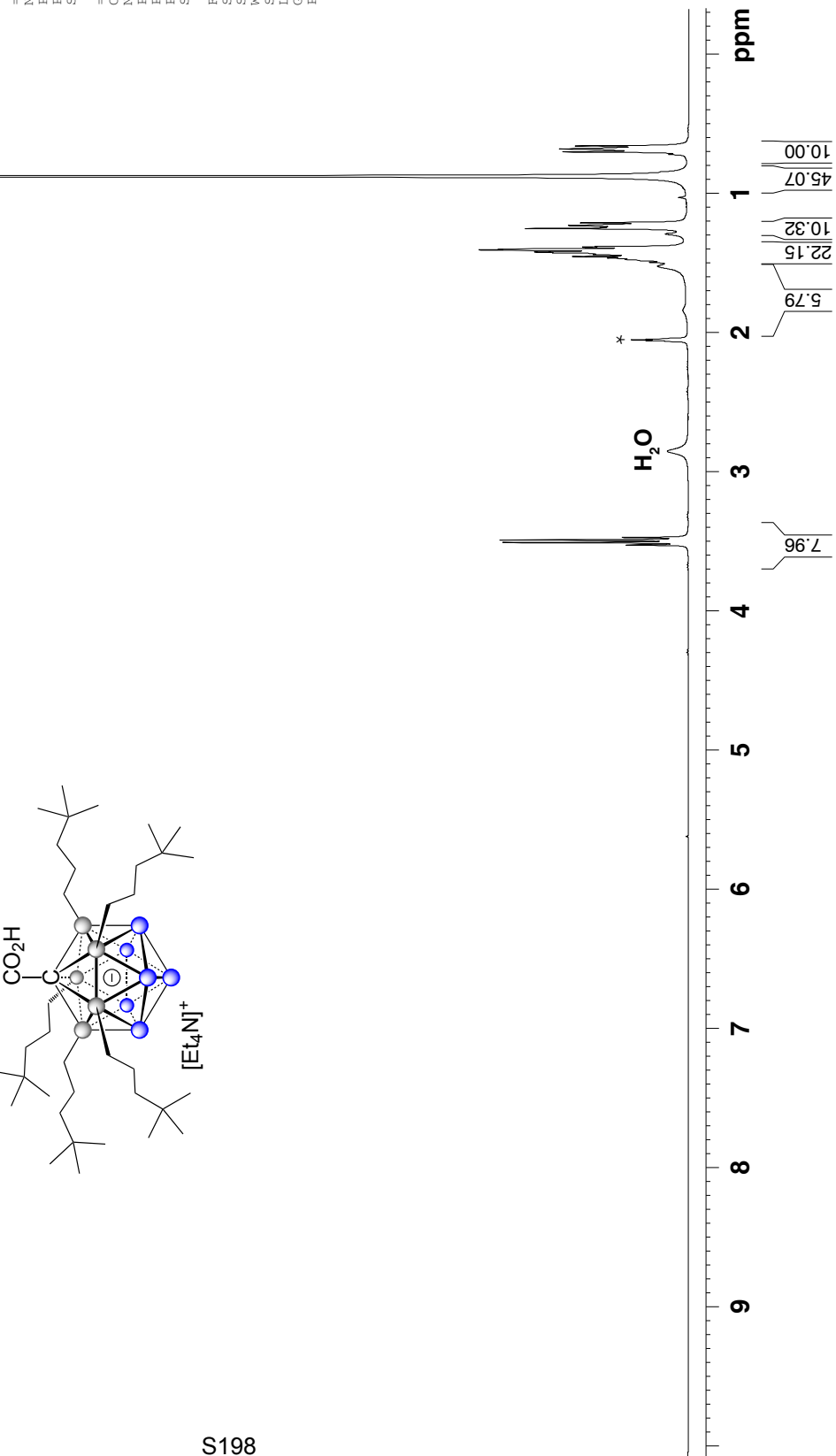
penta-4,4-Dimethylpent-1-en-1-H product, 30 mg in 0.6 ml acetone-d6 *
¹H{¹³B} NMR, 400 MHz, 23 C

Current Data Parameters
 NAME penta-4,4-Dimethylpent-1-ε
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180804
 Time 14:20
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 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 294.9 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1



3.52
3.51
3.49
3.47
2.85
2.06
2.05
2.04
1.84
1.42
1.41
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1.40
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1.23
1.23
1.21
0.87
0.70
0.68
0.66



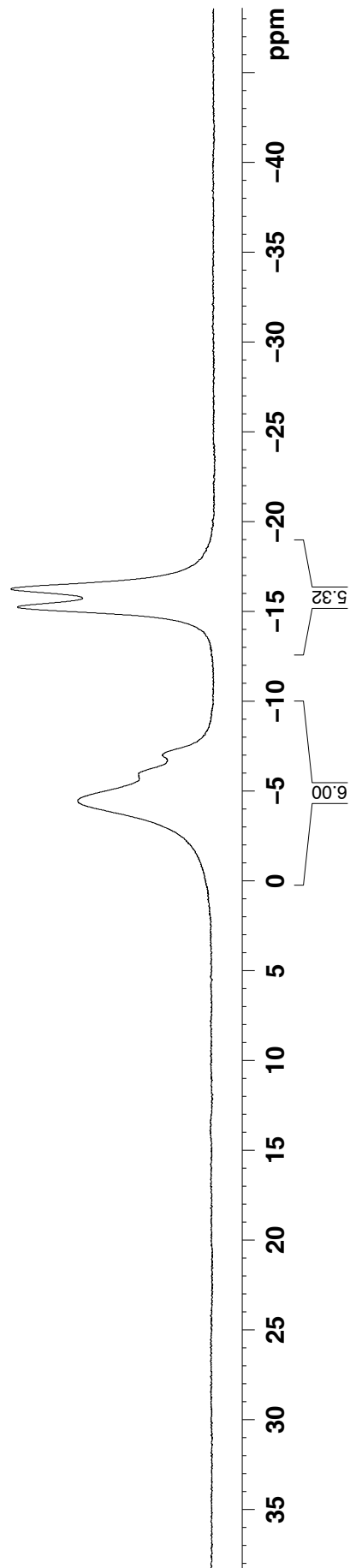
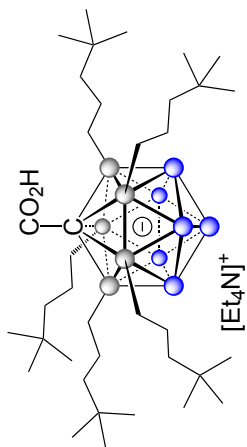
**penta-4,4-Dimethylpent-1-en-1-H product, 30 mg in 0.6 ml acetone-d6
 11B NMR, 128 MHz, 23 C**

Current Data Parameters
 NAME penta-4,4-Dimethylpent-1-en-1-H
 EXPNO 3
 PROCNO 1

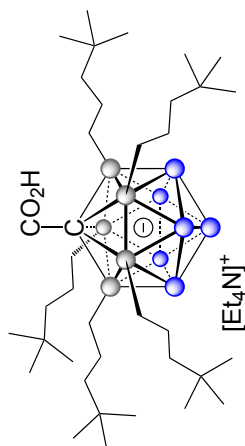
F2 - Acquisition Parameters
 Date_ 20180804
 Time 14.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 294.8 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SF01 128.3776052 MHz

F2 - Processing parameters
 SI 32768
 SF 128.3776050 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



**penta-4,4-Dimethylpent-1-en-1-yl product, 30 mg in 0.6 ml acetone-d6
 11B{1H} NMR, 128 MHz, 23 C**



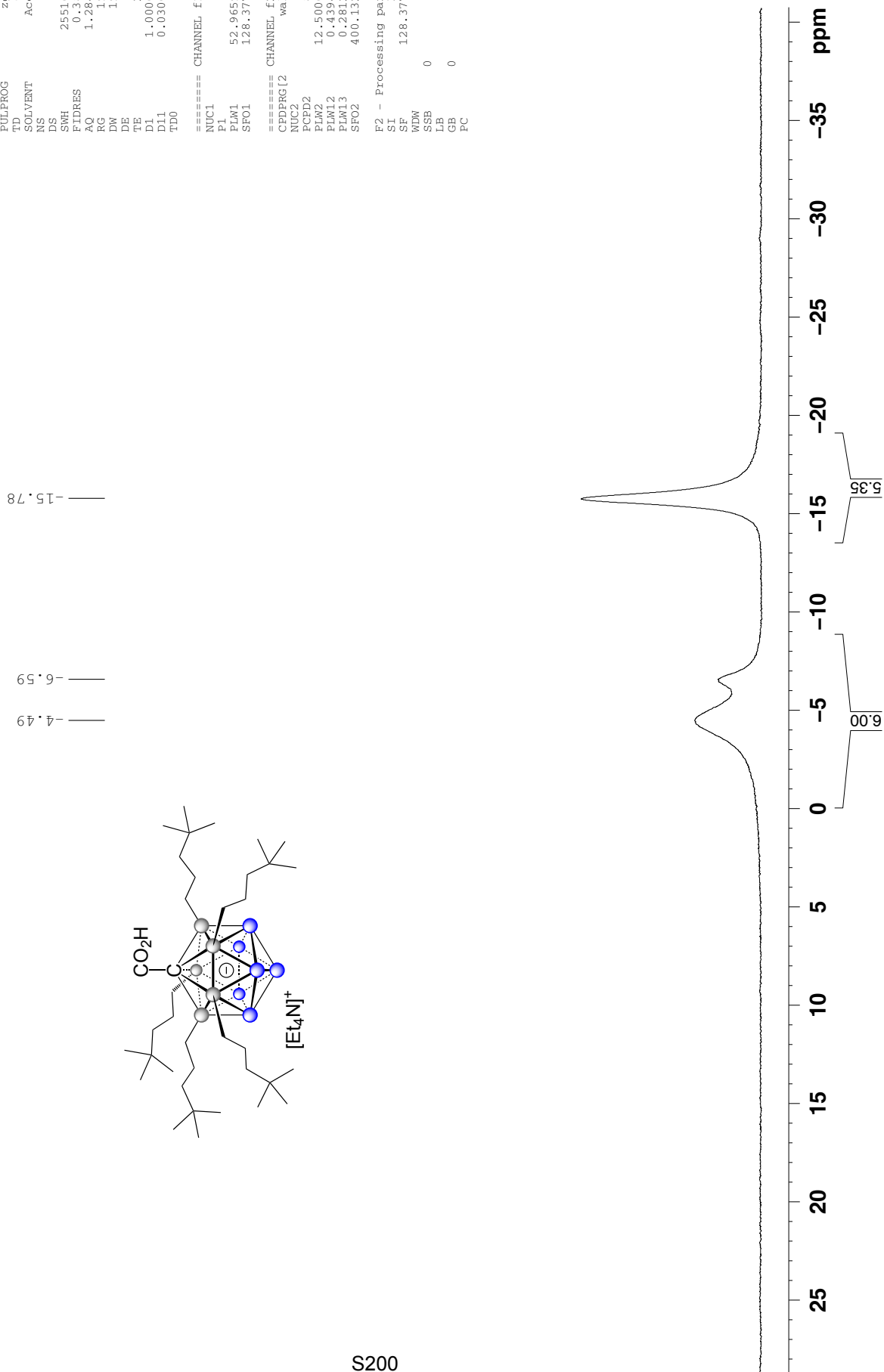
Current Data Parameters
 NAME penta-4,4-Dimethylpent-1-yl
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180804
 Time 14.32
 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 295.5 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 usec
 PLW1 52.9659960 W
 SFO1 128.3776050 MHz

===== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 1H
 P2 80.00 usec
 PLW2 12.5000000 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 4.00 Hz
 GB 0
 PC 1.40



penta-4,4-Dimethylpent-1-en-1-H product, 30 mg in 0.6 ml acetone-d6 *
¹³C{¹H} NMR, 101 MHz, 23 C

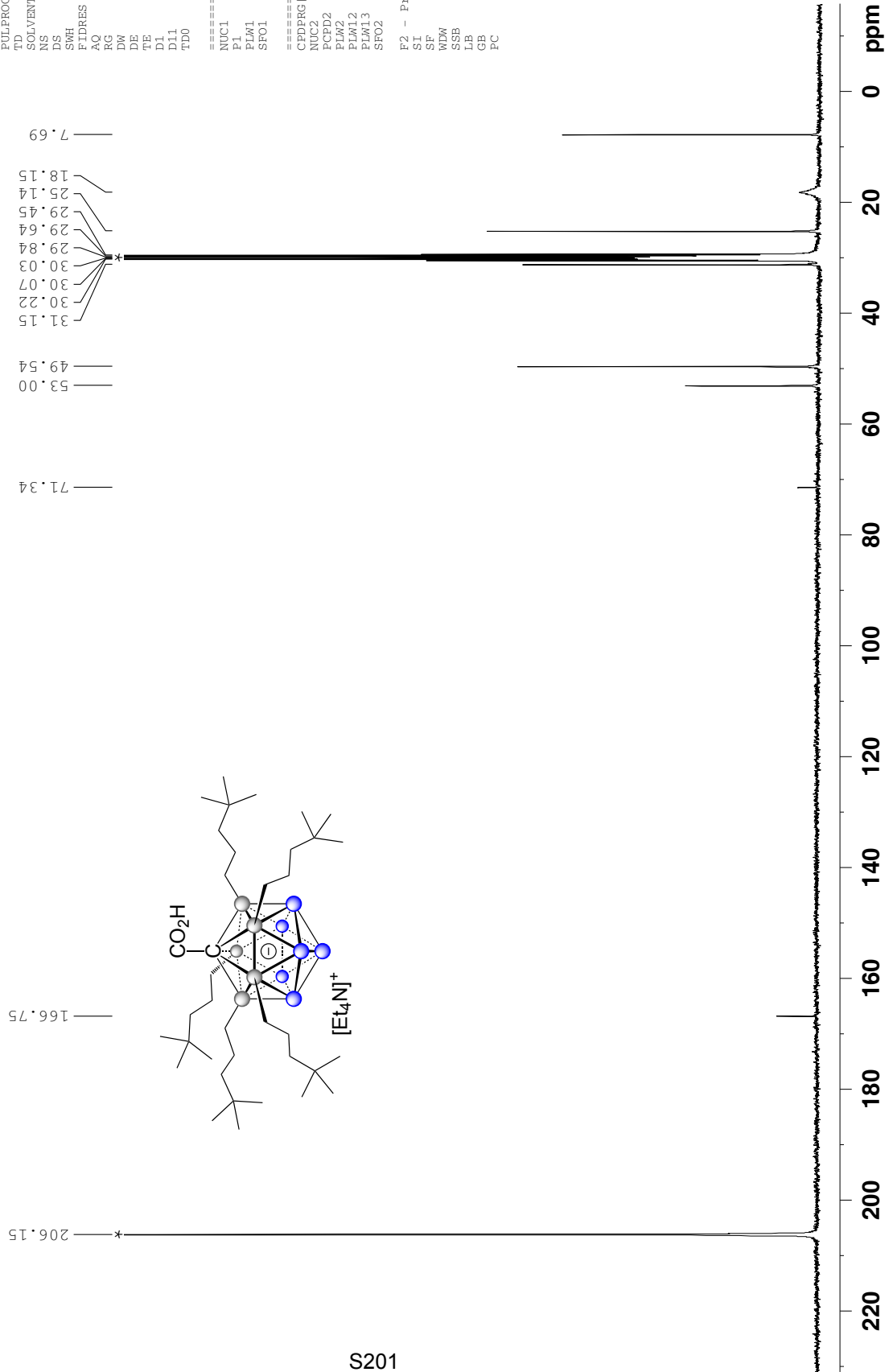
Current Data Parameters
 NAME penta-4,4-Dimethylpent-1-en
 EXPNO 5
 PROCNO 1

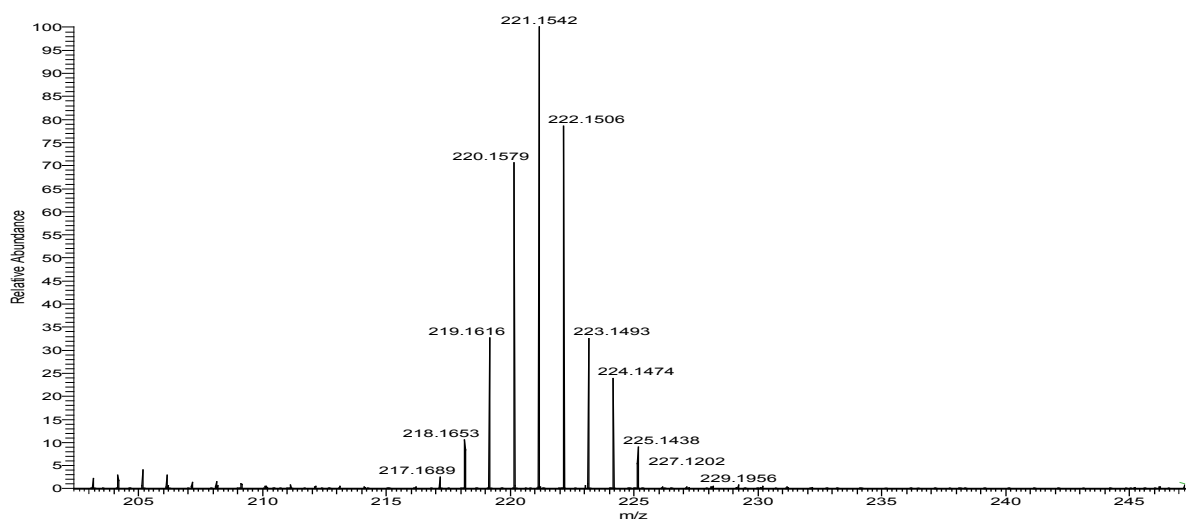
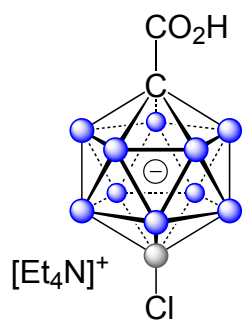
F2 - Acquisition Parameters
 Date_ 20180804
 Time 16.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 3072
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 295.6 K
 D1 1.5000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 53.0000000 W
 SFO1 100.6228293 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 P2 80.00 usec
 PLW2 12.5000000 W
 PLW12 0.43945000 W
 PLW13 0.28125000 W
 SFO2 400.1316005 MHz

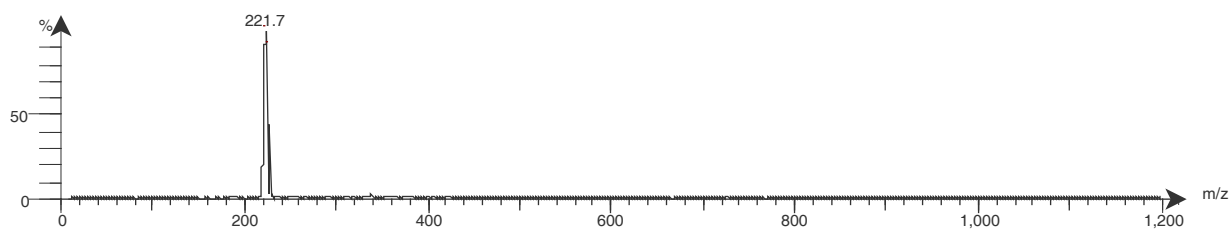
F2 - Processing parameters
 SI 32768
 SF 100.6126817 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



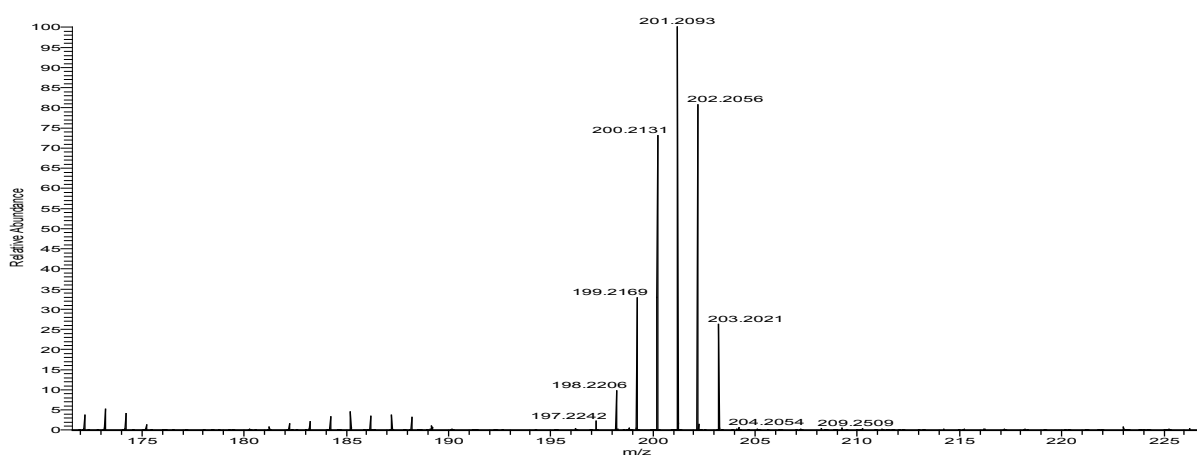
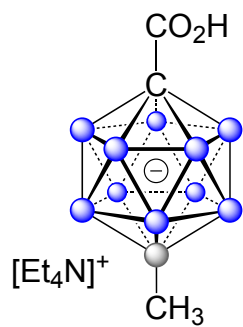


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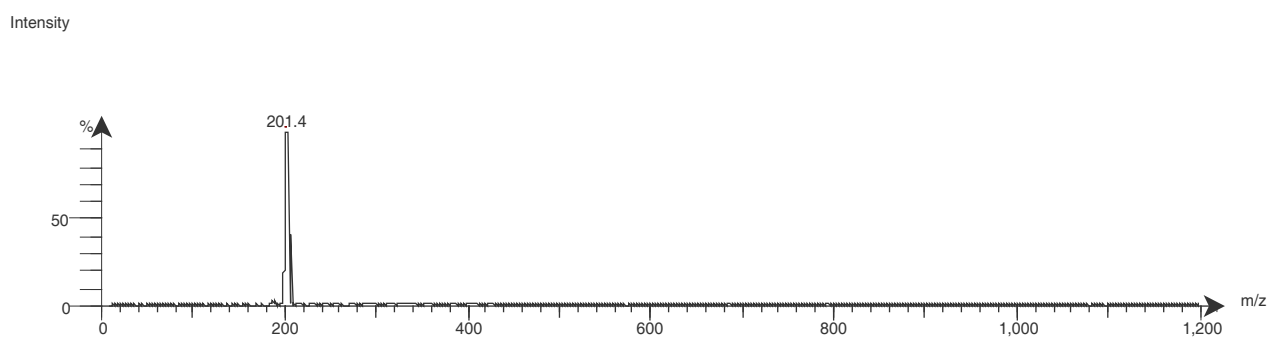
Intensity



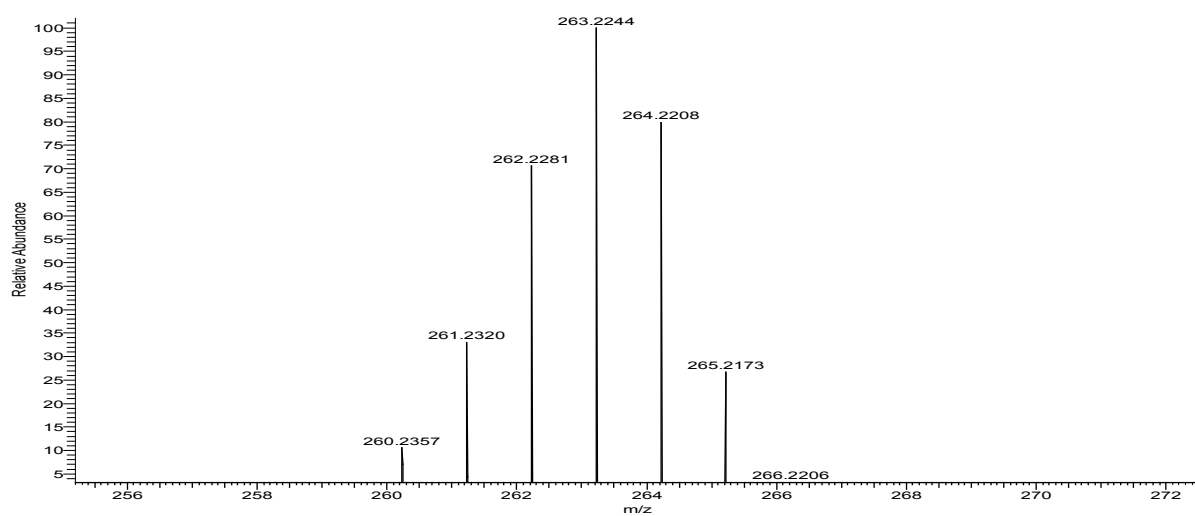
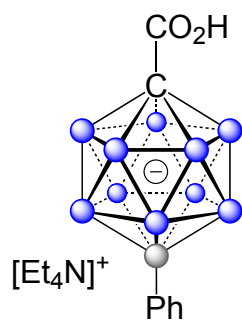
Full-range (-)-ESI-MS Expression CMS



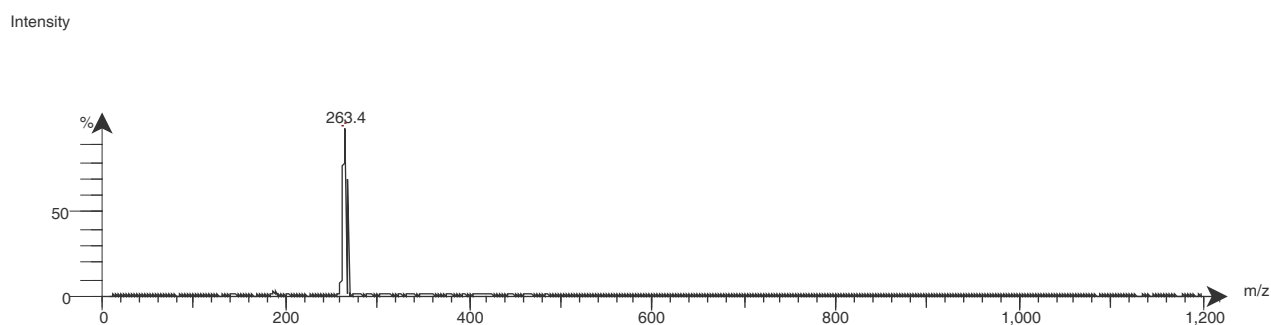
(-)-ESI-HRMS Shimadzu IT-TOF



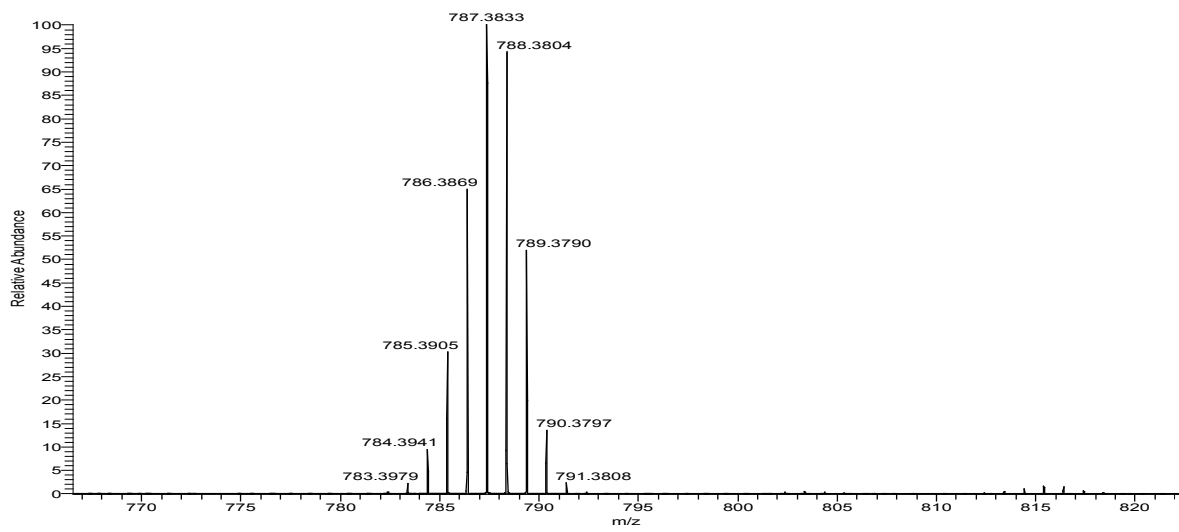
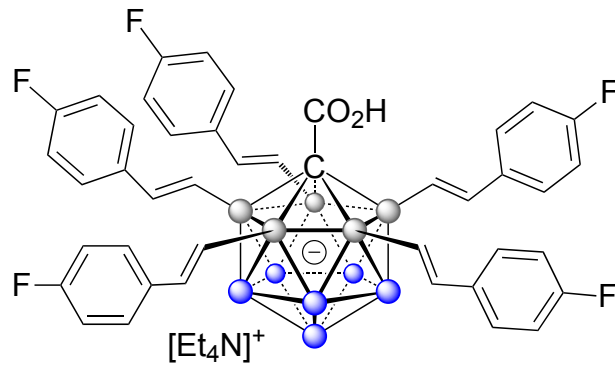
Full-range (-)-ESI-MS Expression CMS



(-)-ESI-HRMS Shimadzu IT-TOF

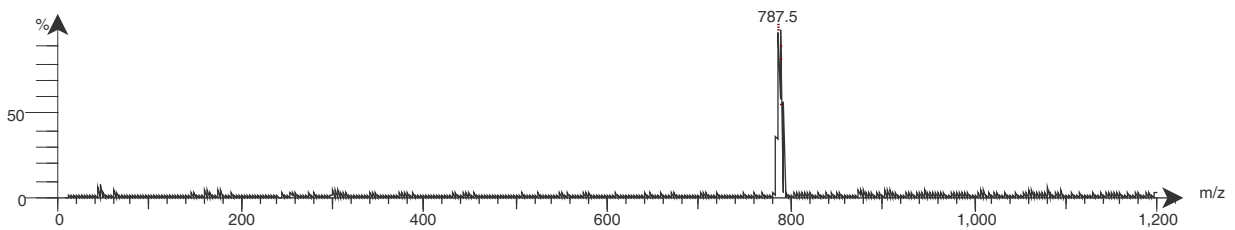


Full-range (-)-ESI-MS Expression CMS

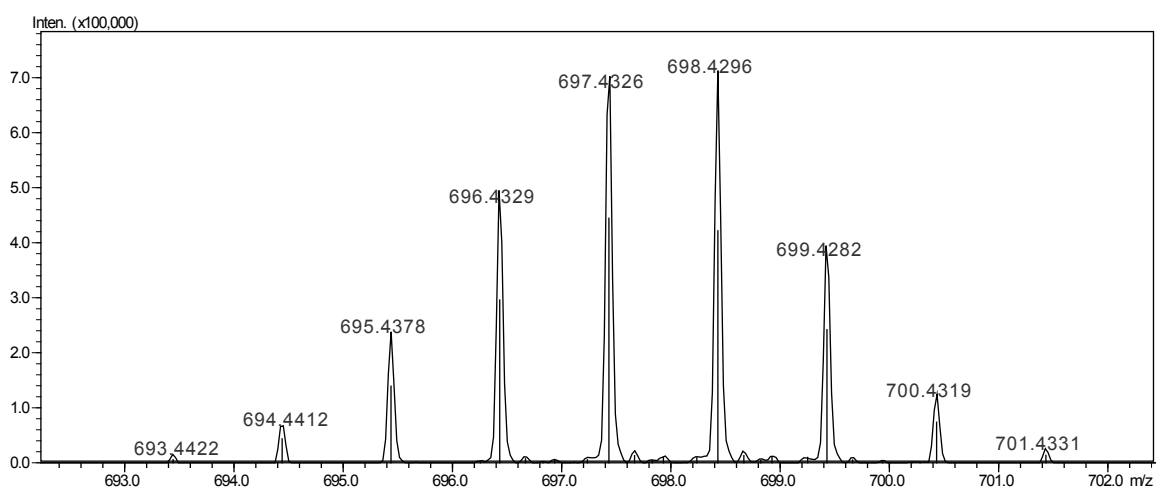
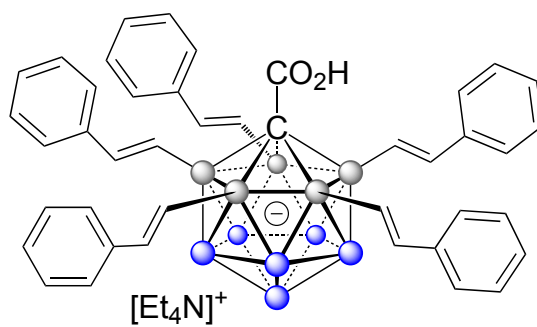


(-)-ESI-HRMS Shimadzu IT-TOF

Intensity

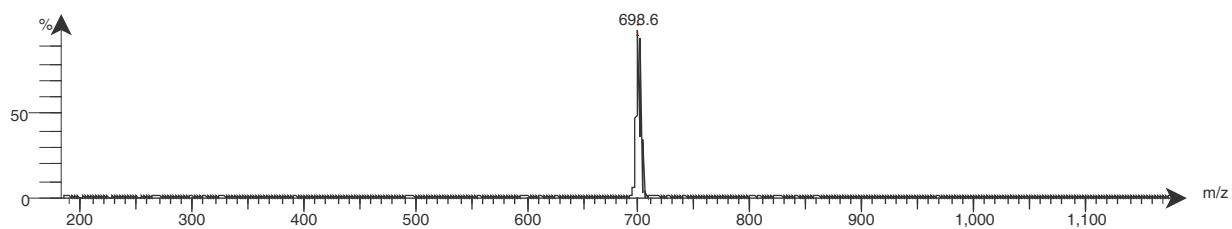


Full-range (-)-ESI-MS Expression CMS

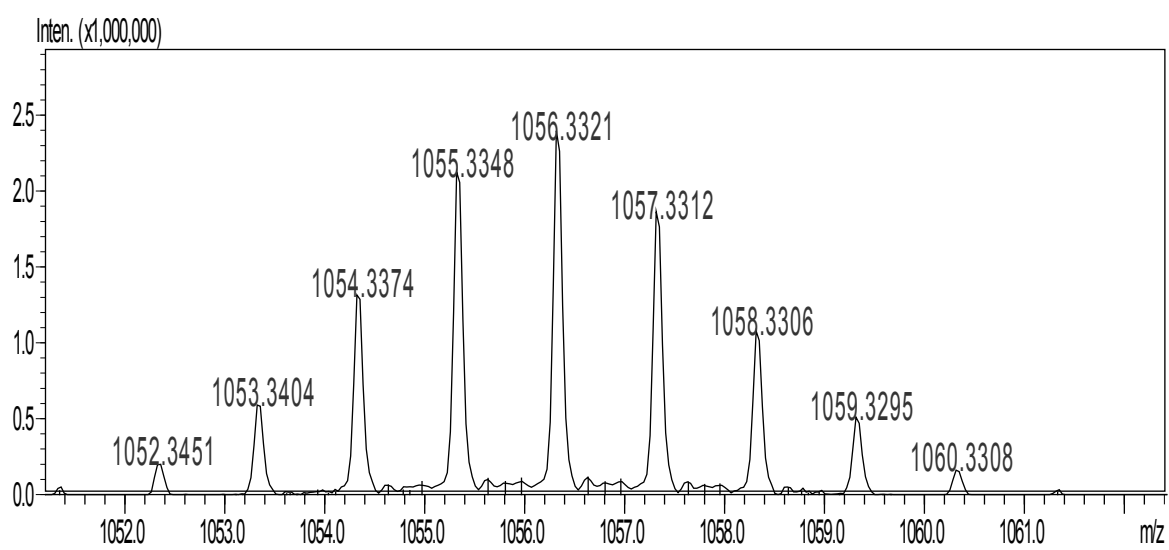
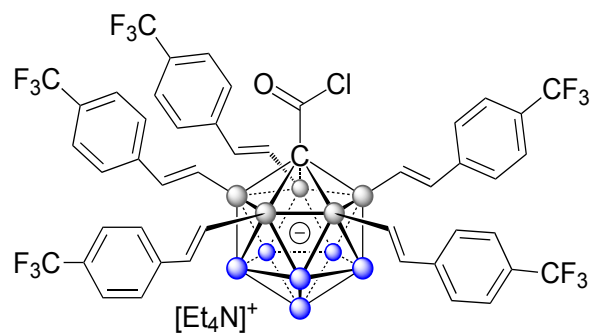


(-)-ESI-HRMS Shimadzu IT-TOF

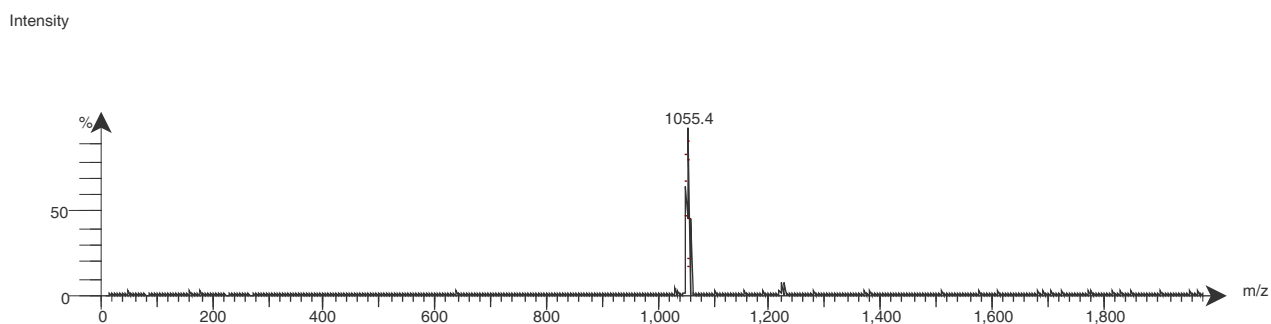
Intensity



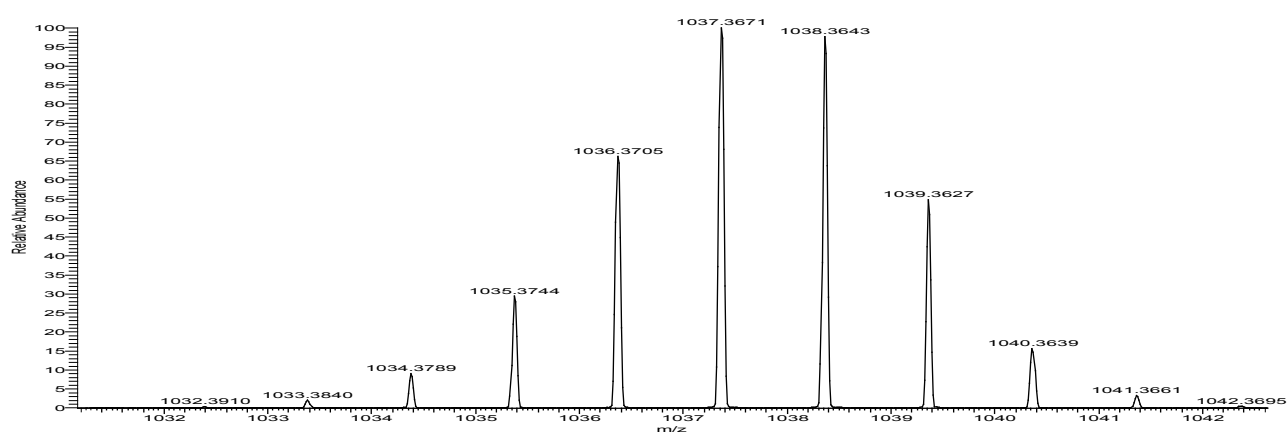
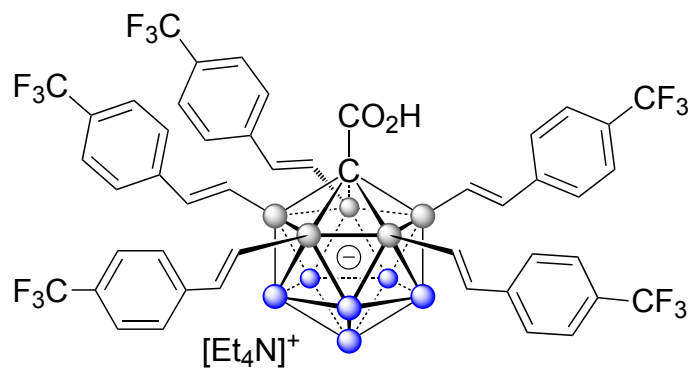
Full-range (-)-ESI-MS Expression CMS



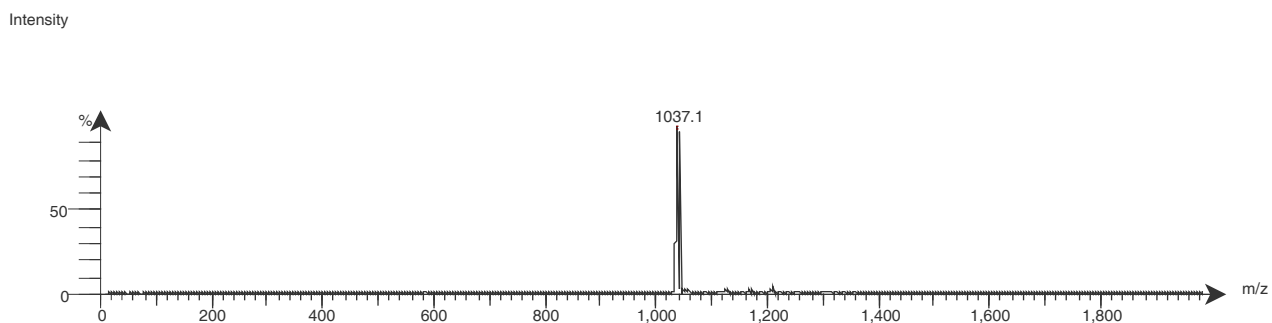
(-)-ESI-HRMS Shimadzu IT-TOF



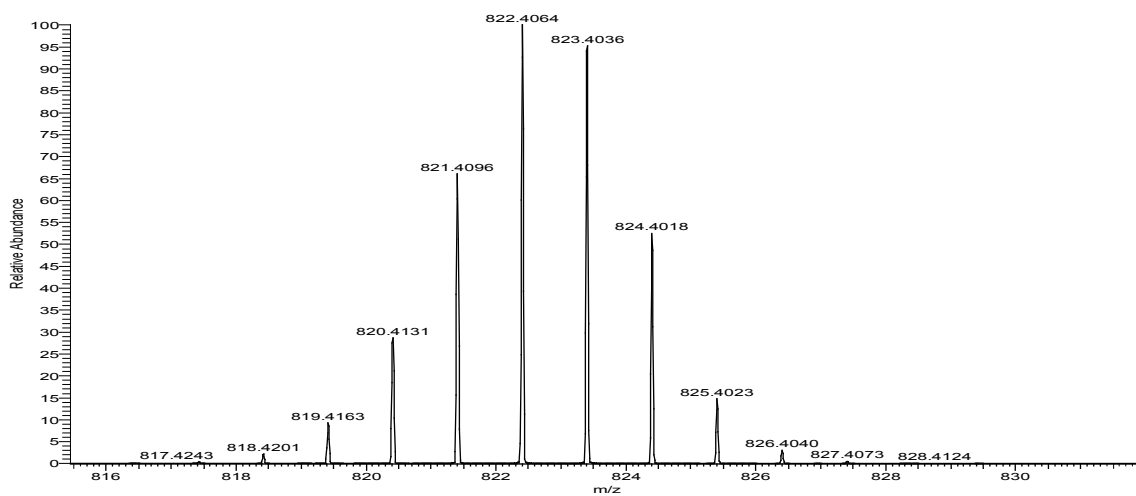
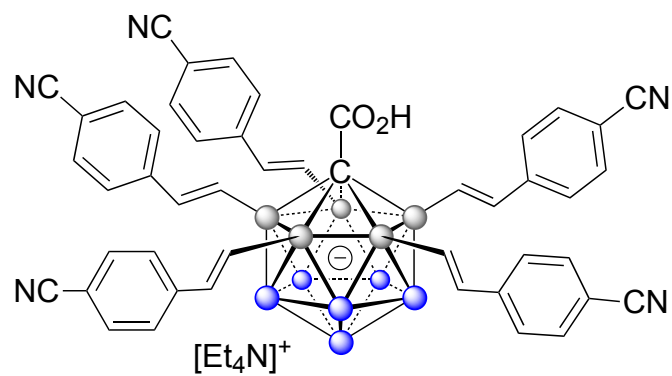
Full-range (-)-ESI-MS Expression CMS



(-)-ESI-HRMS Shimadzu IT-TOF

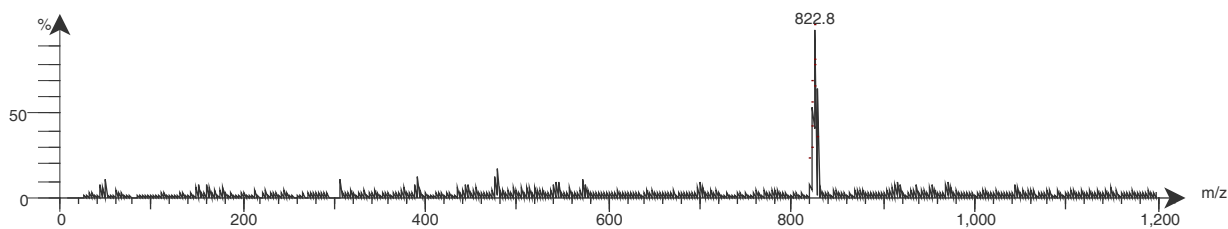


Full-range (-)-ESI-MS Expression CMS

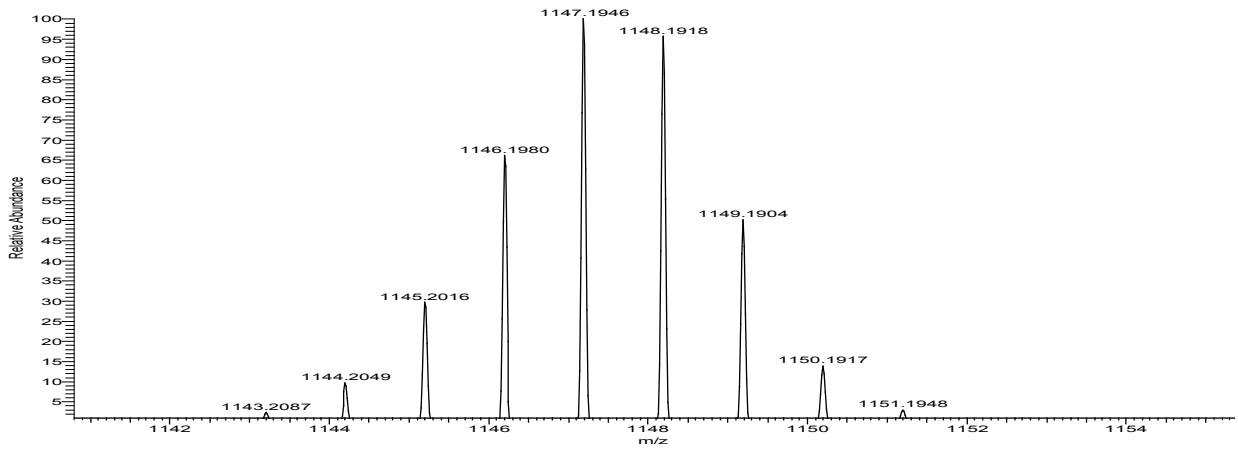
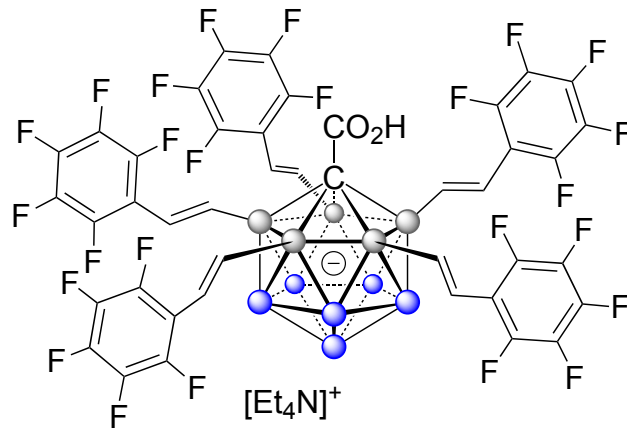


(-)-ESI-HRMS Shimadzu IT-TOF

Intensity

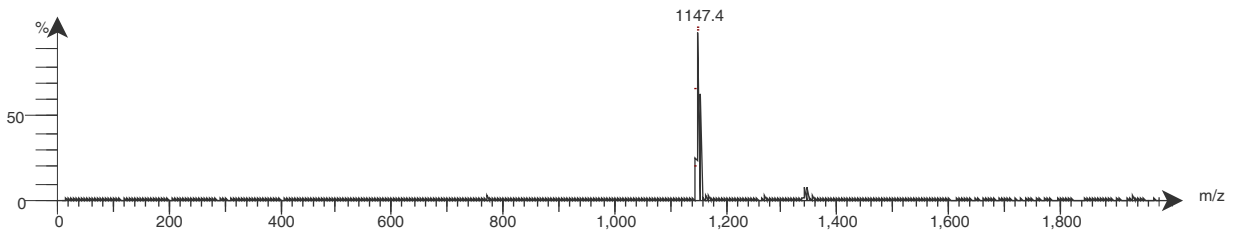


Full-range (-)-ESI-MS Expression CMS

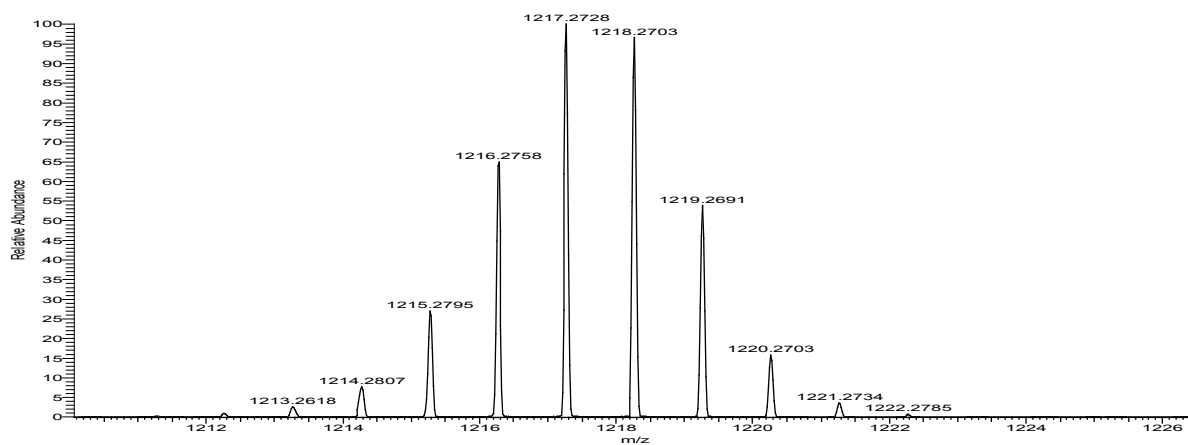
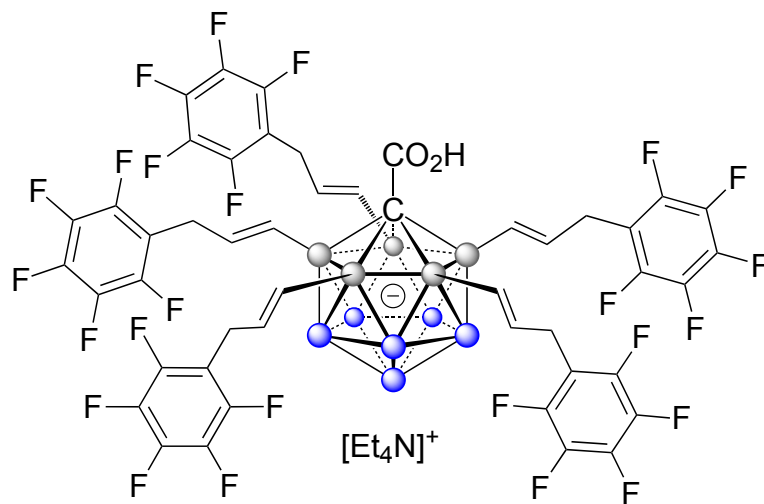


(-)-ESI-HRMS Shimadzu IT-TOF

Intensity

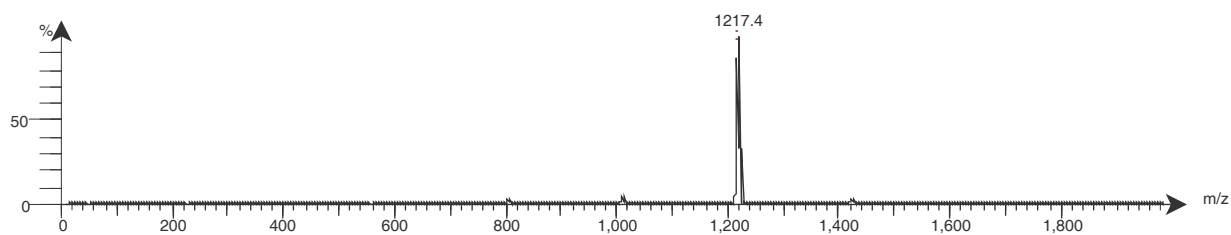


Full-range (-)-ESI-MS Expression CMS

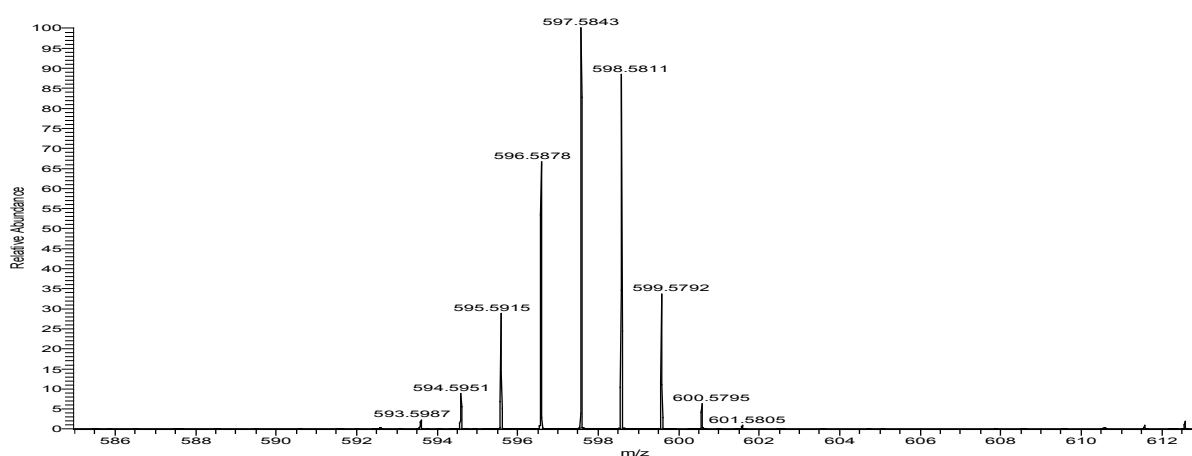
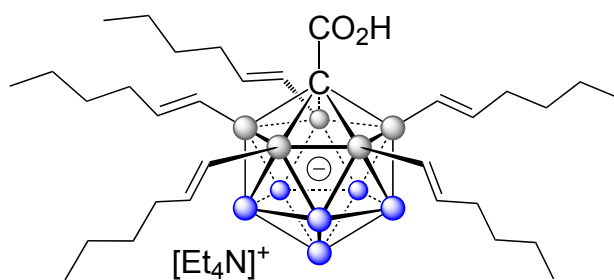


(-)-ESI-HRMS Shimadzu IT-TOF

Intensity

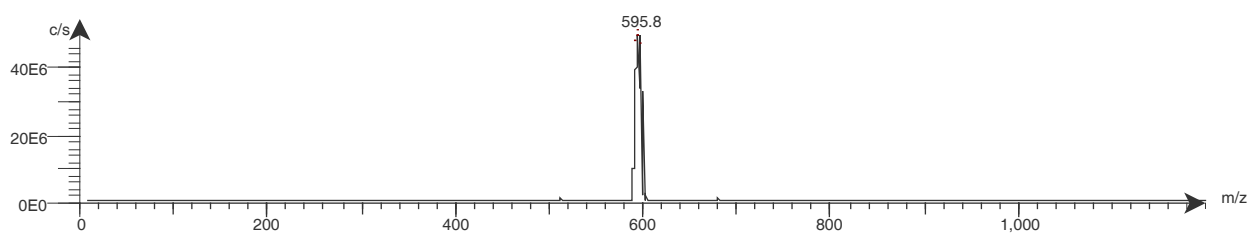


Full-range (-)-ESI-MS Expression CMS

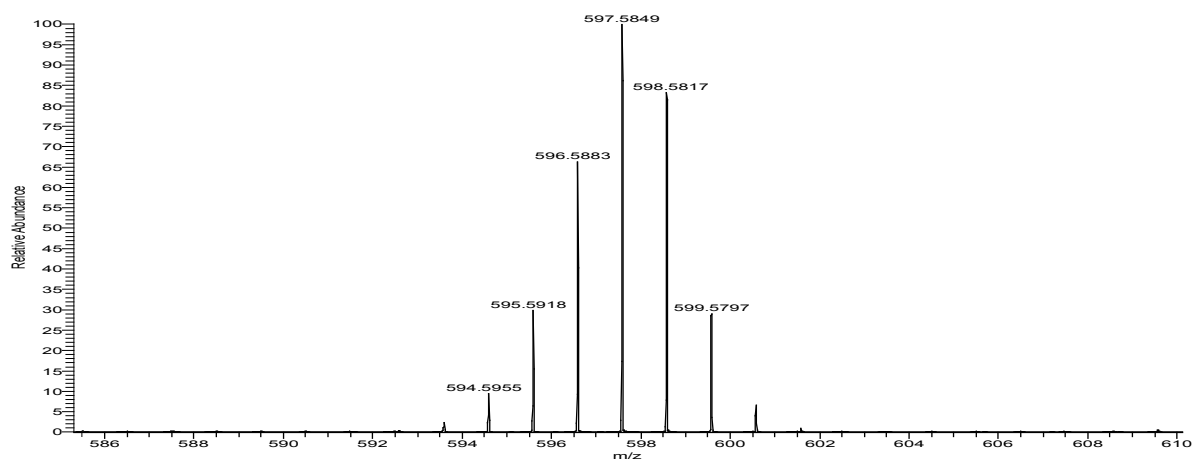
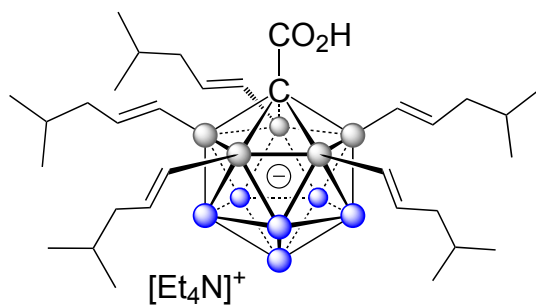


(-)-ESI-HRMS Shimadzu IT-TOF

Intensity

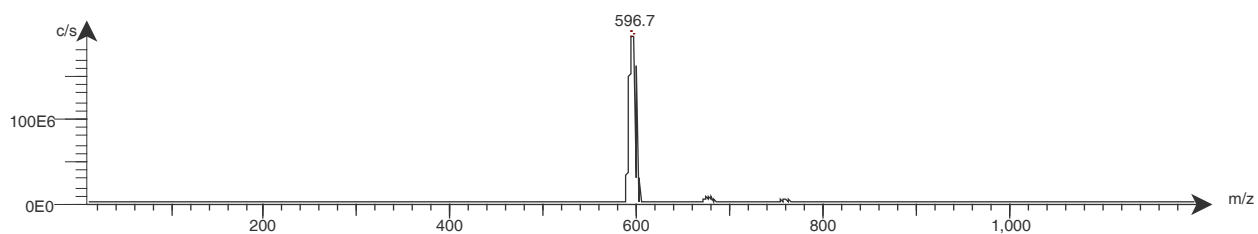


Full-range (-)-ESI-MS Expression CMS

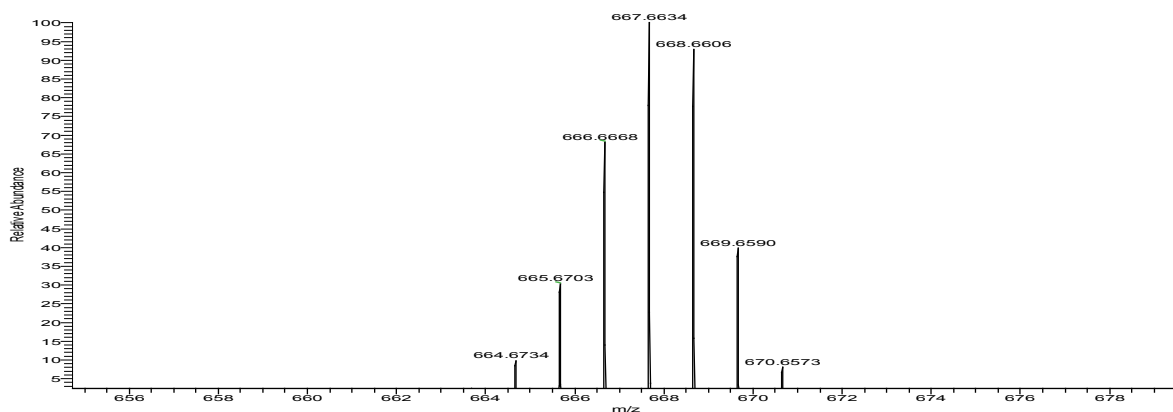
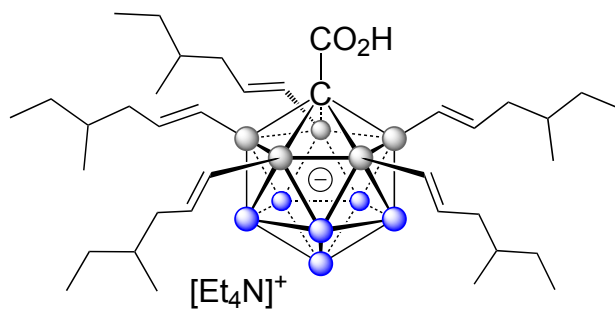


(-)-ESI-HRMS Shimadzu IT-TOF

Intensity

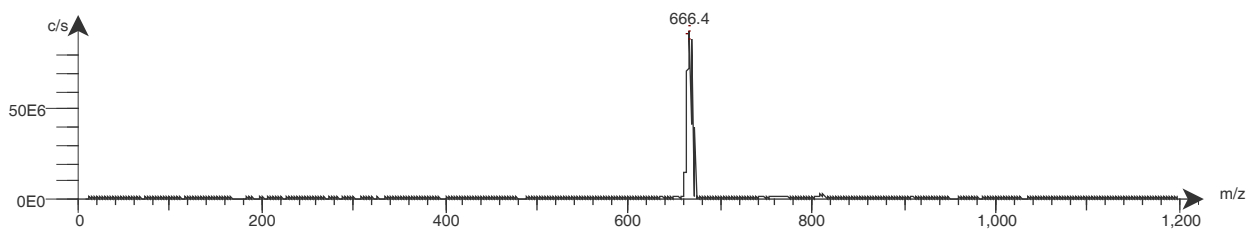


Full-range (-)-ESI-MS Expression CMS

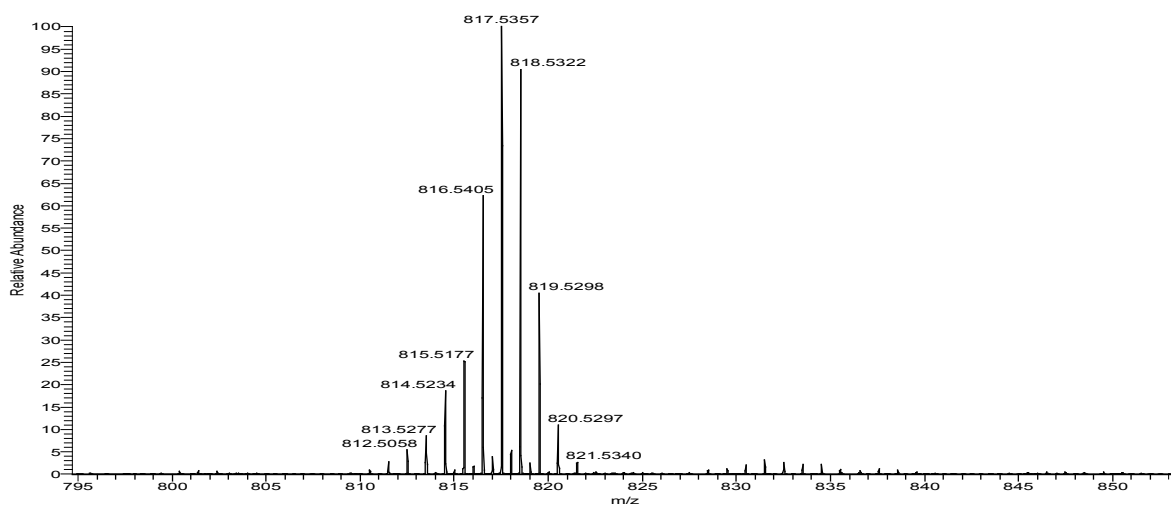
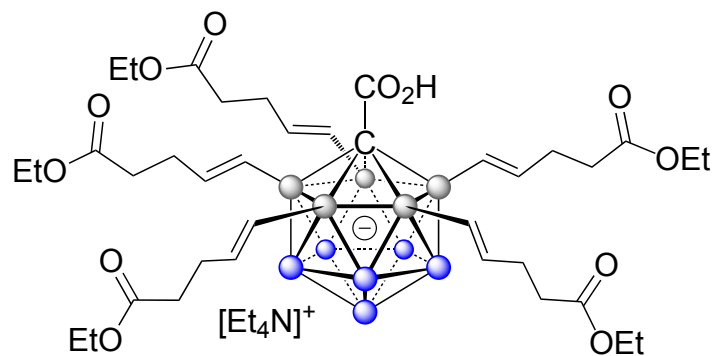


(-)-ESI-HRMS Shimadzu IT-TOF

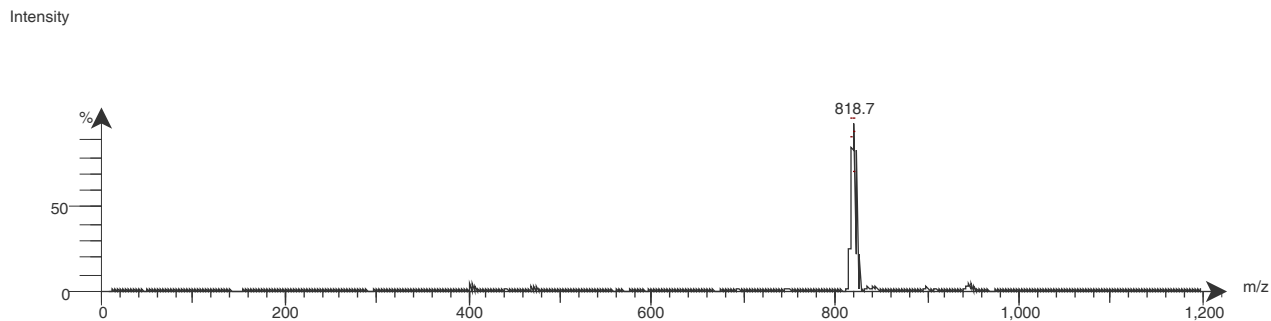
Intensity



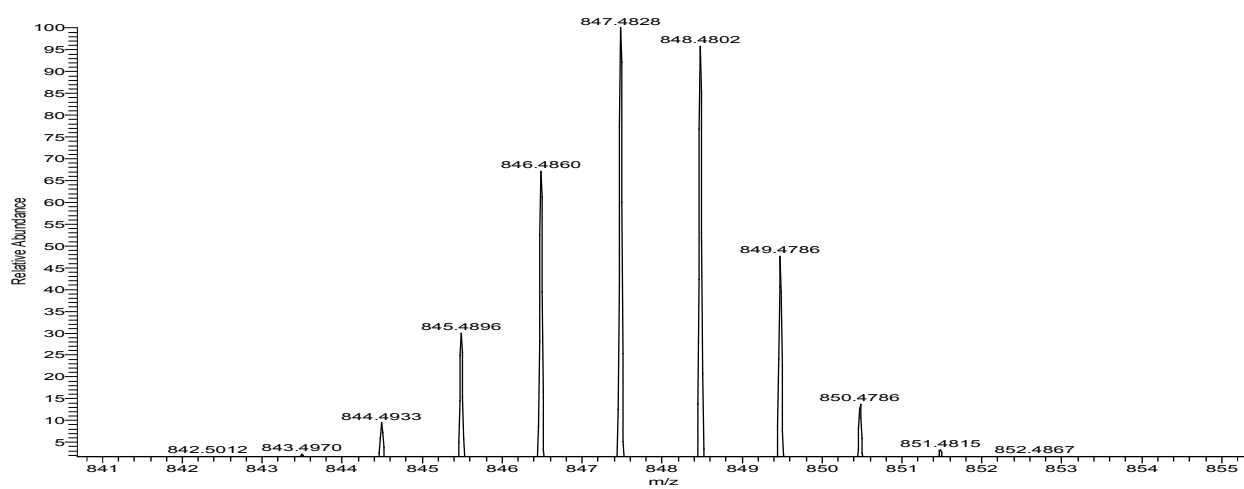
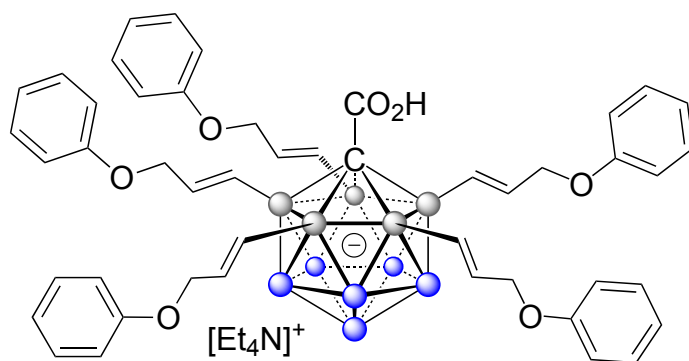
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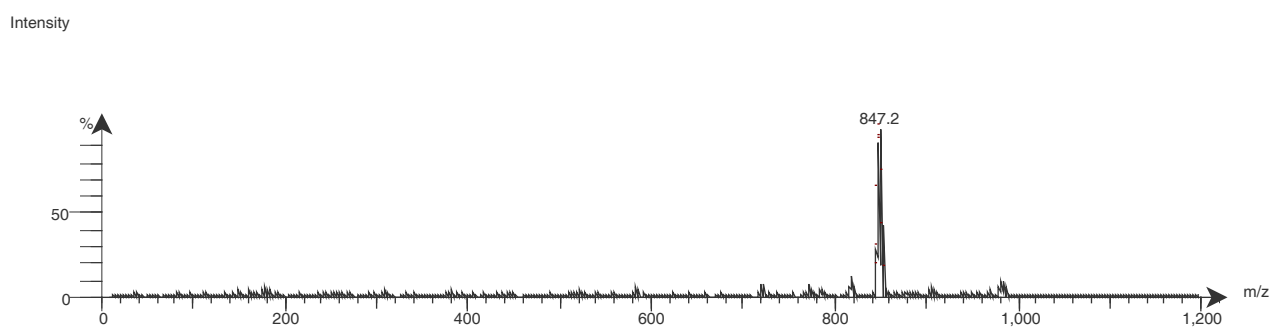
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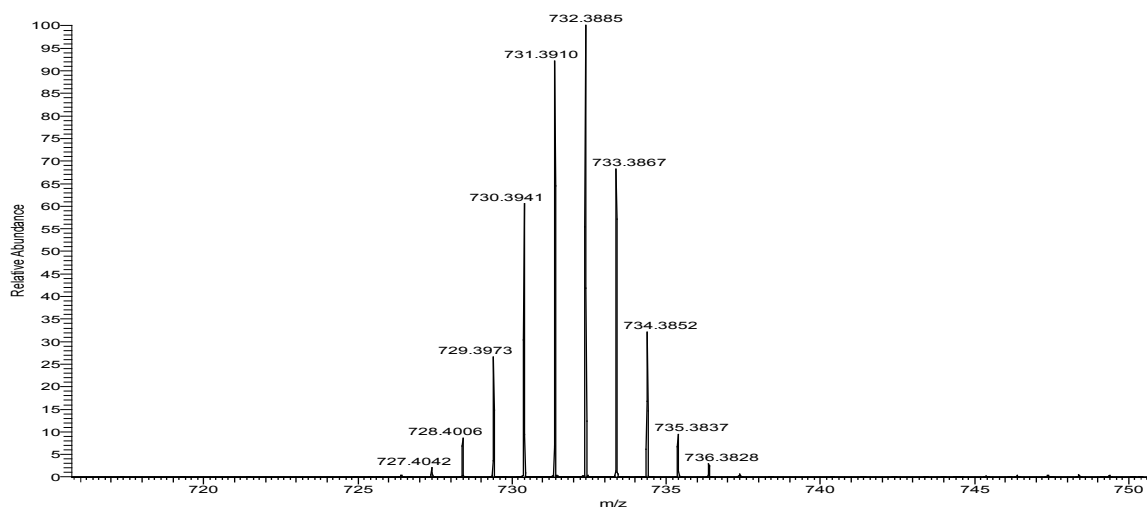
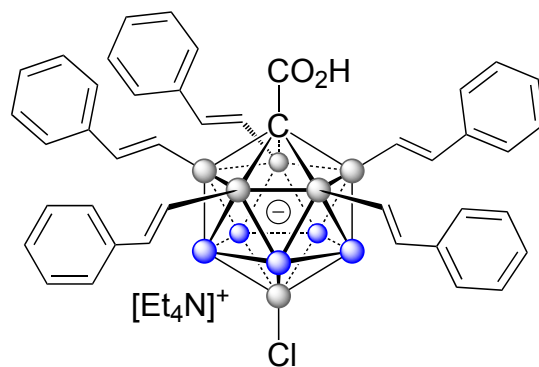
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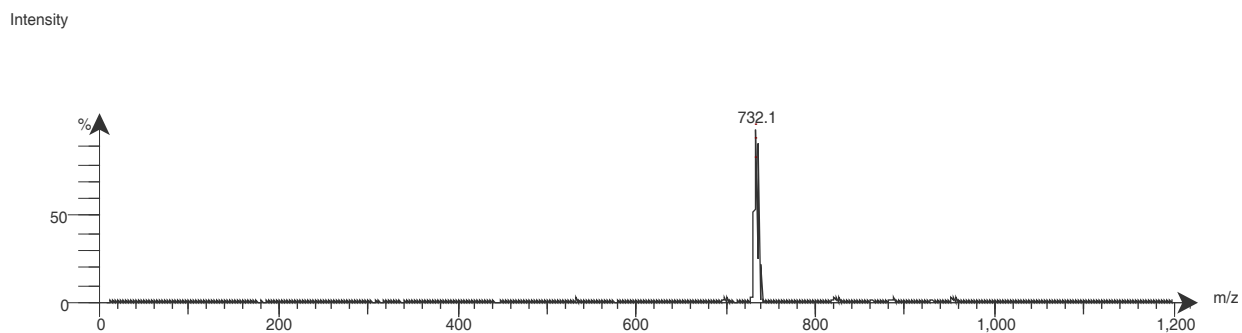
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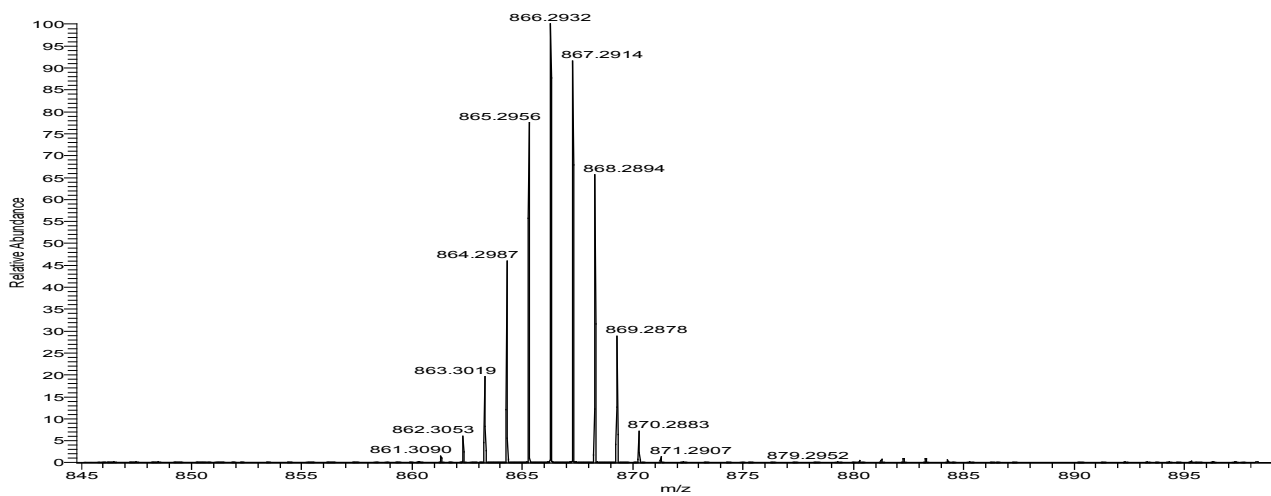
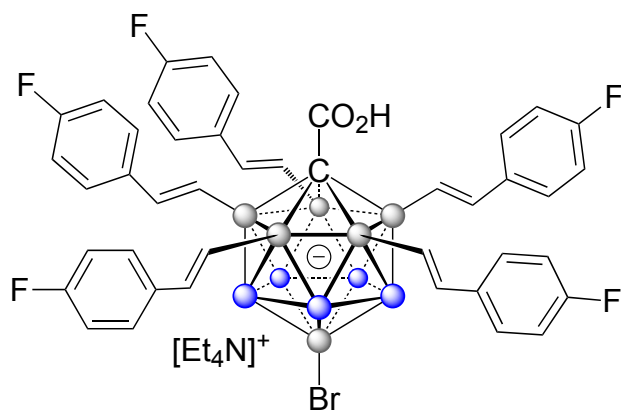
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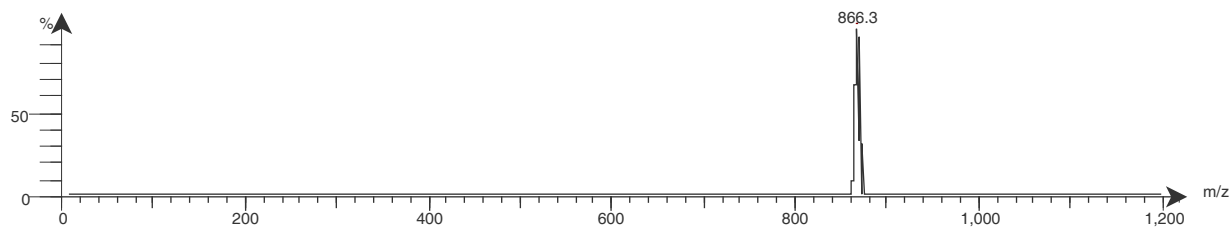


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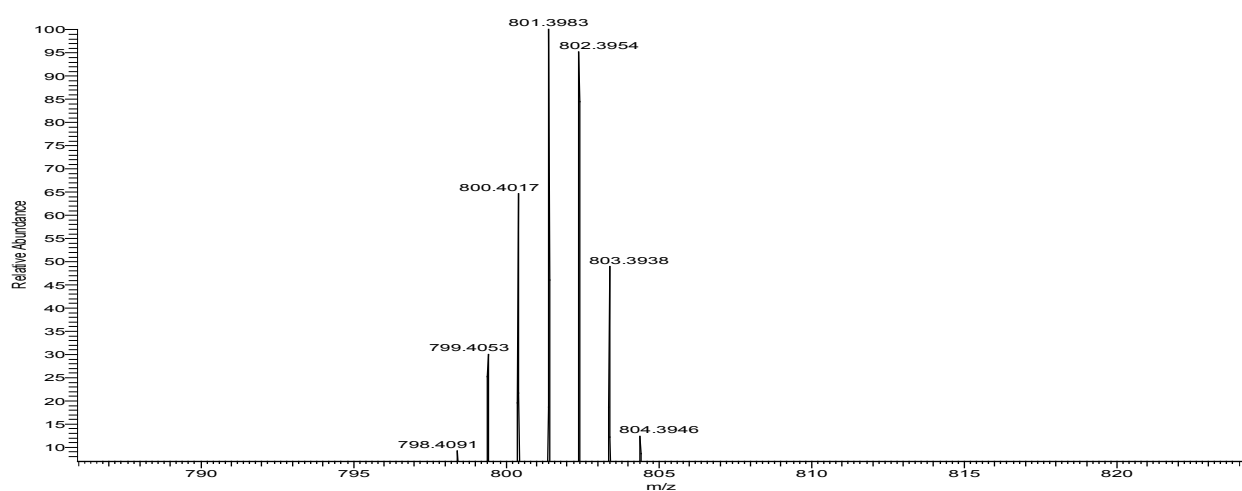
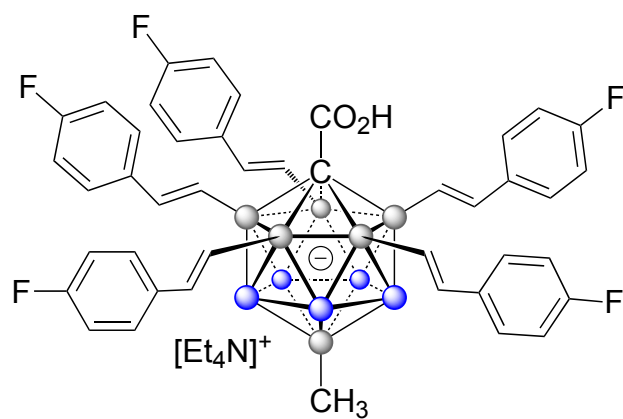


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Intensity

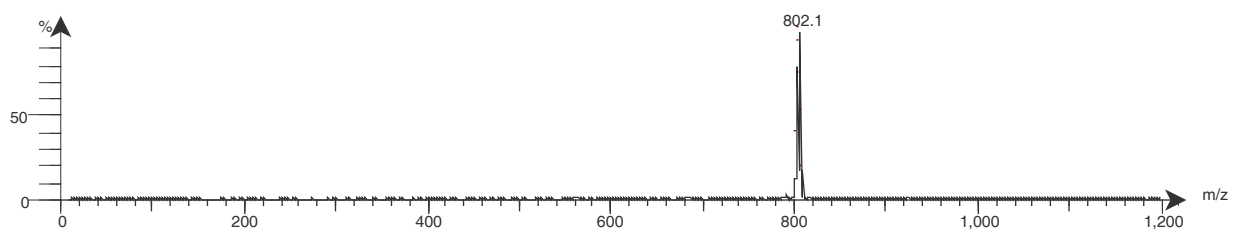


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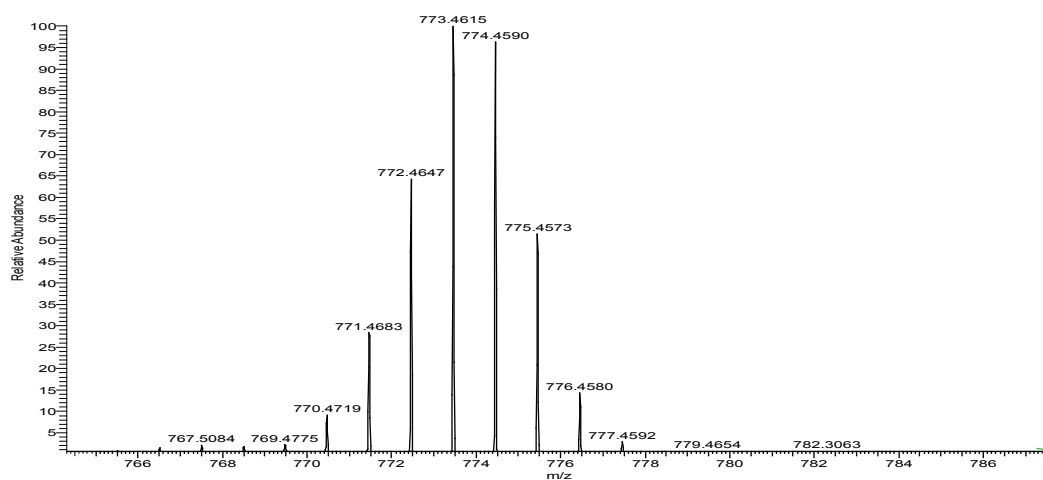
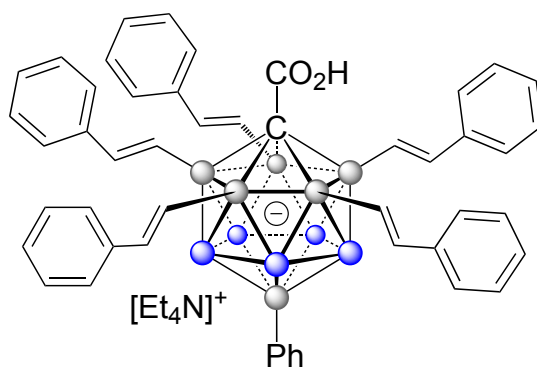


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Intensity

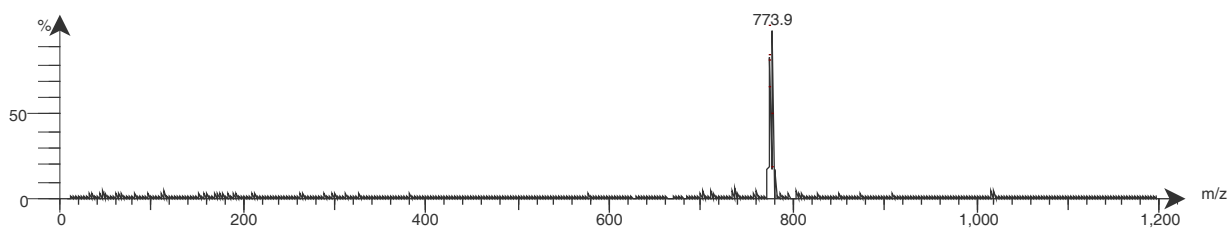


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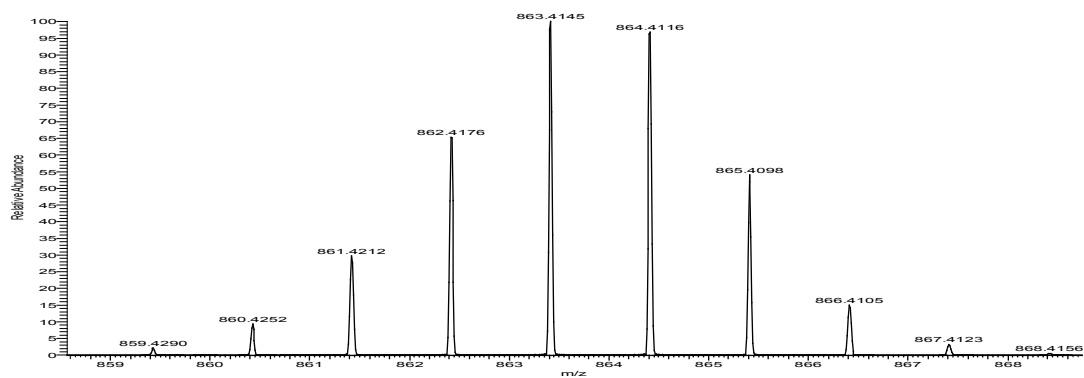
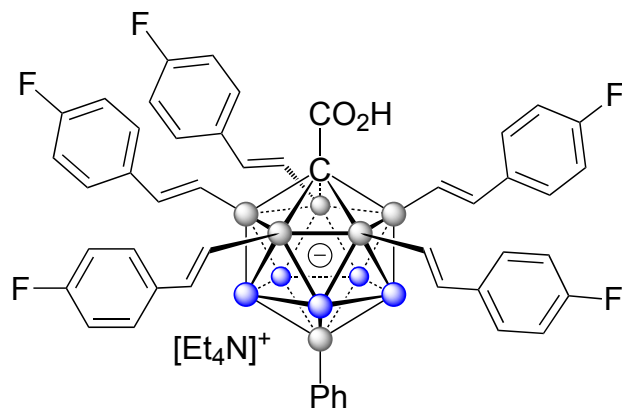


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Intensity

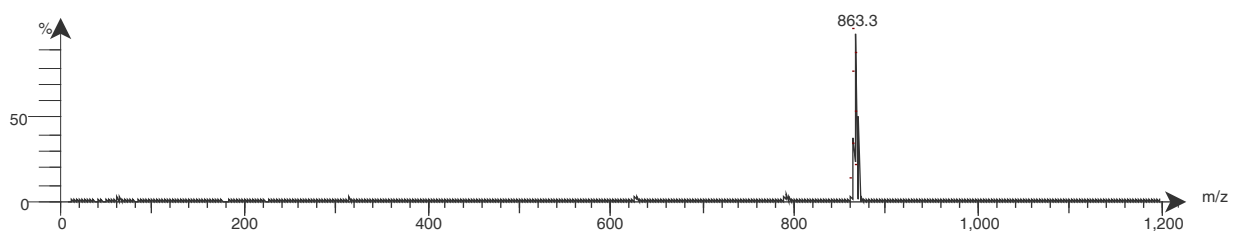


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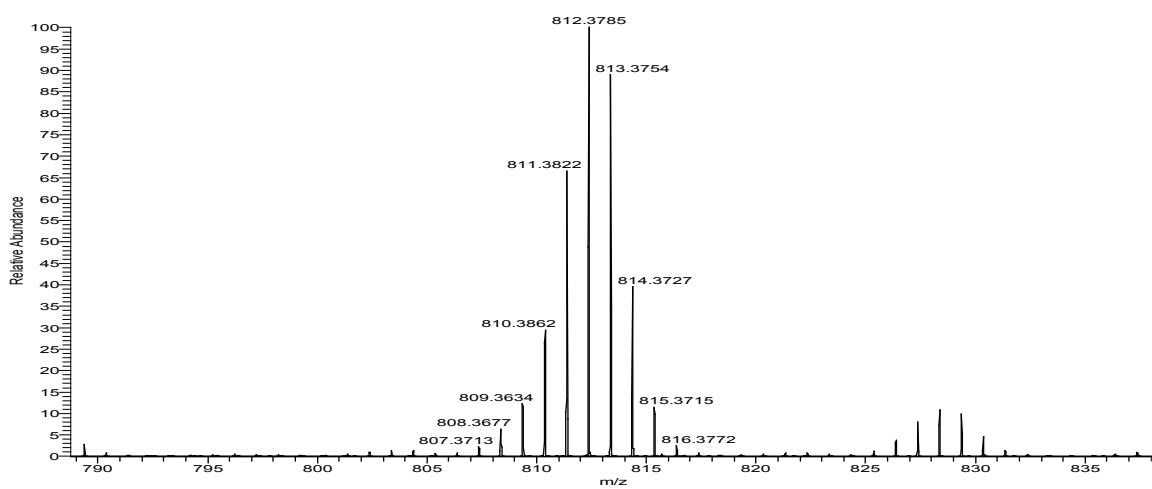
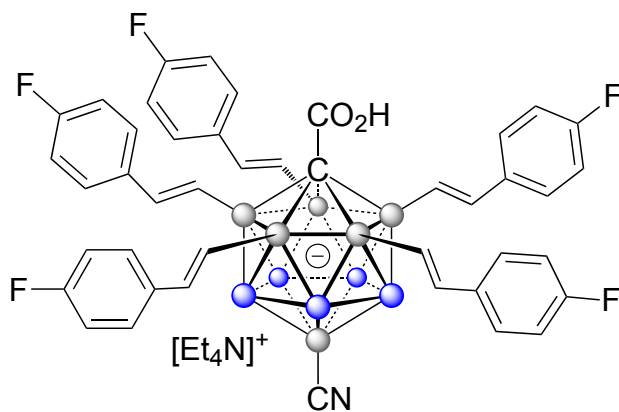


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Intensity

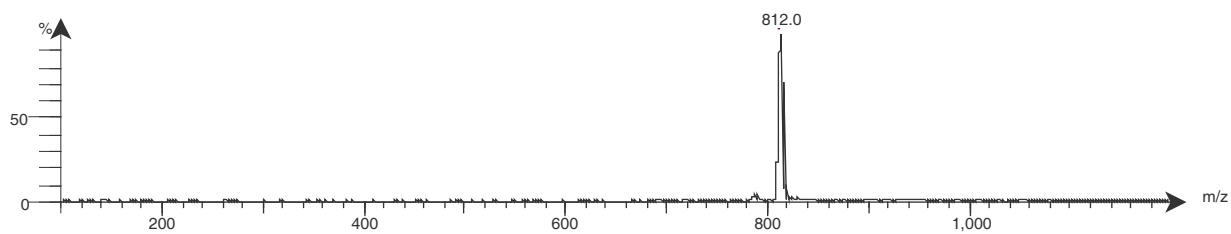


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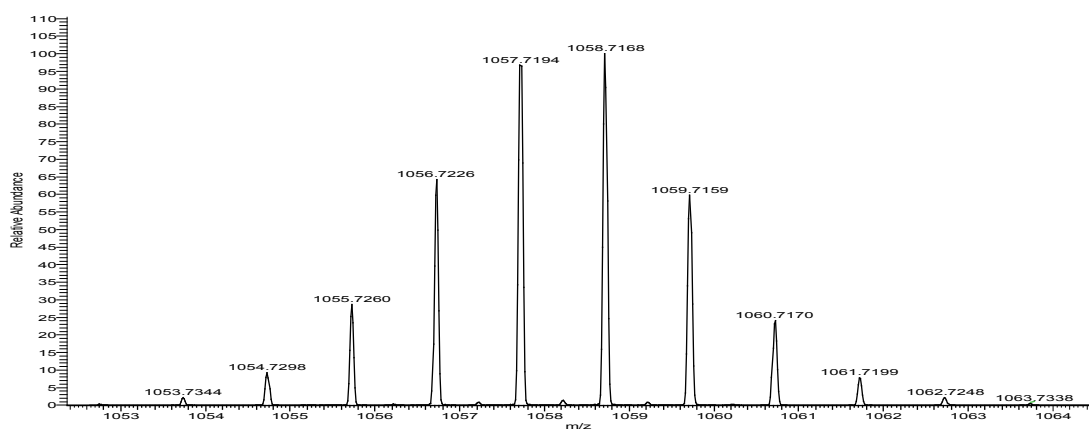
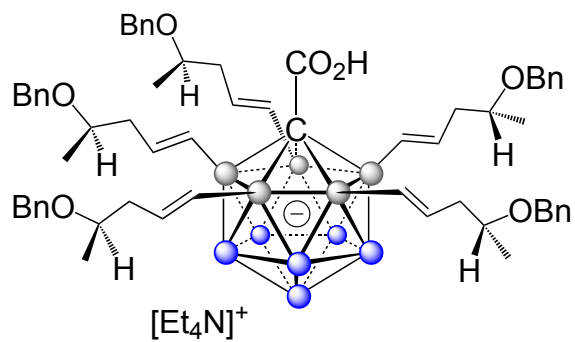


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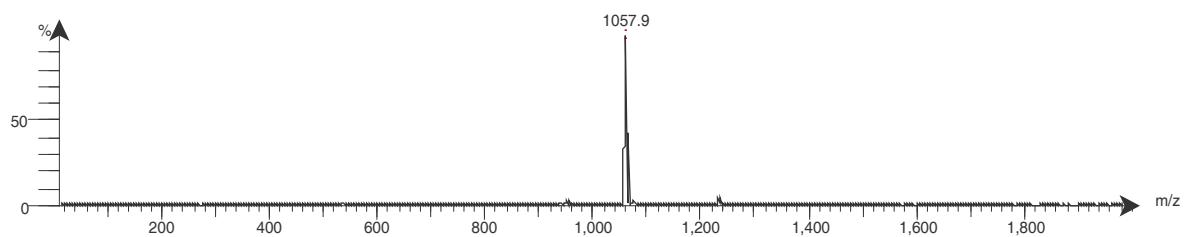


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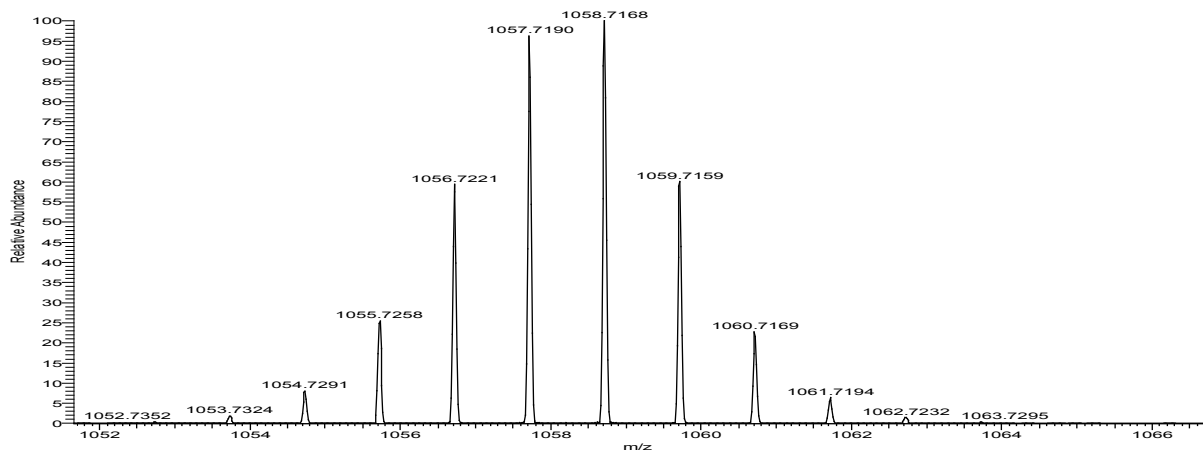
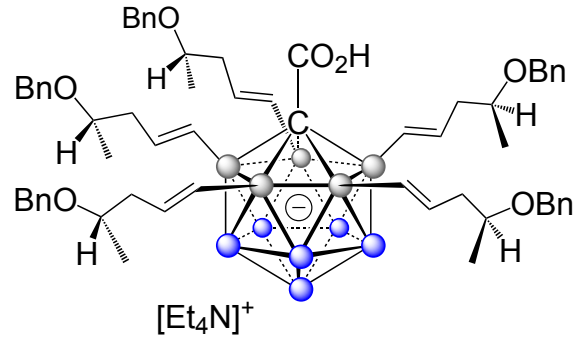


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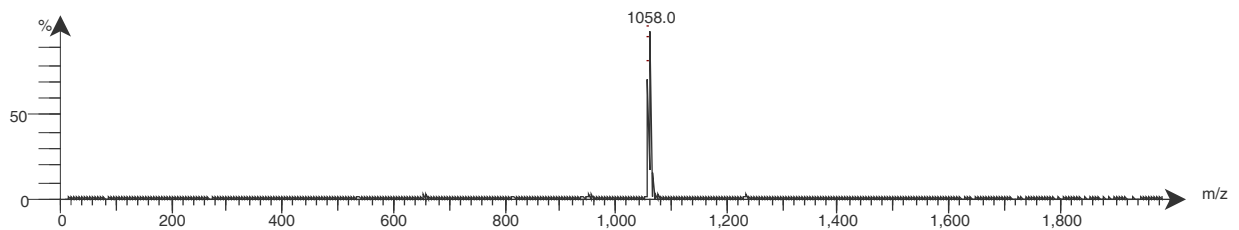


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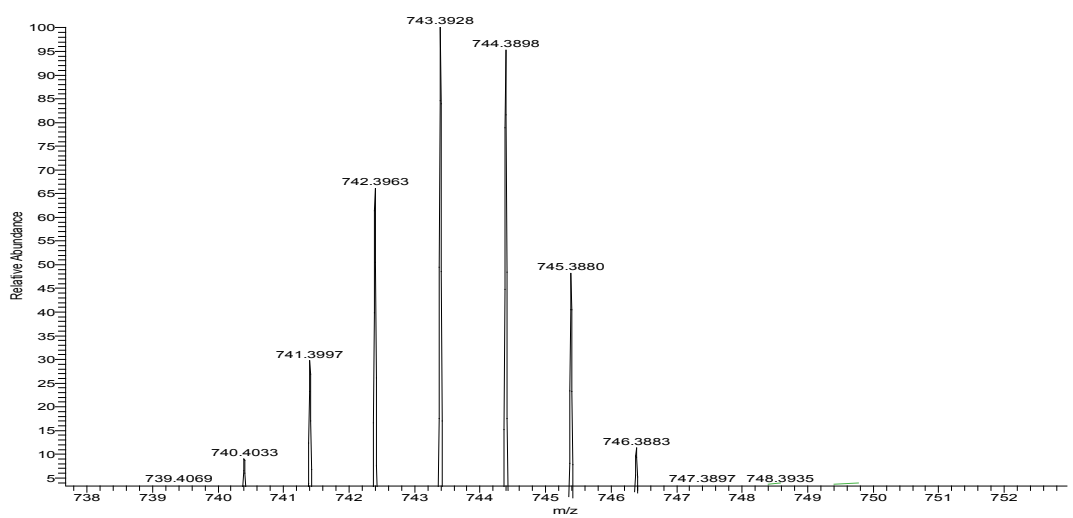
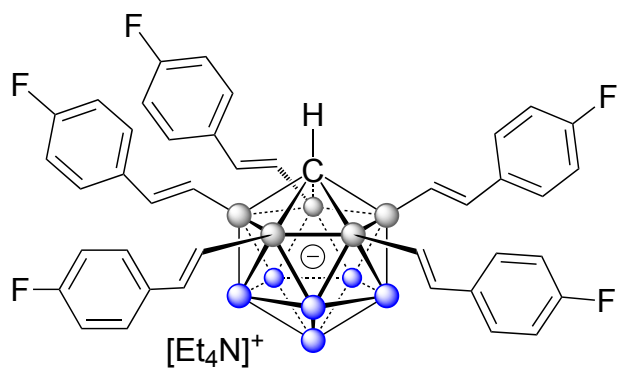


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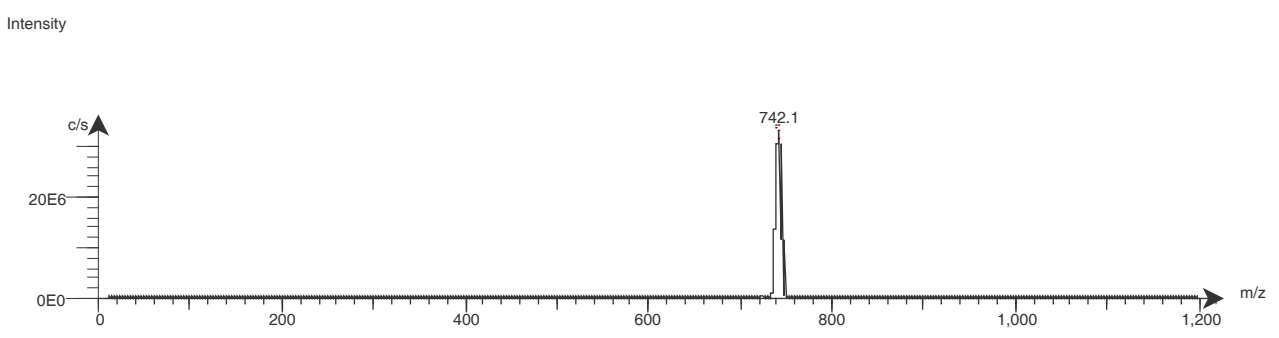
Intensity



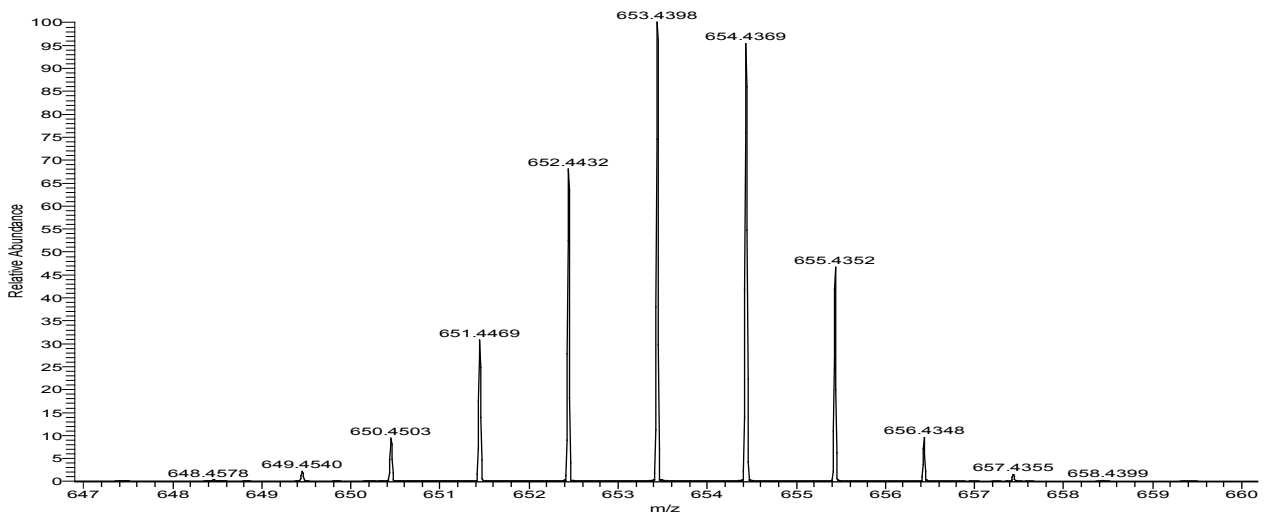
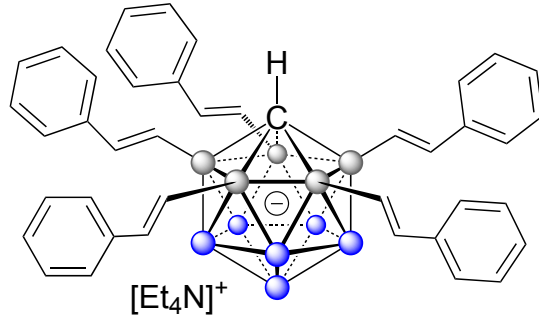
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(-)-ESI-HRMS Shimadzu IT-TOF

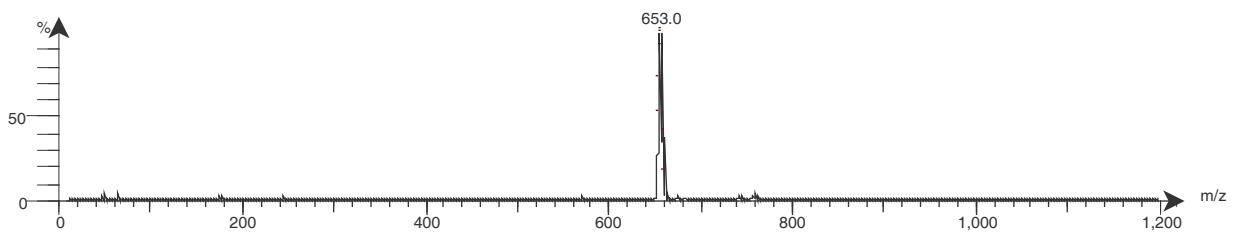


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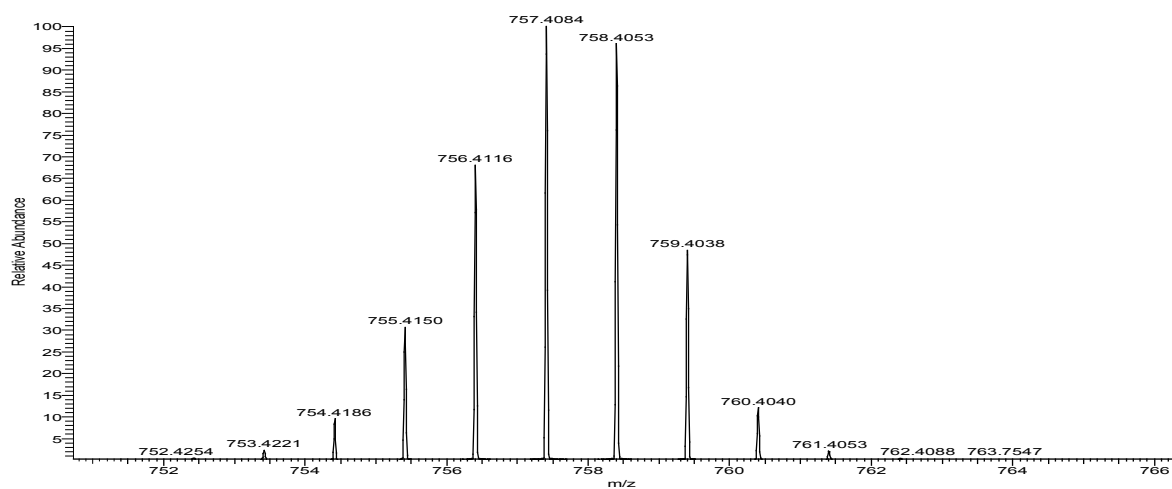
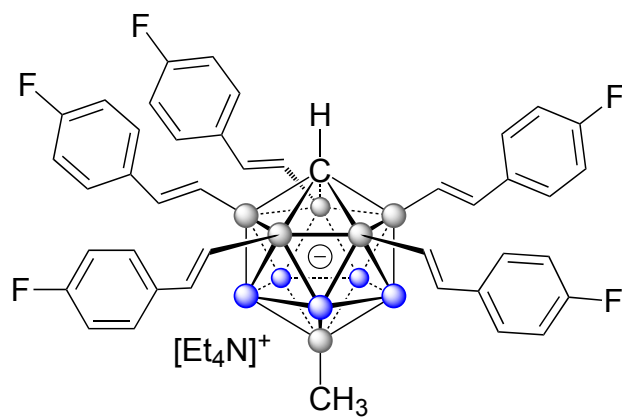


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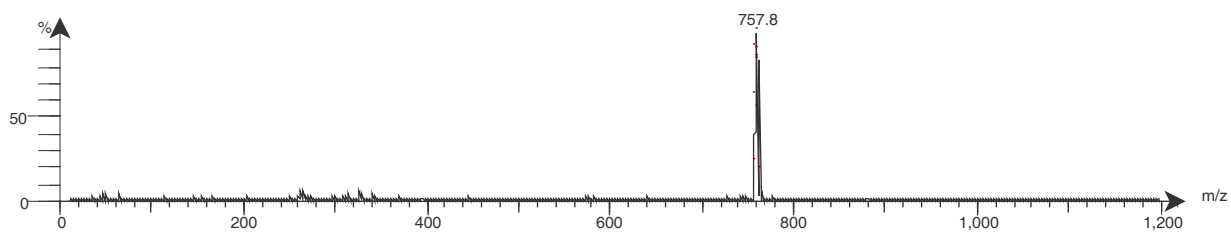


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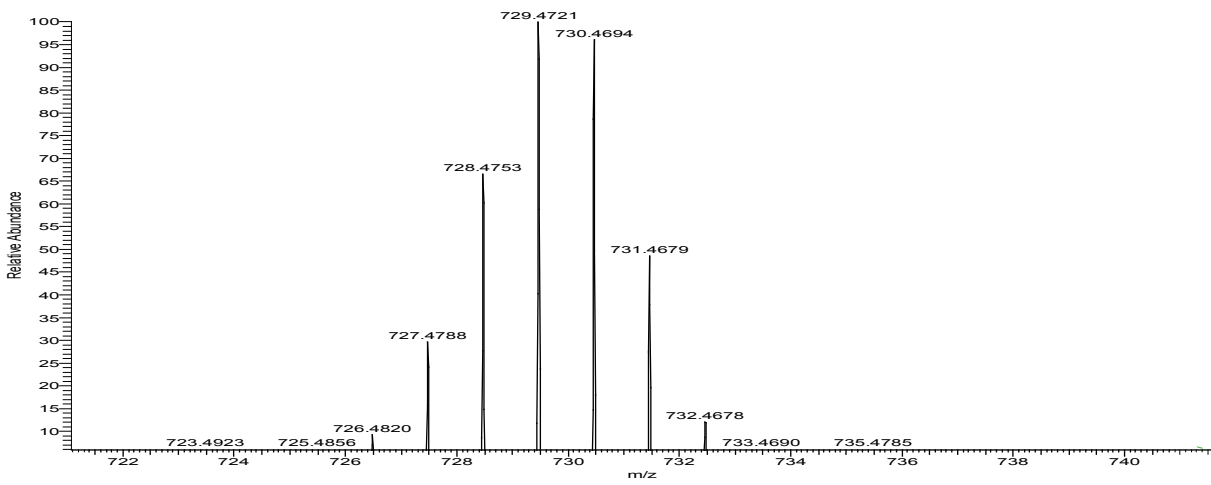
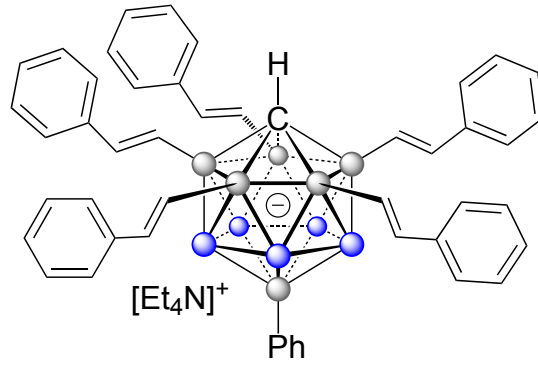


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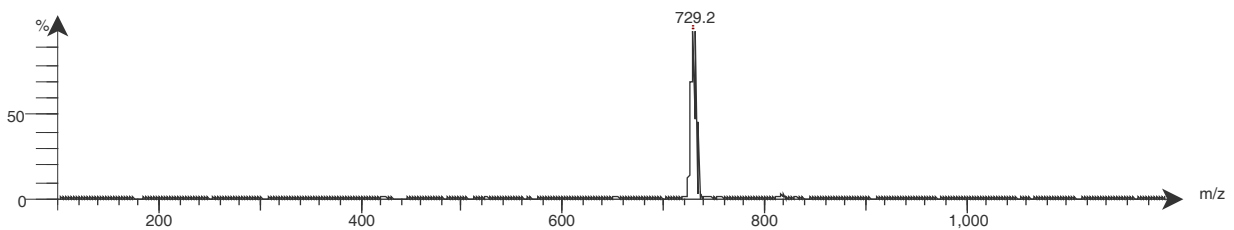


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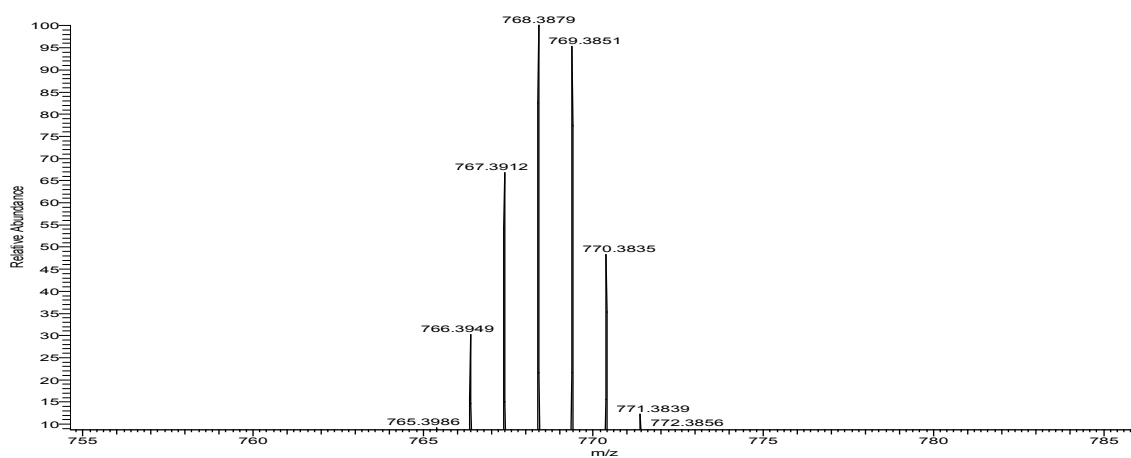
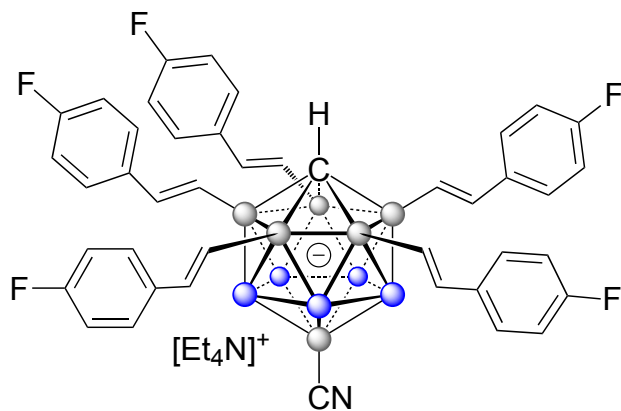


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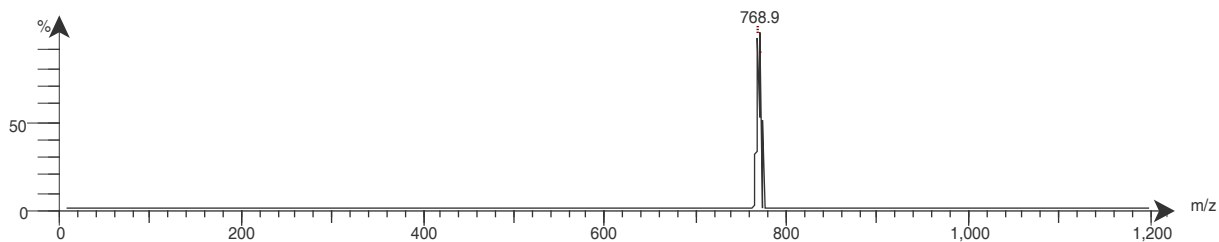


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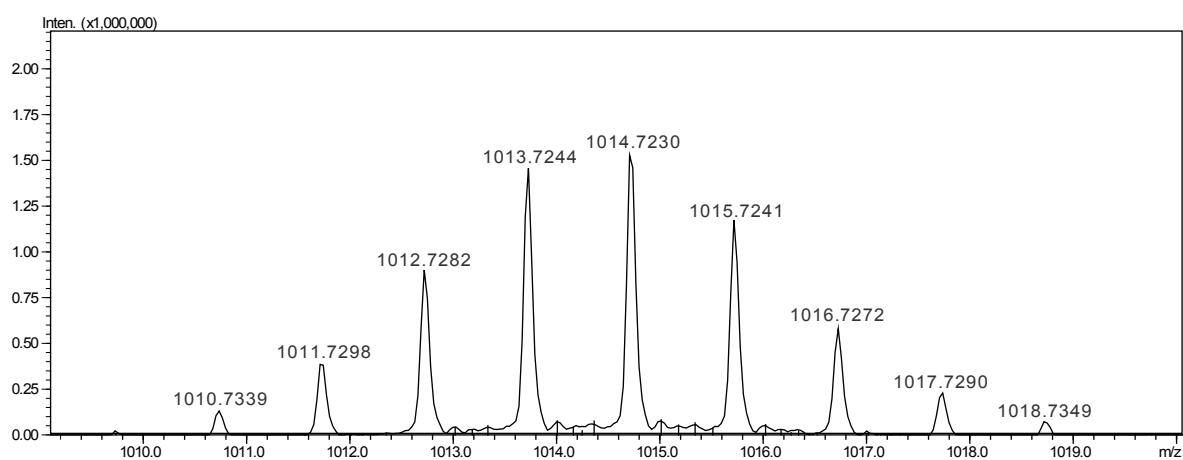
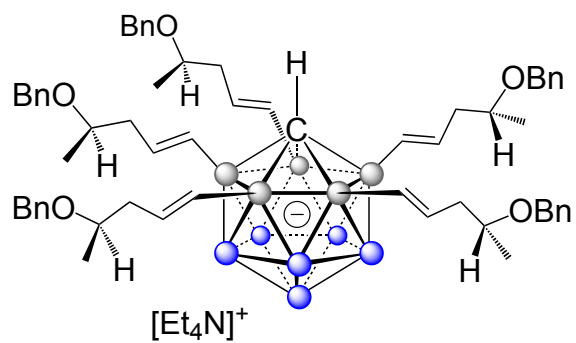


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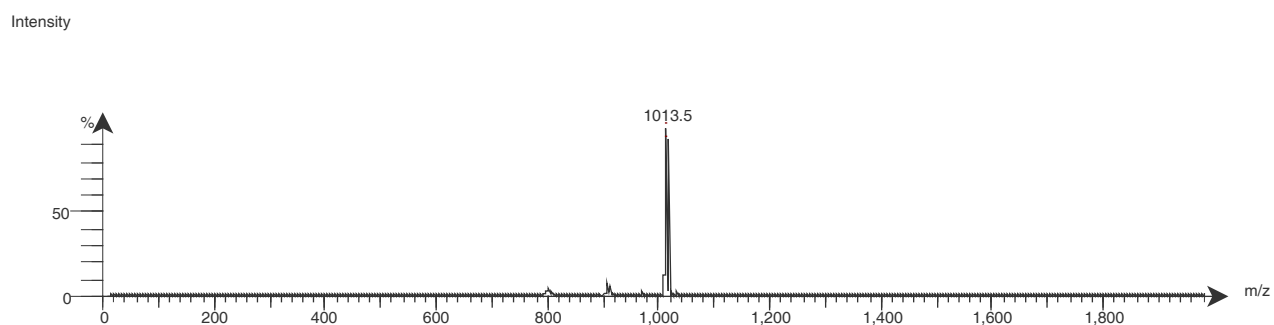
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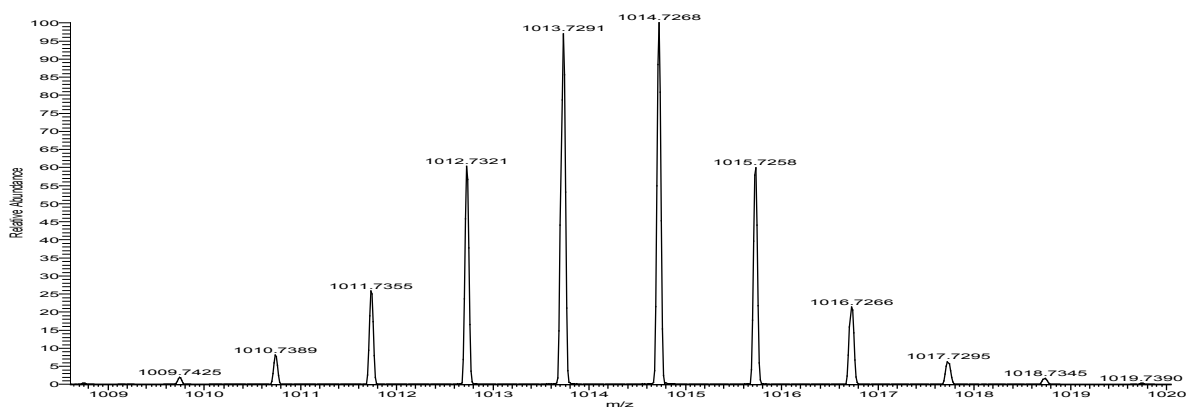
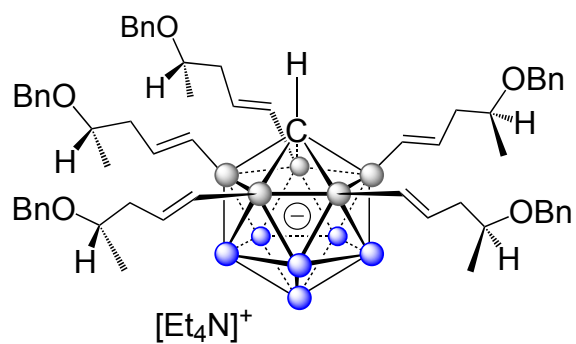
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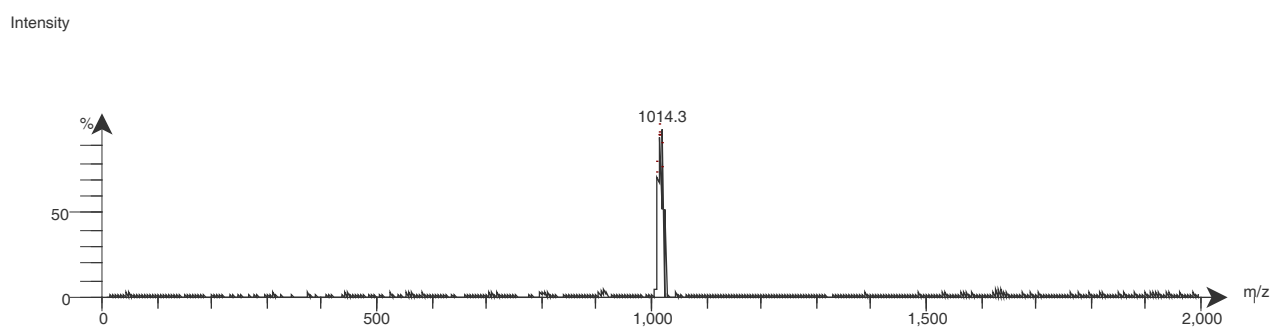
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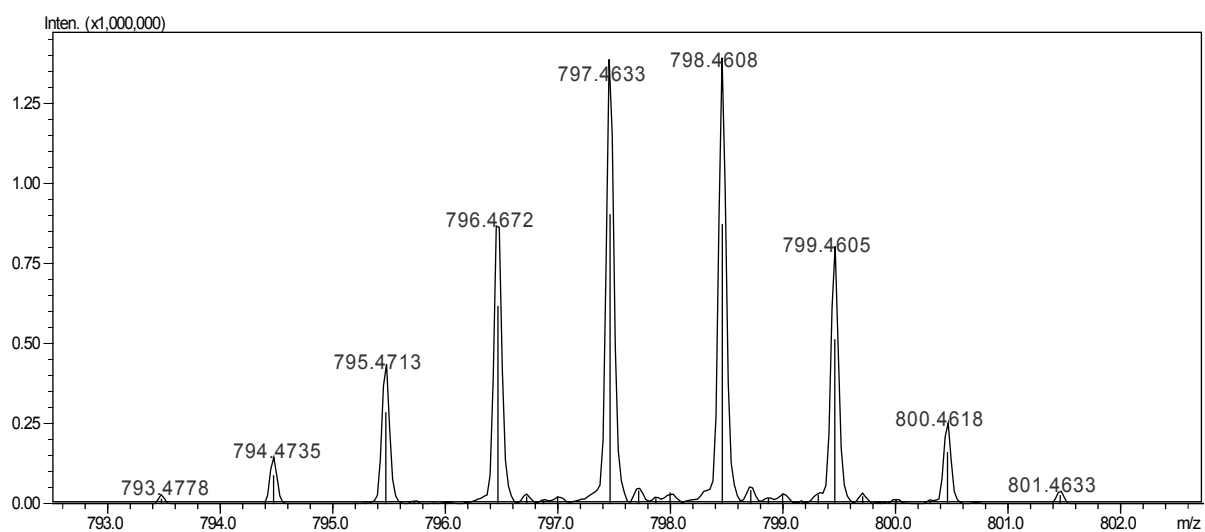
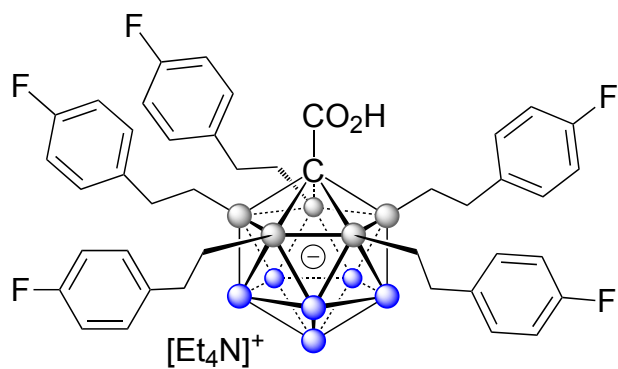
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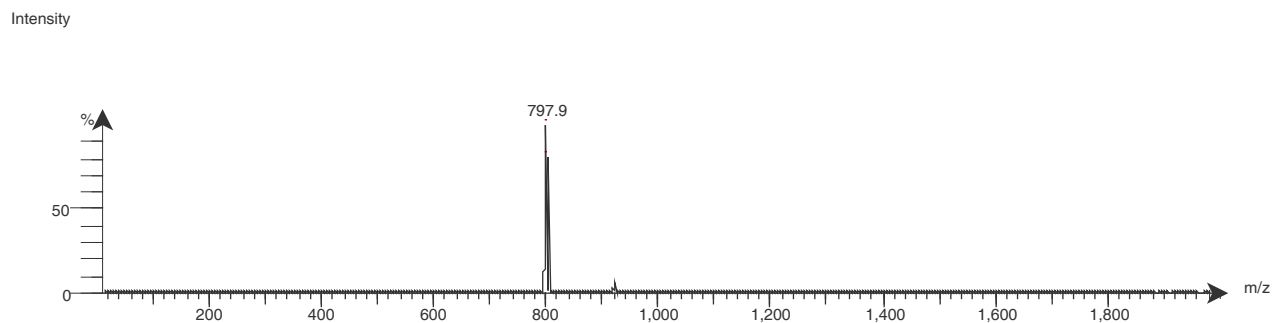
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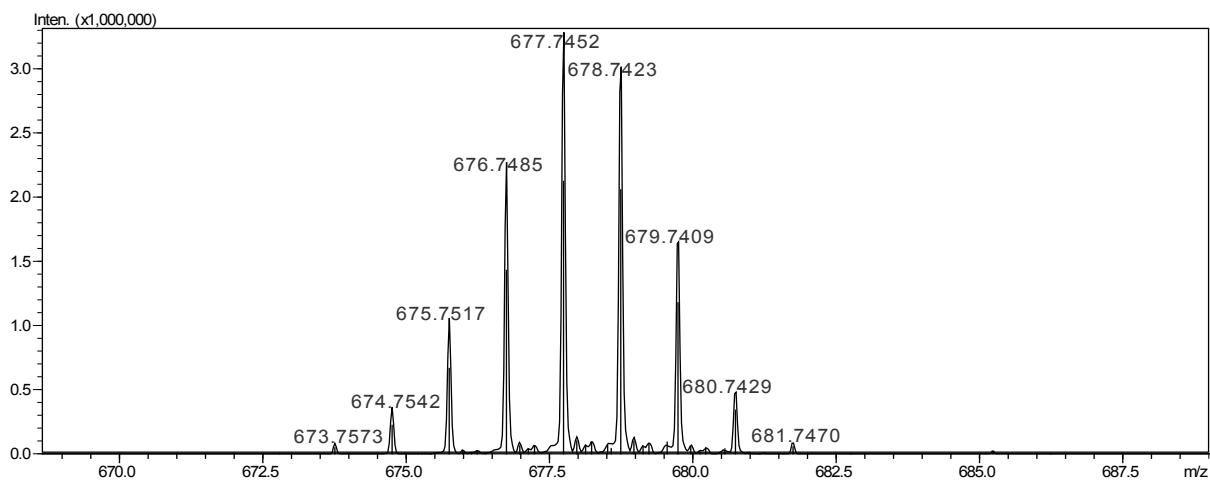
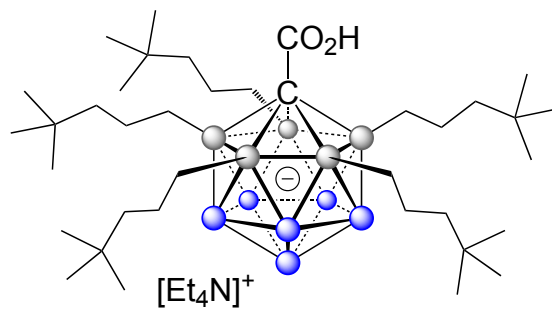
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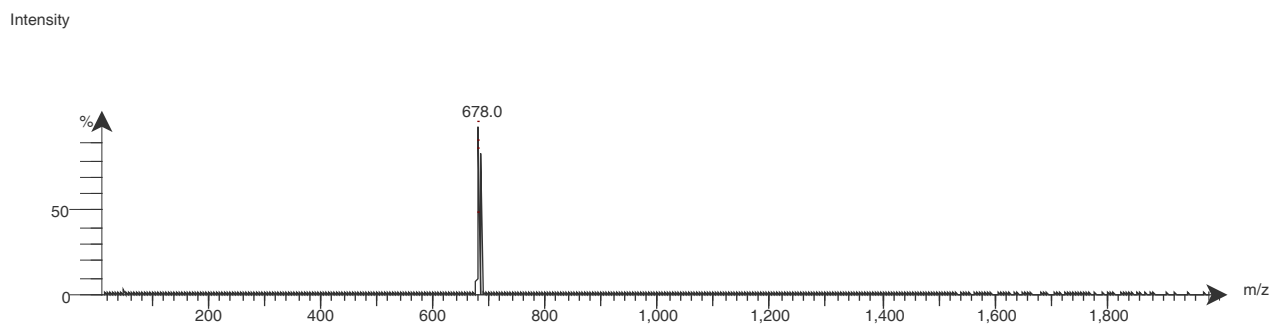
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Full-range (-)-ESI-MS Expression CMS



(-)-ESI-HRMS Shimadzu IT-TOF



Full-range (-)-ESI-MS Expression CMS