

Supporting Information

“Palladium-Catalyzed Selective Five-Fold Cascade Arylation of the 12-Vertex Monocarborane Anion by B–H Activation”

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Table of Contents

I	General Information	p. S2–S3
II	Experimental Section	p. S4–S31
III	X-ray Crystallography	p. S32–S45
IV	Computational details	p. S46–S166
V	References	p. S167–S168
VI	NMR Spectra	p. S169–S317
VII	Mass Spectra	p. S318–S353

I General Information

Chemicals

The starting material [NEt₄][1-COOH-CB₁₁H₁₁] was prepared according to the reported method.^[1] Pd(OAc)₂ was purchased from Energy Chemicals. AgOAc was obtained from Adamas-beta. NaOAc, KOAc and Cu(OAc)₂ were purchased from Aladdin. Aryl iodides were purchased from Energy Chemicals, J & K or Alfa and used as received. HOAc, DMF, CH₃CN, (CH₃)₃CCN, toluene, CH₂Cl₂, 1,2-dichloroethane, EtOAc and hexane were received from Sinopharm. Deuterated solvents were purchased from Cambridge Isotope Laboratories. All reagents were used as received without purification unless noted otherwise. Purification of reaction products was carried out by column chromatography on silica gel 60 (200-30 mesh). Anhydrous solvents were prepared by passing through activated Al₂O₃ and stored over 3 Å molecular sieves. Chemical yields refer to isolated products after chromatography.

Characterization

Thin-layer chromatography (TLC) was carried out using silica gel 60, F254 with a thickness of 0.25 mm. Column chromatography was performed on silica gel 60 (200-30 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 CHD₂S(O)CD₃ = 2.50 ppm, residual CHD₂CN = 1.94 ppm, ¹³C{¹H}: CD₃C(O)CD₃ = 29.84 ppm, CD₃S(O)CD₃ = 39.52 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.^[2]

- The ¹¹B-¹¹B COSY NMR spectrum for **3a** was recorded at 160 MHz (500 MHz for ¹H) under ¹H decoupling. A $^1J_{B-B}$ correlation signal was observed for B12 to B7–11, but not for B7–11 to B2–6. A detailed study by Grimes addressed the phenomenon of missing correlations,^[3] and an explanatory summary is given in the following. The detection of cross peaks requires that several criteria be fulfilled: (a) Sufficient electron density must exist directly between the respective boron atoms; (b) the relaxation times T_1 and T_2 relaxation times must be long enough and (c) the individual ¹¹B resonances in the 1D spectrum are fully or at partially resolved. All of these conditions influence scalar coupling and heavily depend on the number, nature and position of the cage substituents. They cannot be changed by the measurement parameters, except for (c) where recording data at a higher field is beneficial.

- 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.

II Experimental Section

II a) Synthesis of products **3** and **H-3**

General Procedure

In a 20 mL vial, carborane carboxylic acid **1** (0.3 mmol), AgOAc (1.8 mmol), aryl iodide **2** (1.8 mmol), Pd(OAc)₂ (0.025 mmol) and HOAc (1.8 mmol) were dissolved/suspended in DMF (4.8 mL). The resulting mixture was stirred at 25 °C or 60 °C (for **3d**, **3e**, **3p** and **H-3**) for 12–36 h until ESI-MS analysis showed no remaining carborane acid **1**. The turbid reaction mixture was filtered through celite in a glass frit, and the solid on top of the celite was washed with MeCN (3 x 10 mL). The filtrate was concentrated on a rotary evaporator (H₂O bath, 40 °C); most of the MeCN was removed, while the DMF solvent remained. To the remaining solution, an aqueous solution of [Et₄N]Br (80 mL, *c* = ca. 2 g/100 mL), and colorless precipitate formed immediately. The precipitate was then filtered through glass frit, followed by washing with deionized water (3 x 10 mL) and hexane (3 x 20 mL). The solid crude product was dried under air and then purified by column chromatography (silica gel, ca. 80 g, column size: diameter = 30 mm) using a mixture CH₂Cl₂ and MeCN (ratio as given for each product) as the eluent to afford compounds **3** and **H-3**.

A typical monitoring of the reaction **1** → **3a** is shown in Figure S1. After 5 min at 25 °C, primarily starting material **1** and a small amount of **3a** are observed. Within 1 h, conversion to **3a** has proceeded significantly, and only traces of di-, tri-, and tetra-arylated carborane are detected. After 12 h, **3a** has formed cleanly. The fact that **1** and **3a** are observed as the major species during the monitoring is in agreement with the conclusions from the DFT calculations; as soon as the first substitution has occurred, the subsequent steps take place with a decreased barrier of activation.

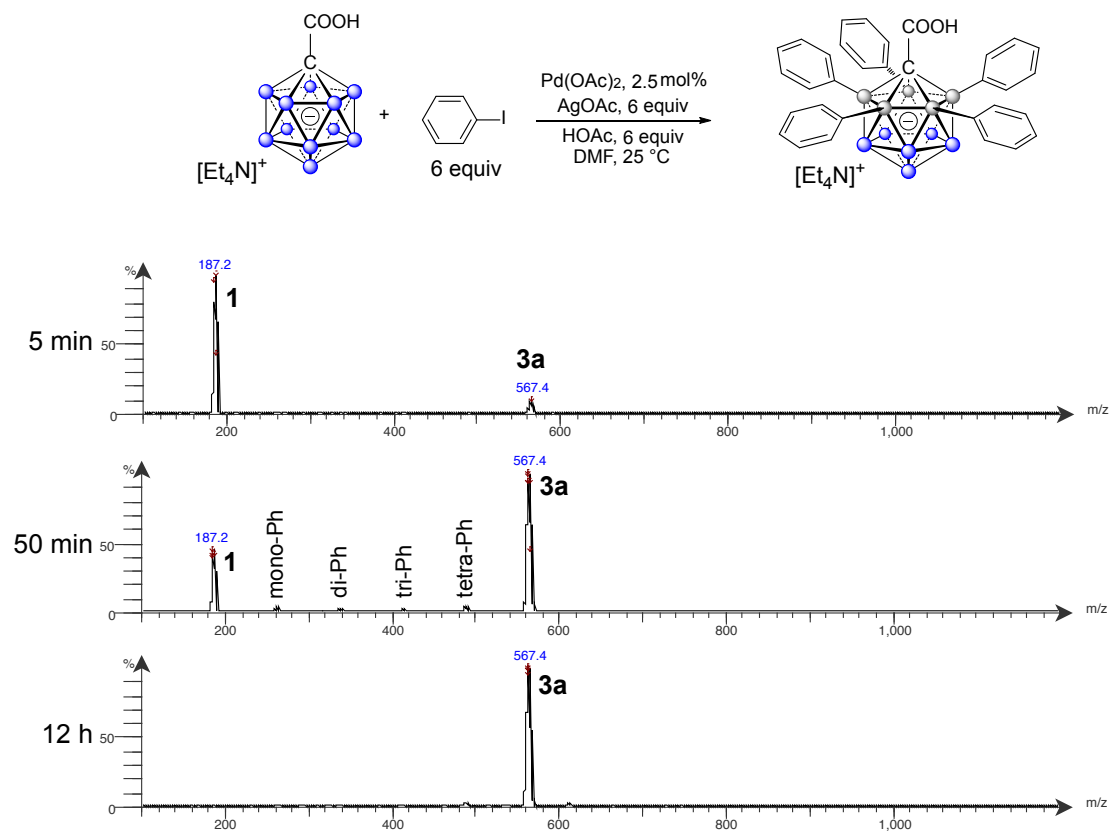
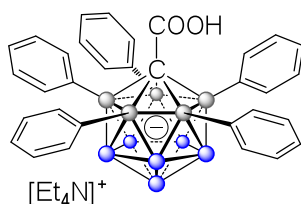


Figure S1. Monitoring of the reaction of **1** $\rightarrow$ **3a** by (–)-ESI-MS.



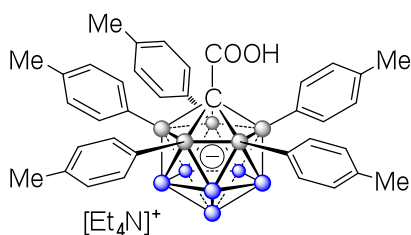
3a: Yield, 86%, colorless solid. Eluent: DCM/MeCN=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6): δ 11.25-10.70 (broad signal, COOH), 7.37-7.15 (m, 10H), 7.10-6.92 (m, 5H), 6.88-6.76 (m, 10H) (phenyl H), 3.42 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.70-1.86 (overlapping broad signals, 6H, BH), 1.35 (tt, 12H, J = 7.3 Hz, 1.9 Hz, CH_3 of cation)

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6): δ -0.20 to -8.05 (overlapping signals, 6B), -11.17 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6): δ 165.31 (carbonyl), 140.51 (broad C-B2-6), 137.29, 126.07, 68.45 (cage C), 52.98 (cation CH_2), 7.65 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{32}\text{H}_{32}\text{B}_{11}\text{O}_2]^-$: 567.3515. Found: 567.3528.



3b: Yield, 91%, colorless solid. Eluent: DCM/MeCN=4:1

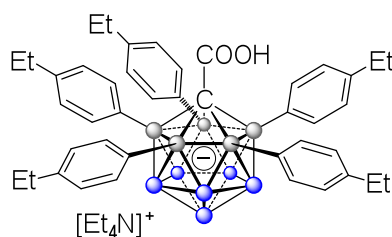
$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6): δ 11.27-9.96 (broad signal, COOH), 7.21-7.09 (m, 10H), 6.69-6.59 (m, 10H) (aryl H), 3.42 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.65-1.83 (overlapping broad signals, 6H, BH), 2.16 (s, 15 H, aryl CH_3), 1.35 (tt, 12H, J = 7.3 Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6): δ 0.35 -7.96 (overlapping signals, 6B), -11.33 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6): δ 165.34 (carbonyl), 137.30, 134.77, 126.93, 68.24 (cage C), 52.98 (cation CH_2), 21.22, 7.65 (cation CH_3). C-B2-6 occurred as a broad signal overlapping with the resonance at 137.30 ppm.

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{37}\text{H}_{42}\text{B}_{11}\text{O}_2]^-$:

637.4299. Found: 637.4307.



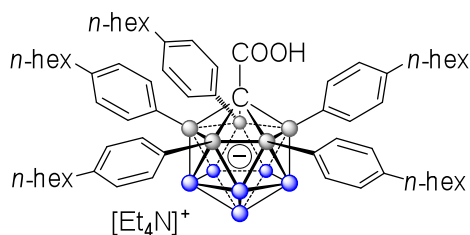
3c: Yield, 87%, colorless solid. Eluent: DCM/MeCN=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 10.90-10.15 (broad signal, COOH), 7.26-7.13 (m, 10H), 6.74-6.63 (m, 10H) (aryl H), 3.40 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.49 (q, J = 7.7 Hz, 10H, CH_2 of ethyl group), 2.65-2.12 (overlapping broad signals, 6H, BH), 1.33 (tt, 12H, J = 7.3 Hz, 1.9 Hz, CH_3 of cation), 1.14 (t, J = 7.7 Hz, 15H, CH_3 of ethyl group),

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ 0.81 to -8.34 (overlapping signals, 6B), -11.27 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6): δ 165.31 (carbonyl), 141.35, 137.33, 125.63, 68.29 (cage C), 53.01 (cation CH_2), 29.11, 15.98, 7.65 (cation CH_3). C-B2-6 occurred as a broad signal overlapping with the resonance at 137.33 ppm.

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{42}\text{H}_{52}\text{B}_{11}\text{O}_2]^-$: 707.5084. Found: 707.5096.



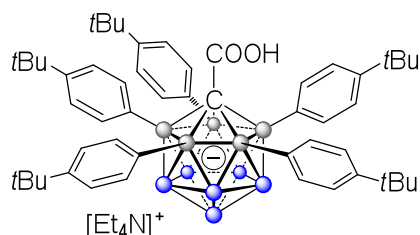
3d: Yield, 86%, colorless solid. Eluent: DCM/MeCN=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 11.20-9.77 (broad signal, COOH), 7.21-7.12 (m, 10H), 6.68-6.63 (m, 10H) (aryl H), 3.46 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.48-2.43 (m, 10H), 2.42-2.12 (overlapping broad signals, 6H, BH), 1.59-1.50 (m, 10H), 1.37 (tt, 12H, J = 7.3 Hz, 1.9 Hz, CH_3 of cation), 1.35-1.22 (m, 30H), 0.91-0.86 (m, 15H).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ 0.24 -7.64 (overlapping signals, 6B), -11.25 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6): δ 165.23 (carbonyl), 139.86, 137.29, 136.26, 68.38 (cage C), 53.00 (cation CH_2), 36.28, 32.52, 32.16, 29.58, 23.35, 14.41, 7.67 (cation CH_3). C-B2-6 occurred as a broad signal overlapping with the resonance at 137.29 ppm.

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{62}\text{H}_{92}\text{B}_{11}\text{O}_2]^-$: 988.8202. Found: 988.8223.



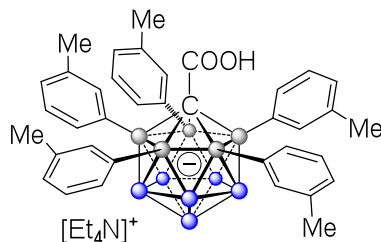
3e: Yield, 85%, colorless solid. Eluent: DCM/MeCN=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 11.37-9.58 (broad signal, COOH), 7.25-7.17 (m, 10H), 6.90-6.83 (m, 10H) (aryl H), 3.44 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.47-2.17 (overlapping broad signals, 6H, BH), 1.35 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation), 1.23 (s, 45H).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ 0.44 to -7.65 (overlapping signals, 6B), -11.13 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6): δ 165.28 (carbonyl), 148.09, 136.99, 122.87, 68.19 (cage C), 53.00 (cation CH_2), 34.56, 31.73, 7.65 (cation CH_3). C-B2-6 occurred as a broad signal overlapping with the resonance at 136.99 ppm.

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{52}\text{H}_{72}\text{B}_{11}\text{O}_2]^-$: 848.6633. Found: 848.6651.



3f: Yield, 88%, colorless solid. Eluent: DCM/MeCN=4:1

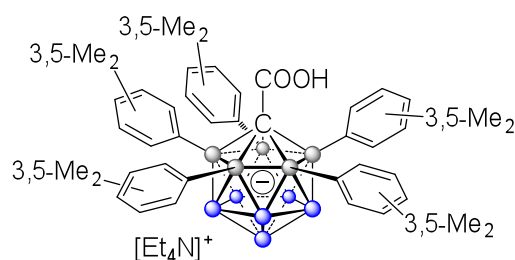
$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 10.85-10.37 (broad signal, COOH), 7.14-7.07 (overlapping m, 10H), 6.82-6.77 (m, 5H), 6.75-6.70 (m, 5H) (aryl H), 3.40 (q, J

= 7.3 Hz, 8H, CH_2 of cation), 2.62-2.19 (overlapping broad signals, 6H, BH), 2.02-1.93 (s, 15H) 1.34 (tt, 12H, J = 7.3 Hz, 1.9 Hz, CH_3 of cation).

$^{11}B\{^1H\}$ NMR (160 MHz, acetone- d_6): δ -0.24 -7.89 (overlapping signals, 6B), -11.22 (5B).

$^{13}C\{^1H\}$ NMR (126 MHz, acetone- d_6): δ 165.15 (carbonyl), 140.40, 138.55, 134.38, 134.29, 126.62, 125.84, 68.64 (cage C), 52.97 (cation CH_2), 21.65, 7.65 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[C_{37}H_{42}B_{11}O_2]^-$: 637.4299. Found: 637.4307.



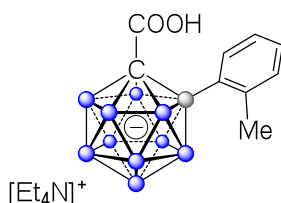
3g: Yield, 88%, colorless solid. Eluent: DCM/MeCN=4:1

$^1H\{^{11}B\}$ NMR (400 MHz, acetone- d_6): δ 10.49-9.61 (broad signal, $COOH$), 7.06-6.98 (m, 10H), 6.67-6.61 (m, 5H) (aryl H), 3.35 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.72-2.18 (overlapping broad signals, 6H, BH), 1.98 (s, 30H, CH_3), 1.38 (tt, 12H, J = 7.3 Hz, 1.9 Hz, CH_3 of cation).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone- d_6): δ 1.23 to -7.71 (overlapping signals, 6B), -11.16 (5B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone- d_6): δ 164.92 (carbonyl), 142.28, 135.52, 134.18, 127.43, 68.46 (cage C), 52.92 (cation CH_2), 21.53, 7.61 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[C_{42}H_{52}B_{11}O_2]^-$: 707.5084. Found: 707.5088.



3h: Applying standard conditions lead to mono-arylation product, however, the conversion was not clean as evidenced by ESI-MS. When the reaction was carried out for 44 h at 25 °C, primarily starting material and the mono-arylated product were

observed by ESI-MS in an estimated 3:2 ratio (we found that the ratio indicated by mass spectra is not always accurate); separation by column chromatography gave **3h** as a colorless solid (12%, purity *ca.* 85%). Impurities were detected in the $^1\text{H}\{^{11}\text{B}\}$ spectrum and could not be identified unambiguously. The low yield is attributed to two factors:

1) According to the proposed mechanism, formation of the first palladium intermediate **1-Pd** with the B2-Pd bond is followed by oxidative addition of the iodoarene. In the case of 1,2-iodomethylbenzene, the oxidative addition is probably slower than with other iodoarenes. Therefore, competitive reaction pathways from **1-Pd** to undesired byproducts occur to a higher degree than with less hindered iodoarenes. We suspect that at least some of the byproducts are not detected clearly by (-)-ESI-MS.

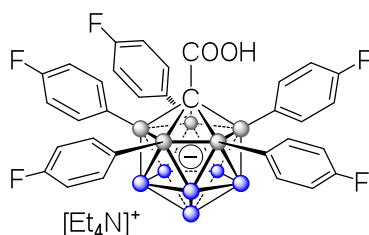
2) Mixed column fractions containing **1** and also **3h**; these fractions were discarded.

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, CD_3CN): δ 7.79 (d, $J = 7.7$ Hz, 1 H, aryl H), 7.10-6.95 (overlapping m, 3H, aryl H), 3.13 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.64, (s, 3 H, aryl- CH_3), 2.43-1.41 (overlapping broad signals, 10, BH), 1.98 (s, 30H, CH_3), 1.19 (tt, 12H, $J = 7.3$ Hz, 1.6 Hz, CH_3 of cation). Additionally, a broad signal at 4.81 ppm was observed, potentially stemming from COOH and hydrogen-bonding residual H_2O .

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6): δ -4.68 (1B), -6.12 (1B), *ca.* -10.6 to -16.5 (overlapping signals with peaks at -11.73 and -13.9, 9B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6): δ 168.57 (carbonyl), 144.71, 138.62, 131.04, 127.83, 125.24, 73.33 (cage C), 53.05 (cation CH_2), 24.44, 7.67 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_9\text{H}_{18}\text{B}_{11}\text{O}_2]^-$: 277.2410. Found: 277.2404.



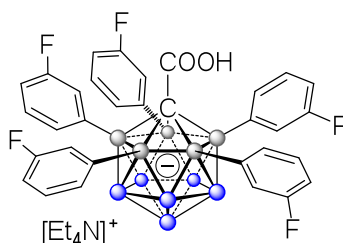
3i: Yield, 93%, colorless solid. Eluent: DCM/MeCN=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6): δ 12.58-10.11 (broad signal, COOH), 7.22-7.14 (m, 10H), 6.68-6.59 (m, 10H) (aryl H), 3.48 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.72-2.14 (overlapping broad signals, 6H, BH), 1.38 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ -1.45 to -6.63 (overlapping signals, 6B), -11.15 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6): δ 165.25 (carbonyl), 162.75 (d, $^1J_{\text{C-F}} = 246$ Hz), 138.83 (d, $^3J_{\text{C-F}} = 8$ Hz), 135.81, 112.93 (d, $^2J_{\text{C-F}} = 20$ Hz), 68.44 (cage C), 52.98 (cation CH_2), 7.64 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{32}\text{H}_{27}\text{B}_{11}\text{F}_5\text{O}_2]^-$: 657.3044. Found: 657.3055.



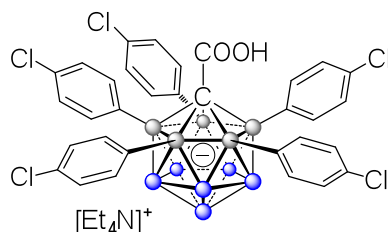
3j: Yield, 92%, colorless solid. Eluent: DCM/MeCN=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6): δ 12.37-11.02 (broad signal, COOH), 7.11-7.03 (m, 5H), 6.99-6.86 (overlapping m, 10H), 6.84-6.73 (m, 5H) (aryl H), 3.46 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.76-2.10 (overlapping broad signals, 6H, BH), 1.36 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation)

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6): δ -0.91 to -7.98 (overlapping signals, 6B), -10.88 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6): δ 164.91 (carbonyl), 162.20 (d, $^1J_{\text{C-F}} = 240$ Hz), 142.74, 132.84 (d, $^4J_{\text{C-F}} = 2$ Hz), 122.95 (d, $^2J_{\text{C-F}} = 20$ Hz), 127.92 (d, $^3J_{\text{C-F}} = 8$ Hz), 113.23 (d, $^2J_{\text{C-F}} = 20$ Hz), 68.19 (cage C), 52.94 (cation CH_2), 7.61 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{32}\text{H}_{27}\text{B}_{11}\text{F}_5\text{O}_2]^-$: 657.3044. Found: 657.3035.



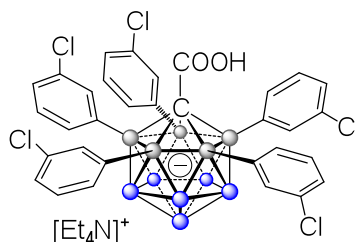
3k: Yield, 89%, colorless solid. Eluent: DCM/MeCN=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 12.30-10.30 (broad signal, COOH), 7.19-7.12 (m, 10H), 6.95-6.88 (m, 10H) (aryl H), 3.47 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.66-1.76 (overlapping broad signals, 6H, BH), 1.38 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ -1.35 to -6.92 (overlapping signals, 6B), -11.01 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6): δ 165.06 (carbonyl), 138.57, 132.60, 126.49, 68.99 (cage C), 52.99 (cation CH_2), 7.65 (cation CH_3). C-B2-6 occurred as a broad signal overlapping with the resonance at 138.57 ppm.

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{32}\text{H}_{27}\text{B}_{11}\text{Cl}_5\text{O}_2]^-$: 739.1541. Found: 739.1552.



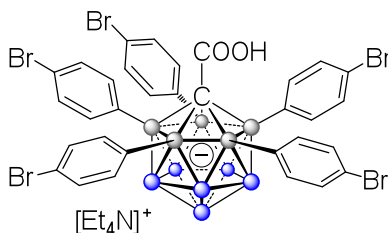
3l: Yield, 86%, colorless solid. Eluent: DCM/MeCN=4:1. Based on the NMR data, this product contained an impurity of about 4%, which could not be removed by column chromatography.

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 12.30-11.16 (broad signal, COOH), 7.25-7.19 (m, 5H), 7.16-7.11 (m, 5H), 7.11-7.05 (m, 5H), 6.95-6.88 (m, 5H) (aryl H), 3.47 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.76-2.01 (overlapping broad signals, 6H, BH), 1.38 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation)

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ -0.55 to -8.15 (overlapping signals, 6B), -10.86 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6): δ 164.77 (carbonyl), 142.17, 136.65, 135.15, 132.50, 128.06, 126.70, 68.35 (cage C), 52.98 (cation CH_2), 7.65 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{32}\text{H}_{27}\text{B}_{11}\text{Cl}_5\text{O}_2]^-$. 739.1541. Found: 739.1554.



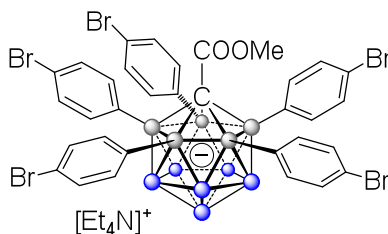
3m: Yield, 94%, colorless solid. Eluent: DCM/MeCN=5:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 7.13-7.03 (overlapping m, 20H) (aryl H), 3.48 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.67-1.80 (overlapping broad signals, 6H, BH), 1.38 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation), the COOH signal could not be detected.

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ -1.56 to -7.17 (overlapping signals, 6B), -11.01 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6): δ 165.03 (carbonyl), 138.92, 129.48, 121.21, 68.22 (cage C), 53.00 (cation CH_2), 7.66 (cation CH_3). C-B2-6 occurred as a broad signal overlapping with the resonance at 138.92 ppm.

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{32}\text{H}_{27}\text{B}_{11}\text{Br}_5\text{O}_2]^-$: 961.8992. Found: 961.9013.



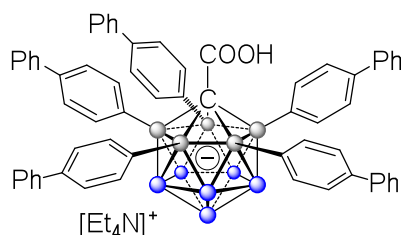
3n: Yield, 86%, colorless solid. Eluent: DCM/MeCN=5:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 7.12-7.07 (m, 10H), 7.00-6.94 (m, 10H) (aryl H), 3.48 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 3.34 (s, 3H, OCH_3), 2.69-2.08 (overlapping broad signals, 6H, BH), 1.39 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation)

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ -0.23 to -7.33 (overlapping signals, 6B), -10.99 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6): δ 164.41 (carbonyl), 138.73, 129.64, 121.35, 67.78 (cage C), 53.01 (cation CH_2), 51.60 (OCH_3), 7.66 (cation CH_3). C-B2-6 occurred as a broad signal overlapping with the resonance at 138.73 ppm.

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{33}\text{H}_{29}\text{B}_{11}\text{Br}_5\text{O}_2]^-$: 975.9150. Found: 975.9116.



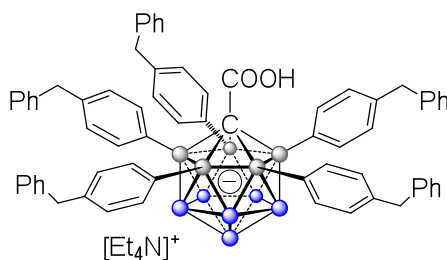
3o: Yield, 88%, colorless solid. Eluent: DCM/MeCN=4:1.

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, DMSO- d_6): δ 13.21-12.65 (broad signal, COOH), 7.69-7.56 (m, 10H), 7.41-7.35 (m, 10H), 7.35-7.29 (m, 10H), 7.29-7.21 (overlapping m, 15H) (aryl H), 3.16 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.47-1.95 (overlapping broad signals, 6H, BH), 1.13 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, DMSO- d_6): two very broad overlapping resonances with peaks at -5.62 ppm and -11.79 ppm.

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, DMSO- d_6): δ 164.75 (carbonyl), 140.32, 138.54, 136.81, 136.47, 128.77, 126.88, 126.25, 123.61, 67.98 (cage C), 51.36 (cation CH_2), 7.07 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{62}\text{H}_{52}\text{B}_{11}\text{O}_2]^-$: 948.5072. Found: 948.5077.



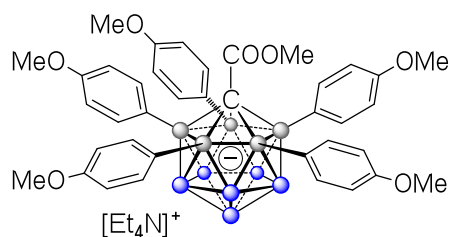
3p: Yield, 78%, colorless solid. Eluent: DCM/MeCN=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 11.35-10.09 (broad signal, COOH), 7.29-7.20 (m, 10H), 7.20-7.11 (overlapping m, 25H), 6.71-6.65 (m, 10H) (aryl H), 3.82 (s, 10H, CH_2), 3.40 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.55-2.11 (overlapping broad signals, 6H, BH), 1.32 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ -0.69 to -7.84 (overlapping signals, 6B), -11.21 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6): δ 165.32 (carbonyl), 143.00, 138.58, 137.42, 129.62, 129.02, 126.87, 126.45, 68.34 (cage C), 52.98 (cation CH_2), 42.25, 7.64 (cation CH_3). C-B2-6 occurred as a broad signal overlapping with the resonance at 138.58 ppm.

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{67}\text{H}_{62}\text{B}_{11}\text{O}_2]^-$: 1018.5857. Found: 1018.5847.



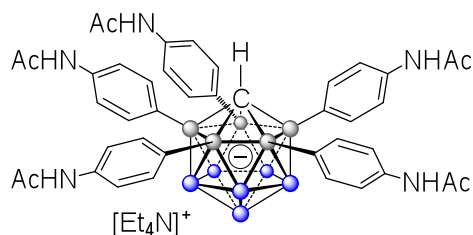
3q: Yield, 76%, colorless solid. Eluent: DCM/MeCN=4:1.

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6): δ 7.06-6.98 (m, 10H), 6.48-6.40 (m, 10H) (aryl H), 3.67 (s, 15H), 3.45 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 3.21 (s, 3H), 2.76-2.11 (overlapping broad signals, 6H, BH), 1.36 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6): δ -0.21 to -7.79 (overlapping signals, 6B), -11.74 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6): δ 164.97 (carbonyl), 158.82, 138.24, 131.65, 111.78, 68.08 (cage C), 54.87, 53.01 (cation CH_2), 50.70, 7.66 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{38}\text{H}_{44}\text{B}_{11}\text{O}_7]^-$: 731.4202. Found: 731.4200.



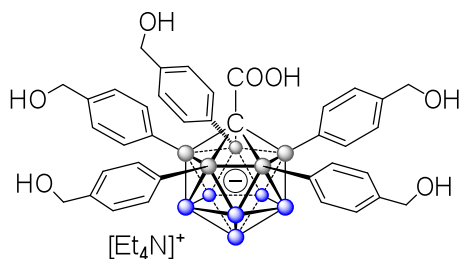
3r: Yield, 70%, colorless solid. Eluent: MeCN/MeOH=10:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, DMSO- d_6): δ 12.73-12.10 (broad signal, COOH), 9.64 (5H, NHCOCH_3), 7.10-7.00 (m, 10H), 7.00-6.89 (m, 10H) (aryl H), 3.17 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.37-1.77 (overlapping broad signals, 6H, BH), 1.98 (s, 15H, NHCOCH_3), 1.14 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, DMSO- d_6): two very broad overlapping signals with peaks at δ -5.68, -12.47.

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, DMSO- d_6): δ 167.85 (acetyl C), 164.71 (COOH), 136.88, 136.03, 133.72, 116.24, 67.72 (cage C), 51.39 (cation CH_2), 24.04, 7.08 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{42}\text{H}_{47}\text{B}_{11}\text{N}_5\text{O}_7]^-$: 852.4593. Found: 852.4556.



3s: Yield, 80%, colorless solid. Eluent: MeCN

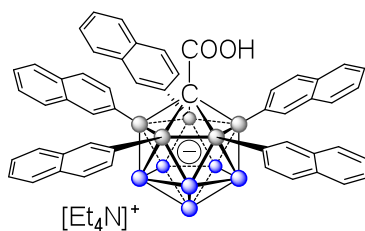
$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, DMSO- d_6): δ 12.97-12.00 (broad signal, COOH), 7.18-6.94 (m, 10H), 6.90-6.67 (m, 10H) (aryl H), 4.97 (t, $J = 5.8$ Hz, 5H, OH), 4.36 (d, $J = 5.8$ Hz, 10H, CH_2OH), 3.18 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.47-1.55 (overlapping broad signals, 6H, BH), 1.15 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, DMSO- d_6): two very broad overlapping signals with peaks at δ -5.00, -11.79.

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, DMSO- d_6): δ 164.78 (carbonyl), 139.05, 137.55, 135.60, 123.74, 67.75 (cage C), 63.14 (CH_2OH), 51.39 (cation CH_2), 7.09 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{37}\text{H}_{42}\text{B}_{11}\text{O}_7]^-$:

717.4046. Found: 717.4047.



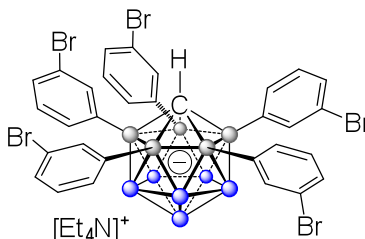
3t: Yield, 59%, colorless solid. Eluent: DCM/MeCN=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, DMSO- d_6): δ 14.00-11.93 (broad signal, COOH), 7.80-7.72 (m, 5H), 7.71-7.63 (m, 5H), 7.40-7.27 (overlapping m, 15H), 7.26-7.18 (m, 5H), 7.18-7.11 (m, 5H) (aryl H), 3.15 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.70-1.45 (overlapping broad signals, 6H, BH), 1.12 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, DMSO- d_6): two very broad overlapping signals with peaks at δ -4.63, -10.92.

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, DMSO- d_6): δ 165.13 (carbonyl), 137.09, 135.64, 133.66, 131.93, 131.67, 127.56, 126.96, 124.96, 124.72, 123.85, 68.23 (cage C), 51.39 (cation CH_2), 7.07 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{52}\text{H}_{42}\text{B}_{11}\text{O}_2]^-$: 818.4285. Found: 818.4280.



H-3u: Yield, 84%, colorless solid. Eluent: MeCN/MeOH=4:1

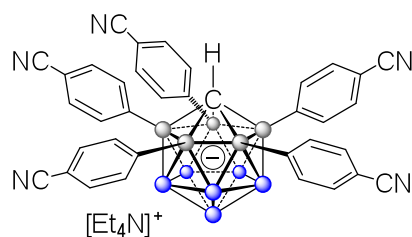
$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 7.70-7.65 (m, 5H), 7.53-7.47 (m, 5H), 7.03-6.99 (m, 5H), 6.85-6.79 (m, 5H) (aryl H), 5.02 (1H, cage CH), 3.46 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.73-2.07 (overlapping broad signals, 6H, BH), 1.37 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ -6.19 (5B), -9.55 (1B), -11.13 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6): δ 144.21, 136.93, 133.24, 129.18, 128.69, 121.61, 53.00 (cation CH_2), 46.32 (cage C), 7.66 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{31}\text{H}_{27}\text{B}_{11}\text{Br}_5]^-$:

917.9093. Found: 917.9091.



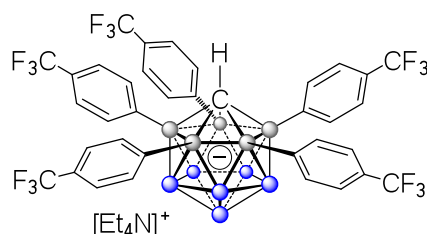
H-3v: Yield, 82%, colorless solid. Eluent: MeCN/MeOH=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetone- d_6): δ 7.68-7.62 (m, 10H), 7.31-7.24 (m, 10H) (aryl H), 5.15 (1H, cage CH), 3.48 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.79-2.09 (overlapping broad signals, 6H, BH), 1.38 (tt, 12H, J = 7.3 Hz, 1.9 Hz, CH_3 of cation)

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetone- d_6): δ -5.87 (5B), -7.96 to -13.53 (overlapping signals with peaks at -8.68 ppm and -10.49 ppm, 6B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6): δ 146.97, 134.86, 130.39, 119.75, 110.22, 52.92 (cation CH_2), 46.34 (cage C), 7.61 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{36}\text{H}_{27}\text{B}_{11}\text{N}_5]^-$: 648.3381. Found: 648.3374.



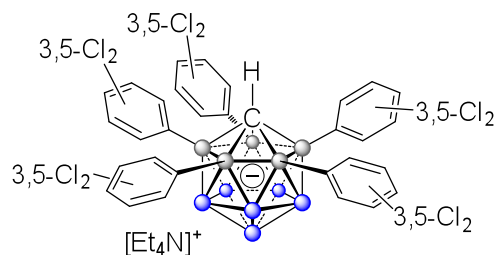
H-3w: Yield, 85%, colorless solid. Eluent: MeCN/MeOH=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 7.76-7.68 (m, 10H), 7.22-7.16 (m, 10H) (aryl H), 5.26 (1H, cage CH), 3.49 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.76-2.10 (overlapping broad signals, 6H, BH), 1.39 (tt, 12H, J = 7.3 Hz, 1.9 Hz, CH_3 of cation)

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ -5.79 (5B), -7.71 to -12.31 (overlapping signals with peaks at -8.88 ppm and -10.64 ppm, 6B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, acetone- d_6): δ 146.19, 134.78, 127.97 (q, $^2J_{\text{C-F}}$ = 31Hz), 125.73 (q, $^1J_{\text{C-F}}$ = 271 Hz), 123.34 (q, $^3J_{\text{C-F}}$ = 4 Hz), 53.01 (cation CH_2), 46.64 (cage C), 7.63 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{36}\text{H}_{27}\text{B}_{11}\text{F}_{15}]^-$: 863.2987. Found: 863.2996.



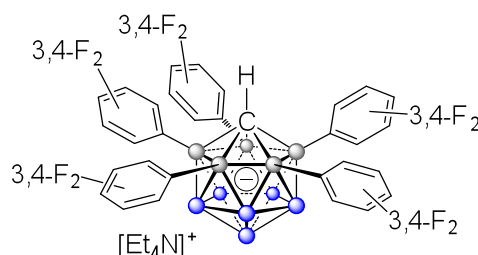
H-3x: Yield, 89%, colorless solid. Eluent: MeCN/MeOH=4:1

¹H{¹¹B} NMR (500 MHz, acetone-*d*₆): δ 7.47 (s, 10H), 7.01 (s, 5H) (aryl H), 5.26 (1H, cage CH), 3.50 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.78-2.09 (overlapping broad signals, 6H, BH), 1.39 (tt, 12H, *J* = 7.3 Hz, 1.9 Hz, CH₃ of cation)

¹¹B{¹H} NMR (160 MHz, acetone-*d*₆): δ -6.55 (5B), -9.00 (1B), -10.81 (5B).

¹³C{¹H} NMR (126 MHz, acetone-*d*₆): δ 144.60, 133.88, 132.37, 126.66, 52.99 (cation CH₂), 45.80 (cage C), 7.65 (cation CH₃).

High-resolution ESI-MS (negative mode, MeOH): *m/z*, calcd for [C₃₁H₂₂B₁₁Cl₁₀]⁻ : 867.9646. Found: 867.9649.



H-3y: Yield, 82%, colorless solid. Eluent: MeCN/MeOH=4:1. Based on the NMR data, this product contained an impurity of about 4%, which could not be removed by column chromatography.

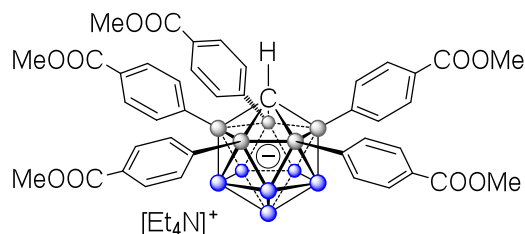
¹H{¹¹B} NMR (500 MHz, acetone-*d*₆): δ 7.34-7.25 (m, 5H), 7.24-7.18 (m, 5H), 6.89-6.80 (m, 5H) (aryl H), 4.75 (1H, cage CH), 3.49 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.64-2.06 (overlapping broad signals, 6H, BH), 1.39 (tt, 12H, *J* = 7.3 Hz, 1.9 Hz, CH₃ of cation)

¹¹B{¹H} NMR (160 MHz, acetone-*d*₆): δ -6.44 (5B), -9.75 (1B), -11.42 (5B).

¹³C{¹H} NMR (101 MHz, acetone-*d*₆): δ 149.73 (d, ¹*J*_{C-F} = 242 Hz, ²*J*_{C-F} coupling not resolved), 149.61 (d, ¹*J*_{C-F} = 242 Hz, ²*J*_{C-F} coupling not resolved), 138.61, 130.84 (dd, ²*J*_{C-F} = 6 Hz ³*J*_{C-F} = 4 Hz), 122.36 (d, ²*J*_{C-F} = 15 Hz, ³*J*_{C-F} coupling not resolved),

115.91 (d, $^2J_{\text{C-F}} = 15$ Hz, $^3J_{\text{C-F}}$ coupling not resolved), 52.96 (cation CH_2), 47.90 (cage C), 7.63 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{31}\text{H}_{22}\text{B}_{11}\text{F}_{10}]^-$: 703.2674. Found: 703.2668.



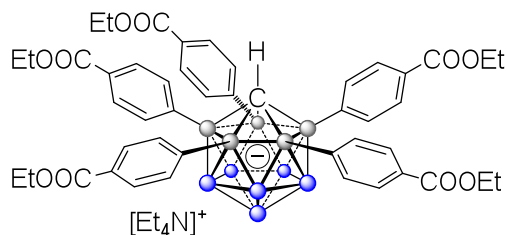
H-3z: Yield, 94%, colorless solid. Eluent: MeCN/MeOH=4:1 to pure MeCN

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, $\text{DMSO-}d_6$): δ 7.65-7.59 (m, 10H), 7.50-7.43 (m, 10H) (aryl H), 5.30 (1H, cage CH), 3.68 (s, 15H, COOMe), 3.19 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.60-1.83 (overlapping broad signals, 6H, BH), 1.14 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, $\text{DMSO-}d_6$): two very broad overlapping signals with a peak at δ -10.89.

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, $\text{DMSO-}d_6$): δ 166.56 (carbonyl), 146.35, 133.47, 126.81, 126.50, 52.69 (COOCH_3), 51.40 (cation CH_2), 45.16 (cage C), 7.08 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{41}\text{H}_{42}\text{B}_{11}\text{O}_{10}]^-$: 813.3895. Found: 813.3886.



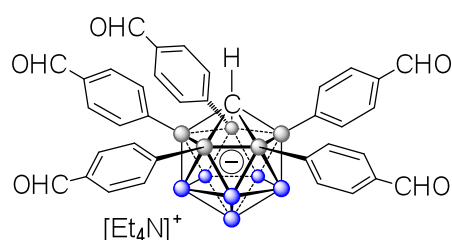
H-3aa: Yield, 99%, colorless solid. Eluent: MeCN/MeOH=4:1

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, $\text{DMSO-}d_6$): δ 7.65-7.57 (m, 10H), 7.48-7.43 (m, 10H) (aryl H), 5.26 (1H, cage CH), 4.16 (q, $J = 7.1$ Hz, 10H, OCH_2CH_3), 3.20 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.47-1.90 (overlapping broad signals, 6H, BH), 1.21 (t, $J = 7.1$ Hz, 15H, OCH_2CH_3), 1.15 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, $\text{DMSO}-d_6$): two very broad overlapping signals with peaks at -6.25 ppm and -10.63 ppm.

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{DMSO}-d_6$): δ 166.03 (carbonyl), 146.26, 133.38, 127.05, 126.44, 60.19 (OCH_2CH_3), 51.37 (cation CH_2), 45.01 (cage C), 14.12 (OCH_2CH_3), 7.05 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{46}\text{H}_{52}\text{B}_{11}\text{O}_{10}]^-$: 883.4680. Found: 883.4709.



H-3ab: Yield, 82%, colorless solid. Eluent: $\text{DCM}/\text{MeCN}=4:1$

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, $\text{acetone}-d_6$): δ 9.73 (s, 5 H, CHO), 7.79-7.74 (m, 10H), 7.43-7.38 (m, 10H) (aryl H), 5.20 (1H, cage CH), 3.50 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.76-2.19 (overlapping broad signals, 6H, BH), 1.39 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, $\text{acetone}-d_6$): δ -5.69 (5B), -8.79 (1B), -10.43 (5B).

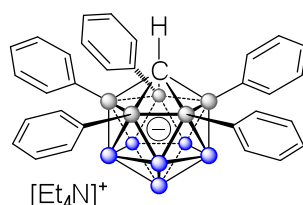
$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{DMSO}-d_6$): δ 193.05 (CHO), 148.00, 133.77 (two overlapping aryl CH), 127.00 (two overlapping aryl CH), 51.02 (cation CH_2), 45.02 (cage C), 7.06 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{36}\text{H}_{32}\text{B}_{11}\text{O}_5]^-$: 663.3364. Found: 663.3355.

II b) Synthesis of products H-3 from isolated 3

General procedure

In a 20 mL flask, compound **3** (0.05 mmol) was dissolved in DMF (2.5 mL) under N₂ atmosphere. The resulting mixture was heated to 100 °C for 18 h. If the reaction was not completed after 18 h, KOAc (0.1 mmol) was added to the mixture to accelerate the reaction. After the reaction period, the mixture was allowed to cool to room temperature and poured into an aqueous solution of [Et₄N]Br (50 mL, *c* = ca. 0.5 g/100 mL) to precipitate the product. Compounds **H-3** were collected by filtration through a glass frit.



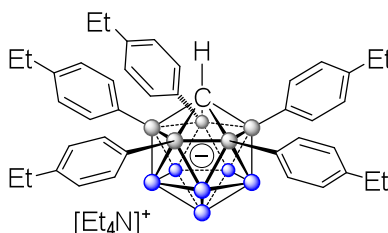
H-3a: Yield, 91%, colorless solid.

¹H{¹¹B} NMR (400 MHz, DMSO-*d*₆): δ 7.41-7.33 (m, 10H), 6.86-6.75 (overlapping m, 15H) (aryl H), 4.62 (1H, cage CH), 3.18 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.50-1.58 (overlapping broad signals, 6H, BH), 1.14 (tt, 12H, *J* = 7.3 Hz, 1.9 Hz, CH₃ of cation).

¹¹B{¹H} NMR (128 MHz, DMSO-*d*₆): two very broad overlapping signals with peaks at -5.81 ppm and -11.71 ppm.

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆): δ 140.47, 133.44, 125.59, 124.89, 51.36 (cation CH₂), 45.41 (cage C), 7.06 (cation CH₃).

High-resolution ESI-MS (negative mode, MeOH): *m/z*, calcd for [C₃₁H₃₂B₁₁]⁻ : 523.3616. Found: 523.3618.



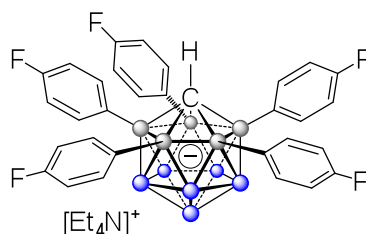
H-3c: Yield, 99%, colorless solid.

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, $\text{DMSO}-d_6$): δ 7.33-7.20 (m, 10H), 6.67-6.60 (m, 10H) (aryl H), 4.42 (1H, cage CH), 3.20 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.31 (q, $J = 7.3$ Hz, 10H, CH_2CH_3), 2.27-1.62 (overlapping broad signals, 6H, BH), 1.15 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation), 0.98 (t, $J = 7.3$ Hz, 15H, CH_2CH_3).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, $\text{DMSO}-d_6$): two very broad overlapping signals with peaks at -5.94 ppm and -11.83 ppm.

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{DMSO}-d_6$): δ 139.40, 137.68, 133.39, 125.19, 51.36 (cation CH_2), 45.01 (cage C), 27.67 (CH_2CH_3), 15.12 (CH_2CH_3), 7.07 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{41}\text{H}_{52}\text{B}_{11}]^-$: 663.5185. Found: 663.5162.



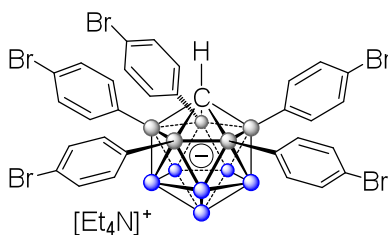
H-3i: Yield, 99%, colorless solid.

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, $\text{DMSO}-d_6$): δ 7.42-7.31 (m, 10H), 6.71-6.59 (m, 10H) (aryl H), 4.75 (1H, cage CH), 3.19 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.45-1.55 (overlapping broad signals, 6H, BH), 1.15 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, $\text{DMSO}-d_6$): two very broad overlapping signals with peaks at -6.05 ppm and -11.65 ppm.

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{DMSO}-d_6$): δ 160.97 (d, $^1J_{\text{C-F}} = 242$ Hz), 136.06, 134.94 (d, $^3J_{\text{C-F}} = 7$ Hz), 112.49 (d, $^2J_{\text{C-F}} = 19$ Hz), 51.36 (cation CH_2), 46.32 (cage C), 7.06 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{31}\text{H}_{27}\text{B}_{11}\text{F}_5]^-$: 613.3145. Found: 613.3136.



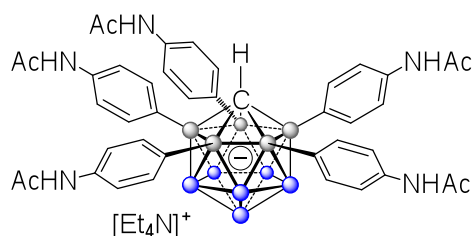
H-3n: Yield, 99%, colorless solid.

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, $\text{DMSO-}d_6$): δ 7.40-7.27 (m, 10H), 7.13-6.98 (m, 10H) (aryl H), 4.93 (1H, cage CH), 3.19 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.43-1.63 (overlapping broad signals, 6H, BH), 1.15 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, $\text{DMSO-}d_6$): two very broad overlapping signals with peaks at -5.88 ppm and -11.27 ppm.

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{DMSO-}d_6$): δ 139.25, 135.33, 128.69, 119.45, 51.36 (cation CH_2), 44.80 (cage C), 7.06 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{31}\text{H}_{27}\text{B}_{11}\text{Br}_5]^-$: 917.9093. Found: 917.9070.



H-3r: Yield, 93%, colorless solid.

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, $\text{DMSO-}d_6$): δ 9.46 (broad s, 5H, NH), 7.26-7.17 (m, 10H), 7.06-6.99 (m, 10H) (aryl H), 4.40 (1H, cage CH), 3.17 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.34-1.62 (overlapping broad signals, 6H, BH), 1.90 (s, 15H, acetyl CH_3), 1.13 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, $\text{DMSO-}d_6$): two very broad overlapping signals with peaks at -5.60 ppm and -12.62 ppm.

$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, $\text{DMSO-}d_6$): δ 167.58 (carbonyl), 136.50, 135.23, 133.49, 116.67, 51.39 (cation CH_2), 45.63 (cage C), 23.92, 7.06 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{41}\text{H}_{47}\text{B}_{11}\text{N}_5\text{O}_5]^-$: 808.4694. Found: 808.4652.

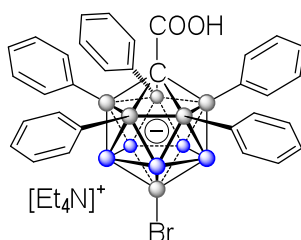
II c) Derivatization of products 3b, H-3v and H-3r

General Procedure for the bromination of the B12 position of 3a and H-3v.

4a and **4b** were synthesized according to the literature.^[4]

To a stirred solution of penta-arylated product **3a** (0.1 mmol) in a mixture of MeCN (1 mL) and MeOH (4 mL) was added *N*-bromosuccinimide (1.1 mmol). The reaction mixture was stirred for 2 h at 25 °C. Aqueous Na₂SO₃ solution (0.1 mmol in 1 mL H₂O) was added to the mixture. The organic solvent was then removed under reduced pressure. The aqueous solution was extracted with DCM (3 x 10 mL). The combined DCM layers were dried in a vacuum to give **4a** as a colorless solid in 98% yield.

Bromination of **H-3v** was conducted in MeCN (4 mL), which was stirred at 60 °C for 17 h. Work-up was the identical to that for **4a**. Product **4b** was obtained in 91% yield.



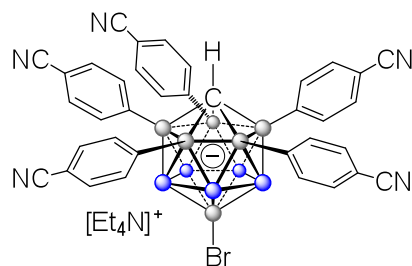
4a: Yield, 98%, colorless solid.

¹H NMR (500 MHz, acetone-*d*₆): δ 7.26-7.22 (m, 10H), 7.01-6.96 (m, 5H), 6.86-6.81 (m, 10H) (phenyl H), 3.42 (q, *J* = 7.3 Hz, 8H, CH₂ of cation), 2.5-2.16 (overlapping broad signals, 5H, BH), 1.35 (tt, 12H, *J* = 7.3 Hz, 1.9 Hz, CH₃ of cation). The COOH signal could not be detected.

¹¹B{¹H} NMR (160 MHz, acetone-*d*₆): δ -0.42 (s, 1B, B12), -4.47 (5B), -10.81 (5B).

¹³C{¹H} NMR (126 MHz, acetone-*d*₆): δ 166.20 (carbonyl), 139.40, 137.25, 126.39, 126.22, 62.73 (cage C), 53.00 (cation CH₂), 7.68 (cation CH₃).

High-resolution ESI-MS (negative mode, MeOH): *m/z*, calcd for [C₃₂H₃₁B₁₁BrO₂]⁻: 646.2609. Found: 646.2639.



4b: Yield, 91%, colorless solid.

$^1\text{H}\{^{11}\text{B}\}$ NMR (500 MHz, acetone- d_6): δ 7.69-7.60 (m, 10H), 7.34-7.23 (m, 10H) (aryl H), 5.16 (cage CH), 3.50 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 3.04-2.47 (overlapping broad signals, 5H, BH), 1.40 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

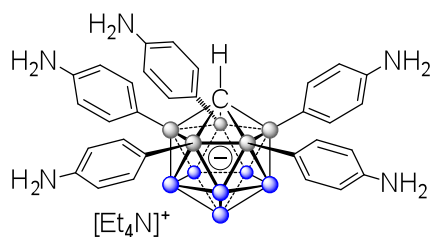
$^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, acetone- d_6): δ -4.35 (s, 1B, B12), -6.50 (5B), -10.21 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetone- d_6): δ 145.55, 135.10, 130.55, 119.65, 110.57, 53.01 (cation CH_2), 40.11 (cage C), 7.70 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{36}\text{H}_{26}\text{B}_{11}\text{BrN}_5]^-$: 727.2475. Found: 727.2462.

General Procedure for deacylation of **H-3r**^[5]

Ammonium bromide (58.8 mg, 0.6 mmol), **H-3r** (93.9 mg, 0.1 mmol), and ethylenediamine (5 mL) were added to 30 mL microwave reaction tube containing a magnetic stir bar. The tube was capped and heated to 80 °C for 22 h under microwave-irradiation conditions (CEM instrument, mode: target temperature). The crude reaction mixture was transferred to 50 mL flask, and most of the ethylenediamine was removed by using a rotary evaporator equipped with a N_2 cooled trap. A solution of 1 g $[\text{Et}_4\text{N}]\text{Br}$ in 30 mL H_2O was then added to the residue to precipitate the deacylated product. The precipitate was collected by filtration through a glass frit, and the solid was washed with H_2O (3 x 10 mL) and hexane (2 x 5 mL). The colorless solid was dried under a vacuum to give **5** (72.4 mg, 99%).



5: Yield, 99%, colorless solid.

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, $\text{DMSO-}d_6$): δ 6.93-6.74 (m, 10H), 6.15-5.95 (m, 10H) (aryl H), 4.33 (broad signal, 10H, NH), 3.58 (cage CH), 3.14 (q, $J = 7.3$ Hz, 8H, CH_2 of cation), 2.05-1.34 (overlapping broad signals, 6H, BH), 1.12 (tt, 12H, $J = 7.3$ Hz, 1.9 Hz, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, $\text{DMSO-}d_6$): very broad overlapping signals with two peaks at -5.92 and -13.31.

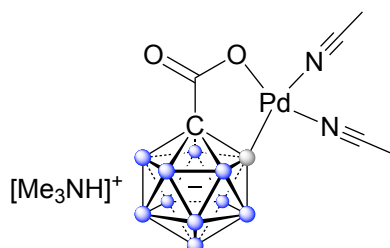
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, $\text{DMSO-}d_6$): δ 145.14, 133.99, 128.16, 112.54, 51.41 (cation CH_2), 46.93 (cage C), 7.08 (cation CH_3).

High-resolution ESI-MS (negative mode, MeOH): m/z , calcd for $[\text{C}_{31}\text{H}_{37}\text{B}_{11}\text{N}_5]^-$: 598.4161. Found: 598.4144.

II d) Preparation of intermediate 1-Pd

For NMR characterization and X-ray diffraction, this complex was obtained starting from the $[\text{Me}_3\text{NH}]^+$ salt according to the following procedure. In a glovebox, $\text{Pd}(\text{OAc})_2$ (91 mg, 0.405 mmol) was added to a stirred solution of $[\text{Me}_3\text{NH}][1\text{-COOH-CB}_{11}\text{H}_{11}]$ (100 mg, 0.405 mmol) in acetonitrile (0.45 mL). The resulting mixture was stirred at 25 °C for 6 h. A pale precipitate formed, which was filtered through a fine glass frit. and washed with hexane (the hexane washing fraction was collected separately and disposed of). The filtrate was left to evaporate slowly at room temperature (evaporation of *ca.* 60% of the solvent over 2 days) to yield colorless crystals, which were collected by filtration. The combined solids were dried at 25 °C in a vacuum to give palladium complex **1-Pd** (151 mg, 86%).

For the catalytic study shown in Figure 3a, the complex was formed in MeCN starting with the $[\text{Et}_4\text{N}]^+$ cation. Upon solvent removal under reduced pressure, it was used directly for the penta-arylation reaction.



1-Pd: yield, 86%, colorless solid.

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, acetonitrile- d_3): δ 9.33 (s, 1H, NH), 2.73 (s, 9H, CH_3 of cation), 1.96 (s, 6H, CH_3CN), 1.22-1.90(m, 10H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, acetonitrile- d_3): δ -7.39, -13.16, -14.23, -15.85, -20.10.

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, acetonitrile- d_3): δ 179.81 (CO), 74.22 (cage C), 45.54 (cation CH_3).

II e) Transformations starting from mono-arylated **3h**

The DFT calculations suggested that the first arylation step at the B2 vertex is followed by substitution at the B3 position rather than at the B4 position. In order to probe the sequence of arylation experimentally, the following transformations starting from mono-arylated **3h** were carried out.

1) Subjecting **3h** to catalytic conditions using iodobenzene as the coupling partner:

5 mg of **3h** were dissolved in DMF, and the catalyst system was added (2.5 mol% Pd(OAc)₂, 6 equiv AgOAc, 6 equiv HOAc). Iodobenzene was added in several portions, and the reaction mixture was first stirred at 25 °C, then at 60 °C (for details, see Fig. S2).

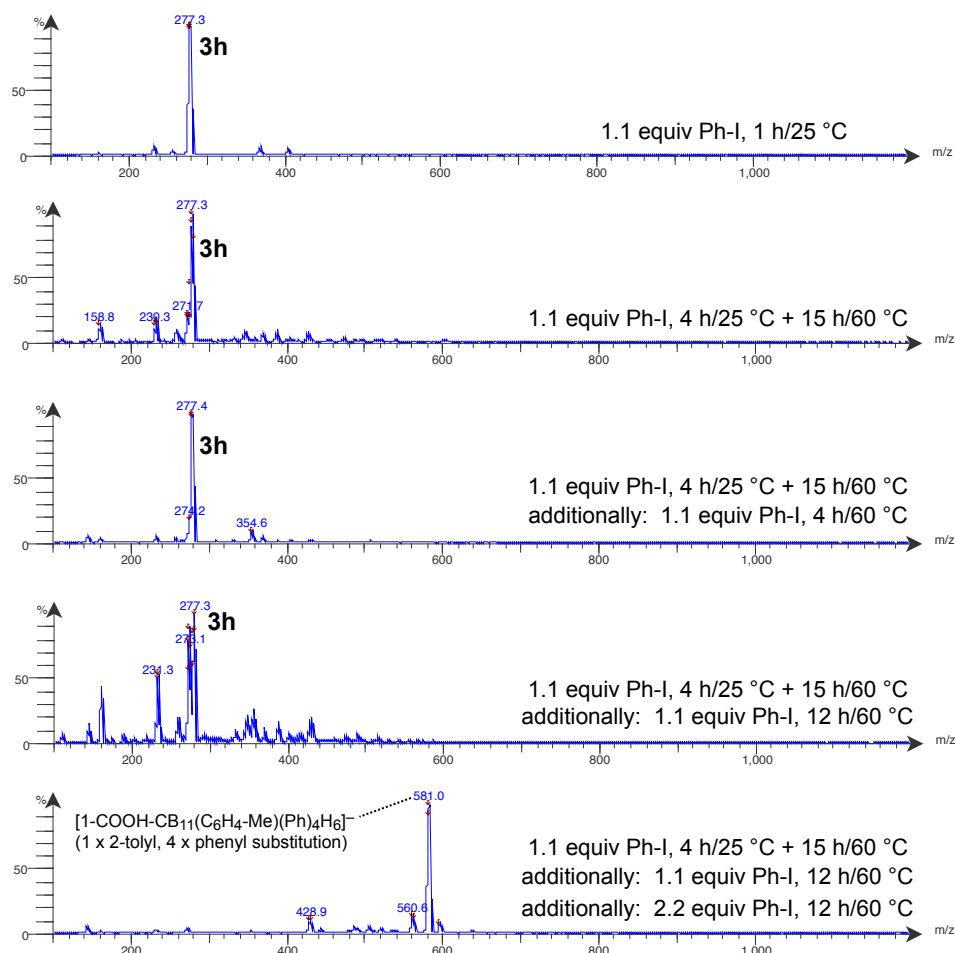


Figure S2. Monitoring of the reaction of **3h** with iodobenzene under catalytic conditions by (–)-ESI-MS.

As evidenced by (–)-ESI-MS, addition of 1.1 equiv of iodobenzene did not lead to a change of the mass spectrum within 4 h at 25 °C plus 15 h at 60 °C. Addition of another 1.1 equiv of iodobenzene and stirring for 12 h at 60 °C resulted in a noisy mass spectrum with multiple signals. Addition of another 2.2 equiv of iodobenzene and stirring for 12 h at 60 °C gave a mass spectrum with the mass of the penta-arylated product $[\text{COOH-CB}_{11}(\text{C}_6\text{H}_4\text{-Me})(\text{Ph})_4\text{H}_6]^-$ as the main signal. Given that products from di-, tri- and tetra-arylation can not be detected clearly, these findings indicate that the entire cascade occurs quickly once the B–H activation process starts. This is consistent with the monitoring displayed in Fig. S1 and the DFT calculations. However, based on this experiment, it is not possible to determine whether the substitution processes occur consecutively at adjacent or at geminal boron vertices.

*2) Treatment of **3h** with a stoichiometric amount of Pd(II):*

In a glovebox, 8 mg of **3h** were dissolved in CD_3CN (0.6 mL) in a 5 mm NMR tube, and $\text{Pd}(\text{OAc})_2$ (1.05 equiv) was added. The mixture was shaken well and kept at 25 °C for 6 h prior to NMR characterization. ^{11}B , $^{11}\text{B}\{^1\text{H}\}$ and ^{11}B - ^{11}B COSY spectra are shown in Figure S3.

The spectra suggested transformation of **3h** to a Pd complex **3h-Pd** with a B–Pd bond, as indicated by the signal at –20 ppm (Fig. S3 a and b). This ^{11}B chemical shift is diagnostic for boron directly bound to Pd (see the characterization of **1-Pd** and also the following reference: Shen, Y.; Liu, J.; Sattasathuchana, T.; Baldrige, K. K.; Duttwyler, S. *Eur. J. Inorg. Chem.* **2017**, 4420). The ^{11}B - ^{11}B COSY spectrum comprised only extremely weak correlations signals (Fig. S3 c). Weak correlation is a common phenomenon in ^{11}B - ^{11}B COSY spectroscopy and has been explained by Grimes.^[3] Based on these results, an unambiguous conclusion about the position where B–H activation of **3h** takes place can therefore not be made.

Attempts to obtain single crystals of **3h-Pd** were not successful because slow decomposition occurred; formation of Pd(0) ("palladium black") and unidentified cage products were observed.

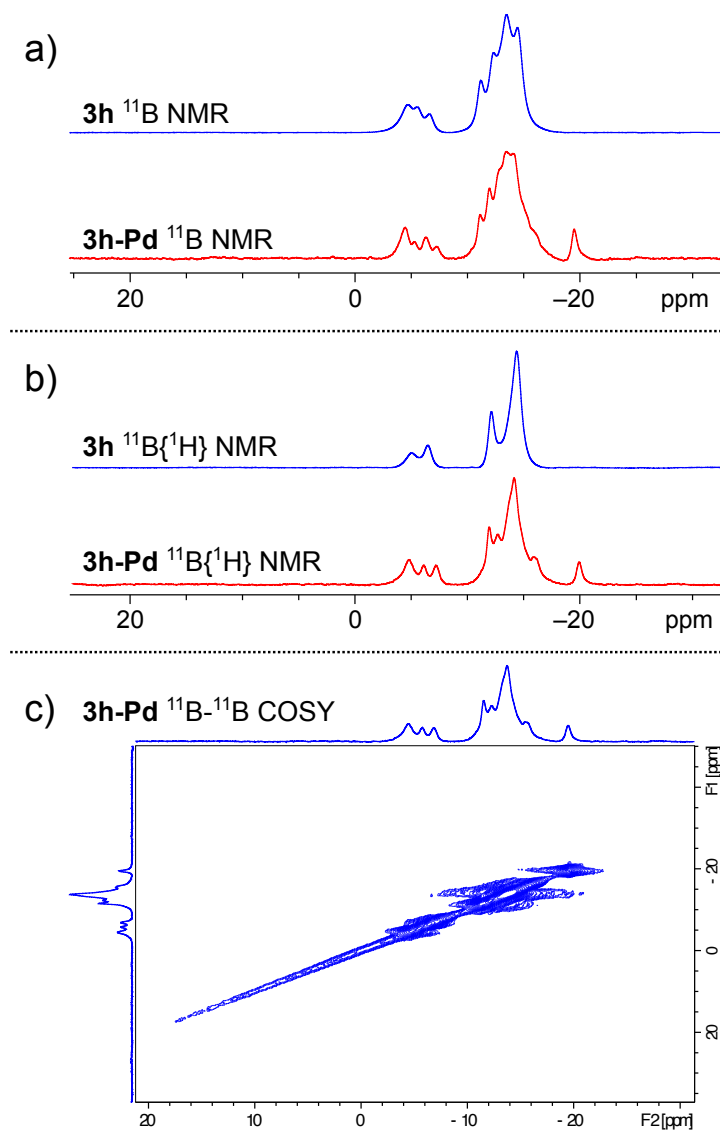


Figure S3. (a) ^{11}B NMR spectra of **3h** and **3h-Pd**; (b) $^{11}\text{B}\{^1\text{H}\}$ NMR spectra of **3h** and **3h-Pd**; (c) ^{11}B - ^{11}B COSY NMR spectrum of **3h-Pd**; conditions: CD_3CN , 23 $^\circ\text{C}$, 160 MHz for ^{11}B .

III X-ray Crystallography

Product 3a

The compound (20 mg) was dissolved in acetone (0.5 mL) in a 1 mL glass vial. The resulting colorless solution was filtered into an 18 cm long glass NMR tube and layered with hexane (1 mL). Colorless crystals of the composition [NEt₄][1-COOH-CB₁₁H₆-Ph₅] suitable for X-ray diffraction grew within 10 d at 13 °C. (CCDC 1854793)

Bond precision:	C-C = 0.0044 Å	Wavelength=1.34139
Cell:	a=11.9001(5)	b=12.2874(6) c=15.7460(7)
	alpha=68.156(3)	beta=80.248(3) gamma=72.507(3)
Temperature:	170 K	
	Calculated	Reported
Volume	2033.95(17)	2033.95(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H32 B11 O2, C8 H20 N	C32 H32 B11 O2, C8 H20 N
Sum formula	C40 H52 B11 N O2	C40 H52 B11 N O2
Mr	697.74	697.73
Dx, g cm ⁻³	1.139	1.139
Z	2	2
Mu (mm ⁻¹)	0.305	0.309
F000	740.0	740.0
F000'	741.34	
h,k,lmax	14,15,19	14,14,19
Nref	7902	7749
Tmin,Tmax	0.971,0.994	0.434,0.751
Tmin'	0.964	
Correction method= # Reported T Limits: Tmin=0.434 Tmax=0.751		
AbsCorr = MULTI-SCAN		
Data completeness=	0.981	Theta(max)= 55.482
R(reflections)=	0.0730(4937)	wR2(reflections)= 0.2215(7749)
S =	1.042	Npar= 495

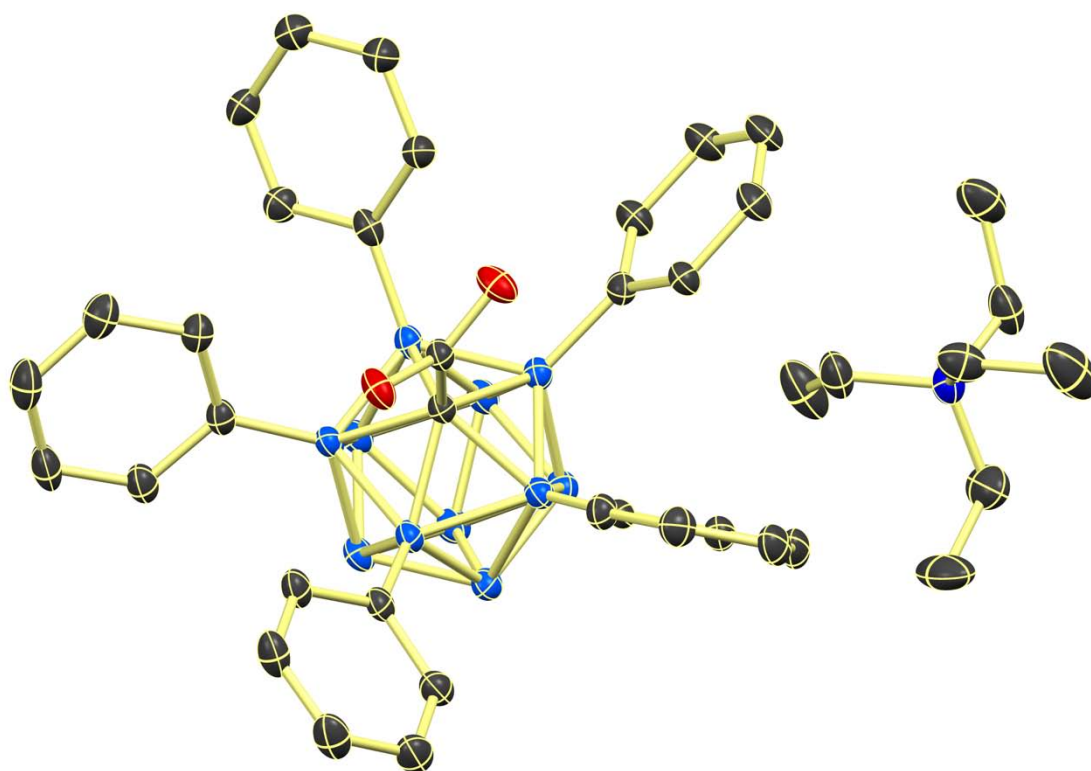


Figure S4. ORTEP representation of [NEt₄][1-COOH-CB₁₁H₆-Ph₅]. Hydrogen atoms are omitted for clarity; 25% displacement ellipsoids.

Product 3b

The compound (20 mg) was dissolved in acetone (0.5 mL) in a 1 mL glass vial. The resulting colorless solution was filtered into an 18 cm long glass NMR tube and layered with hexane (1 mL). Colorless crystals of the composition [NEt₄][1-COOH-CB₁₁H₆-(4-Me-C₆H₄)₅] suitable for X-ray diffraction grew within 10 d at 13 °C. (CCDC 1854794)

Bond precision:	C-C = 0.0032 Å	Wavelength=1.34139
Cell:	a=11.4673 (2) alpha=90	b=16.6842 (3) beta=110.724 (1) c=12.3236 (2) gamma=90
Temperature:	170 K	
	Calculated	Reported
Volume	2205.23 (7)	2205.23 (7)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C37 H42 B11 O2, C8 H20 N	C37 H42 B11 O2, C8 H20 N
Sum formula	C45 H62 B11 N O2	C45 H62 B11 N O2
Mr	767.87	767.86
Dx, g cm ⁻³	1.156	1.156
Z	2	2
Mu (mm ⁻¹)	0.308	0.312
F000	820.0	820.0
F000'	821.47	
h,k,lmax	13,20,15	13,20,15
Nref	8401 [4354]	8373
Tmin,Tmax	0.981,0.997	0.569,0.751
Tmin'	0.963	
Correction method= # Reported T Limits: Tmin=0.569 Tmax=0.751		
AbsCorr = MULTI-SCAN		
Data completeness=	1.92/1.00	Theta(max)= 54.945
R(reflections)=	0.0425 (8196)	wR2(reflections)= 0.1119 (8373)
S =	1.053	Npar= 545

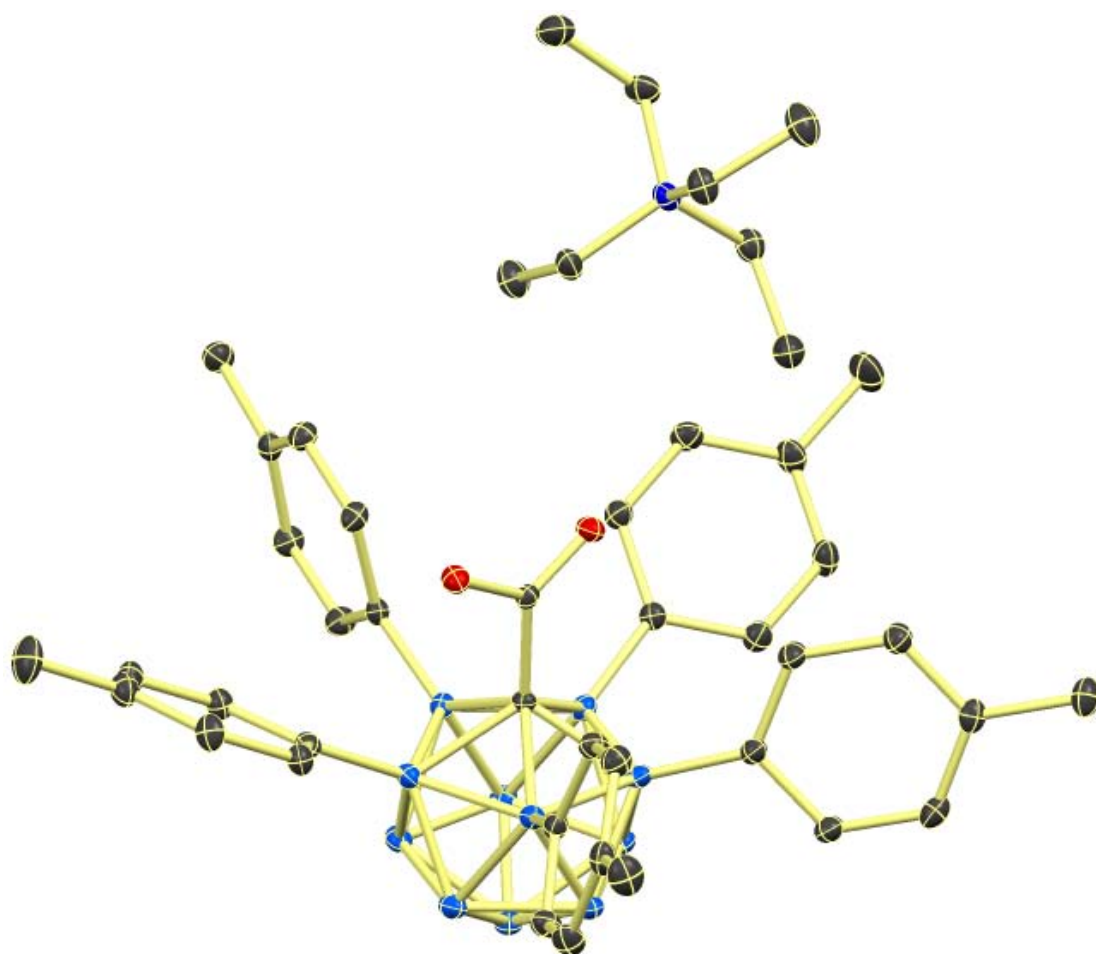


Figure S5. ORTEP representation of $[\text{NEt}_4][1\text{-COOH-CB}_{11}\text{H}_6\text{-(4-Me-C}_6\text{H}_4)_5]$. Hydrogen atoms are omitted for clarity; 25% displacement ellipsoids.

Product 3c

The compound (20 mg) was dissolved in THF (0.5 mL) in a 1 mL glass vial. The resulting colorless solution was filtered into an 18 cm long glass NMR tube and layered with hexane (1 mL). Colorless crystals of the composition [NEt₄][1-COOH-CB₁₁H₆-(3-Me-C₆H₄)₅] suitable for X-ray diffraction grew within 10 d at 13 °C. (CCDC 1854795)

Bond precision:	C-C = 0.0043 Å	Wavelength=0.71073
Cell:	a=18.1297 (9)	b=12.7407 (6) c=23.8742 (13)
	alpha=90	beta=106.874 (5) gamma=90
Temperature:	120 K	
Volume	Calculated 5277.2 (5)	Reported 5277.2 (5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	2 (C37 H42 B11 O2), 0.282 (C8 H16 O2), 2 (C8 H20 N), 2.836 (C4 H8 O)	C37 H42 B11 O2, 1.7 (C4 H8 O), C8 H20 N, 0.3 (C H3 O)
Sum formula	C104.20 H153 B22 N2 O8	C52.09 H76.48 B11 N O4
Mr	1799.51	899.58
Dx, g cm ⁻³	1.133	1.132
Z	2	4
Mu (mm ⁻¹)	0.066	0.066
F000	1932.4	1932.0
F000'	1933.06	
h,k,lmax	21,15,28	21,15,28
Nref	9675	9570
Tmin,Tmax	0.973,0.979	0.949,1.000
Tmin'	0.973	
Correction method= # Reported T Limits: Tmin=0.949 Tmax=1.000		
AbsCorr = MULTI-SCAN		
Data completeness=	0.989	Theta(max)= 25.348
R(reflections)=	0.0735 (6529)	wR2(reflections)= 0.2167 (9570)
S =	1.034	Npar= 666

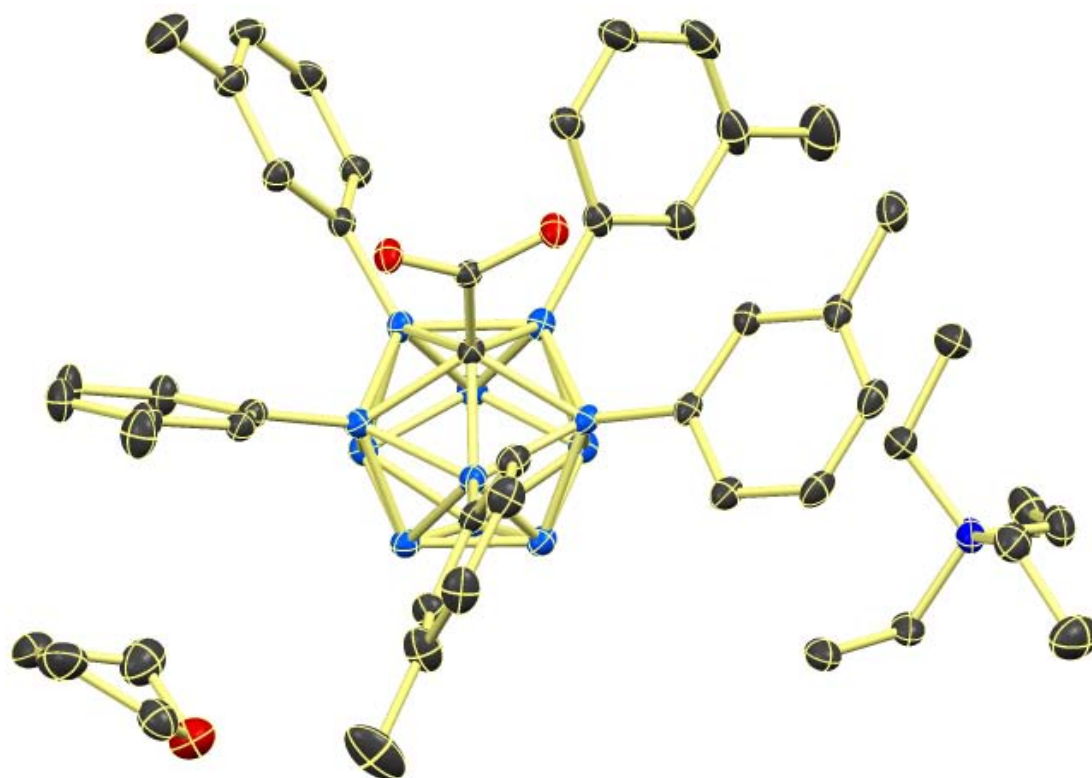


Figure S6. ORTEP representation of $[\text{NEt}_4][1\text{-COOH-CB}_{11}\text{H}_6\text{-(3-Me-C}_6\text{H}_4)_5]$. Hydrogen atoms are omitted for clarity; 25% displacement ellipsoids.

Product 3q

The compound (20 mg) was dissolved in acetone (0.5 mL) in a 1 mL glass vial. The resulting colorless solution was filtered into an 18 cm long glass NMR tube and layered with hexane (1 mL). Colorless crystals of the composition [NEt₄][1-COOMe-CB₁₁H₆-(4-OMe-C₆H₄)₅] suitable for X-ray diffraction grew within 10 d at 13 °C. (CCDC 1854796)

Bond precision:	C-C = 0.0049 Å	Wavelength=0.71073
Cell:	a=23.6242(15) alpha=90	b=19.1081(9) beta=90
		c=22.3852(10) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	10105.0(9)	10105.0(9)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C38 H44 B11 O7, C8 H20 N	C38 H44 B11 O7, 2(C4 H10 N0.5)
Sum formula	C46 H64 B11 N O7	C46 H64 B11 N O7
Mr	861.89	861.89
Dx,g cm ⁻³	1.133	1.133
Z	8	8
Mu (mm ⁻¹)	0.070	0.070
F000	3664.0	3664.0
F000'	3665.45	
h,k,lmax	28,23,26	28,23,26
Nref	9269	9195
Tmin,Tmax	0.967,0.981	0.966,1.000
Tmin'	0.967	
Correction method= # Reported T Limits: Tmin=0.966 Tmax=1.000		
AbsCorr = MULTI-SCAN		
Data completeness=	0.992	Theta(max)= 25.350
R(reflections)=	0.0796(5310)	wR2(reflections)= 0.2654(9195)
S =	1.043	Npar= 614

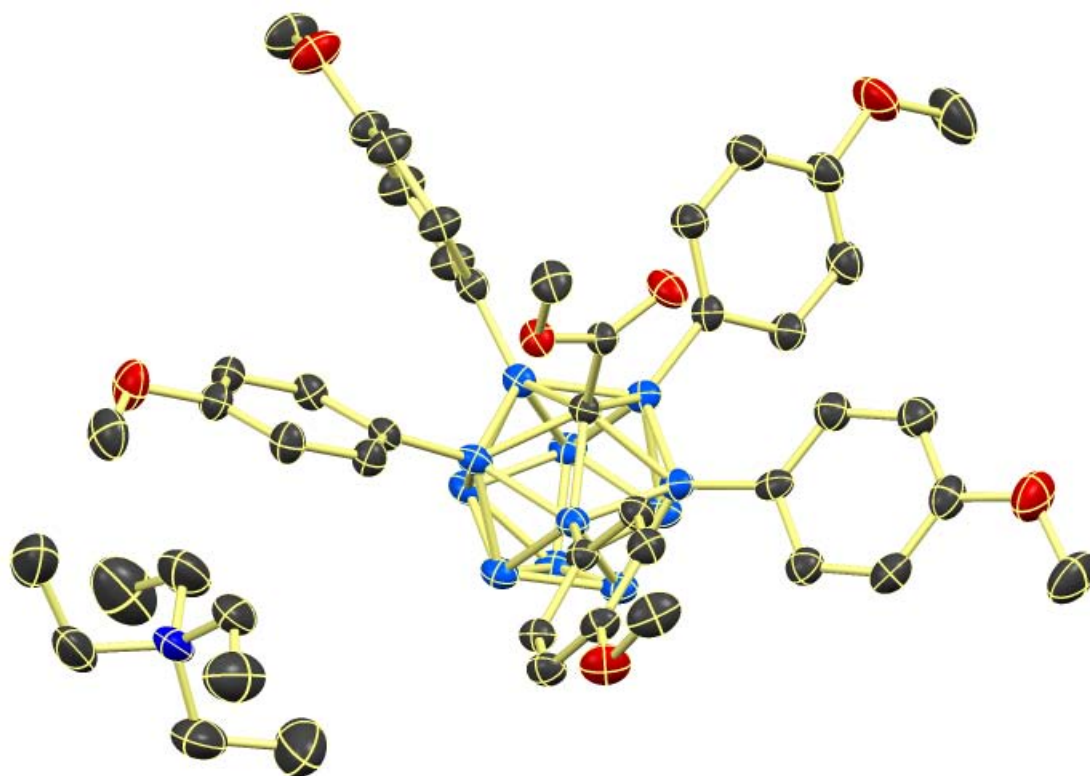


Figure S7. ORTEP representation of $[\text{NEt}_4][1\text{-COOMe-CB}_{11}\text{H}_6\text{-(4-OMe-C}_6\text{H}_4)_5]$. Hydrogen atoms and disordered atoms are omitted for clarity; 25% displacement ellipsoids.

Product H-3u

The compound (20 mg) was dissolved in DCM (0.5 mL) in a 1 mL glass vial. The resulting colorless solution was filtered into an 18 cm long glass NMR tube and layered with hexane (1 mL). Colorless crystals of the composition [NEt₄][CB₁₁H₇-(3-Br-C₆H₄)₅] suitable for X-ray diffraction grew within 10 d at 13 °C. (CCDC 1854797)

Bond precision:	C-C = 0.0160 Å	Wavelength=0.71073
Cell:	a=7.2360 (3) alpha=90	b=26.5714 (13) beta=90
Temperature:	137 K	c=26.8768 (9) gamma=90
	Calculated	Reported
Volume	5167.6 (4)	5167.6 (4)
Space group	P b c m	P b c m
Hall group	-P 2c 2b	-P 2c 2b
Moiety formula	C31 H27 B11 Br5, C8 H20 N, 2(C3 H6 O), C8 H20 N, C31 2(C3 H6 O)	H27 B11 Br5
Sum formula	C45 H59 B11 Br5 N O2	C45 H59 B11 Br5 N O2
Mr	1164.34	1164.39
Dx, g cm ⁻³	1.497	1.497
Z	4	4
Mu (mm ⁻¹)	3.925	3.925
F000	2328.0	2328.0
F000'	2323.11	
h,k,lmax	8,32,32	8,32,32
Nref	4855	4850
Tmin,Tmax	0.384,0.629	0.721,0.909
Tmin'	0.124	
Correction method= # Reported T Limits: Tmin=0.721 Tmax=0.909		
AbsCorr = ANALYTICAL		
Data completeness=	0.999	Theta(max)= 25.348
R(reflections)=	0.0835 (4032)	wR2(reflections)= 0.1600 (4850)
S =	1.184	Npar= 479

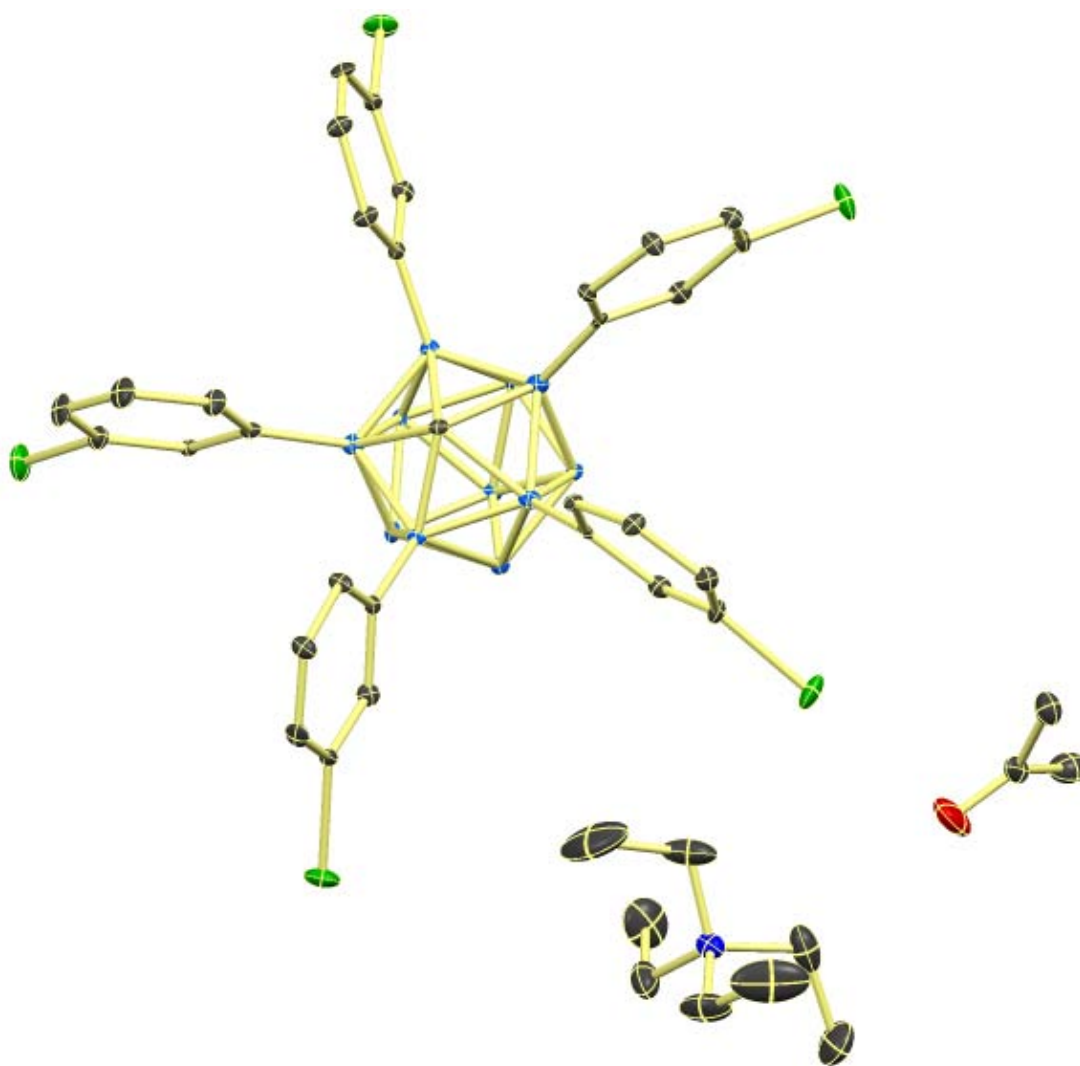


Figure S8. ORTEP representation of [NEt₄][CB₁₁H₇-(3-Br-C₆H₄)₅]. Hydrogen atoms and disordered atoms are omitted for clarity; 25% displacement ellipsoids.

Product H-3x

The compound (20 mg) was dissolved in dichloromethane (0.5 mL) in a 1 mL glass vial. The resulting colorless solution was filtered into an 18 cm long glass NMR tube and layered with hexane (1 mL). Colorless crystals of the composition [NEt₄][CB₁₁H₇-(3,5-Cl₂-C₆H₃)₅] suitable for X-ray diffraction grew within 10 d at 13 °C. (CCDC 1854798)

Bond precision: C-C = 0.0108 Å

Wavelength=0.71073

Cell: a=14.6290 (5) b=14.9866 (5) c=22.4078 (7)
alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	4912.7 (3)	4912.6 (3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	2 (C31 H22 B11 Cl10), 2 (C8.50 H21 Cl N)	2 (C31 H22 B11 Cl10), 2 (C8 H20 N), C H2 Cl2
Sum formula	C79 H86 B22 Cl22 N2	C79 H86 B22 Cl22 N2
Mr	2081.22	2081.21
Dx, g cm ⁻³	1.407	1.407
Z	2	2
Mu (mm ⁻¹)	0.654	0.654
F000	2116.0	2116.0
F000'	2122.95	
h,k,lmax	17,18,26	17,18,26
Nref	8978 [4977]	8913
Tmin,Tmax	0.733,0.833	0.896,1.000
Tmin'	0.719	

Correction method= # Reported T Limits: Tmin=0.896 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.79/0.99 Theta(max)= 25.347

R(reflections)= 0.0609 (7831) wR2(reflections)= 0.1712 (8913)

S = 1.062 Npar= 611

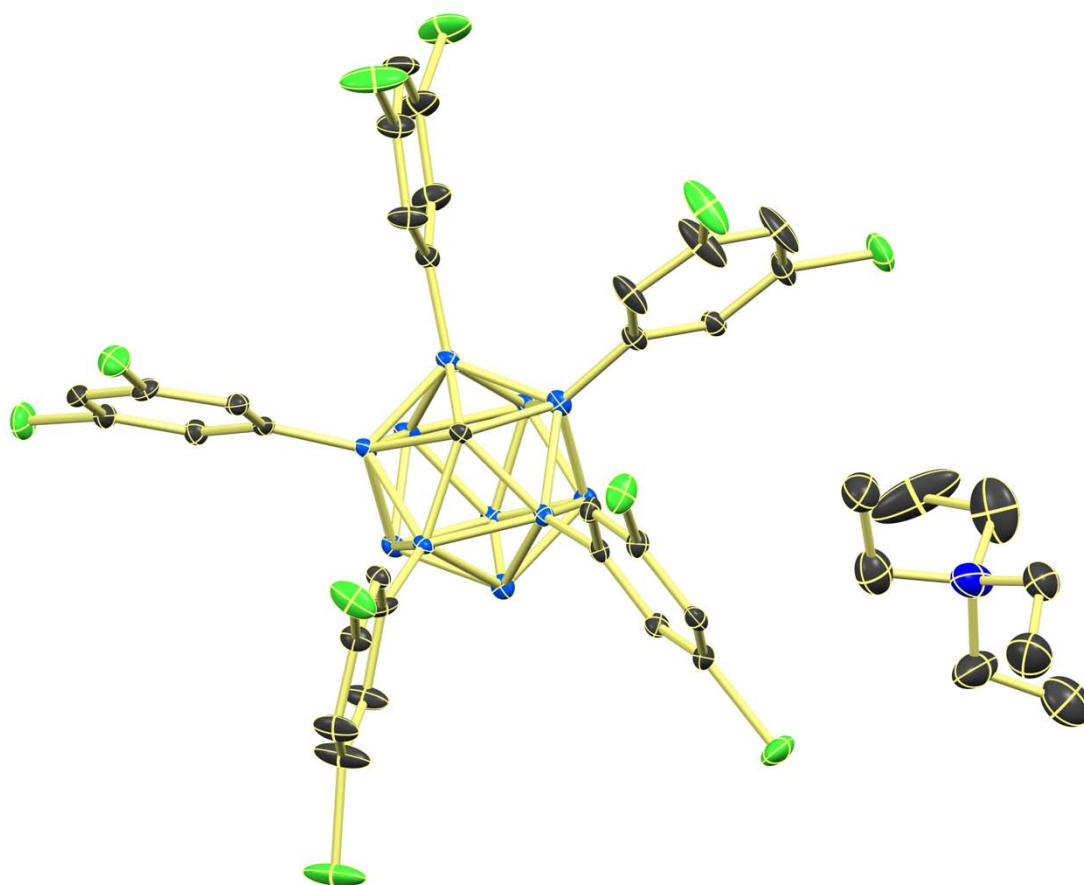


Figure S9. ORTEP representation of [NEt₄][CB₁₁H₇-(3,5-Cl₂-C₆H₃)₅]. Hydrogen atoms are omitted for clarity; 25% displacement ellipsoids.

Palladium complex 1-Pd:

A solution of this complex (50 mg in 0.5 mL MeCN), prepared according to the above procedure, was left to evaporate slowly at room temperature (evaporation of *ca.* 60% of the solvent over 2 days) to yield colorless crystals of the composition [Me₃NH][Pd(MeCN)₂-CB₁₁H₁₀-COO] suitable for X-ray diffraction. (CCDC 1854799)

Bond precision:	C-C = 0.0033 Å		Wavelength=1.34139
Cell:	a=8.7528(1)	b=9.9635(2)	c=24.5410(4)
	alpha=90	beta=96.176(1)	gamma=90
Temperature:	170 K		
	Calculated	Reported	
Volume	2127.76(6)	2127.76(6)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C6 H16 B11 N2 O2 Pd, C3 H10 N	C6 H16 B11 N2 O2 Pd, C3 H10 N	
Sum formula	C9 H26 B11 N3 O2 Pd	C9 H26 B11 N3 O2 Pd	
Mr	433.64	433.64	
Dx,g cm-3	1.354	1.354	
Z	4	4	
Mu (mm-1)	4.794	4.718	
F000	872.0	872.0	
F000'	873.49		
h,k,lmax	11,12,31	11,12,31	
Nref	4882	4865	
Tmin,Tmax	0.844,0.910	0.481,0.752	
Tmin'	0.686		
Correction method= # Reported T Limits: Tmin=0.481 Tmax=0.752			
AbsCorr = MULTI-SCAN			
Data completeness=	0.997	Theta(max)= 60.602	
R(reflections)=	0.0322(4457)	wR2(reflections)= 0.0876(4865)	
S =	1.087	Npar= 240	

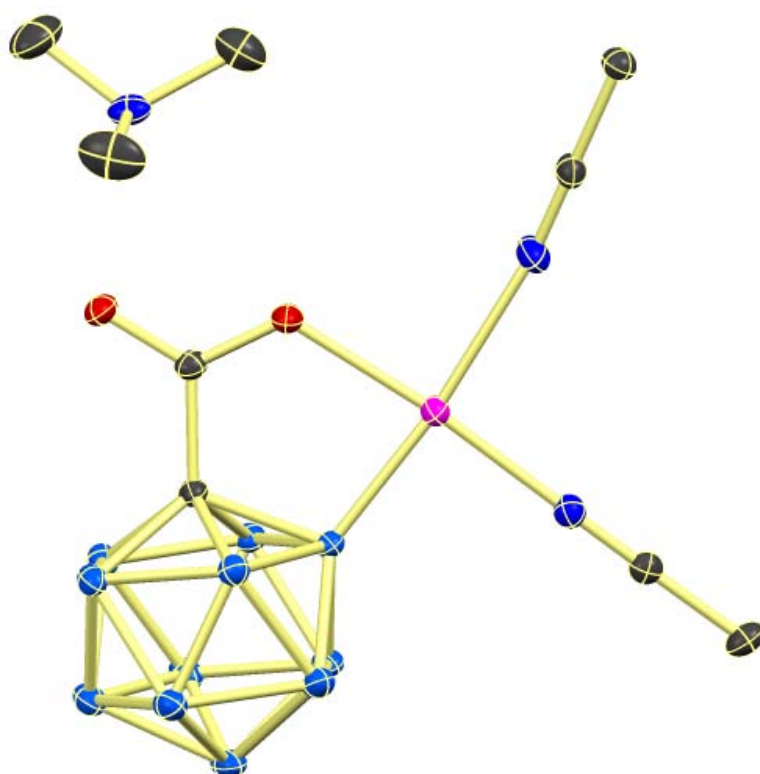


Figure S10. ORTEP representation of $[\text{Me}_3\text{NH}][\text{Pd}(\text{MeCN})_2\text{-CB}_{11}\text{H}_{10}\text{-COO}]$. Hydrogen atoms are omitted for clarity; 25% displacement ellipsoids.

IV Computational Details

We used Gaussian 09 program^[6] to carry out total density functional theory (DFT) calculations. The geometry optimizations were performed by B3LYP functional,^[7] with LANL2DZ basis set^[8] for palladium and silver, and 6-31G(d) basis set for the other elements. The vibrational frequencies calculations were conducted at the same level of theory to be sure whether every optimized stationary point is an energy minimum or a transition state and evaluate the zero-point vibrational energy and thermal corrections at 298 K. Based on the gas-phase optimized structures, the single-point energies and solvent effects were calculated by the M06 functional,^[9] with SDD basis set^[10] for palladium and silver, and 6-311+G(d,p) basis set for other elements. The solvation energies were evaluated by self-consistent reaction field by SMD implicit solvent model.^[11] We used CYLView to generate 3D diagrams of computed species.^[12] In order to adjust the Gibbs free energies from 1 atm to 1 mol/L, a correction of $RT\ln(c_s/c_g)$ (1.9 kcal/mol) is added to energies of all species. c_s represents the standard molar concentration in solution (1 mol/L), c_g represents the standard molar concentration in gas phase (0.0446 mol/L), and R represents the gas constant.

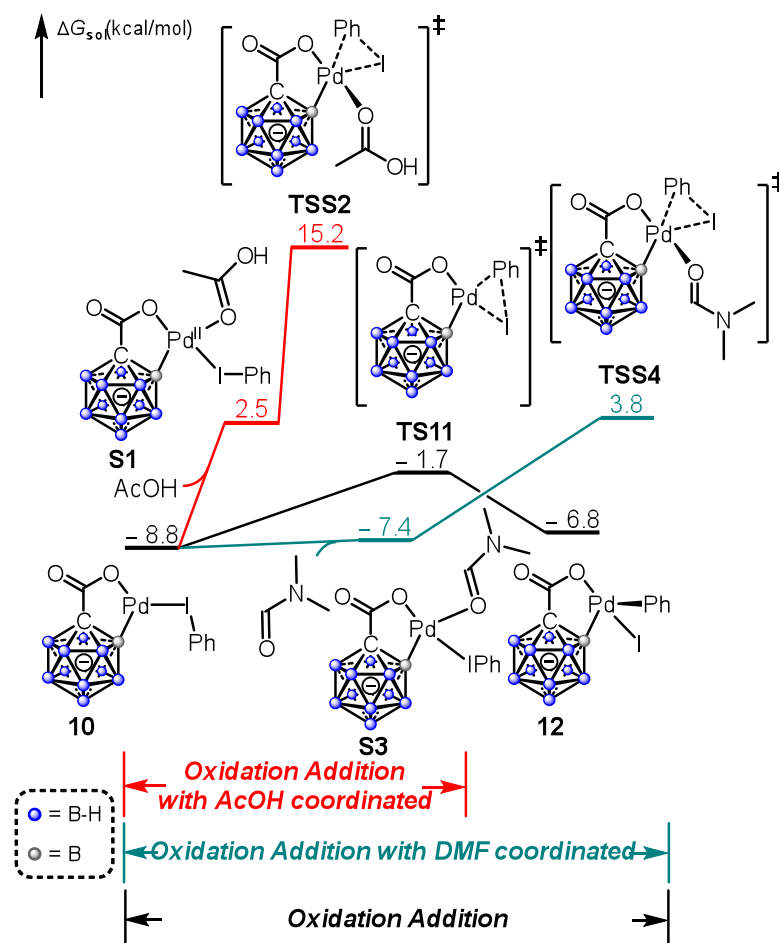


Figure S11. Free energy changes of oxidative additions with the assistance of carboxylic acid or solvent DMF.

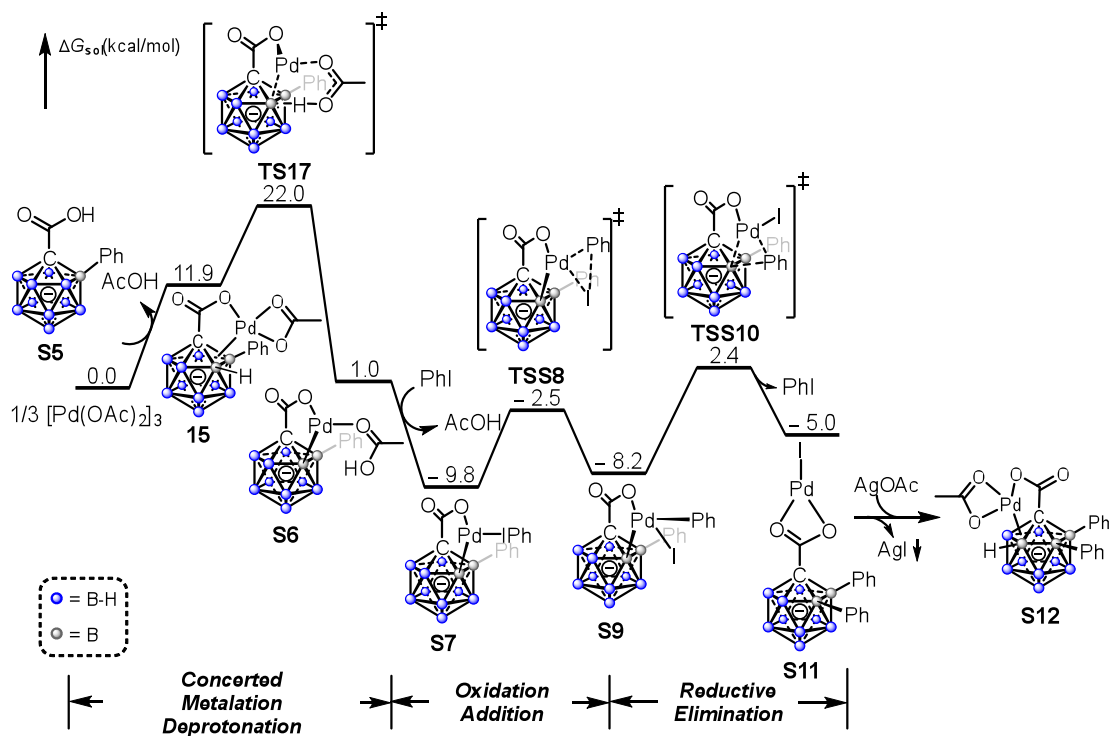


Figure S12. Free energy changes of Pd-catalyzed second arylation of carborane carboxylic acid.

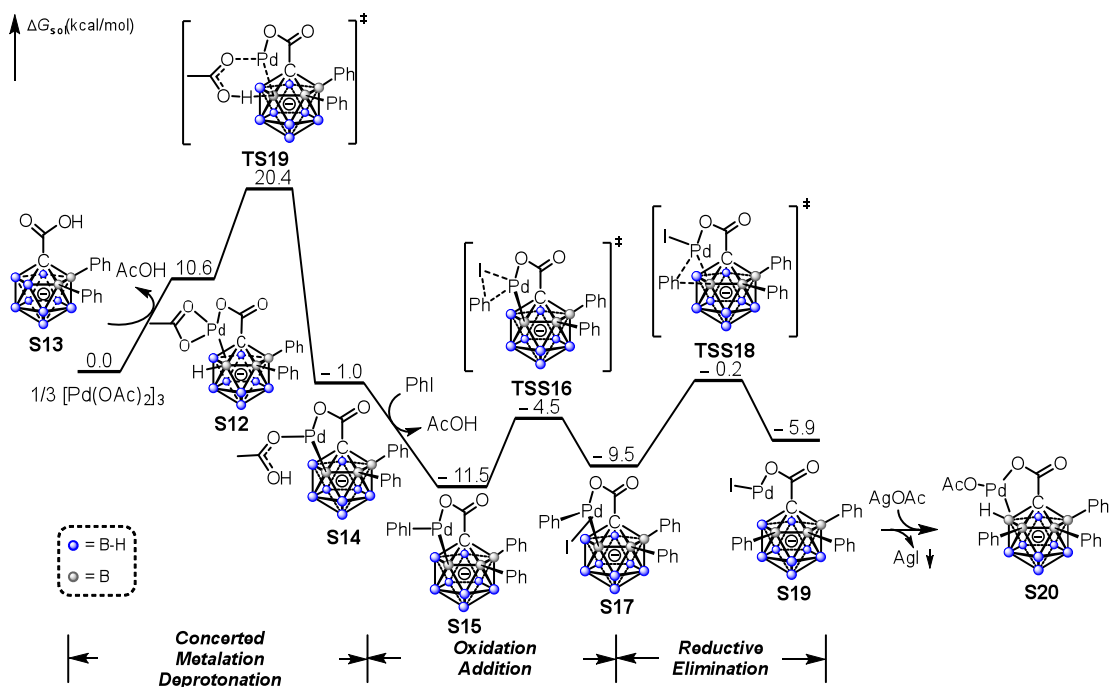


Figure S13. Free energy changes of Pd-catalyzed third arylation of carborane carboxylic acid.

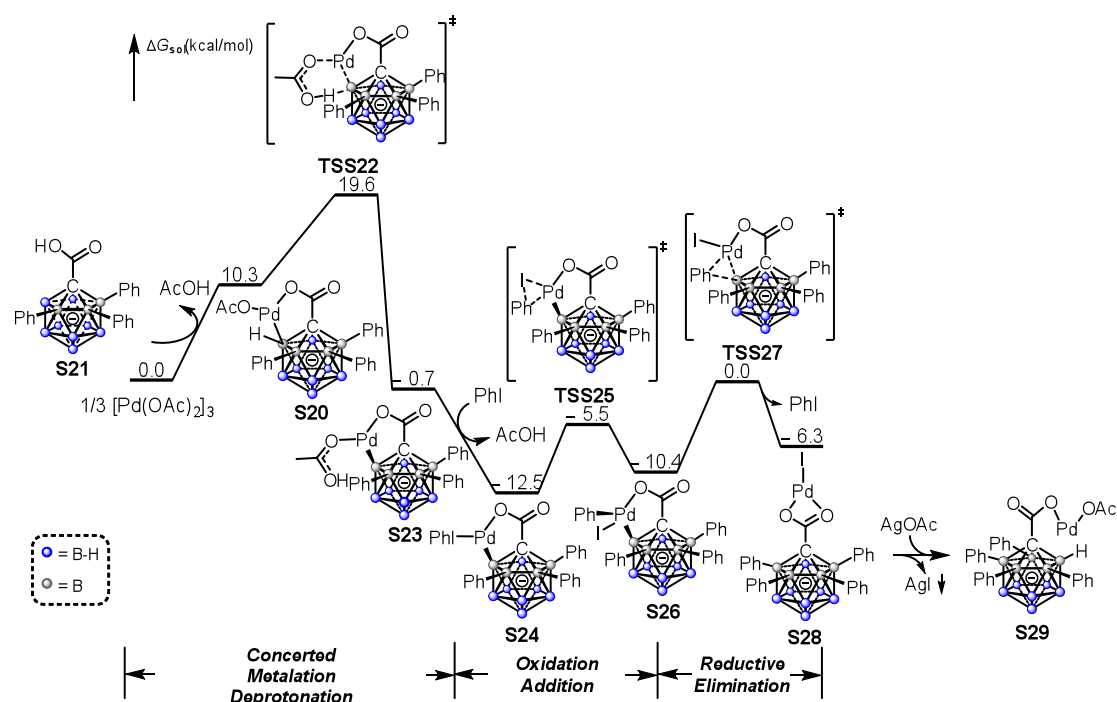


Figure S14. Free energy changes of Pd-catalyzed fourth arylation of carborane carboxylic acid.

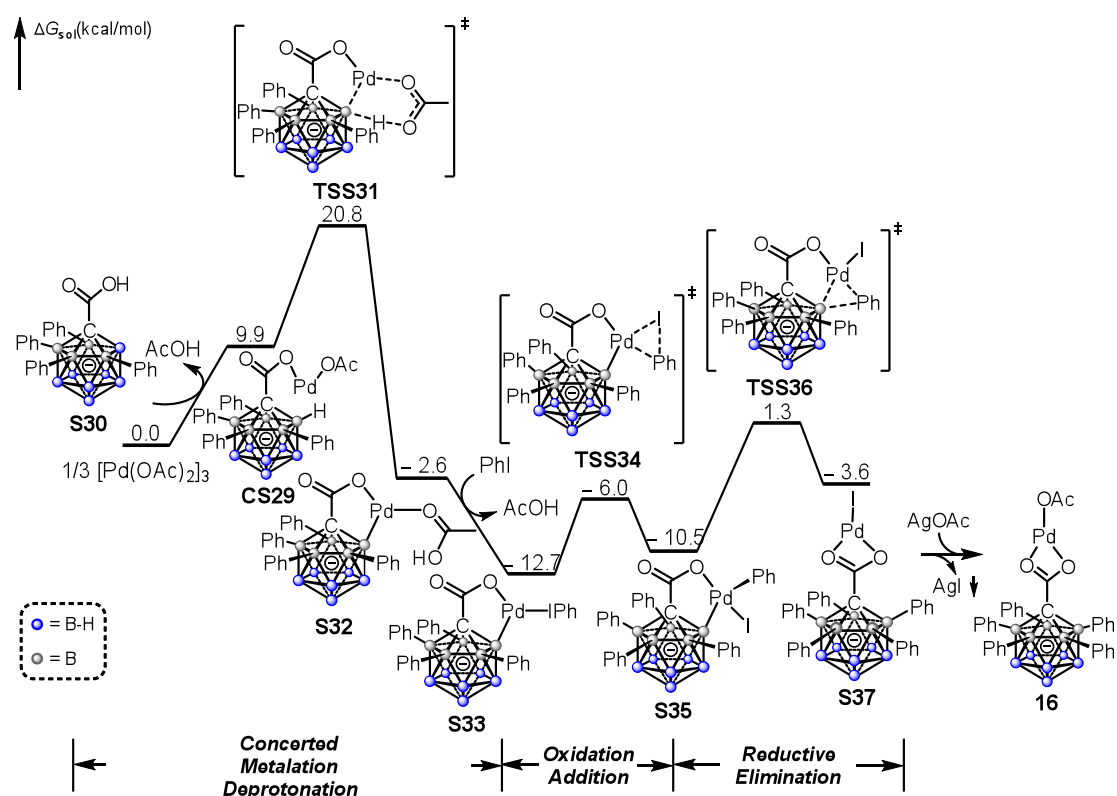


Figure S15. Free energy changes of Pd-catalyzed fifth arylation of carborane carboxylic acid.

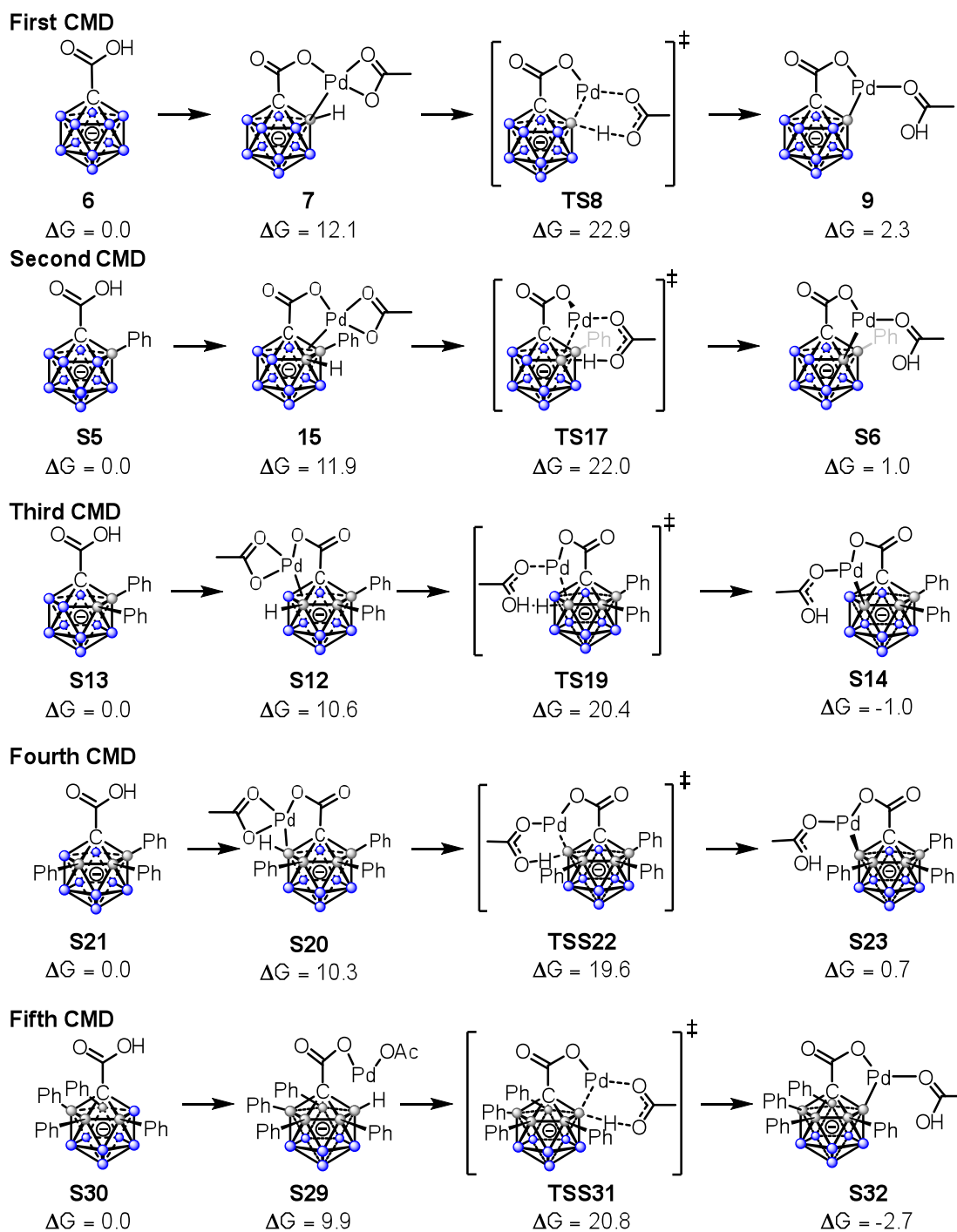


Figure S16. Concerted metalation-deprotonation among five sequential arylations. Gibbs free energies are in kcal/mol.

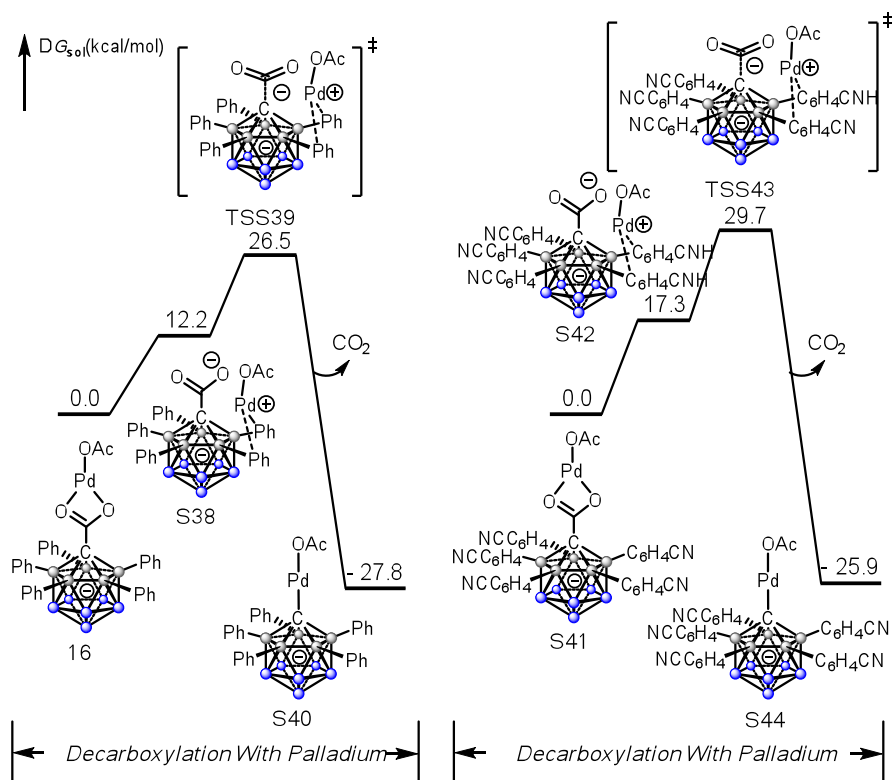


Figure S17. Free energy changes of decarboxylation of penta-arylated carborane with palladium.

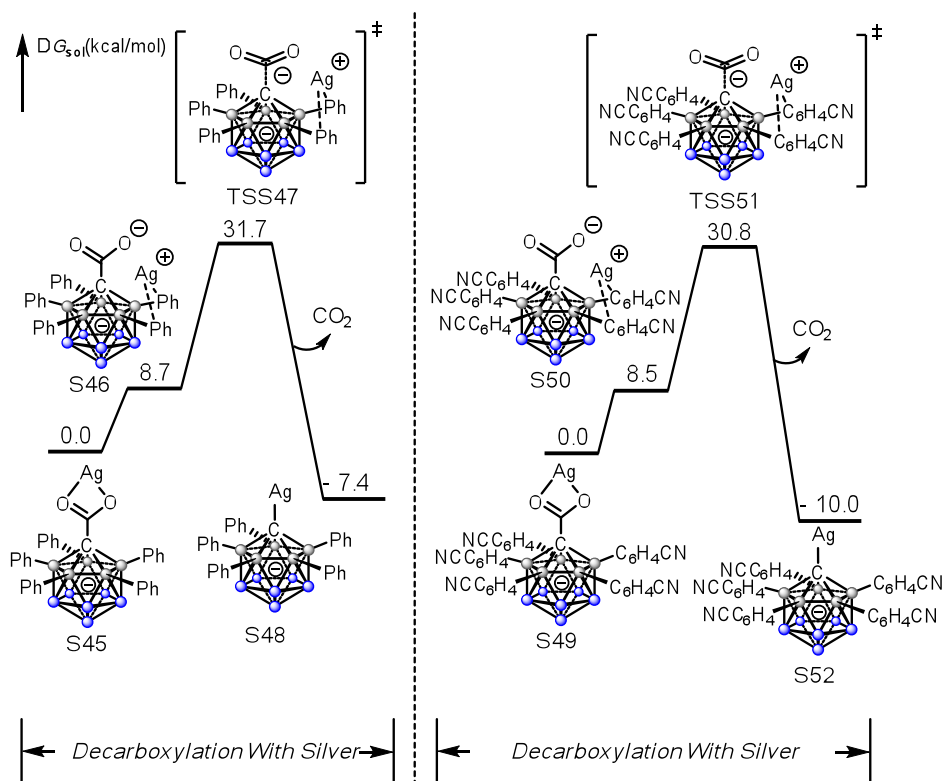


Figure S18. Free energy changes of decarboxylation of penta-arylated carborane with silver.

Table of Energies

Table S1. Zero-point correction (*ZPE*), thermal correction to enthalpy (*TCH*), thermal correction to Gibbs free energy (*TCG*), energies (*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures calculated at the M06/6-311+G(d,p)-SDD-SMD(iodobenzene)//B3LYP/6-31G(d)-LANL2DZ level of theory.

Structures	<i>ZPE</i>	<i>TCH</i>	<i>TCG</i>	<i>E</i>	<i>H</i>	<i>G</i>	Imaginary Frequency
[Pd(OAc) ₂] ₃	0.315942	0.351595	0.2439	-1754.462672	-1754.111077	-1754.218772	-
PhI	0.090288	0.097126	0.058515	-242.907361	-242.810235	-242.848846	-
AcOH	0.062049	0.067543	0.034887	-229.040645	-228.973102	-229.005758	-
DMF	0.103065	0.110090	0.073977	-248.428774	-248.318684	-248.354797	-
CO ₂ (gas phase)	0.011593	0.015184	-0.009126	-188.558460	-188.543276	-188.567586	-
6	0.187959	0.199654	0.152328	-507.473973	-507.274319	-507.321645	-
7	0.228493	0.246781	0.183180	-863.221383	-862.974602	-863.038203	-
TS8	0.224169	0.242393	0.179344	-863.200403	-862.95801	-863.021059	-681.0 <i>i</i>
9	0.230226	0.249	0.185277	-863.239109	-862.990109	-863.053832	-
10	0.25814	0.278919	0.207141	-877.12169	-876.842771	-876.914549	-
TS11	0.257086	0.277297	0.207333	-877.110548	-876.833251	-876.903215	-45.1 <i>i</i>
12	0.25812	0.278737	0.208857	-877.120335	-876.841598	-876.911478	-
TS13	0.25806	0.277841	0.210658	-877.10474	-876.826899	-876.894082	-208.8 <i>i</i>
14	0.259403	0.279808	0.208279	-877.121954	-876.842146	-876.913675	-
15	0.310629	0.333923	0.258740	-1094.161431	-1093.827508	-1093.902691	-
16	0.639569	0.682577	0.563131	-2017.896079	-2017.213502	-2017.332948	-
TS17	0.306516	0.329922	0.254569	-1094.141248	-1093.811326	-1093.886679	-612.4 <i>i</i>
TS18	0.306081	0.329371	0.253985	-1094.13773	-1093.808359	-1093.883745	-674.9 <i>i</i>
TS19	0.388458	0.416852	0.330115	-1325.078113	-1324.661261	-1324.747998	-621.3 <i>i</i>
TS20	0.388176	0.416499	0.329648	-1325.073247	-1324.656748	-1324.743599	-646.0 <i>i</i>
Table4-Entry1-pre	0.583718	0.620021	0.516889	-1661.683643	-1661.063622	-1661.166754	-
Table4-Entry1-ts	0.580155	0.617089	0.510897	-1661.655969	-1661.03888	-1661.145072	-68.8 <i>i</i>
Table4-Entry1-post	0.567206	0.600826	0.503126	-1473.103038	-1472.502212	-1472.599912	-
Table4-Entry2-pre	0.578191	0.623615	0.498466	-2122.768800	-2122.145185	-2122.270334	-
Table4-Entry2-ts	0.575201	0.621099	0.493621	-2122.742752	-2122.121653	-2122.249131	-94.8 <i>i</i>
Table4-Entry2-post	0.562165	0.604853	0.485093	-1934.191106	-1933.586253	-1933.706013	-
Table4-Entry3-pre	0.174003	0.185520	0.138300	-507.004162	-506.818642	-506.865862	-
Table4-Entry3-post	0.157406	0.166098	0.126637	-318.393596	-318.227498	-318.266959	-
S1	0.321936	0.348688	0.261641	-1106.161007	-1105.812319	-1105.899366	-
TSS2	0.320633	0.346853	0.263663	-1106.142687	-1105.795834	-1105.879024	-153.5 <i>i</i>
S3	0.362535	0.391274	0.299233	-1125.563456	-1125.172182	-1125.264223	-
TSS4	0.361929	0.389970	0.302182	-1125.548444	-1125.158474	-1125.246262	-126.3 <i>i</i>
S5	0.269992	0.286623	0.227864	-738.413747	-738.127124	-738.185883	-
S6	0.312309	0.336060	0.260773	-1094.180951	-1093.844891	-1093.920178	-
S7	0.339947	0.365774	0.281842	-1108.062169	-1107.696395	-1107.780327	-
TSS8	0.339110	0.364282	0.283072	-1108.05179	-1107.687508	-1107.768718	-31.5 <i>i</i>

S9	0.340429	0.365949	0.285207	-1108.063023	-1107.697074	-1107.777816	-
TSS10	0.340069	0.364837	0.286515	-1108.047412	-1107.682575	-1107.760897	-208.3 <i>i</i>
S11	0.341419	0.366787	0.284342	-1108.057111	-1107.690324	-1107.772769	-
S12	0.392877	0.421023	0.335571	-1325.099057	-1324.678034	-1324.763486	-
S13	0.352038	0.373557	0.304189	-969.348795	-968.975238	-969.044606	-
S14	0.394177	0.423023	0.335859	-1325.11791	-1324.694887	-1324.782051	-
S15	0.421949	0.452792	0.356893	-1338.998728	-1338.545936	-1338.641835	-
TSS16	0.421165	0.451358	0.358209	-1338.98879	-1338.537432	-1338.630581	-29.2 <i>i</i>
S17	0.422543	0.453057	0.360996	-1338.999638	-1338.546581	-1338.638642	-
TSS18	0.422079	0.451866	0.362249	-1338.985993	-1338.534127	-1338.623744	-207.2 <i>i</i>
S19	0.423558	0.453899	0.360466	-1338.993396	-1338.539497	-1338.63293	-
S20	0.474646	0.507888	0.410503	-1556.034523	-1555.526635	-1555.62402	-
S21	0.434146	0.460684	0.379319	-1200.283895	-1199.823211	-1199.904576	-
TSS22	0.470419	0.503847	0.405220	-1556.014407	-1555.51056	-1555.609187	-584.6 <i>i</i>
S23	0.476264	0.510130	0.410237	-1556.049607	-1555.539477	-1555.63937	-
S24	0.503746	0.539686	0.432089	-1569.935517	-1569.395831	-1569.503428	-
TSS25	0.502980	0.538251	0.433456	-1569.925674	-1569.387423	-1569.492218	-22.5 <i>i</i>
S26	0.504396	0.539973	0.436189	-1569.936213	-1569.39624	-1569.500024	-
TSS27	0.503914	0.538738	0.437646	-1569.921223	-1569.382485	-1569.483577	-210.3 <i>i</i>
S28	0.505511	0.540880	0.436210	-1569.929743	-1569.388863	-1569.493533	-
S29	0.556511	0.594795	0.486051	-1786.970764	-1786.375969	-1786.484713	-
S30	0.556511	0.594795	0.45538	-1431.219972	-1430.625177	-1430.764592	-
TSS31	0.552715	0.591024	0.482439	-1786.949799	-1786.358775	-1786.46736	-614.0 <i>i</i>
S32	0.558015	0.596982	0.485767	-1786.990465	-1786.393483	-1786.504698	-
S33	0.585922	0.626813	0.509195	-1800.873002	-1800.246189	-1800.363807	-
TSS34	0.585520	0.625704	0.510788	-1800.863908	-1800.238204	-1800.35312	-13.3 <i>i</i>
S35	0.586143	0.626763	0.512201	-1800.872467	-1800.245704	-1800.360266	-
TSS36	0.586076	0.625745	0.515185	-1800.856691	-1800.230946	-1800.341506	-213.9 <i>i</i>
S37	0.587628	0.627913	0.513116	-1800.862497	-1800.234584	-1800.349381	-
S38	0.638617	0.681902	0.563438	-2017.877014	-2017.195112	-2017.313576	-
TSS39	0.635013	0.678849	0.559314	-2017.849966	-2017.171117	-2017.290652	-179.6 <i>i</i>
S40	0.623372	0.664175	0.549171	-1829.358887	-1828.694712	-1828.809716	-
S41	0.632764	0.685109	0.542191	-2478.973653	-2478.288544	-2478.431462	-
S42	0.632214	0.684548	0.545459	-2478.949321	-2478.264773	-2478.403862	-
TSS43	0.628365	0.681357	0.539973	-2478.924089	-2478.242732	-2478.384116	-190.1 <i>i</i>
S44	0.616875	0.666795	0.530583	-2290.435714	-2289.768919	-2289.905131	-
S45	1.174990	1.252099	1.057718	-3617.201216	-3615.949117	-3616.143498	-
S46	0.586665	0.624662	0.518672	-1808.578137	-1807.953475	-1808.059465	-
TSS47	0.582995	0.621592	0.513328	-1808.536129	-1807.914537	-1808.022801	-146.2 <i>i</i>
S48	0.571263	0.606810	0.504565	-1620.02202	-1619.41521	-1619.517455	-
S49	1.161232	1.257204	1.015577	-4539.358625	-4538.101421	-4538.343048	-
S50	0.579654	0.627044	0.497714	-2269.655623	-2269.028579	-2269.157909	-
TSS51	0.576383	0.624266	0.493106	-2269.615503	-2268.991237	-2269.122397	-147.2 <i>i</i>
S52	0.564675	0.609539	0.484099	-2081.104013	-2080.494474	-2080.619914	-

Cartesian coordinates of the calculated stationary points

1-Pd

Pd	-1.10676600	-0.06472800	-0.00287100
O	-0.42747900	-2.01824400	-0.00458900
O	1.28890100	-3.45809700	-0.00485500
N	-3.33609700	-0.77735500	-0.00323200
N	-1.62830700	1.90402000	-0.00165600
C	0.84024000	-2.31519900	-0.00358600
C	1.76228900	-1.09299900	-0.00064200
C	-4.40593100	-1.22163900	0.00260900
C	-5.74816800	-1.78249900	0.01069300
H	-6.44878700	-1.06096600	0.44259200
H	-5.76091600	-2.69939100	0.60852200
H	-6.05722500	-2.01621700	-1.01306100
C	-1.93393900	3.02027000	-0.00168300
C	-2.31375900	4.42267300	-0.00151700
H	-1.51892600	5.01855200	-0.46152100
H	-2.46990200	4.76202300	1.02756000
H	-3.23985800	4.55483800	-0.56995700
B	0.88059800	0.37172300	0.00031600
B	1.77916200	-0.16239400	-1.43626200
H	1.19236800	-0.56526700	-2.39007900
B	1.89868400	1.51986800	-0.89007700
H	1.42788600	2.41372900	-1.52765300
B	1.89639600	1.51731800	0.89659800
H	1.42396700	2.40927400	1.53556900
B	1.77547500	-0.16645000	1.43768200
H	1.18621700	-0.57208800	2.38881000
B	3.22497500	-1.04908700	-0.88397400
H	3.57865900	-2.01441300	-1.48062200
B	3.35681900	0.63386800	-1.43921000
H	3.90641200	0.90027600	-2.46609100
B	3.43409000	1.67547900	0.00545000
H	4.05500800	2.69799100	0.00775700
B	3.35307900	0.62973700	1.44694200
H	3.89999400	0.89314100	2.47602700
B	3.22266300	-1.05164600	0.88658800
H	3.57482000	-2.01865500	1.48142300
B	4.25285900	0.08902800	0.00427700
H	5.44259000	-0.02211900	0.00565100

Phi

C	-2.66149500	-1.20711600	0.00000100
C	-1.26394300	-1.21563800	0.00000000

C	-0.58101700	-0.00002300	-0.00000400
C	-1.26392700	1.21562600	-0.00000300
C	-2.66145500	1.20714000	0.00000300
C	-3.36204600	0.00000900	0.00000000
H	-3.19857800	-2.15188800	0.00000500
H	-0.72256800	-2.15540700	-0.00000300
H	-0.72250000	2.15536500	-0.00000400
H	-3.19855300	2.15190400	0.00000800
H	-4.44830800	0.00004200	-0.00000300
I	1.56705300	0.00000000	0.00000000

DMF

O	-1.92413800	-0.15901900	-0.00006500
C	-0.82499400	-0.69028200	-0.00017800
N	0.35768700	-0.01498300	-0.00011100
H	-0.68737200	-1.79053100	-0.00026600
C	0.31010000	1.44304200	0.00015300
C	1.63995000	-0.69351100	0.00010700
H	0.28627175	1.82955720	1.02482528
H	1.19514656	1.82982911	-0.51035500
H	-0.58867286	1.80124441	-0.51346838
H	2.22975200	-0.43636700	-0.88969000
H	2.22910300	-0.43718800	0.89058200
H	1.47481500	-1.77499800	-0.00045900

AcOH

C	0.22068400	0.00179900	0.00016000
O	0.80845400	-1.10877200	-0.00004400
O	0.69605300	1.16624800	-0.00004500
C	-1.35425400	-0.05500900	-0.00004900
H	-1.75052300	0.47067800	0.88144500
H	-1.75055500	0.47383600	-0.87962200
H	-1.73355800	-1.08505800	-0.00178100
H	1.64718686	1.29641861	-0.00006792

[Pd(OAc)₂]₃

Pd	-1.61665200	0.91903200	0.01034200
C	0.05231800	2.60739300	1.88256900
O	-1.05057800	2.42264800	1.28956000
O	1.16183900	2.04079100	1.64715900
C	2.28783400	-1.25442800	-1.89503900
O	1.56608200	-2.11451700	-1.30999600
O	2.35997200	-0.01099600	-1.65809800
C	3.19809000	-1.77986200	-2.98845500

H	3.45798900	-0.97964500	-3.68382600
H	4.12003800	-2.15034500	-2.52511600
H	2.72017400	-2.61049800	-3.51185500
C	0.05383900	3.65118800	2.98286300
H	-0.90794500	3.65644900	3.49986200
H	0.87057900	3.46448400	3.68254000
H	0.20519600	4.63709800	2.52794100
Pd	0.00815300	-1.85797900	-0.00000200
C	2.27453200	-1.34197600	1.85428200
O	2.65995500	-0.29658700	1.25105800
O	1.23396200	-2.02811800	1.62676600
C	-0.07506800	2.60682000	-1.88265500
O	-1.17970300	2.03075200	-1.64721900
O	1.02938200	2.43147200	-1.28971100
C	-0.08578500	3.65093800	-2.98259400
H	0.87717000	3.66762300	-3.49712300
H	-0.89852200	3.45496700	-3.68442000
H	-0.25007000	4.63482500	-2.52776400
C	3.16372300	-1.81495600	2.98827200
H	3.12372900	-1.08076400	3.79996400
H	2.83804400	-2.78900000	3.35540400
H	4.19991300	-1.86677900	2.64170400
Pd	1.60849700	0.93288700	-0.01041700
C	-2.26274200	-1.36179800	-1.85415400
O	-2.65731900	-0.31981000	-1.25095300
O	-1.21621200	-2.03884200	-1.62668800
C	-3.14772600	-1.84249300	-2.98818500
H	-3.11215700	-1.10907600	-3.80079900
H	-2.81483300	-2.81463600	-3.35388400
H	-4.18381000	-1.90113500	-2.64243100
C	-2.27664000	-1.27412300	1.89508900
O	-2.35967400	-0.03139000	1.65811200
O	-1.54749400	-2.12794000	1.31001300
C	-3.18233200	-1.80751100	2.98844000
H	-4.10068500	-2.18668200	2.52498700
H	-2.69690800	-2.63352200	3.51225100
H	-3.44978500	-1.00948500	3.68346200

CO₂

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16915600
O	0.00000000	0.00000000	-1.16915600

B	1.63670100	1.41065900	0.51348400
B	0.14167200	1.47410100	-0.43215700
B	0.11504600	0.87798700	1.24665600
B	1.58864600	-0.06385900	1.52422400
B	0.06921000	-0.91365200	1.19724500
C	-0.70717100	0.03702100	-0.00842200
B	0.10702600	0.05621100	-1.52134400
B	1.58696400	-0.88269500	-1.24966800
B	1.63069800	0.90549600	-1.19969700
B	1.56441600	-1.48015400	0.43400200
B	0.07014100	-1.41819600	-0.51136000
H	2.16750000	2.41688600	0.87811700
H	-0.53719900	1.44951900	2.06103800
H	2.08411700	-0.10620900	2.61076600
H	-0.48694700	2.43897400	-0.71941500
H	-0.60889300	-1.49693200	1.98213300
H	2.15538900	1.55202700	-2.05647700
H	3.73068000	-0.07580000	0.01740600
H	-0.54949700	0.09985900	-2.51433200
H	2.07944100	-1.50835500	-2.14054200
H	2.04344500	-2.52986400	0.74426700
H	-0.59777400	-2.33905700	-0.85238000
B	2.53560100	-0.04578900	0.01011500
C	-2.20944100	0.12360100	-0.00456300
O	-2.86435700	1.14508100	-0.00075600
O	-2.81590900	-1.09257600	0.00074700
H	-3.76906800	-0.88536400	0.00991300

7

C	3.74947500	-0.54921500	-0.18009100
O	2.87279700	-1.35741500	0.28127500
O	3.41836100	0.66251800	-0.38468500
O	0.49129700	1.92677000	0.13781100
C	-0.80429600	2.06247500	-0.08490300
O	-1.30625500	3.15593400	-0.26965900
H	0.18369700	-0.57060200	1.20531800
C	-1.62437200	0.77677500	-0.08583500
B	-3.30574100	0.82956100	0.25443100
B	-2.70533500	0.45484300	-1.37490200
B	-1.17545800	-0.45684200	-1.23245200
B	-2.14673900	0.17192600	1.43560700
B	-0.86465300	-0.61561700	0.49488600
B	-3.99213100	-0.52985900	-0.65050800
B	-3.63984600	-0.70499400	1.09164400

H	-3.80958600	1.88147400	0.46808100
B	-2.67735100	-1.31779000	-1.56813100
H	-2.80901700	1.25818600	-2.24240000
B	-1.50566100	-1.99172400	-0.39477200
B	-2.10519400	-1.60993300	1.25549600
H	-1.85640600	0.78278500	2.41281900
H	-5.10872000	-0.48394700	-1.06834600
B	-3.25404800	-2.03738000	-0.03945600
H	-4.49765300	-0.77474400	1.91791200
H	-2.85456600	-1.81561300	-2.63766100
H	-0.83971900	-2.95624200	-0.61243800
H	-1.85535500	-2.30325600	2.19267000
H	-3.85349900	-3.06933700	-0.01790200
Pd	1.42379100	0.17812000	0.27911600
C	5.13539900	-1.03840600	-0.50522200
H	5.85598200	-0.22262500	-0.40796700
H	5.40478900	-1.87128400	0.14912200
H	5.15475100	-1.39510400	-1.54192500
H	-0.29511700	-0.22638300	-1.99748700

9

C	-3.08631100	-0.89271800	0.13929500
O	-2.95245400	0.12404300	-0.53214600
O	-2.91168000	-0.83980100	1.46443000
O	0.50074200	2.48618100	0.08359800
C	1.70961300	1.98315300	0.17190600
O	2.72246200	2.65026300	0.31529500
C	1.74446400	0.45380000	0.07789400
B	2.96643400	-0.39713300	-0.76680900
B	2.81653500	-0.51137900	0.99845500
B	1.08554500	-0.39566400	1.41902700
B	1.33016100	-0.21056900	-1.45535600
B	0.19345500	-0.20400900	-0.10095300
B	3.04125100	-1.98053600	0.02815300
B	2.12352500	-1.78827800	-1.49191900
H	3.86596600	0.20955700	-1.24887900
B	1.88028400	-1.97540900	1.38383200
H	3.61549900	0.01726300	1.69977700
B	0.23926200	-1.78231400	0.70215500
H	0.75514300	0.21783600	2.38260400
B	0.38247100	-1.66550900	-1.08031700
H	1.16265700	0.52766900	-2.37209800
H	4.05801000	-2.60497300	0.07510500
B	1.44845900	-2.76726600	-0.16032000

H	2.49031100	-2.25969800	-2.52598200
H	2.06806400	-2.58094400	2.39633200
H	-0.71281000	-2.28423500	1.23787000
H	-0.47618600	-2.05457200	-1.81815900
H	1.33074400	-3.95447000	-0.24377700
Pd	-1.15117700	1.33077000	-0.15235600
C	-3.43984700	-2.22163800	-0.47422900
H	-4.09085200	-2.81576200	0.17461300
H	-3.91211800	-2.05953000	-1.44411900
H	-2.50136900	-2.76673700	-0.63775900
H	-2.67591500	-1.71756700	1.81451200

10

O	-1.82878900	-1.75559800	-1.62346700
C	-2.94187300	-1.05691300	-1.57391000
O	-3.91563900	-1.27313600	-2.27692600
C	-2.90881200	0.06876700	-0.53793800
B	-3.61831400	1.60449900	-0.79685300
B	-4.25604200	0.48734400	0.42703100
B	-2.88746600	-0.43907800	1.10809900
B	-1.84927300	1.37991200	-0.88562900
B	-1.43506000	0.13364100	0.29184500
B	-4.00049700	2.19448600	0.83069600
B	-2.51369700	2.74693800	0.01132000
H	-4.22392800	1.79941200	-1.79946900
B	-3.55348700	0.92724300	2.00601000
H	-5.29048300	-0.06618800	0.24477000
B	-1.77790700	0.69058500	1.92494000
H	-3.02335100	-1.59694600	1.34371100
B	-1.13386800	1.82249100	0.68400100
H	-1.30546300	1.40596500	-1.94505600
H	-4.92213000	2.92979100	1.02014900
B	-2.47311800	2.32830800	1.74986900
H	-2.38090400	3.86154000	-0.39682000
H	-4.16364600	0.74972300	3.01687300
H	-1.12916600	0.34614700	2.86642800
H	-0.03034700	2.27560900	0.75467800
H	-2.31286800	3.16133900	2.59118700
Pd	-0.22045800	-1.34144800	-0.44213200
I	2.03834200	-0.99304100	1.01847100
C	3.14617600	0.48211300	-0.10367100
C	4.52587300	0.55603000	0.07220100
C	2.46083700	1.33501800	-0.96360300
C	5.24179700	1.51955500	-0.64395300

H	5.04039500	-0.11827800	0.74947200
C	3.19491400	2.29102600	-1.67232100
H	1.38404100	1.26866800	-1.07686300
C	4.57882900	2.38503000	-1.51576400
H	6.31921700	1.58733400	-0.51605600
H	2.67052500	2.96509100	-2.34379100
H	5.13969400	3.13289200	-2.06987400

12

O	-0.52762700	1.22637600	-1.89702900
C	-1.82749400	1.37517700	-1.69689600
O	-2.52104700	2.10577600	-2.37835400
C	-2.36922500	0.54205800	-0.54361700
B	-3.64964000	1.06499700	0.45195400
B	-3.84237900	-0.31770700	-0.64983400
B	-2.27219500	-1.17458500	-0.75220700
B	-1.96056600	1.08717900	1.04121400
B	-1.18171300	-0.30331200	0.30180200
B	-4.39740500	-0.43308200	1.02877800
B	-3.23645800	0.43825400	2.07024900
H	-4.17982100	2.09764400	0.20728900
B	-3.55341900	-1.81769200	0.27735300
H	-4.49829300	-0.20789800	-1.63225100
B	-1.86001900	-1.81825600	0.86332100
H	-1.88885800	-1.58347600	-1.80415000
B	-1.65673400	-0.40954400	1.97452400
H	-1.38672200	2.11957500	1.14709900
H	-5.56077700	-0.48045200	1.28733100
B	-3.18226800	-1.34645900	1.96445300
H	-3.57253100	1.02252200	3.05393300
H	-4.11186400	-2.82914000	-0.01633300
H	-1.21292800	-2.80838200	0.97443500
H	-0.87293900	-0.42296400	2.87176000
H	-3.48161400	-2.03791700	2.88923800
Pd	0.59214500	-0.09076900	-0.81547100
I	2.27443200	-1.99998700	-0.03652400
C	1.45723200	1.39355000	0.20993600
C	1.74706700	1.29466000	1.56870300
C	1.77086300	2.52556700	-0.53790000
C	2.38511400	2.37356500	2.18998000
H	1.48121400	0.41237200	2.13679000
C	2.42004200	3.58883900	0.10241800
H	1.48799400	2.60062800	-1.58172400
C	2.72693500	3.51460000	1.46127100

H	2.61495300	2.31025700	3.25080200
H	2.66516200	4.48091600	-0.46910100
H	3.22368100	4.34676700	1.95398800

14

O	-0.01404100	-0.76712900	-1.48742000
C	0.49601900	-0.79482400	-0.31742500
O	-0.35850200	-0.65750500	0.64520200
C	1.93777600	-0.97147400	-0.05539900
B	2.41170500	-2.35130300	0.85881500
B	2.73794000	-2.24178800	-0.90424700
B	3.03824900	-0.52428300	-1.29616100
B	2.51826900	-0.70153500	1.53931700
B	2.89882700	0.46088800	0.21538100
B	4.00116400	-2.78107900	0.21031600
B	3.86708400	-1.83014800	1.72054500
H	1.55837500	-3.08296100	1.24568200
B	4.39049500	-1.64979500	-1.12123900
H	2.09531600	-2.90375500	-1.65301400
B	4.48980900	-0.00282800	-0.43244700
H	2.60171100	-0.07177500	-2.30313500
B	4.16962400	-0.11318300	1.32370700
H	1.74474400	-0.38399400	2.38213800
H	4.36090500	-3.91851100	0.20570700
B	5.09503100	-1.39913100	0.49990200
H	4.13189700	-2.28893000	2.78919900
H	5.03063100	-1.97908800	-2.07221700
H	5.20139600	0.83479700	-0.89697200
H	4.65025500	0.64536600	2.10837200
H	6.26109100	-1.55417300	0.70232300
Pd	-1.91261700	-0.50332700	-0.65595500
I	-4.30305200	-0.17118300	0.39091700
C	2.24939700	1.90917000	0.14774600
C	2.60628100	2.79914700	-0.88322500
C	1.32616700	2.37579200	1.10203200
C	2.07391900	4.08713300	-0.95925700
H	3.31818000	2.47333200	-1.63689800
C	0.78273500	3.66083000	1.03017000
H	1.02817700	1.72341100	1.91737100
C	1.15592100	4.52379900	-0.00156000
H	2.37411800	4.74965700	-1.76867000
H	0.06934600	3.98698700	1.78396400
H	0.73605500	5.52593800	-0.05872900

15

C	3.55209400	-1.12292400	-0.45278500
O	2.64276100	-1.28297300	-1.33800500
O	3.20391900	-1.00457100	0.76557500
O	0.20234800	-0.95283800	1.87953800
C	-1.00822400	-0.45415200	2.02753400
O	-1.44307800	-0.14755700	3.12414500
H	-0.19612600	-1.61759700	-0.79717400
C	-1.84321400	-0.30212200	0.75871100
B	-3.54714800	-0.51480200	0.87536800
B	-2.83785600	1.07550300	0.53795000
B	-1.34774200	0.88455300	-0.44620800
B	-2.51856000	-1.74995500	0.11125100
B	-1.20597100	-0.87191300	-0.69009600
B	-4.22253500	0.50126400	-0.40761700
B	-4.01981100	-1.25167200	-0.67175300
H	-4.01652700	-0.73324900	1.94189600
B	-2.87961700	1.35019500	-1.21844700
H	-2.84255700	1.91068900	1.38078100
B	-1.83522900	0.12479500	-1.99205200
B	-2.54439500	-1.49044700	-1.65478800
H	-2.27564000	-2.77280400	0.66487900
H	-5.29691400	1.00505100	-0.28586300
B	-3.60530800	-0.09465100	-1.97171300
H	-4.94234700	-2.00501100	-0.73361400
H	-2.99366600	2.45211000	-1.65991600
H	-1.20752800	0.32721900	-2.98541400
H	-2.39543800	-2.40680200	-2.40250300
H	-4.24460400	-0.02086500	-2.97676400
Pd	1.15022500	-1.13133100	0.14309100
C	4.99980000	-1.04187600	-0.85370100
H	5.16019400	-1.55998500	-1.80224500
H	5.27513500	0.01186300	-0.97970700
H	5.63127000	-1.46824200	-0.06984800
C	-0.09727900	1.84212000	-0.22792400
C	0.17019100	2.46815300	1.00468100
C	0.76994300	2.13746700	-1.29755700
C	1.25108400	3.33718300	1.16404100
H	-0.47396500	2.27097200	1.85686800
C	1.84854400	3.01143500	-1.14736000
H	0.59109500	1.67711800	-2.26524200
C	2.09514000	3.61550700	0.08733100
H	1.43171300	3.79786100	2.13278100
H	2.49493800	3.22128900	-1.99739500

H	2.93539500	4.29603200	0.20898200
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16

B	0.67177000	-0.05419600	-3.68244900
B	1.13918400	0.60366700	-2.09156600
B	0.33061400	-1.02562800	-2.23674700
B	-0.89017700	-0.88119200	-3.52674200
B	-1.43673300	-0.77451000	-1.83484300
C	-0.20678100	0.19089700	-1.04886300
B	-0.12303400	1.85710400	-1.62794300
B	-1.30323200	1.90093400	-2.95867300
B	0.41303800	1.66108100	-3.32048400
B	-2.10838100	0.32486900	-3.07333300
B	-1.72467400	1.00190600	-1.47770400
H	1.50854800	-0.42701000	-4.44515100
H	-1.17278200	-1.83732600	-4.17751700
H	1.07986100	2.50737000	-3.82874900
H	-1.03937900	0.95519300	-5.36899000
H	-1.85475000	2.92482400	-3.21444500
H	-3.25026300	0.23111900	-3.39909700
B	-0.81738900	0.74945800	-4.21508800
C	0.08167200	-0.06887700	0.38952600
O	0.95097500	-0.92964600	0.77531800
C	2.64720900	0.77607000	-1.60164100
C	3.02430300	1.25618900	-0.33316100
C	3.69292300	0.48243900	-2.49922100
C	4.36401000	1.41669300	0.02734600
H	2.26500400	1.53370100	0.39042300
C	5.03454400	0.64483000	-2.15062900
H	3.44692400	0.11249500	-3.48951700
C	5.37876800	1.10965100	-0.88007200
H	4.61076100	1.79215600	1.01806900
H	5.81117100	0.40388000	-2.87371800
H	6.42316600	1.23522800	-0.60217100
C	0.28267500	3.12569000	-0.74534000
C	-0.31031100	3.46560100	0.48670900
C	1.25837100	4.01653600	-1.23882900
C	0.05486000	4.61904600	1.18641300
H	-1.07031800	2.82397700	0.91251300
C	1.62419800	5.17285700	-0.54924100
H	1.74471600	3.79725800	-2.18328300
C	1.02434800	5.48080800	0.67297700
H	-0.42945800	4.84290900	2.13466000
H	2.38347300	5.83057700	-0.96767200

H	1.30795200	6.38015600	1.21615400
C	-2.87932200	1.48540900	-0.48259700
C	-3.39234100	0.72619800	0.58689000
C	-3.49845300	2.72919900	-0.72038800
C	-4.45228700	1.18192900	1.37365700
H	-2.96373200	-0.24078800	0.81769900
C	-4.56050300	3.19168800	0.05876800
H	-3.13865300	3.35061700	-1.53364200
C	-5.04420900	2.41878100	1.11481500
H	-4.81642600	0.56163800	2.19002400
H	-5.00622900	4.15990000	-0.16064900
H	-5.87062500	2.77438500	1.72700300
C	1.05972800	-2.41824000	-1.94077700
C	2.29815900	-2.55232000	-1.28327200
C	0.48646800	-3.60329600	-2.44574100
C	2.92558200	-3.79168500	-1.13992900
H	2.78319000	-1.67770000	-0.87084300
C	1.10704500	-4.84601100	-2.30820500
H	-0.46890700	-3.55224100	-2.95677500
C	2.33451200	-4.94728100	-1.65273500
H	3.88219400	-3.84961800	-0.62475900
H	0.62657400	-5.73478300	-2.71244200
H	2.82334600	-5.91329400	-1.54172100
C	-2.28306800	-1.90636500	-1.09649700
C	-1.77266800	-2.74576000	-0.08687200
C	-3.62207000	-2.12361800	-1.47943800
C	-2.55770600	-3.73021800	0.51948200
H	-0.73766600	-2.65322700	0.22229400
C	-4.40921600	-3.11115600	-0.88606300
H	-4.05695400	-1.50072100	-2.25441200
C	-3.88222200	-3.91848900	0.12356100
H	-2.12341000	-4.35783700	1.29481000
H	-5.43909300	-3.24519600	-1.21091700
H	-4.49410800	-4.68696400	0.59142500
C	1.03033900	-0.93036700	5.12533700
O	0.16402000	-0.06154800	4.77157600
O	1.65091700	-1.55711100	4.20191600
Pd	0.55974400	-0.49611600	2.75241200
O	-0.51661400	0.54963300	1.33896600
C	1.28395100	-1.23028600	6.57438100
H	0.59733600	-2.02043700	6.90115400
H	2.30809500	-1.58540200	6.71165000
H	1.09786600	-0.34083700	7.18120700

S1

O	0.01731800	-1.36707500	-0.08104000
C	-0.89666500	-2.30635100	-0.19306400
O	-0.63545800	-3.48357100	-0.38755900
C	-2.32169000	-1.77677200	-0.05238000
B	-3.63759500	-2.39921000	-0.95022700
B	-3.53745800	-2.61859000	0.80854700
B	-2.74224100	-1.17816400	1.50710000
B	-2.90605500	-0.82087600	-1.35544500
B	-2.36032100	-0.09035300	0.16521700
B	-5.05735400	-2.08818000	0.06763900
B	-4.66375300	-0.98103100	-1.27572800
H	-3.45693300	-3.32125900	-1.67674400
B	-4.49778400	-1.33783700	1.58956700
H	-3.28805100	-3.68879400	1.25920200
B	-3.75640500	0.24746200	1.19310200
H	-1.96607300	-1.31932600	2.39695400
B	-3.86261800	0.46211100	-0.58287700
H	-2.23893800	-0.71931800	-2.33688600
H	-6.01208500	-2.80471400	0.03155700
B	-5.19756600	-0.32232000	0.29884900
H	-5.32336400	-0.91441100	-2.26980600
H	-5.04172300	-1.53227400	2.63465000
H	-3.77783700	1.17261800	1.94770800
H	-3.98276200	1.54490400	-1.08238200
H	-6.25712800	0.21677500	0.42344500
Pd	-0.43561400	0.59791400	0.19458400
C	3.88826300	-0.60949700	-0.03378700
C	5.28129400	-0.62794000	-0.09321100
C	3.11894000	-1.75582700	-0.21222200
C	5.92499300	-1.84321400	-0.34222000
H	5.85828800	0.27955900	0.05168400
C	3.78626100	-2.96099800	-0.46080200
H	2.03073300	-1.73475700	-0.16474200
C	5.17945200	-3.00971400	-0.52620400
H	7.01111700	-1.87078300	-0.39024000
H	3.19159400	-3.85968500	-0.60102600
H	5.68472200	-3.95286100	-0.71890200
I	2.90160200	1.26977700	0.36262500
O	-0.87847900	2.70617500	0.41267900
C	-1.31505500	3.42526100	-0.47415600
O	-1.70241200	4.66739400	-0.12763000
C	-1.46168500	3.02217200	-1.91761400
H	-2.07178500	5.12191200	-0.90173900

H	-0.66633300	2.31990500	-2.17594700
H	-2.41237800	2.48668500	-2.02706000
H	-1.44435500	3.88246800	-2.59607200

S3

O	-1.17186200	2.15715000	0.45012700
C	-2.42704900	1.98126700	0.80006500
O	-3.11076400	2.84580700	1.32764200
C	-2.95100800	0.58412000	0.47898200
B	-4.03732700	-0.25068800	1.50368500
B	-4.53570200	0.31342100	-0.10355700
B	-3.11979300	0.21587900	-1.19082300
B	-2.31111800	-0.70180100	1.41970300
B	-1.76334900	-0.40946200	-0.23971100
B	-4.92829300	-1.33367600	0.41877800
B	-3.55169000	-1.95879700	1.36863400
H	-4.44455200	0.29269600	2.47862100
B	-4.36313900	-1.03784400	-1.25015800
H	-5.27807800	1.23543800	-0.20524000
B	-2.63052300	-1.48637800	-1.34015900
H	-2.93671200	1.08378800	-1.98472000
B	-2.12825100	-2.05773400	0.28469200
H	-1.59672300	-0.43794900	2.33755200
H	-6.05449800	-1.65452200	0.65575200
B	-3.75486500	-2.44887000	-0.33768900
H	-3.69452600	-2.70912700	2.28772900
H	-5.08670400	-1.13331000	-2.19604500
H	-2.12972600	-1.89899200	-2.34377100
H	-1.27067100	-2.87668300	0.43600300
H	-4.05172800	-3.56736100	-0.63780700
Pd	-0.02832600	0.65947900	-0.39445600
I	1.52356200	-1.32326600	-1.44780900
C	2.38044000	-2.18318800	0.33054100
C	3.61381300	-2.82560800	0.24379300
C	1.68018500	-2.09090800	1.53083300
C	4.16113500	-3.39146900	1.39886900
H	4.14525500	-2.88630100	-0.70071300
C	2.24379300	-2.66157900	2.67576900
H	0.71769100	-1.59239800	1.57680800
C	3.47894100	-3.30944100	2.61396200
H	5.12362200	-3.89403600	1.34219700
H	1.70308600	-2.59804800	3.61606200
H	3.90819200	-3.75069600	3.50969800
O	1.85312700	2.29854000	-0.37140000

C	1.45623600	3.36075200	0.12061100
N	2.23903400	4.45892900	0.29301100
H	0.41552400	3.47601600	0.45594500
C	3.63499200	4.45386700	-0.10266800
C	1.69961700	5.67243200	0.87657600
H	3.82638400	5.22440900	-0.86184800
H	4.28390100	4.65126800	0.76139600
H	3.86703100	3.47131100	-0.51501100
H	2.23880400	5.93901800	1.79606500
H	1.77970100	6.51476000	0.17553800
H	0.64537500	5.52154800	1.12163300

S5

B	-1.03008400	-1.63336000	-1.15804000
B	-0.97552200	0.10743400	-1.45863700
B	-0.00641100	-0.60226300	-0.12284500
B	-1.00158300	-1.88483100	0.61107400
B	-0.92619400	-0.30408000	1.39482400
C	-0.96397100	0.83159100	0.10040400
B	-2.44259100	0.84534500	-0.77590100
B	-3.41566900	-0.43892300	-0.04034100
B	-2.52347400	-0.74193400	-1.56007900
B	-2.47494700	-1.15343200	1.30097700
B	-2.41459800	0.58949300	0.99676800
H	-0.51847500	-2.39806700	-1.91869400
H	-0.47579900	-2.83506100	1.10912200
H	-0.41344500	0.65929200	-2.34615700
H	-0.32101800	-0.03197800	2.37919700
H	-3.07590500	-0.87116400	-2.61074500
H	-3.12285900	-3.01632500	-0.41488700
H	-2.82744000	1.88437600	-1.20748800
H	-4.60643000	-0.35300700	-0.00792500
H	-2.99269400	-1.57909200	2.28947200
H	-2.78397300	1.46226200	1.71576700
B	-2.54427800	-1.97986800	-0.27762100
C	-0.25389500	2.15278300	0.22935800
O	0.06381100	2.87871100	-0.69022600
O	0.01505200	2.49194600	1.51439000
H	0.47756600	3.34831200	1.44836400
C	1.58379000	-0.53907600	-0.11205700
C	2.31934100	-1.32329000	0.79679600
C	2.32328600	0.26910000	-0.99604800
C	3.71493900	-1.30890800	0.82234000
H	1.78201700	-1.95936700	1.49496100

C	3.72004900	0.29555800	-0.97330100
H	1.79663200	0.89297000	-1.71211400
C	4.42445800	-0.49595600	-0.06454400
H	4.24909300	-1.93183500	1.53768300
H	4.25795900	0.93487300	-1.67104800
H	5.51264200	-0.48017000	-0.04740800

S6

C	-3.13369700	1.67240200	-0.49053700
O	-2.11606000	2.23320500	-0.10190300
O	-3.85904000	0.94470300	0.36582500
O	0.58760200	0.10050000	2.34083500
C	1.11032500	-1.03886800	1.96391000
O	1.98236300	-1.63753100	2.57848500
C	0.52396600	-1.58010100	0.65319600
B	1.42236700	-2.45015900	-0.51338900
B	0.15602600	-3.24030500	0.44179300
B	-1.13099200	-2.04609300	0.75457900
B	0.95902300	-0.74018500	-0.80896500
B	-0.62257000	-0.52953600	-0.00704700
B	0.23670400	-3.49940600	-1.31052700
B	0.72515100	-1.96422500	-2.07759400
H	2.56538100	-2.69257100	-0.30252300
B	-1.34231300	-3.25017000	-0.51955500
H	0.45090900	-4.00925400	1.29685900
B	-1.83383100	-1.55305400	-0.79614500
H	-1.66481900	-2.02229900	1.81625700
B	-0.55576700	-0.75324100	-1.75839000
H	0.55428500	-4.55588700	-1.76695900
B	-0.98980500	-2.45500700	-2.08029500
H	1.39495000	-1.92347500	-3.06452600
H	-2.14773400	-4.12362100	-0.39908100
H	-2.99094800	-1.24615200	-0.89214500
H	-0.80808400	0.12664900	-2.52930400
H	-1.55251200	-2.76724400	-3.08800700
Pd	-0.74663200	1.11606200	1.18984400
C	-3.60361500	1.75975000	-1.91854600
H	-4.69541900	1.77736400	-1.99504200
H	-3.17531100	2.64635200	-2.38786700
H	-3.22090900	0.87541600	-2.44398500
H	-4.43008200	0.31834900	-0.11197300
C	2.05838600	0.40897600	-0.84349000
C	3.21871400	0.37657300	-0.04731500
C	1.92227300	1.49541300	-1.72808300

C	4.18580500	1.38128000	-0.12436100
H	3.36463900	-0.43987800	0.65373300
C	2.88769400	2.50010000	-1.81584300
H	1.04222200	1.55152300	-2.36309000
C	4.02717300	2.44852600	-1.01039600
H	5.06690700	1.32716400	0.51194700
H	2.74866300	3.32399600	-2.51388600
H	4.78189700	3.23030800	-1.07270400

S7

O	1.29662700	0.14029800	2.31422200
C	2.18029700	1.05272200	1.98823600
O	3.07764500	1.43531600	2.72478200
C	1.99079600	1.60908800	0.57413000
B	2.16082900	3.27673800	0.22096400
B	3.27372100	2.07324400	-0.45232900
B	2.38253700	0.54048100	-0.74447500
B	0.54766700	2.52549100	0.35371200
B	0.70714100	0.87245700	-0.24209100
B	2.58544700	3.32743700	-1.49876000
B	0.89769700	3.60942200	-0.99204200
H	2.52792700	4.01009100	1.07936900
B	2.71823900	1.64944500	-2.09071100
H	4.38899700	2.00371300	-0.05061200
B	1.10591600	0.88161700	-1.95391300
B	-0.02474200	2.09825800	-1.27347000
H	-0.12804800	2.75006000	1.30785600
H	3.26560900	4.20296200	-1.94124000
B	1.24315700	2.59888800	-2.42510800
H	0.37777500	4.68227200	-1.05574200
H	3.49601400	1.32755300	-2.93658100
H	0.73169600	0.03279200	-2.70519200
H	-1.18939200	2.09549500	-1.53940100
H	0.96717600	2.95749400	-3.53051600
Pd	-0.11340200	-0.53268100	1.00088600
I	-2.10937100	-1.54847000	-0.52934200
C	-3.75800500	-0.22695200	-0.08497400
C	-5.05543000	-0.67576200	-0.31987200
C	-3.49163600	1.04460900	0.41390900
C	-6.12206600	0.18358700	-0.04117900
H	-5.24125800	-1.67146700	-0.70986200
C	-4.57195600	1.88909100	0.68723300
H	-2.47262000	1.37672800	0.58178400
C	-5.88214000	1.46330000	0.46223500

H	-7.13963600	-0.15491100	-0.21913600
H	-4.37613300	2.88554300	1.07316400
H	-6.71477200	2.12776300	0.67686200
C	3.08202000	-0.87087600	-0.52020800
C	4.06705500	-1.08438900	0.46239700
C	2.76106300	-1.96229400	-1.34957600
C	4.69062700	-2.32463600	0.61453600
H	4.34558900	-0.27222500	1.12724600
C	3.38481400	-3.20361900	-1.20795100
H	2.01392700	-1.83075600	-2.12788700
C	4.35408900	-3.39181700	-0.22048700
H	5.44356600	-2.45472100	1.38927400
H	3.11477000	-4.02328200	-1.87170400
H	4.84255000	-4.35748600	-0.10481800

S9

O	-0.26707400	-0.62211400	2.02040900
C	-1.25063700	-1.47878000	1.82130000
O	-1.85500300	-2.02178200	2.72883100
C	-1.57219500	-1.71672000	0.35027800
B	-2.07618200	-3.23593600	-0.24253700
B	-3.16933400	-1.83745100	-0.24487100
B	-2.21292400	-0.34007800	-0.51856000
B	-0.41074000	-2.64958500	-0.52202200
B	-0.54800700	-0.90776300	-0.70819400
B	-3.02866900	-2.85478900	-1.68582000
B	-1.32334700	-3.35718800	-1.85416000
H	-2.24751800	-4.11986400	0.52971900
B	-3.11448700	-1.07976800	-1.85572100
H	-4.07168000	-1.79213800	0.52479600
B	-1.45393800	-0.47131800	-2.14034100
B	-0.33409000	-1.88594200	-2.13464300
H	0.48967900	-3.12632200	0.08372800
H	-3.92828000	-3.55726900	-2.03135400
B	-1.96718000	-2.02220100	-2.85364400
H	-1.00940900	-4.41643200	-2.30219000
H	-4.06822500	-0.51974900	-2.30058300
H	-1.22320400	0.50361800	-2.78005300
H	0.67197600	-1.89229000	-2.77263000
H	-2.10891100	-2.13145500	-4.03288700
Pd	0.61577800	0.39634700	0.48199100
I	1.80100000	2.12489000	-1.17240200
C	2.26496200	-0.72156500	0.69528100
C	2.97646400	-1.24810600	-0.37932300

C	2.66449800	-0.91262900	2.01547600
C	4.13497000	-1.98488200	-0.11099600
H	2.64352100	-1.10088400	-1.39877300
C	3.83495300	-1.64176400	2.26098900
H	2.06733000	-0.53922100	2.83978500
C	4.56892300	-2.17690700	1.20231700
H	4.69761300	-2.40393500	-0.94171800
H	4.15386800	-1.80134700	3.28831200
H	5.47210800	-2.74909400	1.39959900
C	-2.52432500	1.01813000	0.25023300
C	-3.23945200	1.04964600	1.46488100
C	-2.10712200	2.25385700	-0.28265100
C	-3.52325300	2.25179800	2.11119600
H	-3.57132600	0.11882700	1.91500100
C	-2.38954400	3.46269500	0.36206200
H	-1.56407600	2.27266600	-1.22227700
C	-3.09913000	3.46578500	1.56198100
H	-4.07584900	2.24088800	3.04806000
H	-2.04984400	4.39739600	-0.07776600
H	-3.32014300	4.40339700	2.06745800

S11

O	-0.36317300	1.22477300	1.34020800
C	0.10971200	1.05861500	0.16632400
O	-0.76292800	0.67986600	-0.71062000
C	1.52507100	1.30228700	-0.18595600
B	1.87992300	1.79238600	-1.79729600
B	1.89885100	2.96743300	-0.44636000
B	2.46569900	2.10430000	1.01524000
B	2.42633700	0.18480300	-1.20526800
B	2.78345100	0.37965600	0.58547500
B	3.20661700	2.95371700	-1.63650400
B	3.53807700	1.25864500	-2.08736100
H	0.98931100	1.84482600	-2.58028800
B	3.56930500	3.14354400	0.10435800
H	1.00806700	3.74976800	-0.35101500
B	4.11639300	1.56097100	0.72275800
H	1.96329500	2.33743200	2.06392600
B	4.09377500	0.39584200	-0.62398100
H	3.31725900	3.84896700	-2.41642400
B	4.58602700	2.08917300	-0.91114800
H	3.89190700	0.94680800	-3.18202500
H	3.94435400	4.17326000	0.57452800
H	4.89614200	1.47802900	1.62136200

H	4.85838100	-0.51769800	-0.67827100
H	5.71651800	2.36873800	-1.17158400
Pd	-2.26073600	0.67093800	0.66567600
I	-4.66413600	-0.00271200	-0.16294400
C	2.46128800	-0.75766000	1.64999100
C	3.29158800	-0.91121000	2.77678700
C	1.37390400	-1.64499200	1.54162400
C	3.05151900	-1.89038100	3.74205900
H	4.14088200	-0.24553800	2.89913300
C	1.12095900	-2.62353900	2.50551400
H	0.71625000	-1.59198100	0.67900700
C	1.96034900	-2.75170900	3.61293100
H	3.71705900	-1.97719100	4.59869200
H	0.26984700	-3.29001300	2.38344600
H	1.76778100	-3.51446700	4.36449100
C	1.84840200	-1.16804800	-1.81068200
C	2.51205800	-2.38589700	-1.56512800
C	0.73047200	-1.21571700	-2.66495600
C	2.08312900	-3.58638300	-2.13355800
H	3.38239100	-2.39124000	-0.91597900
C	0.28972400	-2.41369500	-3.23233400
H	0.19504800	-0.30056500	-2.89354700
C	0.96501600	-3.60654900	-2.96944200
H	2.62214200	-4.50703100	-1.91957800
H	-0.58107700	-2.41110000	-3.88441600
H	0.62486700	-4.54057100	-3.41185900

S12

C	4.32706100	0.54695700	0.23085700
O	3.89863400	-0.37274500	-0.54866200
O	3.64853000	0.82970000	1.26952800
O	0.80142500	-0.46652300	2.06999900
C	-0.48468200	-0.69145400	1.90420000
O	-1.28446100	-0.47706400	2.80018100
H	1.52734700	-2.02823400	-0.04628600
C	-0.90977900	-1.27761500	0.55633300
B	-2.32016000	-2.26095700	0.48653200
B	-2.27893600	-0.68701400	-0.36087100
B	-0.57510600	-0.41721700	-0.94663900
B	-0.70130200	-2.98680900	0.46354000
B	0.33381900	-1.85727900	-0.42759000
B	-2.89180400	-2.15065200	-1.18191500
B	-1.92951600	-3.55748200	-0.66586600
H	-2.98122400	-2.37136800	1.46442500

B	-1.81694700	-1.03098700	-2.05789400
B	-0.18563300	-1.74233400	-2.09510000
B	-0.25271100	-3.31231900	-1.23219000
H	-0.26667000	-3.53783700	1.42203600
H	-4.05337100	-2.23372400	-1.43601400
B	-1.61659400	-2.79208000	-2.24859000
H	-2.39941200	-4.64591200	-0.53899000
H	-2.20729800	-0.33071300	-2.94003500
H	0.58977700	-1.55671200	-2.98065800
H	0.48889500	-4.20632000	-1.49877600
H	-1.87154200	-3.33740900	-3.27861700
Pd	2.17209200	-0.59793500	0.63598300
C	5.58530600	1.30076000	-0.10123600
H	6.23763100	0.69151100	-0.73154700
H	5.31606700	2.20958100	-0.65222500
H	6.10102100	1.59644900	0.81604600
C	0.06497600	1.03980200	-0.99459000
C	-0.15690500	2.01655300	-0.00418700
C	0.86702100	1.41385600	-2.09108000
C	0.40286300	3.29227600	-0.09612000
H	-0.78179500	1.78544200	0.85244400
C	1.42445400	2.68974400	-2.19260800
H	1.05774900	0.68949600	-2.87741100
C	1.19654800	3.63637100	-1.19149700
H	0.21195500	4.01829900	0.69067500
H	2.03534200	2.94331000	-3.05688100
H	1.62885100	4.63210400	-1.26616100
C	-3.21155000	0.52600600	0.07534400
C	-3.79408700	0.62710100	1.35346600
C	-3.54744700	1.52539200	-0.85836400
C	-4.66357300	1.67033800	1.67948100
H	-3.54309800	-0.10802400	2.10884600
C	-4.41938100	2.56830500	-0.54069800
H	-3.11983300	1.48434100	-1.85574100
C	-4.98362100	2.64579800	0.73369300
H	-5.09096000	1.71890900	2.67909600
H	-4.65510400	3.32146100	-1.29010200
H	-5.66236900	3.45792900	0.98725600

S13

B	1.92412100	-1.69455700	0.35392700
B	0.50780600	-0.99035100	-0.48529400
B	1.13724100	-0.11201600	-1.90039100
B	0.72147800	0.82499500	-0.43807100

C	1.29013300	-0.17820600	0.86180100
B	2.99885500	-0.38024500	0.90709100
B	3.60563900	0.47143000	-0.52185000
B	3.39375200	-1.30269000	-0.55104200
B	2.20940500	1.19855300	-1.35579600
B	2.27076000	1.16852800	0.40418900
H	1.71348500	-2.66751700	-2.03422300
H	0.46751600	-0.00869100	-2.88280100
H	4.31807100	-2.05812500	-0.55583600
H	3.49441100	-0.36926100	-2.99729900
H	4.68063800	0.99024400	-0.50857300
H	2.30401900	2.23031800	-1.94913800
B	2.90867200	-0.32126900	-1.95739600
C	0.62197100	-0.16097800	2.21237300
O	0.07602900	-1.10476300	2.74739500
C	-0.51011800	1.82009500	-0.26481100
C	-1.63293500	1.54047000	0.53715300
C	-0.50860600	3.05769800	-0.93634200
C	-2.68873600	2.44487400	0.67026900
H	-1.69821900	0.59080500	1.05993900
C	-1.56140500	3.96644100	-0.81443900
H	0.34014200	3.31264100	-1.56425000
C	-2.65916800	3.66545600	-0.00601100
H	-3.53922200	2.18942400	1.29947900
H	-1.52156300	4.91297500	-1.35053900
H	-3.48156700	4.37128700	0.09350800
B	1.87417200	-1.66258900	-1.41153400
O	0.69645100	1.04226400	2.83039100
H	1.76560800	-2.63486400	1.06084500
H	3.51637300	-0.46527900	1.97583500
H	2.32690200	2.10723100	1.12570100
C	-0.93199500	-1.67068400	-0.43824400
C	-1.26481600	-2.71495600	0.44535500
C	-1.91960800	-1.28780400	-1.36699800
C	-2.51352600	-3.33946000	0.40646000
H	-0.53728000	-3.03527300	1.18219100
C	-3.16904800	-1.90871900	-1.41520100
H	-1.70175000	-0.48755600	-2.06781900
C	-3.47342400	-2.94039000	-0.52545500
H	-2.73486800	-4.14273700	1.10689800
H	-3.90499500	-1.58393200	-2.14837000
H	-4.44625900	-3.42760600	-0.55833300
H	0.22690400	0.91393700	3.67584700

S14

C	-4.42817200	-0.05194800	0.60145100
O	-3.84672200	0.93024700	0.15718800
O	-4.72075300	-1.07359500	-0.21094900
O	-0.50124600	0.43204500	-2.36597900
C	0.51430300	-0.32946800	-2.05697500
O	1.47951700	-0.50909000	-2.78917900
C	0.38264900	-1.01265400	-0.68551600
B	0.91149500	-2.62041000	-0.41274900
B	1.66426700	-1.26367900	0.47181700
B	0.36917800	-0.01415800	0.73924000
B	-0.80808500	-2.25996800	-0.69847100
B	-1.12444000	-0.66945400	0.01337200
B	1.15436100	-2.74032800	1.33763200
B	-0.34846000	-3.35560300	0.60731600
H	1.53113200	-3.17370000	-1.26022800
B	0.81330100	-1.14007700	2.04375200
B	-0.90572300	-0.75949600	1.75693600
B	-1.62549600	-2.13499000	0.86853300
H	-1.30149900	-2.55312000	-1.73921500
H	1.97777100	-3.46944500	1.79930100
B	-0.41078600	-2.43257300	2.13281300
H	-0.59611100	-4.52111900	0.53402900
H	1.37883000	-0.72967800	3.01090900
H	-2.77596900	-2.44810500	1.00074000
H	-0.70591100	-2.94276500	3.17273000
Pd	-2.13036900	0.64269800	-1.17161100
C	-4.82215500	-0.16561700	2.05055400
H	-4.03875500	-0.74211900	2.55910700
H	-4.85624400	0.82937900	2.49583300
H	-5.78244500	-0.67498000	2.18042900
H	-4.90983700	-1.87828800	0.30176900
C	0.70776200	1.54012300	0.71481800
C	1.56202200	2.12840300	-0.23703300
C	0.16974500	2.39149400	1.69861300
C	1.84976400	3.49456400	-0.21621900
H	2.01738800	1.51462200	-1.00746700
C	0.45662700	3.75749500	1.72939500
H	-0.48721000	1.97328700	2.45646500
C	1.29808600	4.31818900	0.76655000
H	2.51223900	3.91288000	-0.97104500
H	0.02179700	4.38342000	2.50682500
H	1.52413400	5.38267500	0.78437100
H	-1.54777000	-0.09582300	2.51730500

C	3.18864100	-0.86238800	0.25458700
C	3.92197200	-0.28769000	1.31036000
C	3.88665400	-1.11523600	-0.94225900
C	5.27945100	0.01435700	1.18734600
H	3.41855300	-0.07470300	2.24886500
C	5.24376200	-0.81193700	-1.07321900
H	3.34900300	-1.52427000	-1.78950000
C	5.94961200	-0.24844300	-0.00867000
H	5.81190700	0.45826700	2.02667500
H	5.74961500	-1.01606500	-2.01515300
H	7.00756600	-0.01310600	-0.11094900

S15

O	0.45374700	-0.00979500	-2.27342800
C	1.47257400	-0.74985700	-1.91551200
O	2.35884700	-1.09969200	-2.68340900
C	1.44288500	-1.17124600	-0.43928200
B	1.91547800	-2.73702500	0.06968800
B	2.81219800	-1.29846900	0.63272800
B	1.60755400	0.05833800	0.78147200
B	0.19476100	-2.32349400	-0.12824100
B	0.03054100	-0.62581000	0.32386700
B	2.31098100	-2.56644300	1.78627200
B	0.71779800	-3.20242600	1.30609100
H	2.42379600	-3.46649500	-0.71674300
B	2.11541600	-0.85017800	2.22269000
B	0.39751600	-0.41555100	2.02298200
B	-0.47528800	-1.87632500	1.45456200
H	-0.40686000	-2.75318400	-1.06066300
H	3.13738000	-3.25613700	2.30003100
B	0.84280600	-2.02795400	2.64347500
H	0.41336600	-4.34633700	1.45822600
H	2.78879800	-0.31642700	3.04998000
H	-0.13691400	0.41116100	2.69741700
H	-1.62570900	-2.06507000	1.71459100
H	0.62746900	-2.33164000	3.77801500
Pd	-1.03050100	0.52875200	-0.98229500
I	-3.17614100	1.29077600	0.49685900
C	-4.60107500	-0.26680000	0.04399600
C	-5.96025400	0.03116300	0.10461900
C	-4.13364200	-1.53420600	-0.29171300
C	-6.88113400	-0.98042400	-0.18331200
H	-6.30344000	1.02717300	0.36583300
C	-5.07023300	-2.53199900	-0.57793000

H	-3.07047100	-1.74639400	-0.32792700
C	-6.43826200	-2.25930900	-0.52511900
H	-7.94484900	-0.76039400	-0.14169500
H	-4.71737100	-3.52559400	-0.83968800
H	-7.15814100	-3.04172800	-0.74965100
C	2.00231600	1.56362500	0.44798900
C	2.79578100	1.92547200	-0.65713800
C	1.58009300	2.60449200	1.29742500
C	3.13633200	3.25622100	-0.90806900
H	3.16086800	1.15930800	-1.33329100
C	1.92087000	3.93689000	1.05601400
H	0.97616500	2.36237000	2.16780600
C	2.70024400	4.27038900	-0.05362100
H	3.74983400	3.49727400	-1.77351300
H	1.57883900	4.71399500	1.73743800
H	2.96866700	5.30720800	-0.24687200
C	4.32670700	-1.03506200	0.22321900
C	4.90402500	-1.53749000	-0.95909300
C	5.17584700	-0.32753100	1.09581000
C	6.25670100	-1.34509500	-1.24935700
H	4.27681700	-2.05897100	-1.67254100
C	6.52944300	-0.13529800	0.81368300
H	4.76800700	0.07785500	2.01711400
C	7.07876500	-0.64621200	-0.36349600
H	6.66781200	-1.74352200	-2.17507700
H	7.15363700	0.41630700	1.51444200
H	8.13338100	-0.49828700	-0.58910000

S17

O	-0.11270000	-0.75125500	-1.80747800
C	0.98504800	-1.34312500	-1.38542800
O	1.75832700	-1.91189900	-2.13786000
C	1.18648900	-1.27188900	0.12681000
B	1.93621400	-2.52903000	1.00144700
B	2.69040300	-0.90545000	0.93288300
B	1.32986500	0.30674400	0.85969400
B	0.15717500	-2.37048200	0.97915200
B	-0.15515300	-0.64350600	0.92954700
B	2.52414600	-1.77032400	2.48443000
B	0.98648400	-2.67275300	2.50364000
H	2.43126100	-3.42264100	0.39875500
B	2.15230600	-0.02854200	2.39963700
B	0.37922600	0.15748700	2.38386400
B	-0.35621200	-1.48681300	2.44199900

H	-0.49160500	-3.12450100	0.33434600
H	3.49943100	-2.17541600	3.03673100
B	1.12455400	-1.12049000	3.37349700
H	0.87387000	-3.72535300	3.05126400
H	2.84659800	0.80509600	2.89288400
H	-0.17712400	1.10211000	2.84131500
H	-1.42250700	-1.68137400	2.93523800
H	1.10504000	-1.05630300	4.56404100
Pd	-1.38735100	0.22736100	-0.54462400
I	-3.12724800	1.83327600	0.68360200
C	-2.72509800	-1.24863400	-0.77308800
C	-3.45236800	-1.79137500	0.28297900
C	-2.88428600	-1.68607600	-2.08562100
C	-4.37508600	-2.80483400	0.00227500
H	-3.30825900	-1.44713400	1.29905900
C	-3.82380000	-2.69137100	-2.34647000
H	-2.27152700	-1.28703400	-2.88604900
C	-4.56731400	-3.25050100	-1.30691300
H	-4.94602200	-3.23918000	0.81937200
H	-3.95272700	-3.04386900	-3.36708500
H	-5.28876700	-4.03690400	-1.51454700
C	1.38817000	1.62870600	-0.02952500
C	2.08568600	1.70184600	-1.25384500
C	0.75499200	2.80604100	0.41842100
C	2.15275900	2.88802300	-1.98391500
H	2.59263800	0.82398600	-1.64043000
C	0.82299000	3.99797200	-0.30771500
H	0.20287400	2.78813700	1.35236000
C	1.52339600	4.04341400	-1.51266100
H	2.70201000	2.90906200	-2.92228100
H	0.32163700	4.88597900	0.06982100
H	1.57747800	4.96869300	-2.08225700
C	4.07580200	-0.64975800	0.19824800
C	4.56273400	-1.47542100	-0.83347500
C	4.90557400	0.40937200	0.61446100
C	5.81285400	-1.25404900	-1.41557500
H	3.94246700	-2.28387600	-1.20241900
C	6.15770600	0.63318200	0.03965700
H	4.56447700	1.06987300	1.40616400
C	6.61884700	-0.20051200	-0.98063300
H	6.15564700	-1.90896200	-2.21407700
H	6.77123400	1.46141800	0.38875500
H	7.59353600	-0.02907100	-1.43331200

S19

O	0.32555900	-0.68632300	0.59138900
C	0.13622300	-0.16184600	-0.55440400
O	1.22345800	0.10679800	-1.20282300
C	-1.18981900	0.13253800	-1.14450800
B	-1.52194500	-0.65350000	-2.64641400
B	-2.43925200	-1.09394300	-1.15516700
B	-2.61293000	0.42215300	-0.14729900
B	-1.12319100	1.07999600	-2.59191400
B	-1.76655500	1.77796300	-1.05652200
B	-3.27850000	-0.81557900	-2.70348500
B	-2.46608600	0.50729900	-3.58399700
H	-0.71231000	-1.42048700	-3.05465900
B	-3.94264000	-0.14403900	-1.18955800
B	-3.53578500	1.58817600	-1.13374000
B	-2.62903700	1.99072100	-2.60822600
H	-0.06215200	1.44891300	-2.97100500
H	-3.78018200	-1.74405200	-3.25733000
B	-3.96782700	0.82427700	-2.68444000
H	-2.38538700	0.52944200	-4.77308900
H	-4.93296100	-0.57147600	-0.68155500
H	-4.24295100	2.38751900	-0.60409900
H	-2.68308000	3.07077300	-3.10985600
H	-4.99361400	1.08423600	-3.23527600
Pd	2.40293700	-0.56108400	0.30457100
I	4.99925700	-0.43198100	-0.06935600
C	-0.92171900	2.91238400	-0.32599300
C	-0.30980400	2.74918100	0.93188500
C	-0.74828100	4.16012500	-0.95618800
C	0.43974200	3.76949100	1.52344700
H	-0.42436900	1.81542100	1.47239400
C	-0.00894600	5.18723700	-0.36848400
H	-1.19922900	4.32564000	-1.93008800
C	0.59335700	4.99581000	0.87660700
H	0.89812100	3.60298600	2.49592900
H	0.10205000	6.13673200	-0.88833900
H	1.17557100	5.79183400	1.33585200
C	-2.68125700	0.41282700	1.44894500
C	-3.35617200	1.46324200	2.10406600
C	-2.16700300	-0.60943800	2.27056900
C	-3.50907300	1.49686500	3.49086000
H	-3.76962100	2.27418700	1.51377900
C	-2.31221500	-0.58150700	3.65995200
H	-1.64086400	-1.44310800	1.82432400

C	-2.98528100	0.47168400	4.27974000
H	-4.03556300	2.32916800	3.95354400
H	-1.89874300	-1.39219000	4.25640700
H	-3.09949100	0.49371100	5.36162800
C	-2.27456500	-2.54649000	-0.52795500
C	-1.14079100	-3.35335000	-0.73661000
C	-3.32450100	-3.11121800	0.22123900
C	-1.05032800	-4.64647600	-0.21710100
H	-0.31330900	-2.97592700	-1.33148800
C	-3.24688600	-4.40519800	0.73890000
H	-4.21894600	-2.52243800	0.40145200
C	-2.10524100	-5.17974600	0.52543900
H	-0.15671200	-5.23931700	-0.40074800
H	-4.08008000	-4.80683700	1.31190400
H	-2.03992200	-6.18801200	0.92879900

S20

C	-4.89780300	-0.89887400	-0.68960800
O	-4.38071900	-1.28712900	0.41547800
O	-4.13660900	-0.74411300	-1.69664600
O	-0.90658100	-1.12001400	-1.67002800
C	0.31342100	-0.77888000	-1.31681400
O	1.17134600	-0.56439200	-2.15792000
H	-1.57731000	-2.06254900	0.76109100
C	0.60170900	-0.70850500	0.18754400
B	2.20460400	-1.06836800	0.81762500
B	1.48711600	0.59266500	0.95718300
B	-0.31953600	0.42747100	1.17745800
B	0.85797100	-2.23960900	0.93880700
B	-0.63356100	-1.32232200	1.17327400
B	2.24693400	-0.19840900	2.36961900
B	1.87114700	-1.93696900	2.34779300
B	0.72738500	0.69635400	2.58418500
B	-0.59846800	-0.47976700	2.70385000
B	0.10970900	-2.11639100	2.55587500
H	0.83557100	-3.20245100	0.24451600
H	3.27754500	0.22382500	2.79360800
B	0.97909200	-0.84411600	3.43872600
H	2.63726700	-2.76803500	2.72441600
H	0.67346600	1.73847100	3.15834200
H	-1.58974500	-0.28913800	3.33598400
H	-0.39572800	-3.07189200	3.05688100
H	1.11737200	-0.88278500	4.62273900
Pd	-2.46126800	-1.24958800	-0.43781300

C	-6.36859500	-0.59680700	-0.77355100
H	-6.91990900	-1.18819000	-0.03832600
H	-6.52322300	0.46568100	-0.55158800
H	-6.73720400	-0.79439800	-1.78326900
C	-1.32478300	1.50100600	0.56799000
C	-1.13768200	2.11721100	-0.68460400
C	-2.44683600	1.90774800	1.31768700
C	-2.02887100	3.07675900	-1.16852500
H	-0.28003500	1.85364200	-1.29484600
C	-3.33839700	2.87088700	0.84217900
H	-2.62382700	1.45992700	2.29099600
C	-3.13446600	3.45940700	-0.40762100
H	-1.85263500	3.52745600	-2.14235300
H	-4.19114300	3.16282700	1.45215800
H	-3.82676200	4.21057800	-0.78220100
C	2.10396600	1.86631000	0.22239500
C	2.74706000	1.82095200	-1.03060300
C	2.06424200	3.11811000	0.86924000
C	3.31320600	2.96277100	-1.60317400
H	2.78793300	0.88494700	-1.57257300
C	2.63184200	4.26089700	0.30412800
H	1.57760600	3.19973300	1.83579600
C	3.26128600	4.18904900	-0.93958400
H	3.79834500	2.88745300	-2.57418300
H	2.57814100	5.20846900	0.83676600
H	3.70359100	5.07773900	-1.38587000
C	3.48646100	-1.39572800	-0.06516500
C	3.48976300	-2.35785700	-1.09138000
C	4.71231200	-0.76550000	0.21826600
C	4.65093400	-2.67490500	-1.79726300
H	2.56666800	-2.86501200	-1.35260900
C	5.88024100	-1.07741100	-0.48086000
H	4.75247900	-0.01598100	1.00295600
C	5.85507500	-2.03594900	-1.49461900
H	4.61281900	-3.42176300	-2.58764300
H	6.80917600	-0.56766300	-0.23298100
H	6.76191900	-2.28150500	-2.04379800

S21

O	0.74249700	-1.35567800	2.75349700
C	0.00928600	-0.60906200	1.89410200
O	-0.58747900	0.37465600	2.28287500
H	1.53547500	-3.07134000	1.08577000
C	0.02200400	-1.14031100	0.48240900

B	-1.45636300	-1.04395200	-0.45267000
B	-0.01151600	-0.02464100	-0.87939000
B	1.48111100	-1.00016000	-0.45621300
B	-0.84096100	-2.60334200	0.20641600
B	0.93475900	-2.58552900	0.18825700
B	-0.88581200	-0.94281900	-2.13368300
B	-1.41074900	-2.50919600	-1.46584900
B	0.89286600	-0.91697600	-2.13681200
B	1.46715400	-2.46495200	-1.48349100
B	0.04734600	-3.45350700	-1.06620600
H	-1.41005100	-3.09311200	1.12891700
H	-1.52284000	-0.35009900	-2.94979600
B	0.02299000	-2.42389500	-2.51616100
H	-2.43956100	-3.02154200	-1.78484800
H	1.51658100	-0.32188000	-2.96034600
H	2.49711400	-2.95752000	-1.83127300
H	0.06502800	-4.64635700	-1.09699100
H	0.02646100	-2.88059800	-3.61942800
C	2.79576900	-0.32799900	0.14146600
C	2.78283100	0.82137900	0.95429900
C	4.05639600	-0.89190800	-0.13410300
C	3.95829300	1.37166600	1.47090200
H	1.83990200	1.30844100	1.18205000
C	5.23683300	-0.34507300	0.37167300
H	4.10968900	-1.78036400	-0.75640300
C	5.19400100	0.79157200	1.18158200
H	3.90509900	2.26144000	2.09523000
H	6.19168500	-0.81079400	0.13454400
H	6.11166700	1.22041500	1.57956000
C	0.00240800	1.57262600	-0.80255500
C	-0.85227600	2.34380500	0.01009700
C	0.88029400	2.28785900	-1.64308700
C	-0.83009000	3.74069600	-0.01559300
H	-1.53570200	1.84803500	0.68561000
C	0.90613300	3.68285500	-1.67696400
H	1.56013100	1.73831400	-2.28581600
C	0.04769200	4.42057100	-0.86028200
H	-1.50721300	4.29663300	0.63017200
H	1.60202200	4.19182600	-2.34130300
H	0.06440400	5.50873600	-0.88094000
C	-2.83505600	-0.44782000	0.07906500
C	-3.39995000	-0.79735400	1.31938300
C	-3.59355600	0.41129900	-0.73871800
C	-4.64431400	-0.31387400	1.72717000

H	-2.86101600	-1.46773000	1.98231200
C	-4.84116200	0.89759200	-0.34268500
H	-3.19608600	0.70386000	-1.70599300
C	-5.37395800	0.53839700	0.89635700
H	-5.04530800	-0.60700100	2.69564300
H	-5.39593700	1.55982400	-1.00458500
H	-6.34528000	0.91586700	1.20998000
H	0.66000700	-0.89354300	3.60886900

S23

C	-4.65389000	-1.48659000	0.62679900
O	-4.43864400	-0.55416800	-0.13703200
O	-4.40283900	-2.73958300	0.23089000
O	-0.86513400	-0.25562300	-2.34295500
C	0.31324100	-0.17711700	-1.77754500
O	1.33592900	0.07659300	-2.39934400
C	0.29215900	-0.41849300	-0.25615800
B	1.42418500	-1.47865400	0.57494600
B	1.33346000	0.29678900	0.93972900
B	-0.39860400	0.84640800	0.74520100
B	-0.24459200	-2.00683200	0.15685400
B	-1.31746900	-0.60694300	0.26969600
B	1.33940100	-0.90947200	2.26065200
B	0.38072000	-2.31831300	1.77174500
B	0.25335300	0.48659400	2.36253700
B	-1.39564900	-0.04924700	1.93707500
B	-1.30414900	-1.79671700	1.56903800
H	-0.39290200	-2.79291600	-0.72065200
H	2.28827000	-1.02210700	2.97352900
B	-0.31896900	-1.11423800	2.87862200
H	0.63501500	-3.42899900	2.12279500
H	0.45637500	1.37164100	3.13471200
H	-2.21777900	-2.54483700	1.77097600
H	-0.53667100	-1.36591500	4.02636400
Pd	-2.59786400	-0.46558700	-1.30262600
C	-5.18222700	-1.27305600	2.02068400
H	-4.31572100	-1.20784200	2.69110800
H	-5.71432500	-0.32178400	2.06356100
H	-5.83328600	-2.08840400	2.35166200
H	-4.38382000	-3.34405000	0.99222900
C	-0.75257700	2.33134700	0.26757000
C	-1.05396100	2.71153700	-1.05528800
C	-0.80066500	3.35106400	1.23919200
C	-1.37893500	4.02997600	-1.38602100

H	-1.04054100	1.97263300	-1.84794100
C	-1.13013100	4.66863800	0.91736600
H	-0.57222000	3.10679000	2.27166200
C	-1.42129500	5.01783700	-0.40208800
H	-1.59915400	4.28057700	-2.42197200
H	-1.15412500	5.42363800	1.70105700
H	-1.67510400	6.04438700	-0.65943900
H	-2.37507400	0.46467100	2.39021000
C	2.53809900	1.30416900	0.67046400
C	3.56450700	1.41420300	1.62898000
C	2.62752100	2.15125400	-0.45032500
C	4.62178900	2.31366600	1.48118500
H	3.53397400	0.78084300	2.51039600
C	3.68260200	3.05260700	-0.60613200
H	1.87486700	2.09550200	-1.22617900
C	4.68688700	3.14062000	0.35880700
H	5.39604300	2.36510600	2.24464600
H	3.71646500	3.68762500	-1.48916200
H	5.50979100	3.84263300	0.23714000
C	2.69974800	-2.17815200	-0.07465900
C	3.52290000	-1.57555700	-1.04553500
C	3.07820400	-3.46240900	0.36596900
C	4.65469200	-2.22250400	-1.54765900
H	3.25967000	-0.59949500	-1.43159500
C	4.20966800	-4.11262800	-0.12921400
H	2.47434700	-3.96394000	1.11583000
C	5.00758100	-3.49348200	-1.09272200
H	5.26235200	-1.72486500	-2.30094200
H	4.46601700	-5.10450400	0.23953500
H	5.89084200	-3.99558000	-1.48370200

S24

O	0.10144300	0.13668800	-2.17529200
C	1.24719900	-0.22603200	-1.66003500
O	2.24436600	-0.44773400	-2.33475800
C	1.22190600	-0.37365700	-0.12893000
B	2.00812400	-1.67562600	0.72639100
B	2.48929700	0.04860000	0.99527500
B	0.99635900	1.08020500	0.80899100
B	0.24566200	-1.69893400	0.39255700
B	-0.33928000	-0.04070800	0.45967400
B	2.18360000	-1.03781500	2.37997800
B	0.82423000	-2.12114200	2.00018000
B	1.57045700	0.62883400	2.42639500

B	-0.17530600	0.59042400	2.08275700
B	-0.64282500	-1.11824400	1.81523300
H	-0.17017000	-2.44068200	-0.43921700
H	3.09241600	-1.38276600	3.07085600
B	0.56831200	-0.70547500	3.05228300
H	0.77513800	-3.24899200	2.38439700
H	2.03125500	1.46405100	3.14128500
H	-0.93762400	1.38530300	2.54002000
H	-1.73676900	-1.52512900	2.06629500
H	0.33775300	-0.81703800	4.21817400
Pd	-1.56277000	0.52208200	-1.07183600
I	-3.92062400	1.04703500	0.16827500
C	-4.90776200	-0.87262100	0.14290500
C	-6.29483500	-0.91136100	0.26290200
C	-4.14134200	-2.02777500	0.02033100
C	-6.93282500	-2.15508700	0.25747700
H	-6.87433400	0.00141200	0.35764500
C	-4.79786100	-3.26217300	0.01594500
H	-3.06116300	-1.97454400	-0.06358800
C	-6.18720500	-3.32863300	0.13342900
H	-8.01503100	-2.19904400	0.34948700
H	-4.20967400	-4.17096700	-0.07530400
H	-6.68805500	-4.29292200	0.13011900
C	1.06333300	2.54048900	0.17970700
C	1.84117200	2.86501600	-0.94768700
C	0.34267600	3.59161700	0.77955300
C	1.88529400	4.16486500	-1.45615900
H	2.42875500	2.09673500	-1.43896700
C	0.38549800	4.89455000	0.27978900
H	-0.25874100	3.38380000	1.66018600
C	1.15685400	5.18762700	-0.84660500
H	2.49712500	4.37616800	-2.33046400
H	-0.18232200	5.68121800	0.77359000
H	1.19395000	6.20129800	-1.24078800
C	3.93582700	0.60217900	0.62170700
C	4.65223900	0.21908200	-0.52951900
C	4.58423300	1.48527300	1.50817800
C	5.94098800	0.69737200	-0.77969000
H	4.18377300	-0.44201900	-1.24803200
C	5.87312700	1.96249900	1.26541200
H	4.06847600	1.80500300	2.40831000
C	6.56087500	1.56957300	0.11591500
H	6.46105600	0.38138800	-1.68192700
H	6.33813000	2.64392900	1.97563200

H	7.56583700	1.93974900	-0.07907300
C	2.97382900	-2.74389000	0.05135000
C	2.67131200	-3.40136800	-1.15492300
C	4.16758700	-3.11770600	0.69611700
C	3.51072300	-4.38090700	-1.68803500
H	1.76752900	-3.13929400	-1.69523000
C	5.01210000	-4.09871500	0.17263100
H	4.43922100	-2.62932700	1.62729500
C	4.68668900	-4.73724600	-1.02496800
H	3.24510100	-4.86436100	-2.62613400
H	5.92689400	-4.36061900	0.70091600
H	5.34255900	-5.50102000	-1.43853700

S26

O	0.38963600	0.38505400	-1.76931500
C	-0.85751700	0.47979700	-1.36115000
O	-1.77899700	0.69545500	-2.13108400
C	-1.03696800	0.30897100	0.14905100
B	-2.22166800	1.16683300	1.08865800
B	-2.27365100	-0.64177100	0.93237000
B	-0.55056700	-1.23804800	0.81078000
B	-0.49502300	1.66901400	1.07129400
B	0.45575500	0.20641800	0.93737200
B	-2.41926600	0.14001800	2.52899800
B	-1.34758800	1.56026200	2.60736600
B	-1.41283000	-1.31565300	2.35871300
B	0.29327800	-0.80771800	2.34475500
B	0.34187400	0.98488700	2.49019400
H	-0.18532400	2.64661100	0.47721900
H	-3.46036200	0.10399700	3.10751400
B	-0.86818300	0.03405100	3.39366000
H	-1.63802900	2.54794200	3.20634700
H	-1.72572100	-2.37334400	2.80797900
H	1.17364100	-1.49133600	2.75416000
H	1.25835300	1.55373800	2.99409900
H	-0.81300400	-0.07535900	4.57949200
Pd	1.95060600	-0.03943700	-0.52515000
I	4.19157700	-0.84003700	0.67839200
C	2.58363300	1.85567300	-0.69563800
C	3.01473800	2.61835900	0.38610200
C	2.57658100	2.34998400	-1.99744500
C	3.45900500	3.92259500	0.14321200
H	3.00330300	2.22117500	1.39300000
C	3.03865400	3.65330400	-2.22010700

H	2.19095800	1.75718500	-2.81931600
C	3.47839600	4.43847400	-1.15417100
H	3.79487500	4.52966900	0.98036100
H	3.03340700	4.05147900	-3.23197600
H	3.82831200	5.45227000	-1.33218400
C	-0.10158200	-2.43310900	-0.14385100
C	-0.76618000	-2.74809800	-1.34748300
C	0.99527200	-3.24415600	0.21300900
C	-0.35982800	-3.81643200	-2.14583400
H	-1.61700600	-2.15539500	-1.66556300
C	1.40556500	-4.31692600	-0.58407500
H	1.53279200	-3.03825100	1.13274900
C	0.72863300	-4.60748300	-1.76762200
H	-0.89756700	-4.03142200	-3.06630900
H	2.25779200	-4.91806600	-0.27633900
H	1.04495300	-5.44045000	-2.39173200
C	-3.46821200	-1.40364700	0.20647500
C	-4.14072200	-0.91099800	-0.92982800
C	-3.93506200	-2.61977300	0.74445800
C	-5.21526900	-1.60057000	-1.49705000
H	-3.80591700	0.01156100	-1.38726400
C	-5.01147400	-3.30952200	0.18480100
H	-3.44626900	-3.03426500	1.62055100
C	-5.65884000	-2.80196500	-0.94295100
H	-5.70741500	-1.19047600	-2.37645300
H	-5.34163500	-4.24576600	0.63060600
H	-6.49745300	-3.33698600	-1.38433600
C	-3.34033900	2.11795600	0.48051200
C	-3.06915800	3.10826700	-0.48085800
C	-4.66373400	2.03326800	0.95160700
C	-4.06352400	3.96933000	-0.94743900
H	-2.06484700	3.20790400	-0.87956600
C	-5.66437800	2.89221400	0.49309700
H	-4.91406500	1.27962500	1.69231700
C	-5.36818900	3.86668900	-0.46100500
H	-3.81676600	4.72116300	-1.69417700
H	-6.67643300	2.79661000	0.88123400
H	-6.14482300	4.53753300	-0.82278000

S28

O	-0.27466800	0.01003300	1.09495500
C	-0.11608100	0.00394600	-0.17027300
O	-1.21815600	0.07440000	-0.84419700
C	1.19620900	-0.08949100	-0.85202400

B	1.77940600	1.33431800	-1.71941100
B	2.61797700	0.70546500	-0.21247200
B	2.46551900	-1.12009700	-0.18140700
B	1.12381800	-0.10057400	-2.57618700
B	1.50538900	-1.60893200	-1.66916200
B	3.54362300	1.13142900	-1.67659700
B	2.62336200	0.64868200	-3.12562400
B	3.95137000	-0.34135500	-0.76946400
B	3.27879000	-1.73485500	-1.64621900
B	2.45927200	-1.12223700	-3.09773500
H	0.06050900	-0.02366000	-3.09475900
H	4.24802100	2.09272300	-1.65385700
B	3.96497100	-0.36212200	-2.54700100
H	2.64758800	1.27201600	-4.14071600
H	4.94827600	-0.43730600	-0.12413800
H	3.79943700	-2.80587700	-1.62691900
H	2.38262600	-1.75757000	-4.10310700
H	4.98480600	-0.46625800	-3.15669700
Pd	-2.35088900	0.14617100	0.84253300
I	-4.95208200	0.33601700	0.53584900
C	0.43924100	-2.79123000	-1.66151900
C	-0.24675600	-3.22513700	-0.51099400
C	0.14455300	-3.46335300	-2.86362800
C	-1.17952100	-4.26425000	-0.55733000
H	-0.04530000	-2.75730600	0.44729000
C	-0.77894800	-4.50804800	-2.91768400
H	0.64842600	-3.15744100	-3.77544000
C	-1.44974100	-4.91331900	-1.76227500
H	-1.68927000	-4.56842700	0.35422300
H	-0.97845400	-5.00202700	-3.86649300
H	-2.17411600	-5.72401000	-1.80079200
C	2.38846000	-1.96531600	1.17095400
C	2.77539600	-3.32112700	1.14610700
C	2.02097700	-1.44076400	2.42561700
C	2.79522400	-4.10817600	2.29830600
H	3.06530900	-3.77047200	0.20214300
C	2.03370000	-2.22339600	3.58302500
H	1.71772000	-0.40523300	2.50615900
C	2.42206200	-3.56225300	3.52737600
H	3.09939500	-5.15076200	2.23195800
H	1.74245700	-1.77788700	4.53198500
H	2.43364400	-4.17179300	4.42865600
C	2.67621700	1.57683800	1.12240800
C	1.63821500	2.41244800	1.57699400

C	3.85744500	1.56775000	1.89087300
C	1.76321600	3.18124500	2.73637800
H	0.71334100	2.48071100	1.01614100
C	3.99390400	2.33658700	3.04768700
H	4.68541400	0.94037100	1.57670900
C	2.94318300	3.14709400	3.48037600
H	0.93591200	3.81366000	3.05120600
H	4.92316300	2.29807000	3.61240000
H	3.04344700	3.74621300	4.38297000
C	1.01844100	2.73113500	-1.74081100
C	-0.32276200	2.87425900	-2.14487200
C	1.71341200	3.91237500	-1.41449100
C	-0.94245400	4.12526800	-2.20395900
H	-0.89436400	1.99591400	-2.42528500
C	1.10472500	5.16632900	-1.47985900
H	2.75126700	3.84528700	-1.10304800
C	-0.23091700	5.27873600	-1.87120000
H	-1.98162700	4.19517400	-2.51801000
H	1.67480700	6.05602100	-1.22052800
H	-0.71047900	6.25414200	-1.91929900

S29

C	-4.85147400	-1.38179500	-0.52287000
O	-4.23526200	-1.63447400	0.57078900
O	-4.16548800	-1.06908600	-1.54736400
O	-0.93651700	-0.70328200	-1.60319000
C	0.21871400	-0.16112100	-1.27648800
O	1.00828500	0.19101900	-2.13691800
H	-1.31531800	-1.77208600	0.85444500
C	0.51206000	-0.01797200	0.22108400
B	2.14418700	0.03609700	0.86979200
B	1.06702200	1.49872900	0.91820000
B	-0.65570500	0.94593500	1.15028700
B	1.10735900	-1.44363500	1.06298500
B	-0.56343300	-0.82979000	1.24319000
B	1.95987400	0.98541600	2.37296600
B	1.98672000	-0.78322800	2.45529200
B	0.27958100	1.52431200	2.53563500
B	-0.74638000	0.08673200	2.72323000
B	0.31298600	-1.34973200	2.67690900
H	2.85941900	1.65293900	2.77701300
B	0.85874700	0.13622700	3.47976300
H	2.91985100	-1.37448700	2.90045600
H	-0.01427600	2.56079400	3.04262600

H	-1.76640200	0.07880200	3.33750600
H	0.03038700	-2.36227400	3.23607700
H	0.99102800	0.19536300	4.66336900
Pd	-2.39533000	-1.17454900	-0.32835800
C	-6.35337800	-1.41831200	-0.57484400
H	-6.74315100	-2.09808600	0.18677400
H	-6.73728600	-0.41127700	-0.37354000
H	-6.68855100	-1.72064300	-1.57028000
C	-1.87115800	1.74118500	0.49385500
C	-1.80883100	2.35918600	-0.77048100
C	-3.06651300	1.90322400	1.22364700
C	-2.88497600	3.08486100	-1.28425300
H	-0.90589200	2.28262400	-1.36666700
C	-4.14393700	2.63300800	0.71805400
H	-3.15209800	1.45010200	2.20660700
C	-4.05898500	3.22629200	-0.54309800
H	-2.79960000	3.54395600	-2.26629900
H	-5.04797500	2.74078100	1.31434800
H	-4.89579100	3.79622700	-0.94144600
C	1.39635300	2.83164400	0.10827100
C	2.10192700	2.86215900	-1.11088800
C	1.02105900	4.07606000	0.65397300
C	2.40975300	4.06714200	-1.74730900
H	2.39860600	1.93231400	-1.57790000
C	1.33031800	5.28304300	0.02553300
H	0.47482600	4.10079200	1.59133800
C	2.02853700	5.28485500	-1.18302700
H	2.95347000	4.04825900	-2.68951300
H	1.02126000	6.22182800	0.48111800
H	2.27057400	6.22306400	-1.67869300
C	3.49851700	-0.00533900	0.02997200
C	3.70889400	-0.82772300	-1.09296600
C	4.59241300	0.77318100	0.45613700
C	4.93899000	-0.86995000	-1.75186900
H	2.90044100	-1.44042800	-1.47105400
C	5.82628500	0.73544900	-0.19569600
H	4.47515300	1.42436400	1.31639600
C	6.00675400	-0.08927400	-1.30661500
H	5.05930700	-1.51751400	-2.61778300
H	6.64497000	1.35472600	0.16565400
H	6.96583500	-0.12197200	-1.81988800
C	1.43779300	-2.84141200	0.37146500
C	0.76772000	-3.36411600	-0.75155900
C	2.44292700	-3.64965800	0.93969900

C	1.08478200	-4.61939100	-1.27783800
H	-0.00876100	-2.78674100	-1.24080900
C	2.76103800	-4.90563800	0.42266900
H	2.98652300	-3.28512800	1.80527600
C	2.08213400	-5.39920100	-0.69279600
H	0.54637600	-4.98358700	-2.15024600
H	3.54426200	-5.49738200	0.89206400
H	2.32876500	-6.37714300	-1.10085500

S30

O	-0.26297000	-1.83777300	-2.02164100
C	-0.05251500	-0.61911500	-1.46870900
O	0.08149400	0.36240900	-2.17003000
H	-0.11022700	-3.16284900	0.14330300
C	-0.02778900	-0.64473900	0.03980300
B	0.91754200	0.54236200	0.91537300
B	-0.90310900	0.60975400	0.91851400
B	-1.51078500	-1.11550800	0.83490500
B	1.42429000	-1.21151400	0.84719900
B	-0.07463300	-2.18930800	0.81644700
B	0.00983500	0.75188600	2.43839600
B	1.41740200	-0.32827400	2.39191300
B	-1.45711800	-0.24640900	2.38689700
B	-0.95627900	-1.94672400	2.31792200
B	0.81989700	-2.00456100	2.32400900
H	0.02378600	1.79856600	3.00839400
B	-0.03574800	-0.79646300	3.30513000
H	2.44824400	-0.03493500	2.91528100
H	-2.46847600	0.08532100	2.92292400
H	-1.61237100	-2.82561900	2.78725700
H	1.42979700	-2.92379700	2.77680900
H	-0.04236200	-0.83871000	4.49797900
C	-2.81591000	-1.52366500	0.01595500
C	-3.27618800	-0.83054900	-1.12022300
C	-3.58068900	-2.63100900	0.43052800
C	-4.42787600	-1.22205300	-1.80658700
H	-2.73602800	0.04119300	-1.47624800
C	-4.73665900	-3.02613200	-0.24505600
H	-3.25976700	-3.19453400	1.30152000
C	-5.16703800	-2.32296200	-1.37175700
H	-4.75014600	-0.65781700	-2.67955100
H	-5.29996400	-3.88743900	0.10930200
H	-6.06722900	-2.62766400	-1.90196700
C	-1.73008800	1.81713600	0.27677700

C	-1.23810800	2.68467000	-0.71837800
C	-3.02108700	2.09642800	0.77128000
C	-1.99047600	3.76349000	-1.19011300
H	-0.25773600	2.51058000	-1.14058800
C	-3.77666700	3.17423100	0.30789400
H	-3.44301700	1.45432600	1.53736100
C	-3.26369600	4.01716900	-0.67932000
H	-1.57246700	4.40900500	-1.96010400
H	-4.76892500	3.35171000	0.71835400
H	-3.84863600	4.85887400	-1.04554100
C	1.82257300	1.69407600	0.27724900
C	2.58298300	1.55704100	-0.90009000
C	1.93480000	2.92472200	0.95505000
C	3.39805900	2.58588300	-1.37666400
H	2.54260200	0.63295500	-1.46319400
C	2.74882100	3.95805800	0.48799400
H	1.36777300	3.07623800	1.86775900
C	3.48666600	3.79475000	-0.68517500
H	3.96766300	2.43692500	-2.29179800
H	2.80294800	4.89277800	1.04282500
H	4.12187400	4.59728500	-1.05510200
C	2.73466700	-1.68638200	0.07535300
C	2.72330200	-2.66557300	-0.93637600
C	3.99333600	-1.17338500	0.44580100
C	3.89977000	-3.10070900	-1.55210900
H	1.77862100	-3.10180600	-1.24439200
C	5.17381800	-1.60778200	-0.15849300
H	4.04506900	-0.41764300	1.22351900
C	5.13299600	-2.57415300	-1.16564600
H	3.85093100	-3.85972500	-2.33081600
H	6.12676300	-1.18735700	0.15651000
H	6.05099400	-2.91413700	-1.64094500
H	-0.28638700	-1.67169200	-2.98292600

S32

C	4.59905000	-0.73743000	1.02328100
O	4.09984700	-1.38070300	0.10940500
O	4.79669300	0.57698800	0.87819500
O	0.78288900	-0.12879400	-2.14735300
C	-0.38256200	0.10453800	-1.60602900
O	-1.39230700	0.33870300	-2.26025600
C	-0.37668200	0.06248200	-0.06641700
B	-1.20960200	1.21703600	0.96433800
B	-1.65181900	-0.54184800	0.96325900

B	-0.14343800	-1.52179000	0.66522400
B	0.57980600	1.34151300	0.65691400
B	1.17881000	-0.33604800	0.49156600
B	-1.39295400	0.33584300	2.50080100
B	-0.04498800	1.46821600	2.30940100
B	-0.76377100	-1.30860600	2.31840500
B	0.98935000	-1.20493200	2.01215100
B	1.42811900	0.52284500	2.00543200
H	-2.31244200	0.58654000	3.21647400
B	0.21077100	-0.07863500	3.14840200
H	0.00672000	2.51457100	2.87774300
H	-1.25840800	-2.23163000	2.88744100
H	2.50689600	0.89701500	2.36483300
H	0.42519100	-0.12604600	4.32279700
Pd	2.43209800	-0.64934200	-1.07372800
C	4.98329400	-1.37383000	2.33314100
H	4.13907500	-1.24122600	3.02186400
H	5.13335900	-2.44386100	2.18498400
H	5.87911400	-0.92184900	2.77126300
H	5.01426300	0.99163000	1.72984700
C	-0.18538800	-2.93528200	-0.08311000
C	-0.09554200	-3.14162200	-1.47380900
C	-0.30014900	-4.09200700	0.71461200
C	-0.12717800	-4.42281300	-2.03150300
H	0.01258200	-2.29709300	-2.14339300
C	-0.32654300	-5.37478100	0.16550600
H	-0.37313400	-3.98401800	1.79210900
C	-0.24184200	-5.54899300	-1.21653700
H	-0.06056700	-4.53459500	-3.11196700
H	-0.41726500	-6.23858000	0.82157200
H	-0.26580000	-6.54646700	-1.65102400
H	1.75499600	-2.05799900	2.35063100
C	-3.07684800	-1.08640000	0.50235500
C	-4.12754700	-1.11169500	1.44072100
C	-3.35735900	-1.61284700	-0.77275400
C	-5.38639200	-1.62781000	1.12922400
H	-3.95438000	-0.71889600	2.43788700
C	-4.61461900	-2.13036800	-1.09232300
H	-2.59283200	-1.60169700	-1.53888900
C	-5.63774500	-2.14218200	-0.14356100
H	-6.17092000	-1.62616100	1.88380400
H	-4.79113300	-2.52583700	-2.09058900
H	-6.61747800	-2.54556400	-0.39268600
C	-2.21845700	2.35316500	0.48397200

C	-3.16134800	2.18439600	-0.54879900
C	-2.23227400	3.59119400	1.15732100
C	-4.06407400	3.19550300	-0.88693800
H	-3.17313200	1.25994200	-1.11079800
C	-3.13363600	4.60398600	0.82634100
H	-1.52227100	3.76558200	1.95959900
C	-4.05846900	4.41057500	-0.20105400
H	-4.77560600	3.02704200	-1.69289400
H	-3.10996200	5.54571600	1.37186900
H	-4.76338200	5.19718800	-0.46431400
C	1.18456400	2.56846200	-0.16038400
C	0.59499700	3.10221300	-1.32209200
C	2.34086600	3.21596300	0.31527500
C	1.14160200	4.20559000	-1.98045600
H	-0.30971100	2.65912100	-1.72327600
C	2.89069800	4.32310100	-0.33290900
H	2.81621600	2.84657800	1.21928900
C	2.29391800	4.82273500	-1.49168500
H	0.65695500	4.58558300	-2.87714000
H	3.78454800	4.79712100	0.06954200
H	2.71757500	5.68503800	-2.00280100

S33

O	-0.25208300	-0.48655400	-2.07745700
C	-1.36053000	-0.02038300	-1.56342200
O	-2.32950600	0.30107900	-2.23979200
C	-1.33407200	0.09395700	-0.03091400
B	-2.06281900	1.35374200	0.92807400
B	-2.66705100	-0.35454200	1.01910800
B	-1.24208700	-1.46269400	0.77814400
B	-0.26316500	1.31700800	0.63795900
B	0.17619400	-0.40639900	0.57029200
B	-2.33589900	0.56282900	2.50837700
B	-0.90024300	1.57285300	2.27633300
B	-1.83979400	-1.13537500	2.41099000
B	-0.08473400	-1.18185900	2.11969400
B	0.50494600	0.50292500	2.03604100
H	-3.24222900	0.90339000	3.20324000
B	-0.77325000	0.05583000	3.19144600
H	-0.80464900	2.64643300	2.78547000
H	-2.38134500	-2.00081900	3.02511000
H	0.61122900	-2.06615800	2.51327700
H	1.61344500	0.80812700	2.35552800
H	-0.57514900	0.04396700	4.36825000

Pd	1.38447700	-0.99894800	-0.96342100
I	3.66748600	-1.73658000	0.30710500
C	4.85870600	0.06524200	0.32154000
C	6.23867300	-0.05535700	0.46931700
C	4.22899700	1.29905400	0.19673800
C	7.01199400	1.10869500	0.49013400
H	6.70954000	-1.02851400	0.56529000
C	5.02040100	2.45216500	0.21693800
H	3.15294400	1.37896500	0.08707200
C	6.40529300	2.35979800	0.36275800
H	8.09018500	1.02948600	0.60418600
H	4.53173300	3.41667600	0.11669200
H	7.01217800	3.26118500	0.37781700
C	-1.37536900	-2.85210100	0.00917000
C	-2.21852300	-3.05153000	-1.10037200
C	-0.65330500	-3.97185200	0.46710000
C	-2.32317900	-4.29563000	-1.72578700
H	-2.80657600	-2.22687800	-1.48807700
C	-0.75736200	-5.22041500	-0.14909100
H	-0.00299500	-3.86386100	1.33043900
C	-1.59305300	-5.38795400	-1.25492800
H	-2.98350300	-4.40845700	-2.58283500
H	-0.18690600	-6.06274900	0.23834100
H	-1.67795500	-6.35843300	-1.73987300
C	-4.13304400	-0.76839200	0.55161800
C	-4.83279600	-0.13934500	-0.49665100
C	-4.81853300	-1.78135900	1.25199500
C	-6.14134800	-0.50284500	-0.82385800
H	-4.34053500	0.62833100	-1.07867700
C	-6.12692000	-2.14673400	0.93207200
H	-4.31712500	-2.29425200	2.06660800
C	-6.79808600	-1.50655500	-0.11100500
H	-6.64710500	0.00565200	-1.64225200
H	-6.61979600	-2.93478500	1.49850100
H	-7.81825300	-1.78804600	-0.36565300
C	-2.93961400	2.57501700	0.39908300
C	-2.88333600	3.09544600	-0.90775300
C	-3.78989200	3.23787700	1.30622100
C	-3.63503300	4.20992400	-1.28679900
H	-2.26224800	2.61365900	-1.65208600
C	-4.54367600	4.35241800	0.93525900
H	-3.86144800	2.87243800	2.32596900
C	-4.46991200	4.84671500	-0.36783200
H	-3.56516500	4.57899700	-2.30806800

H	-5.18984300	4.83327900	1.66734200
H	-5.05584300	5.71503500	-0.66315600
C	0.48960600	2.47424200	-0.17356600
C	1.03158900	3.54323600	0.57065300
C	0.68677900	2.52124100	-1.56870400
C	1.72059000	4.59727100	-0.03378700
H	0.90334200	3.55243200	1.64821400
C	1.37335000	3.57389800	-2.18089100
H	0.31118700	1.72333600	-2.19773200
C	1.89527500	4.61988200	-1.41927000
H	2.11015700	5.40677700	0.58092200
H	1.49596300	3.57162300	-3.26198600
H	2.42429900	5.44194600	-1.89715100

S35

O	0.42538800	-0.09345100	-1.76753500
C	-0.83682100	-0.01374600	-1.42526000
O	-1.72820700	0.10337200	-2.25520500
C	-1.08645800	-0.07750000	0.08635500
B	-2.34965400	0.71494900	0.99117100
B	-2.30556300	-1.09647600	0.85144500
B	-0.55691100	-1.60586300	0.79211400
B	-0.62882400	1.34355400	1.01523600
B	0.38151000	-0.11374200	0.92981900
B	-2.53006700	-0.31906000	2.43601600
B	-1.53022900	1.14297600	2.53286600
B	-1.45411500	-1.72000600	2.30984600
B	0.22188400	-1.12887100	2.34148500
B	0.18450600	0.66003300	2.47168400
H	-3.58861300	-0.39660600	2.97606800
B	-1.00567900	-0.34326900	3.34887400
H	-1.88837100	2.11734200	3.11614400
H	-1.72607700	-2.79172200	2.75079400
H	1.12382100	-1.76501700	2.77702000
H	1.05641100	1.27450100	3.00074500
H	-0.98062100	-0.43708200	4.53692300
Pd	1.93743800	-0.50075800	-0.44240000
I	4.11538300	-1.23847100	0.91552600
C	2.74563200	1.29133900	-0.82575800
C	3.13631000	2.19376700	0.15730500
C	2.91582700	1.54601300	-2.18351500
C	3.72262100	3.39772100	-0.24650000
H	2.99105100	1.97757500	1.20828400
C	3.52067100	2.74974500	-2.56558200

H	2.56460600	0.84689700	-2.93510300
C	3.92256500	3.67319500	-1.60047800
H	4.02314000	4.11795800	0.51000500
H	3.65698100	2.96309000	-3.62317400
H	4.38254100	4.61075100	-1.90251100
C	-0.03412900	-2.80626700	-0.12155900
C	1.04606500	-3.59967300	0.31759900
C	-0.63387600	-3.16460100	-1.34819800
C	1.50582500	-4.69178400	-0.42490200
H	1.52926700	-3.36672200	1.26015700
C	-0.17818100	-4.25184300	-2.09121400
H	-1.47331700	-2.59253400	-1.72726400
C	0.89552000	-5.02154700	-1.63343000
H	2.34365100	-5.27686600	-0.05365100
H	-0.66676100	-4.49999400	-3.03047700
H	1.24997800	-5.86969700	-2.21509200
C	-3.43460100	-1.93099500	0.10134300
C	-4.12299100	-1.48067000	-1.04203600
C	-3.82748800	-3.17871700	0.62694500
C	-5.14348500	-2.23503000	-1.62587900
H	-3.84712300	-0.53727100	-1.49364000
C	-4.84868900	-3.93490000	0.05044000
H	-3.32499100	-3.56530400	1.50766200
C	-5.51435200	-3.46554400	-1.08306600
H	-5.65022200	-1.85297800	-2.50957200
H	-5.12161400	-4.89304800	0.48821900
H	-6.31062700	-4.05193200	-1.53724400
C	-3.53887800	1.62803000	0.44924500
C	-3.67282800	2.11679800	-0.86397000
C	-4.52565400	2.02792400	1.37365200
C	-4.73093000	2.95151100	-1.23217600
H	-2.95441000	1.82498200	-1.61924300
C	-5.58554200	2.86026000	1.01269300
H	-4.46118500	1.68100100	2.40012500
C	-5.69437000	3.32940200	-0.29723700
H	-4.79824500	3.30572100	-2.25882800
H	-6.32594800	3.14228400	1.75869100
H	-6.51845800	3.97940500	-0.58440400
C	-0.29359000	2.78448000	0.43066900
C	-0.30836400	3.14760800	-0.92784100
C	0.00399800	3.80471000	1.35620700
C	-0.03803700	4.45447200	-1.33963100
H	-0.53090700	2.41139000	-1.69079500
C	0.27520800	5.11218700	0.95255100

H	0.01703500	3.56953100	2.41619600
C	0.25530600	5.44506000	-0.40263000
H	-0.05905000	4.69460700	-2.40021400
H	0.49749400	5.87124000	1.69990800
H	0.46366200	6.46338600	-0.72394400

S37

O	0.06390600	0.06951100	-1.51856800
C	0.01438100	0.01530100	-0.24643500
O	-1.18684300	-0.03152900	0.23317600
C	1.21490000	0.01533300	0.62691400
B	0.98155700	-0.23010500	2.37163200
B	1.75592000	-1.50630400	1.31611000
B	2.71722400	-0.66719400	-0.00793400
B	1.44885700	1.39701900	1.67779900
B	2.53140300	1.13491400	0.21469900
B	2.49171200	-1.03215100	2.86617900
B	2.29721100	0.71703100	3.09185900
B	3.52417200	-1.29102400	1.44796700
B	3.98111800	0.29468700	0.80130800
B	3.21594600	1.53452500	1.81387200
H	2.47877100	-1.79855300	3.77729300
B	3.85488800	0.05645500	2.55424100
H	2.13750000	1.19729300	4.17044300
H	4.24531400	-2.23362700	1.34726400
H	5.02229700	0.49117900	0.25792800
H	3.70706300	2.60498300	1.98997300
H	4.81897400	0.07106500	3.25601500
Pd	-2.02940400	0.01066800	-1.62387100
I	-4.64949800	-0.06413700	-1.77206100
C	2.53047600	2.18361900	-0.98947900
C	2.33746400	1.84699900	-2.34375600
C	2.81595100	3.53681800	-0.71390200
C	2.41784900	2.80346600	-3.35916900
H	2.12217400	0.82236400	-2.61589500
C	2.90260300	4.49726700	-1.72245400
H	2.97228000	3.84556800	0.31411700
C	2.70150500	4.13517200	-3.05519100
H	2.26303500	2.49960500	-4.39238900
H	3.12352000	5.53053800	-1.46298600
H	2.76574200	4.88036100	-3.84549000
C	2.92093600	-1.35280800	-1.43643900
C	4.13947700	-1.15082300	-2.11555800
C	1.99399600	-2.21223700	-2.05683100

C	4.41559700	-1.75967500	-3.34091400
H	4.88689100	-0.49850000	-1.67606200
C	2.25955200	-2.82251600	-3.28464000
H	1.04641300	-2.42381800	-1.57640300
C	3.47317500	-2.59934800	-3.93597300
H	5.36932300	-1.57341700	-3.83046700
H	1.51433900	-3.48043700	-3.72662700
H	3.68226400	-3.07516900	-4.89181100
C	1.05874000	-2.91321500	1.03630700
C	-0.33303300	-3.10812400	0.93595200
C	1.86684300	-4.06049400	0.90334000
C	-0.88462000	-4.37020800	0.69824000
H	-1.00797700	-2.26983900	1.06109500
C	1.32324400	-5.32522200	0.67657800
H	2.94476900	-3.95745200	0.97318600
C	-0.05910600	-5.48690500	0.56679500
H	-1.96485200	-4.47589200	0.62687700
H	1.98354500	-6.18451200	0.57930000
H	-0.48689900	-6.47049700	0.38476700
C	-0.40076700	-0.50855200	3.12564100
C	-1.52385600	0.34211900	3.08431300
C	-0.50005600	-1.63690000	3.96424800
C	-2.67712800	0.07830400	3.82767600
H	-1.50465600	1.22886900	2.46472700
C	-1.64646400	-1.90557000	4.71354400
H	0.33791400	-2.32240800	4.03075500
C	-2.74580400	-1.04735600	4.64806400
H	-3.52159500	0.76069500	3.76245000
H	-1.67969000	-2.79030200	5.34596000
H	-3.64274800	-1.25404600	5.22813300
C	0.47261400	2.65433600	1.72997400
C	-0.25469000	3.14146400	0.62755400
C	0.34078900	3.36814000	2.93774100
C	-1.08472000	4.26032300	0.72694700
H	-0.16005000	2.66121600	-0.34118400
C	-0.47864200	4.49258400	3.04443500
H	0.88716700	3.02894100	3.81228200
C	-1.20270600	4.94200700	1.93864300
H	-1.63103600	4.60205500	-0.14916900
H	-0.55424700	5.01470500	3.99598300
H	-1.84710800	5.81469100	2.01874100
S38			
O	0.86633300	0.00759600	-1.49198600

C	-0.38317300	0.00115600	-1.33590100
O	-1.24344300	-0.00481300	-2.23605000
C	-0.88399100	0.00055200	0.16850000
B	0.13242600	0.88646700	1.27189500
B	-2.60160600	0.00157200	0.68768700
B	0.13105500	-0.88657600	1.27139300
B	0.08313600	-0.00021700	2.81154700
B	-0.91929700	1.43614200	2.58213600
B	-1.54382700	1.45793400	0.89264200
C	1.44246200	1.70600900	0.83883200
B	-1.54620600	-1.45633100	0.89270000
B	-2.56491800	0.88933600	2.24010600
B	-2.56618500	-0.88605600	2.24020100
C	-3.97320700	0.00280900	-0.14880400
C	1.43959300	-1.70752800	0.83647900
B	-0.92119000	-1.43512800	2.58195200
H	1.02436700	-0.00113700	3.54746600
B	-1.57259700	0.00091900	3.40909800
H	-0.67270900	2.45843600	3.14593300
C	-1.84746100	2.82428600	0.12574800
C	2.61286400	1.67042700	1.66259400
C	1.44218000	2.68851200	-0.20215500
C	-1.85217100	-2.82318700	0.12741600
H	-3.51409900	1.53604200	2.55688700
H	-3.51636100	-1.53127200	2.55703700
C	-4.12499500	0.00256900	-1.54831900
C	-5.16912000	0.00438600	0.60372500
C	1.43694000	-2.68751500	-0.20657800
C	2.61051900	-1.67589800	1.65970700
H	-0.67574200	-2.45764400	3.14579400
H	-1.81390000	0.00106000	4.57810500
C	-2.04646900	2.93068900	-1.26558100
C	-1.97241400	4.01151400	0.87558800
C	3.67681200	2.59544000	1.49622300
H	2.59904600	1.06593800	2.56133200
C	2.48216800	3.58037100	-0.35500600
H	0.59098900	2.74796900	-0.86615100
C	-2.05219900	-2.93142400	-1.26362100
C	-1.97905200	-4.00904000	0.87916100
C	-5.38485700	0.00389100	-2.15434900
H	-3.23634900	0.00112100	-2.16375700
C	-6.42945200	0.00567400	0.00563300
H	-5.11517300	0.00459800	1.68689400
C	2.47480700	-3.58164700	-0.36146300

H	0.58537600	-2.74395400	-0.87043800
C	3.67223300	-2.60292200	1.49115300
H	2.59844100	-1.07306100	2.55961900
C	-2.33723700	4.15670300	-1.87042400
H	-1.96577600	2.04482000	-1.88583400
C	-2.26738100	5.23741300	0.27711900
H	-1.83989800	3.97275300	1.95250900
C	3.60953700	3.54427000	0.49958400
H	4.52775800	2.55115700	2.17092900
H	2.43279400	4.32733700	-1.14299100
C	-2.34571700	-4.15784000	-1.86634400
H	-1.96989100	-2.04654500	-1.88507000
C	-2.27674700	-5.23530800	0.28280700
H	-1.84598800	-3.96893500	1.95595000
C	-6.54717600	0.00546500	-1.38496600
H	-5.45068400	0.00364000	-3.24117800
H	-7.32022100	0.00685500	0.63158700
C	3.60236000	-3.54993100	0.49284500
H	2.42337700	-4.32697900	-1.15086900
H	4.52353700	-2.56185300	2.16562500
C	-2.44881800	5.31791600	-1.10477700
H	-2.48321700	4.19777600	-2.94804900
H	-2.35644100	6.13024900	0.89349600
H	4.41379100	4.26341300	0.36632800
C	-2.45914600	-5.31764100	-1.09884900
H	-2.49243900	-4.20029800	-2.94382200
H	-2.36722300	-6.12697000	0.90067400
H	-7.52766900	0.00650500	-1.85816100
H	4.40482600	-4.27079500	0.35810200
H	-2.67845600	6.27143100	-1.57669600
H	-2.69097800	-6.27145400	-1.56910900
Pd	2.92736800	-0.00012900	0.00523600
O	4.07859700	-1.09431000	-1.42534800
C	4.42586500	-0.00332600	-1.98845000
O	4.08947800	1.09073000	-1.42620000
C	5.16489900	-0.00836500	-3.29525400
H	4.43189900	-0.00992900	-4.11047900
H	5.78219300	0.88923700	-3.38580300
H	5.77948000	-0.90838700	-3.38049000
S40			
Pd	-0.15322100	-0.54476100	1.31099900
B	1.40363600	0.72992200	-1.42332700
B	1.24592400	-1.06681200	-1.48393600

B	0.45280200	-1.50621900	-3.03164600
B	-0.51052600	-1.43676200	-1.54961400
C	0.05181400	-0.07513700	-0.67006200
B	-0.25491500	1.45288900	-1.45387800
B	-0.99729700	0.97911500	-3.01883500
B	0.73197100	1.35383500	-2.95288200
B	-1.17209200	-0.79380100	-3.06626000
B	-1.45051000	0.10194600	-1.54306600
H	2.71520800	-0.28255000	-3.44228000
H	0.69190000	-2.55029700	-3.55787700
H	1.18294100	2.34416600	-3.43957000
H	0.19766800	0.02718500	-5.12951800
H	-1.77539500	1.71705800	-3.53999100
H	-2.09624700	-1.33220600	-3.59777300
B	0.15623200	-0.00959200	-3.93666000
C	2.61117400	1.44441400	-0.66512500
C	2.47242900	2.10464900	0.57084300
C	3.89109000	1.46444000	-1.25353400
C	3.55456100	2.73717700	1.18928200
H	1.50821000	2.13131400	1.06304800
C	4.97477600	2.09924000	-0.64428900
H	4.04101400	0.96882600	-2.20766000
C	4.81292000	2.73880100	0.58617000
H	3.40575100	3.23810800	2.14402600
H	5.94770200	2.09090300	-1.13228600
H	5.65514600	3.23407700	1.06576600
C	-0.56808600	2.84482000	-0.73686700
C	-1.51717400	3.00163700	0.28959000
C	0.08416300	4.01538000	-1.17288500
C	-1.80241300	4.25012400	0.84698400
H	-2.04911500	2.13674400	0.66541500
C	-0.19461100	5.26761100	-0.62348500
H	0.82755100	3.94304200	-1.96013400
C	-1.14373000	5.39281000	0.39252700
H	-2.54602700	4.32599800	1.63812300
H	0.33327100	6.14590100	-0.99029700
H	-1.36579000	6.36710700	0.82400400
C	-2.92959600	0.18444900	-0.93216100
C	-3.31337100	-0.19108600	0.36909200
C	-3.96615000	0.64006000	-1.77278400
C	-4.63517200	-0.10690400	0.81334800
H	-2.56552600	-0.56261900	1.06634300
C	-5.29125800	0.72497900	-1.34288800
H	-3.72597200	0.93742800	-2.78830300

C	-5.63601700	0.35345900	-0.04239300
H	-4.87798200	-0.40683000	1.83082100
H	-6.05561300	1.08564600	-2.02856600
H	-6.66735700	0.42054800	0.29791100
C	2.29891800	-2.01772200	-0.74625100
C	2.98446900	-1.65902700	0.43194600
C	2.60389000	-3.28051300	-1.29081600
C	3.90936500	-2.51363400	1.03732300
H	2.80265000	-0.68876800	0.88274400
C	3.53005100	-4.13937800	-0.69539400
H	2.10368400	-3.59551600	-2.20149000
C	4.18721600	-3.76144100	0.47683600
H	4.41761600	-2.19619300	1.94542100
H	3.73586200	-5.10708900	-1.14889200
H	4.90788600	-4.42853500	0.94538300
C	-1.10570500	-2.58661900	-0.63213700
C	-0.52345900	-2.84161100	0.63284000
C	-2.29606700	-3.27012500	-0.93435800
C	-1.12733400	-3.70007400	1.57111400
H	0.52173000	-2.55065700	0.81241500
C	-2.87527600	-4.15183700	-0.02396200
H	-2.78141600	-3.08526800	-1.88820200
C	-2.30438600	-4.35953500	1.24077600
H	-0.65582100	-3.85168800	2.53831300
H	-3.79445700	-4.66977200	-0.28972700
H	-2.77574800	-5.03538900	1.94998300
B	1.62897900	-0.17430000	-2.96244500
O	-0.32358000	-0.61814100	3.55075200
O	-0.00206200	1.26950000	2.45227100
C	-0.15925100	0.63769900	3.55373200
C	-0.14171000	1.42500200	4.84320900
H	0.83578800	1.90395600	4.96587300
H	-0.89290300	2.22029300	4.79842200
H	-0.34032700	0.76946700	5.69387100

S41

B	0.38429700	-1.42350200	-3.52811400
B	1.19444700	-0.92801700	-2.01611100
B	-0.55036700	-1.45511300	-2.02065200
B	-1.27997000	-0.81029600	-3.51366800
B	-1.55925000	0.06003200	-1.98694900
C	-0.01033500	0.01118700	-1.16942900
B	1.26966300	0.90128400	-2.01149800
B	0.49087400	1.44701000	-3.50933200

B	1.47586300	-0.02713600	-3.52314000
B	-1.21279700	0.96033700	-3.49245600
B	-0.44220700	1.51025700	-1.98939900
H	0.66996300	-2.45614900	-4.04703500
H	-2.18105600	-1.39278400	-4.02735700
H	2.54605800	-0.07423100	-4.04119800
H	-0.04448600	0.04730400	-5.63778500
H	0.86770200	2.45244000	-4.02206400
H	-2.05773100	1.63738100	-3.98693700
B	-0.03527400	0.03701200	-4.44713000
C	0.01796900	-0.01031300	0.32473800
O	-0.23966100	-1.06844500	0.99809100
C	2.33699700	-1.76927600	-1.29172800
C	2.92268000	-1.41512900	-0.06032300
C	2.84326100	-2.92202200	-1.92660200
C	3.93758200	-2.17064600	0.52035600
H	2.60346600	-0.51684300	0.45708200
C	3.86114000	-3.68739700	-1.36762600
H	2.42472300	-3.22751300	-2.87978500
C	4.41595000	-3.31932800	-0.13037000
H	4.36939100	-1.87100400	1.47032800
H	4.22914400	-4.57136000	-1.87957000
C	2.49471500	1.66751300	-1.32836000
C	2.36320400	2.68294500	-0.35982200
C	3.80447300	1.38362800	-1.76994400
C	3.46420900	3.37185200	0.14250500
H	1.38428400	2.94212000	0.01856900
C	4.91722700	2.06141500	-1.28339300
H	3.95760900	0.61302700	-2.51693500
C	4.75540200	3.06701400	-0.31654600
H	3.32790600	4.14951800	0.88787100
H	5.91139400	1.81687600	-1.64500200
C	-0.88057700	2.88054600	-1.29531300
C	-1.69208300	2.97823600	-0.14792700
C	-0.49976900	4.09528400	-1.90260700
C	-2.09383800	4.20467800	0.37301900
H	-2.02857200	2.08153900	0.35689500
C	-0.89161700	5.33197600	-1.40055200
H	0.12065600	4.07127500	-2.79164800
C	-1.69508300	5.39789500	-0.25069900
H	-2.71994300	4.24417400	1.25911900
H	-0.57903600	6.24843900	-1.89184700
C	-1.06626700	-2.82539400	-1.37483500
C	-0.33509500	-3.60781700	-0.45908000

C	-2.29857000	-3.35540300	-1.81014900
C	-0.79562900	-4.83962900	-0.00451000
H	0.61263000	-3.24989600	-0.08073000
C	-2.77882600	-4.58438700	-1.36842300
H	-2.89922400	-2.79357700	-2.51634700
C	-2.02638400	-5.34222000	-0.45739900
H	-0.20599000	-5.41697600	0.70110000
H	-3.73316800	-4.96108600	-1.72381700
C	-2.96596400	0.11612600	-1.23644700
C	-3.26706000	-0.59543700	-0.05713400
C	-4.00516100	0.89074300	-1.79259400
C	-4.52238600	-0.52984100	0.54327600
H	-2.51525700	-1.22499500	0.40312300
C	-5.26692500	0.96331000	-1.21253200
H	-3.81861300	1.45229800	-2.70147500
C	-5.53650200	0.25292700	-0.03075500
H	-4.72421800	-1.09078800	1.45081800
H	-6.04597000	1.56954300	-1.66475100
C	0.09167400	-0.07585300	5.22628100
O	0.36505600	0.98483100	4.56615500
O	-0.18905000	-1.12160000	4.54552400
Pd	0.06258800	-0.04475700	2.77930800
O	0.31027800	1.02483300	1.01677400
C	0.07068100	-0.08512100	6.72319200
H	-0.93768800	0.17308500	7.06792600
H	0.31804800	-1.08199900	7.09579300
H	0.76992400	0.65843700	7.11295900
C	-2.10565300	6.66613400	0.27578600
N	-2.43862200	7.69748400	0.70116600
C	-6.83226700	0.32341000	0.57822700
N	-7.88490100	0.38166200	1.07205500
C	-2.50738900	-6.61162200	0.00255200
N	-2.89861600	-7.64340100	0.37404400
C	5.46249400	-4.10336900	0.45655800
N	6.31240700	-4.74160600	0.93149400
C	5.89392700	3.77378200	0.19248600
N	6.81950200	4.34756400	0.60426100

S42

O	-0.85703900	0.00004000	-1.39275200
C	0.37338400	-0.00006400	-1.13035800
O	1.31243900	-0.00025700	-1.94750000
C	0.73821200	0.00001200	0.41074000
B	-0.37197400	-0.88763300	1.41647800

B	2.39815300	0.00030600	1.08107300
B	-0.37235900	0.88729900	1.41641400
B	-0.46183200	-0.00016800	2.95439300
B	0.55865500	-1.43672400	2.81801700
B	1.33133500	-1.45270300	1.19119100
C	-1.63004900	-1.71542700	0.86303600
B	1.33084800	1.45295900	1.19121700
B	2.22773700	-0.88664800	2.62497000
B	2.22740400	0.88721200	2.62491600
C	3.83706700	0.00062800	0.36964200
C	-1.63075300	1.71470100	0.86314900
B	0.55811200	1.43670500	2.81800200
H	-1.46588800	-0.00045000	3.59985600
B	1.13172500	0.00008900	3.70094300
H	0.26372200	-2.46110000	3.35122900
C	1.71607400	-2.81519000	0.45569700
C	-2.87449200	-1.67183000	1.56743000
C	-1.53747300	-2.68896000	-0.18062400
C	1.71493800	2.81558100	0.45564800
H	3.14626200	-1.53299300	3.01960800
H	3.14566300	1.53390800	3.01960400
C	4.11060200	0.00073300	-1.01224900
C	4.96029800	0.00083700	1.22847800
C	-1.53855700	2.68824600	-0.18057800
C	-2.87504500	1.67091800	1.56777900
H	0.26288400	2.46096300	3.35128200
H	1.26744900	0.00011700	4.88462400
C	2.01759500	-2.92552400	-0.91762800
C	1.81369700	-3.99266800	1.22637500
C	-3.92987200	-2.57402400	1.28847300
H	-2.94709700	-1.07766800	2.47010900
C	-2.56329600	-3.56440000	-0.45515900
H	-0.62725200	-2.75482500	-0.76007300
C	2.01637900	2.92594300	-0.91769700
C	1.81196600	3.99316800	1.22621600
C	5.41266000	0.00106000	-1.50817100
H	3.28067700	0.00054800	-1.70527200
C	6.26614600	0.00115800	0.75272500
H	4.81141100	0.00075100	2.30190000
C	-2.56458400	3.56348400	-0.45494500
H	-0.62846900	2.75422500	-0.76021600
C	-3.93063400	2.57291400	1.28900300
H	-2.94740200	1.07671300	2.47044500
C	2.37731200	-4.14220000	-1.49294700

H	1.96306100	-2.04718300	-1.55129800
C	2.17504600	-5.21463700	0.66949100
H	1.60479200	-3.94914100	2.29019200
C	-3.77849900	-3.51725600	0.28386300
H	-4.84448500	-2.53194900	1.87087400
H	-2.45337600	-4.30442000	-1.24130200
C	2.37543100	4.14275700	-1.49313400
H	1.96229200	2.04753200	-1.55130400
C	2.17265700	5.21528200	0.66921600
H	1.60309900	3.94961800	2.29004100
C	6.50740300	0.00128400	-0.63094800
H	5.58527100	0.00114300	-2.58060700
H	7.10249200	0.00131300	1.44555900
C	-3.77963500	3.51613800	0.28433500
H	-2.45496600	4.30349600	-1.24113600
H	-4.84512000	2.53069800	1.87159300
C	2.45704700	-5.30137900	-0.70429000
H	2.60240900	-4.19832100	-2.55383000
H	2.24085200	-6.10433900	1.28877600
C	2.45456600	5.30205200	-0.70457800
H	2.60046400	4.19891400	-2.55402900
H	2.23800800	6.10507000	1.28842500
Pd	-3.06156600	-0.00038300	-0.09899100
O	-4.03373800	1.08792600	-1.63275200
C	-4.32250300	-0.00068200	-2.23746400
O	-4.03288100	-1.08903600	-1.63260100
C	-4.93034000	-0.00109700	-3.60382400
H	-4.12289900	-0.00211100	-4.34559900
H	-5.53532000	-0.89991100	-3.74770800
H	-5.53418800	0.89829700	-3.74877500
C	7.84886900	0.00162900	-1.13471000
N	8.93991500	0.00190900	-1.54221800
C	2.81502900	6.55917400	-1.29097300
N	3.10126900	7.58341000	-1.76523600
C	-4.83820500	4.43673300	-0.00902700
N	-5.69673500	5.18606600	-0.24441400
C	-4.83685000	-4.43804500	-0.00968900
N	-5.69520400	-5.18752800	-0.24523700
C	2.81819600	-6.55835500	-1.29057300
N	3.10500600	-7.58247100	-1.76475100

S44

Pd	0.12706900	-0.59242300	-1.09823800
B	-1.38880800	0.76044700	1.62250100

B	-1.23218100	-1.02841900	1.73804000
B	-0.42472200	-1.42044900	3.29244400
B	0.52029300	-1.40054100	1.79770700
C	-0.05066400	-0.06787800	0.87333200
B	0.26562600	1.47945800	1.61014100
B	1.02560700	1.06179000	3.18139600
B	-0.70420600	1.43502400	3.12345400
B	1.19995600	-0.70826700	3.28471700
B	1.45792000	0.13370300	1.72855900
H	-2.68346200	-0.18434800	3.68239100
H	-0.65707300	-2.44795100	3.84997900
H	-1.15060100	2.44152500	3.57698200
H	-0.14533500	0.18014900	5.33447200
H	1.81058400	1.81616800	3.66439400
H	2.13072100	-1.23004400	3.81828400
B	-0.11787000	0.10486800	4.14523900
C	-2.60279900	1.45581300	0.85823300
C	-2.48396100	2.05521700	-0.41135000
C	-3.86609200	1.52627300	1.48010400
C	-3.56319800	2.67774700	-1.03404400
H	-1.53388100	2.04127700	-0.93062300
C	-4.95470700	2.14664300	0.87609300
H	-3.99951800	1.08281800	2.46113000
C	-4.81264600	2.72864800	-0.39492300
H	-3.44160500	3.13337000	-2.01235400
H	-5.91633800	2.18335900	1.37932100
C	0.56985000	2.84649900	0.84375900
C	1.50412600	2.96813800	-0.20181100
C	-0.07803300	4.03032300	1.25256400
C	1.78304800	4.19005500	-0.80688300
H	2.03035300	2.09271000	-0.55915800
C	0.18445000	5.26212700	0.66265100
H	-0.80599300	3.98579900	2.05518600
C	1.12378000	5.35304600	-0.37801600
H	2.51174200	4.25066300	-1.60975100
H	-0.33238000	6.15545800	1.00028200
C	2.93033900	0.19301300	1.10165700
C	3.30093600	-0.22415700	-0.19191800
C	3.97489800	0.66947000	1.92241600
C	4.61363900	-0.16512500	-0.65202300
H	2.54685000	-0.60887800	-0.87416200
C	5.29417400	0.73631300	1.48738800
H	3.74557500	0.99841600	2.92990600
C	5.62854300	0.31875200	0.18853000

H	4.85742200	-0.49489700	-1.65753800
H	6.07083200	1.11158900	2.14704400
C	-2.29945100	-1.99714500	1.04757100
C	-2.98215000	-1.68591600	-0.14647500
C	-2.62760700	-3.22270100	1.66177700
C	-3.92572300	-2.54385100	-0.70597400
H	-2.78333800	-0.74517400	-0.64918700
C	-3.56946500	-4.09320200	1.12217600
H	-2.13381000	-3.49891300	2.58748400
C	-4.22751000	-3.76134400	-0.07392200
H	-4.43574400	-2.27385500	-1.62572600
H	-3.79986200	-5.03112200	1.61859300
C	1.10468500	-2.58841200	0.92419000
C	0.53060000	-2.87701400	-0.33656100
C	2.27732400	-3.28574700	1.26609800
C	1.11677100	-3.77532800	-1.23903800
H	-0.50469000	-2.56360300	-0.54411100
C	2.85184300	-4.20801900	0.40022700
H	2.75365400	-3.08242500	2.22018300
C	2.28511800	-4.44990300	-0.86987800
H	0.65979900	-3.95822500	-2.20616400
H	3.75541200	-4.73874400	0.68508500
B	-1.60143200	-0.09184900	3.19293200
O	0.27665400	-0.72701500	-3.30893800
O	-0.01480800	1.18675400	-2.26036800
C	0.11993500	0.52913000	-3.35578400
C	0.06658800	1.27313900	-4.66381800
H	-0.97147600	1.55342800	-4.87719100
H	0.65153300	2.19484500	-4.59610500
H	0.43943500	0.64218600	-5.47328100
C	6.98497200	0.38212500	-0.26926000
N	8.08798200	0.43248300	-0.63857200
C	1.40579300	6.61590800	-0.99410300
N	1.63549100	7.64161400	-1.49524800
C	-5.92816800	3.36729000	-1.02868200
N	-6.83561100	3.88455800	-1.54334800
C	-5.19589700	-4.65415800	-0.63917400
N	-5.98119800	-5.38222400	-1.09587800
C	2.89652300	-5.39025500	-1.76315500
N	3.39492600	-6.15842200	-2.48116100

S45

O	2.13573400	1.11825800	0.00039100
C	2.71695200	-0.00469200	-0.02838200

O	2.15820700	-1.14026400	-0.06720400
Ag	-0.01034300	1.41107400	-0.02221800
O	-2.13572000	-1.11823700	0.00073000
C	-2.71695100	0.00470600	-0.02798300
O	-2.15821600	1.14028300	-0.06687200
Ag	0.01034800	-1.41113400	-0.02221400
C	-4.24757600	-0.01513700	0.01490200
B	-5.10389200	-1.38960100	-0.68217900
B	-5.15918000	0.26695800	-1.44997100
B	-5.01857600	-1.16850500	1.11679000
B	-6.56703400	-1.54534700	0.33066300
B	-6.64963900	-0.69853000	-1.22123600
C	-4.45571300	-2.62725700	-1.46203900
B	-5.13082500	1.52750800	-0.14184000
B	-6.66787300	1.04259800	-0.90013600
C	-4.50058000	0.51712000	-2.88313400
B	-5.01610800	0.63222200	1.43880100
B	-6.51116300	-0.32227400	1.61221300
C	-4.27636700	-2.17658500	2.11376600
H	-7.06691900	-2.61309700	0.50859900
B	-7.52747400	-0.06363500	0.18325600
H	-7.20437100	-1.17791200	-2.16195600
C	-3.35637800	-2.53828200	-2.33802300
C	-5.04990100	-3.89883600	-1.33580800
B	-6.57892700	1.27752500	0.85407700
C	-4.52318100	2.98770900	-0.39744400
H	-7.23614400	1.80380700	-1.62046500
C	-3.32340900	1.26222300	-3.09403300
C	-5.12955700	-0.00281300	-4.03206900
C	-4.22557100	1.21687700	2.69608200
H	-6.96486200	-0.51754100	2.69747500
C	-3.40046600	-3.20058200	1.70208700
C	-4.56259400	-2.11778300	3.49282900
H	-8.72030200	-0.08243800	0.24380300
C	-2.86821000	-3.64931300	-3.02930000
H	-2.86842500	-1.58417300	-2.49418800
C	-4.57079500	-5.01613000	-2.02321500
H	-5.90422900	-4.01737500	-0.67703800
H	-7.08056100	2.21736200	1.39102800
C	-3.61563200	3.63715800	0.46230100
C	-4.97353700	3.73357600	-1.50428600
C	-2.79639400	1.46117200	-4.37319500
H	-2.81111800	1.70382800	-2.24738300
C	-4.61478200	0.19871100	-5.31346100

H	-6.03867400	-0.58419800	-3.91622300
C	-2.94897500	0.78203300	3.10148900
C	-4.83327300	2.20802700	3.49179900
C	-2.83990600	-4.10297500	2.60962900
H	-3.15176200	-3.29699600	0.65402900
C	-4.00691000	-3.01443400	4.40764200
H	-5.23385600	-1.34875800	3.86010600
C	-3.47081000	-4.89918400	-2.87368300
H	-2.01801500	-3.53214100	-3.69836600
H	-5.05884200	-5.97989400	-1.88887400
C	-3.18264800	4.94431500	0.23119600
H	-3.23354400	3.11276000	1.32805400
C	-4.54450100	5.04084300	-1.74707100
H	-5.67438400	3.27993800	-2.19700900
C	-3.43895600	0.92975900	-5.49190600
H	-1.88327800	2.04098800	-4.49187900
H	-5.13140900	-0.22394700	-6.17337700
C	-2.30357600	1.32157000	4.21666400
H	-2.44847600	-0.00872800	2.55296400
C	-4.20045500	2.74786200	4.61299500
H	-5.81975400	2.56926800	3.21755200
C	-3.13734600	-4.01421000	3.97060700
H	-2.17199600	-4.88202400	2.24646100
H	-4.25241700	-2.92544400	5.46430900
H	-3.09090600	-5.76592900	-3.41099500
C	-3.64262900	5.65612100	-0.87905700
H	-2.48520200	5.40788000	0.92668200
H	-4.91544900	5.57452700	-2.62029600
H	-3.02967200	1.08421500	-6.48833700
C	-2.92570200	2.31194100	4.97882600
H	-1.31624500	0.95822400	4.49371100
H	-4.70390800	3.51575700	5.19763500
H	-2.69849100	-4.71465900	4.67864800
H	-3.30372700	6.67412600	-1.06213900
H	-2.42473700	2.73338100	5.84779800
C	4.24757800	0.01514700	0.01442900
B	5.10387800	1.38954800	-0.68278400
B	5.15915300	-0.26707300	-1.45043900
B	5.01859700	1.16860500	1.11620600
B	6.56703800	1.54538300	0.33001900
B	6.64961800	0.69843700	-1.22181000
C	4.45568900	2.62713100	-1.46275200
B	5.13082600	-1.52751500	-0.14220700
B	6.66786000	-1.04266400	-0.90056700

C	4.50052600	-0.51734100	-2.88357200
B	5.01613300	-0.63209900	1.43836000
B	6.51119000	0.32241600	1.61167300
C	4.27640200	2.17676900	2.11310400
H	7.06692200	2.61315000	0.50785600
B	7.52747800	0.06366000	0.18271900
H	7.20433100	1.17774000	-2.16258100
C	3.35626900	2.53809500	-2.33862300
C	5.04997100	3.89869200	-1.33676900
B	6.57894300	-1.27744700	0.85366600
C	4.52317800	-2.98773800	-0.39768100
H	7.23611900	-1.80393200	-1.62084300
C	3.32338200	-1.26250700	-3.09440200
C	5.12945700	0.00255200	-4.03255000
C	4.22561300	-1.21665600	2.69569800
H	6.96490400	0.51777300	2.69691300
C	3.40017500	3.20046200	1.70136500
C	4.56295500	2.11837700	3.49211700
H	8.72030700	0.08246900	0.24324300
C	2.86810600	3.64905400	-3.03001900
H	2.86824100	1.58399400	-2.49460400
C	4.57087000	5.01591400	-2.02429500
H	5.90437100	4.01727300	-0.67810000
H	7.08058800	-2.21723900	1.39068600
C	3.61566500	-3.63713000	0.46214500
C	4.97349300	-3.73368200	-1.50448800
C	2.79634800	-1.46155200	-4.37354200
H	2.81112800	-1.70408500	-2.24771700
C	4.61466200	-0.19906600	-5.31392000
H	6.03855100	0.58398200	-3.91675600
C	2.94892600	-0.78193600	3.10095100
C	4.83340500	-2.20759800	3.49160600
C	2.83962000	4.10296100	2.60880500
H	3.15119200	3.29654100	0.65334200
C	4.00728400	3.01514100	4.40682800
H	5.23447600	1.34960000	3.85943600
C	3.47079700	4.89891000	-2.87464300
H	2.01784200	3.53183600	-3.69898900
H	5.05899100	5.97966700	-1.89014500
C	3.18267900	-4.94430600	0.23115100
H	3.23360800	-3.11267500	1.32787600
C	4.54445300	-5.04096800	-1.74716400
H	5.67431000	-3.28009100	-2.19727200
C	3.43886300	-0.93017400	-5.49229700

H	1.88325400	-2.04141300	-4.49217300
H	5.13125200	0.22356400	-6.17387100
C	2.30353700	-1.32138500	4.21617500
H	2.44834200	0.00865400	2.55225700
C	4.20059800	-2.74733800	4.61285300
H	5.81995200	-2.56874500	3.21747300
C	3.13739700	4.01461200	3.96973700
H	2.17144600	4.88176200	2.24559200
H	4.25305600	2.92647800	5.46346100
H	3.09089600	5.76560000	-3.41204700
C	3.64261900	-5.65618900	-0.87907000
H	2.48526400	-5.40782500	0.92669800
H	4.91536900	-5.57471100	-2.62036500
H	3.02956400	-1.08470500	-6.48871100
C	2.92576200	-2.31153900	4.97853900
H	1.31613400	-0.95814000	4.49310000
H	4.70412500	-3.51506800	5.19764800
H	2.69854900	4.71514500	4.67770000
H	3.30371400	-6.67420900	-1.06206600
H	2.42480500	-2.73290900	5.84755000

S46

O	-0.58201900	-0.84368700	-1.81336100
C	0.18116900	0.08639700	-1.35920500
O	0.71012200	0.97783000	-2.02691200
C	0.42695300	0.08887000	0.18835500
B	-0.54679100	-1.00319100	1.21184900
B	2.02426800	0.39166900	0.85107500
B	-0.82667300	0.79407700	1.16346400
B	-0.78636400	-0.09656100	2.71414900
B	0.47996100	-1.33573500	2.61173100
B	1.22776100	-1.23970700	0.98253800
C	-1.65791500	-2.06845900	0.74018100
B	0.74931600	1.66258900	0.97118100
B	2.02623800	-0.49734800	2.40242400
B	1.72548500	1.24610200	2.39838200
C	3.40492800	0.53443000	0.05617700
C	-2.16257200	1.45822800	0.57306900
B	-0.01498900	1.48876300	2.58273500
H	-1.79162400	-0.26761000	3.33767700
B	0.79092500	0.18558700	3.47311800
H	0.38326700	-2.39396900	3.15522900
C	1.90491600	-2.50095200	0.26891900
C	-3.04494200	-1.81268400	0.92711200

C	-1.33614100	-3.33779700	0.21508300
C	0.81125800	3.09169500	0.25919800
H	3.05268100	-0.95843100	2.79519800
H	2.51930100	2.03719000	2.80418200
C	3.61262100	0.23655600	-1.30440800
C	4.54130400	0.93566000	0.78869400
C	-2.33316700	1.86908100	-0.77593900
C	-3.24720600	1.70847600	1.44093000
H	-0.48020900	2.44677100	3.11933000
H	0.92104600	0.22000700	4.65931800
C	1.87050900	-2.78565900	-1.11073700
C	2.61377500	-3.41159700	1.07948100
C	-4.03671400	-2.74503900	0.56186900
H	-3.35452000	-0.90633800	1.43709200
C	-2.31423900	-4.27437200	-0.12148100
H	-0.29644200	-3.59754500	0.06653700
C	1.75307900	3.43238500	-0.73102500
C	-0.04775100	4.12312700	0.68739900
C	4.87452800	0.33664400	-1.89572000
H	2.77549900	-0.05061700	-1.92632800
C	5.80475500	1.03968500	0.20513500
H	4.43275800	1.16971200	1.84302400
C	-3.54133300	2.43350900	-1.22722500
H	-1.48863800	1.84209600	-1.45979500
C	-4.43616900	2.29295000	1.00079500
H	-3.14551400	1.44280300	2.48908100
C	2.51288400	-3.90500700	-1.64699500
H	1.30427900	-2.14751800	-1.77892200
C	3.25465100	-4.53331900	0.55150900
H	2.66573300	-3.23352200	2.14901400
C	-3.67226100	-3.98213900	0.03104100
H	-5.08349000	-2.50546400	0.73768100
H	-2.00946400	-5.24154200	-0.51499100
C	1.83213300	4.72213500	-1.25799200
H	2.42805100	2.67454100	-1.10414500
C	0.01984600	5.41581400	0.16174600
H	-0.78342300	3.91522600	1.45779400
C	5.98021100	0.73843500	-1.14616400
H	4.98849200	0.09752100	-2.95129200
H	6.65246300	1.35551200	0.81057900
C	-4.59993600	2.64205500	-0.34192500
H	-3.62216700	2.74877700	-2.26515100
H	-5.24009500	2.47392500	1.71122100
C	3.21069800	-4.78616700	-0.82050300

H	2.46240700	-4.08594800	-2.71897100
H	3.79117500	-5.20862500	1.21540200
H	-4.43115800	-4.71205200	-0.24057400
C	0.96446400	5.72348400	-0.81712100
H	2.57596000	4.94225800	-2.02130400
H	-0.66601200	6.18056800	0.52216800
H	6.96301600	0.81598000	-1.60739800
H	-5.52720000	3.09257500	-0.68768300
H	3.71133600	-5.65746000	-1.23832100
H	1.02509800	6.72885400	-1.23027600
Ag	-2.74189600	-0.61426800	-1.27102000

S48

B	1.49111100	0.25176700	2.68455800
B	1.36552100	-0.68746900	1.16519100
B	1.07550200	1.08644900	1.16448700
B	0.22212800	1.49585300	2.68496600
B	-0.70079600	1.35901400	1.16529800
C	0.00000000	-0.00004900	0.35770000
B	-0.23211300	-1.51073900	1.16546800
B	-1.05814300	-1.07858100	2.68597100
B	0.69956200	-1.33959400	2.68535200
B	-1.35320400	0.67368100	2.68557100
B	-1.50877700	-0.24593200	1.16559900
H	2.55116300	0.44016300	3.19994800
H	0.37099900	2.56179800	3.20084400
H	1.20556600	-2.28993400	3.20103300
H	0.00133200	0.00118000	4.81022100
H	-1.80522500	-1.85338900	3.20234200
H	-2.32121200	1.14466700	3.20136700
B	0.00080100	0.00083600	3.61550500
C	2.63085700	-1.31153800	0.41288500
C	2.54170600	-2.05556900	-0.77923500
C	3.92266700	-1.14101200	0.94737100
C	3.67086300	-2.58097200	-1.41383700
H	1.56566800	-2.25506600	-1.21268800
C	5.05726100	-1.66535900	0.32542000
H	4.03848500	-0.57700500	1.86774300
C	4.93892300	-2.38599900	-0.86488200
H	3.55443700	-3.15591900	-2.33088400
H	6.03742100	-1.50514800	0.77062800
H	5.82112100	-2.79488400	-1.35347500
C	-0.43607900	-2.90658000	0.41320300
C	-1.17423600	-3.05228400	-0.77712500

C	0.12901300	-4.08162900	0.94545800
C	-1.32448000	-4.28867500	-1.41188200
H	-1.66884400	-2.18607100	-1.20773200
C	-0.01862200	-5.32259400	0.32343000
H	0.70422800	-4.01686700	1.86395100
C	-0.74385800	-5.43359200	-0.86470100
H	-1.91018100	-4.35646900	-2.32700300
H	0.43966700	-6.20468100	0.76670800
H	-0.85985300	-6.39903400	-1.35321800
C	-2.89981000	-0.48347600	0.41335200
C	-3.26227200	0.16633300	-0.78203200
C	-3.84772300	-1.37566700	0.95108100
C	-4.48430800	-0.07229400	-1.41719600
H	-2.58766500	0.89815200	-1.21759900
C	-5.07389500	-1.61779800	0.32903500
H	-3.61226700	-1.89679200	1.87391800
C	-5.39862500	-0.97031800	-0.86488600
H	-4.72566600	0.45798600	-2.33678700
H	-5.77500000	-2.31973600	0.77662000
H	-6.35253700	-1.15800200	-1.35374900
C	2.06076000	2.09638000	0.41142400
C	2.73702200	1.78491100	-0.78376600
C	2.30263500	3.37524800	0.94985500
C	3.58621800	2.69674700	-1.41725100
H	2.62145900	0.79715800	-1.22106700
C	3.15294400	4.29227100	0.32946000
H	1.80537900	3.65851400	1.87246900
C	3.79788600	3.96008900	-0.86364500
H	4.09406100	2.41042800	-2.33660400
H	3.30718000	5.27187700	0.77798500
H	4.46011000	4.67288600	-1.35104300
C	-1.35787800	2.60703000	0.41231000
C	-0.84758900	3.15860400	-0.77863300
C	-2.50631900	3.22477500	0.94416900
C	-1.45344900	4.24659600	-1.41360800
H	0.06101900	2.74881900	-1.21079400
C	-3.11765000	4.31444400	0.32152300
H	-2.93347000	2.83441100	1.86279900
C	-2.59662500	4.83088100	-0.86663800
H	-1.01991500	4.64539100	-2.32909800
H	-4.00736800	4.75782700	0.76470400
H	-3.07108100	5.67951500	-1.35541100
Ag	0.00193700	-0.00194900	-1.80396000

S49

O	2.12019100	-0.28037300	1.13096900
C	2.72140300	-0.00975000	0.05142500
O	2.18393000	0.26909900	-1.06045200
Ag	-0.03598700	-0.32795300	1.37985700
O	-2.11789200	0.24514700	-1.13794000
C	-2.71857000	0.00869000	-0.04992700
O	-2.18021500	-0.23036700	1.07042100
Ag	0.03868000	0.31691800	-1.37987500
C	-4.24892700	-0.00179400	-0.10127200
B	-5.07520900	1.13345400	-1.15777100
B	-5.15144200	1.29367600	0.65672000
B	-5.02105800	-0.62794900	-1.56957300
B	-6.55019000	0.26588400	-1.67363600
B	-6.62780200	1.43558900	-0.34878200
C	-4.39753300	2.28760700	-2.03056900
B	-5.15799200	-0.36504300	1.38524000
B	-6.68049500	0.54031600	1.17692800
C	-4.50354700	2.55044300	1.40102700
B	-5.05242400	-1.54391600	0.00613800
B	-6.53448500	-1.35590100	-0.96284200
C	-4.29761900	-1.22741000	-2.86493400
H	-7.02669600	0.47379100	-2.74495100
B	-7.53566800	-0.08406000	-0.24246200
H	-7.15654300	2.49359100	-0.48746000
C	-3.28239100	3.05132000	-1.63140200
C	-4.99967200	2.64792300	-3.25387500
B	-6.61660200	-1.18845700	0.79866100
C	-4.58454600	-0.66007700	2.85105500
H	-7.24874400	0.96712000	2.13166000
C	-3.38296800	2.48333200	2.25422700
C	-5.11581100	3.81362300	1.26187300
C	-4.30666200	-2.94866000	0.12794300
H	-6.99412000	-2.30150100	-1.52153500
C	-3.44504300	-0.48957900	-3.71141700
C	-4.60679600	-2.54005100	-3.27710500
H	-8.72594600	-0.11272100	-0.29384600
C	-2.79111400	4.10477200	-2.39823000
H	-2.78939500	2.83734700	-0.69104100
C	-4.52509700	3.69475500	-4.03710600
H	-5.86446700	2.09262400	-3.60026300
H	-7.13473000	-2.00360100	1.49558100
C	-3.68685000	-1.69946900	3.16820700
C	-5.07895900	0.09163100	3.93641200

C	-2.90046300	3.60236100	2.93036300
H	-2.88372000	1.53449700	2.40694800
C	-4.65255400	4.94106300	1.93057100
H	-5.98043900	3.91385600	0.61532400
C	-3.03246200	-3.22988600	-0.40479100
C	-4.97970300	-4.01815700	0.75424000
C	-2.94196400	-1.01546900	-4.89848100
H	-3.17490600	0.52278200	-3.44440500
C	-4.11174900	-3.08796200	-4.45659800
H	-5.26102800	-3.14894200	-2.66366000
C	-3.41083500	4.43750400	-3.61432500
H	-1.93872100	4.68313600	-2.05416700
H	-5.01283900	3.94500000	-4.97447600
C	-3.31283500	-1.98437000	4.47823800
H	-3.26909900	-2.30747400	2.37690900
C	-4.71614900	-0.17157800	5.25399000
H	-5.77211900	0.90334000	3.74739900
C	-3.53572900	4.84494800	2.77710900
H	-2.04160700	3.51676100	3.58967700
H	-5.14890000	5.89848300	1.80373700
C	-2.45263200	-4.49299800	-0.30900500
H	-2.48408700	-2.45772500	-0.93357200
C	-4.42059100	-5.28706100	0.85796000
H	-5.96622300	-3.84799900	1.17167700
C	-3.27487900	-2.32430800	-5.28549800
H	-2.30244800	-0.41315900	-5.53740200
H	-4.37242700	-4.10228300	-4.74327600
C	-3.82882900	-1.22092400	5.53948300
H	-2.63090100	-2.80350700	4.68769400
H	-5.11845000	0.42840000	6.06476500
C	-3.14402300	-5.53707300	0.32688300
H	-1.47384500	-4.68277000	-0.73986800
H	-4.96396700	-6.08969200	1.34744200
C	4.25178700	-0.03861500	0.09487200
B	5.07185700	0.55115700	1.53130500
B	5.15255100	1.45749100	-0.04947400
B	5.02353500	-1.22110800	1.16827800
B	6.54899800	-0.44901700	1.64175200
B	6.62573900	1.16800500	0.92800200
C	4.38669000	1.23019100	2.80509000
B	5.16460900	0.25517700	-1.40443800
B	6.68457000	0.99282500	-0.83228700
C	4.50439200	2.91005500	-0.20241400
B	5.06026700	-1.39227000	-0.64649600

B	6.53989900	-1.62468200	0.31696600
C	4.29951300	-2.31010700	2.09053400
H	7.02267300	-0.70748800	2.70340100
B	7.53848000	-0.16612700	0.19862800
H	7.15083300	2.07181100	1.49854500
C	3.25975500	2.07494100	2.75838600
C	4.98900400	1.05594500	4.06830200
B	6.62474200	-0.73566400	-1.21191700
C	4.59299800	0.59842700	-2.86013700
H	7.25426600	1.78024600	-1.51946700
C	3.39722700	3.20820600	-1.02244600
C	5.10418200	3.99676000	0.46776300
C	4.31782100	-2.61592900	-1.35025100
H	7.00192800	-2.71627200	0.42936400
C	3.44262100	-1.99787600	3.16576100
C	4.61352000	-3.67359400	1.91526300
H	8.72873300	-0.21142800	0.23717200
C	2.75817600	2.70727600	3.89315700
H	2.76478800	2.26302800	1.81336100
C	4.50491500	1.67640800	5.21518600
H	5.86207100	0.41822100	4.15349800
H	7.14714600	-1.18350500	-2.18409600
C	3.68597000	-0.20801500	-3.57675100
C	5.09556900	1.72814500	-3.53785600
C	2.91554600	4.50750400	-1.17090300
H	2.90899800	2.41113100	-1.56889800
C	4.64131800	5.30053800	0.33069700
H	5.95850400	3.81528600	1.11031100
C	3.03932400	-3.08986900	-0.99307100
C	4.99336900	-3.32460700	-2.36554400
C	2.94004000	-2.97463400	4.02132800
H	3.16881200	-0.96764400	3.34721900
C	4.11899100	-4.66719300	2.75464200
H	5.27110200	-3.96706400	1.10511400
C	3.37959400	2.51303600	5.13804800
H	1.89634100	3.36401800	3.81984500
H	4.99331100	1.52039100	6.17243300
C	3.31036700	0.07922300	-4.88589000
H	3.26189300	-1.08563900	-3.10696400
C	4.73105200	2.03821900	-4.84471800
H	5.79608300	2.38249900	-3.03180100
C	3.53801600	5.56972300	-0.49606200
H	2.06771400	4.70747400	-1.81961700
H	5.12781200	6.11533600	0.85846700

C	2.45915000	-4.19386800	-1.61388700
H	2.48695400	-2.60826900	-0.19319100
C	4.43396600	-4.43089300	-2.99554300
H	5.98213400	-2.99778300	-2.66888100
C	3.27751600	-4.32417500	3.82465700
H	2.29727400	-2.69776200	4.85210600
H	4.38345500	-5.70740700	2.59031600
C	3.83402200	1.20963100	-5.53662100
H	2.62071100	-0.57305000	-5.41389800
H	5.13891700	2.91723100	-5.33478600
C	3.15402600	-4.87684800	-2.62539500
H	1.47724300	-4.54348500	-1.30845400
H	4.97959600	-4.95506700	-3.77440300
C	3.07055600	6.91537500	-0.65564400
N	2.70650900	8.01372000	-0.78396600
C	3.47335800	1.50736400	-6.89143000
N	3.19374900	1.75079700	-7.99519000
C	2.58094100	-6.02349100	-3.26671600
N	2.13394900	-6.95998900	-3.79404900
C	2.78961100	-5.33579800	4.71535500
N	2.40743500	-6.15895600	5.44459700
C	2.88862600	3.16812500	6.31445000
N	2.50486500	3.69895600	7.27700500
C	-2.57124000	-6.84751100	0.42278600
N	-2.12435600	-7.91924600	0.50376300
C	-3.47090900	-1.51603500	6.89557400
N	-3.19320700	-1.75559200	8.00067800
C	-3.06751500	6.00081600	3.48383700
N	-2.70297600	6.94502800	4.05907400
C	-2.93017800	5.52885300	-4.40933100
N	-2.55476200	6.41720200	-5.06158300
C	-2.78669700	-2.86699500	-6.51916600
N	-2.40439800	-3.30664600	-7.52715200

S50

O	-0.42965200	-0.96686000	-1.53719100
C	0.14502900	0.09033400	-1.08401300
O	0.50769300	1.06704000	-1.74245900
C	0.35478800	0.12633300	0.46272800
B	-0.47095000	-1.11127100	1.43725800
B	1.86104700	0.65806200	1.17595800
B	-1.01911600	0.61881300	1.39929700
B	-0.89586100	-0.27939200	2.94277700
B	0.55022500	-1.30865600	2.86905800

B	1.32391000	-1.07438600	1.26936700
C	-1.38076900	-2.31515200	0.88909500
B	0.40813400	1.71559900	1.26828700
B	1.95555800	-0.23979600	2.71798300
B	1.39253700	1.43663200	2.72130400
C	3.21792000	1.02492500	0.41702700
C	-2.41363200	1.08679300	0.76643900
B	-0.36967000	1.40777700	2.85455100
H	-1.88394100	-0.61485100	3.52261800
B	0.59810300	0.22909800	3.75606600
H	0.60185000	-2.37801000	3.39349800
C	2.21233800	-2.20303100	0.56522200
C	-2.79966600	-2.23072800	0.89045600
C	-0.84123800	-3.54339400	0.45990500
C	0.27345700	3.14557600	0.56677100
H	3.02846700	-0.54078000	3.13807400
H	2.04436300	2.33431500	3.15366900
C	3.49396600	0.78642200	-0.94400300
C	4.25940700	1.59167000	1.18219500
C	-2.60113600	1.48258800	-0.58518900
C	-3.55047600	1.15339200	1.59957500
H	-0.99294200	2.27557000	3.38080900
H	0.68652900	0.26611700	4.94365400
C	2.24865500	-2.48624700	-0.81566300
C	3.04738800	-2.98538000	1.39165600
C	-3.61699100	-3.26885300	0.41855600
H	-3.28226900	-1.37055800	1.34161000
C	-1.63596300	-4.59421400	0.00960800
H	0.23141600	-3.68334700	0.47147100
C	1.15549600	3.62372100	-0.42237800
C	-0.72540500	4.03947600	1.00430200
C	4.72763200	1.09496500	-1.51124300
H	2.72599900	0.38097100	-1.58876700
C	5.49710000	1.90950100	0.63405200
H	4.09527600	1.78886200	2.23613000
C	-3.86268900	1.84292000	-1.08162200
H	-1.74123600	1.60556600	-1.23929200
C	-4.80445000	1.53072100	1.12674000
H	-3.44397900	0.89858900	2.64937500
C	3.07070900	-3.47909300	-1.34298000
H	1.59680300	-1.95104600	-1.49524100
C	3.87159400	-3.98432500	0.88457600
H	3.05157300	-2.80452600	2.46114400
C	-3.03372300	-4.46210000	-0.04090800

H	-4.69851100	-3.17194400	0.45240600
H	-1.17599700	-5.52242000	-0.31569100
C	1.05516200	4.91057500	-0.94084800
H	1.92846600	2.97426600	-0.80766500
C	-0.84822400	5.32913800	0.49545000
H	-1.42398700	3.72360700	1.77151300
C	5.74439500	1.66157300	-0.72619100
H	4.90771900	0.90080100	-2.56431500
H	6.27568600	2.34797500	1.25116100
C	-4.98014900	1.85656800	-0.22871200
H	-3.96840200	2.15767400	-2.11582200
H	-5.65559500	1.56828300	1.80004800
C	3.89265100	-4.24025100	-0.49651000
H	3.07508000	-3.67294700	-2.41151400
H	4.50095000	-4.56823400	1.54952500
C	0.04781900	5.77868100	-0.48691800
H	1.75233600	5.24866200	-1.70155800
H	-1.63032500	5.99128600	0.85511600
Ag	-2.65013300	-0.99672900	-1.35044600
C	-6.27415200	2.21405400	-0.73003900
N	-7.32797400	2.49429900	-1.13697700
C	-0.06619200	7.10490300	-1.01790100
N	-0.16263000	8.18308700	-1.44730200
C	7.01541800	1.98563900	-1.30326000
N	8.04864600	2.25154200	-1.76990600
C	4.73090600	-5.27241700	-1.03103700
N	5.40702500	-6.11622100	-1.46307900
C	-3.85704800	-5.52972100	-0.52605900
N	-4.53114700	-6.39197100	-0.92225200

S52

B	1.40495300	0.55225900	2.95821200
B	1.47460200	-0.39176000	1.43711800
B	0.82707100	1.27997200	1.43744500
B	-0.09358300	1.50576100	2.95787500
B	-0.96287600	1.18094300	1.43627500
C	0.00059700	-0.00114200	0.61973400
B	0.08498300	-1.52434100	1.43579800
B	-0.81165900	-1.27719800	2.95601500
B	0.96120600	-1.16750400	2.95725100
B	-1.46361500	0.37526600	2.95632500
B	-1.42179100	-0.55235000	1.43514200
H	2.40364700	0.95622800	3.46893000
H	-0.16946900	2.58050400	3.46827200

H	1.65441700	-1.99231200	3.46740600
H	-0.00187300	-0.00329900	5.08096300
H	-1.38209300	-2.19188700	3.46501100
H	-2.50973500	0.63521200	3.46554500
B	-0.00121100	-0.00273600	3.88867000
C	2.84304300	-0.74657300	0.69273800
C	2.91329000	-1.48741300	-0.50374600
C	4.07032900	-0.32812000	1.24531800
C	4.12264900	-1.78099800	-1.12898900
H	2.00095000	-1.86982100	-0.95190800
C	5.29109700	-0.61166100	0.64144800
H	4.06485700	0.23994300	2.16962900
C	5.32851400	-1.34014100	-0.55980100
H	4.14229900	-2.36041200	-2.04748200
H	6.21916700	-0.26956800	1.08965800
C	0.16966100	-2.93505000	0.69054100
C	-0.51346100	-3.22980600	-0.50601700
C	0.94541500	-3.97413800	1.24305800
C	-0.42122200	-4.47098700	-1.13100100
H	-1.15793800	-2.47941500	-0.95417200
C	1.05089400	-5.22302500	0.63936100
H	1.48412200	-3.79465900	2.16755900
C	0.36890200	-5.48287000	-0.56167100
H	-0.96675000	-4.66796400	-2.04933400
H	1.66164600	-6.00092900	1.08778400
C	-2.73778300	-1.06789700	0.69017100
C	-3.22866700	-0.50919700	-0.50643200
C	-3.48774400	-2.12520300	1.24367800
C	-4.38168000	-0.97882700	-1.13063800
H	-2.71253100	0.33442300	-0.95509200
C	-4.64405000	-2.60978900	0.64084900
H	-3.15095300	-2.58178100	2.16843200
C	-5.10149600	-2.04136200	-0.56029400
H	-4.73715900	-0.52088700	-2.04914600
H	-5.19643700	-3.42973600	1.09007100
C	1.58819000	2.47141900	0.69348600
C	2.31535500	2.30838900	-0.50235200
C	1.56908100	3.76830800	1.24516700
C	2.96898400	3.36735100	-1.12768800
H	2.39748400	1.32220600	-0.94970800
C	2.21673200	4.84122300	0.64119600
H	1.02642400	3.93927100	2.16896100
C	2.92210200	4.65078900	-0.55933100
H	3.52678900	3.20634400	-2.04565600

H	2.17802700	5.82985800	1.08878800
C	-1.86009300	2.27339800	0.69198300
C	-1.47955300	2.91528400	-0.50320800
C	-3.09903200	2.65687100	1.24393200
C	-2.28391500	3.86517300	-1.12803100
H	-0.51605300	2.68858900	-0.95012500
C	-3.91852800	3.60532900	0.64046200
H	-3.42943900	2.19404800	2.16787800
C	-3.51888800	4.21766700	-0.55969700
H	-1.95783200	4.34646700	-2.04550600
H	-4.87042000	3.87473300	1.08830700
Ag	0.00057700	-0.00002800	-1.54438700
C	-6.28924300	-2.53475800	-1.19229700
N	-7.25348100	-2.93613800	-1.70690700
C	-4.35661000	5.19301400	-1.19258600
N	-5.03765700	5.98422300	-1.70819400
C	3.58914500	5.74942200	-1.19311000
N	4.13015300	6.64185200	-1.70941000
C	6.57976200	-1.63425800	-1.19343200
N	7.59591400	-1.87243500	-1.70956700
C	0.47310300	-6.76434500	-1.19459600
N	0.55822600	-7.80490800	-1.71002700

table4-entry1-pre

B	-0.65951100	-1.33853200	2.37961200
B	-1.34816100	-0.70699300	0.84870000
B	0.26499800	-1.52589400	0.87057300
B	1.08235300	-1.02143400	2.37586200
B	1.50258300	-0.21916200	0.83427100
C	-0.01347300	-0.00363600	-0.00445300
B	-1.11623200	1.08878800	0.84650500
B	-0.26910500	1.50387100	2.35529500
B	-1.49058100	0.22262200	2.36809100
B	1.31987300	0.72919000	2.34720500
B	0.65836000	1.38540100	0.82724400
H	-1.12441800	-2.30559200	2.90782900
H	1.86846100	-1.74609000	2.90887300
H	-2.55526100	0.35837800	2.89292700
H	0.00597000	0.04034600	4.49968300
H	-0.46723400	2.56687700	2.86505300
H	2.26801000	1.25477500	2.85124000
B	0.00040400	0.02848800	3.30182200
C	-0.06893900	-0.04421600	-1.59429100
O	0.16819900	-1.15515900	-2.11487000

C	-2.63470200	-1.33006700	0.13412900
C	-3.09098800	-0.92676400	-1.13710500
C	-3.40518800	-2.30049600	0.80393100
C	-4.24279500	-1.47449600	-1.70730100
H	-2.54309600	-0.16945700	-1.68815600
C	-4.56011100	-2.84891100	0.24189700
H	-3.08570500	-2.63366900	1.78738300
C	-4.98546900	-2.43935300	-1.02344100
H	-4.56095500	-1.13870700	-2.69298500
H	-5.12529000	-3.60008200	0.79316100
H	-5.88397900	-2.86476700	-1.46961600
C	-2.20084200	2.08551100	0.21085400
C	-1.89683900	3.08192300	-0.73845000
C	-3.52911600	2.05879400	0.68067000
C	-2.85391600	4.00153700	-1.17284800
H	-0.90394200	3.11350900	-1.16396400
C	-4.49555400	2.97012400	0.24625600
H	-3.81548500	1.30374800	1.40541300
C	-4.16129800	3.95511900	-0.68333700
H	-2.57327300	4.75601600	-1.90686900
H	-5.51118600	2.90470100	0.63592000
H	-4.90839700	4.67115200	-1.02589700
C	1.37527300	2.65578700	0.16552700
C	1.94778300	2.67771400	-1.12159200
C	1.53008600	3.82457600	0.93804000
C	2.62628900	3.79896900	-1.60524400
H	1.83524300	1.81694400	-1.76722000
C	2.20499700	4.95093600	0.46152800
H	1.11038300	3.84935000	1.93925800
C	2.76060100	4.94498800	-0.81883300
H	3.05168500	3.77268400	-2.60746000
H	2.29551500	5.83350800	1.09451900
H	3.28931900	5.81919000	-1.19809400
C	0.53385000	-2.98537100	0.25979400
C	-0.30240400	-3.61879000	-0.68118200
C	1.61418700	-3.74891100	0.74195000
C	-0.08560800	-4.93395100	-1.09407700
H	-1.12068100	-3.06299800	-1.11690300
C	1.84658500	-5.06418500	0.32739700
H	2.29497200	-3.30269700	1.45962600
C	0.99129400	-5.66986800	-0.59227500
H	-0.75975800	-5.38213400	-1.82307600
H	2.70123200	-5.61092500	0.72538400
H	1.16346000	-6.69531200	-0.91938600

C	2.92326900	-0.41300700	0.12199700
C	3.09593100	-1.05644400	-1.12063200
C	4.09331500	0.03011000	0.77128700
C	4.36476600	-1.23669000	-1.67896200
H	2.21826500	-1.40701900	-1.65567400
C	5.36342900	-0.15122200	0.21994700
H	4.00398800	0.53071500	1.73076100
C	5.50743700	-0.78778100	-1.01446500
H	4.45597500	-1.73675100	-2.64239300
H	6.24105600	0.21002800	0.75575300
H	6.49575000	-0.93045900	-1.45137500
O	-0.36778100	1.03533800	-2.15011900

table4-entry1-ts

O	0.84411300	-1.05906500	-2.79886800
C	0.10421200	-0.14680200	-2.71409400
O	-0.61642200	0.74603200	-2.98519500
C	-0.00743600	-0.00145800	0.12296700
B	1.13015300	-0.99994100	1.00060900
B	-0.34248200	1.46838800	0.99368400
B	-0.60250800	-1.37621400	0.98896300
B	0.32390800	-1.47247500	2.52857700
B	1.48567500	-0.13081900	2.53645800
B	1.28100100	0.76373700	0.99607700
C	2.24854100	-1.95520100	0.34530500
B	-1.51101300	0.14198000	0.99352900
B	0.57450700	1.38729900	2.53027700
B	-1.15199000	0.98942800	2.52837400
C	-0.63382800	2.88404200	0.29740600
C	-1.22448300	-2.67039800	0.27517600
B	-1.30482100	-0.77604100	2.52563300
H	0.57055700	-2.52540500	3.04614700
B	-0.01749600	-0.00072500	3.46696800
H	2.55740100	-0.21441200	3.06547600
C	2.51330800	1.49174700	0.27241800
C	1.97535700	-2.91654500	-0.64697700
C	3.58172100	-1.90631200	0.80337700
C	-2.94883400	0.28352500	0.29509500
H	0.98861400	2.38655500	3.04749700
H	-1.97705600	1.68954700	3.04388600
C	-0.09797200	3.25175300	-0.95109900
C	-1.42098800	3.85664700	0.94587100
C	-1.82714400	-2.62096800	-0.99626300
C	-1.22995100	-3.92382600	0.91840000

H	-2.22591800	-1.34495300	3.04009700
H	-0.01975100	-0.00201900	4.66728500
C	3.01397300	1.07730400	-0.97727700
C	3.17310300	2.57937400	0.87760400
C	2.95993400	-3.77472700	-1.14450500
H	0.97211900	-2.99397000	-1.04565000
C	4.57494400	-2.75778600	0.31434300
H	3.84429500	-1.17892300	1.56518900
C	-3.14266500	0.94178600	-0.93457500
C	-4.10732300	-0.22059300	0.91976800
C	-0.33399100	4.50532900	-1.52117800
H	0.51446100	2.53778900	-1.48819400
C	-1.66355700	5.11367400	0.38725200
H	-1.85368100	3.61586000	1.91272000
C	-2.39012700	-3.74996200	-1.59638700
H	-1.86557600	-1.67023300	-1.51796200
C	-1.78966400	-5.06007800	0.32943100
H	-0.77799800	-4.00450200	1.90325100
C	4.09689100	1.71303200	-1.59067600
H	2.55122000	0.23068300	-1.47247500
C	4.25771100	3.22150100	0.27526700
H	2.81902700	2.93064300	1.84276800
C	4.26942900	-3.70414300	-0.66604600
H	2.69751100	-4.50195700	-1.91234200
H	5.59150900	-2.67769300	0.69954400
C	-4.40940900	1.08340900	-1.50830000
H	-2.28373100	1.34890100	-1.45315400
C	-5.37823100	-0.08365000	0.35668800
H	-4.00448000	-0.73489000	1.87094600
C	-1.11984400	5.44807700	-0.85511100
H	0.10187900	4.74516300	-2.49050200
H	-2.28182300	5.83327900	0.92424900
C	-2.37327700	-4.98136000	-0.93732100
H	-2.84855700	-3.66449200	-2.58104000
H	-1.76715600	-6.01132600	0.86130200
C	4.72741300	2.79269600	-0.96832400
H	4.45237300	1.35676200	-2.55709200
H	4.73453900	4.06308500	0.77793400
C	-5.53887800	0.57131300	-0.86652200
H	-4.51092200	1.60083900	-2.46185100
H	-6.24556500	-0.49316000	0.87490100
H	5.57217200	3.29083600	-1.44368300
H	-1.30584100	6.42698300	-1.29674600
H	-6.52789200	0.68063200	-1.31145500

H	-2.81071600	-5.86462500	-1.40207700
H	5.03918900	-4.37221200	-1.05249900

table4-entry1-post

B	-1.48092700	0.29951600	2.40326600
B	-1.01199300	1.10166100	0.86667600
B	-1.36057300	-0.62221700	0.86662200
B	-0.74264500	-1.31620400	2.40305900
B	0.17123800	-1.48636800	0.86647100
C	0.00004500	-0.00011200	0.01543200
B	0.73516600	1.30282200	0.86664300
B	1.37450200	0.62788600	2.40309000
B	-0.17253500	1.50098700	2.40322100
B	1.02217600	-1.11325000	2.40299900
B	1.46643500	-0.29658400	0.86644700
H	-2.54758000	0.51531100	2.90946400
H	-1.27752000	-2.26406300	2.90901500
H	-0.29686600	2.58219600	2.90924500
H	0.00023600	-0.00042000	4.54289100
H	2.36442000	1.08028300	2.90900700
H	1.75838500	-1.91487600	2.90890300
B	0.00016500	-0.00029600	3.34181800
C	-1.96670300	2.14168200	0.11647300
C	-2.03643600	2.21955800	-1.28639100
C	-2.78589400	3.03272200	0.83553700
C	-2.87175700	3.13011700	-1.93755100
H	-1.41370900	1.54214900	-1.86403000
C	-3.62579100	3.94820400	0.19670600
H	-2.75935200	3.00234700	1.92208500
C	-3.67429300	4.00304300	-1.19875800
H	-2.89662700	3.15888700	-3.02694100
H	-4.24486800	4.62148500	0.79016500
C	1.42923800	2.53222200	0.11648800
C	1.48094900	2.62308500	-1.28634100
C	2.02404000	3.58633100	0.83560400
C	2.08867000	3.69899400	-1.93748300
H	1.02859500	1.82173100	-1.86384000
C	2.63500400	4.66814100	0.19681700
H	2.00397200	3.55127200	1.92214800
C	2.67141900	4.73166700	-1.19865200
H	2.10771700	3.73192500	-3.02687300
H	3.08447300	5.46470400	0.79029700
C	2.85028600	-0.57685300	0.11633500
C	2.95300400	-0.59792200	-1.28650900

C	4.03652900	-0.81667500	0.83560900
C	4.16417200	-0.84344900	-1.93742500
H	2.05135500	-0.41520700	-1.86438100
C	5.25428000	-1.06353100	0.19705300
H	3.99686200	-0.80822800	1.92214100
C	5.32623000	-1.07862000	-1.19838800
H	4.20158900	-0.85137200	-3.02680900
H	6.15064800	-1.24479500	0.79070300
C	-2.64488300	-1.20850600	0.11644500
C	-2.74052800	-1.25093900	-1.28639400
C	-3.74555900	-1.71191100	0.83555600
C	-3.86483100	-1.76370500	-1.93748900
H	-1.90373000	-0.86832900	-1.86403100
C	-4.87597200	-2.22749100	0.19682500
H	-3.70844800	-1.69598200	1.92208900
C	-4.94316700	-2.25681100	-1.19863300
H	-3.89990000	-1.77857400	-3.02687900
H	-5.70769800	-2.60789700	0.79035500
C	0.33221800	-2.88892800	0.11612500
C	0.34399200	-2.99274200	-1.28675100
C	0.47002500	-4.09147100	0.83509900
C	0.48436600	-4.22037500	-1.93798100
H	0.23948500	-2.07855000	-1.86435300
C	0.61124000	-5.32576700	0.19621700
H	0.46555800	-4.05143500	1.92163600
C	0.61927900	-5.39847000	-1.19924500
H	0.48844800	-4.25812500	-3.02737500
H	0.71538000	-6.23449100	0.78962000
H	0.72900700	-6.35876000	-1.70295900
H	-5.82264800	-2.65782700	-1.70224400
H	-4.32763700	4.71535500	-1.70242300
H	3.14676800	5.57327500	-1.70230200
H	6.27362700	-1.27069200	-1.70184800

table4-entry2-pre

B	0.64166100	1.34745800	2.64212300
B	1.34032900	0.73099000	1.10927000
B	-0.28676300	1.51186600	1.13371400
B	-1.09264200	0.99042600	2.64031700
B	-1.49452400	0.18369300	1.09735500
C	0.02242600	0.00453900	0.25601800
B	1.14719900	-1.06359500	1.10160000
B	0.31521100	-1.50410200	2.61055900
B	1.50769300	-0.19544100	2.62599200

B	-1.28964500	-0.76423900	2.60771600
B	-0.61658900	-1.39659600	1.08333100
H	1.08490000	2.32455900	3.16606200
H	-1.89481200	1.69582800	3.17126400
H	2.57644700	-0.30825300	3.14371400
H	0.01124900	-0.05185600	4.75721400
H	0.53622800	-2.56654700	3.10800000
H	-2.22521000	-1.31341900	3.10565400
B	0.01467400	-0.03677000	3.56252500
C	0.08051500	0.05714000	-1.33094000
O	-0.22104900	1.15458800	-1.84338800
C	2.60868700	1.38218100	0.39139100
C	3.06799700	0.99613400	-0.88570400
C	3.36033300	2.36310500	1.07051300
C	4.20341800	1.56402900	-1.45670800
H	2.53360700	0.23463900	-1.44416100
C	4.49913800	2.93885800	0.51831400
H	3.03803000	2.68153300	2.05693200
C	4.93267100	2.54333000	-0.75949200
H	4.53337000	1.24956500	-2.44254700
H	5.05681500	3.69452400	1.06473200
C	2.25083500	-2.03360000	0.46079600
C	1.96810300	-3.03534600	-0.49076200
C	3.57866200	-1.97472800	0.93277500
C	2.93633400	-3.93410900	-0.92597700
H	0.97813200	-3.09025600	-0.91887300
C	4.56559000	-2.85738900	0.50467400
H	3.84761300	-1.21713200	1.66026100
C	4.25012500	-3.85727700	-0.42986100
H	2.68317100	-4.69720400	-1.65659400
H	5.57885300	-2.77934400	0.88909900
C	-1.31265100	-2.67701400	0.42289300
C	-1.79650700	-2.75070300	-0.89978500
C	-1.53688800	-3.80547200	1.24042500
C	-2.45943000	-3.87738000	-1.37829600
H	-1.61618200	-1.92895800	-1.58023100
C	-2.19350400	-4.94150100	0.78058900
H	-1.18532600	-3.78891100	2.26681300
C	-2.66640700	-4.98839600	-0.54220400
H	-2.81819800	-3.90368700	-2.40327600
H	-2.34523600	-5.79445100	1.43647000
C	-0.58493200	2.96192700	0.51912000
C	0.22820900	3.60439300	-0.43751500
C	-1.67227200	3.70759800	1.01744400

C	-0.00801500	4.90982400	-0.85151200
H	1.04661700	3.06123100	-0.88716000
C	-1.93531500	5.01252700	0.60981100
H	-2.33285000	3.25445300	1.74822900
C	-1.09581300	5.63354300	-0.32865800
H	0.64108700	5.37521400	-1.58785000
H	-2.78591800	5.55467100	1.01380100
C	-2.91952000	0.34585000	0.38895100
C	-3.11196300	0.97681200	-0.85815500
C	-4.07525600	-0.11556100	1.05423100
C	-4.38113500	1.13368400	-1.40976200
H	-2.24549900	1.33875100	-1.40369100
C	-5.34993100	0.03438900	0.51973000
H	-3.97001300	-0.60496400	2.01679500
C	-5.51614600	0.66533900	-0.72571300
H	-4.49958500	1.62362800	-2.37220500
H	-6.22029300	-0.33351900	1.05624700
O	0.44978100	-1.00035700	-1.88600300
C	-3.34563900	-6.15265300	-1.02535300
N	-3.89755800	-7.10406700	-1.41147600
C	-6.82575800	0.83013000	-1.28167600
N	-7.89454300	0.96449600	-1.72716700
C	-1.34394800	6.98121500	-0.74300800
N	-1.54555000	8.08112900	-1.07310000
C	6.10573900	3.12940900	-1.33527900
N	7.06276500	3.60952600	-1.79594400
C	5.25162800	-4.78301600	-0.86612100
N	6.06829000	-5.53869300	-1.21420500

table4-entry2-ts

O	-0.86336600	0.99380400	-2.42429200
C	-0.08763300	0.11291500	-2.29654400
O	0.66820800	-0.75039000	-2.57817800
C	0.00307900	0.01091900	0.37698100
B	-1.15164100	0.99707200	1.24334600
B	0.35467700	-1.44407500	1.26230000
B	0.57277900	1.39777900	1.23741800
B	-0.36452200	1.49323500	2.77141100
B	-1.50389400	0.13311800	2.78329100
B	-1.27699500	-0.76565800	1.25128700
C	-2.28007500	1.93424300	0.58538600
B	1.50302300	-0.10341900	1.25989800
B	-0.56841300	-1.36930100	2.79371500
B	1.15003000	-0.94290500	2.79834900

C	0.66902300	-2.86032600	0.58317800
C	1.18213900	2.69301900	0.52240100
B	1.27413500	0.82405200	2.78415100
H	-0.63335000	2.54605000	3.27235100
B	-0.00551400	0.03512100	3.72358100
H	-2.57970900	0.20158300	3.30049100
C	-2.49626100	-1.51544200	0.53370700
C	-2.01925000	2.90508300	-0.40297400
C	-3.61233600	1.86270100	1.04770000
C	2.94866800	-0.22912500	0.57921800
H	-0.96597800	-2.37207900	3.31116200
H	1.98304800	-1.62629600	3.31823800
C	0.12282100	-3.26469500	-0.65108600
C	1.48944900	-3.79965700	1.24308800
C	1.79969300	2.64686200	-0.74359900
C	1.16261800	3.94694500	1.16810500
H	2.18193500	1.41279700	3.29425700
H	-0.01047200	0.04513500	4.92031800
C	-3.01408000	-1.11151100	-0.71430600
C	-3.13152800	-2.61200900	1.15310600
C	-3.00675300	3.75373300	-0.89406300
H	-1.02044300	2.99722000	-0.80773700
C	-4.61743400	2.69766900	0.57227200
H	-3.86409600	1.13088700	1.80760900
C	3.17805900	-0.92882800	-0.62277500
C	4.08275400	0.33105900	1.20493300
C	0.37147600	-4.51921700	-1.19931900
H	-0.50756300	-2.57639100	-1.19928900
C	1.75390000	-5.05867500	0.71581100
H	1.93047500	-3.52925100	2.19704000
C	2.35608900	3.77379900	-1.34047400
H	1.85482100	1.69817200	-1.26612400
C	1.71008300	5.08774700	0.59194800
H	0.69974400	4.02206700	2.14715200
C	-4.08988900	-1.75848200	-1.31559600
H	-2.56941000	-0.26317900	-1.22182200
C	-4.20746700	-3.27400600	0.57201900
H	-2.76483000	-2.95262000	2.11625800
C	-4.32254700	3.66165100	-0.40795200
H	-2.76621900	4.49111900	-1.65493800
H	-5.63182600	2.61120400	0.95244400
C	4.45012100	-1.06276800	-1.17235200
H	2.34035900	-1.37260600	-1.14445000
C	5.36259400	0.21068500	0.67514600

H	3.95217600	0.87610400	2.13411100
C	1.19290300	-5.43484500	-0.51802100
H	-0.06724600	-4.79875900	-2.15315500
H	2.39288400	-5.75763000	1.24900600
C	2.31422400	5.01310600	-0.67651700
H	2.82849500	3.70414100	-2.31637400
H	1.67471200	6.04118200	1.11232200
C	-4.70038400	-2.85212300	-0.67614100
H	-4.46778600	-1.41978400	-2.27639300
H	-4.67208600	-4.11906600	1.07311800
C	5.56138600	-0.49273100	-0.52663800
H	4.59107400	-1.61011300	-2.10036200
H	6.21408700	0.65743100	1.18167300
C	1.45446200	-6.73071700	-1.06695700
N	1.66913000	-7.78825300	-1.50848900
C	6.87550300	-0.62623700	-1.07851100
N	7.94802000	-0.73374800	-1.52301100
C	2.88118100	6.18226500	-1.27712600
N	3.34149100	7.13771200	-1.76135100
C	-5.34540700	4.53487100	-0.89816400
N	-6.18029100	5.24708700	-1.29216300
C	-5.81043100	-3.52459300	-1.28026700
N	-6.71611500	-4.07414600	-1.76706800

table4-entry2-post

B	-0.71537600	1.33028600	2.78873000
B	0.20070800	1.47864400	1.25141500
B	-1.34431200	0.64796200	1.25152100
B	-1.48613700	-0.26916600	2.78890000
B	-1.03153900	-1.07817100	1.25128700
C	-0.00000800	0.00007800	0.39586700
B	1.46832300	0.26596100	1.25148000
B	1.36062500	-0.65566300	2.78887200
B	1.04396000	1.09142900	2.78889400
B	-0.20330200	-1.49660200	2.78862600
B	0.70669200	-1.31418600	1.25143000
H	-1.23140500	2.28991500	3.28684800
H	-2.55811800	-0.46358800	3.28738800
H	1.79703600	1.87876300	3.28724900
H	-0.00007400	-0.00009400	4.92573900
H	2.34226400	-1.12852000	3.28700100
H	-0.35003100	-2.57626700	3.28676700
B	-0.00004800	-0.00001100	3.72810300
C	0.39022200	2.87471400	0.50351000

C	0.40510900	2.97968900	-0.90062600
C	0.55184100	4.07114800	1.23083500
C	0.57061600	4.19789800	-1.55097900
H	0.28197800	2.07047900	-1.48131200
C	0.71896000	5.30118900	0.60458300
H	0.54527700	4.02752300	2.31615600
C	0.73012400	5.37750900	-0.80077600
H	0.57825800	4.25033800	-2.63652000
H	0.84161700	6.20885800	1.18974900
C	2.85487400	0.51719100	0.50384500
C	2.95956700	0.53523100	-0.90024300
C	4.04259100	0.73321300	1.23131300
C	4.16931900	0.75446500	-1.55049300
H	2.05700200	0.37080700	-1.48099700
C	5.26409400	0.95468400	0.60521500
H	3.99889800	0.72598400	2.31659400
C	5.34032600	0.96764500	-0.80014100
H	4.22172100	0.76323000	-2.63603100
H	6.16512400	1.11871100	1.19051100
C	1.37390600	-2.55526600	0.50369300
C	1.42415200	-2.64893300	-0.90044000
C	1.94575700	-3.61838400	1.23118800
C	2.00659100	-3.73175500	-1.55058000
H	0.98942600	-1.84115600	-1.48137100
C	2.53383100	-4.71173400	0.60517500
H	1.92494800	-3.57930700	2.31647600
C	2.57049000	-4.77990400	-0.80017100
H	2.03171400	-3.77863900	-2.63611500
H	2.96770600	-5.51824200	1.19051300
C	-2.61367800	1.25966300	0.50403700
C	-2.70946100	1.30530900	-0.90004400
C	-3.70084800	1.78439700	1.23152100
C	-3.81700900	1.83898100	-1.55035200
H	-1.88292300	0.90667700	-1.48045000
C	-4.81916600	2.32329000	0.60534900
H	-3.66077100	1.76556000	2.31682100
C	-4.88902300	2.35621000	-0.80002000
H	-3.86501300	1.86166200	-2.63588800
H	-5.64403100	2.72132900	1.19057700
C	-2.00559300	-2.09633200	0.50342700
C	-2.07978800	-2.17238500	-0.90069700
C	-2.83931600	-2.96941000	1.23086800
C	-2.92971800	-3.06077000	-1.55091900
H	-1.44609700	-1.50909200	-1.48157500

C	-3.69749600	-3.86643600	0.60478200
H	-2.80810500	-2.93792500	2.31615900
C	-3.75174400	-3.92156300	-0.80056900
H	-2.96698900	-3.09864600	-2.63645800
H	-4.32998200	-4.52879300	1.19008000
C	3.17371700	-5.90132300	-1.45355100
N	3.66615100	-6.81688800	-1.98170800
C	-4.63197500	-4.84166900	-1.45398800
N	-5.35062300	-5.59282400	-1.98220200
C	-6.03612600	2.90894300	-1.45346800
N	-6.97265400	3.36026700	-1.98159900
C	0.90153700	6.63918900	-1.45433100
N	1.04150600	7.66927900	-1.98255600
C	6.59321600	1.19481200	-1.45360600
N	7.61608700	1.38023600	-1.98185900

table4-entry3-pre

B	-1.57647900	-1.49229800	0.28868200
B	-0.06866500	-1.36568200	-0.64413800
B	-0.05615300	-1.03239400	1.08992900
B	-1.56550900	-0.19157800	1.50991400
B	-0.05673600	0.73094600	1.31033900
C	0.76612300	0.00282800	-0.00836800
B	-0.07010900	0.19090500	-1.49354200
B	-1.58717400	1.03704000	-1.10055200
B	-1.58345100	-0.73324100	-1.32422900
B	-1.58040700	1.37158400	0.64986200
B	-0.07499300	1.48638900	-0.28678700
H	-2.09146100	-2.55829100	0.49565200
H	-2.07089500	-0.32804600	2.59200300
H	-2.10109100	-1.25748100	-2.27401500
H	-3.72118000	-0.00618700	0.01704600
H	-2.10771200	1.77871500	-1.89040900
H	-2.09761300	2.35226500	1.11384800
B	-2.51825600	-0.00392600	0.01050300
C	2.36633000	0.00060600	-0.00381700
O	2.89185000	-1.13506200	0.00113100
O	2.89601800	1.13419800	0.00029200
H	0.53837700	2.48552500	-0.48321200
H	0.55053900	0.31779000	-2.50643400
H	0.54901400	-2.28245100	-1.08364200
H	0.57167700	-1.72211200	1.83148600
H	0.57234600	1.21785800	2.19949100

table4-entry3-post

C	-0.00194700	0.00628900	-1.64979800
B	-0.16586300	-1.47137400	-0.79043400
B	0.99949200	1.09944000	-0.78229000
B	-1.45518300	-0.29591400	-0.78424500
B	-1.02225300	-1.12474400	0.74486300
B	0.75153000	-1.32248800	0.74194200
B	1.35132600	-0.60961600	-0.78866800
B	-0.73461500	1.29307800	-0.77960600
B	1.48812300	0.30318000	0.74715900
B	0.16924100	1.50549800	0.75290100
B	-1.38199800	0.62350100	0.75177200
H	-1.75634400	-1.93147600	1.26382900
B	0.00192900	-0.00646500	1.68847200
H	1.29013600	-2.27182900	1.25943600
H	2.55568100	0.52033000	1.26891700
H	0.29129500	2.58598300	1.27900000
H	-2.37346700	1.07211100	1.27594800
H	0.00309300	-0.01068500	2.89678900
H	-2.49071400	-0.50650200	-1.37054800
H	-0.28425100	-2.51939200	-1.38056300
H	2.31282100	-1.04460100	-1.37753200
H	1.71172300	1.88278100	-1.36506200
H	-1.25692800	2.21506000	-1.36075300

TS8

C	3.19814500	0.94331100	-0.22010100
O	2.92264500	0.02327500	0.64613800
O	2.50415100	1.21239300	-1.21716100
O	-0.18419200	-2.38562600	-0.25787500
C	-1.46641300	-2.06341500	-0.24071000
O	-2.35975100	-2.88330700	-0.33781500
H	1.11556600	0.23827700	-0.83973900
C	-1.71609200	-0.56693400	-0.09594700
B	-3.04623400	0.19619900	-0.84830500
B	-2.95848000	0.03265300	0.91713200
B	-1.24614100	0.14930200	1.41504600
B	-1.38350000	0.40456200	-1.47294900
B	-0.30596000	0.38381100	-0.06433300
B	-3.41264700	1.58403400	0.18927700
B	-2.43702100	1.80882700	-1.28980300
H	-3.80836800	-0.46822800	-1.46930300
B	-2.30361500	1.54819000	1.58997400
H	-3.65980200	-0.74496300	1.47576500

B	-0.63102800	1.76264800	0.98004100
H	-0.84502900	-0.56389700	2.27831000
B	-0.71702800	1.93346000	-0.80944400
H	-1.04949300	-0.13511800	-2.47689000
H	-4.52497900	2.00667400	0.27809500
B	-1.98234400	2.65060000	0.22449600
H	-2.85162200	2.37672900	-2.25352100
H	-2.62918100	1.92362500	2.67458200
H	0.23111100	2.27887700	1.62141800
H	0.07235300	2.57269400	-1.42505700
H	-2.08033700	3.83514800	0.33454800
Pd	1.26136000	-1.07735200	0.16028400
C	4.45360000	1.74831400	0.07641000
H	4.20783700	2.50993000	0.82557000
H	5.23629200	1.10821600	0.49196000
H	4.80480500	2.24727700	-0.82867400

TS11

O	0.90884700	1.87466900	-1.50761700
C	2.20216000	1.86608600	-1.28018400
O	2.98609500	2.67654600	-1.74708500
C	2.63845300	0.72509000	-0.36257900
B	4.08704600	-0.15555400	-0.57191300
B	3.84007600	0.88744300	0.84361700
B	2.10693300	0.84630900	1.27074500
B	2.50880500	-0.85514300	-1.03779600
B	1.33301300	-0.22919000	0.10948200
B	4.47912700	-0.75226500	1.05030300
B	3.66138800	-1.82622500	-0.11828700
H	4.84451600	0.17216900	-1.42544000
B	3.25638500	-0.12637300	2.19092100
H	4.43006900	1.91365400	0.93720600
B	1.66543200	-0.81709900	1.73183000
H	1.56088600	1.84542500	1.61579000
B	1.91877200	-1.87736500	0.29600900
H	2.22487200	-0.95485900	-2.18828000
H	5.61007500	-0.93679700	1.38575000
B	3.14437300	-1.80854200	1.59445100
H	4.21083300	-2.75705600	-0.62492400
H	3.51506600	0.15111600	3.32307200
H	0.80103100	-1.02998600	2.53035600
H	1.23838200	-2.83333000	0.08750500
H	3.32913600	-2.74264900	2.31593900
Pd	-0.42643400	0.55935400	-0.65279000

C	-2.40425700	0.25061400	0.39538500
C	-2.04625600	0.50825600	1.73075500
C	-3.27472700	1.11299400	-0.29817700
C	-2.52811300	1.66476700	2.34701800
H	-1.38520400	-0.16852800	2.26007100
C	-3.74130500	2.26271200	0.34210100
H	-3.57727900	0.88596900	-1.31489000
C	-3.37611000	2.53856700	1.66204800
H	-2.22897900	1.88024400	3.36915900
H	-4.40090200	2.93849300	-0.19627900
H	-3.74799100	3.43323700	2.15346800
I	-2.12818700	-1.81021900	-0.41844400

TS13

O	-0.61731800	-0.20784800	2.32799100
C	-1.90673300	-0.42171300	2.11702000
O	-2.69757700	-0.57439500	3.02832600
C	-2.30501800	-0.42719800	0.64865800
B	-3.26686200	-1.69205700	-0.00590300
B	-3.89887900	-0.04362500	0.17123200
B	-2.55982600	1.10785300	-0.08223300
B	-1.52363800	-1.58192400	-0.37277200
B	-1.10252600	0.14991400	-0.41975500
B	-4.14556500	-0.93406000	-1.34250400
B	-2.66974100	-1.88529400	-1.67393100
H	-3.63595000	-2.55304600	0.72288700
B	-3.71131900	0.79462600	-1.38608600
H	-4.69901000	0.19766400	1.01288300
B	-1.96600500	0.92359300	-1.75417300
H	-2.49047800	2.07680800	0.59793500
B	-1.30955200	-0.73825900	-1.92747300
H	-0.79892500	-2.38932000	0.12323200
H	-5.22846900	-1.32160300	-1.65769400
B	-2.94818200	-0.34497900	-2.52826500
H	-2.69447100	-2.94975800	-2.21003700
H	-4.47797800	1.64616200	-1.71719700
H	-1.50530100	1.85203100	-2.33794300
H	-0.38634500	-0.98657700	-2.63688300
H	-3.17808700	-0.30956800	-3.69859300
Pd	0.75031400	-0.42102700	0.84766900
C	0.50295300	1.46061400	0.09401100
C	1.09330700	1.85316100	-1.12500800
C	0.26409100	2.42799300	1.09053000
C	1.38469200	3.19680600	-1.35393000

H	1.28176800	1.11920500	-1.89754400
C	0.57086600	3.76658600	0.85178100
H	-0.17351300	2.12756800	2.03522000
C	1.12874300	4.15417200	-0.36938000
H	1.81585700	3.49260900	-2.30684000
H	0.37118800	4.50679400	1.62255900
H	1.36385900	5.19983400	-0.55310500
I	2.97271000	-1.14953000	-0.45386700

TS17

C	3.56505800	-0.75134500	-0.25908500
O	2.88017700	0.35974500	-0.18858700
O	3.25083000	-1.82386700	0.26089000
O	-0.32772600	0.43495300	2.23998600
C	-1.53319600	-0.00804700	1.93256300
O	-2.52387600	0.22624900	2.60011000
H	1.39114000	-1.26433900	0.80298600
C	-1.57093500	-0.84362900	0.65537600
B	-2.61280900	-2.18979300	0.48420800
B	-2.84214300	-0.72255200	-0.48127100
B	-1.24896200	0.02019600	-0.83904700
B	-0.86313500	-2.41062300	0.75699600
B	-0.06220000	-1.06764400	-0.06971200
B	-2.90689800	-2.31304000	-1.25799600
B	-1.67797200	-3.35459800	-0.48917900
H	-3.36597500	-2.44234200	1.36536800
B	-2.06806800	-0.95866500	-2.06712600
H	-3.75537200	-0.00293200	-0.24255300
B	-0.30698200	-1.16289900	-1.80323000
B	-0.06417900	-2.65422100	-0.82854800
H	-0.46377100	-2.77547000	1.81400800
H	-3.93377000	-2.75188600	-1.67704100
B	-1.34337300	-2.58962100	-2.07249400
H	-1.82955200	-4.52886900	-0.34879600
H	-2.49855200	-0.42724500	-3.04401200
H	0.51165500	-0.78576400	-2.58258800
H	0.92004300	-3.31385200	-0.92121400
H	-1.25728000	-3.23158800	-3.07451300
Pd	1.21246200	0.30164400	0.96216700
C	4.83033700	-0.62215600	-1.09952800
H	4.54853400	-0.55751400	-2.15668000
H	5.37190300	0.29383600	-0.84520200
H	5.46843500	-1.49524500	-0.95135800
C	-1.05022600	1.60063800	-0.84487600

C	-1.96688400	2.47687500	-0.23332200
C	0.06316900	2.18267000	-1.48415400
C	-1.78163700	3.86058200	-0.25467400
H	-2.83291200	2.07035800	0.28029500
C	0.25226600	3.56704800	-1.51202300
H	0.79166500	1.54084600	-1.97142900
C	-0.67121400	4.41354500	-0.89573700
H	-2.50730700	4.50708400	0.23412800
H	1.12252600	3.98116800	-2.01689800
H	-0.52670000	5.49172000	-0.91362400

TS18

C	4.35890600	0.10909400	0.52637000
O	3.62953300	-0.77805500	1.12434000
O	4.06072100	0.67412500	-0.53992800
O	0.39878500	-2.06354800	-0.91124000
C	-0.67693700	-1.36834900	-1.23099700
O	-1.61406100	-1.84409600	-1.84550900
H	2.39943600	0.10438000	-0.67656500
C	-0.62147500	0.08869500	-0.78356000
B	-1.44951300	1.32117700	-1.62193900
B	-1.94498500	0.87123200	0.03567100
B	-0.44351700	0.40120900	0.91340100
B	0.31619400	1.11815500	-1.78884000
B	0.90945200	0.56815100	-0.21013100
B	-1.74093200	2.58588500	-0.42151600
B	-0.36218600	2.72854500	-1.54397600
H	-2.13637600	1.02388200	-2.54238100
B	-1.11881400	2.00968700	1.14926800
B	0.65232600	1.80384900	1.00902300
B	1.12513400	2.26145200	-0.66607300
H	0.77211600	0.66220200	-2.78608100
H	-2.69214500	3.30052000	-0.50039800
B	-0.16227700	3.15828900	0.18090900
H	-0.33649600	3.52956000	-2.42707600
H	-1.62670400	2.30709000	2.18640700
H	1.39148900	1.93437100	1.93480000
H	2.19041100	2.71730700	-0.92536400
H	0.00345200	4.28663600	0.53207200
Pd	1.94761600	-1.29349100	0.07971300
C	5.64529100	0.47018300	1.25263400
H	5.40278900	1.16732500	2.06305500
H	6.10068900	-0.41777000	1.69916000
H	6.34201300	0.95600200	0.56715900

H	-0.49485100	-0.51613400	1.66770300
C	-3.32010500	0.14913400	0.36729000
C	-3.79651100	0.11633100	1.69136000
C	-4.13576400	-0.43653800	-0.61875900
C	-5.02492500	-0.46103000	2.01887300
H	-3.19398300	0.55817300	2.48025600
C	-5.36425500	-1.01790400	-0.29944100
H	-3.79218300	-0.45728600	-1.64657800
C	-5.81753300	-1.03075800	1.02110800
H	-5.36141000	-0.46566900	3.05401500
H	-5.96725700	-1.46588800	-1.08677400
H	-6.77573500	-1.48284800	1.27022900

TS19

C	-4.48785700	-0.11271900	0.34016700
O	-3.63964200	0.86300900	0.15649800
O	-4.35986300	-1.26463400	-0.08266600
O	-0.53512900	0.18139800	-2.30558200
C	0.56608600	-0.47785000	-2.00879300
O	1.51378200	-0.55937100	-2.77147300
H	-2.47872200	-1.06985800	-0.69327500
C	0.53300300	-1.15347400	-0.63754500
B	1.33327400	-2.63743500	-0.34846900
B	1.85319300	-1.15757900	0.50804400
B	0.36709800	-0.14213900	0.78559100
B	-0.42711600	-2.58770700	-0.61800100
B	-0.99179400	-1.07387800	0.10153100
B	1.61047800	-2.68644900	1.39662800
B	0.22492000	-3.56088200	0.69712100
H	2.02474700	-3.08478700	-1.20213200
B	1.01111200	-1.15583000	2.09025500
B	-0.75283500	-1.08506400	1.83273500
B	-1.24748900	-2.58210900	0.97276100
H	-0.88148800	-2.95869000	-1.65019900
H	2.55269700	-3.25699400	1.85200700
B	0.02931900	-2.63886700	2.21524600
H	0.18384600	-4.75073100	0.63890000
H	1.51304400	-0.64037500	3.04069500
H	-1.49170700	-0.52323700	2.57896300
H	-2.32840900	-3.05706000	1.10333500
H	-0.15221100	-3.17714800	3.26411000
Pd	-2.03659700	0.42737000	-1.00346200
C	-5.69135400	0.28704100	1.18522600
H	-5.37599500	0.36637900	2.23192600

H	-6.07262500	1.26543100	0.87893300
H	-6.47351100	-0.47004500	1.10459600
C	0.40580500	1.44978800	0.70481700
C	1.23274000	2.15507300	-0.19207300
C	-0.39651900	2.21832700	1.57219900
C	1.25293300	3.55091100	-0.22458200
H	1.87622900	1.61026500	-0.87518500
C	-0.37711800	3.61440300	1.54774200
H	-1.04890800	1.71119200	2.27666600
C	0.44896200	4.28856000	0.64636300
H	1.90384400	4.06018800	-0.93163800
H	-1.01000500	4.17359600	2.23367700
H	0.46661800	5.37616300	0.62349800
C	3.28147200	-0.50428400	0.25945700
C	4.01720900	-0.69041700	-0.92688600
C	3.89761700	0.24300800	1.28188500
C	5.29903400	-0.15779400	-1.08131100
H	3.56807900	-1.23683500	-1.74783600
C	5.18039100	0.77381100	1.13565500
H	3.36250900	0.40899500	2.21217500
C	5.88951800	0.57487800	-0.05012100
H	5.83675500	-0.31739300	-2.01381500
H	5.62389900	1.34480900	1.94908400
H	6.88923100	0.98805100	-0.16986000

TS20

C	5.02606600	0.39413000	0.23873600
O	4.54656200	-0.71265200	-0.24374100
O	4.42826100	1.47972300	0.26061500
O	1.02327400	-0.46784200	-2.16037000
C	-0.17380100	-0.32014400	-1.62455800
O	-1.19717900	-0.47311400	-2.26574100
H	2.77407900	0.86659700	-0.25002900
C	-0.14864000	0.04278200	-0.13944700
B	-1.30535500	1.10555800	0.61923700
B	-1.23358100	-0.66068000	1.02471500
B	0.48483400	-1.18230200	0.91377200
B	0.38465500	1.62768500	0.25805000
B	1.44472900	0.22488100	0.46074800
B	-1.29528800	0.56003900	2.32015600
B	-0.30479600	1.95774700	1.84469700
B	-0.21546000	-0.84793500	2.49294700
B	1.45317000	-0.31624400	2.13152500
B	1.39441500	1.43544700	1.73558900

H	-2.27288700	0.69120500	2.98965500
B	0.33783700	0.76266300	3.00446100
H	-0.57099300	3.07244200	2.16971700
H	-0.44458600	-1.74053400	3.24859800
H	2.41371000	-0.82939800	2.61405300
H	2.30059600	2.17224000	1.94764500
H	0.50377200	1.03925200	4.15283700
Pd	2.70786600	-0.51971500	-1.10129800
C	6.41863200	0.26318200	0.83785400
H	6.33179500	-0.21076900	1.82238800
H	7.05038500	-0.37575000	0.21466300
H	6.87084000	1.24922200	0.95808400
H	0.71942700	-2.25094500	0.44910600
C	-2.52458600	1.81149500	-0.12363600
C	-3.42784900	1.13934800	-0.96980100
C	-2.76258100	3.18316600	0.09429200
C	-4.50809800	1.80025000	-1.55862500
H	-3.27151800	0.09213600	-1.19077200
C	-3.84106000	3.84964100	-0.48974300
H	-2.08912500	3.74171300	0.73699300
C	-4.72376800	3.15826300	-1.32085400
H	-5.18170200	1.24658700	-2.20952400
H	-3.98880100	4.91032200	-0.29510400
H	-5.56616400	3.67229100	-1.78003900
H	0.57767900	2.39387900	-0.62747400
C	-2.39135800	-1.69196800	0.67180200
C	-2.23203500	-2.75403000	-0.23663900
C	-3.63067000	-1.60198800	1.33305900
C	-3.25252300	-3.67609000	-0.47491300
H	-1.29606600	-2.86453200	-0.77479300
C	-4.65600200	-2.52145800	1.10412200
H	-3.79360300	-0.79497600	2.04136900
C	-4.47169100	-3.56540100	0.19625800
H	-3.09318000	-4.48205500	-1.18828100
H	-5.60041500	-2.41893500	1.63492800
H	-5.26844700	-4.28341100	0.01264800

TSS2

O	-0.31846000	-1.05890800	-1.75511200
C	-1.57741700	-1.39786300	-1.93252400
O	-1.95938700	-2.14370100	-2.81920600
C	-2.52693100	-0.77707500	-0.90868400
B	-4.08520500	-0.18956500	-1.30431600
B	-3.87198700	-1.60993800	-0.26045300

B	-2.37809200	-1.38834600	0.69495700
B	-2.72519000	0.92682500	-1.00187800
B	-1.70608400	0.16557600	0.22180600
B	-5.00332800	-0.32833800	0.20634400
B	-4.29512400	1.24250000	-0.25906400
H	-4.48775100	-0.31894800	-2.41371100
B	-3.94731500	-1.07497200	1.43838000
H	-4.13482800	-2.69129900	-0.67365900
B	-2.57276000	0.03637200	1.74722500
H	-1.65590000	-2.31355700	0.87925200
B	-2.79451100	1.47187500	0.69175300
H	-2.23092600	1.50933400	-1.91754600
H	-6.18315400	-0.51012600	0.19541800
B	-4.21004800	0.69180800	1.44087500
H	-4.95780600	2.16992300	-0.61589100
H	-4.37098100	-1.79790400	2.28836900
H	-2.02258800	0.10644000	2.80300700
H	-2.40577700	2.55816600	1.01176400
H	-4.83004700	1.23574800	2.30509200
Pd	0.30600500	0.24252100	-0.27376400
C	1.80142900	-1.14448000	0.64854900
C	1.99393700	-0.84389400	1.99796900
C	1.63495400	-2.45210600	0.18859800
C	1.93640300	-1.89255800	2.92179400
H	2.15038500	0.17702300	2.32406400
C	1.58602800	-3.47863200	1.13369200
H	1.49225500	-2.65014200	-0.86649400
C	1.73829800	-3.20684700	2.49649700
H	2.05201500	-1.66828800	3.97957800
H	1.42059500	-4.49776000	0.79278400
H	1.70181900	-4.01554600	3.22147400
I	3.17249800	0.27518400	-0.88676100
O	0.66079800	1.94533400	1.15655300
C	0.43997900	3.11391600	0.88010900
O	0.53909300	4.01781800	1.87134800
C	0.07271100	3.60580800	-0.49714400
H	0.29582200	4.89680700	1.53971400
H	0.75090700	3.15244500	-1.22544600
H	-0.94001700	3.25972300	-0.72761700
H	0.11289500	4.69628800	-0.58863900
TSS4			
O	0.02230800	1.99053300	0.66090400
C	-1.16094900	2.52377600	0.86893600

O	-1.32996600	3.63068800	1.35745800
C	-2.31010000	1.62384200	0.42482100
B	-3.79027200	1.52431500	1.27452300
B	-3.70461500	2.24272400	-0.34647400
B	-2.44225100	1.37760100	-1.27214500
B	-2.58094600	0.21123400	1.36349100
B	-1.77034200	0.13623900	-0.20573700
B	-4.98139000	1.07645700	0.04042900
B	-4.28471500	-0.17708400	1.10402100
H	-3.95641100	2.21742900	2.22468500
B	-4.14686300	0.99441500	-1.53685800
H	-3.81234100	3.41774800	-0.48314200
B	-2.93196700	-0.32092800	-1.45856500
H	-1.72255700	1.99664000	-1.99068000
B	-3.01863400	-1.04463900	0.18180400
H	-1.95098500	0.06049600	2.36173600
H	-6.12250800	1.41711100	0.13155400
B	-4.50865600	-0.50676000	-0.63879500
H	-4.92047400	-0.71829300	1.95842500
H	-4.68357400	1.29132100	-2.56164500
H	-2.61104700	-0.95407700	-2.41737000
H	-2.77369700	-2.19865500	0.37636400
H	-5.31817000	-1.29520500	-1.02756900
Pd	0.29595100	0.12378800	-0.20457300
I	0.69657600	-2.29707000	-1.45743700
C	1.06423100	-1.94492000	0.78103500
C	0.10135900	-2.41114600	1.67948000
C	2.38888800	-1.72175300	1.17231300
C	0.46993900	-2.60126600	3.01285600
H	-0.91764000	-2.58575600	1.35659000
C	2.73235000	-1.92242800	2.51119500
H	3.12014700	-1.36252600	0.45933800
C	1.78029300	-2.36238900	3.43338200
H	-0.28327900	-2.93310700	3.72270900
H	3.75537700	-1.73251400	2.82795600
H	2.05742300	-2.51810000	4.47268700
O	2.74068400	0.90094500	-0.53422400
C	2.81599600	2.08748800	-0.19750200
N	3.91983700	2.86141800	-0.37397200
H	1.96366400	2.59664600	0.27490200
C	5.11368500	2.33030300	-1.00488500
C	3.92454300	4.25459400	0.03068100
H	5.35113500	2.89055500	-1.91930300
H	5.97470400	2.39610500	-0.32590500

H	4.92747200	1.28608000	-1.25813700
H	4.71338600	4.44566900	0.77122500
H	4.09702900	4.91257300	-0.83212000
H	2.95881800	4.50862800	0.47458800

TSS8

O	0.61802400	-0.56209100	2.21007200
C	1.76315100	-1.16231300	2.00040800
O	2.56009100	-1.45380300	2.88049900
C	2.01999800	-1.46429900	0.52366800
B	3.55036100	-1.40455600	-0.22817200
B	2.69755900	-2.94342700	-0.01391000
B	0.94678300	-2.63153700	-0.15434400
B	2.35068100	-0.09204000	-0.49665000
B	0.76987300	-0.90335900	-0.45260900
B	3.43531900	-2.55035200	-1.57516800
B	3.22061100	-0.80464700	-1.87245100
H	4.50883400	-1.15917000	0.42838900
B	1.82249400	-3.31293700	-1.52313200
H	3.07963000	-3.72609900	0.79288300
B	0.59547200	-2.03177700	-1.79031100
B	1.46650500	-0.47347400	-2.00766100
H	4.39621400	-3.13805200	-1.97025500
B	2.14565100	-1.98431400	-2.67457800
H	4.02763000	-0.14977100	-2.45862100
H	1.63326600	-4.44204400	-1.86094400
H	-0.45700800	-2.24547800	-2.31613100
H	1.02851400	0.39526800	-2.69662900
H	2.18918000	-2.16894100	-3.85375500
Pd	-0.72534500	-0.08755000	0.71622900
C	-2.92543900	-0.01704300	0.09736700
C	-3.10710800	-1.36134200	-0.27512600
C	-3.52529600	0.49815000	1.26193600
C	-3.86145200	-2.19443600	0.55340700
H	-2.64857800	-1.74490300	-1.17958000
C	-4.27252900	-0.35866400	2.07352800
H	-3.40767000	1.54431700	1.52312900
C	-4.44792500	-1.69865900	1.72051100
H	-3.98148600	-3.23938400	0.28102000
H	-4.72490500	0.03230400	2.98118400
H	-5.03522500	-2.35566200	2.35572900
I	-2.15893800	1.41925000	-1.39685500
H	0.18981300	-3.18787500	0.57508100
C	2.59217200	1.36711700	0.08789400

C	3.27163200	1.59920700	1.29871700
C	2.16711600	2.49896600	-0.63262500
C	3.50572100	2.89325100	1.76848500
H	3.61622300	0.75655600	1.89054300
C	2.40320000	3.79611600	-0.17274500
H	1.64749300	2.35828600	-1.57650800
C	3.07402500	3.99990000	1.03474700
H	4.02952400	3.03461000	2.71173400
H	2.06353800	4.64781200	-0.75959000
H	3.25954800	5.00877700	1.39846400

TSS10

O	-0.67922500	-0.06124000	2.26384400
C	-1.88007100	-0.55073100	2.02744800
O	-2.59120200	-1.00789200	2.90517400
C	-2.30600700	-0.47311400	0.56594000
B	-3.03516900	-1.79804400	-0.24978100
B	-3.97033300	-0.35577900	0.16847400
B	-2.89817500	1.06315100	0.06033100
B	-1.34513600	-1.31896000	-0.61852800
B	-1.29249300	0.48034800	-0.42402800
B	-4.10270300	-1.06083900	-1.45186700
B	-2.48530100	-1.63728000	-1.93472200
H	-3.19210900	-2.81020000	0.34999000
B	-4.02165400	0.70617000	-1.25574600
H	-4.76381200	-0.39946000	1.04858700
B	-2.35432200	1.23332400	-1.62494200
H	-2.99452000	1.92137900	0.87225900
B	-1.38902200	-0.21978000	-2.03710400
H	-5.09698500	-1.61790200	-1.80273400
B	-3.09713300	-0.08663800	-2.55785700
H	-2.31812500	-2.60234300	-2.61452500
H	-4.95380400	1.42438600	-1.44855300
H	-2.11079600	2.30423500	-2.08070000
H	-0.47073500	-0.17264500	-2.79535200
H	-3.37497100	0.05896000	-3.70901100
Pd	0.69271700	0.17254700	0.76717600
C	0.01511300	2.02465200	0.24573200
C	0.45552700	2.68408100	-0.92208200
C	-0.39399500	2.79328400	1.35596600
C	0.43052300	4.07570900	-0.98906000
H	0.77154200	2.10828500	-1.78192800
C	-0.40207700	4.18427200	1.28052600
H	-0.71824300	2.29231500	2.26051000

C	0.00742600	4.82801500	0.10898900
H	0.74774400	4.57081600	-1.90318300
H	-0.73103400	4.76560000	2.13831400
H	-0.00339300	5.91397000	0.05263700
I	3.04450000	0.34056000	-0.51913300
C	-0.16495300	-2.32920300	-0.25097100
C	-0.02969000	-2.96344800	1.00415800
C	0.74217200	-2.71723300	-1.26041000
C	0.96617000	-3.91693700	1.23923200
H	-0.73084000	-2.74437000	1.80298700
C	1.72807500	-3.67415100	-1.03308800
H	0.66678400	-2.25582400	-2.24015700
C	1.84878300	-4.27666000	0.22208900
H	1.03739600	-4.38492600	2.21838100
H	2.40977600	-3.94488500	-1.83587900
H	2.62131700	-5.02080700	0.40220600

TSS18

O	0.00336200	-0.58738800	-2.13944800
C	-1.09545500	-1.21262000	-1.77555800
O	-1.92778900	-1.59687500	-2.58039000
C	-1.20145900	-1.46804000	-0.27413700
B	-2.60420900	-1.08677400	0.70436400
B	-2.15974800	-2.76653500	0.29935100
B	-0.38858400	-2.91312000	0.19696300
B	-1.05322800	-0.15154600	0.85642700
B	0.29741900	-1.31331600	0.54681700
B	-2.57547600	-2.34698400	1.96564200
B	-1.87816900	-0.74489100	2.30492700
B	-1.23484100	-3.46859800	1.64435000
H	-2.81724700	-3.36929900	-0.48151000
B	0.29942000	-2.56801200	1.79869900
H	0.08192500	-3.58607500	-0.65814400
B	-0.09611500	-0.86904200	2.20146000
H	-3.60191900	-2.70414100	2.45450600
B	-1.05712100	-2.21046500	2.88927100
H	-2.39104600	0.04216100	3.03908300
H	-1.29870600	-4.63530500	1.88073700
H	1.31031600	-3.08534600	2.15022600
H	0.62784100	-0.18289400	2.85245500
H	-0.99924000	-2.46813600	4.05252400
Pd	1.22315100	0.35078600	-0.78928200
C	2.23548000	-1.36984000	-0.35234700
C	3.14561000	-1.45426100	0.72324200

C	2.41148900	-2.21465400	-1.46852500
C	4.17065000	-2.39791500	0.69858400
H	3.02206600	-0.81316300	1.58615700
C	3.44731900	-3.14600900	-1.48632000
H	1.72446200	-2.14369400	-2.30371400
C	4.32712200	-3.24097800	-0.40386000
H	4.85004900	-2.46939900	1.54399800
H	3.56592100	-3.79955900	-2.34701600
H	5.13274900	-3.97127200	-0.42017300
I	3.02896900	2.02502900	0.28261300
C	-1.01003500	1.39724600	0.46649000
C	-1.29753500	1.92407300	-0.81425400
C	-0.72462700	2.33180900	1.48628600
C	-1.27553100	3.30302200	-1.06151400
H	-1.59053400	1.26551900	-1.62369400
C	-0.71328600	3.70182000	1.24469800
H	-0.50289100	1.96727300	2.48434900
C	-0.98238300	4.19638300	-0.03563700
H	-1.50657700	3.66839600	-2.05921300
H	-0.48529100	4.38876200	2.05639500
H	-0.96716300	5.26700500	-0.22540000
C	-3.91058900	-0.38447900	0.13693100
C	-4.50027900	0.68096700	0.84380100
C	-4.56180800	-0.81180900	-1.03613600
C	-5.68131500	1.28651000	0.41160200
H	-4.02516000	1.04073500	1.75174100
C	-5.74086200	-0.20656800	-1.47687600
H	-4.12776700	-1.61438000	-1.62161700
C	-6.30923200	0.84356200	-0.75390700
H	-6.10855400	2.10666600	0.98525800
H	-6.21543800	-0.55912400	-2.39043300
H	-7.22910700	1.31379700	-1.09609100

TSS22

C	-4.71705400	-1.61414200	0.32245500
O	-4.32869700	-0.47277600	-0.18061000
O	-4.05047800	-2.65163900	0.34566000
O	-0.83422800	-0.41515100	-2.15529300
C	0.36900300	-0.34776300	-1.62592800
O	1.36873700	-0.16744400	-2.30063900
H	-2.33119100	-1.82726900	-0.24324800
C	0.39605300	-0.54133500	-0.10667200
B	1.68545200	-1.37465200	0.72189200
B	1.36656500	0.38511100	1.01481400

B	-0.43045400	0.66933300	0.86570300
B	0.10622700	-2.16494600	0.39830800
B	-1.14446700	-0.92671800	0.51163200
B	1.58727400	-0.74162800	2.38279300
B	0.82958900	-2.30492200	1.99657900
B	0.30759800	0.49127700	2.46442400
B	-1.25136400	-0.30439800	2.13850600
B	-0.93120600	-2.04522300	1.85093300
H	0.03372800	-2.99770900	-0.44453200
H	2.56634100	-0.66219500	3.05736900
B	0.00024500	-1.15128400	3.07637700
H	1.28079400	-3.34525000	2.36117300
H	0.37030900	1.43459800	3.18921600
H	-2.27985800	0.07104500	2.60508600
H	-1.73085300	-2.88792000	2.09698700
H	-0.13740400	-1.36599300	4.24130100
Pd	-2.50948300	-0.47772300	-1.06965200
C	-6.10973300	-1.55768900	0.93824100
H	-6.05148600	-1.02308100	1.89331000
H	-6.79809200	-1.00632100	0.29128200
H	-6.48072200	-2.56850500	1.11722000
C	-1.02392900	2.00773500	0.23473100
C	-0.40047600	2.70882200	-0.81642700
C	-2.21731600	2.55609300	0.74756000
C	-0.94238800	3.88814400	-1.33178500
H	0.52596100	2.33617400	-1.24053500
C	-2.76102800	3.73773500	0.23974300
H	-2.72912100	2.04729900	1.55881800
C	-2.12541300	4.40995600	-0.80584600
H	-0.43224400	4.40051200	-2.14426900
H	-3.68298500	4.13095600	0.66298800
H	-2.54630300	5.33057300	-1.20458600
C	2.41487800	1.52188300	0.63217800
C	3.25947500	1.47139200	-0.49458300
C	2.56776700	2.62906000	1.49094800
C	4.19828100	2.47450600	-0.74856700
H	3.16576100	0.64853200	-1.19173200
C	3.50801500	3.63061700	1.24525800
H	1.93859700	2.70787500	2.37183700
C	4.33073800	3.55851700	0.12003400
H	4.82987500	2.40215500	-1.63157500
H	3.59420700	4.46903700	1.93381200
H	5.06405400	4.33808700	-0.07753900
C	3.00865200	-1.91301700	0.02448300

C	3.00299000	-2.64626100	-1.17590300
C	4.25665300	-1.71999000	0.64556700
C	4.17747900	-3.15899300	-1.72858200
H	2.06587300	-2.81724800	-1.69555100
C	5.43651000	-2.23191800	0.10215200
H	4.30440600	-1.15835800	1.57381600
C	5.40263500	-2.95518900	-1.09085100
H	4.13339800	-3.71805300	-2.66095900
H	6.38277200	-2.06196000	0.61192300
H	6.31967600	-3.35438700	-1.51960500

TSS25

O	0.25278500	-0.54533200	-1.84698700
C	-0.99701100	-0.57611600	-1.46811700
O	-1.92774500	-0.75939700	-2.24249600
C	-1.17984200	-0.38136200	0.04430700
B	-2.44259600	0.49494900	0.86800300
B	-2.29413000	-1.30297800	1.02120100
B	-0.54926900	-1.70928200	0.95178400
B	-0.76132400	1.18363900	0.69032300
B	0.34133800	-0.20489900	0.76630500
B	-2.50102500	-0.29069800	2.47052200
B	-1.57491600	1.21140500	2.26795400
B	-1.35670000	-1.65262400	2.51267100
B	0.29519300	-0.98880000	2.33763400
H	-0.20854100	-2.67585200	0.34954300
B	0.15309000	0.79466700	2.18939500
H	-3.52428000	-0.30829200	3.08295700
B	-0.92707300	-0.10356100	3.28364300
H	-1.92866600	2.25278900	2.72782400
H	-1.57436100	-2.65580500	3.11926600
H	1.25747300	-1.51407200	2.81222200
H	1.00560000	1.52744800	2.58299200
H	-0.84034700	0.01078900	4.46865600
Pd	1.87181900	-0.33779600	-0.59692300
C	4.07358200	-0.94666600	-0.26972700
C	3.86454900	-2.22353900	0.28365800
C	4.53459600	-0.79803200	-1.59119300
C	4.09274400	-3.34907700	-0.51034500
H	3.51857800	-2.32598300	1.30601400
C	4.74983500	-1.94223300	-2.36469200
H	4.72275100	0.18891300	-1.99945500
C	4.53902800	-3.21362000	-1.82749200
H	3.91185000	-4.33526000	-0.09182900

H	5.09300200	-1.83073000	-3.38976300
H	4.71480400	-4.09639600	-2.43548200
I	4.11387700	0.80036600	1.05357400
C	-0.47213900	2.45294100	-0.22405000
C	-1.04784800	2.64254900	-1.49445300
C	0.37379700	3.47396500	0.25029200
C	-0.78341300	3.78418600	-2.25396400
H	-1.71869100	1.89387000	-1.90207800
C	0.63912400	4.62024200	-0.50107300
H	0.82985700	3.36841400	1.23053100
C	0.06218900	4.77992400	-1.76245300
H	-1.24671800	3.89448400	-3.23205300
H	1.29615500	5.38929900	-0.09877400
H	0.26553900	5.67134300	-2.35270800
C	-3.70609800	1.19059700	0.19259700
C	-4.33677200	0.71483900	-0.97406900
C	-4.28189600	2.31820300	0.81121800
C	-5.47439800	1.33759200	-1.49385600
H	-3.91686700	-0.13937200	-1.49128900
C	-5.42090400	2.94118200	0.29885500
H	-3.82842500	2.71568500	1.71398500
C	-6.02519700	2.45251000	-0.86082000
H	-5.93151200	0.94310300	-2.39928100
H	-5.83422500	3.81071600	0.80685500
H	-6.91294700	2.93537200	-1.26545000
C	-3.38265200	-2.30355700	0.43609700
C	-3.09700300	-3.25336800	-0.56144000
C	-4.68919000	-2.30475900	0.95900900
C	-4.06003900	-4.15832000	-1.01089600
H	-2.10647100	-3.28377700	-1.00348900
C	-5.65832000	-3.20825500	0.51861000
H	-4.95058800	-1.58245700	1.72675200
C	-5.34748300	-4.14227400	-0.47081900
H	-3.80286800	-4.87590300	-1.78759400
H	-6.65810200	-3.17844300	0.94762200
H	-6.09988500	-4.84722000	-0.81939100

TSS27

O	0.22006500	-0.52365000	-1.96776800
C	-1.00988100	-0.50061500	-1.50529200
O	-1.97831900	-0.51657900	-2.24780400
C	-1.11126000	-0.51205600	0.02138800
B	-2.08838200	0.58092800	0.98493100
B	-2.51757200	-1.16895400	0.83052300

B	-0.98424600	-2.09294300	0.69428900
B	-0.27270000	0.71379700	0.93335000
B	0.37933800	-0.96562800	0.76656700
B	-2.48247400	-0.38575700	2.43005300
B	-1.11578400	0.74394900	2.48564900
B	-1.82875100	-2.02560900	2.24259200
B	-0.05190000	-1.91402600	2.19679100
H	-0.94296500	-3.01116600	-0.05418700
B	0.39841000	-0.18936500	2.33998000
H	-3.49520500	-0.16819500	3.01884200
B	-0.97989800	-0.84500200	3.26587400
H	-1.14049200	1.75979500	3.10750700
H	-2.38064500	-2.99515000	2.66039400
H	0.64770000	-2.79359900	2.58262900
H	1.41682500	0.16704400	2.84374200
H	-0.92814400	-0.95476200	4.45225100
Pd	1.83953900	-0.07699800	-0.80700300
C	1.99485300	-2.00337500	-0.13503100
C	2.86969200	-2.35592800	0.91612800
C	1.68452000	-2.96638300	-1.11898900
C	3.37108300	-3.65278300	1.00386000
H	3.11744200	-1.63003300	1.67931900
C	2.19895400	-4.25755300	-1.02502200
H	1.03063100	-2.69786500	-1.94028100
C	3.04111900	-4.60399800	0.03573300
H	4.02411600	-3.91702100	1.83153500
H	1.94147900	-4.99376900	-1.78238400
H	3.43943700	-5.61335900	0.10691800
I	4.28583700	0.71340200	-0.03782100
C	0.40671800	2.01666200	0.30553800
C	0.23469200	2.46302000	-1.02524100
C	1.18497200	2.83644600	1.15253100
C	0.82488700	3.64773100	-1.48373100
H	-0.40631700	1.91716400	-1.70770200
C	1.76330100	4.01881000	0.70169100
H	1.33739500	2.53188200	2.18305500
C	1.59211000	4.42874700	-0.62441600
H	0.66316600	3.95902500	-2.51287300
H	2.35807700	4.62040800	1.38496300
H	2.04875800	5.35014300	-0.97795700
C	-2.98119800	1.75938000	0.39689700
C	-3.13441900	2.94410900	1.14457200
C	-3.67681300	1.68473600	-0.82602000
C	-3.93360800	3.99859100	0.70112900

H	-2.61730200	3.04257000	2.09399700
C	-4.47351600	2.73999700	-1.27739900
H	-3.58756000	0.79427100	-1.43657200
C	-4.60838600	3.90206500	-0.51712400
H	-4.02585600	4.89698600	1.30835100
H	-4.99332200	2.64670200	-2.22869100
H	-5.23109400	4.72250000	-0.86853000
C	-3.84171700	-1.67383000	0.10843000
C	-3.84593200	-2.64487500	-0.90892800
C	-5.09481800	-1.20141400	0.54056900
C	-5.03371000	-3.12138100	-1.46476000
H	-2.90332900	-3.03310900	-1.28065600
C	-6.28923600	-1.67322600	-0.00795500
H	-5.13590100	-0.44962700	1.32295700
C	-6.26436600	-2.63814300	-1.01548000
H	-4.99649900	-3.87100800	-2.25259300
H	-7.23888200	-1.28320300	0.35276400
H	-7.19211200	-3.00854600	-1.44703300

TSS31

C	-4.66471300	-1.05208200	0.73000000
O	-4.32751800	0.04598700	0.10767700
O	-3.96266600	-2.06074900	0.83281600
O	-0.88962200	0.01872500	-1.98038200
C	0.33418800	0.08992000	-1.49551600
O	1.31288400	0.20131300	-2.21357400
H	-2.32120800	-1.28296300	0.08680400
C	0.40512900	0.01431100	0.03278800
B	1.72154000	-0.65816400	0.95268900
B	1.36914600	1.12211800	1.00451400
B	-0.43190700	1.34292800	0.84427000
B	0.14874100	-1.56786400	0.76522800
B	-1.11289000	-0.30445700	0.73182600
B	1.62474400	0.21337900	2.50956800
B	0.90038700	-1.39584500	2.36625800
B	0.32606400	1.41955200	2.43706400
B	-1.21644300	0.54975400	2.25384900
B	-0.86502400	-1.20640900	2.21740800
H	2.60758200	0.40513900	3.15456000
B	0.06146600	-0.12260200	3.28288900
H	1.38946700	-2.34351800	2.89597500
H	0.37824300	2.45998000	3.01388700
H	-2.24995800	0.96774600	2.67075400
H	-1.64144400	-2.01846000	2.60081900

H	-0.05230000	-0.17405200	4.46869500
Pd	-2.53554800	0.00699700	-0.83420900
C	-6.04179800	-0.97911900	1.37741400
H	-5.98481500	-0.32684900	2.25626900
H	-6.77034100	-0.54277400	0.68783200
H	-6.36138900	-1.97479100	1.68976100
C	-1.07807200	2.55840000	0.03292400
C	-0.42236500	3.21926100	-1.02459200
C	-2.36277200	3.02868200	0.37827000
C	-1.01614400	4.28683300	-1.70048600
H	0.56648600	2.89710400	-1.33110400
C	-2.96050900	4.09847900	-0.29300200
H	-2.90355500	2.54984600	1.18868000
C	-2.28798100	4.73392500	-1.33808300
H	-0.47862600	4.76925000	-2.51365100
H	-3.95194400	4.43293900	0.00488700
H	-2.74926700	5.56714900	-1.86393200
C	2.40144200	2.20304600	0.45285400
C	3.26172000	1.98730500	-0.64205300
C	2.52619200	3.43651400	1.12410400
C	4.18765100	2.95277200	-1.04476400
H	3.19258800	1.06226100	-1.19919600
C	3.45308600	4.40220300	0.72921400
H	1.88509600	3.64476500	1.97476500
C	4.29098100	4.16495200	-0.36160300
H	4.83215400	2.74985700	-1.89749600
H	3.51739600	5.34159900	1.27493700
H	5.01415500	4.91549200	-0.67486400
C	3.07729000	-1.24687900	0.35894500
C	3.17414400	-1.92791400	-0.86916200
C	4.25906300	-1.14168200	1.11820200
C	4.38194900	-2.46748700	-1.31574700
H	2.29883100	-2.03595100	-1.49698700
C	5.46988800	-1.68041400	0.68003000
H	4.23072300	-0.62655200	2.07323300
C	5.53822900	-2.34758600	-0.54372200
H	4.41457200	-2.98492200	-2.27219000
H	6.36024900	-1.57527300	1.29689700
H	6.47978200	-2.76830300	-0.89119500
C	0.06546500	-2.95035700	-0.02781100
C	0.47414600	-4.12336700	0.63786800
C	-0.41687400	-3.10755400	-1.34186700
C	0.40551700	-5.37864200	0.03338300
H	0.85445500	-4.05112700	1.65136200

C	-0.48322300	-4.36142700	-1.95510700
H	-0.74480700	-2.24396000	-1.90871500
C	-0.07399900	-5.50556600	-1.27112500
H	0.73062300	-6.25853000	0.58471100
H	-0.85921900	-4.43777100	-2.97317900
H	-0.12784600	-6.48249500	-1.74696400

TSS34

O	-0.31094000	-0.21304900	-1.78446100
C	0.93132700	0.02996600	-1.49181200
O	1.77710800	0.26345900	-2.35387200
C	1.23453400	-0.00007800	0.01821900
B	2.63094800	-0.72427800	0.79804400
B	2.30707900	1.05817400	0.92101200
B	0.50144200	1.30309200	0.93743900
B	1.02480900	-1.59028700	0.73656600
B	-0.21963400	-0.32190600	0.84495000
B	2.69240300	0.10132400	2.37782800
B	1.92408100	-1.49447500	2.26080200
B	1.41362300	1.32766600	2.45614200
B	-0.15255700	0.49192200	2.39624400
B	0.16267300	-1.25899500	2.27468000
H	3.74845400	0.25393600	2.90937500
B	1.20183800	-0.23207200	3.28647700
H	2.41857400	-2.48372600	2.70447700
H	1.54490500	2.36251000	3.03357600
H	-1.13174300	0.91460600	2.92802400
H	-0.59395900	-2.06052900	2.72981100
H	1.19178900	-0.31682300	4.47715900
Pd	-1.81847900	-0.46632400	-0.42240300
C	-4.21884600	0.12954700	-0.43907400
C	-4.08257500	1.52008000	-0.55074700
C	-4.62800300	-0.65875700	-1.52178400
C	-4.34764400	2.11958600	-1.78253200
H	-3.73571500	2.11614400	0.28539000
C	-4.89187300	-0.03128900	-2.74484400
H	-4.73858300	-1.73212700	-1.41572400
C	-4.75785700	1.35059100	-2.87532300
H	-4.20231900	3.19098500	-1.88289400
H	-5.20246200	-0.63610400	-3.59248100
H	-4.95805700	1.82764000	-3.83048400
I	-3.94979700	-0.82446800	1.50324200
C	0.80803600	-2.91740800	-0.11792900
C	1.35999800	-3.12953500	-1.39490700

C	0.05286500	-3.97388400	0.42848200
C	1.16118400	-4.32359700	-2.09110400
H	1.95834300	-2.35564100	-1.86171200
C	-0.14745000	-5.17225300	-0.25898800
H	-0.38226200	-3.85635800	1.41644400
C	0.40541700	-5.35286500	-1.52825200
H	1.60449600	-4.44736800	-3.07686700
H	-0.73414000	-5.96578200	0.20046200
H	0.25327100	-6.28496800	-2.06898200
C	3.95155700	-1.30248600	0.11669200
C	4.35735700	-1.06405000	-1.21038100
C	4.81823800	-2.08185500	0.91054700
C	5.55325500	-1.58152700	-1.71556000
H	3.72331600	-0.47264200	-1.85964800
C	6.01461300	-2.59902900	0.41285500
H	4.55059500	-2.28552000	1.94255100
C	6.39036800	-2.35185600	-0.90872000
H	5.82972600	-1.37457000	-2.74772600
H	6.65381400	-3.19577200	1.06110500
H	7.32283400	-2.75268500	-1.30188100
C	3.30419300	2.16846800	0.36090400
C	3.56162500	2.43848900	-0.99647200
C	3.99848500	2.95644600	1.30256100
C	4.45419100	3.44010900	-1.38854900
H	3.06382700	1.85101500	-1.75851600
C	4.89225400	3.95599200	0.91785000
H	3.83519300	2.78094300	2.36134600
C	5.12512300	4.20612700	-0.43582400
H	4.62545700	3.61620600	-2.44893900
H	5.40737800	4.53947500	1.67880800
H	5.82127900	4.98486400	-0.74181200
C	-0.19484400	2.58896100	0.29851900
C	-0.00791600	3.03823800	-1.02225400
C	-1.04612000	3.36380600	1.11343900
C	-0.64921800	4.18089200	-1.50748600
H	0.65095200	2.49913200	-1.69268300
C	-1.68884000	4.50869800	0.63749300
H	-1.20083600	3.06501400	2.14599000
C	-1.49734200	4.92223800	-0.68332000
H	-0.47522100	4.49387500	-2.53479900
H	-2.33031400	5.08336300	1.30345400
H	-1.98874600	5.81794900	-1.05856400

TSS36

O	-0.27742200	0.23016800	-1.91470600
C	0.90974900	-0.10485600	-1.47400900
O	1.84899900	-0.32483600	-2.22672100
C	1.02275600	-0.16387600	0.05109300
B	1.70625700	-1.51708800	0.94869200
B	2.52945400	0.09524000	0.92094900
B	1.24562500	1.39156000	0.83444300
B	-0.08707100	-1.24006500	0.87522600
B	-0.34896200	0.55352200	0.82056900
B	2.27109400	-0.76905400	2.46214600
B	0.69068900	-1.57024200	2.42662000
B	1.99050000	0.97325300	2.39277600
B	0.24322100	1.26634200	2.31957700
B	-0.57446600	-0.31553100	2.33586600
H	3.20852800	-1.23256700	3.03250300
B	0.88524800	-0.05439400	3.31915700
H	0.49147800	-2.62267800	2.94785900
H	2.71327000	1.76405300	2.91134200
H	-0.25872300	2.23970500	2.78061600
H	-1.66223100	-0.46789300	2.79459900
H	0.83348600	-0.01012300	4.50964300
Pd	-1.96904400	0.04660600	-0.75292200
C	-1.76742500	1.94236000	-0.01351500
C	-2.52125600	2.41048800	1.08610800
C	-1.38073700	2.85541100	-1.01747300
C	-2.83163200	3.76329600	1.19447400
H	-2.82972800	1.72296600	1.86290600
C	-1.72057500	4.20364300	-0.91032000
H	-0.81183700	2.50582700	-1.86975700
C	-2.44346600	4.65930300	0.19356300
H	-3.39237400	4.11459700	2.05692300
H	-1.40440600	4.89701500	-1.68455500
H	-2.70242900	5.71223700	0.27729900
I	-4.50674500	-0.26417000	0.05366700
C	-1.05347900	-2.31725000	0.18198400
C	-1.14753400	-2.60706900	-1.20176600
C	-1.88632100	-3.07480000	1.03691300
C	-2.03286300	-3.57859000	-1.69336300
H	-0.49623800	-2.11807100	-1.91508800
C	-2.75515900	-4.04521900	0.55088700
H	-1.84855700	-2.88948600	2.10493500
C	-2.84041600	-4.29955300	-0.82248200
H	-2.06771200	-3.77011300	-2.76309000
H	-3.37833700	-4.60249700	1.24636000

H	-3.52598700	-5.05363500	-1.20112600
C	2.31466400	-2.86608000	0.35591100
C	2.30378500	-3.25616400	-0.99684800
C	2.87736000	-3.78004300	1.26990900
C	2.82267700	-4.48524200	-1.41179700
H	1.91288600	-2.58261400	-1.74974600
C	3.39843200	-5.00870700	0.86287100
H	2.90627500	-3.52255700	2.32413700
C	3.37212700	-5.37080400	-0.48474500
H	2.79722900	-4.74617100	-2.46775400
H	3.82506900	-5.68327900	1.60246700
H	3.77625600	-6.32801800	-0.80747600
C	3.96601600	0.34901600	0.27662900
C	4.76581700	1.39829400	0.77240800
C	4.53667000	-0.45501100	-0.72798400
C	6.05919400	1.63056600	0.30268700
H	4.36755300	2.05085000	1.54210500
C	5.83001800	-0.22946200	-1.20365000
H	3.96325400	-1.26561400	-1.15510800
C	6.60100800	0.81397500	-0.69066400
H	6.64070600	2.45366800	0.71323800
H	6.23274800	-0.87523400	-1.98126000
H	7.60886400	0.99033100	-1.06156400
C	1.58127500	2.76198400	0.09989100
C	1.38970500	3.96329100	0.81005600
C	2.12727000	2.86769300	-1.19357600
C	1.69834800	5.20519300	0.25463700
H	0.98620400	3.92390000	1.81719400
C	2.42966600	4.10879900	-1.75915800
H	2.34006000	1.97434700	-1.76977100
C	2.21411200	5.28532900	-1.04043400
H	1.53480800	6.11077500	0.83542800
H	2.84802000	4.15011300	-2.76242700
H	2.45610600	6.25139500	-1.47880700

TSS39

O	1.01793900	0.55577400	-1.94330300
C	-0.04395000	0.09204200	-2.18013500
O	-0.93134700	-0.35323000	-2.82366800
C	-0.98006300	0.03123100	0.24246800
B	0.08286000	0.88812200	1.30561400
B	-2.63247800	0.07689100	0.78624800
B	0.02628200	-0.86612400	1.30173000
B	0.04397900	0.00487200	2.86402300

B	-0.92159700	1.48296300	2.65247900
B	-1.55817700	1.49068200	0.96317600
C	1.43030800	1.67993700	0.93722000
B	-1.64770100	-1.39439100	0.99387100
B	-2.59392700	0.98031200	2.33461500
B	-2.64367400	-0.79807600	2.35344700
C	-3.94399000	0.11426400	-0.12648000
C	1.28806300	-1.73079200	0.79820500
B	-1.00486500	-1.39437500	2.67004000
H	0.99495400	-0.02342300	3.58945100
B	-1.60096000	0.06559700	3.49067800
H	-0.63725000	2.50131800	3.20870100
C	-1.83368300	2.85021100	0.17224200
C	2.61711800	1.45530900	1.71552000
C	1.49290200	2.75876400	0.01211000
C	-2.01280500	-2.76602100	0.25519600
H	-3.52664300	1.65032800	2.66062200
H	-3.61565500	-1.40730800	2.68434300
C	-3.94987200	0.10582100	-1.53266100
C	-5.20461400	0.16265200	0.50263400
C	1.22283900	-2.57788300	-0.34717000
C	2.45168000	-1.87644500	1.61755700
H	-0.77674500	-2.42135900	3.23695400
H	-1.81327700	0.09537500	4.66684100
C	-1.94381500	2.92526500	-1.22869300
C	-1.99414600	4.05787200	0.87975400
C	3.74926900	2.31785400	1.62341000
H	2.54678300	0.81400300	2.58559800
C	2.60998300	3.56733200	-0.08829200
H	0.63232100	2.96634300	-0.60965700
C	-2.21297500	-2.88871000	-1.13277900
C	-2.19429200	-3.93672200	1.01904000
C	-5.13697800	0.14507200	-2.26928800
H	-3.01010400	0.06124500	-2.06820500
C	-6.39602200	0.20212500	-0.22272000
H	-5.25074700	0.16946500	1.58754900
C	2.18806600	-3.53573300	-0.60101000
H	0.36158400	-2.50657300	-0.99955800
C	3.43513600	-2.86260000	1.35148500
H	2.48040800	-1.36201400	2.57198100
C	-2.18405800	4.13267100	-1.88957900
H	-1.85017100	2.01848400	-1.81579600
C	-2.23632300	5.26964300	0.23023400
H	-1.92646100	4.04400300	1.96370200

C	3.74861500	3.35971800	0.72515100
H	4.59971300	2.14343700	2.27766600
H	2.60903100	4.38812300	-0.80175700
C	-2.56030600	-4.10561800	-1.72580200
H	-2.09434700	-2.01817300	-1.76477700
C	-2.54354400	-5.15643600	0.43666600
H	-2.06232300	-3.88806300	2.09560400
C	-6.36978600	0.19427800	-1.61881800
H	-5.09353800	0.13576800	-3.35709700
H	-7.34733200	0.23923100	0.30545800
C	3.30099000	-3.68869200	0.25258700
H	2.08019500	-4.18866400	-1.46333000
H	4.28162900	-2.96516600	2.02574200
C	-2.32921800	5.31526200	-1.16244800
H	-2.26439700	4.14556400	-2.97492600
H	-2.35328900	6.18072400	0.81450600
H	4.60610900	4.02195100	0.63986300
C	-2.72675500	-5.24969000	-0.94442500
H	-2.70743500	-4.15387500	-2.80326800
H	-2.67430200	-6.03566900	1.06531300
H	-7.29612900	0.22510200	-2.18960500
H	4.04540900	-4.45236000	0.04246900
H	-2.51769600	6.25768200	-1.67298800
H	-2.99997600	-6.19820800	-1.40309700
Pd	3.01591900	-0.12073000	0.11414200
O	4.02852500	-1.17271500	-1.53505000
C	4.48446500	-0.05903400	-1.94193800
O	4.24302600	0.99105500	-1.25636700
C	5.26289000	0.03987300	-3.22688800
H	4.57513000	0.30862700	-4.03733500
H	6.02293000	0.82247200	-3.15164600
H	5.72470900	-0.92118500	-3.46646900

TSS43

O	-0.98013500	-0.41487800	-1.86590700
C	0.14672600	-0.07307900	-1.98691700
O	1.13846600	0.25621400	-2.54227200
C	0.81844800	-0.03952300	0.49169100
B	-0.35925200	-0.87682800	1.44691200
B	2.40068800	-0.11170400	1.21492300
B	-0.27647600	0.87459700	1.45224900
B	-0.46922100	0.00425900	3.00273100
B	0.48789900	-1.48686000	2.89321300
B	1.29504700	-1.50319800	1.27863700

C	-1.66746300	-1.65205900	0.93136900
B	1.42502800	1.36942100	1.31605500
B	2.19059200	-1.01094700	2.75182400
B	2.26753900	0.76513000	2.77487100
C	3.80181700	-0.17248400	0.45013900
C	-1.46875900	1.76174300	0.83611200
B	0.61575100	1.38908300	2.92010900
H	-1.49109000	0.04779500	3.62182200
B	1.09744900	-0.07985600	3.80025400
H	0.13101200	-2.50121200	3.41120900
C	1.63657300	-2.86967400	0.52844000
C	-2.91794900	-1.44944400	1.60541300
C	-1.64982500	-2.69435200	-0.03967600
C	1.89625500	2.72655300	0.61543500
H	3.07414300	-1.69594300	3.16725600
H	3.21024800	1.36146700	3.19689100
C	3.95886000	-0.17894000	-0.94823100
C	4.98518200	-0.23231000	1.21631500
C	-1.28822600	2.61674400	-0.29110300
C	-2.71167400	1.89722500	1.53115800
H	0.34634800	2.42273400	3.45312600
H	1.18659800	-0.10866500	4.98984200
C	1.88340500	-2.95917100	-0.85554300
C	1.72492800	-4.06894500	1.26457800
C	-4.04291900	-2.28553700	1.37399700
H	-2.93404000	-0.82830200	2.49261700
C	-2.74997100	-3.48901900	-0.28321000
H	-0.73733200	-2.88627800	-0.58768000
C	2.21642300	2.83786200	-0.75204500
C	2.05319200	3.89031900	1.39669300
C	5.21127800	-0.24344900	-1.55404300
H	3.08463500	-0.12829900	-1.58356200
C	6.24581800	-0.29698200	0.63395700
H	4.91330800	-0.22872900	2.29883600
C	-2.22277500	3.56659400	-0.64989900
H	-0.36494500	2.55330100	-0.85258500
C	-3.67067000	2.87235300	1.16964200
H	-2.83951900	1.38166800	2.47662200
C	2.18198200	-4.16757700	-1.47957100
H	1.84844000	-2.06116700	-1.46118000
C	2.02265200	-5.28732400	0.66339400
H	1.55507700	-4.04297600	2.33625200
C	-3.96602900	-3.29598900	0.43019300
H	-4.95277800	-2.13523300	1.94623800

H	-2.69627000	-4.28242100	-1.02230900
C	2.65257200	4.03405200	-1.31612200
H	2.12080800	1.97159700	-1.39392700
C	2.48854300	5.09508800	0.85483400
H	1.83055800	3.84764300	2.45784000
C	6.37141200	-0.30422900	-0.76595400
H	5.29763400	-0.24655200	-2.63679100
H	7.13706800	-0.34272200	1.25298600
C	-3.42983100	3.70583700	0.08421200
H	-2.03899500	4.22499800	-1.49294400
H	-4.58444500	2.97397100	1.74622900
C	2.24968100	-5.34903700	-0.72246700
H	2.36858800	-4.20398600	-2.54884500
H	2.08042700	-6.19527700	1.25660300
C	2.79044400	5.17960600	-0.51526000
H	2.89283600	4.08655100	-2.37405000
H	2.59771000	5.97435200	1.48304200
Pd	-3.13894500	0.15522000	-0.02573100
O	-3.96687200	1.22863300	-1.70649000
C	-4.38579500	0.13053300	-2.19933400
O	-4.19297300	-0.93344000	-1.51507200
C	-5.04862400	0.07258300	-3.54211900
H	-4.29209000	-0.16067900	-4.30067600
H	-5.80278700	-0.71872600	-3.55661200
H	-5.49902800	1.03840400	-3.78329400
C	7.66466400	-0.37268700	-1.37873100
N	8.71648200	-0.42887800	-1.87578800
C	3.22961900	6.41805500	-1.08652900
N	3.58027300	7.42693800	-1.55074200
C	-4.39380500	4.69649900	-0.29454100
N	-5.17648400	5.50154100	-0.60004200
C	-5.09438100	-4.14210900	0.17541800
N	-6.00884500	-4.83186200	-0.02929700
C	2.54302600	-6.60125200	-1.35402200
N	2.77392100	-7.62116900	-1.86646900

TSS47

O	-0.29295500	-0.52532600	-2.81327300
C	0.37631300	0.38085500	-2.40559300
O	1.02077800	1.36149500	-2.46026700
C	0.34365500	0.01164200	0.25503300
B	-0.74933100	-0.92726200	1.26296100
B	1.93265000	0.07171400	0.97069500
B	-0.80306600	0.85663000	1.25123300

B	-0.91948600	-0.03604500	2.79953300
B	0.16274800	-1.43496200	2.70191600
B	0.94462000	-1.40941000	1.07553100
C	-1.96928800	-1.81827100	0.69426400
B	0.84963600	1.48869700	1.08657500
B	1.81546900	-0.82260600	2.52646700
B	1.75066200	0.94939900	2.53072900
C	3.33751700	0.05883500	0.19734600
C	-2.06806300	1.62691600	0.61569200
B	0.05493300	1.43293700	2.70242000
H	-1.94314200	-0.06676500	3.41924900
B	0.66468000	0.01860700	3.58460300
H	-0.09761500	-2.47670900	3.22625000
C	1.37915100	-2.78237700	0.37455900
C	-3.14179700	-2.00416700	1.46729800
C	-1.94672600	-2.49282300	-0.56087200
C	1.14068500	2.92556600	0.42936400
H	2.76439200	-1.42487800	2.93036100
H	2.63633300	1.62507800	2.95956200
C	3.51566000	-0.33522600	-1.14044700
C	4.50915400	0.41884600	0.89561100
C	-2.04049000	2.23394300	-0.67468000
C	-3.27968200	1.76083100	1.33434500
H	-0.27873500	2.44254700	3.24593600
H	0.77908000	0.02571200	4.77451400
C	1.40631300	-3.00785200	-1.01397300
C	1.77923700	-3.86464900	1.18459700
C	-4.20394300	-2.79401500	1.03365000
H	-3.19889000	-1.52778200	2.44006900
C	-3.03164700	-3.27360100	-1.00973300
H	-1.03155000	-2.49982000	-1.14216900
C	2.23099500	3.18909700	-0.42226000
C	0.34663700	4.03778800	0.77783300
C	4.77112000	-0.35953100	-1.75284200
H	2.65564200	-0.63889800	-1.72342000
C	5.76944100	0.39923000	0.29682700
H	4.42690000	0.72357700	1.93411700
C	-3.16279900	2.90140800	-1.20794300
H	-1.09486100	2.29937800	-1.20518700
C	-4.38081900	2.43996800	0.81565200
H	-3.33903500	1.33147200	2.32940200
C	1.79948200	-4.23063100	-1.56548800
H	1.10838900	-2.21164600	-1.68675100
C	2.17536400	-5.09026800	0.64711100

H	1.78151800	-3.73812300	2.26284900
C	-4.16296300	-3.42630800	-0.21489300
H	-5.07552600	-2.91707100	1.67331100
H	-2.95591500	-3.78540700	-1.96665100
C	2.50529000	4.47168600	-0.90231100
H	2.88200500	2.37660500	-0.71973000
C	0.60847600	5.32435600	0.30157100
H	-0.49294300	3.89678700	1.45182200
C	5.90955200	0.01083800	-1.03706000
H	4.85659300	-0.67335200	-2.79166000
H	6.64469400	0.68828800	0.87610500
C	-4.33528000	3.00484100	-0.46465400
H	-3.08627900	3.37179200	-2.18578200
H	-5.28637600	2.52738900	1.41243900
C	2.18738300	-5.28282600	-0.73603900
H	1.80615900	-4.35570000	-2.64700000
H	2.47736700	-5.89724200	1.31245500
H	-4.99570400	-4.03960800	-0.55088500
C	1.69372400	5.54991900	-0.54632000
H	3.36082300	4.62552800	-1.55748700
H	-0.03439500	6.15079800	0.60040800
H	6.89002400	-0.00615800	-1.50919600
H	-5.19778900	3.53132900	-0.86606200
H	2.49710900	-6.23629900	-1.15955700
H	1.90643800	6.55031300	-0.91919800
Ag	-2.25691000	-0.15325800	-1.24440400

TSS51

O	-0.33431800	-0.50347900	-2.58254000
C	0.35799100	0.39360500	-2.19612000
O	1.02737200	1.35515300	-2.25819100
C	0.32400400	0.05074200	0.45907200
B	-0.71158900	-0.98890500	1.42652800
B	1.86932800	0.25768600	1.24587200
B	-0.93288100	0.77522600	1.41468300
B	-1.02577400	-0.12873600	2.95966000
B	0.18653200	-1.41664800	2.90205700
B	1.02265200	-1.30328900	1.30619400
C	-1.82148900	-1.99268400	0.82732700
B	0.65482400	1.55791100	1.31330700
B	1.77810500	-0.64893600	2.79473100
B	1.54477200	1.11018600	2.79615800
C	3.30155300	0.37689100	0.53667900
C	-2.24140500	1.43634600	0.75183600

B	-0.19452500	1.42672400	2.89874500
H	-2.06545100	-0.25780000	3.53494600
B	0.51217900	0.07581600	3.80670100
H	0.00846800	-2.48232400	3.40965300
C	1.60794800	-2.62147200	0.61507800
C	-2.96826200	-2.31950900	1.59435100
C	-1.72382300	-2.63653600	-0.44079500
C	0.83653100	3.01047400	0.65454500
H	2.76347600	-1.16091400	3.23048300
H	2.34384400	1.86684500	3.25511900
C	3.57559800	0.00075800	-0.79130300
C	4.40172100	0.83933200	1.29108200
C	-2.24310600	2.05280200	-0.53454700
C	-3.47155500	1.46719400	1.45454300
H	-0.64370800	2.39880700	3.42464100
H	0.57837700	0.08944900	4.99777800
C	1.68484100	-2.83349000	-0.77483300
C	2.09125900	-3.66477700	1.43252400
C	-3.94109600	-3.20354400	1.14747500
H	-3.07672900	-1.87442100	2.57680600
C	-2.71108200	-3.51821700	-0.91276800
H	-0.81808000	-2.52701200	-1.02559900
C	1.89754000	3.34952900	-0.20867400
C	-0.04026500	4.05995900	1.00375800
C	4.84941500	0.08354600	-1.34637400
H	2.77380300	-0.36734500	-1.41615000
C	5.68352300	0.93276900	0.76053500
H	4.24511000	1.13353300	2.32311600
C	-3.39839400	2.63617000	-1.08271800
H	-1.30060000	2.18663500	-1.05719400
C	-4.61503500	2.05725600	0.93113800
H	-3.51129600	1.02786200	2.44538300
C	2.19658300	-4.00503800	-1.32667100
H	1.33051800	-2.06346700	-1.45072500
C	2.60809100	-4.84386900	0.90672100
H	2.06035700	-3.54484000	2.51040300
C	-3.82972500	-3.80545900	-0.12139000
H	-4.79865900	-3.43469400	1.77234200
H	-2.58939500	-4.00292700	-1.87690200
C	2.07109600	4.63831600	-0.70476700
H	2.60932600	2.59028100	-0.50429000
C	0.11005900	5.35546300	0.51911400
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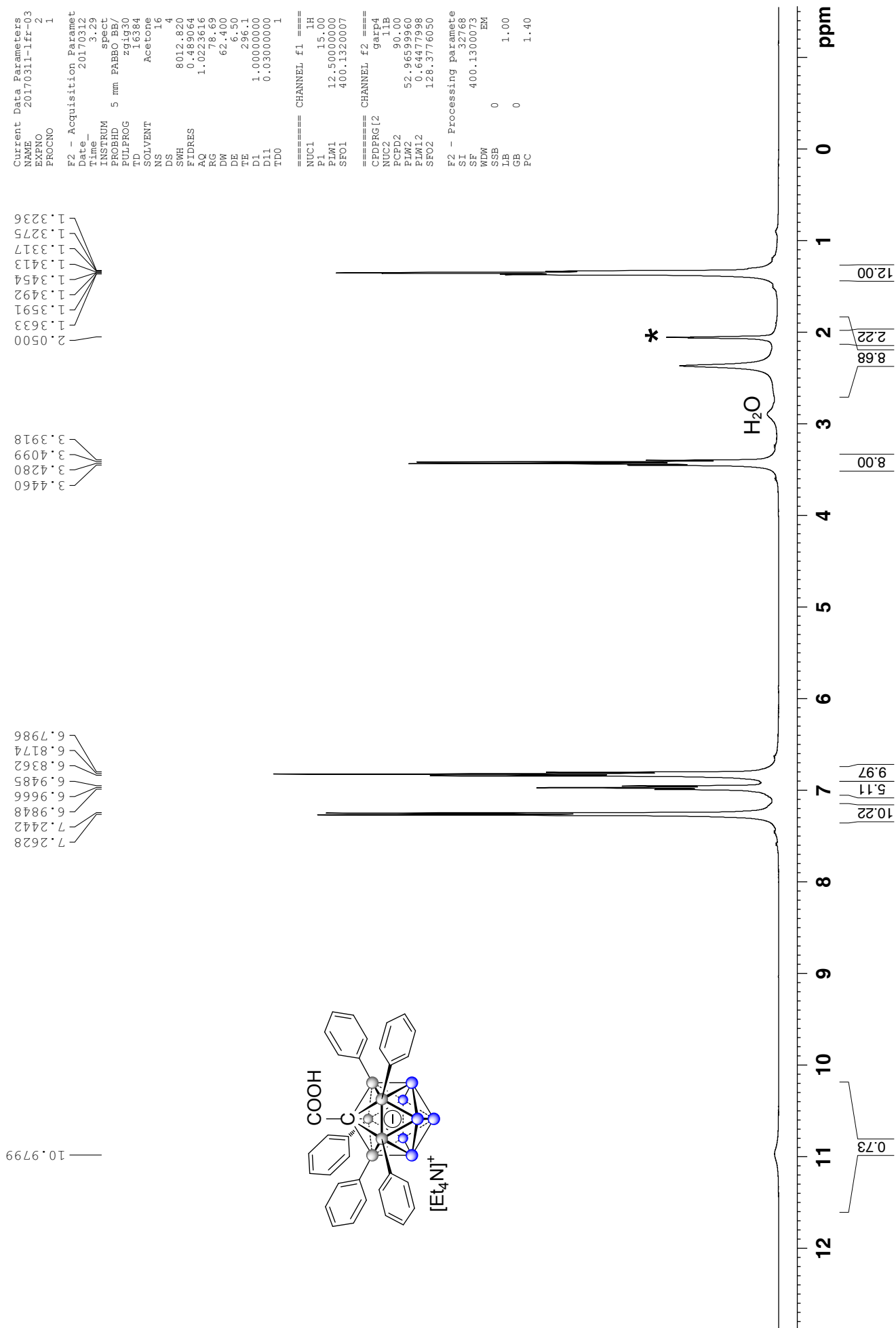
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C	2.66337900	-5.02792000	-0.48579900
H	2.24005300	-4.13411800	-2.40434600
H	2.97046100	-5.62780500	1.56522400
C	1.17301700	5.65763600	-0.34811700
H	2.90118600	4.86216600	-1.36830200
H	-0.58526900	6.13739800	0.81049700
Ag	-2.34718500	-0.35209100	-1.12359900
C	-5.77813600	3.23330900	-0.89876600
N	-6.74288300	3.70996900	-1.34195500
C	1.33732700	6.98658400	-0.85789600
N	1.46570800	8.06704100	-1.27325400
C	7.23669500	0.64884700	-1.13208800
N	8.30561600	0.72681100	-1.58785100
C	3.18334600	-6.24241700	-1.03999900
N	3.60059400	-7.23145800	-1.49152700
C	-4.84421600	-4.70211300	-0.59188300
N	-5.67306000	-5.42469500	-0.97315000

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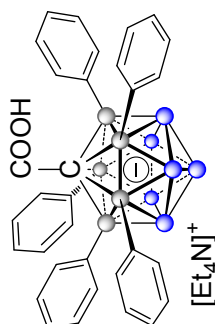
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20170311-lfr-0358 [NEt₄][COOH-CB₁₁H₆-Ph₅]
400 MHz, ¹H{¹B} NMR, ca. 24 mg dissolved in 0.55 mL acetone-d₆*



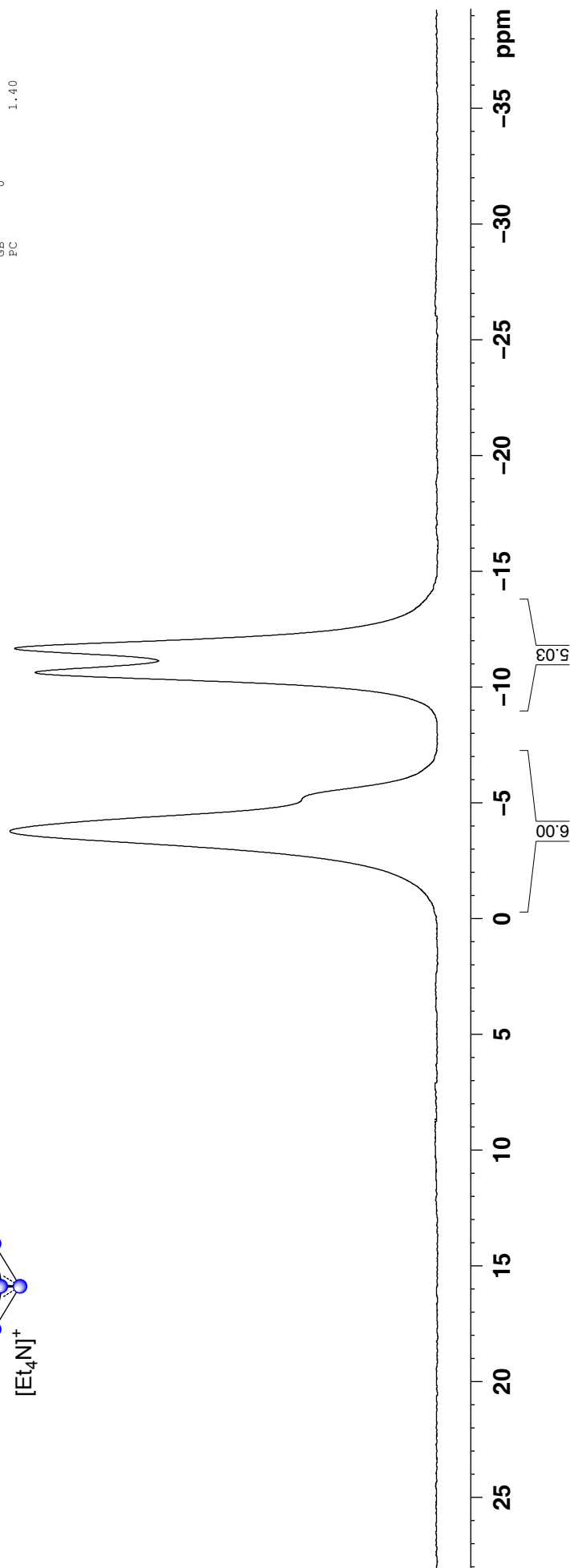
20170311-lfr-0358 [NEt₄][COOH-CB₁₁H₆-Ph₅]
 128 MHz, ¹¹B NMR, ca. 24 mg dissolved in 0.55 mL acetone-d₆

— 10.6561 — 11.6942
 — 3.8013 — 5.3307

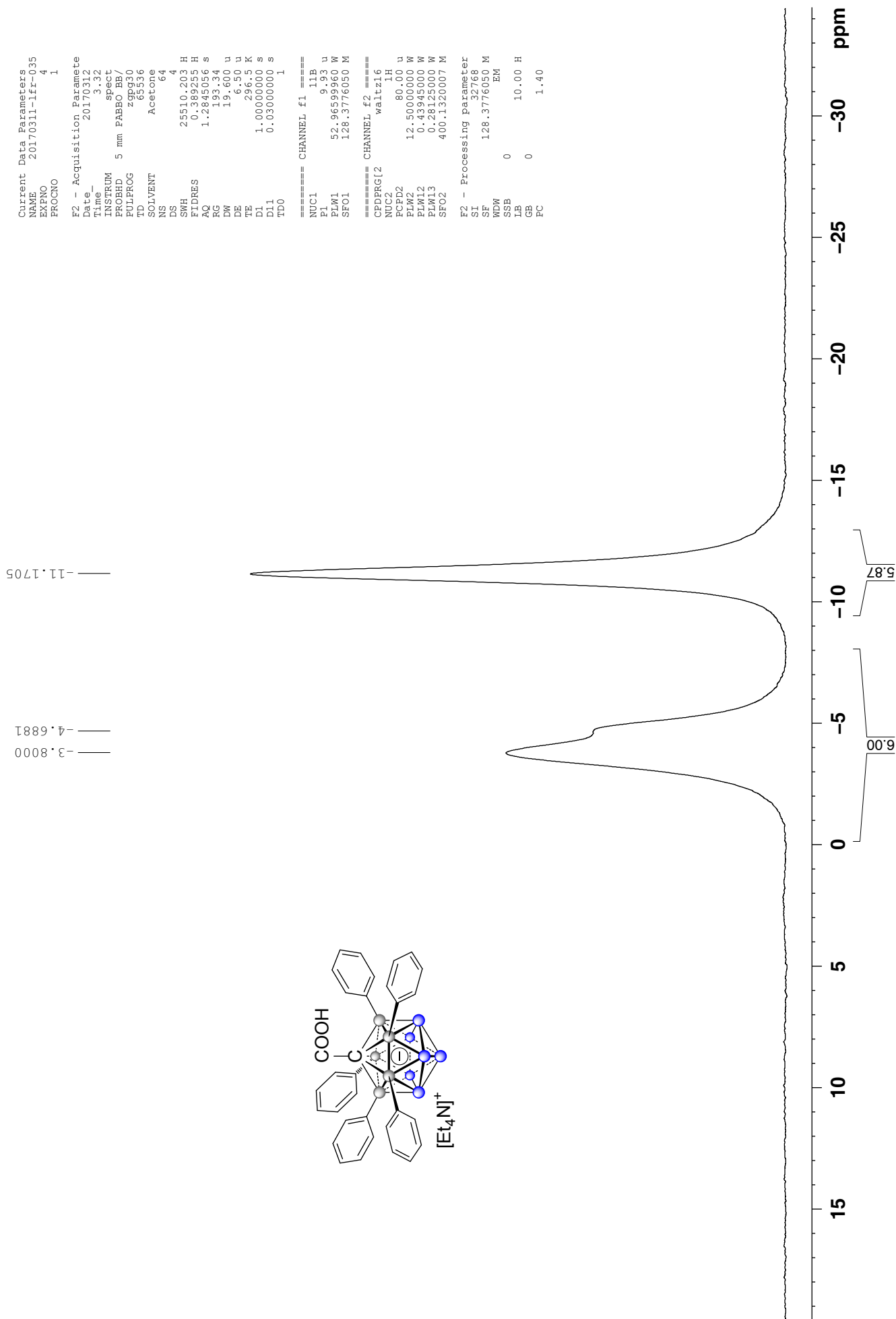


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 PROCNO 1
 F2 - Acquisition Parameters
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 Time 3.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg
 TD 65536
 SOLVENT Acetone
 NS 64
 DS 4
 SWH 25510.203 H
 FIDRES 0.389255 H
 AQ 1.2845056 s
 RG 193.34
 DW 19.600 u
 DE 6.50 u
 TE 295.8 K
 D1 1.00000000 s
 TD0 1

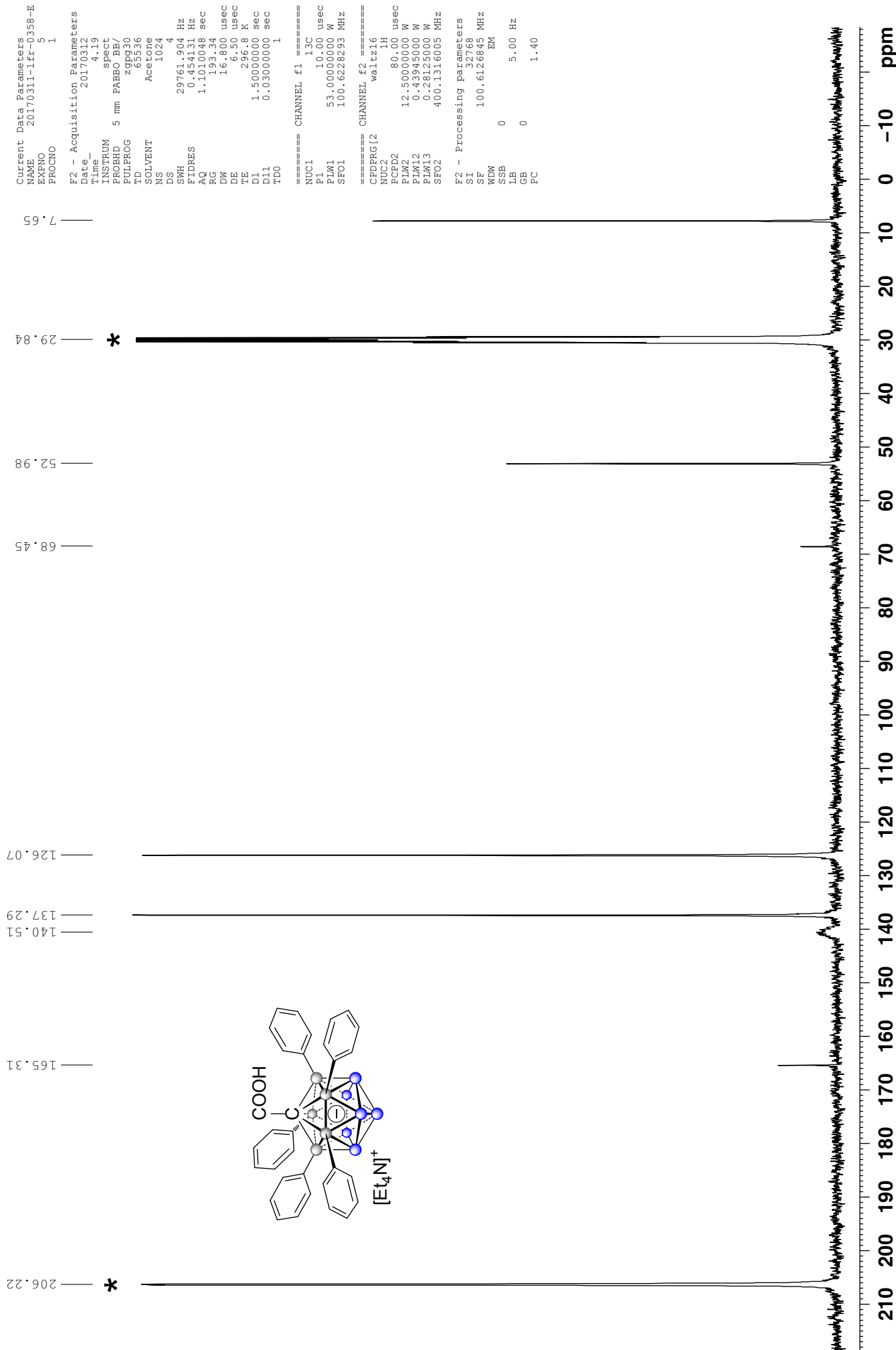
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 P1 9.93 u
 PLW1 52.9659960 W
 SFO1 128.3776052 M
 F2 - Processing parameters
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 SF 128.3776050 M
 WDW EM
 SSB 0
 LB 10.00 H
 GB 0
 PC 1.40



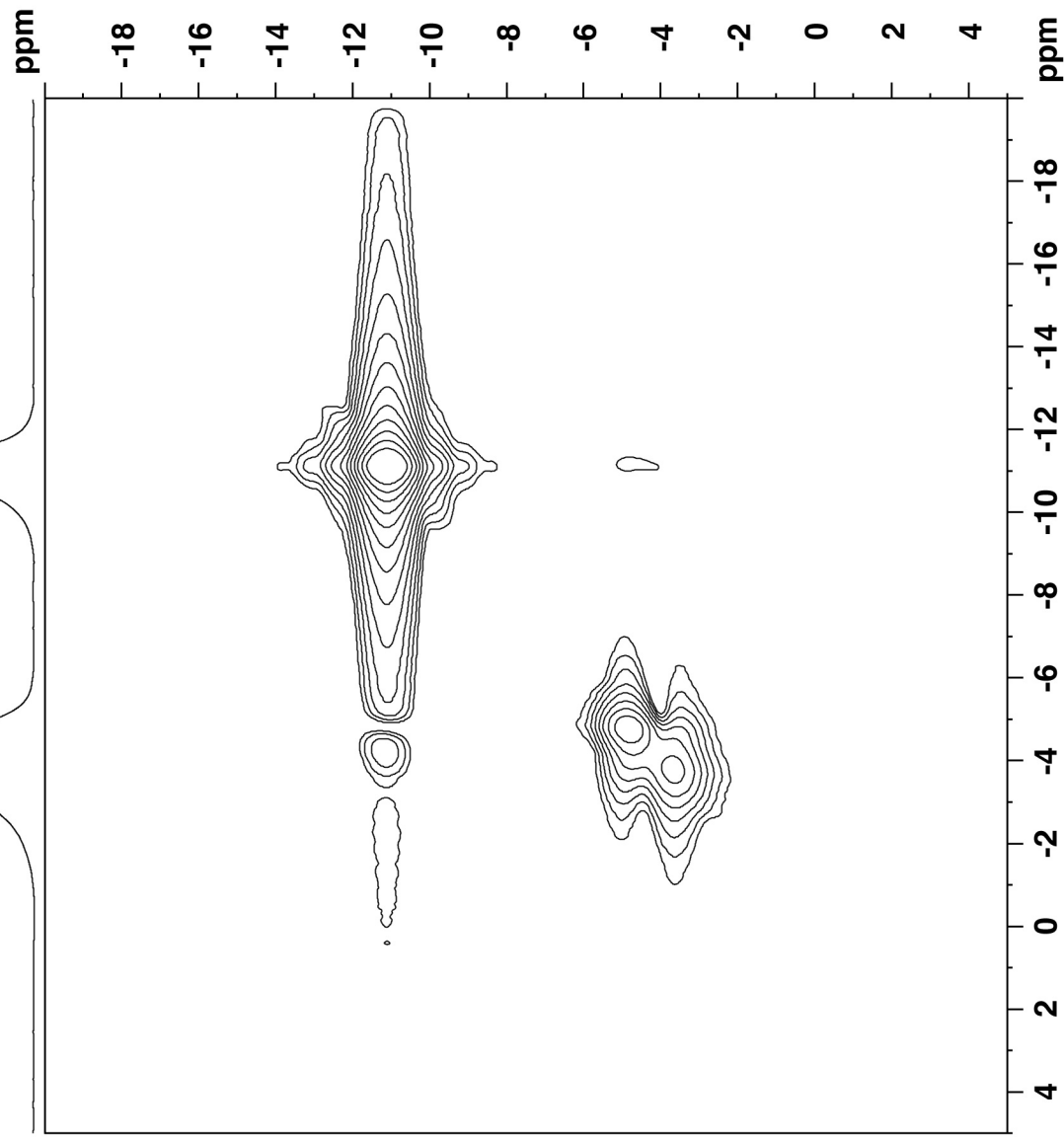
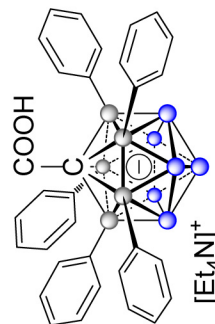
20170311-lfr-0358 [NEt₄][COOH-CB₁₁H₆-Ph₅]
 128 MHz, ¹B{¹H} NMR, ca. 24 mg dissolved in 0.55 mL acetone-d₆



20170311-lfr-0358 [NEt₄][COOH-CB₁₁H₆-Ph₅]
101 MHz, ¹³C{¹H} NMR, ca. 24 mg dissolved in 0.55 mL acetone-d₆*



20170311-lfr-0358 [NEt₄][COOH-CB₁₁H₆-Ph₅]
 160 MHz, ¹¹B{¹H}-¹¹B{¹H} COSY NMR, ca. 24 mg dissolved in 0.55 mL acetone-d₆



```

Current Data Parameters
NAME      20170311-lfr-0358-E4
EXPNO     11
PROCNO    1

F2 - Acquisition Parameters
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Time_     16.37
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PULPROG   cosygpqfdec
TD        2566
SOLVENT   Acetone
NS        32
DS        16
SWH        6421.233 Hz
FIDRES     2.502429 Hz
AQ         0.1998059 sec
RG         203
DM         77.867 usec
DE         6.50 usec
TE         294.9 K
D0         0.00000300 sec
D1         0.30000001 sec
D11        0.03000000 sec
D13        0.00000400 sec
D16        0.00020000 sec
IN0        0.00013550 sec

===== CHANNEL f1 =====
NUC1       11B
P0         13.10 usec
PL1        13.10 usec
PLW1       95.00000000 W
SFO1       160.4615790 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
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PCPD2      80.10 usec
PLW2       19.00000000 W
PLW12      0.40639001 W
SFO2       500.1312000 MHz

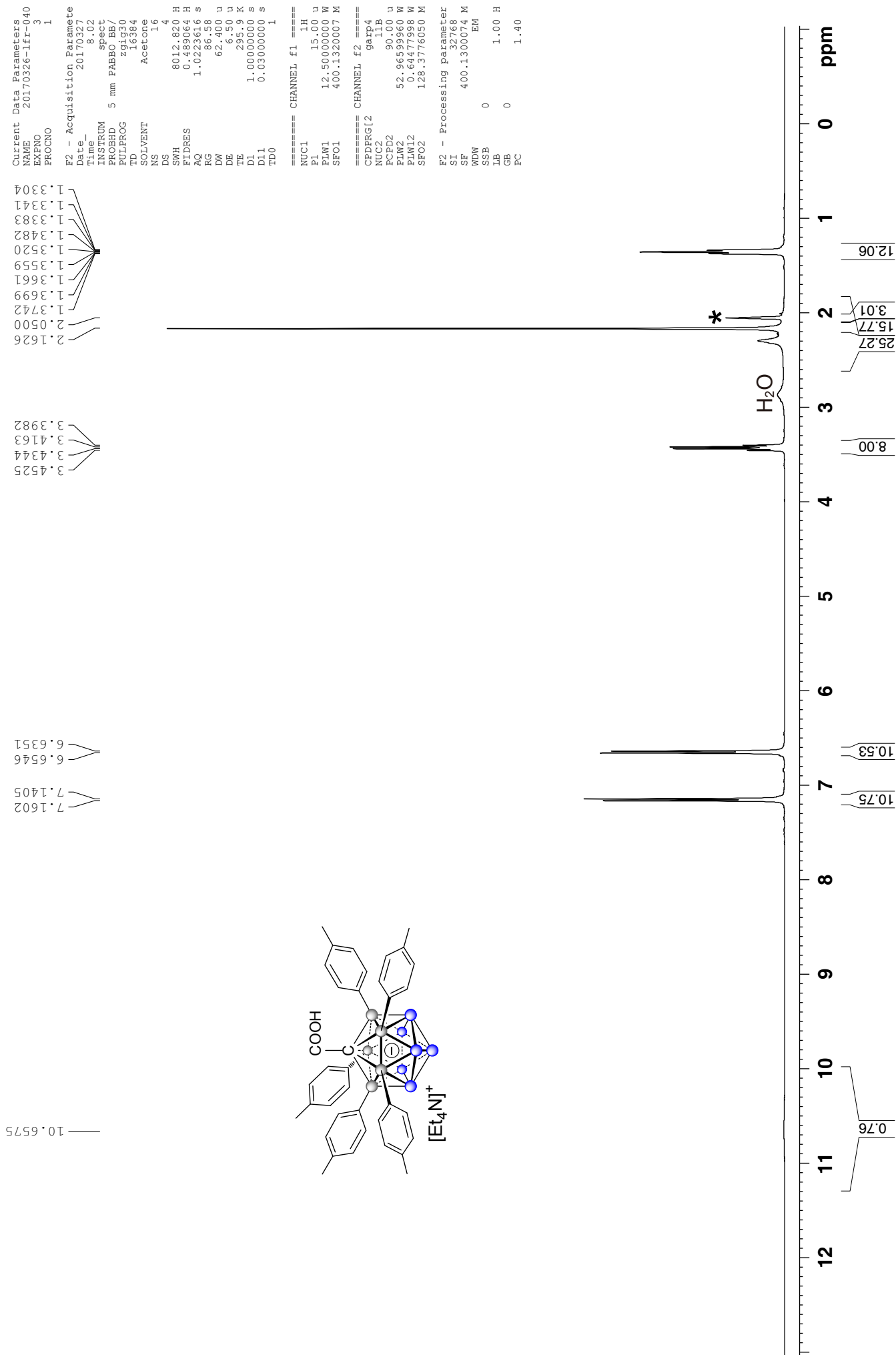
===== GRADIENT CHANNEL =====
GPNAM[1]   SMSQ10.100
GPZ1       10.00 %
P16        1000.00 usec

F1 - Acquisition parameters
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SFO1       160.4616 MHz
FIDRES     115.331413 Hz
SW         46.000 ppm
FhMODE     QF

F2 - Processing parameters
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SF         160.4615766 MHz
WDW        EM
SSB        0
LB         20.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        QF
SF         160.4615703 MHz
WDW        SINE
SSB        0 Hz
LB         0
GB         0
  
```

20170326-lfr-0403 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Me)₅]
 400 MHz, ¹H{¹B} NMR, 24 mg dissolved in 0.55 mL acetone-d₆*

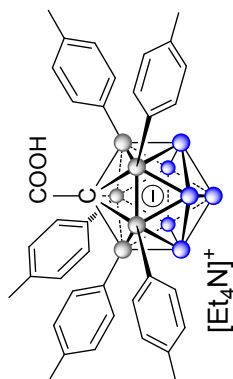


20170326-lfr-0403 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Me)₅]
 128 MHz, ¹¹B NMR, 24 mg dissolved in 0.55 mL acetone-d₆

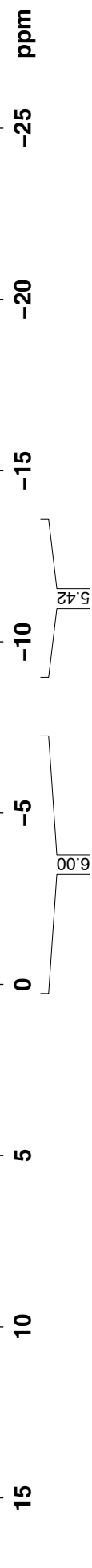
3.8184

10.8319

11.8350



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 PULPROG zg
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 H
 FIDRES 0.389255 H
 AQ 1.2845056 s
 RG 193.34
 DW 19.600 u
 DE 6.50 u
 TE 295.6 K
 D1 1.0000000 s
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 u
 PLW1 52.9659960 W
 SFO1 128.3776052 M
 F2 - Processing parameters
 SI 32768
 SF 128.3776050 M
 WDW EM
 SSB 0
 LB 10.00 H
 GB 0
 PC 1.40



20170326-lfr-0403 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Me)₅]
 128 MHz, ¹B{¹H} NMR, 24 mg dissolved in 0.55 mL acetone-d₆

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Current Data Parameters
NAME      20170326-lfr-040
EXPNO     4
PROCNO    1

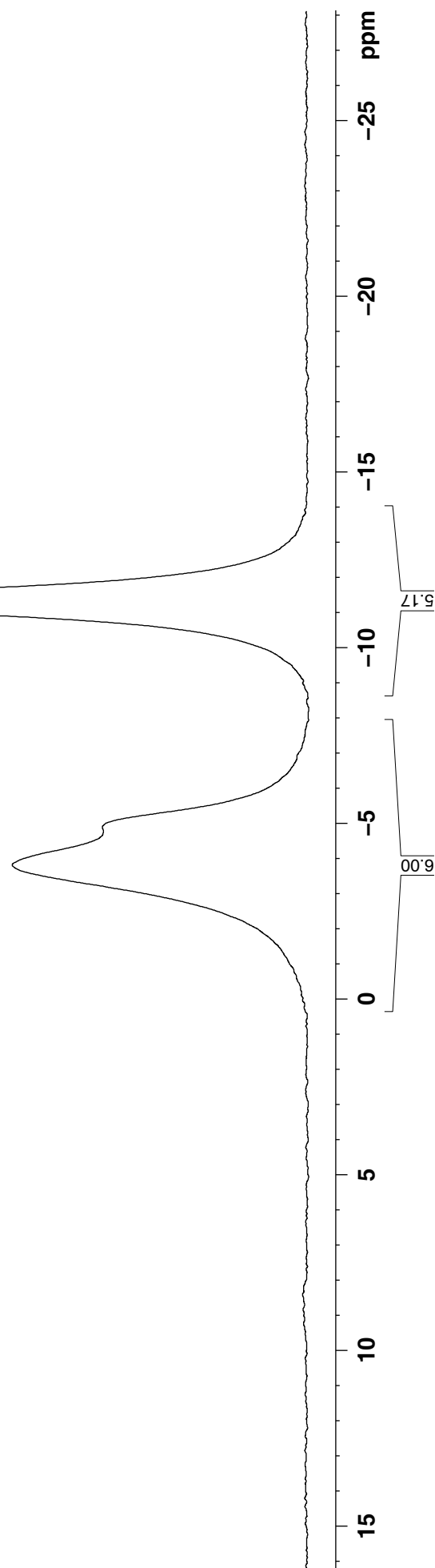
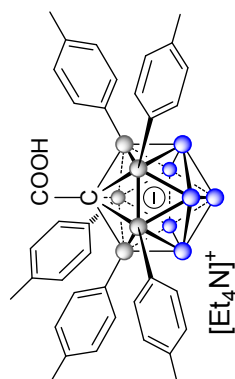
F2 - Acquisition Parameters
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Time      8.08
INSTRUM   spect
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PULPROG   zgpg30
TD        65536
SOLVENT   Acetone
NS        128
DS        4
SWH       25510.203 H
FIDRES    0.389255 H
AQ        1.2845056 s
RG        193.34
DW        19.600 u
DE        6.50 u
TE        296.4 K
D1        1.0000000 s
D11       0.0300000 s
TD0       1

===== CHANNEL f1 =====
NUC1      11B
P1        9.93 u
PLW1     52.9659960 W
SFO1     128.3776050 M

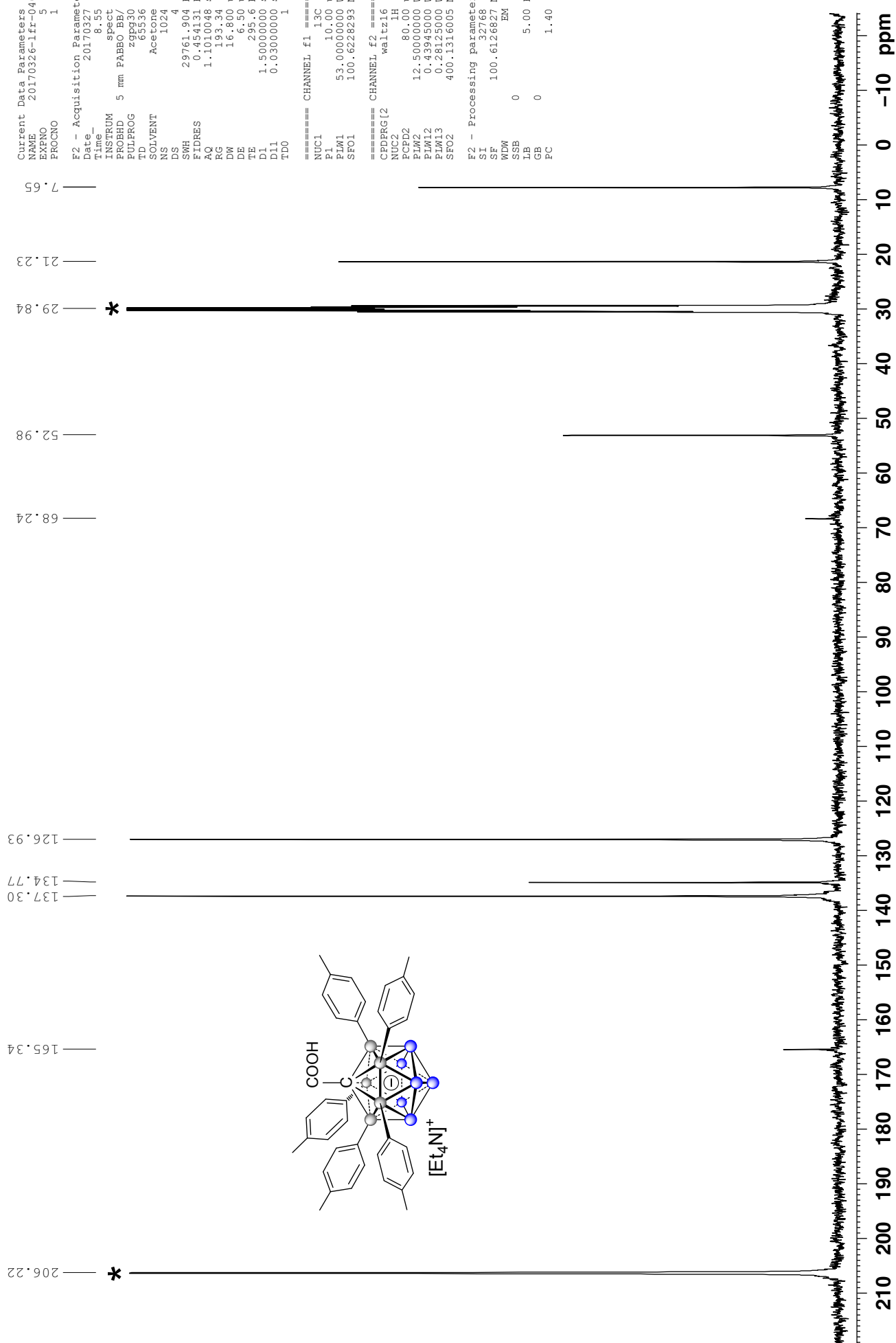
===== CHANNEL f2 =====
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PCPD2     80.00 u
PLW2     12.5000000 W
PLW12    0.4394500 W
PLW13    0.2812500 W
SFO2     400.1320007 M

F2 - Processing parameters
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SF        128.3776050 M
WDW       EM
SSB       0
LB        10.00 H
GB        0
PC        1.40
  
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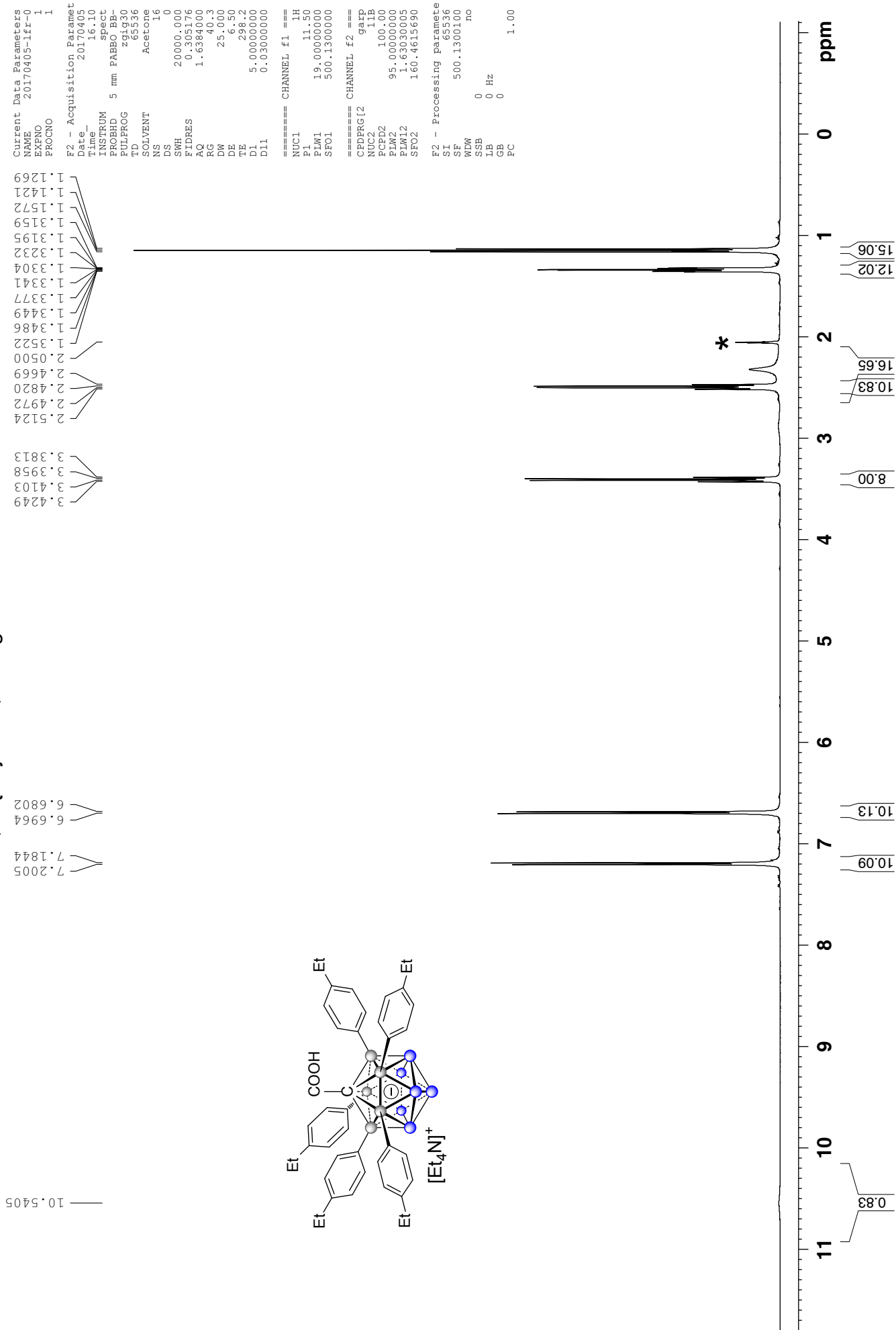
— 4.9878 —
 — 3.8278 —
 — 11.3321 —



20170326-lfr-0403 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Me)₅]
 101 MHz, ¹³C{¹H} NMR, 24 mg dissolved in 0.55 mL acetone-d₆*



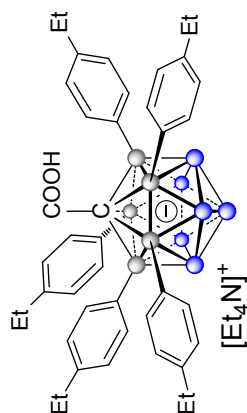
20170405-lfr-0410 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Et)₅]
500 MHz, ¹H{¹B} NMR, 35 mg dissolved in acetone-d₆*



20170405-lfr-0410 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Et)₅]
128 MHz, ¹¹B NMR, 35 mg dissolved in acetone-d₆

— -3.9262

— -11.0482
— -11.8185

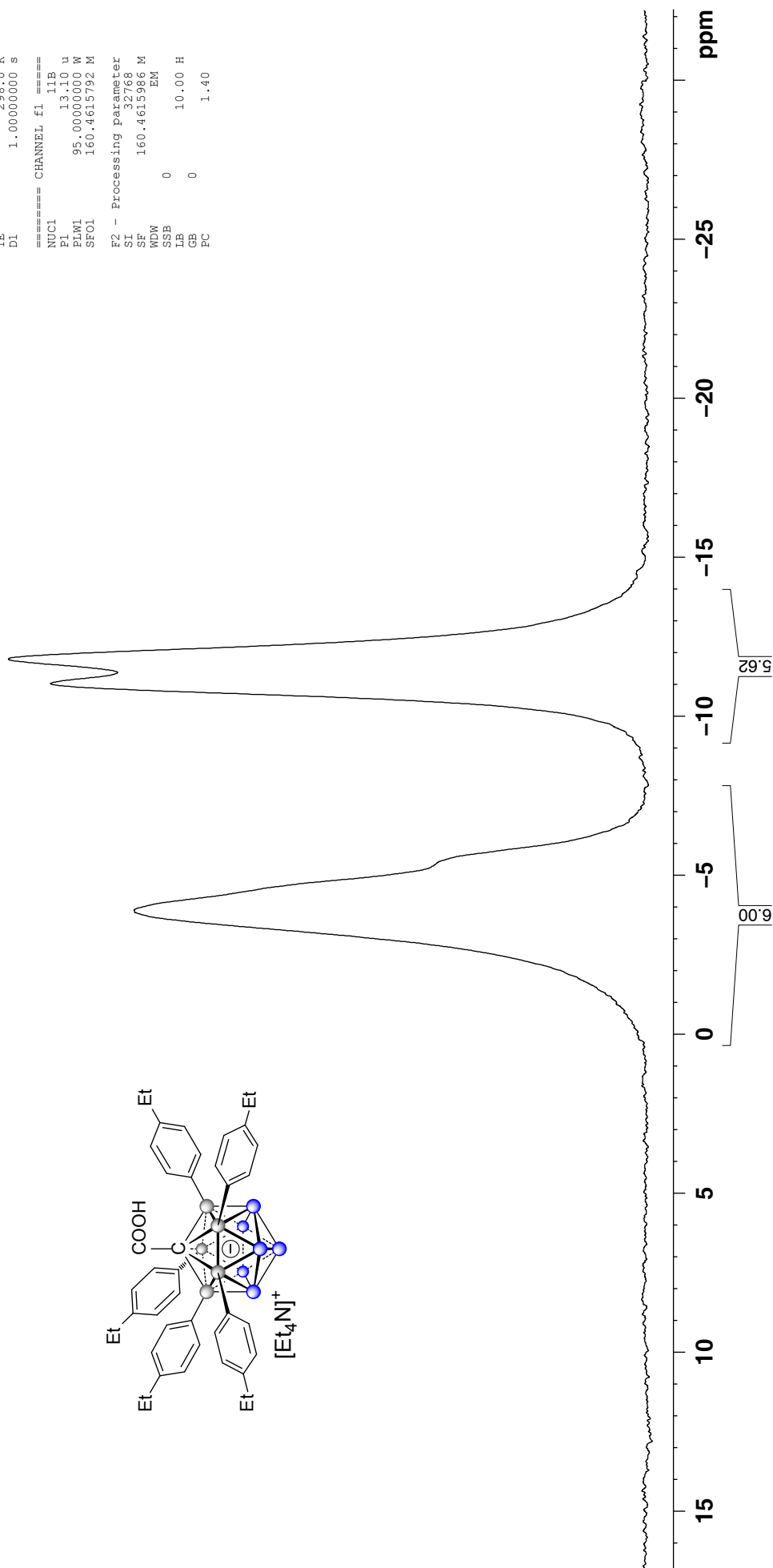


Current Data Parameters
NAME 20170405-lfr-041
EXPNO 2
PROCNO 1

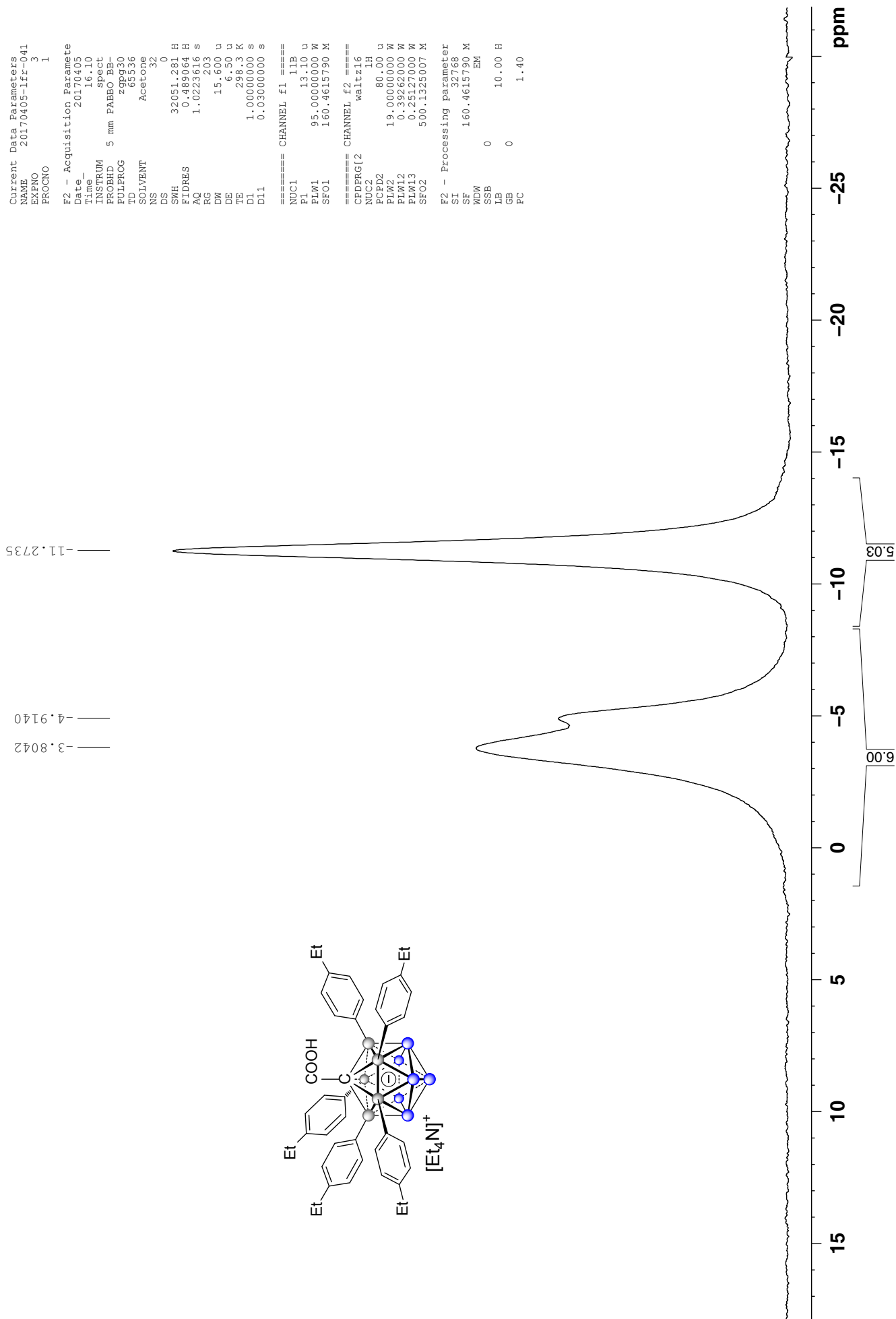
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Time_ 16.08
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SOLVENT Acetone
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DS 0
SWH 32051.281 H
FIDRES 0.500036 H
AQ 0.9999288 S
RG 203
DW 15.600 u
DE 6.50 u
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D1 1.00000000 S

===== CHANNEL f1 =====
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P1 13.10 u
PLW1 95.00000000 W
SFO1 160.4615792 M

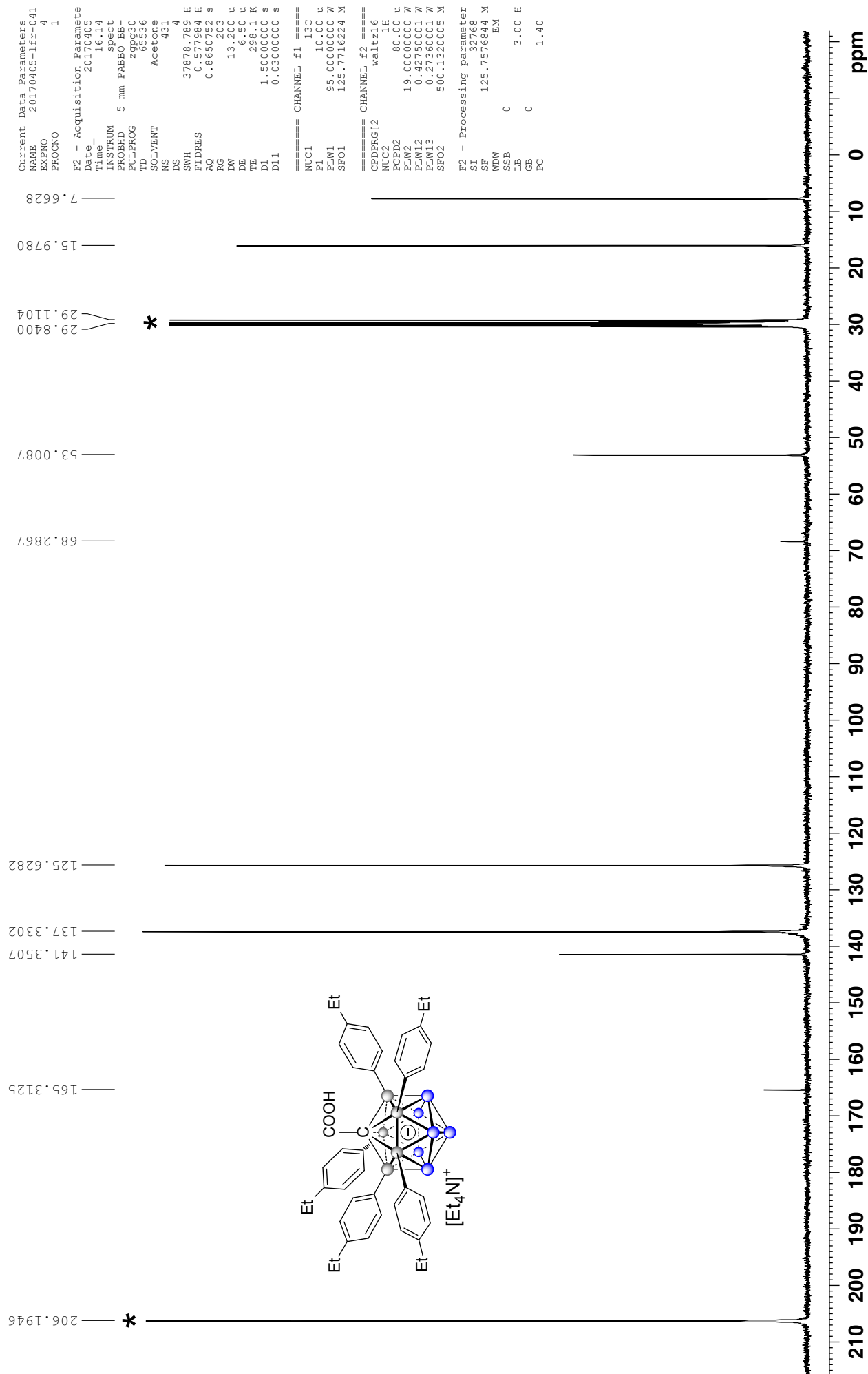
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SSB 0
LB 10.00 H
GB 0
PC 1.40



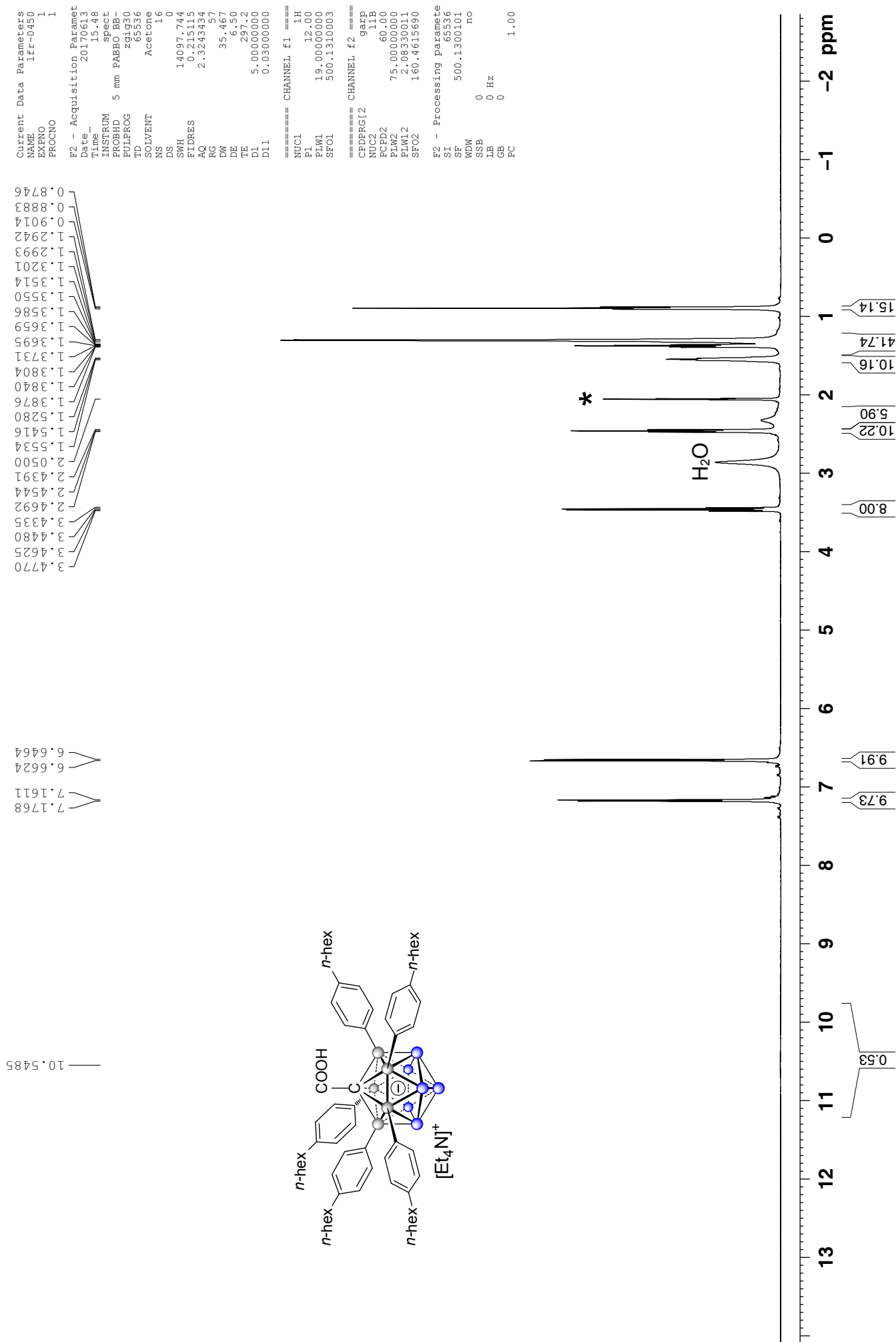
20170405-lfr-0410 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Et)₅]
128 MHz, ¹B{¹H} NMR, 35 mg dissolved in acetone-d₆



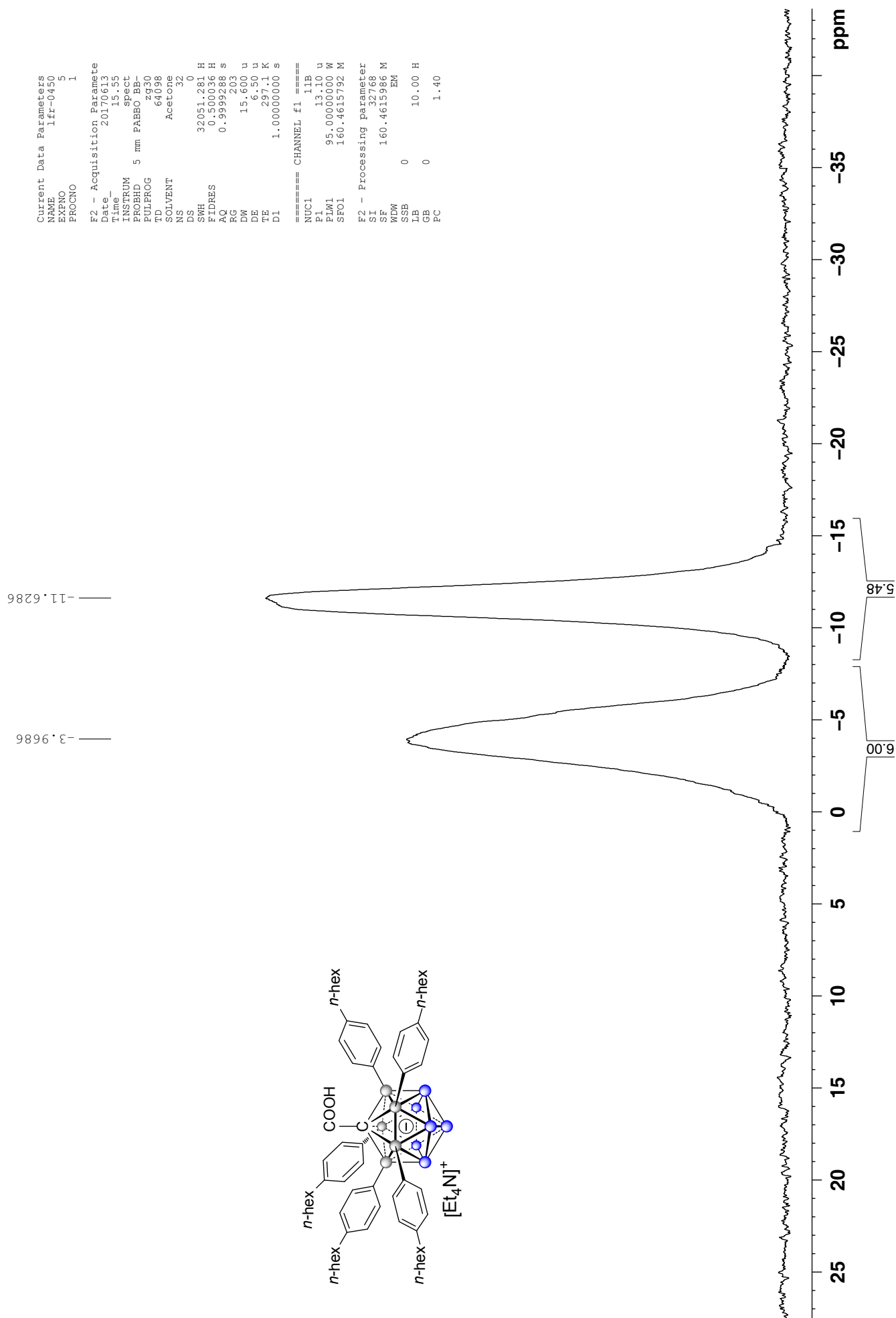
20170405-lfr-0410 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Et)₅]
 126 MHz, ¹³C{¹H} NMR, 35 mg dissolved in acetone-d₆*



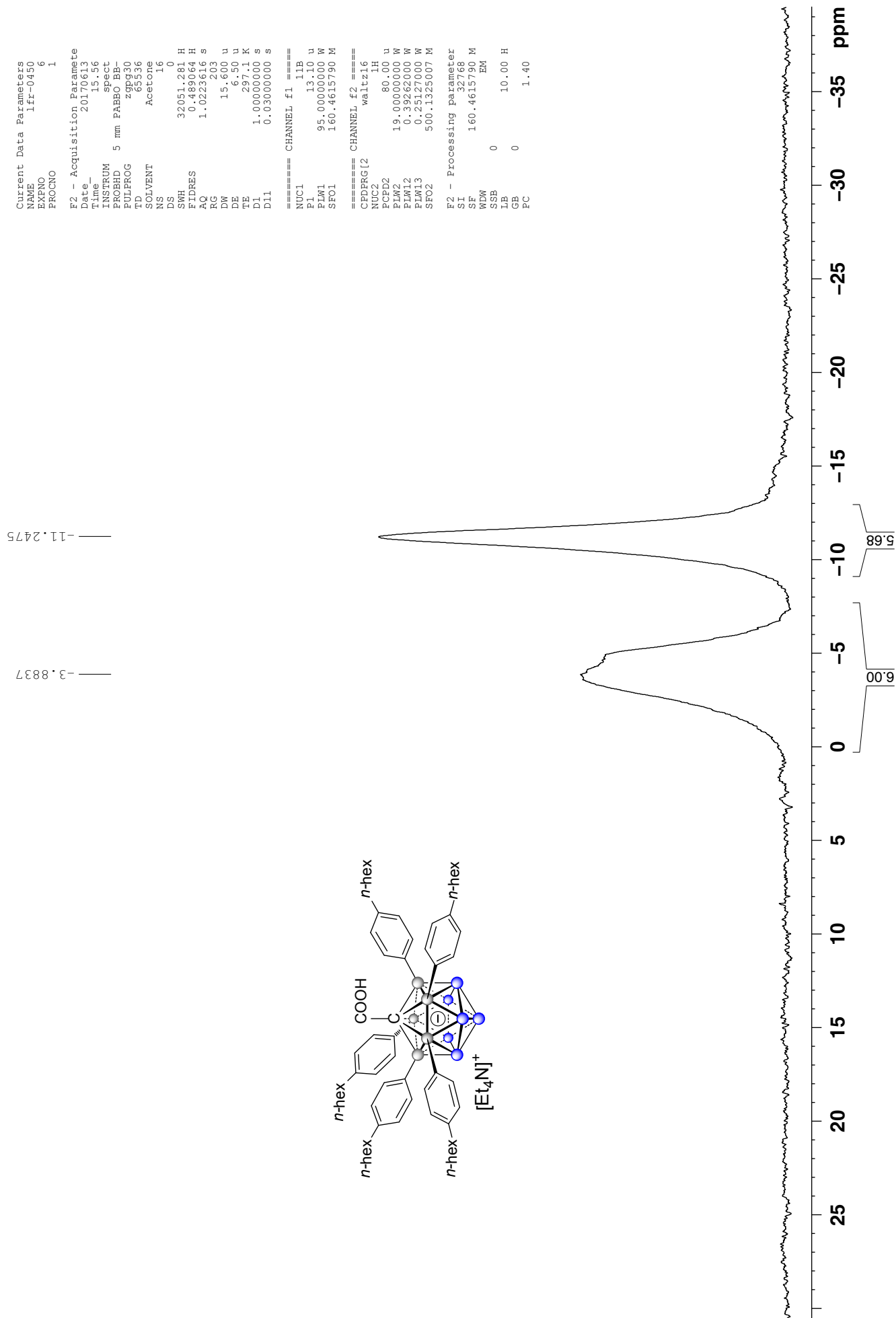
20170612-lfr-0450 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-n-Hex)₅]
 500 MHz, ¹H{¹B} NMR, 15 mg dissolved in 0.55 mL acetone-d₆*



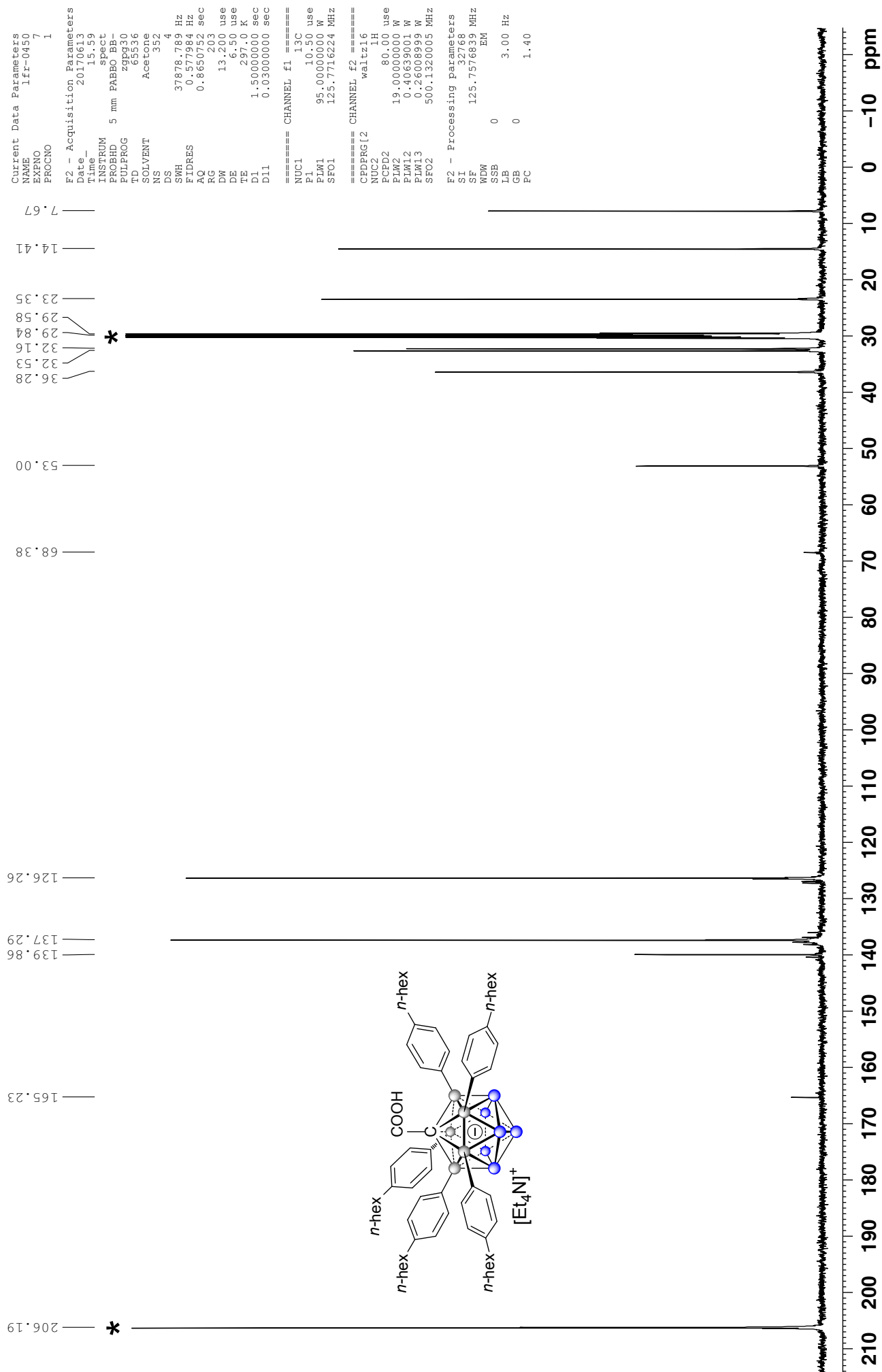
20170612-lfr-0450 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-n-Hex)₅]
 160 MHz, ¹¹B NMR, 40 mg dissolved in 0.55 mL acetone-d₆



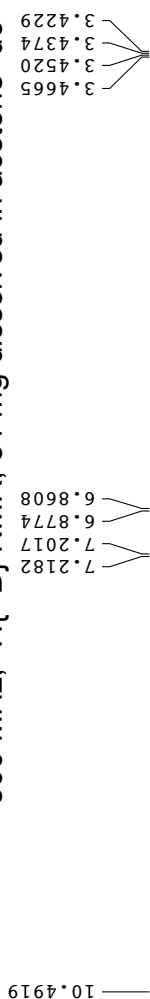
20170612-lfr-0450 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-n-Hex)₅]
 160 MHz, ¹¹B{¹H} NMR, 40 mg dissolved in 0.55 mL acetone-d₆



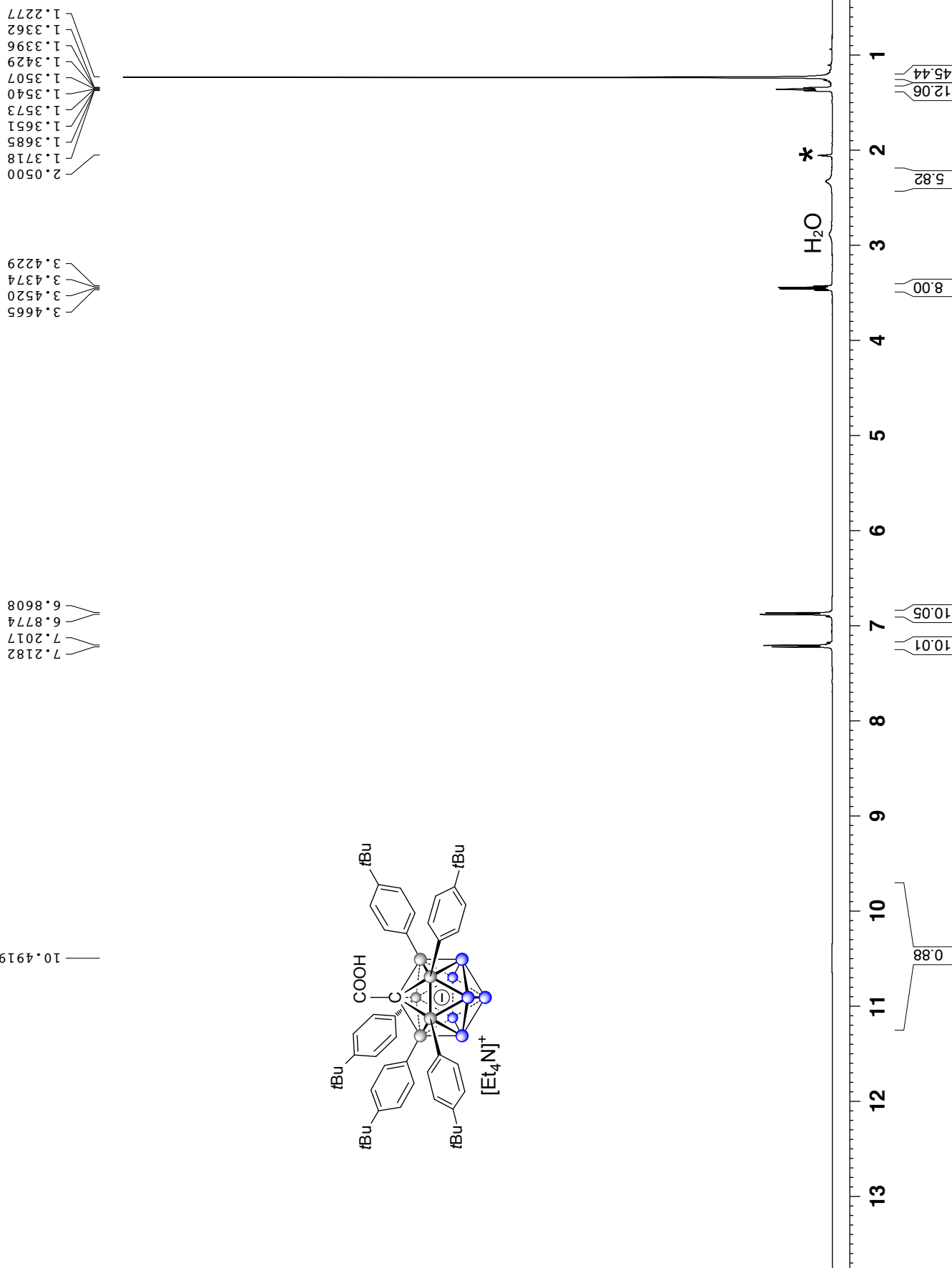
20170612-lfr-0450 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-n-Hex)₅]
 126 MHz, ¹³C{¹H} NMR, 40 mg dissolved in 0.55 mL acetone-d₆*



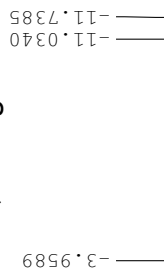
20170511-lfr-0428 [NEt₄][COOH-CB₁₁H₅-(C₆H₄-p-tBu)₅]
500 MHz, ¹H{¹B} NMR, 31 mg dissolved in acetone-d₆*



Current Data Parameters
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PROCNO 1
F2 - Acquisition Parameters
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Time_ 16.03
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PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 20000.000
FIDRES 0.305176
AQ 1.6384000
RG 40.3
DW 25.000
DE 6.50
TE 295.4
D1 5.00000000
D11 0.03000000
===== CHANNEL f1 =====
NUC1 1H
P1 11.70
PLW1 19.00000000
SFO1 500.1300000
===== CHANNEL f2 =====
CPDPRG[2] garp
NUC2 11B
PCPD2 100.00
PLW2 95.00000000
PLW12 1.63030005
SFO2 160.4615690
F2 - Processing Parameters
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SF 500.1300102
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



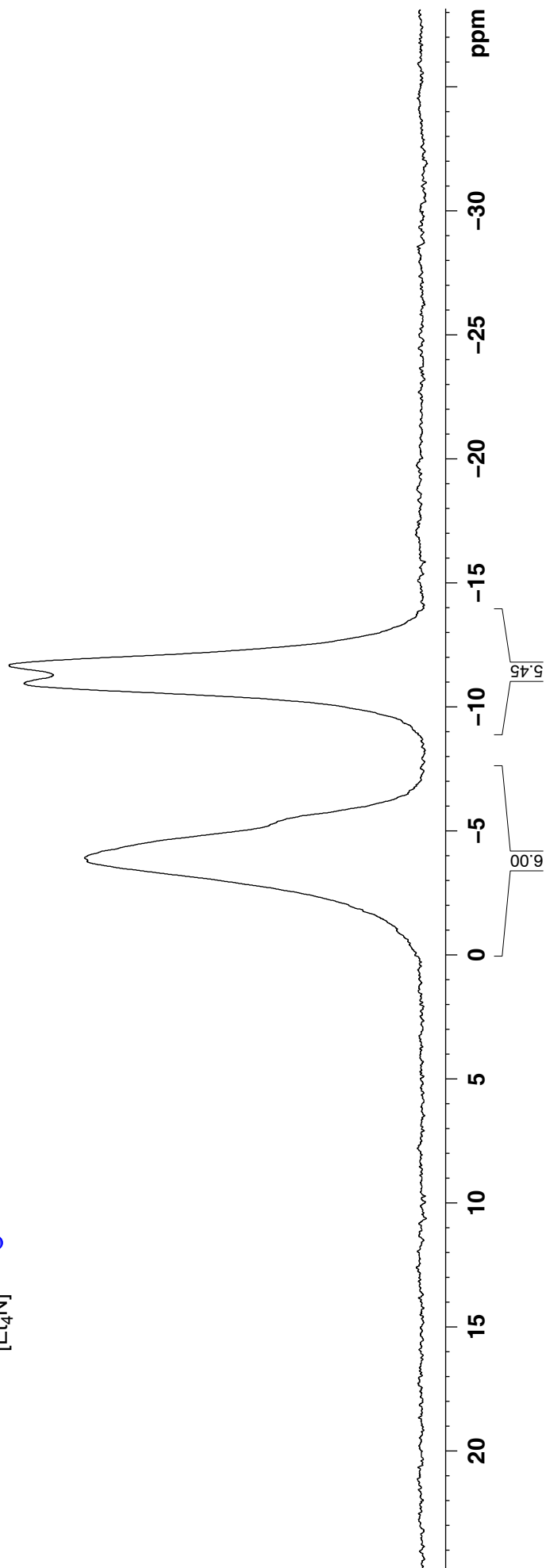
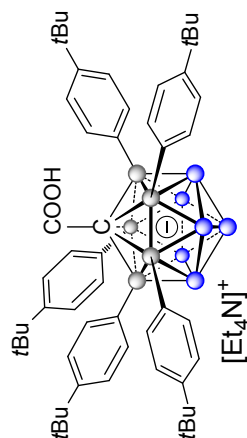
20170511-lfr-0428 [NEt₄][COOH-CB₁₁H₅-(C₆H₄-p-tBu)₅]
160 MHz, ¹¹B NMR, 31 mg dissolved in acetone-d₆



Current Data Parameters
NAME 20170511-lfr-0428
EXPNO 2
PROCNO 1

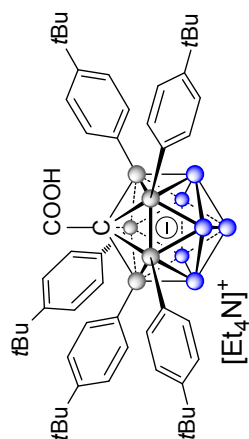
F2 - Acquisition Parameter
Date_ 20170511
Time_ 16.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 64098
SOLVENT Acetone
NS 32
DS 0
SWH 32051.281 H
FIDRES 0.500036 H
AQ 0.9999288 s
RG 203
DW 15.600 u
DE 6.50 u
TE 295.4 K
D1 0.5000000 s

===== CHANNEL f1 =====
NUC1 11B
P1 13.10 u
PLW1 95.0000000 W
SF01 160.4615792 M
F2 - Processing parameter
SI 32768
SF 160.4615986 M
WDW EM
SSB 0
LB 10.00 H
GB 0
PC 1.40

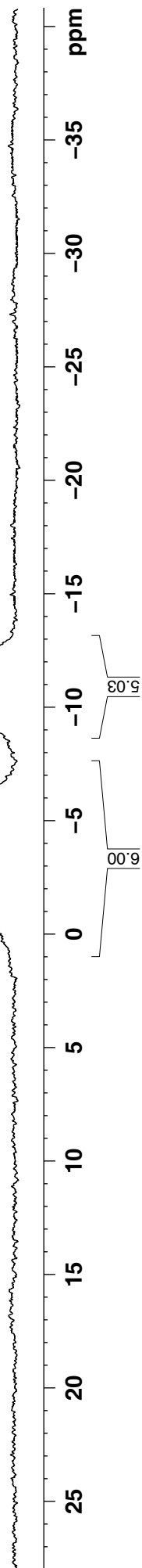


20170511-lfr-0428 [NEt₄][COOH-CB₁₁H₅-(C₆H₄-p-tBu)₅]
160 MHz, ¹¹B{¹H} NMR, 31 mg dissolved in acetone-d₆

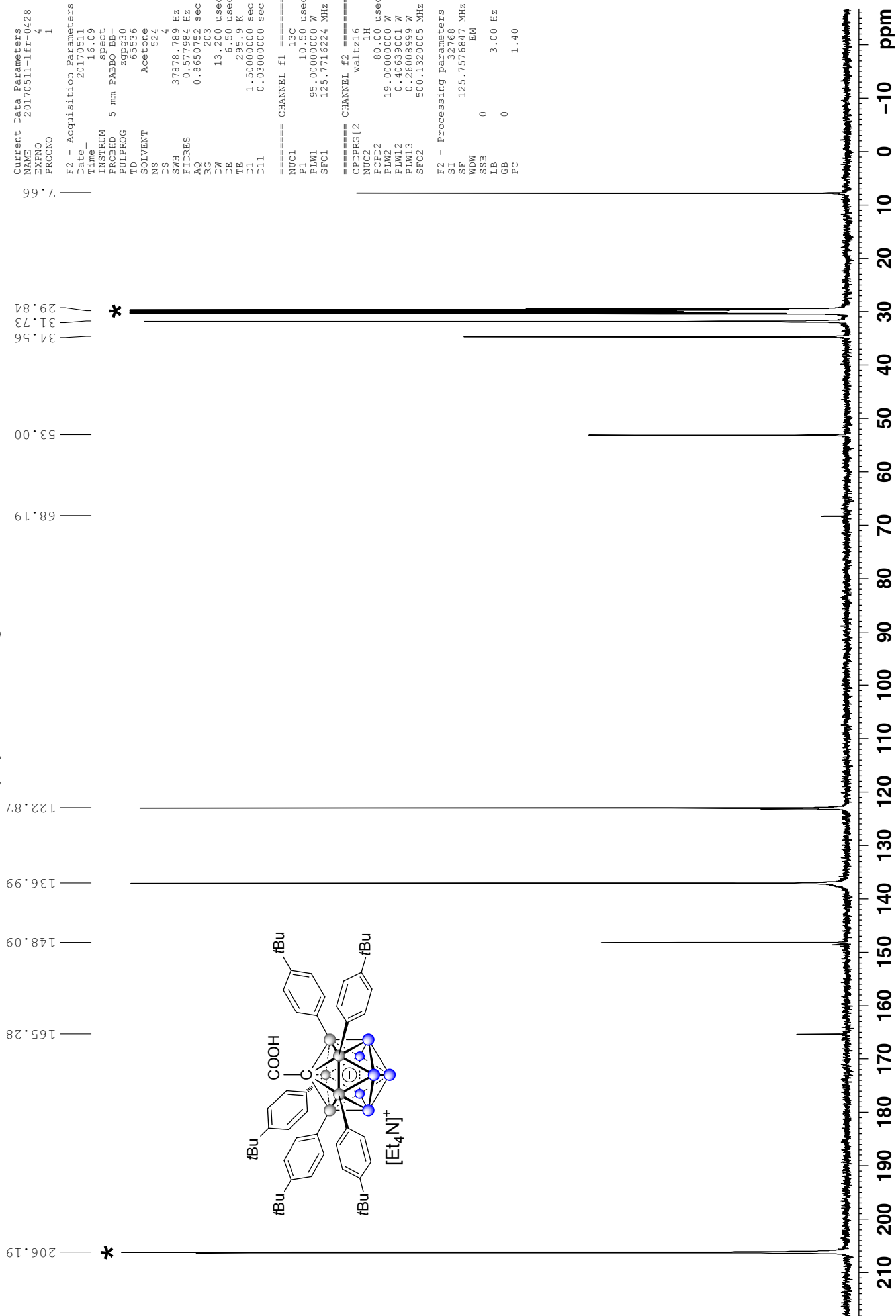
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— -4.8367
— -11.1303



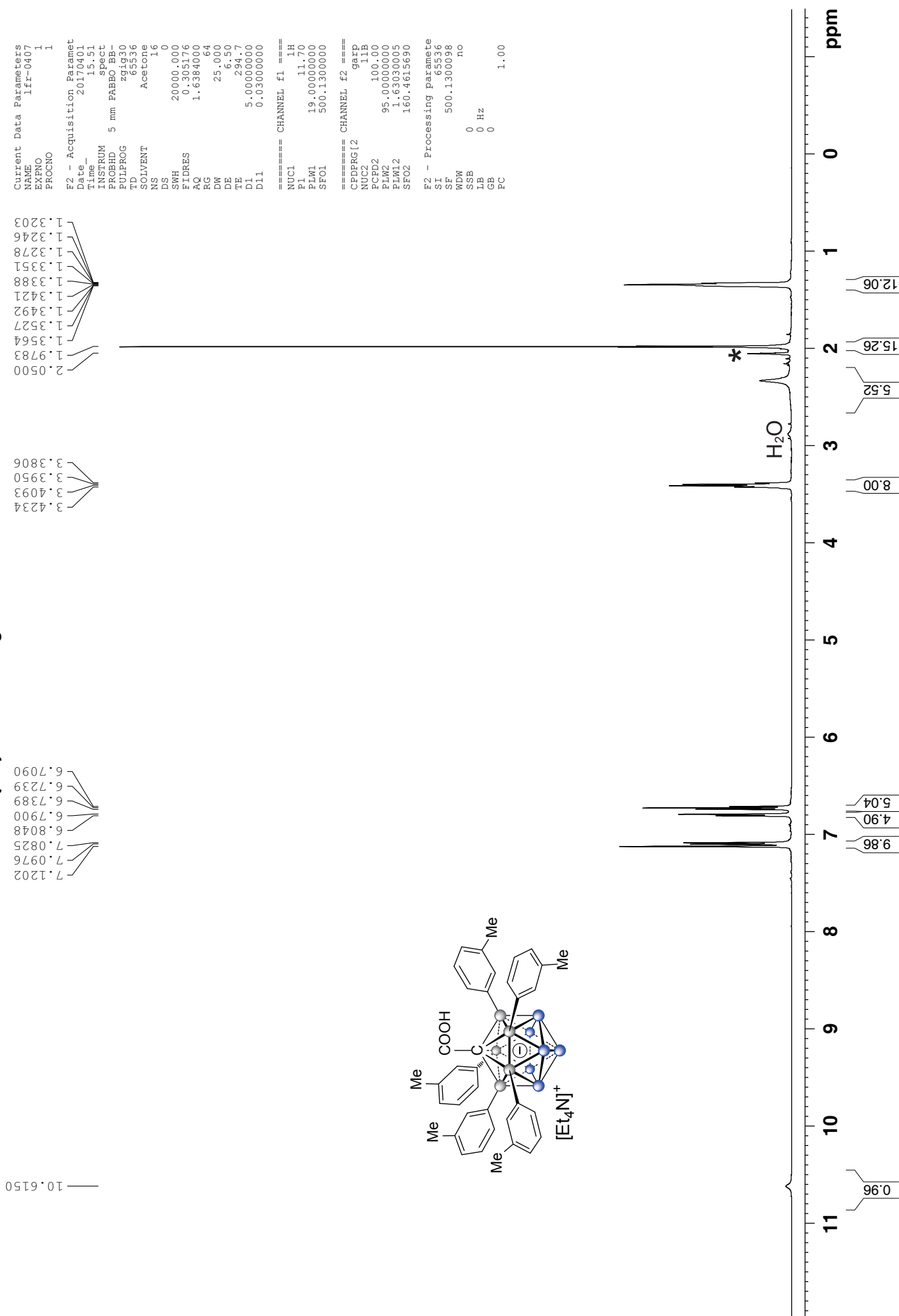
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NAME 20170511-lfr-042
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170511
Time_ 16.06
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 32051.281 H
FIDRES 0.489064 H
AQ 1.0223616 s
RG 203
DW 15.600 u
DE 6.50 u
TE 295.6 K
D1 1.00000000 s
D11 0.03000000 s
===== CHANNEL f1 =====
NUC1 11B
P1 13.10 u
PLW1 95.00000000 W
SFO1 160.4615790 M
===== CHANNEL f2 =====
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 u
PLW2 19.00000000 W
PLW12 0.39262000 W
PLW13 0.25127000 W
SFO2 500.1325007 M
F2 - Processing parameters
SI 32768
SF 160.4615790 M
WDW EM
SSB 0
LB 10.00 H
GB 0
FC 1.40



20170511-lfr-0428 [NEt₄][COOH-CB₁₁H₅-(C₆H₄-p-tBu)₅]
126 MHz, ¹³C{¹H} NMR, 31 mg dissolved in acetone-d₆*



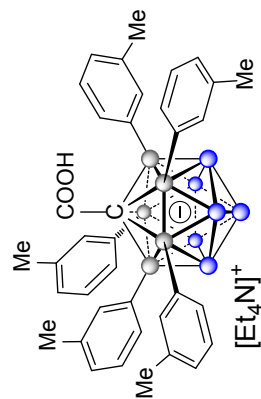
20170401-lfr-0407 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-Me)₅]
500 MHz, ¹H{¹B} NMR, 28 mg dissolved in acetone-d₆*



20170401-lfr-0407 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-Me)₅]
160 MHz, ¹¹B NMR, 28 mg dissolved in acetone-d₆

— -3.9344

— -10.9678
— -11.7923

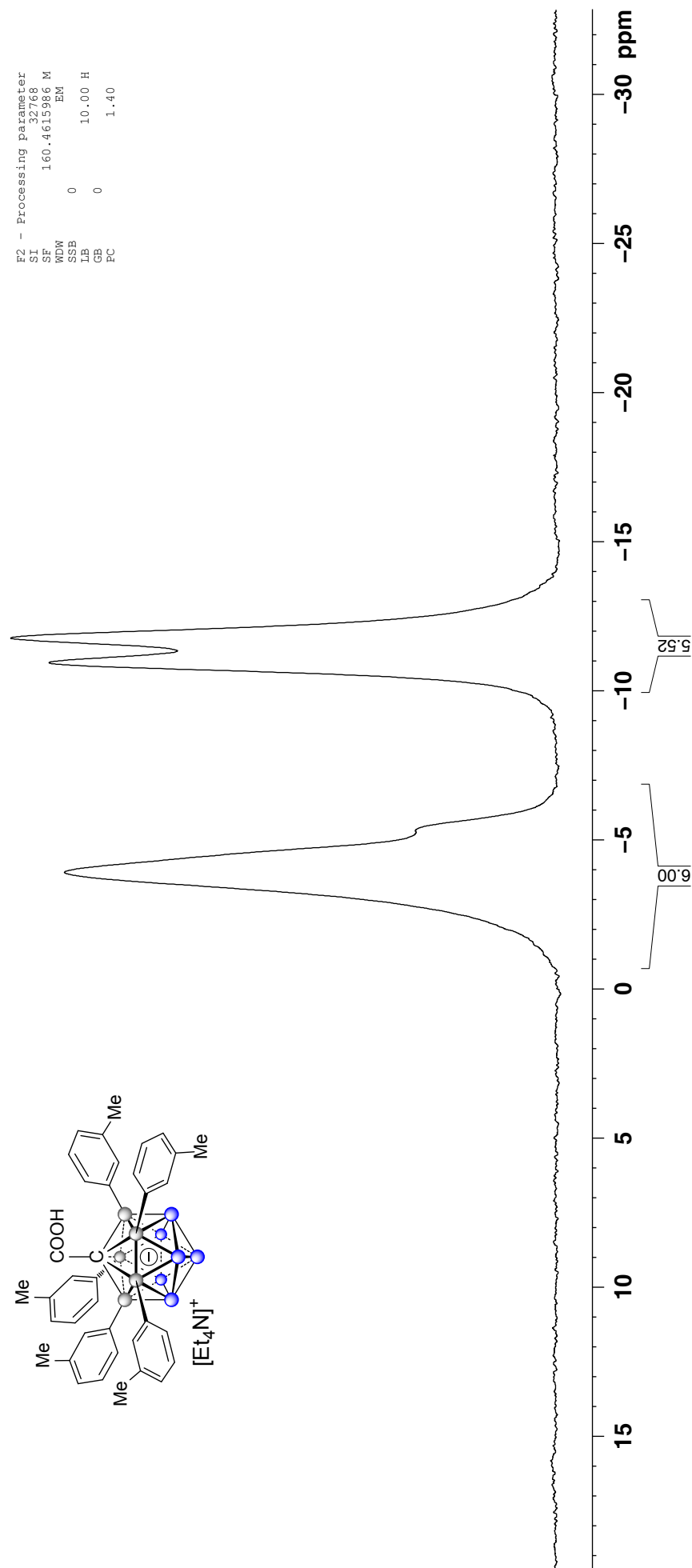


Current Data Parameters
NAME 20170401-lfr-040
EXPNO 2
PROCNO 1

F2 - Acquisition Parameter
Date_ 20170401
Time_ 15.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 64098
SOLVENT Acetone
NS 32
DS 0
SWH 32051.281 H
FIDRES 0.500036 H
AQ 0.9999288 s
RG 203
DW 15.600 u
DE 6.50 u
TE 294.6 K
D1 1.00000000 s

===== CHANNEL f1 =====
NUC1 11B
P1 13.10 u
PLW1 95.00000000 W
SFO1 160.4615792 M

F2 - Processing parameter
SI 32768
SF 160.4615986 M
WDW EM
SSB 0
LB 10.00 H
GB 0
PC 1.40



20170401-lfr-0407 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-Me)₅]
 160 MHz, ¹¹B{¹H} NMR, 28 mg dissolved in acetone-d₆

```

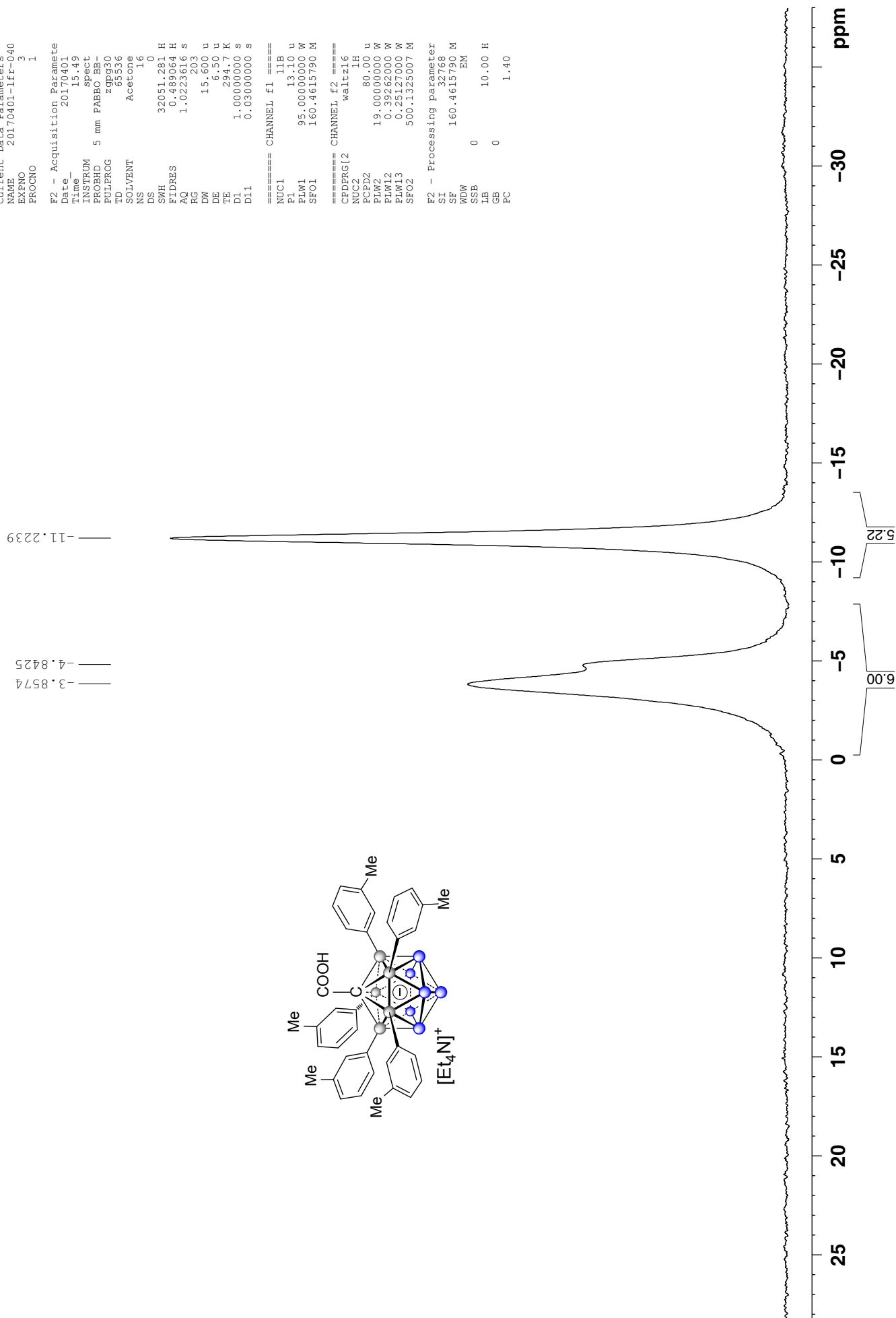
Current Data Parameters
NAME      20170401-lfr-040
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20170401
Time      15.49
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         16
DS         0
SWH        32051.281 H
FIDRES     0.489064 H
AQ          1.0223616 s
RG          203
DW          15.600 u
DE          6.50 u
TE         294.7 K
D1          1.00000000 s
D11         0.03000000 s

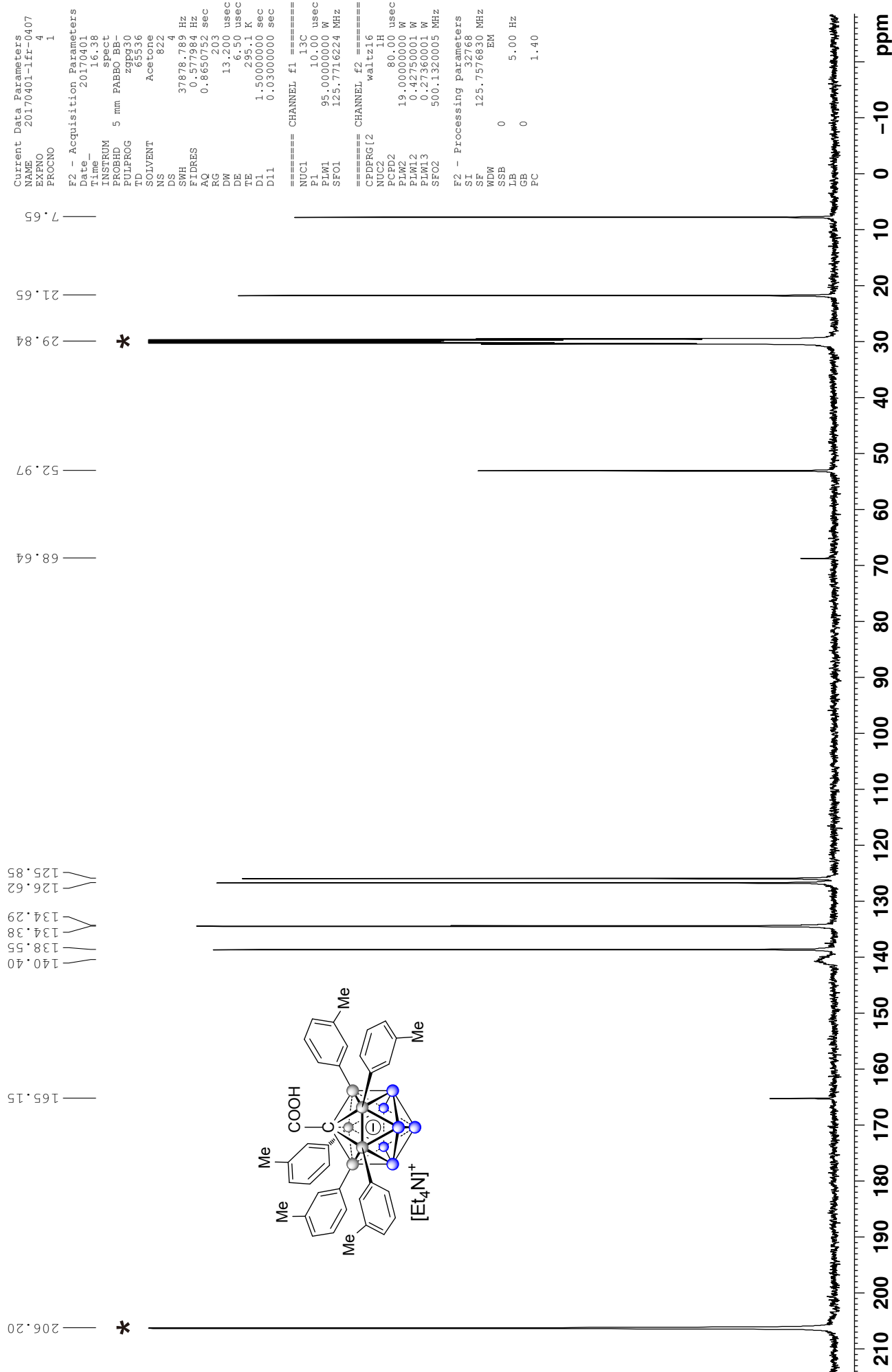
===== CHANNEL f1 =====
NUC1       11B
P1         13.10 u
PLW1       95.00000000 W
SFO1       160.4615790 M

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       80.00 u
PLW2       19.00000000 W
PLW12      0.39262000 W
PLW13      0.25127000 W
SFO2       500.1325007 M

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



20170401-lfr-0407 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-Me)₅]
 126 MHz, ¹³C{¹H} NMR, 28 mg dissolved in acetone-d₆*



20180903-lfr-0550 [NEt₄][1-COOH-CB₁₁H₁₀-(C₆H₄-2-Me)]
400 MHz, ¹H{¹³B} NMR, 15 mg in 0.55 mL MeCN-d₃*

Current Data Parameters
NAME 20180903-lfr-055
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180904
Time_ 11.48
INSTRUM spect
PROBHD 5 mm PABBO1BB/
PULPROG zgpg30
TD 65536
SOLVENT CD₃CN
NS 16
DS 4
SWH 8012.820 H
FIDRES 0.489064 H
AQ 1.0223616 s
RG 66.58
DM 62.400 u
DE 6.50 u
TE 296.0 K
D1 1.0000000 s
D11 0.0300000 s
TD0 1

===== CHANNEL f1 =====
NUC1 ¹H
P1 15.00 u
PLW1 12.5000000 W
SF01 400.1320007 M

===== CHANNEL f2 =====
CPDPRG[2] garp4
NUC2 ¹³B
PCPD2 90.00 u
PLW2 52.96599960 W
PLW12 0.64477998 W
SF02 128.3776050 M

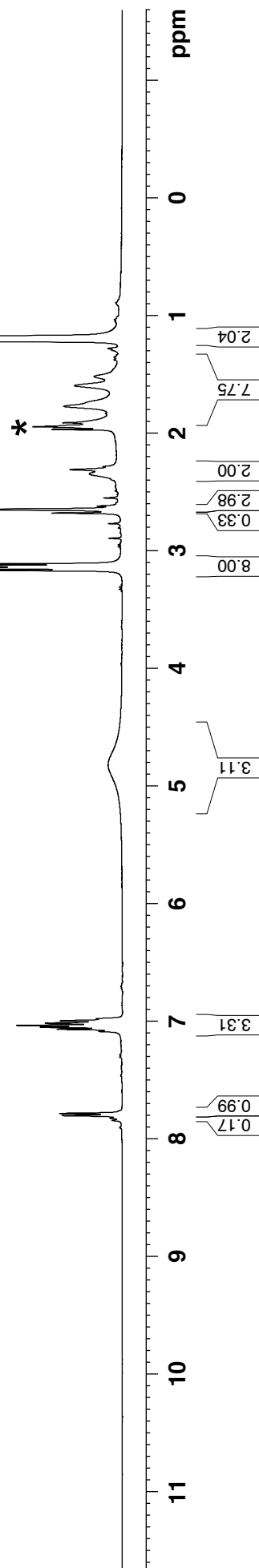
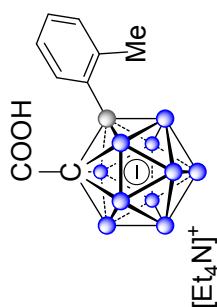
F2 - Processing parameters
SI 32768
SF 400.1300116 M
WDW EM
SSB 0
LB 1.00 H
GB 0
PC 1.40

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1.2068
1.1969
1.1929
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1.1790
1.1750
1.1711

2.6445
3.1074
3.1256
3.1437
3.1618

4.8143

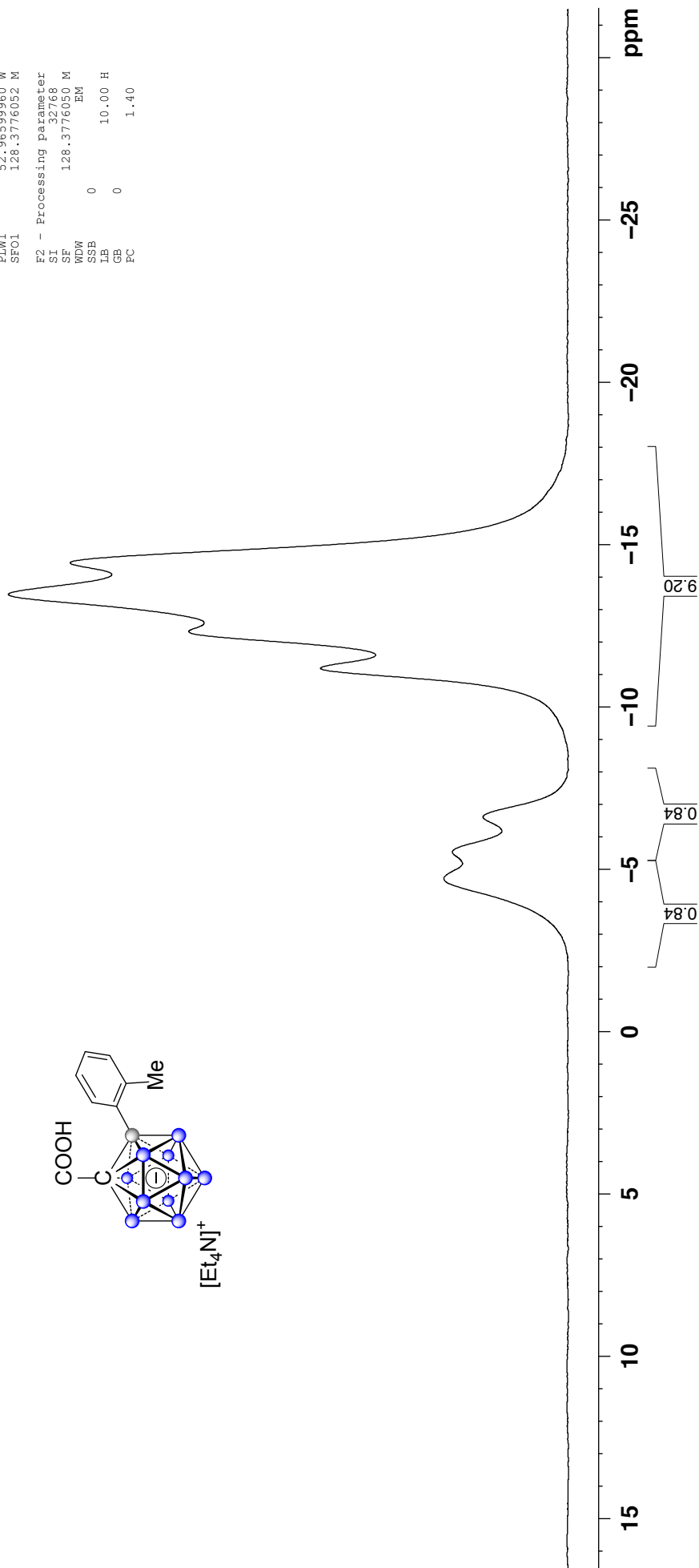
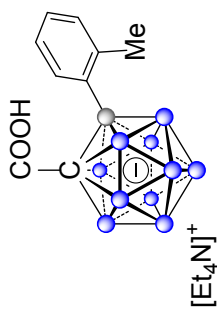
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7.7789
7.0809
7.0632
7.0454
7.0306
7.0119
6.9923
6.9758



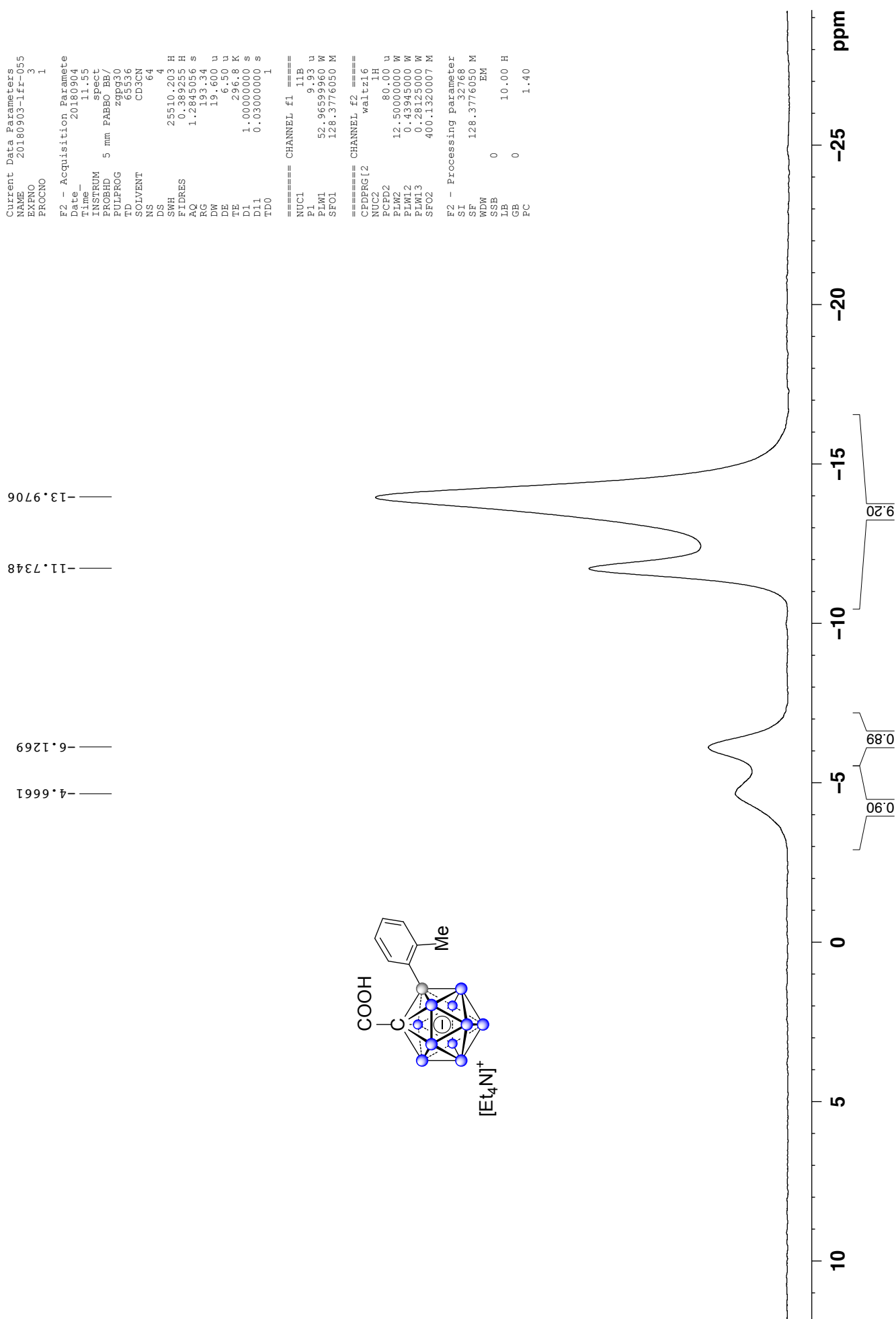
20180903-lfr-0550 [NEt₄][1-COOH-CB₁₁H₁₀-(C₆H₄-2-Me)]
128 MHz, ¹¹B NMR, 15 mg in 0.55 mL MeCN-d₃

Current Data Parameters
NAME 20180903-lfr-055
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180904
Time_ 11.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 6536
SOLVENT CD3CN
NS 64
DS 4
SWH 25510.203 H
FIDRES 0.389255 H
AQ 1.2845056 S
RG 193.34
DW 19.600 u
DE 6.50 u
TE 296.0 K
D1 1.00000000 S
TD0 1
===== CHANNEL f1 =====
NUC1 11B
P1 9.93 u
PLW1 52.9659960 W
SFO1 128.3776032 M
F2 - Processing parameters
SI 32768
SF 128.3776030 M
WDW EM
SSB 0
LB 10.00 H
GB 0
PC 1.40

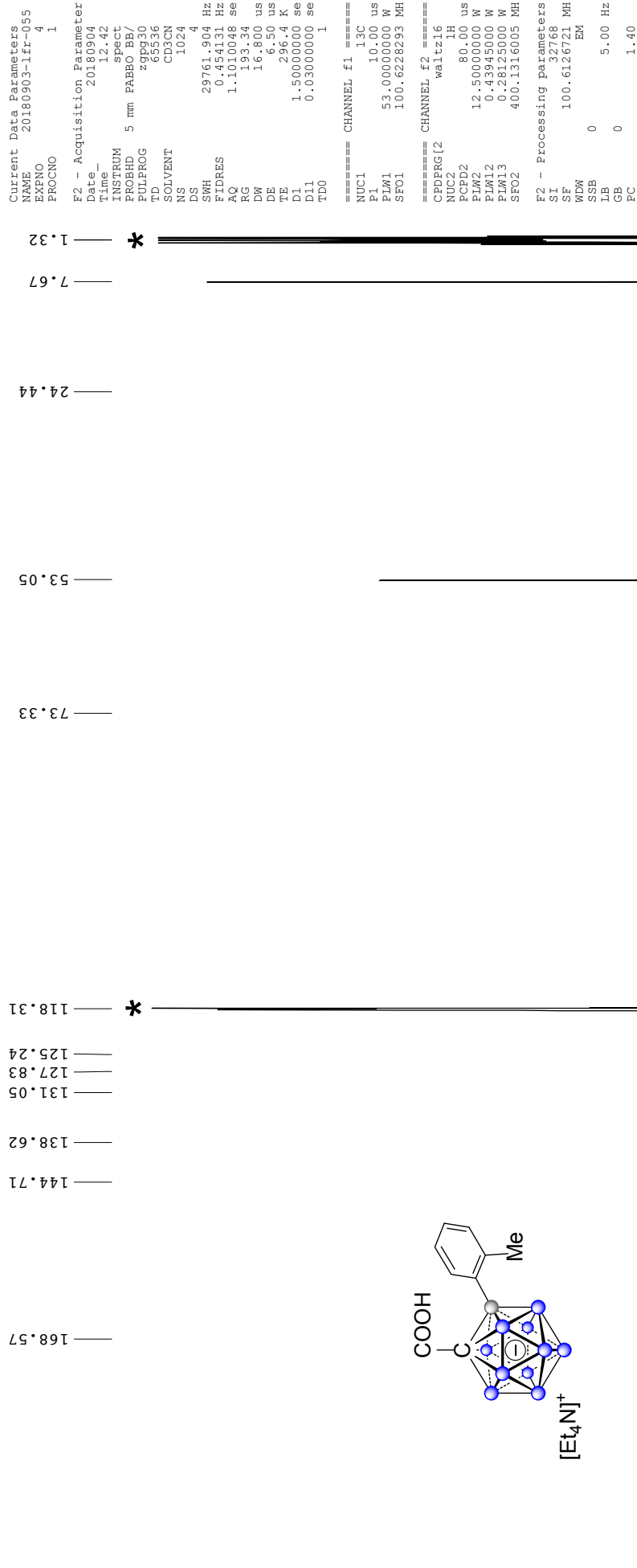
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— -6.6210
— -11.2109
— -12.3412
— -13.4874
— -14.4589



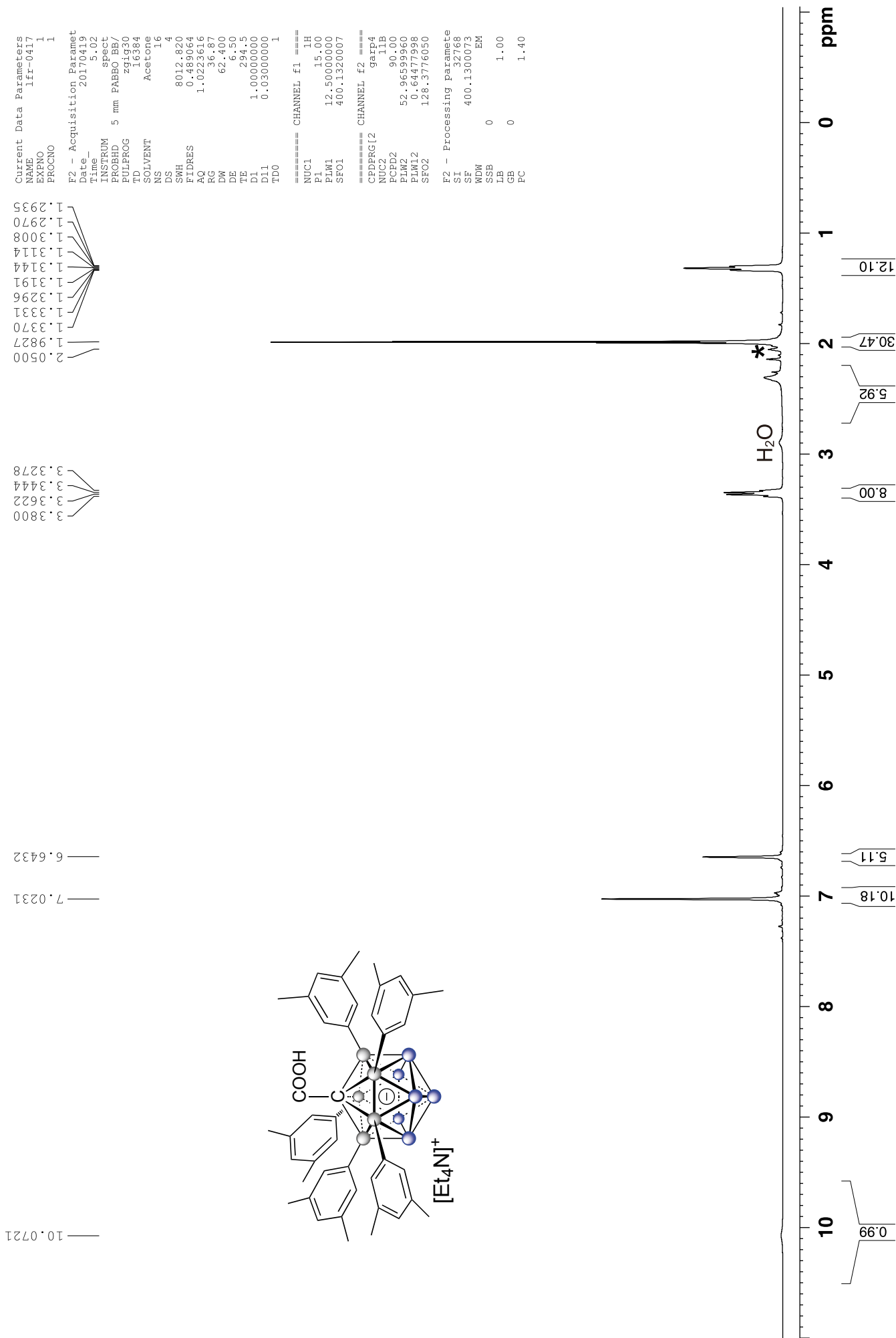
20180903-lfr-0550 [NEt₄][1-COOH-CB₁₁H₁₀-(C₆H₄-2-Me)]
 128 MHz, ¹B{¹H} NMR, 15 mg in 0.55 mL MeCN-d₃



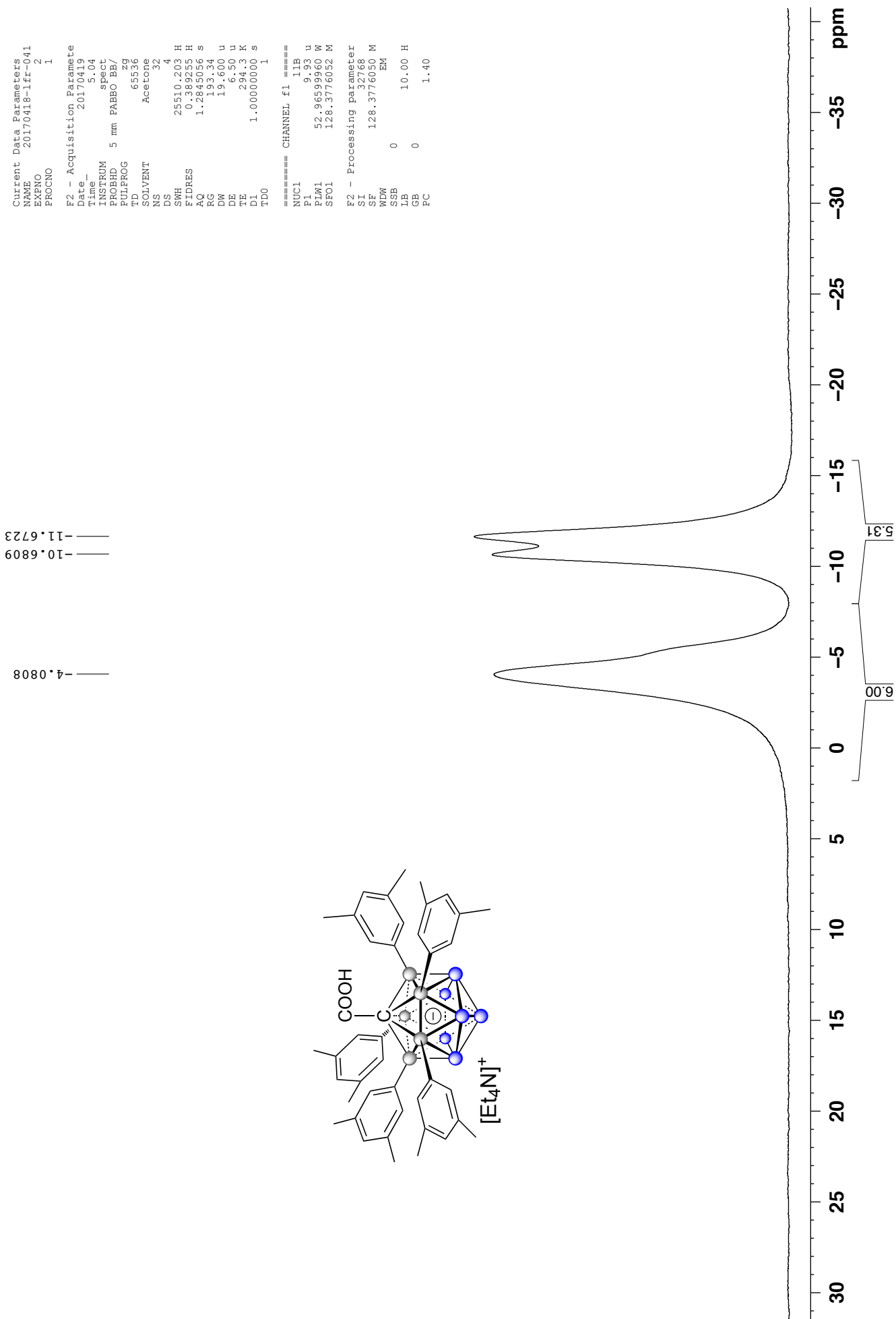
20180903-lfr-0550 [NEt₄][1-COOH-CB₁₁H₁₀-(C₆H₄-2-Me)]
 101 MHz, ¹H{¹³B} NMR, 15 mg in 0.55 mL MeCN-d₃*



20170418-lfr-0417 [NEt₄][COOH-CB₁₁H₆-(C₆H₃-3,5-Me)₅]
 400 MHz, ¹H{¹¹B} NMR, 40 mg dissolved in 0.55 mL acetone-d₆*



20170418-lfr-0417 [NEt₄][COOH-CB₁₁H₆-(C₆H₃-3,5-Me)₅]
 128 MHz, ¹¹B NMR, 40 mg dissolved in 0.55 mL acetone-d₆



20170418-lfr-0417 [NEt₄][COOH-CB₁₁H₆-(C₆H₃-3,5-Me)₅]
 128 MHz, ¹¹B{¹H} NMR, 40 mg dissolved in 0.55 mL acetone-d₆

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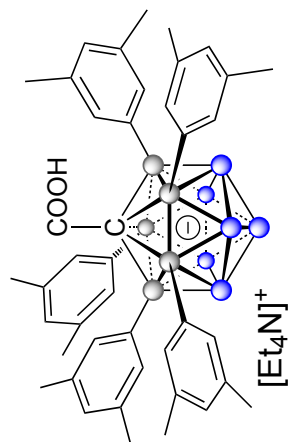
Current Data Parameters
NAME      20170418-lfr-041
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20170419
Time      5.06
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   Acetone
NS        32
DS        4
SWH       25510.203 H
FIDRES    0.389255 H
AQ        1.2845056 s
RG        193.34
DW        19.600 u
DE        6.50 u
TE        295.0 K
D1        1.00000000 s
D11       0.03000000 s
TDO       1

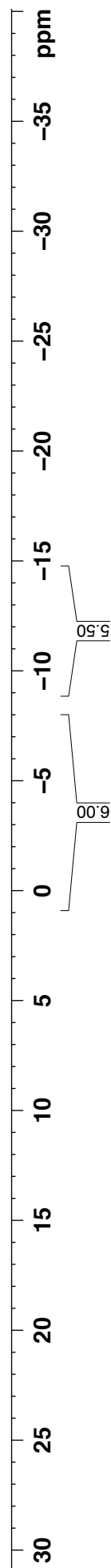
===== CHANNEL f1 =====
NUC1      11B
P1        9.93 u
PLW1     52.9659960 W
SF01     128.3776050 M

===== CHANNEL f2 =====
CPDPRG[2  waltz16
NUC2      1H
PCPD2     80.00 u
PLW2     12.50000000 W
PLW12    0.43945000 W
PLW13    0.28125000 W
SF02     400.1320007 M

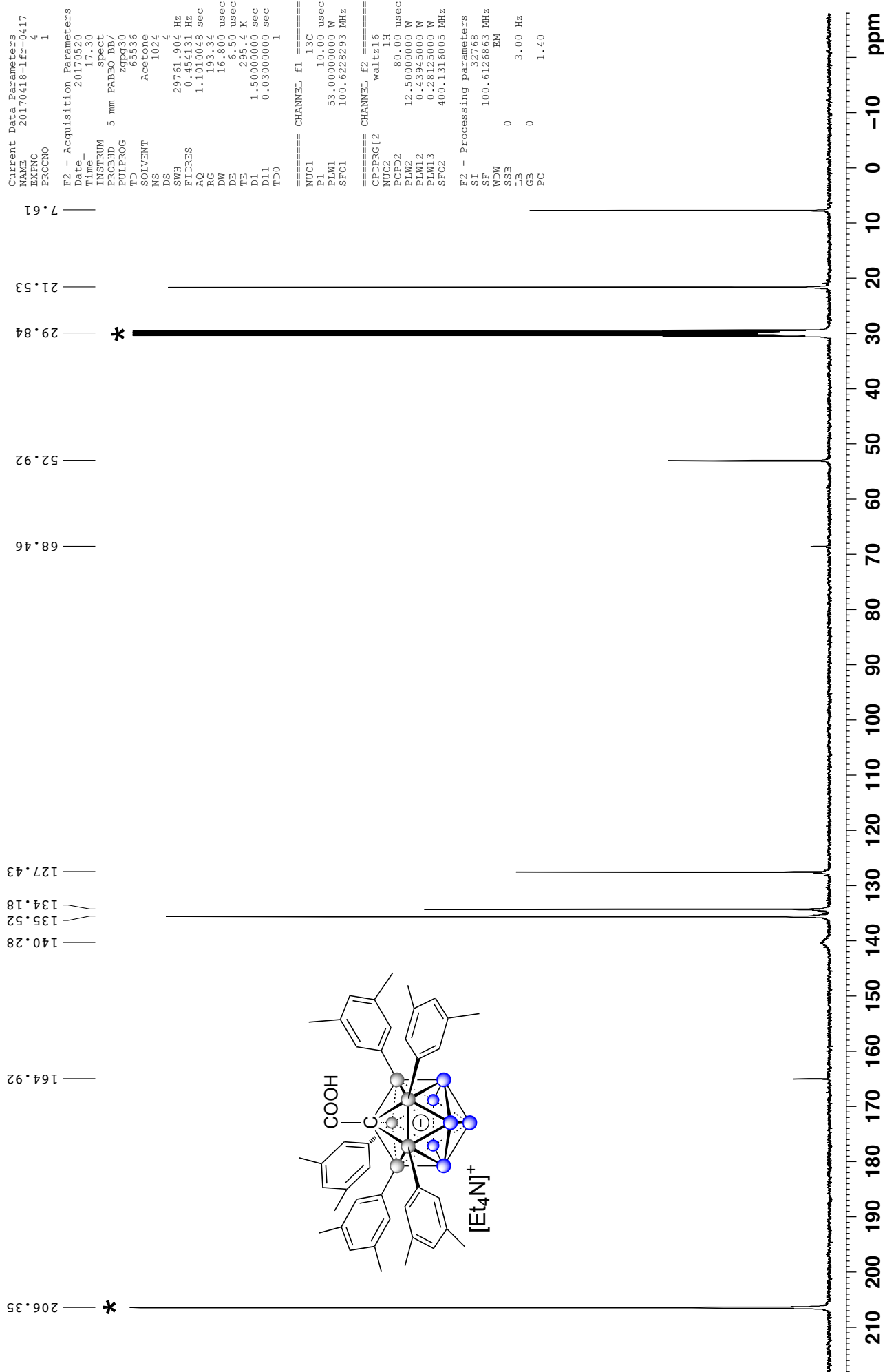
F2 - Processing parameters
SI        32768
SF        128.3776050 M
WDW       EM
SSB       0
LB        10.00 H
GB        0
PC        1.40
  
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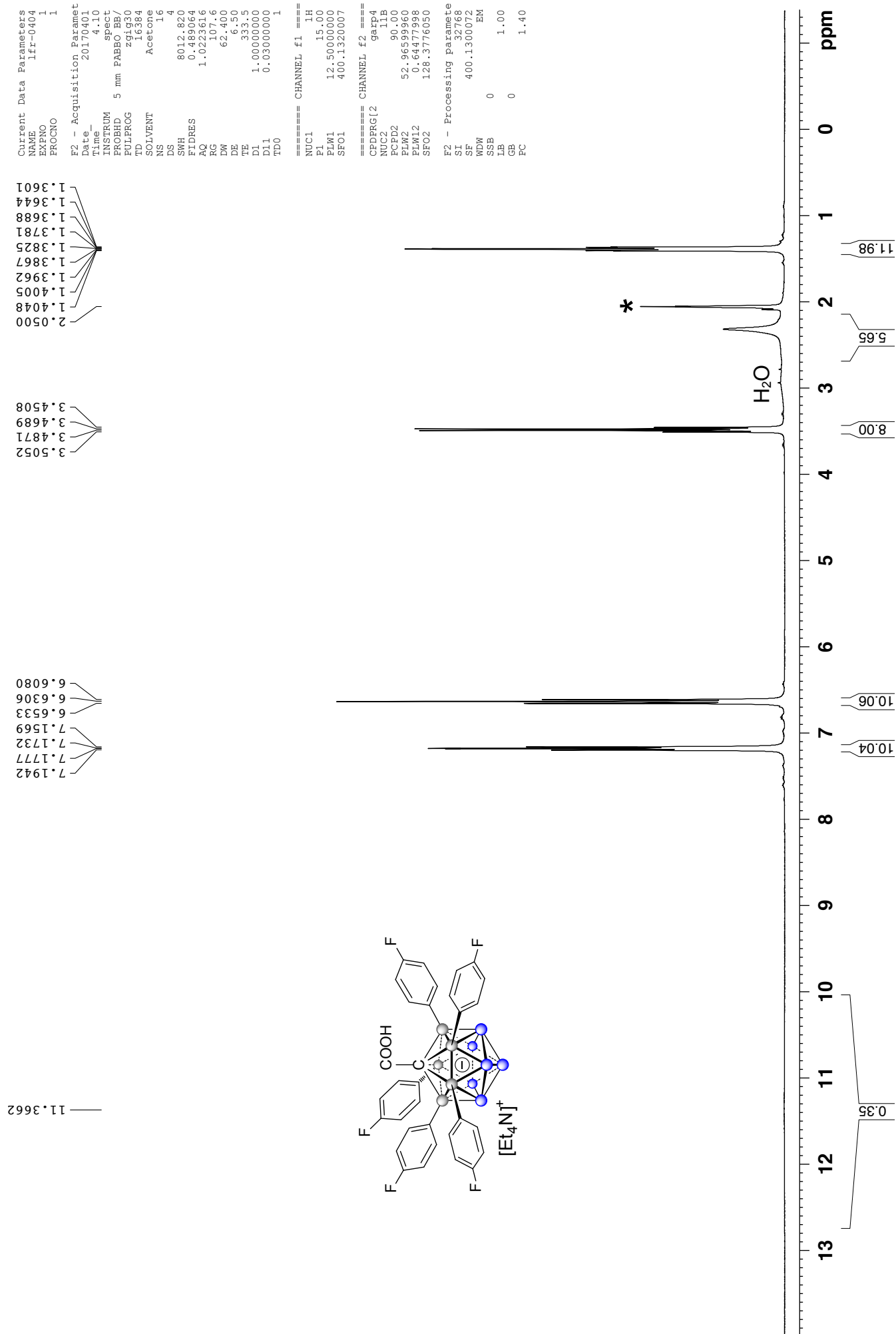
— -4.1154
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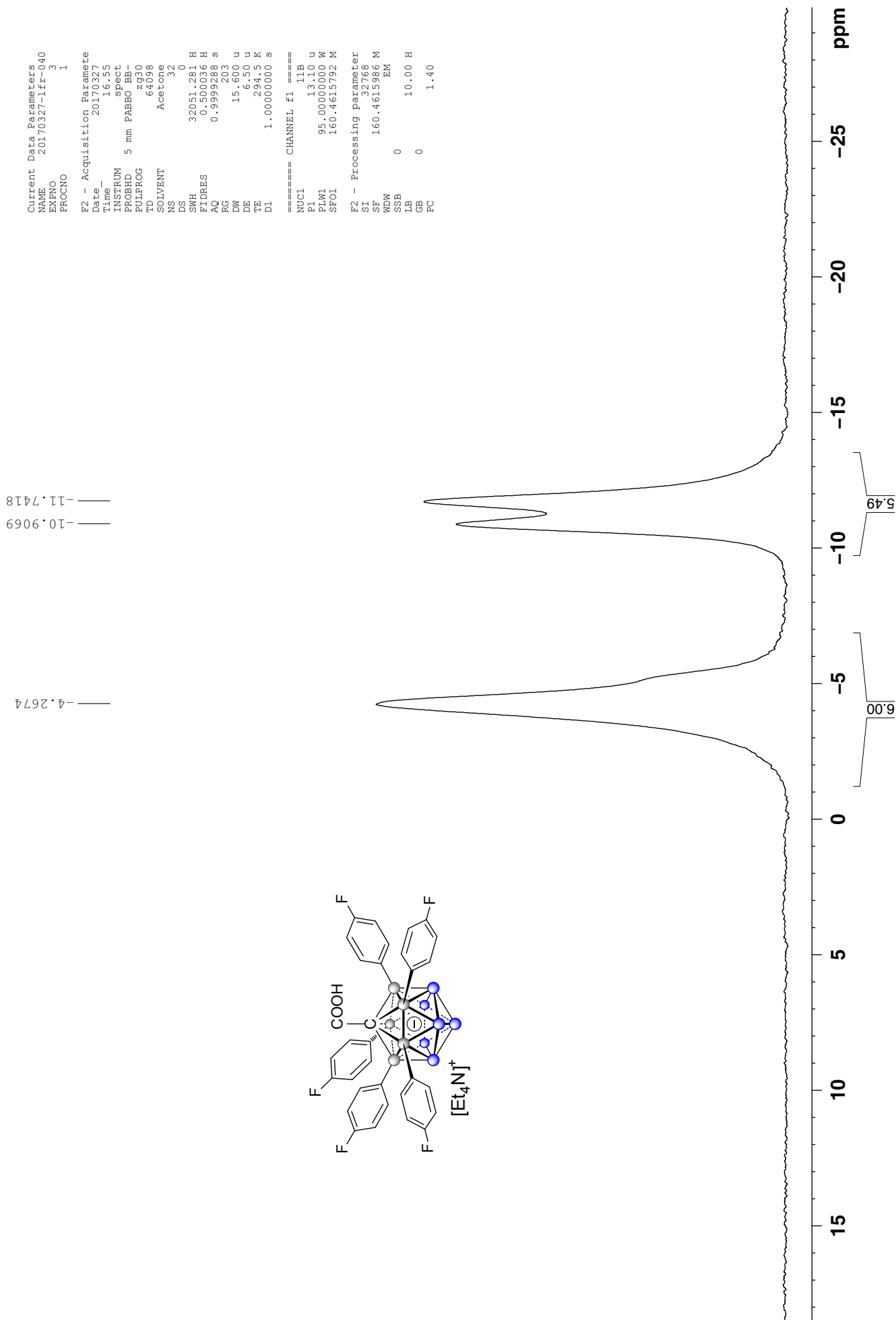
20170418-lfr-0417 [NEt₄][COOH-CB₁₁H₆-(C₆H₃-3,5-Me)₅]
101 MHz, ¹³C{¹H} NMR, 40 mg dissolved in 0.55 mL acetone-d₆*



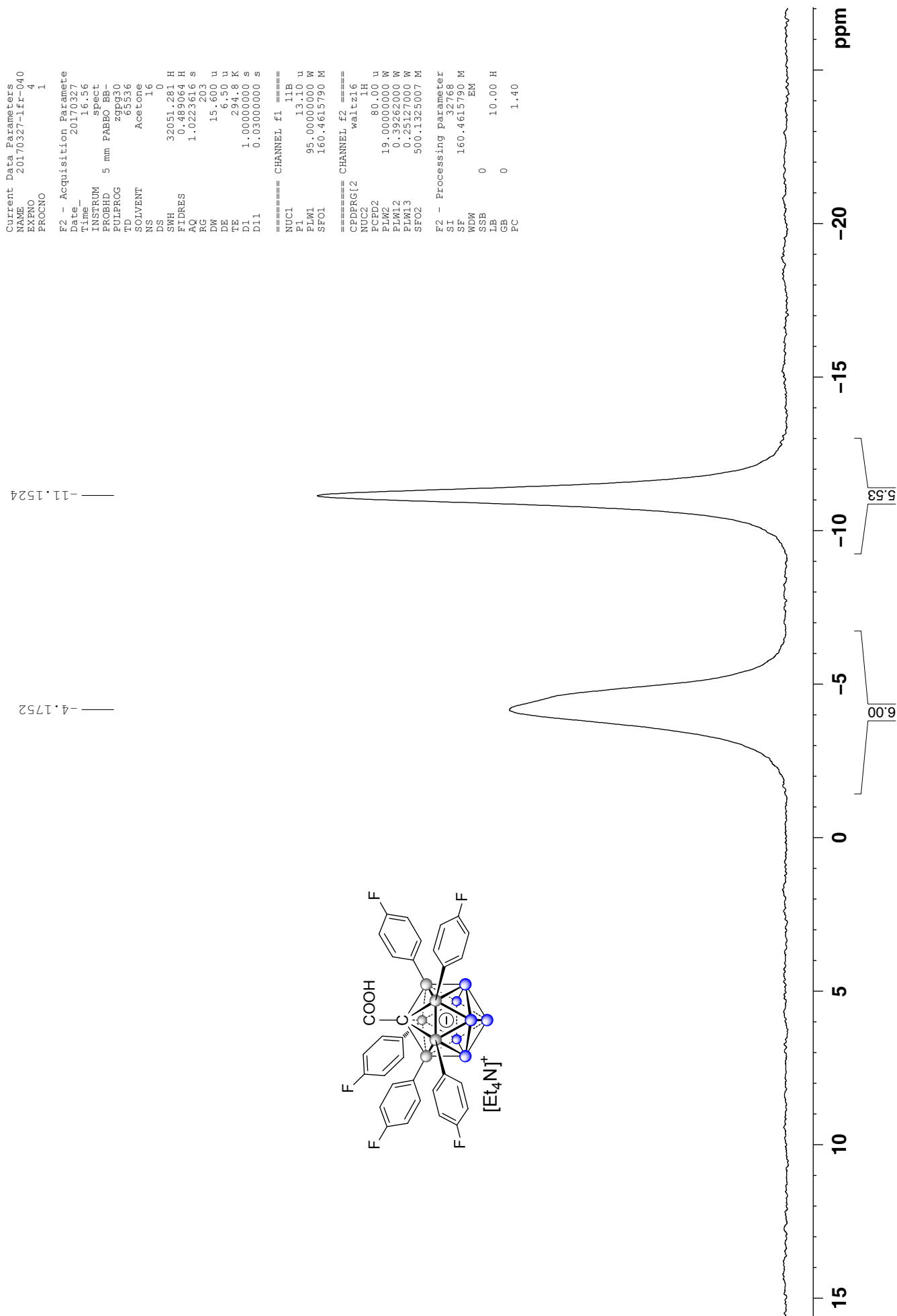
20170327-lfr-0404 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-F)₅]
 500 MHz, ¹H{¹B} NMR, 24 mg dissolved in 0.55 mL acetone-d₆*



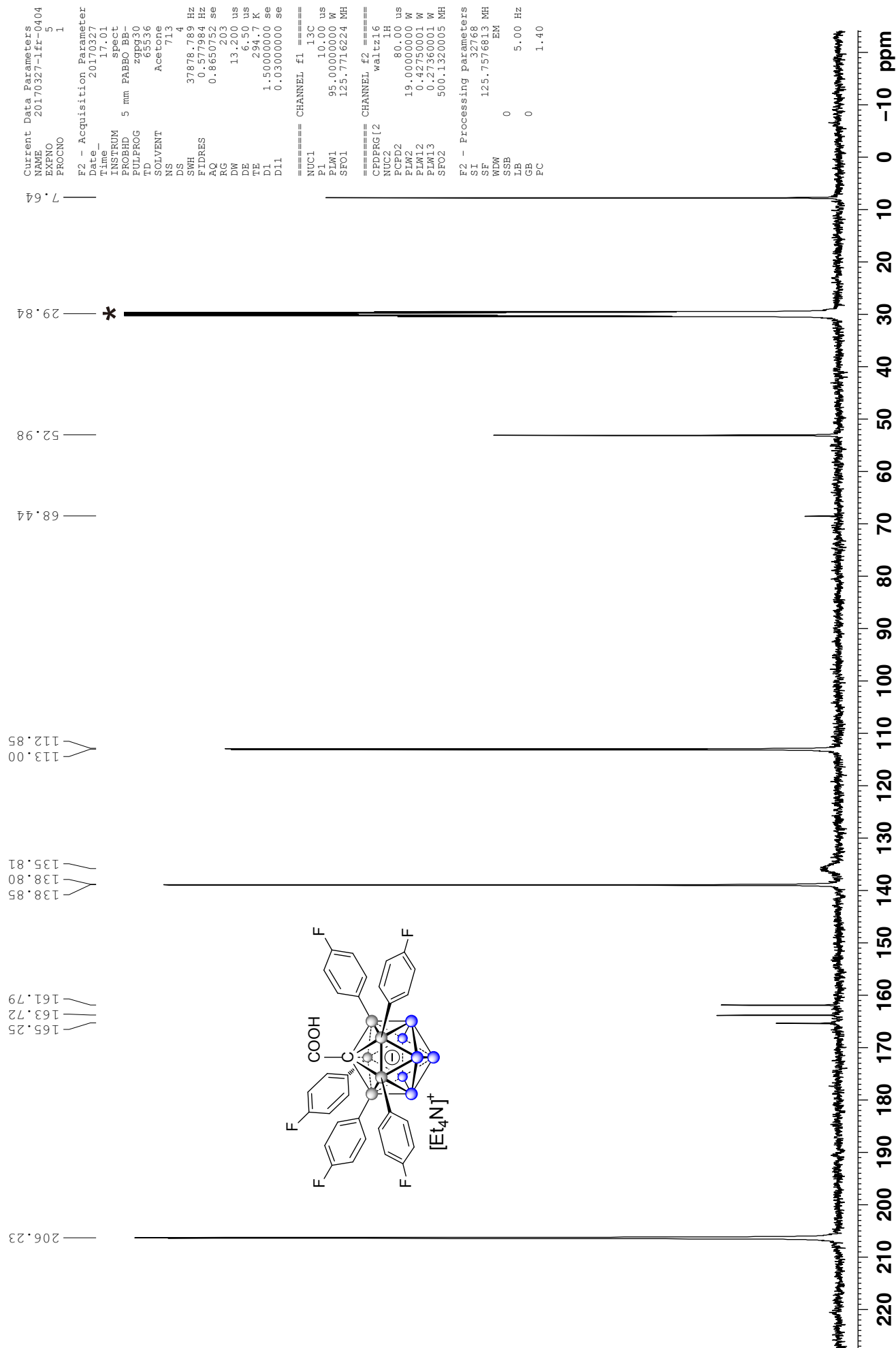
20170327-lfr-0404 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-F)₅]
 160 MHz, ¹¹B NMR, 24 mg dissolved in 0.55 mL acetone-d₆



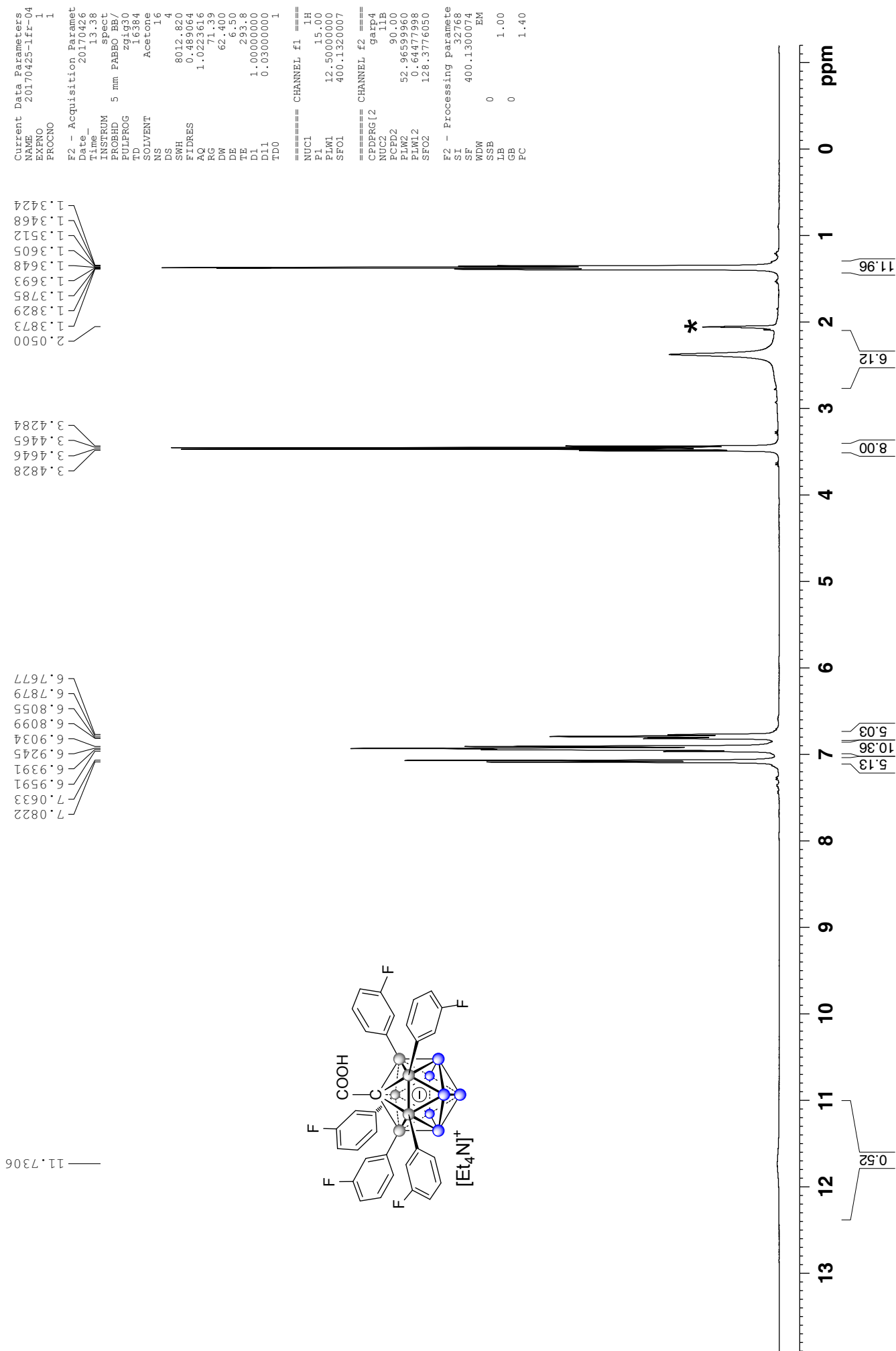
20170327-lfr-0404 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-F)₅]
 160 MHz, ¹¹B{¹H} NMR, 24 mg dissolved in 0.55 mL acetone-d₆



20170327-lfr-0404 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-F)₅]
 126 MHz, ¹³C{¹H} NMR, 24 mg dissolved in 0.55 mL acetone-d₆*



20170425-lfr-0418 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-F)₅]
400 MHz, ¹H{¹B} NMR, 40 mg dissolved in 0.55 mL acetone-d₆*



20170425-lfr-0418 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-F)₅]
 128 MHz, ¹¹B NMR, 40 mg dissolved in 0.55 mL acetone-d₆

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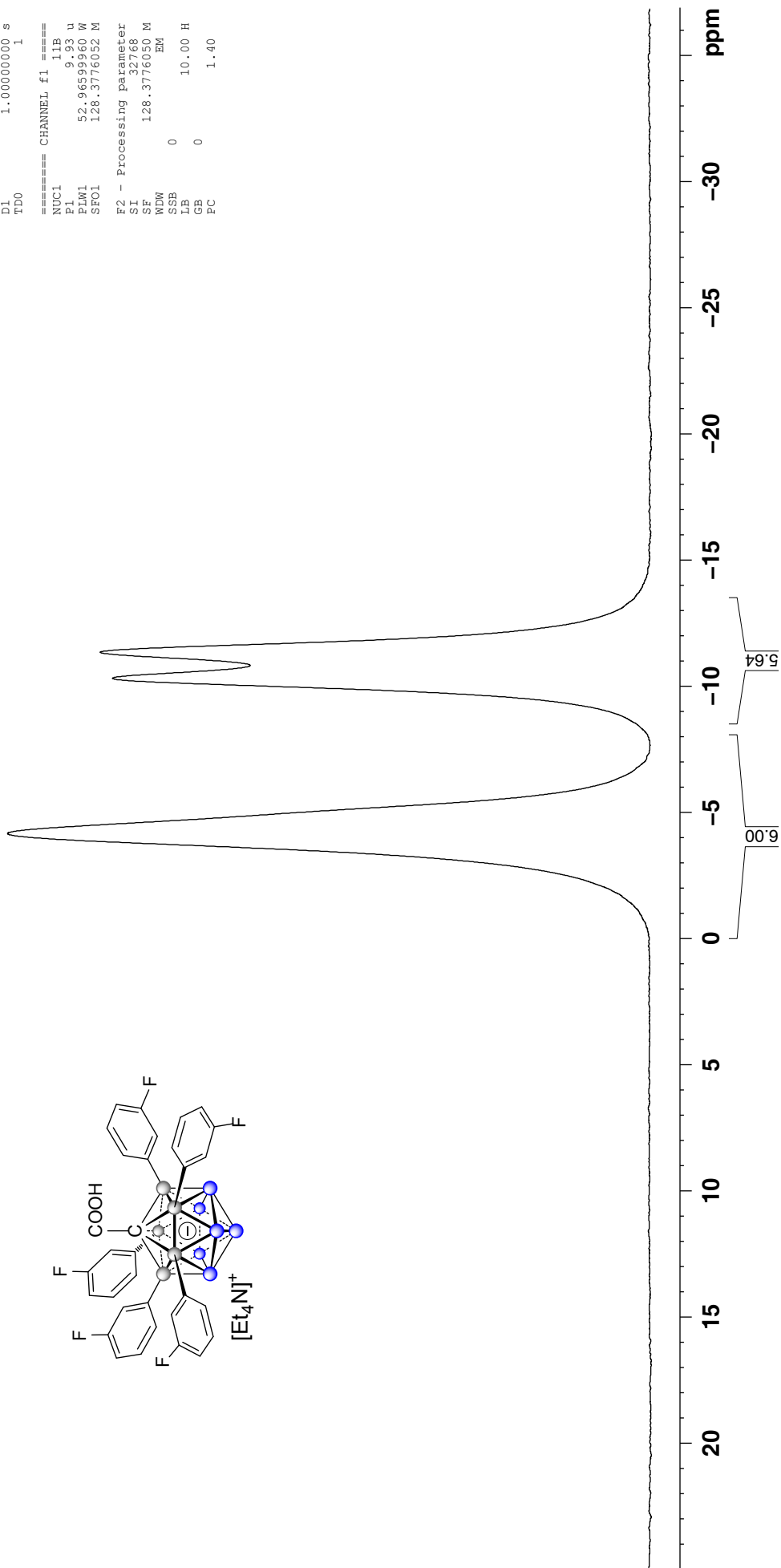
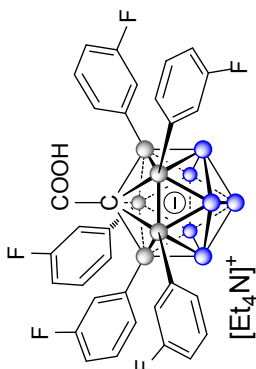
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NAME      20170425-lfr-041
EXPNO     2
PROCNO    1

F2 - Acquisition Parameter
Date_     20170426
Time      13.40
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg
TD         65536
SOLVENT   Acetone
NS         32
DS         4
SWH        25510.203 H
FIDRES     0.389235 H
AQ         1.2845056 s
RG         193.34
DW         19.600 u
DE         6.50 u
TE         283.4 K
D1         1.00000000 s
TD0        1

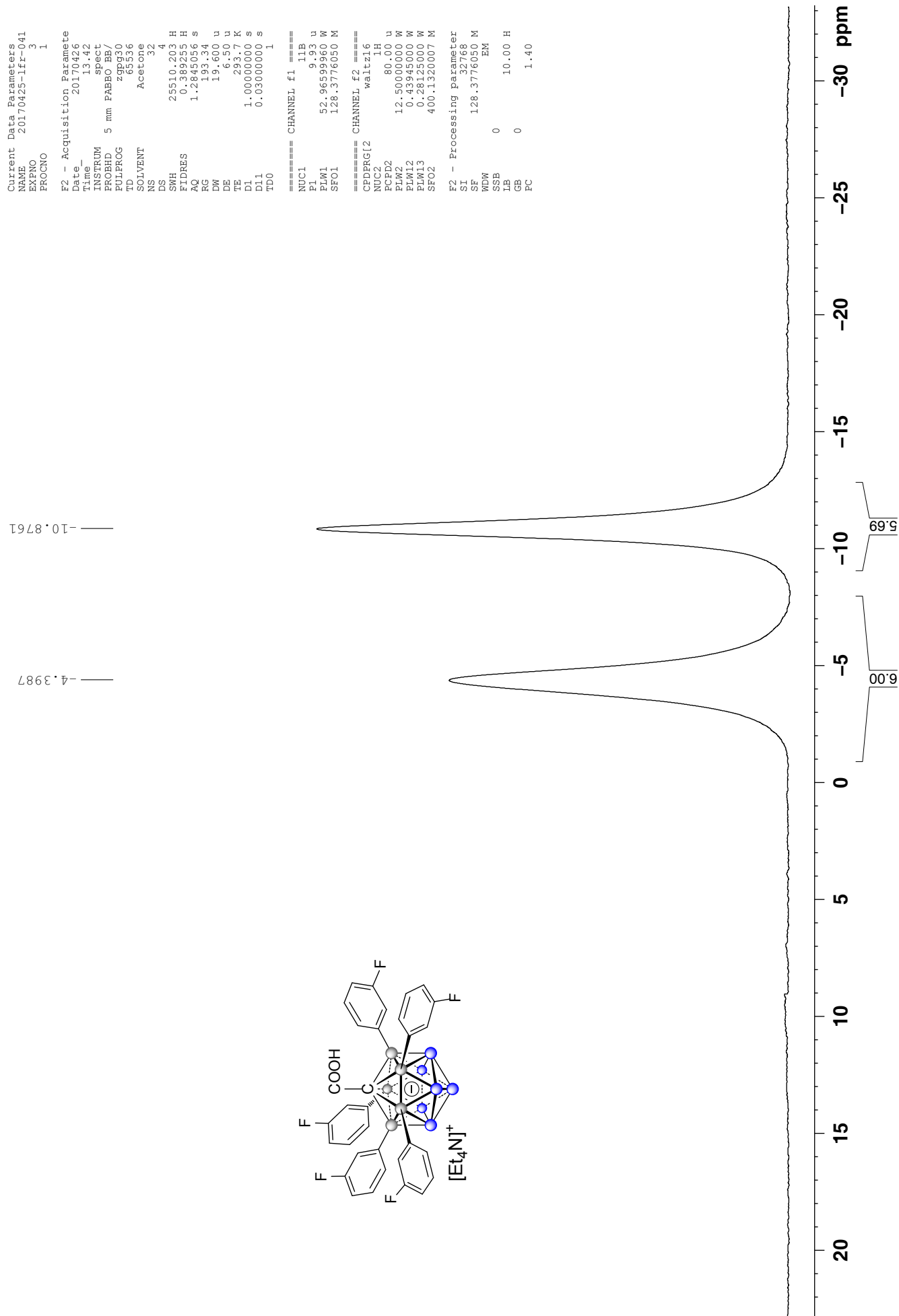
===== CHANNEL f1 =====
NUC1       11B
P1         9.93 u
PLW1       52.9659960 W
SFO1       128.3776052 M

F2 - Processing parameter
SI         32768
SF         128.3776050 M
WDW        EM
SSB        0
LB         10.00 H
GB         0
PC         1.40
  
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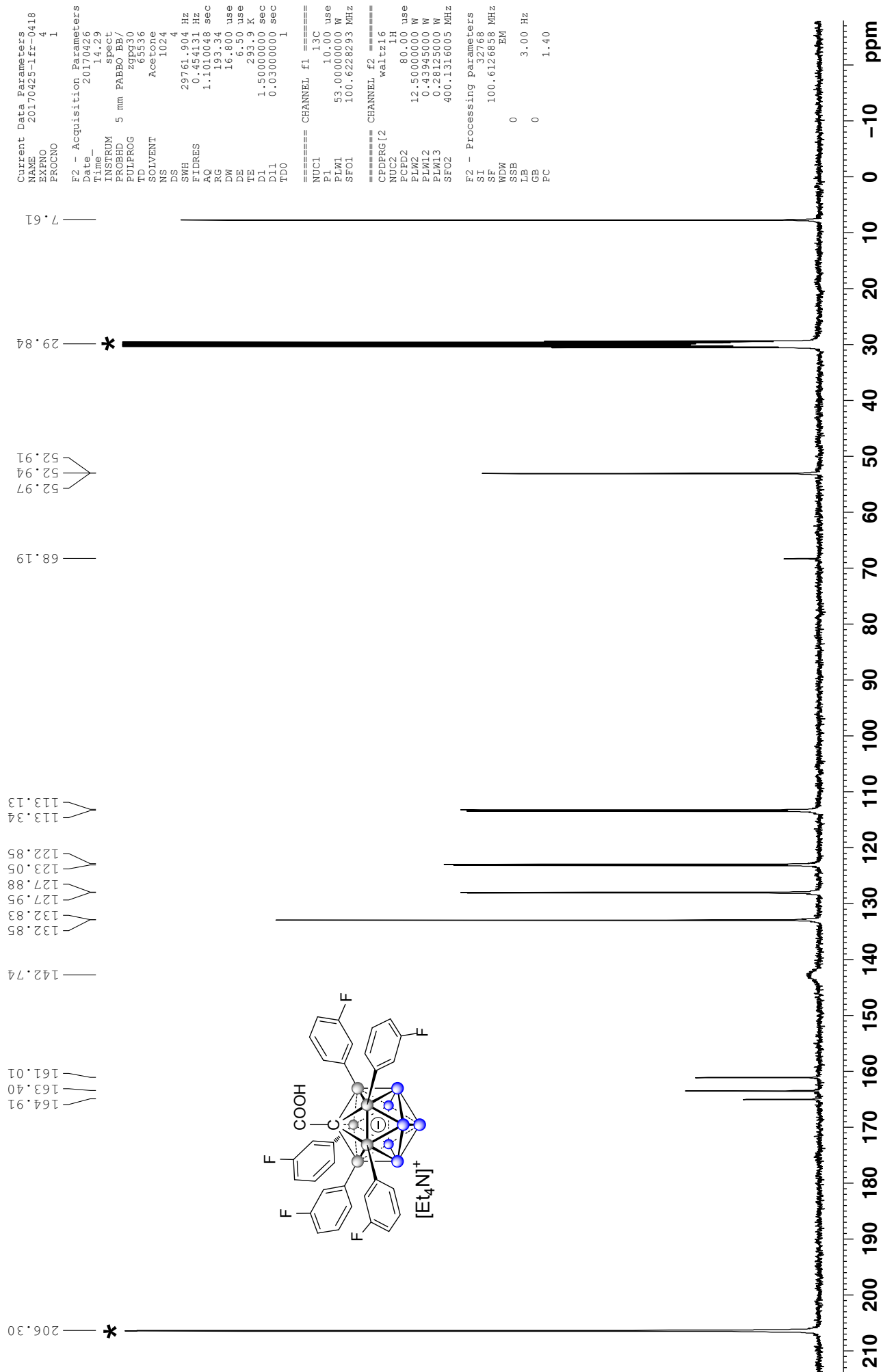
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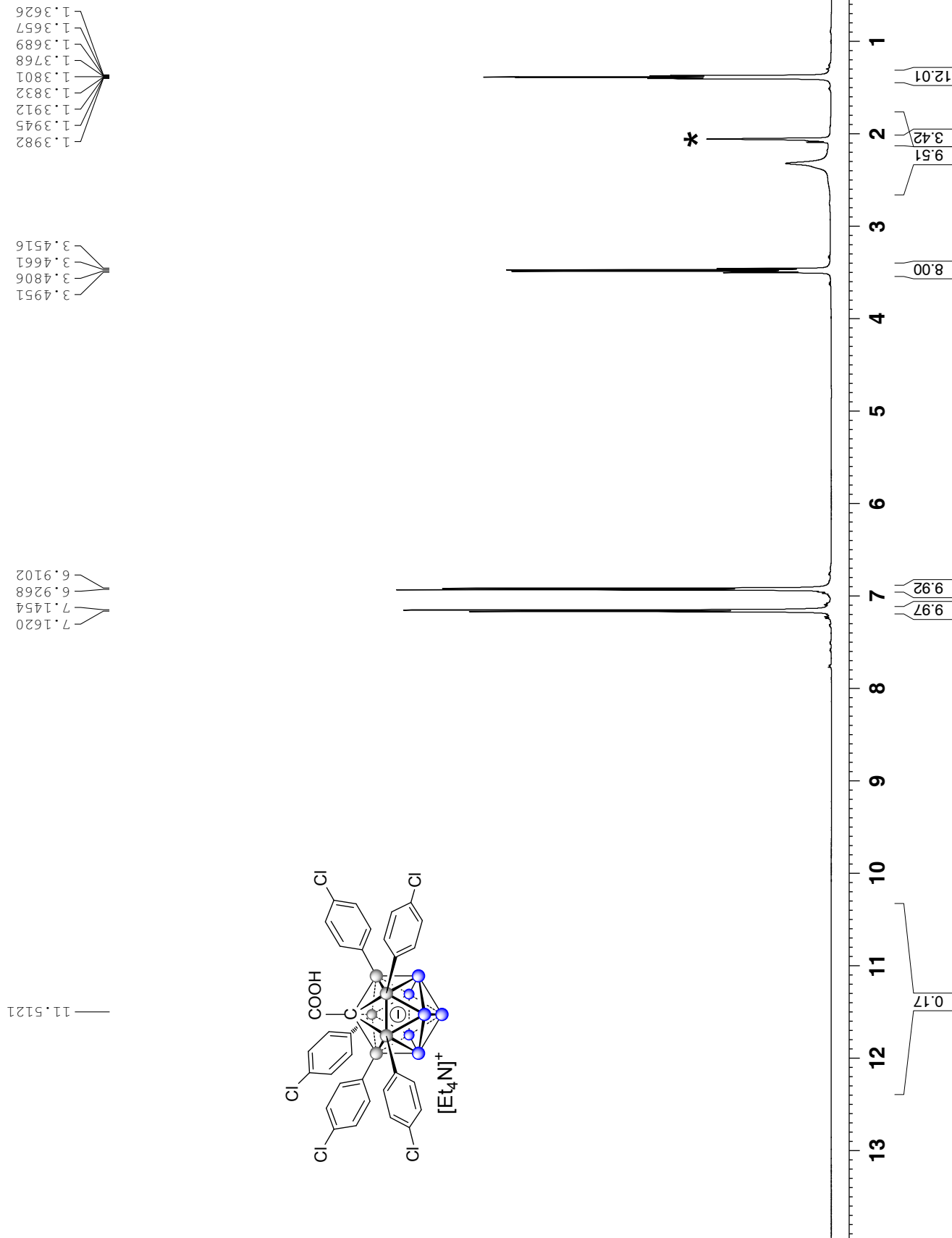
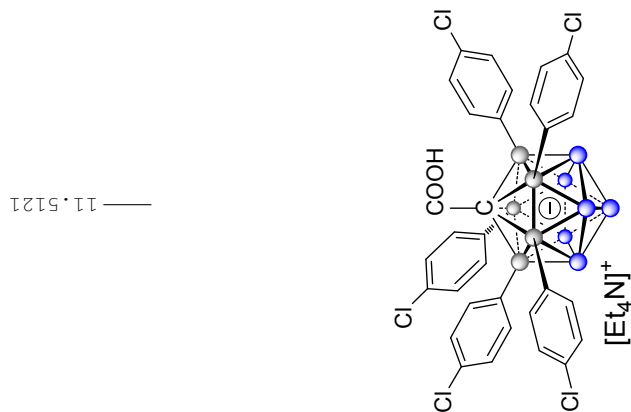
20170425-lfr-0418 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-F)₃]
 128 MHz, ¹H{¹H} NMR, 40 mg dissolved in 0.55 mL acetone-d₆



20170425-lfr-0418 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-F)₅]
 101 MHz, ¹³C{¹H} NMR, 40 mg dissolved in 0.55 mL acetone-d₆*

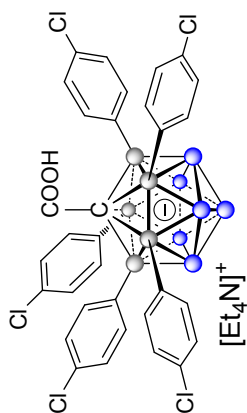


20170329-lfr-0402 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Cl)₅]
 500 MHz, ¹H{¹B} NMR, 30 mg dissolved in 0.55 mL acetone-d₆*



Current Data Parameters
 NAME 20170329-lfr-0402
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20170330
 Time_ 4.08
 INSTRUM spect
 PROHD 5 mm PABBO-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 12500.000 H
 SWH 0.190735 H
 FIDRES 2.621439 S
 AQ 64
 RG 40.000 u
 DW 6.50 u
 DE 296.2 K
 TE 5.0000000 S
 D1 0.0300000 S
 D11
 ===== CHANNEL f1 =====
 NUC1 ¹H
 F1 11.70 u
 FLW1 19.0000000 W
 SF01 500.1335009 M
 ===== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 ¹¹B
 F2 100.00 u
 FLW2 95.0000000 W
 SF02 1.6303005 W
 SFO2 160.4615690 M
 F2 - Processing parameters
 SI 65536
 SF 500.1300100 M
 WDW EM
 SSB 0
 LB 1.00 H
 GB 0
 FC 1.00

20170329-lfr-0401 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Cl)₅]
 160 MHz, ¹¹B NMR, 30 mg dissolved in 0.55 mL acetone-d₆



```

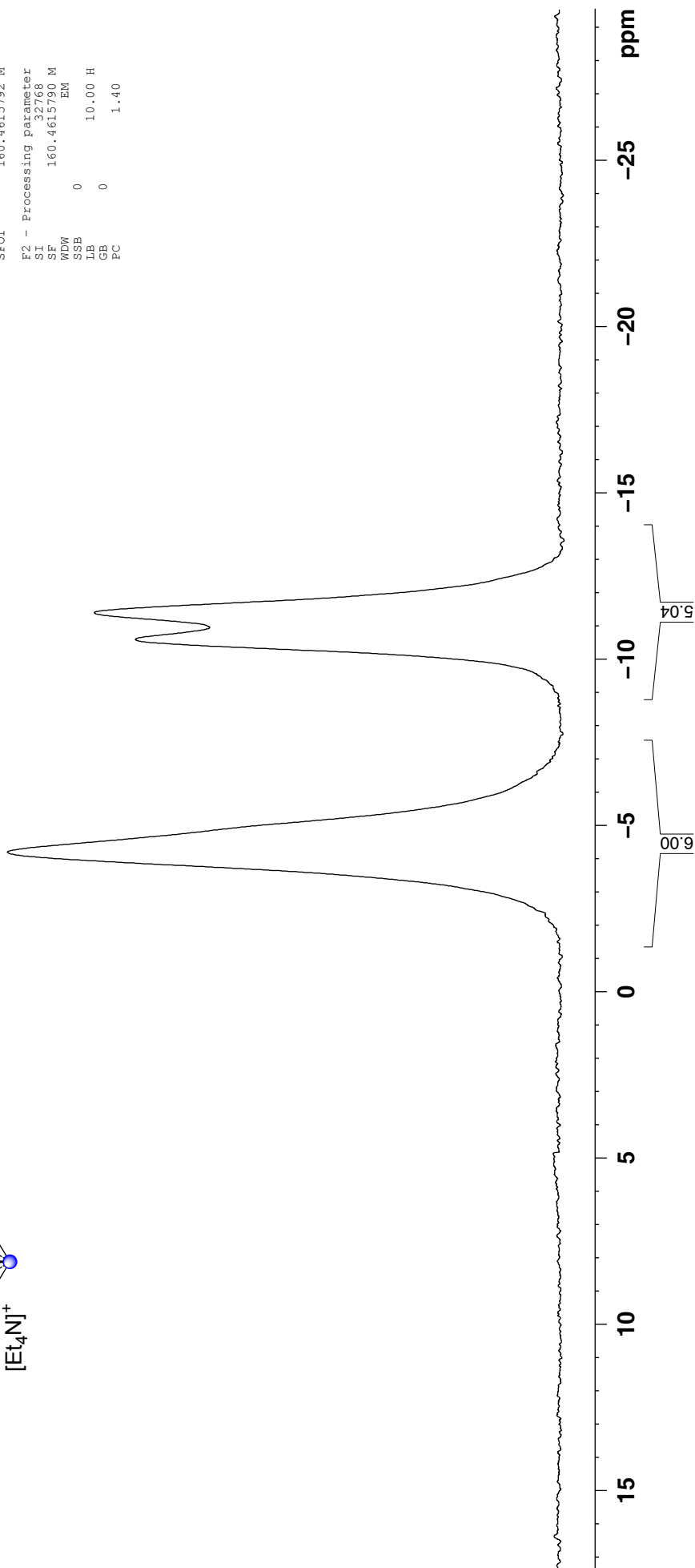
Current Data Parameters
NAME      20170329-lfr-0401
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20170330
Time      4.10
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        64098
SOLVENT   Acetone
NS        32
DS        0
SWH       32051.281 H
FIDRES    0.500036 H
AQ        0.9999288 s
RG        203
DE        15.600 u
TE        295.9 K
D1        1.00000000 s

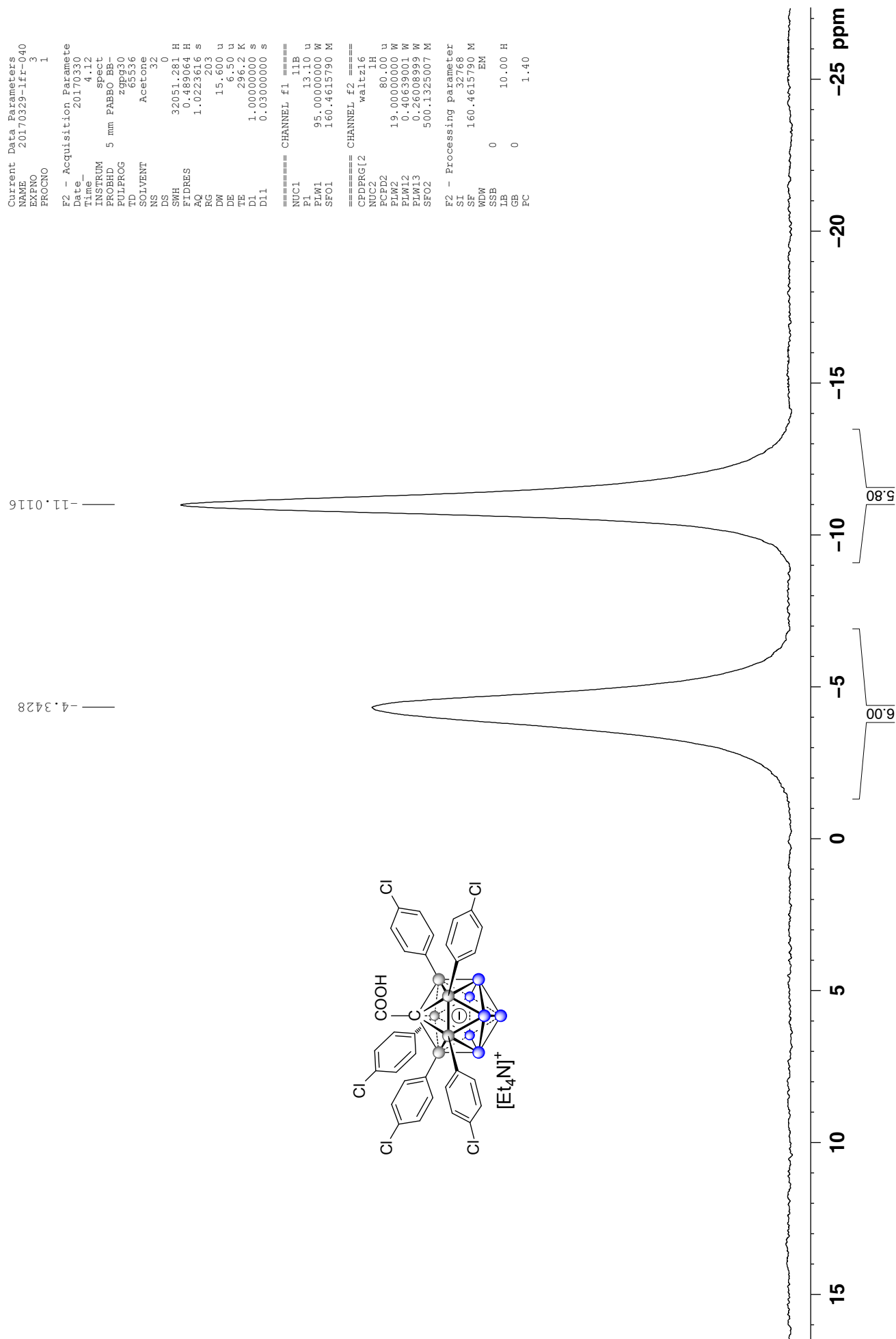
===== CHANNEL f1 =====
NUC1      11B
P1        13.10 u
PLWL      95.0000000 W
SFO1      160.4615792 M

F2 - Processing parameters
SI        32768
SF        160.4615790 M
WDW       EM
SSB       0
LB        0
GB        0
PC        1.40
    
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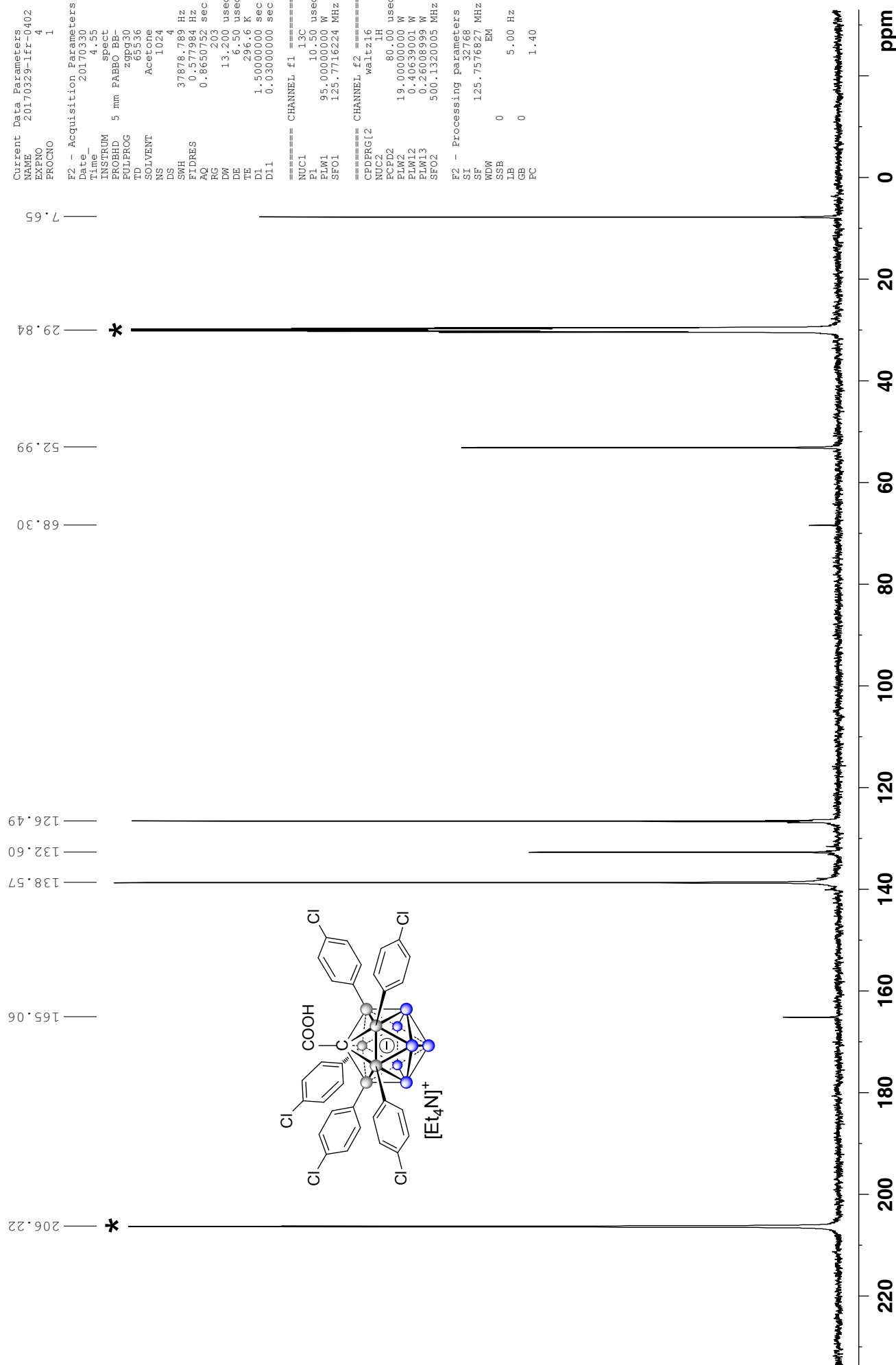
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 -11.4186



20170329-lfr-0401 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Cl)₅]
 160 MHz, ¹¹B{¹H} NMR, 30 mg dissolved in 0.55 mL acetone-d₆



20170329-lfr-0401 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Cl)₅]
 126 MHz, ¹³C{¹H} NMR, 30 mg dissolved in 0.55 mL acetone-d₆*



20170401-lfr-0408 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-Cl)₅]
500 MHz, ¹H{¹³B} NMR, 29 mg dissolved in acetone-d₆*

11.7908

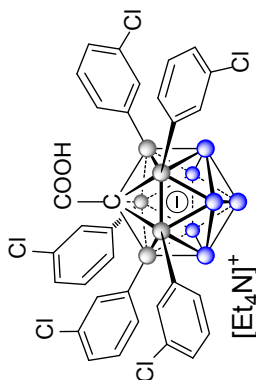
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7.1256
7.0873
7.0856
7.0715
7.0696
6.9337
6.9182
6.9026

3.4897
3.4753
3.4608
3.4463

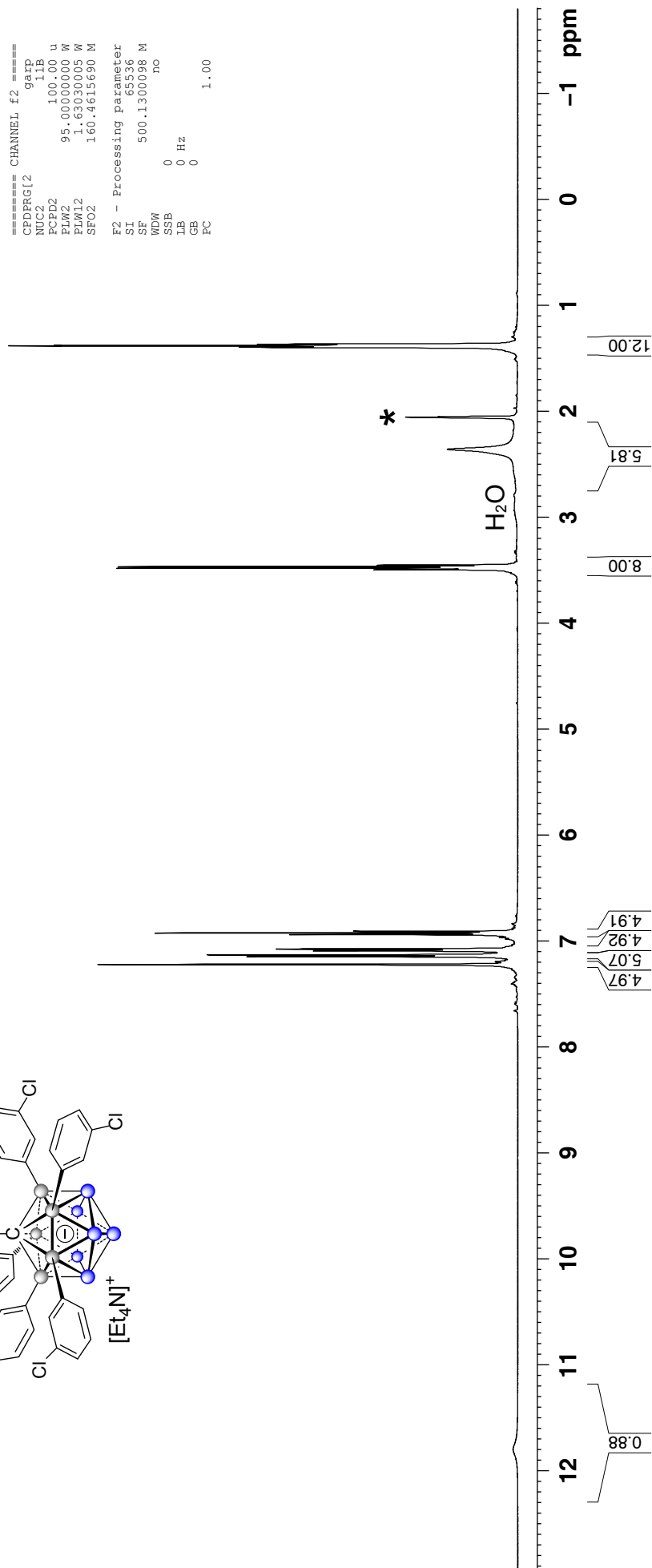
2.0500
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1.3732
1.3650
1.3622
1.3588

Current Data Parameters
NAME 20170401-lfr-040
EXPNO 1
PROCNO 1

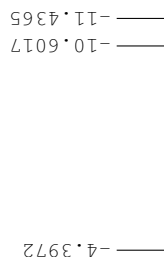
F2 - Acquisition Parameters
Date_ 20170401
Time 15.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgig30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 20000.000 H
FIDRES 0.305176 H
AQ 1.6384000 s
RG 64
DW 25.000 u
DE 6.50 u
TE 295.3 K
D1 5.0000000 s
D11 0.0300000 s



===== CHANNEL f1 =====
NUC1 1H
P1 11.50 u
PLW1 19.0000000 W
SFO1 500.1300000 M
===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 11B
PCPD2 100.00 u
PLW2 95.0000000 W
PLW12 1.63030005 W
SFO2 160.4615690 M
F2 - Processing parameters
SI 65536
SF 500.1300098 M
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



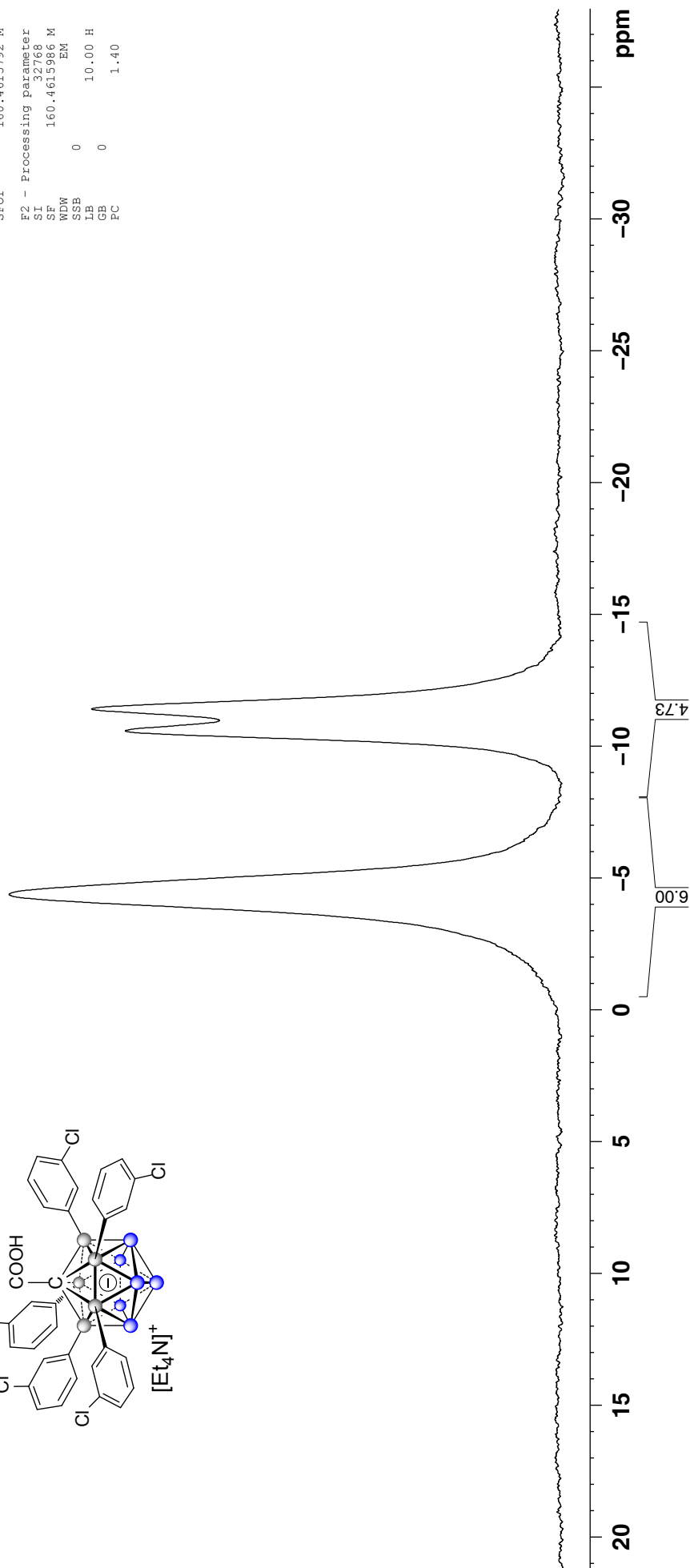
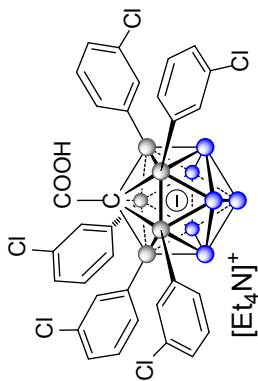
20170401-lfr-0408 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-Cl)₅]
 160 MHz, ¹¹B NMR, 29 mg dissolved in acetone-d₆



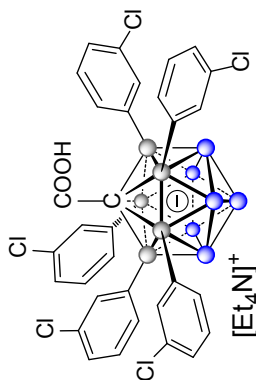
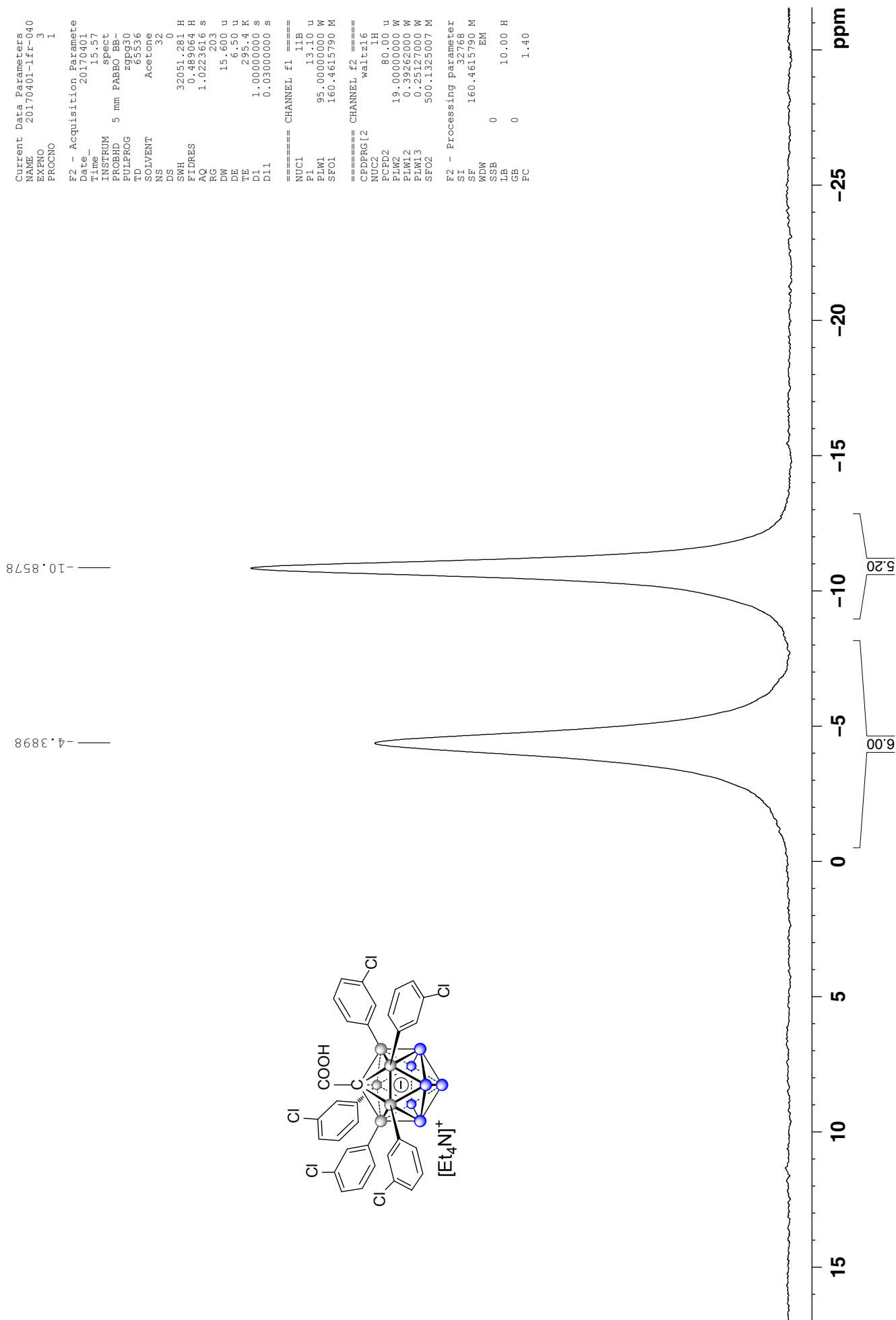
Current Data Parameters
 NAME 20170401-lfr-040
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameter
 Date_ 20170401
 Time_ 15:55
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zg30
 TD 64098
 SOLVENT Acetone
 NS 32
 DS 0
 SWH 32051.281 H
 FIDRES 0.500036 H
 AQ 0.9999288 S
 RG 203
 DW 15.600 u
 DE 650 u
 TE 295.0 K
 D1 1.0000000 S

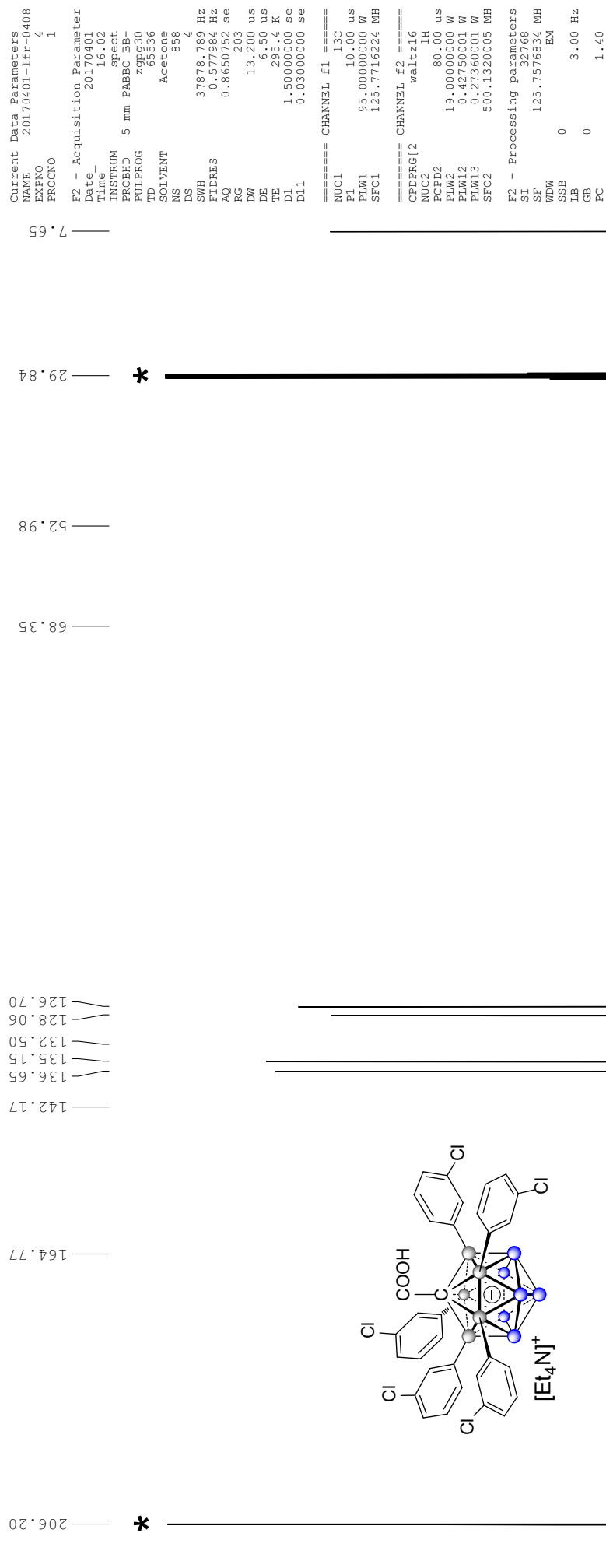
===== CHANNEL f1 =====
 NUC1 11B
 FL 13.10 u
 FLW1 95.0000000 W
 SFO1 160.4615792 M
 F2 - Processing parameter
 SI 32768
 SF 160.4615986 M
 WDW EM
 SSB 0
 LB 10.00 H
 GB 0
 PC 1.40



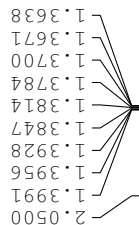
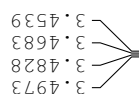
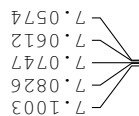
20170401-lfr-0408 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-Cl)₅]
 160 MHz, ¹¹B{¹H} NMR, 29 mg dissolved in acetone-d₆



20170401-lfr-0408 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-m-Cl)₅]
126 MHz, ¹³C{¹H} NMR, 29 mg dissolved in acetone-d₆*

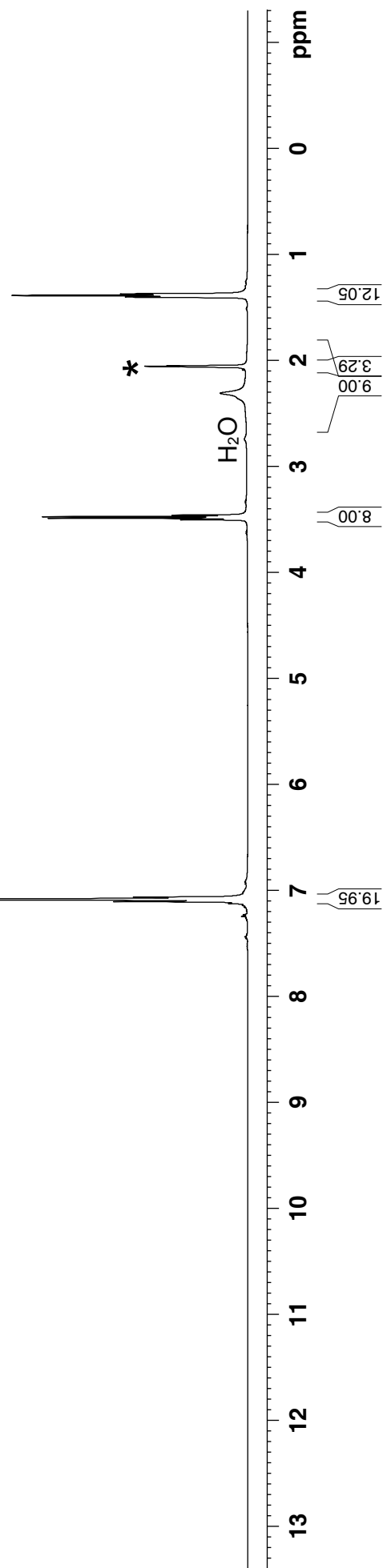


20170329-lfr-0401 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Br)₅]
 500 MHz, ¹H{¹B} NMR, 30 mg dissolved in 0.55 mL acetone-d₆*

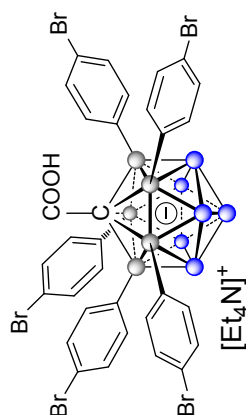


Current Data Parameters
 NAME 20170329-lfr-04
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Paramet
 Date_ 20170330
 Time_ 3.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgig30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 0
 SWH 12500.000
 FIDRES 0.190735
 AQ 2.6214399
 RG 71.8
 DW 40.000
 DE 6.50
 TE 296.1
 D1 5.00000000
 D11 0.03000000

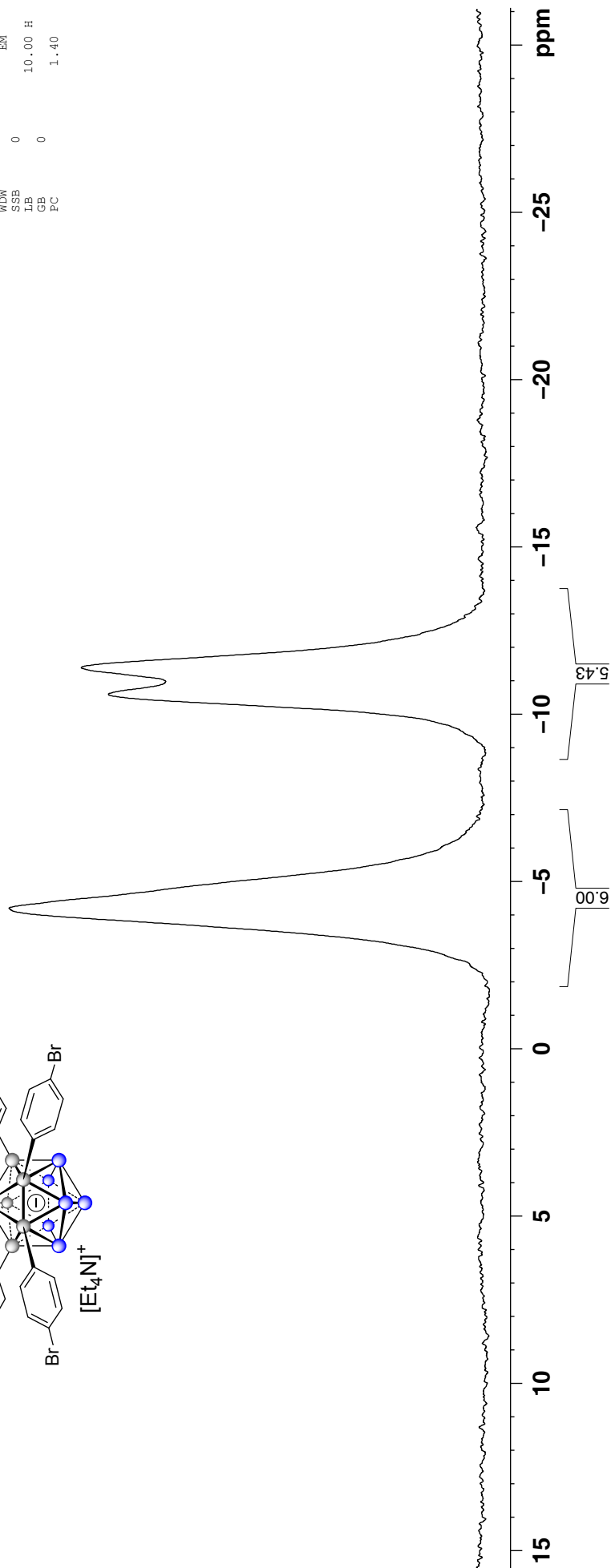
===== CHANNEL f1 =====
 NUC1 1H
 P1 11.70
 PLW1 19.00000000
 SFO1 500.1335009
 ===== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 11B
 PCPD2 100.00
 PLW2 95.00000000
 PLW12 1.63030005
 SFO2 160.4615690
 F2 - Processing Paramete
 SI 65536
 SF 500.1300101
 WDW 0
 SSB 0
 LB 1.00
 GB 0
 PC 1.00



20170329-lfr-0401 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Br)₅]
 160 MHz, ¹¹B NMR, 30 mg dissolved in 0.55 mL acetone-d₆



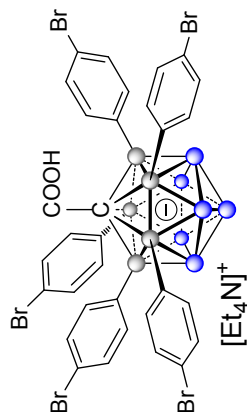
Current Data Parameters
 NAME 20170329-lfr-040
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameter
 Date_ 20170330
 Time_ 3.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 64098
 SOLVENT Acetone
 NS 32
 DS 0
 SWH 32051.281 H
 FIDRES 0.500036 H
 AQ 0.9999288 s
 RG 203
 DW 15.600 u
 DE 6.50 u
 TE 295.9 K
 D1 1.00000000 s
 ===== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 u
 PLW1 95.00000000 W
 SFO1 160.4615792 M
 F2 - Processing parameter
 SI 32768
 SF 160.4615790 M
 MDW 0
 SSB 0
 LB 10.00 H
 GB 0
 PC 1.40



20170329-lfr-0401 [NEt₄][COOH-CB₁₁H₆⁻-(C₆H₄-p-Br)₅]
 160 MHz, ¹¹B{¹H} NMR, 30 mg dissolved in 0.55 mL acetone-d₆

— -4.3810

— -11.0102

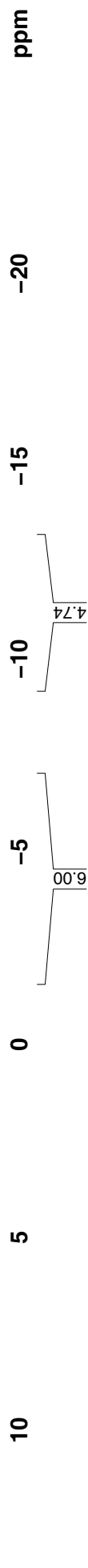


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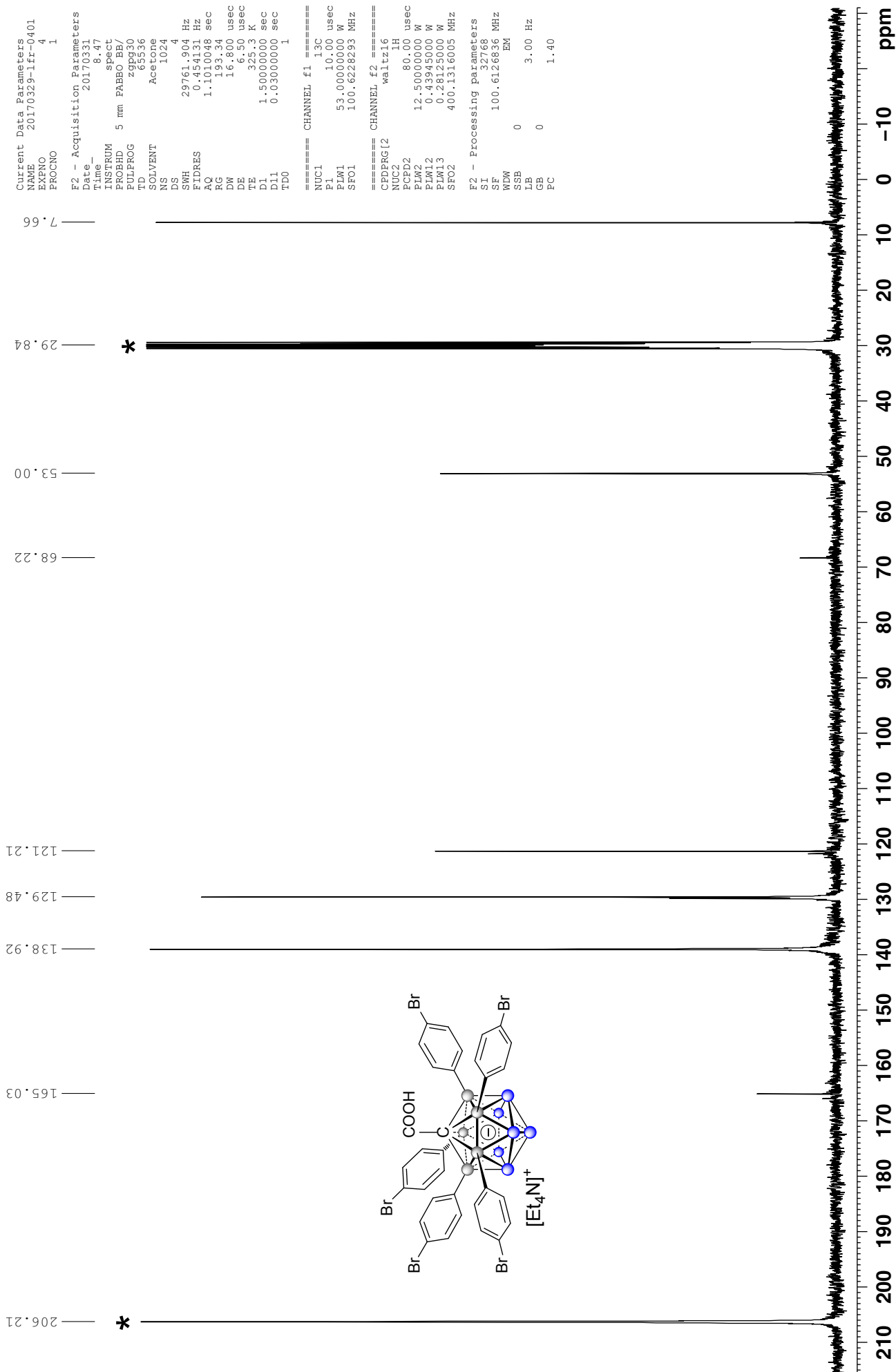
Current Data Parameters
NAME      20170329-lfr-040
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20170330
Time      4.02
INSTRUM   spect
PROBHD    5 mm FABBO B5
PULPROG   zgpg30
TD        65536
SOLVENT   Acetone
NS         32
DS         0
SWH        32051.281 H
FIDRES     0.489064 H
AQ         1.0223616 s
RG          203
DW         15.600 u
DE         6.50 u
TE         296.2 K
D1         1.00000000 s
D11        0.03000000 s
===== CHANNEL f1 =====
NUC1       11B
P1         13.10 u
PLW1       95.00000000 W
SFO1       160.4615790 M
===== CHANNEL f2 =====
CPDPRG[2   waltz16
NUC2       1H
PCPD2      80.00 u
PLW2       19.00000000 W
PLW12      0.40639001 W
PLW13      0.26008999 W
SFO2       500.1325007 M

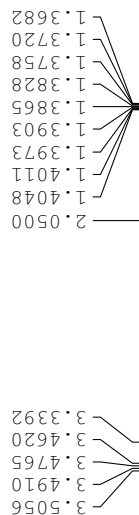
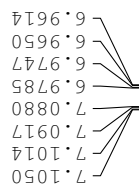
F2 - Processing parameters
SI          32768
SF          160.4615790 M
WDW         EM
SSB         0
LB          10.00 H
GB          0
PC          1.40
  
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20170329-lfr-0401 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-p-Br)₅]
 101 MHz, ¹³C{¹H} NMR, 30 mg dissolved in 0.55 mL acetone-d₆*

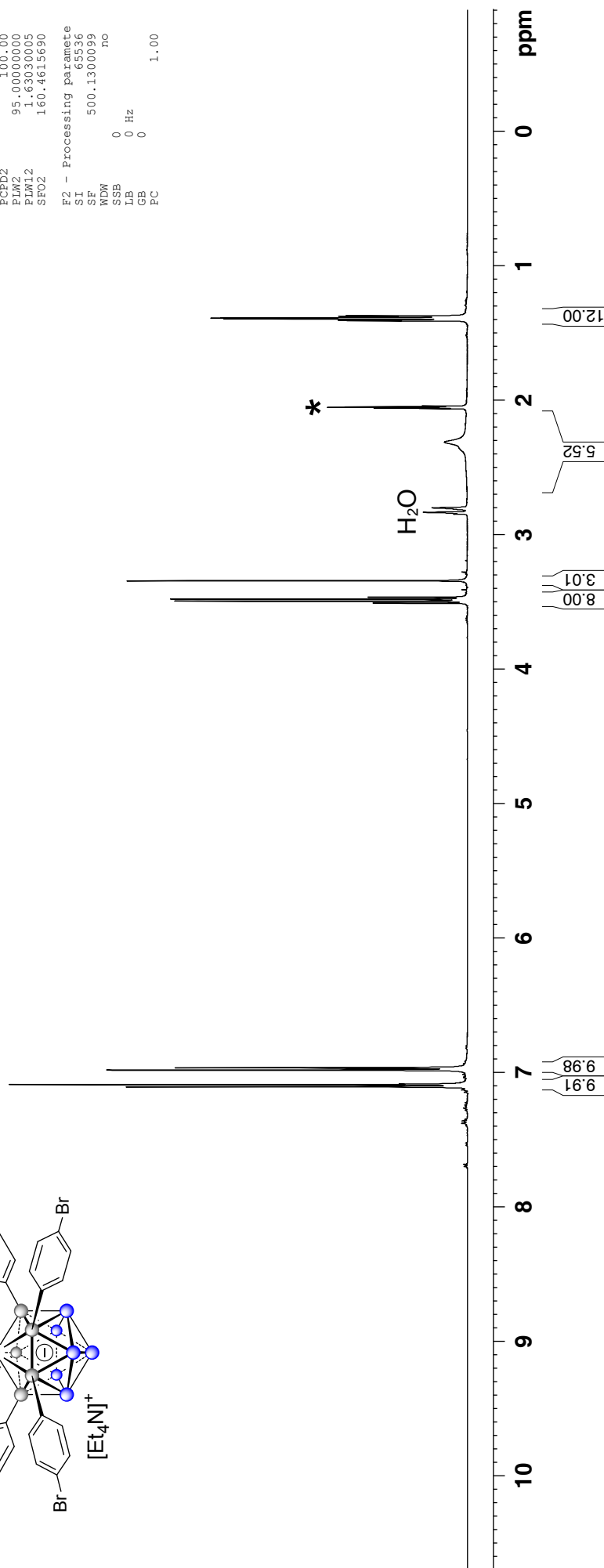


20171030-lfr-0470 [NEt₄][COOMe-CB₁₁H₆-(4-Br-C₆H₄)₅]
 500 MHz, ¹H{¹B} NMR, ca. 26 mg dissolved in 0.55 mL acetone-d₆*



Current Data Parameters
 NAME lfr-0470-2
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20171030
 Time 15.57
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 0
 SWH 12500.000
 FIDRES 0.190735
 AQ 2.6214399
 RG 80.6
 DW 40.000
 DE 6.50
 TE 296.5
 D1 5.00000000
 D11 0.03000000

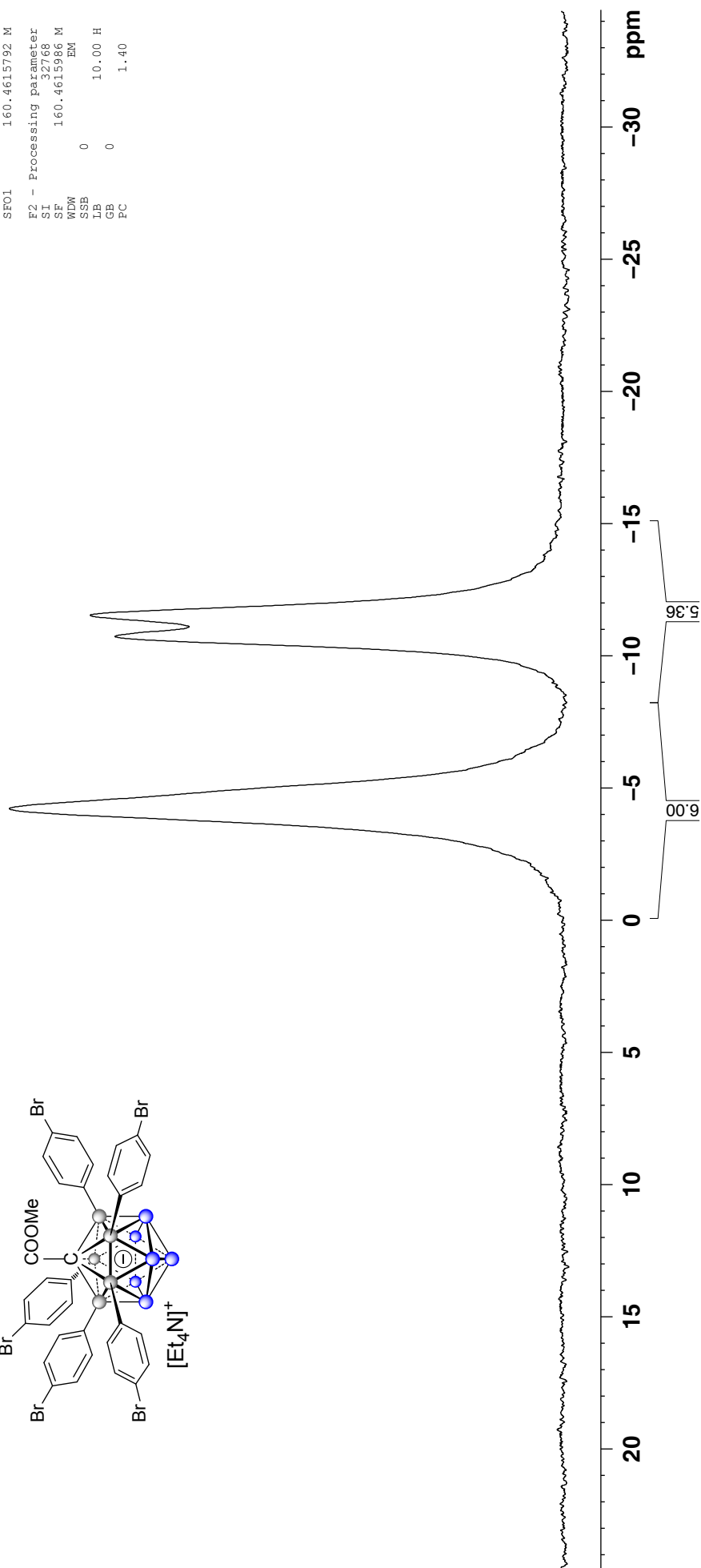
===== CHANNEL f1 =====
 NUC1 1H
 P1 11.70
 PLW1 19.00000000
 SFO1 500.1335009
 ===== CHANNEL f2 =====
 CPDPRG[2] garp
 NUC2 11B
 P1 100.00
 PLW2 95.00000000
 PLW12 1.63030005
 SFO2 160.4615690
 F2 - Processing parameters
 SI 65536
 SF 500.1300099
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



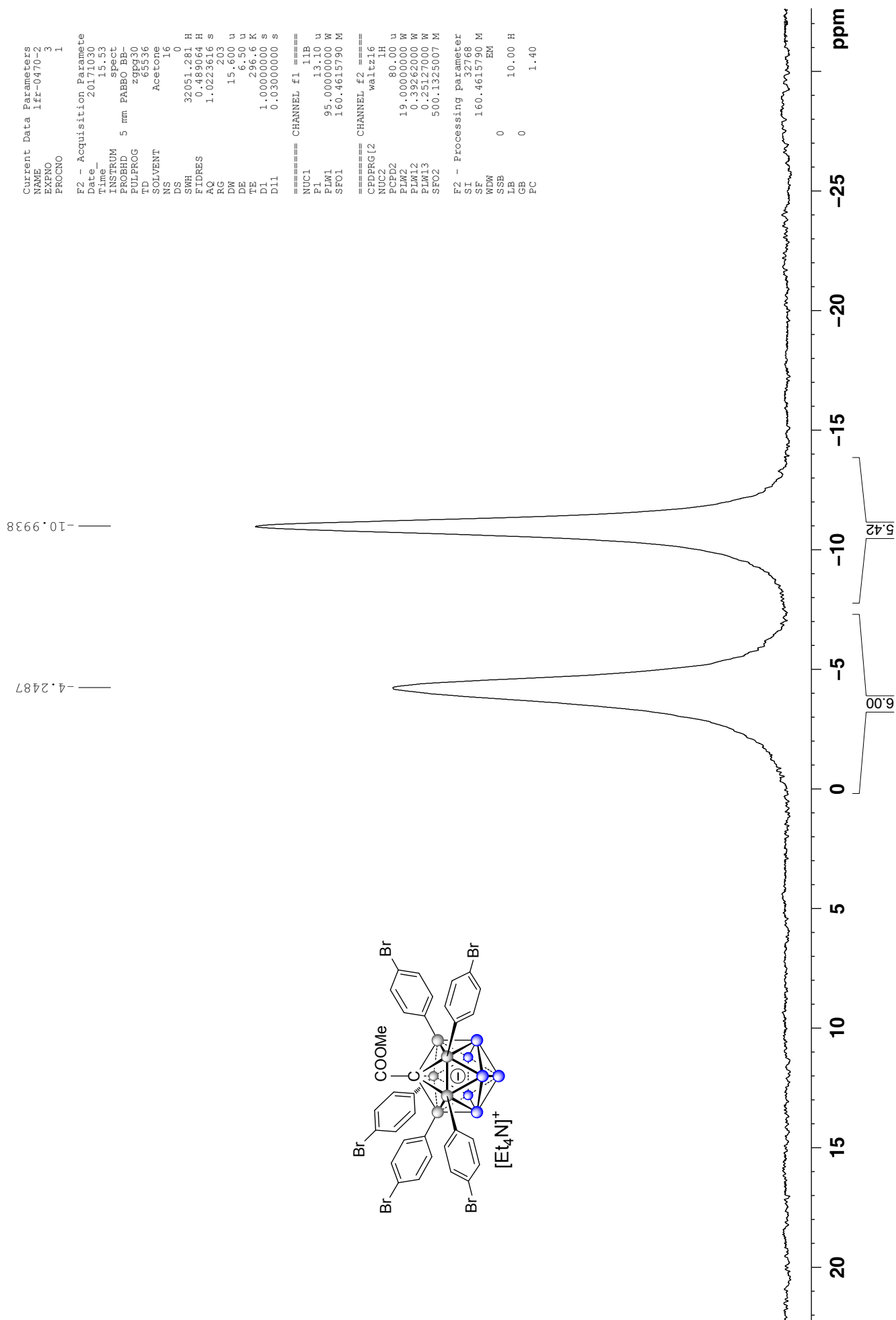
20171030-lfr-0470 [NEt₄][COOMe-CB₁₁H₆-(4-Br-C₆H₄)₅]
 160 MHz, ¹¹B NMR, ca. 26 mg dissolved in 0.55 mL acetone-d₆



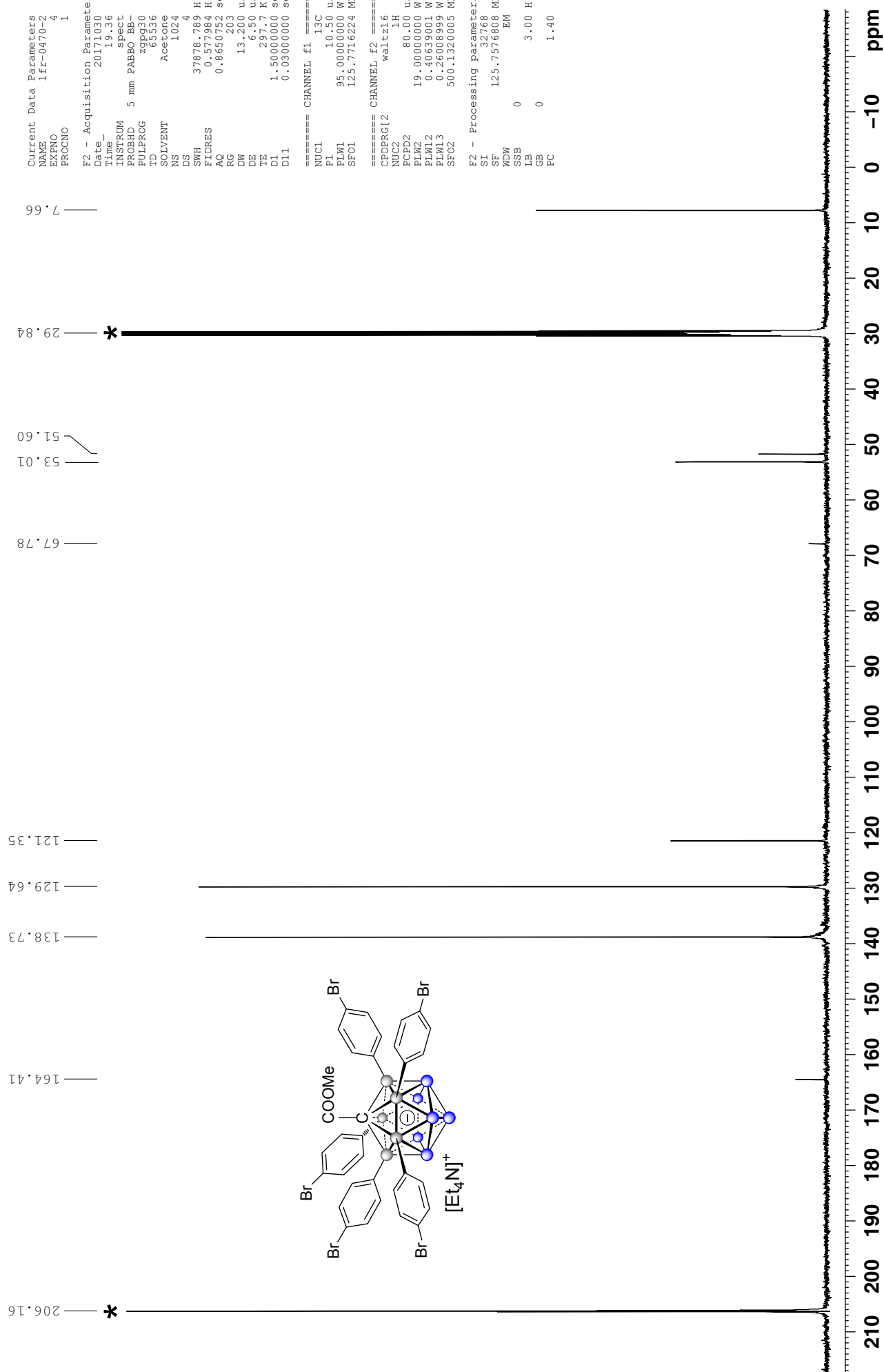
Current Data Parameters
 NAME lfr-0470-2
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20171030
 Time_ 15.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 64098
 SOLVENT Acetone
 NS 32
 DS 0
 SWH 32051.281 H
 FIDRES 0.500036 H
 AQ 0.9999288 S
 RG 203
 DW 15.600 u
 DE 6.50 u
 TE 296.5 K
 D1 1.00000000 S
 ===== CHANNEL f1 =====
 NUC1 11B
 P1 13.10 u
 PL1 95.00000000 W
 SF01 160.4615792 M
 F2 - Processing parameters
 SI 32768
 SF 160.4615986 M
 WDW EM
 SSB 0
 LB 10.00 H
 GB 0
 PC 1.40



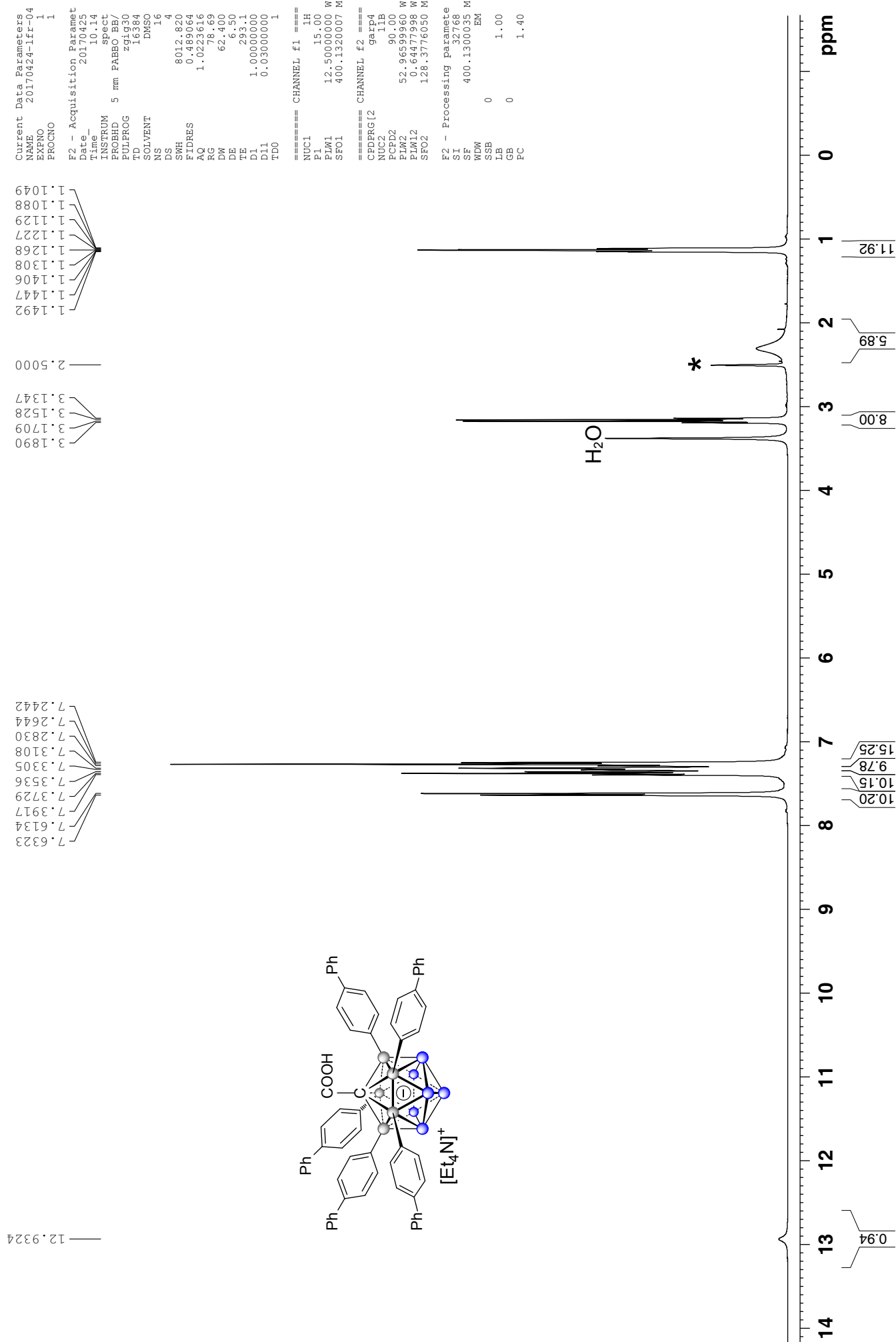
20171030-lfr-0470 [NEt₄][COOMe-CB₁₁H₆-(4-Br-C₆H₄)₅]
 160 MHz, ¹B{¹H} NMR, ca. 26 mg dissolved in 0.55 mL acetone-d₆



20171030-lfr-0470 [NEt₄][COOMe-CB₁₁H₆-(4-Br-C₆H₄)₅]
 126 MHz, ¹³C{¹H} NMR, ca. 26 mg dissolved in 0.55 mL acetone-d₆*



20170424-lfr-0411 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-Ph)₅]
 400 MHz, ¹H{¹B} NMR, 30 mg dissolved in 0.55 mL dmsO-d₆*



20170424-lfr-0411 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-Ph)₅]
 128 MHz, ¹¹B NMR, 30 mg dissolved in 0.55 mL dmsO-d₆

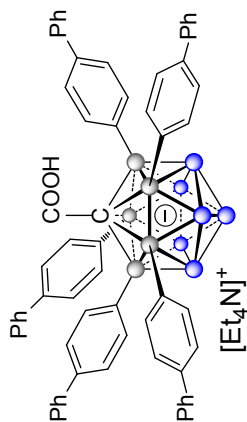
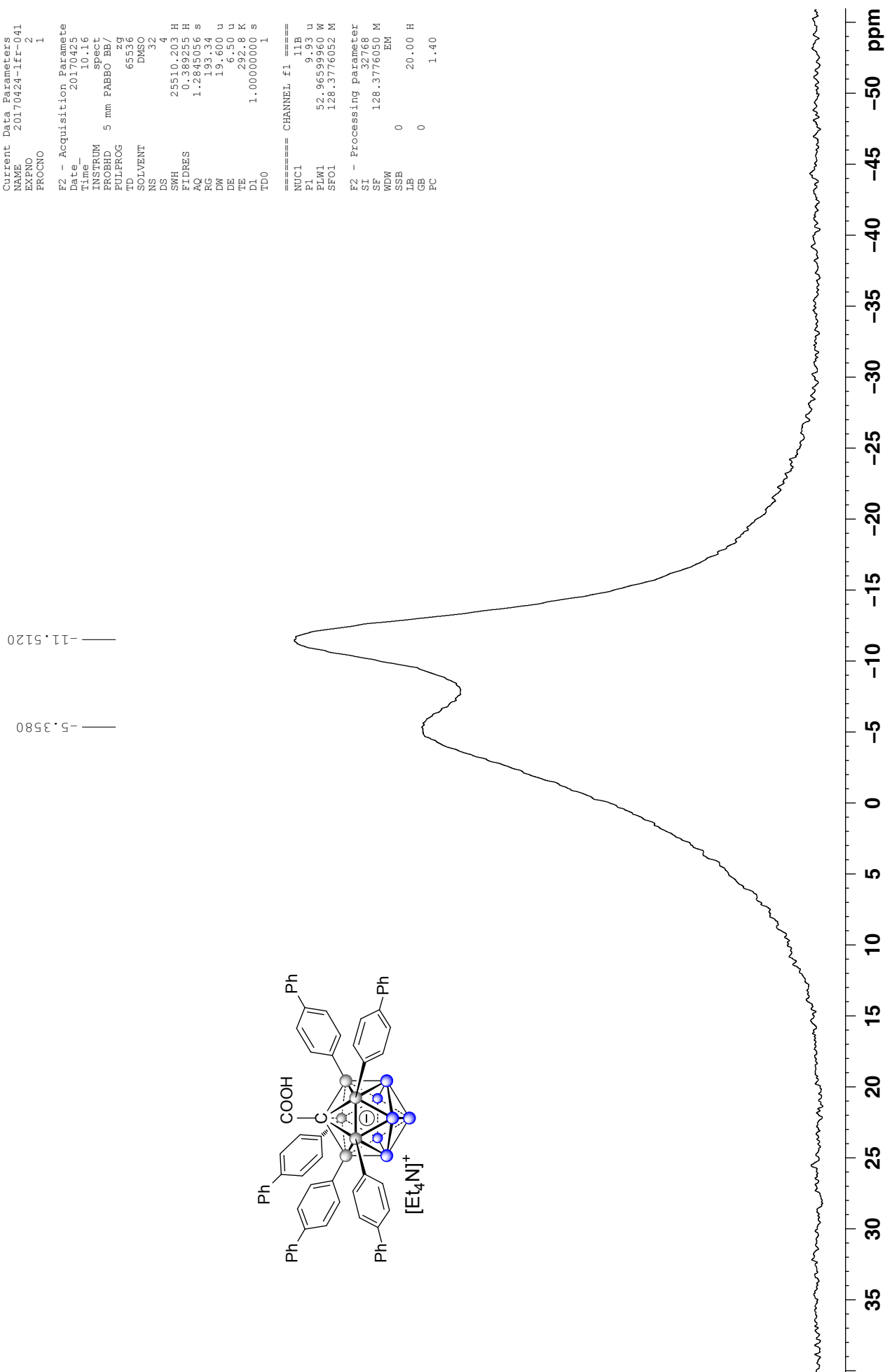
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Current Data Parameters
NAME      20170424-lfr-041
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20170425
Time      10.16
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg
TD         65536
SOLVENT   DMSO
NS         32
DS         4
SWH        25510.203 H
FIDRES     0.389255 H
AQ         1.2845056 s
RG         193.34
DW         19.600 u
DE         6.50 u
TE         292.8 K
D1         1.0000000 s
TD0        1

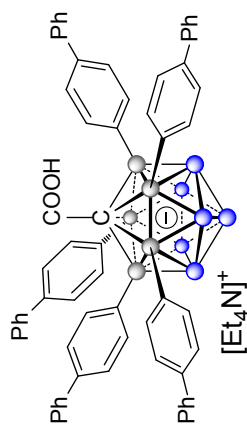
===== CHANNEL f1 =====
NUC1       11B
P1         9.93 u
PLW1       52.9659960 W
SFO1       128.3776052 M

F2 - Processing parameters
SI         32768
SF         128.3776050 M
WDW        EM
SSB        0
LB         20.00 H
GB         0
PC         1.40
    
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20170424-lfr-0411 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-Ph)₅]
 128 MHz, ¹B{¹H} NMR, 30 mg dissolved in 0.55 mL dmsO-d₆

— -5.6179
 — -11.7926



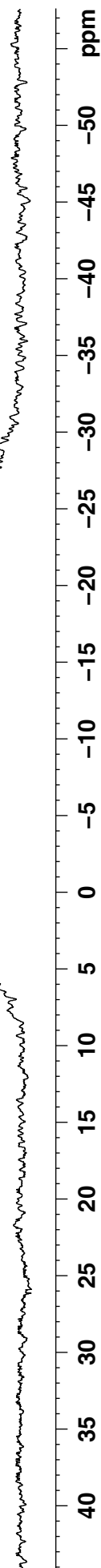
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Current Data Parameters
NAME      20170424-lfr-0411
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20170425
Time      10.18
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         32
DS         4
SWH        25510.203 H
FIDRES     0.389255 H
AQ         1.2845056 s
RG         193.34
DW         19.600 u
DE         6.50 u
TE         293.5 K
D1         1.00000000 s
D11        0.03000000 s
TD0        1

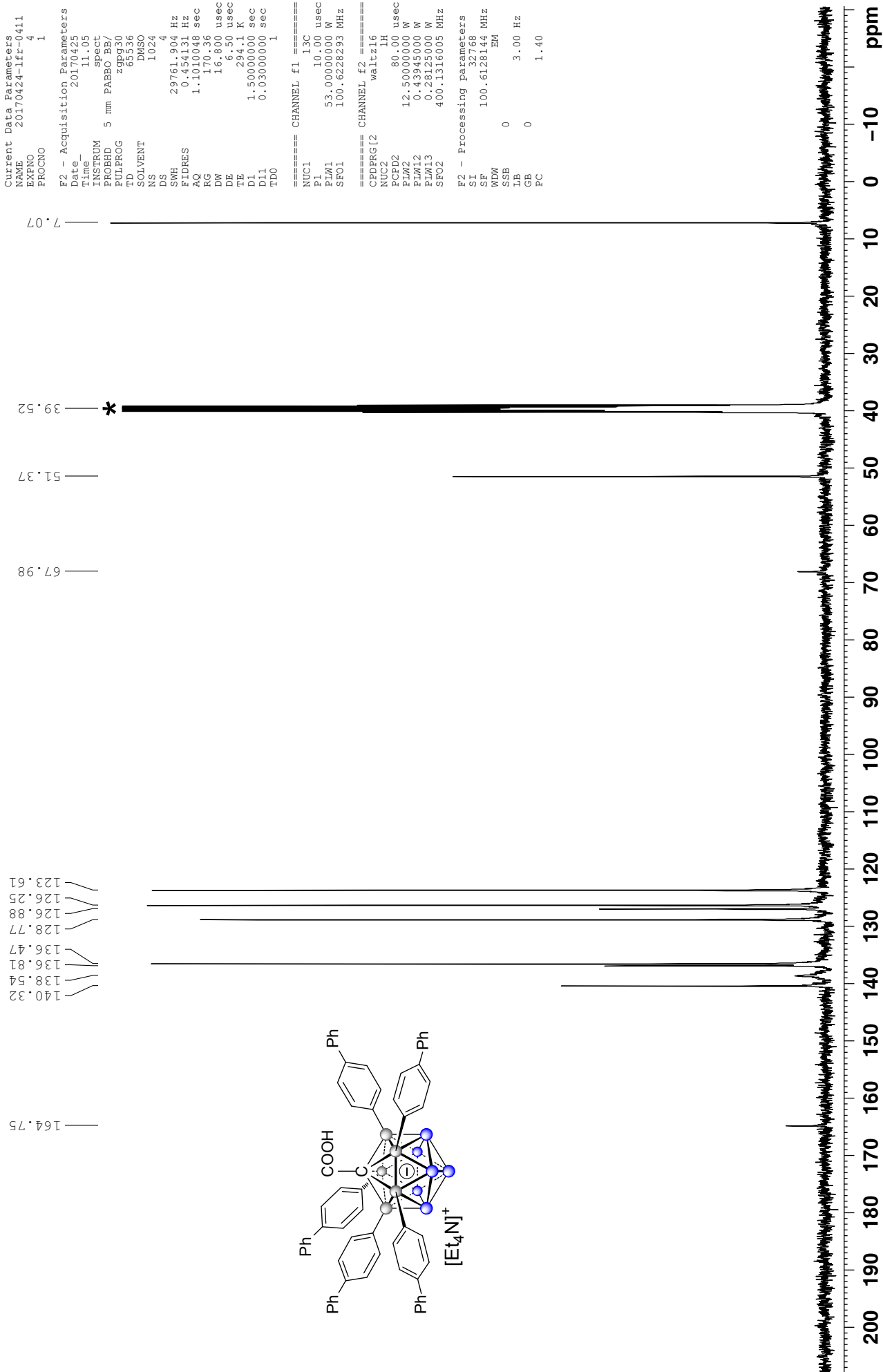
===== CHANNEL f1 =====
NUC1       11B
P1         9.93 u
PLW1       52.96599960 W
SFO1       128.3776050 M

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 u
PLW2       12.50000000 W
PLW12      0.43945000 W
PLW13      0.28135000 W
SFO2       400.1320007 M

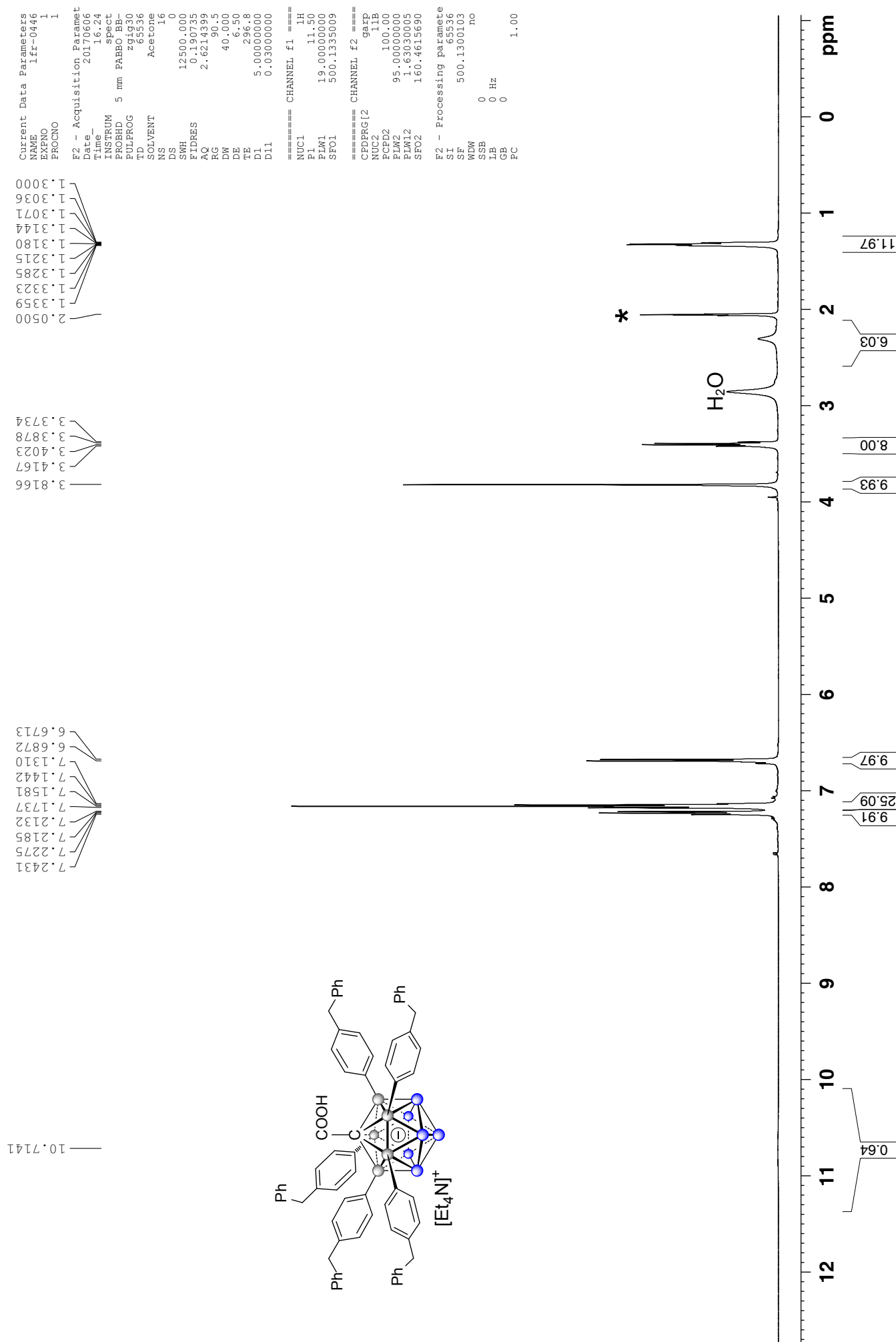
F2 - Processing parameter
SI         32768
SF         128.3776050 M
WDW        EM
SSB        0
LB         20.00 H
GB         0
FC         1.40
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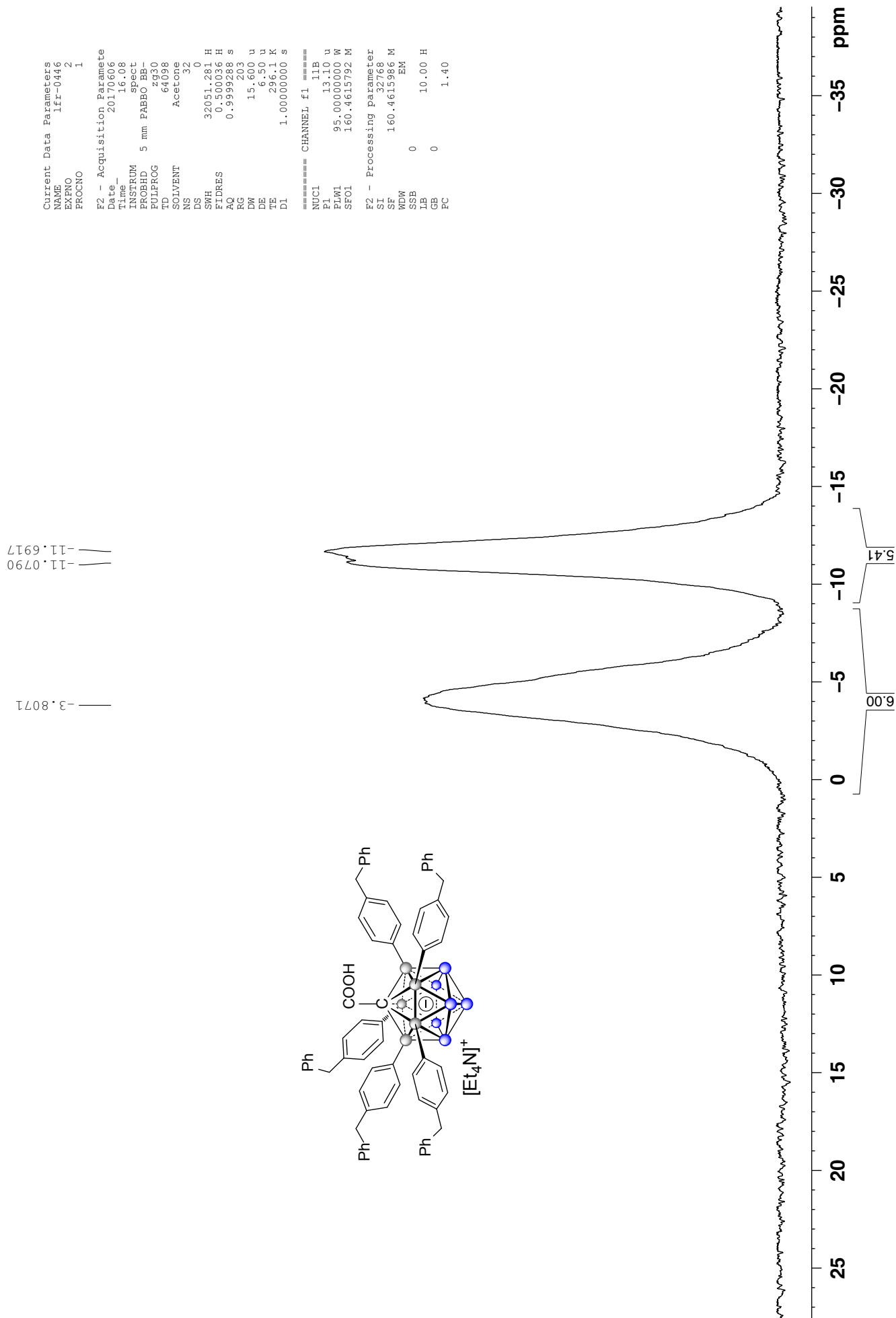
20170424-lfr-0411 [NEt₄][COOH-CB₁₁H₆-(C₆H₄-Ph)₅]
 101 MHz, ¹³C{¹H} NMR, 30 mg dissolved in 0.55 mL dmsO-d6*



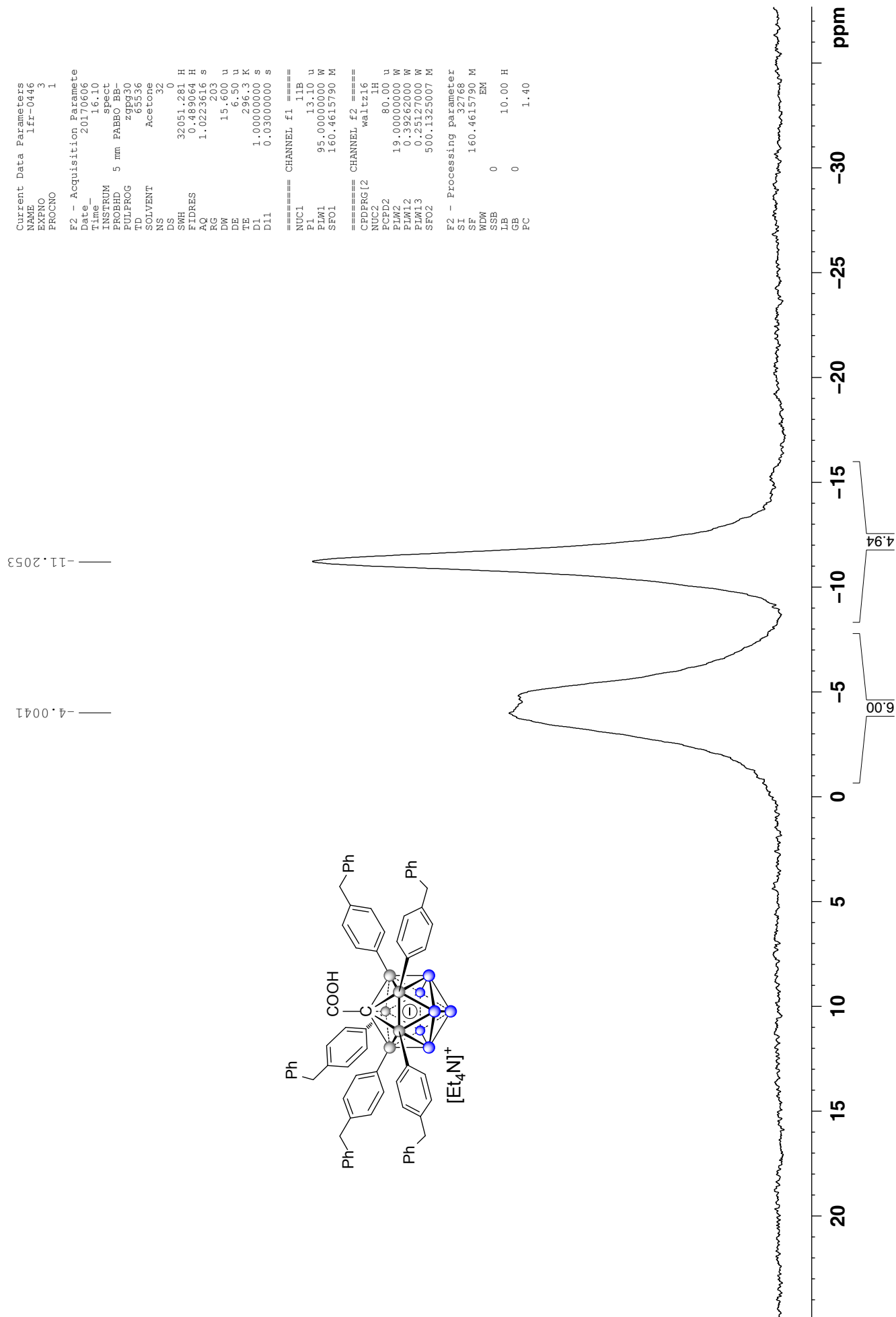
20170606-lfr-0446 [NEt₄][COOH-CB₁₁H₆-(4-PhCH₂-C₆H₄)₅]
500 MHz, ¹H{¹B} NMR, ca. 16 mg dissolved in 0.55 mL acetone-d₆*



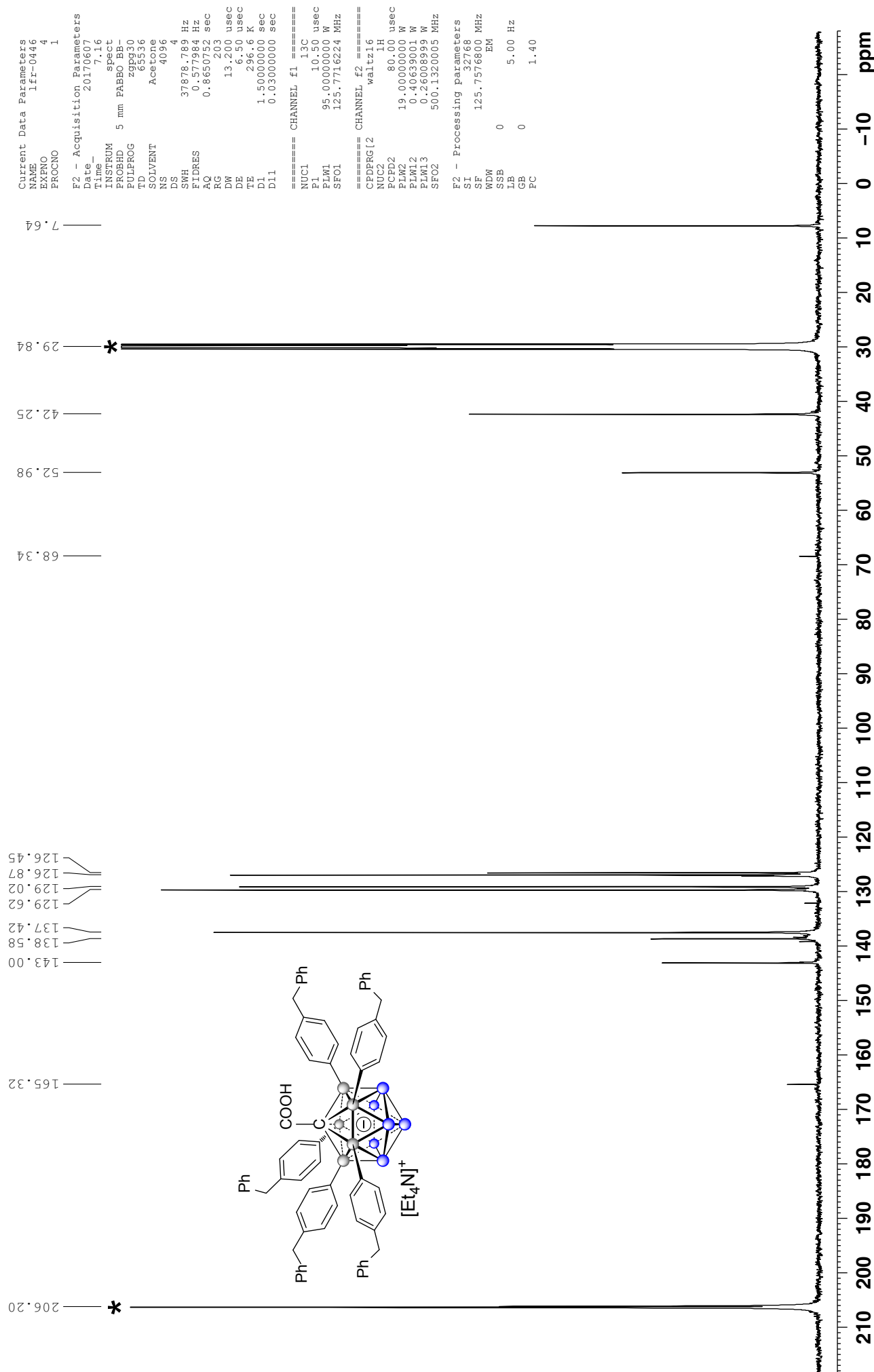
20170606-lfr-0446 [NEt₄][COOH-CB₁₁H₆-(4-PhCH₂-C₆H₄)₅]
160 MHz, ¹¹B NMR, ca. 16 mg dissolved in 0.55 mL acetone-d₆



20170606-lfr-0446 [NEt₄][COOH-CB₁₁H₆-(4-PhCH₂-C₆H₄)₅]
 160 MHz, ¹B{¹H} NMR, ca. 16 mg dissolved in 0.55 mL acetone-d₆

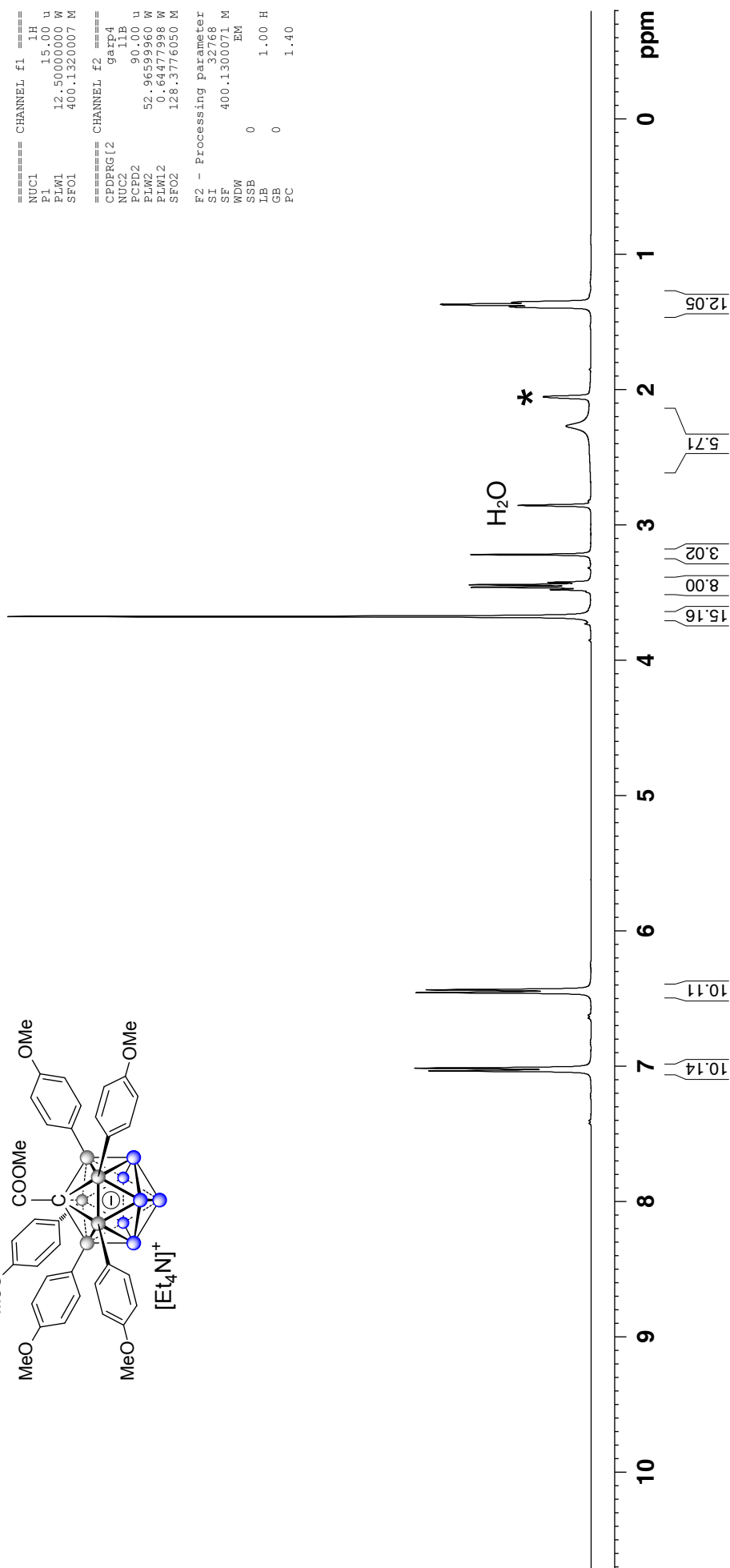
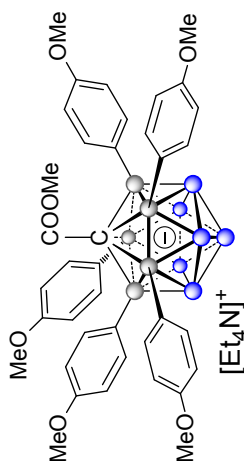
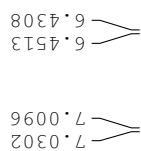
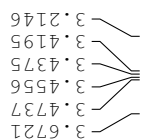
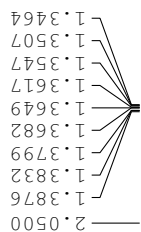


20170606-lfr-0446 [NEt₄][COOH-CB₁₁H₆-(4-PhCH₂-C₆H₄)₅]
 126 MHz, ¹³C{¹H} NMR, ca. 16 mg dissolved in 0.55 mL acetone-d₆

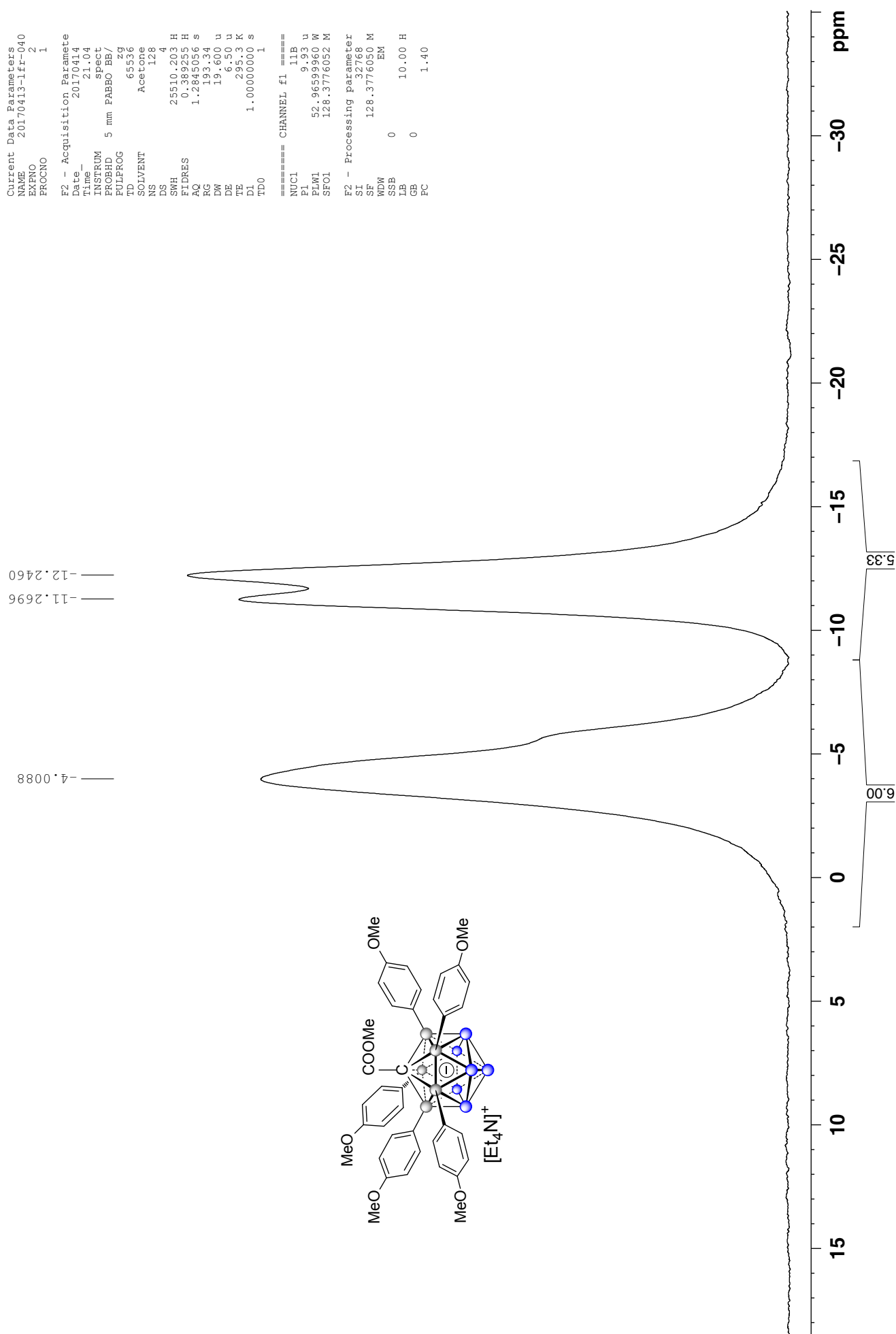


20170413-lfr-0409-Me [NEt₄][COOMe-CB₁₁H₆-(C₆H₄-p-OMe)₅]
 400 MHz, ¹H{¹B} NMR, 17 mg dissolved in 0.55 mL acetone-d₆*

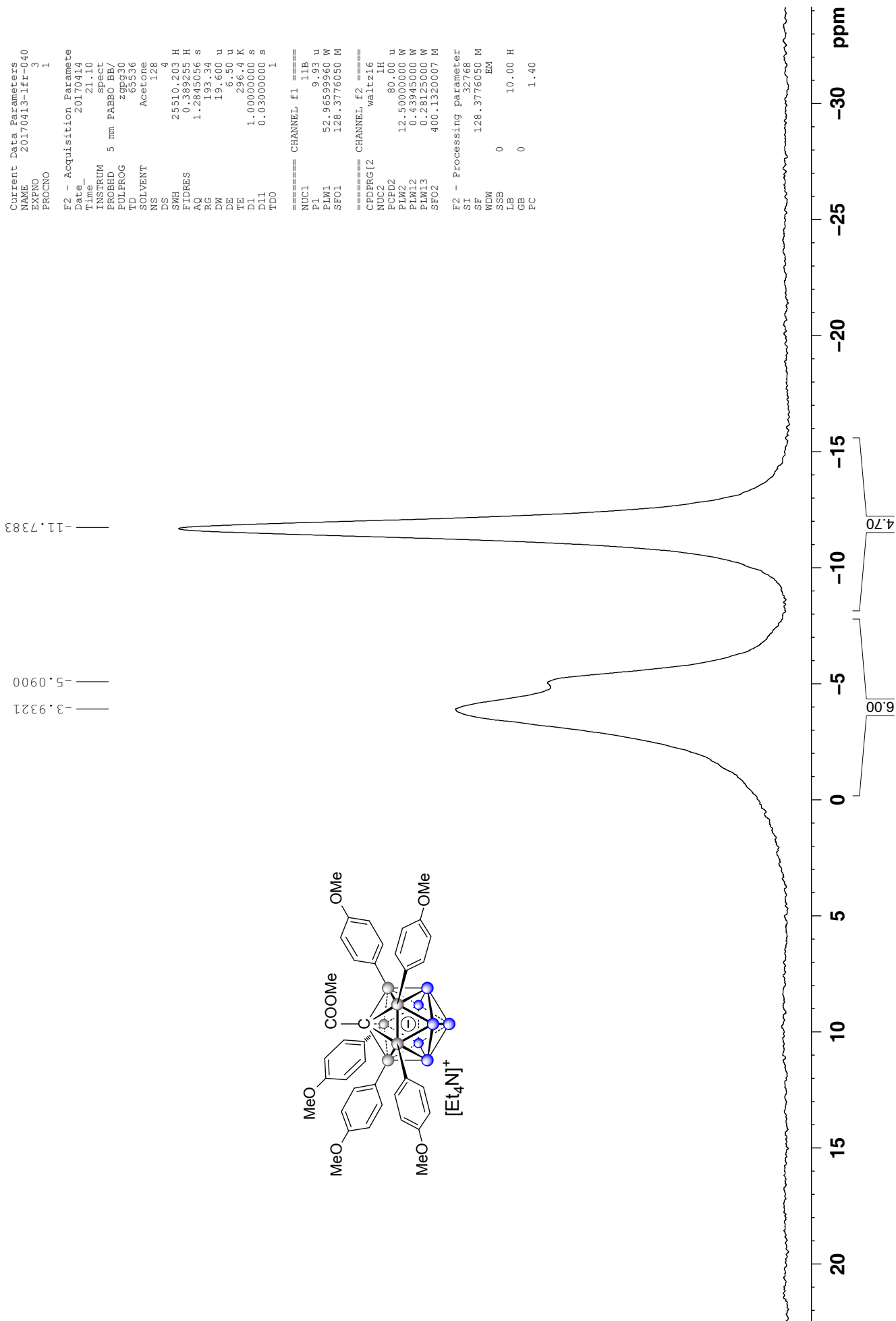
Current Data Parameters
 NAME 20170413-lfr-040
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20170414
 Time_ 5.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 H
 FIDRES 0.489064 H
 AQ 1.0223616 s
 RG 107.6
 DW 62.400 u
 DE 6.50 u
 TE 294.2 K
 D1 1.0000000 s
 D11 0.0300000 s
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 u
 PLW1 12.5000000 W
 SFO1 400.1320007 M
 ===== CHANNEL f2 =====
 CPDPRG[2] garp4
 NUC2 ¹¹B
 P2 90.00 u
 PLW2 52.96599960 W
 PLW12 0.64477998 W
 SFO2 128.3776050 M
 F2 - Processing parameters
 SI 32768
 SF 400.1300071 M
 WDW EM
 SSB 0
 LB 1.00 H
 GB 0
 PC 1.40



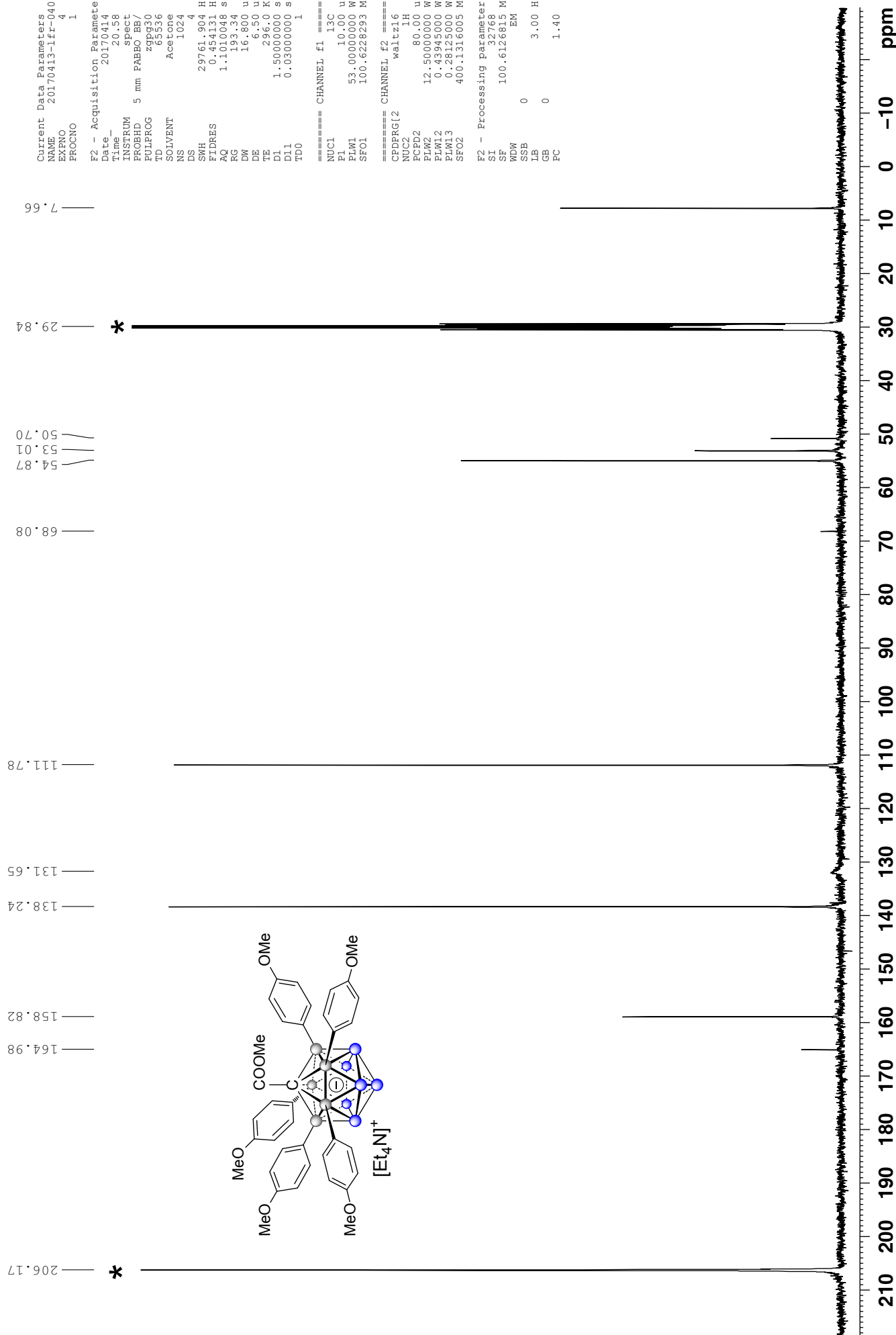
20170413-lfr-0409-Me [NEt₄][COOMe-CB₁₁H₆-(C₆H₄-p-OMe)₅]
 128 MHz, ¹¹B NMR, 17 mg dissolved in 0.55 mL acetone-d₆



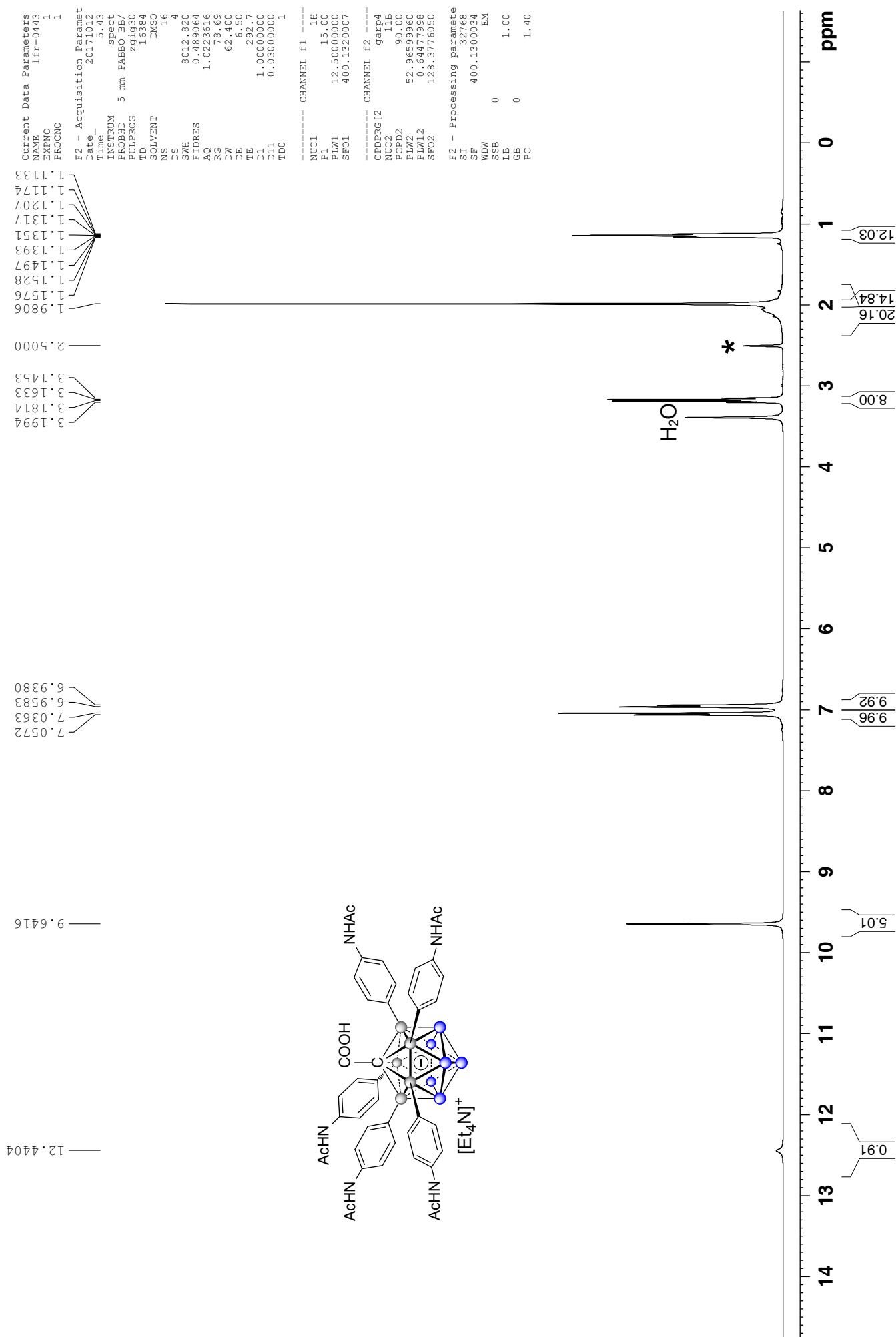
20170413-lfr-0409-Me [NEt₄][COOMe-CB₁₁H₆-(C₆H₄-p-OMe)₅]
 128 MHz, ¹¹B{¹H} NMR, 17 mg dissolved in 0.55 mL acetone-d₆



20170413-lfr-0409-Me [NEt₄][COOMe-CB₁₁H₆-(C₆H₄-p-OMe)₅]
101 MHz, ¹³C{¹H} NMR, 17 mg dissolved in 0.55 mL acetone-d₆*

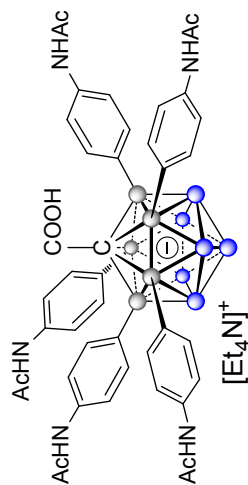


20171011-lfr-0443 [NEt₄][COOH-CB₁₁H₆-(4-NHAc-C₆H₄)₅]
400 MHz, ¹H{¹B} NMR, ca. 28 mg dissolved in 0.55 mL dmsO-d₆*



20171011-lfr-0443 [NEt₄][COOH-CB₁₁H₆-(4-NHAc-C₆H₄)₅]
 128 MHz, ¹¹B NMR, ca. 28 mg dissolved in 0.55 mL dmsO-d₆

— -6.2036
 — -12.4126

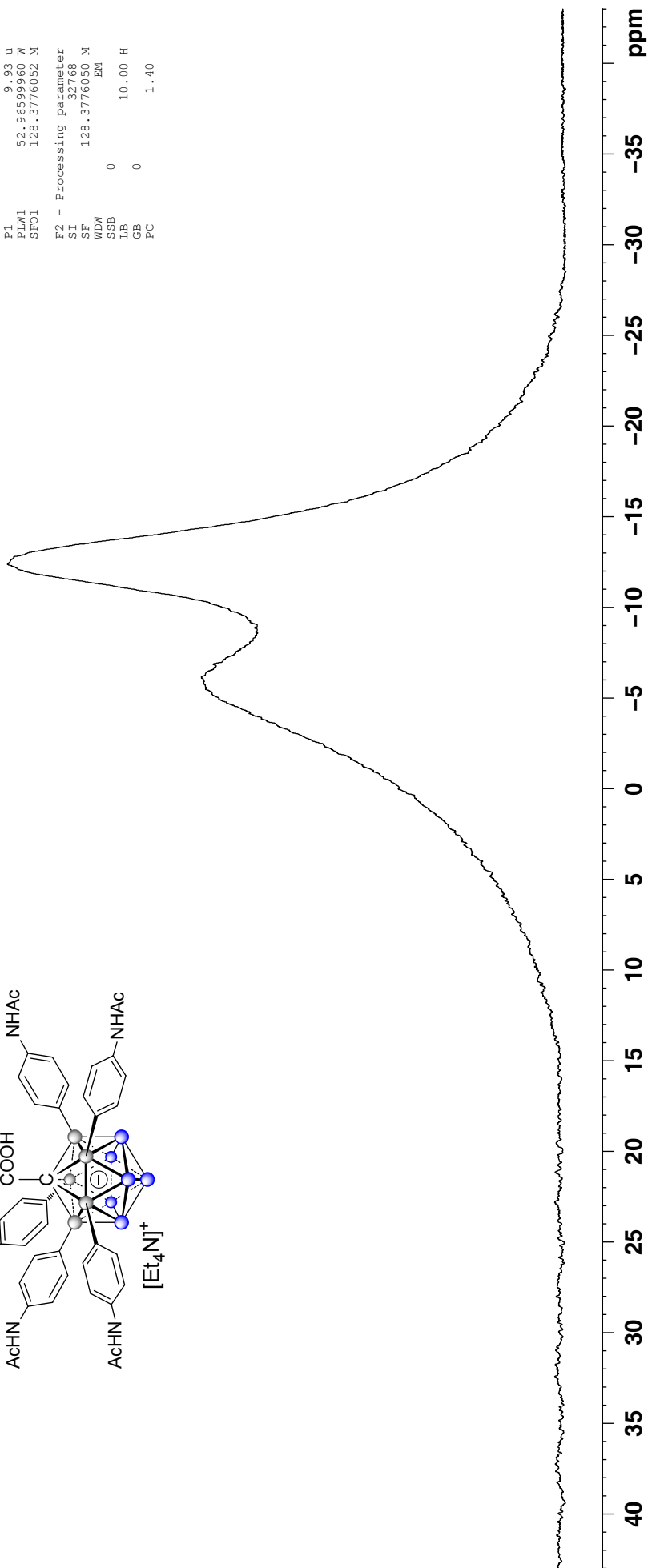


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Current Data Parameters
NAME      lfr-0443
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20171012
Time      5.48
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg
TD         65536
SOLVENT   DMSO
NS         128
DS         4
SWH        25510.203 H
FIDRES     0.389255 H
AQ         1.2845056 s
RG         193.34
DW         19.600 u
DE         6.50 u
TE         293.0 K
D1         1.0000000 s
TD0        1

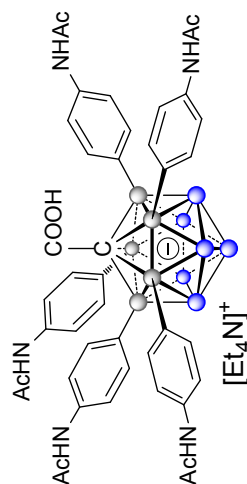
===== CHANNEL f1 =====
NUC1       11B
P1         9.93 u
PLM1       52.9659960 M
SFO1       128.3776052 M

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



20171011-lfr-0443 [NEt₄][COOH-CB₁₁H₆-(4-NHAc-C₆H₄)₅]
 128 MHz, ¹¹B{¹H} NMR, ca. 28 mg dissolved in 0.55 mL dmsO-d₆

— -5.6836 —
 — -12.4730 —



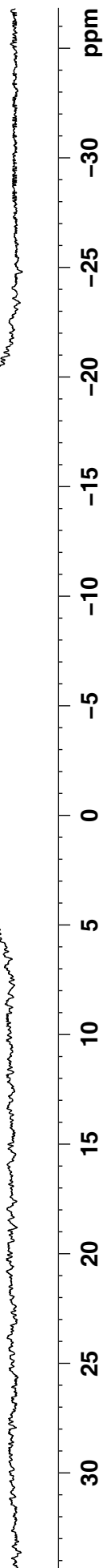
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Current Data Parameters
NAME      lfr-0443
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20171012
Time      5.55
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS         128
DS         4
SWH        25510.203 H
FIDRES     0.389255 H
AQ         1.2845056 s
RG         193.34
DE         19.600 u
TE         6.50 u
D1         293.6 K
D11        1.0000000 s
D11        0.0300000 s
TD0        1

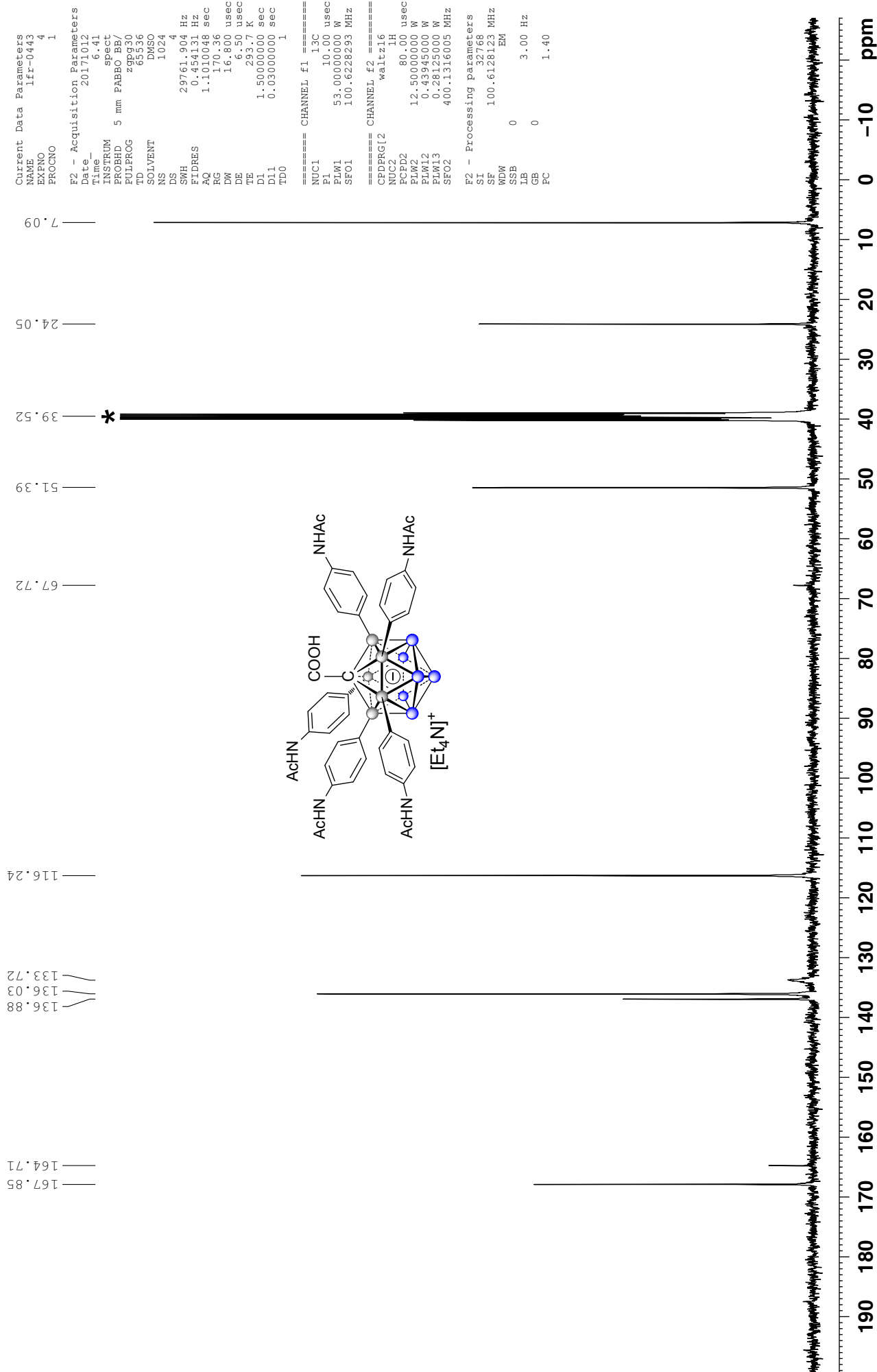
===== CHANNEL f1 =====
NUC1       11B
P1         9.93 u
PLW1       52.9659960 W
SFO1       128.3776050 M

===== CHANNEL f2 =====
CPDPRG[2   waltz16
NUC2       1H
PCPD2      80.00 u
PLW2       12.5000000 W
PLW12      0.43945000 W
PLW13      0.28125000 W
SFO2       400.1320007 M

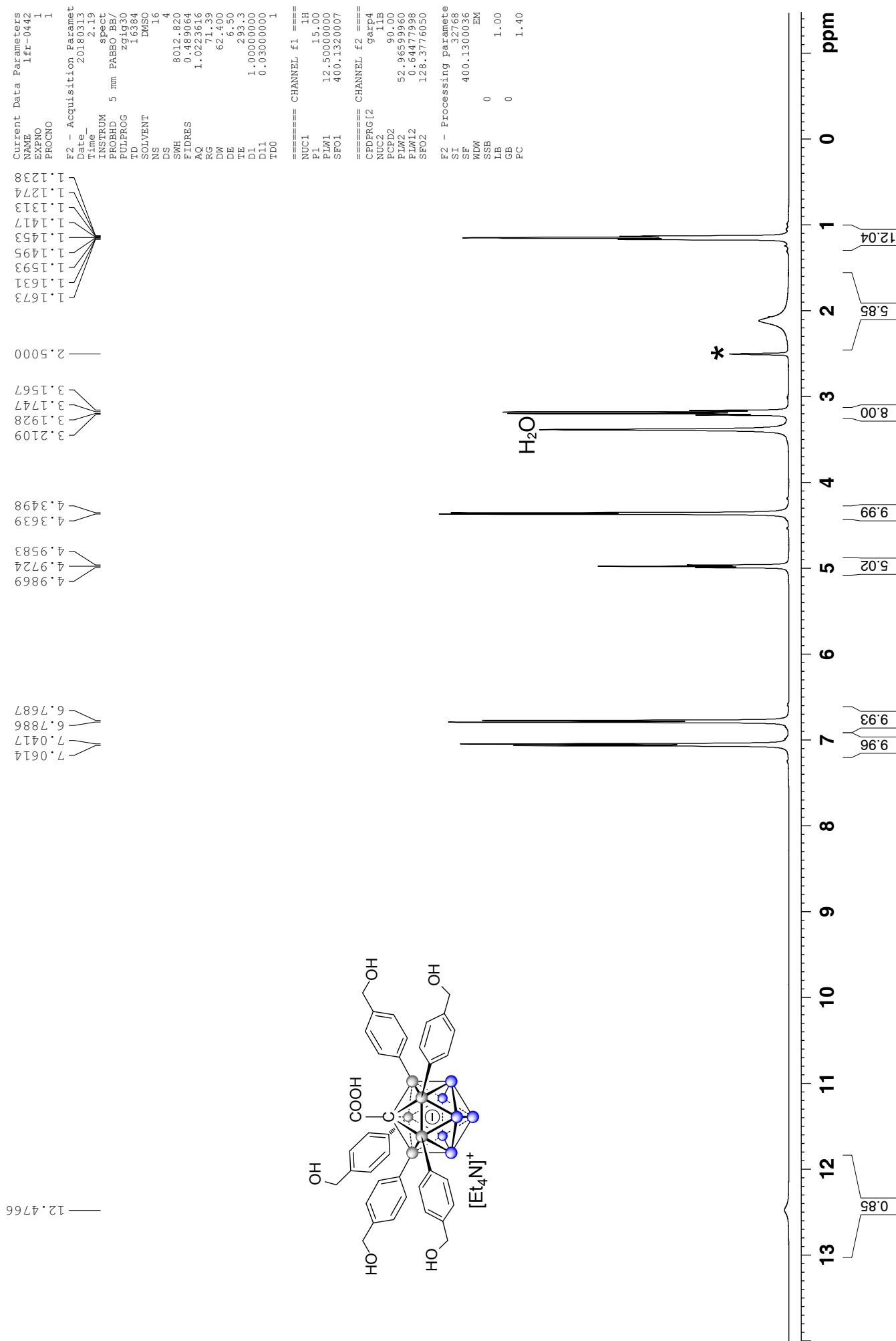
F2 - Processing parameters
SI         32768
SF         128.3776050 M
WDW        EM
SSB        0
LB         10.00 H
GB         0
PC         1.40
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20171011-lfr-0443 [NEt₄][COOH-CB₁₁H₆-(4-NHAc-C₆H₄)₅]
101 MHz, ¹³C{¹H} NMR, ca. 28 mg dissolved in 0.55 mL dmsO-d₆*



20180311-lfr-0442 [NEt₄][COOH-CB₁₁H₆-(4-CH₂OH-C₆H₄)₅]
 400 MHz, ¹H{¹B} NMR, ca. 24 mg dissolved in 0.55 mL dmsO-d6*



20180311-lfr-0442 [NEt₄][COOH-CB₁₁H₆-(4-CH₂OH-C₆H₄)₅]
 128 MHz, ¹¹B NMR, ca. 24 mg dissolved in 0.55 mL dmsO-d₆

```

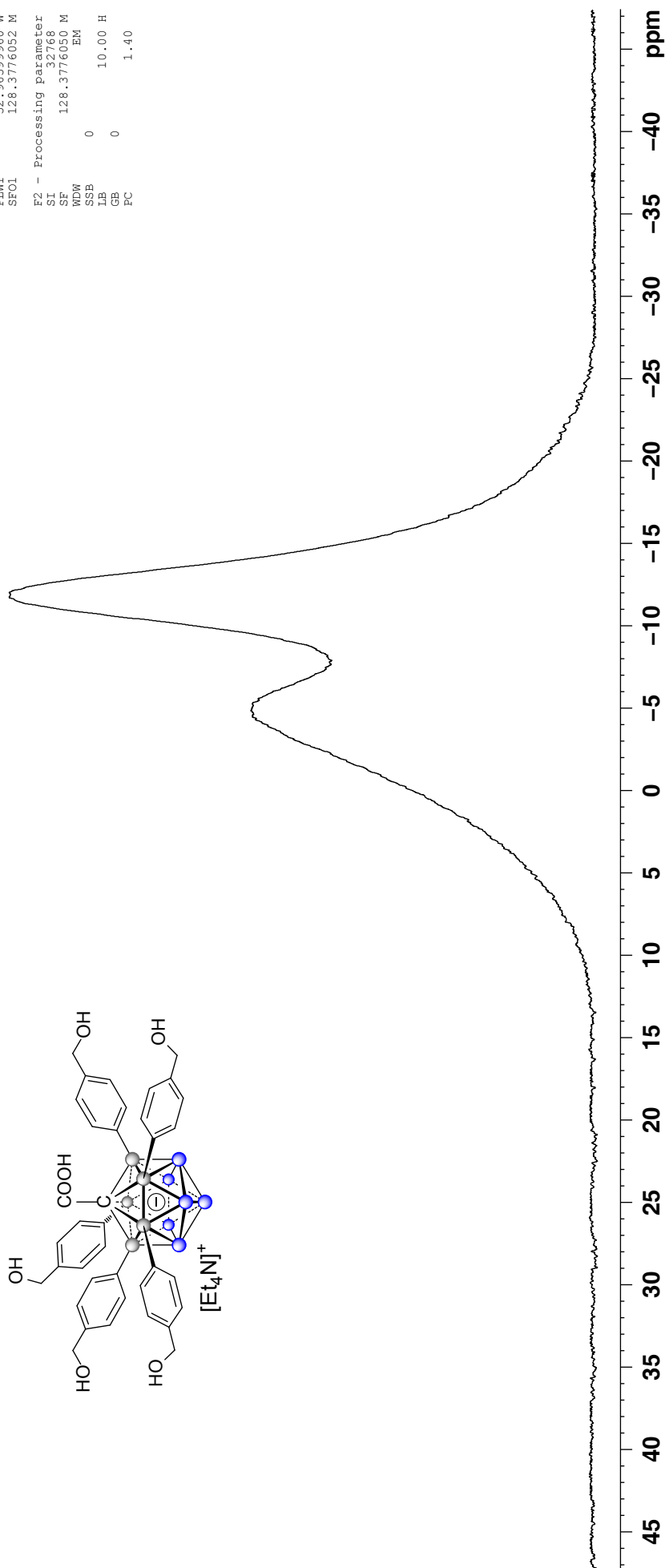
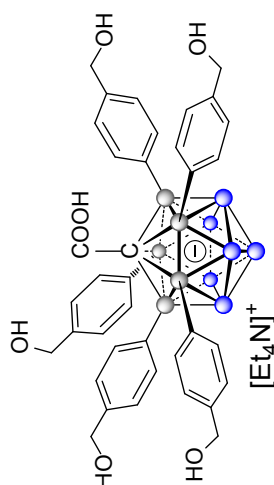
Current Data Parameters
NAME      lfr-0442
EXNO      2
PROCNO    1

F2 - Acquisition Parameter
Date_     20180310
Time      2.48
INSTRUM   spect
PROBHD    5 mm F4BBO BB/
PULPROG   zg
TD         65536
SOLVENT   DMSO
NS         128
DS         4
SWH        25510.203 H
FIDRES     0.389255 H
AQ         1.2845056 s
RG         193.34
DW         19.600 u
DE         6.50 u
TE         292.9 K
D1         1.0000000 s
TD0        1

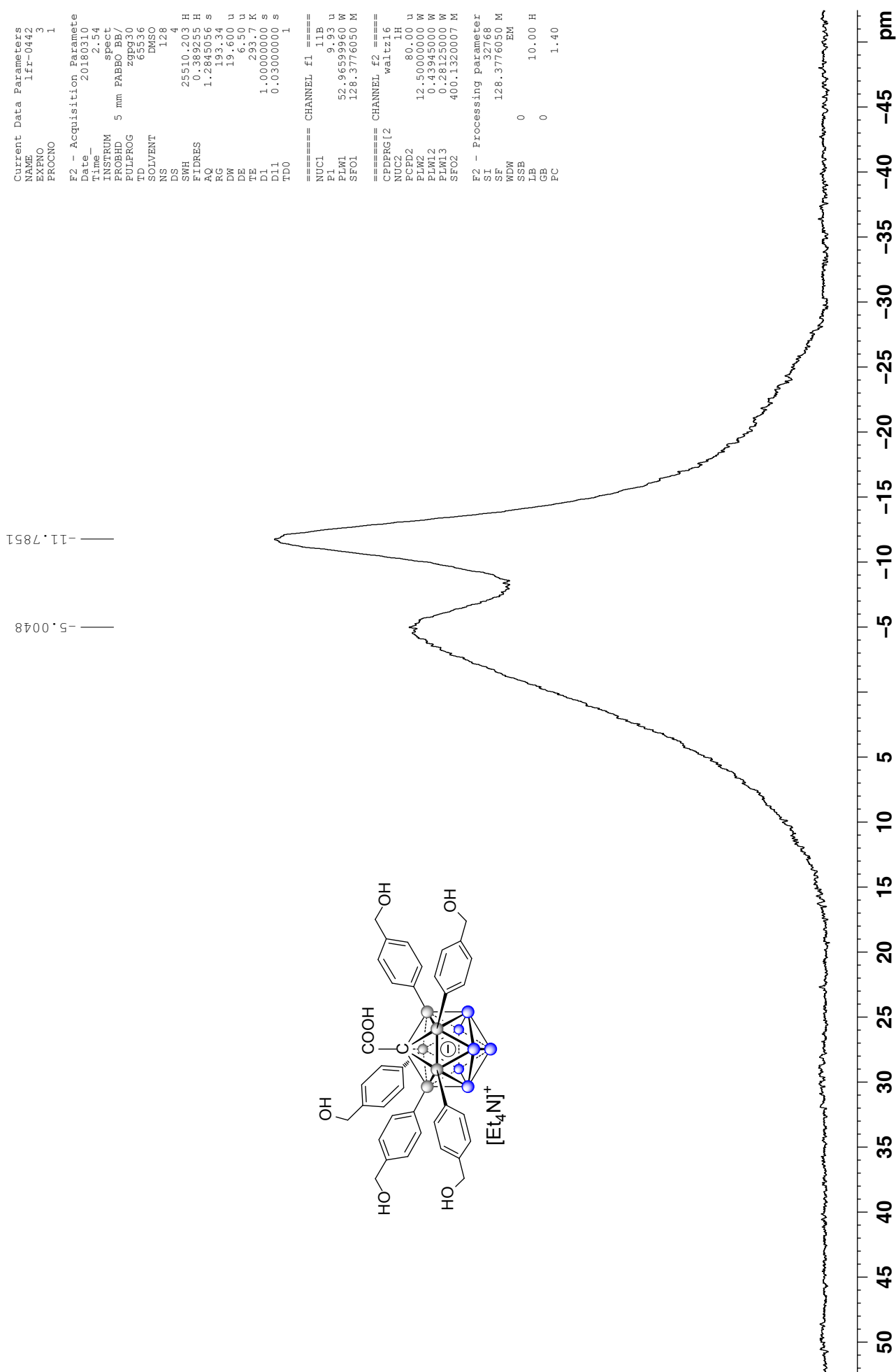
===== CHANNEL f1 =====
NUC1       11B
P1         9.93 u
PLW1       52.9659960 W
SFO1       128.3776052 M

F2 - Processing parameter
SI         32768
SF         128.3776050 M
WDW        EM
SSB        0
LB         10.00 H
GB         0
PC         1.40
  
```

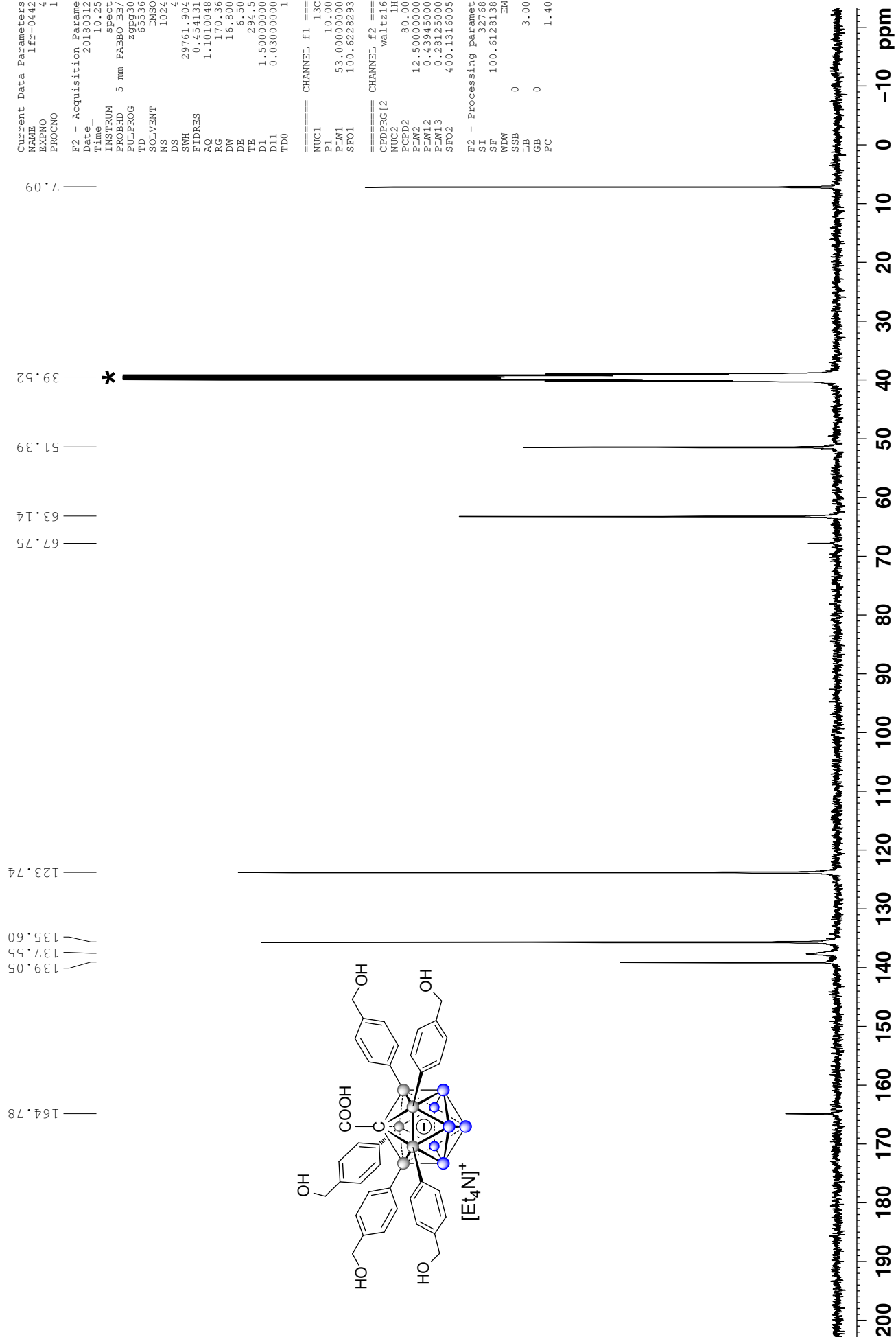
— -4.8861
 — -12.0585



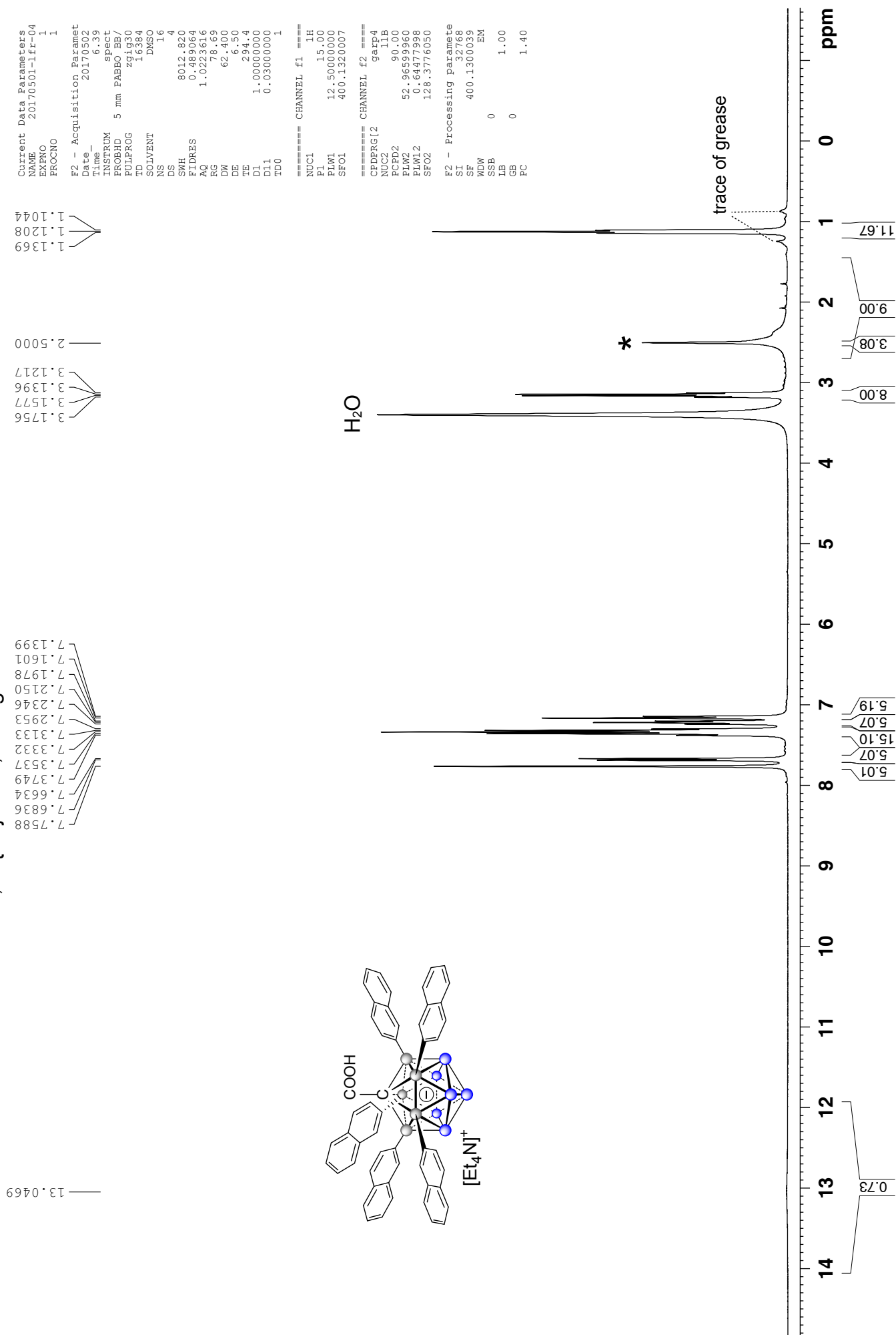
20180311-lfr-0442 [NEt₄][COOH-CB₁₁H₆-(4-CH₂OH-C₆H₄)₅]
 128 MHz, ¹¹B{¹H} NMR, ca. 24 mg dissolved in 0.55 mL dmsO-d₆



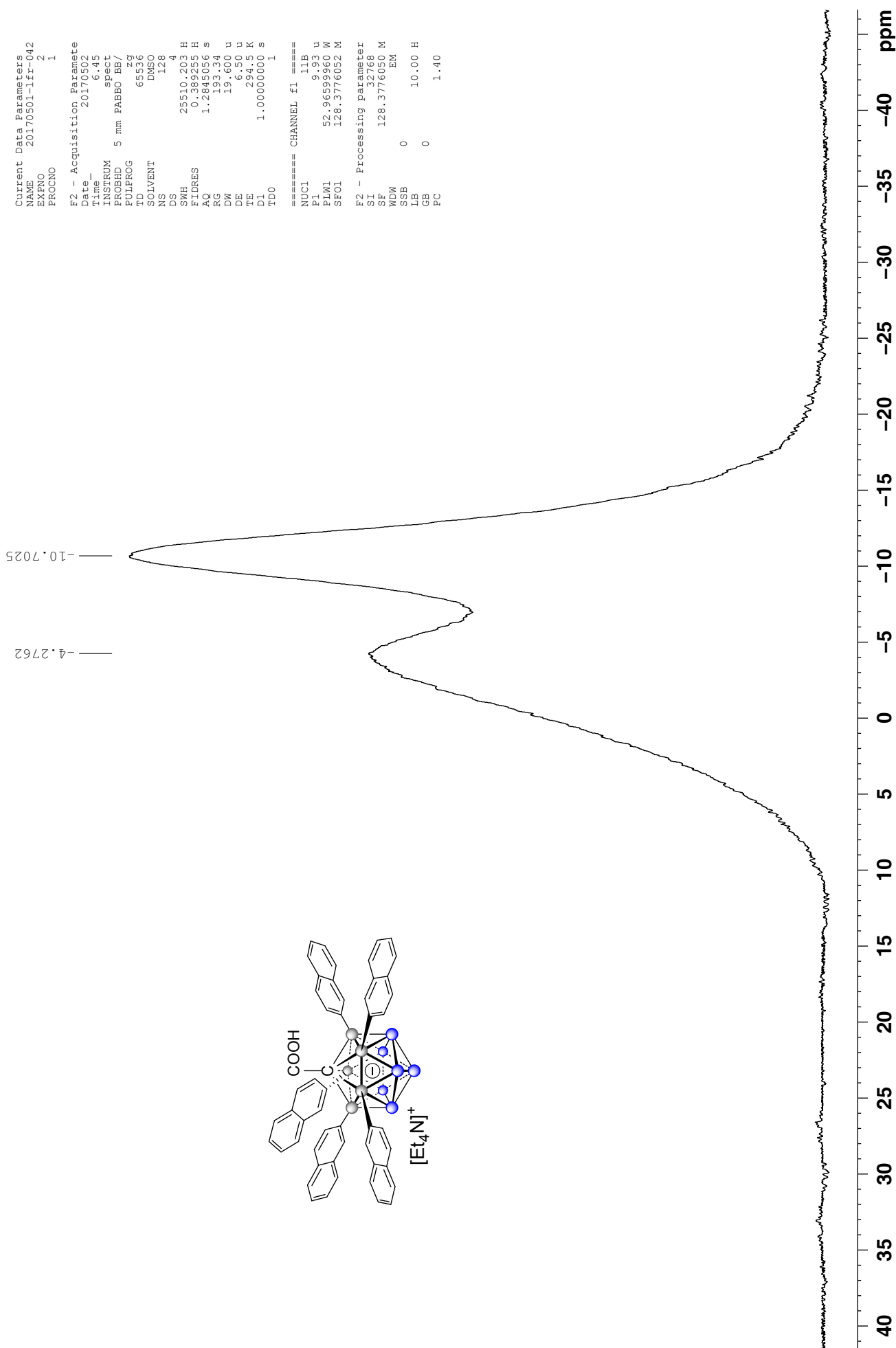
20180311-lfr-0442 [NEt₄][COOH-CB₁₁H₆-(4-CH₂OH-C₆H₄)₅]
 101 MHz, ¹³C{¹H} NMR, ca. 24 mg dissolved in 0.55 mL dmsO-d₆*



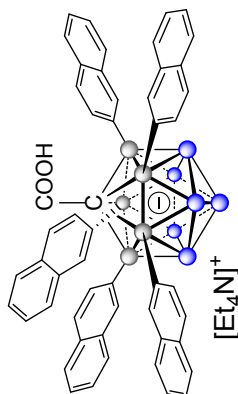
20170501-lfr-0424 [NEt₄][COOH-CB₁₁H₆-(2-Nap)₅]
400 MHz, ¹H{¹B} NMR, 21 mg dissolved in 0.55 mL dmsO-d6*



20170501-lfr-0424 [NEt₄][COOH-CB₁₁H₆-(2-Nap)₅]
 128 MHz, ¹B NMR, 21 mg dissolved in 0.55 mL dmsO-d6



20170501-lfr-0424 [NEt₄][COOH-CB₁₁H₆-(2-Nap)₅]
 128 MHz, ¹B{¹H} NMR, 21 mg dissolved in 0.55 mL dmsO-d6



— -4.6312 — -10.9169

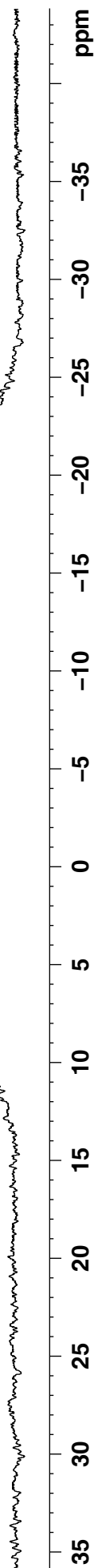
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Current Data Parameters
NAME      20170501-lfr-042
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20170502
Time      6.51
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS         128
DS         4
SWH        25510.203 H
FIDRES     0.389255 H
AQ         1.2845056 s
RG         193.34
DW         19.600 u
DE         6.50 u
TE         295.0 K
D1         1.0000000 s
D11        0.0300000 s
TD0        1

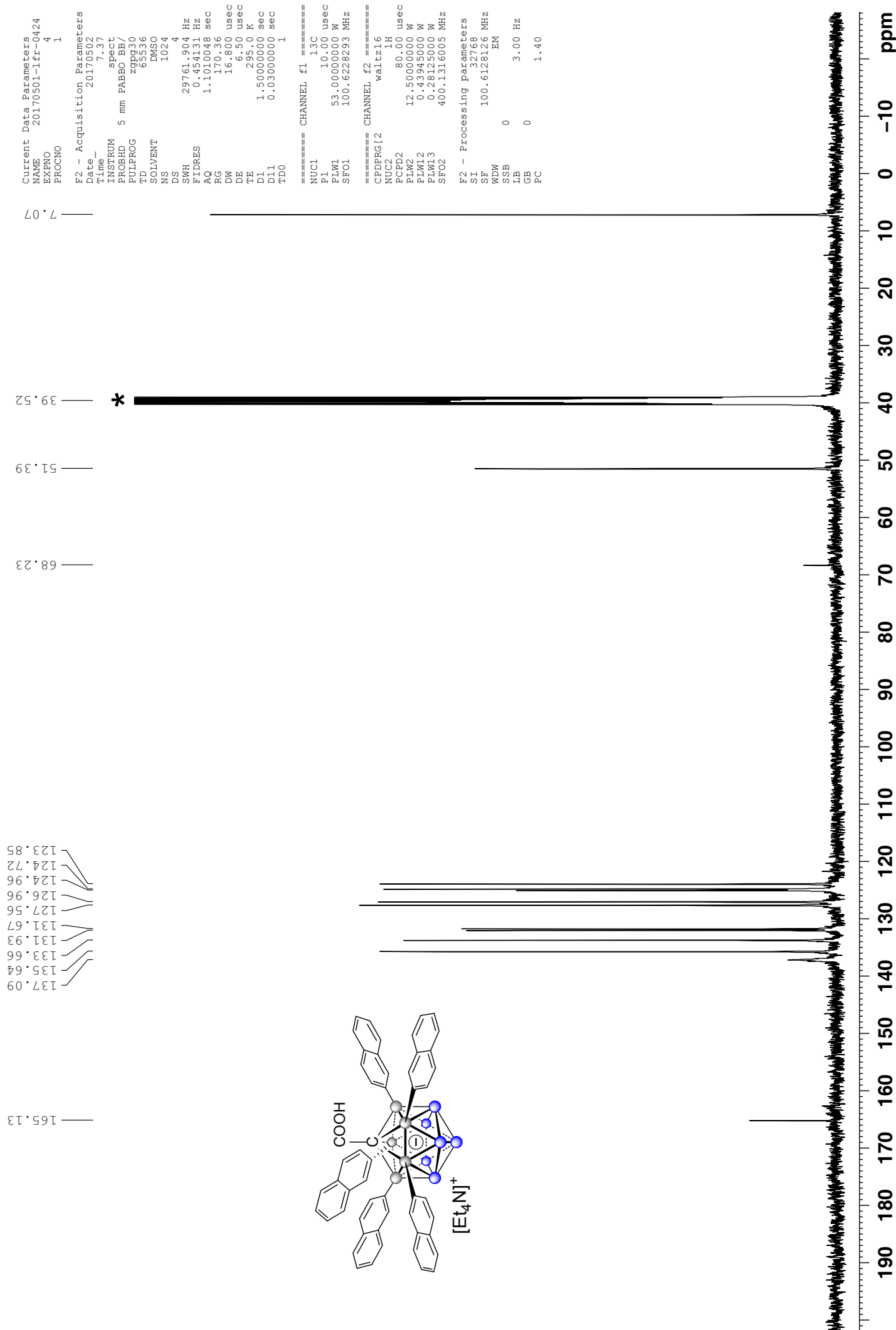
===== CHANNEL f1 =====
NUC1       11B
P1         9.93 u
PLW1       52.9659960 W
SFO1       128.3776050 M

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2       1H
PCPD2      80.00 u
PLW2       12.5000000 W
PLW12      0.43945000 W
PLW13      0.28125000 W
SFO2       400.1320007 M

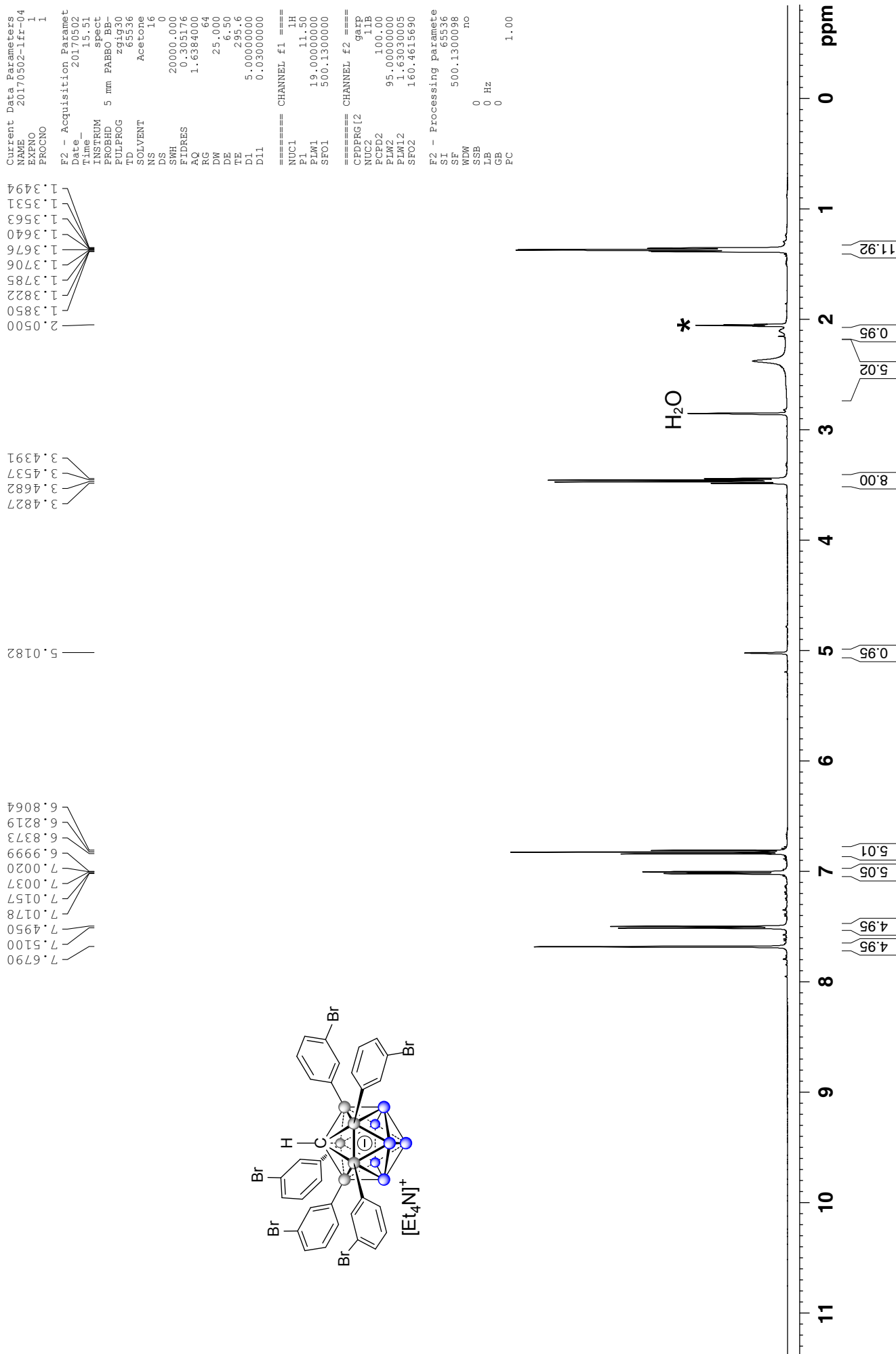
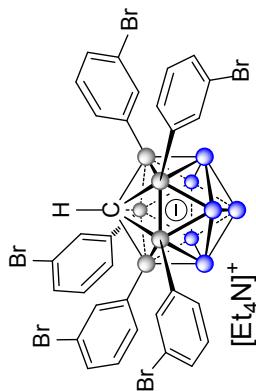
F2 - Processing parameters
SI         32768
SF         128.3776050 M
WDW        EM
SSB        0
LB         10.00 H
GB         0
PC         1.40
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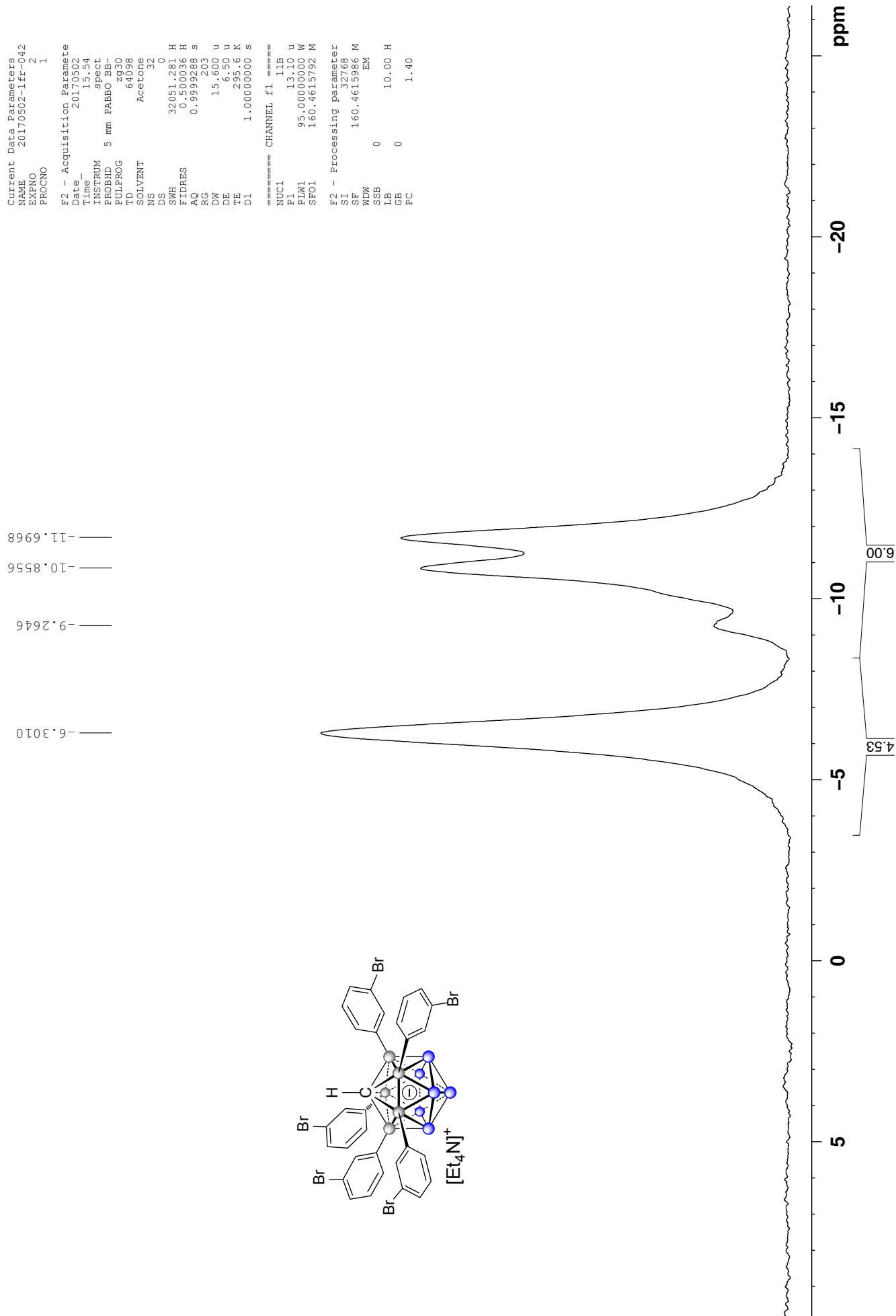
20170501-lfr-0424 [NEt₄][COOH-CB₁₁H₆-(2-Nap)₅]
101 MHz, ¹³C{¹H} NMR, 21 mg dissolved in 0.55 mL dmsO-d6*



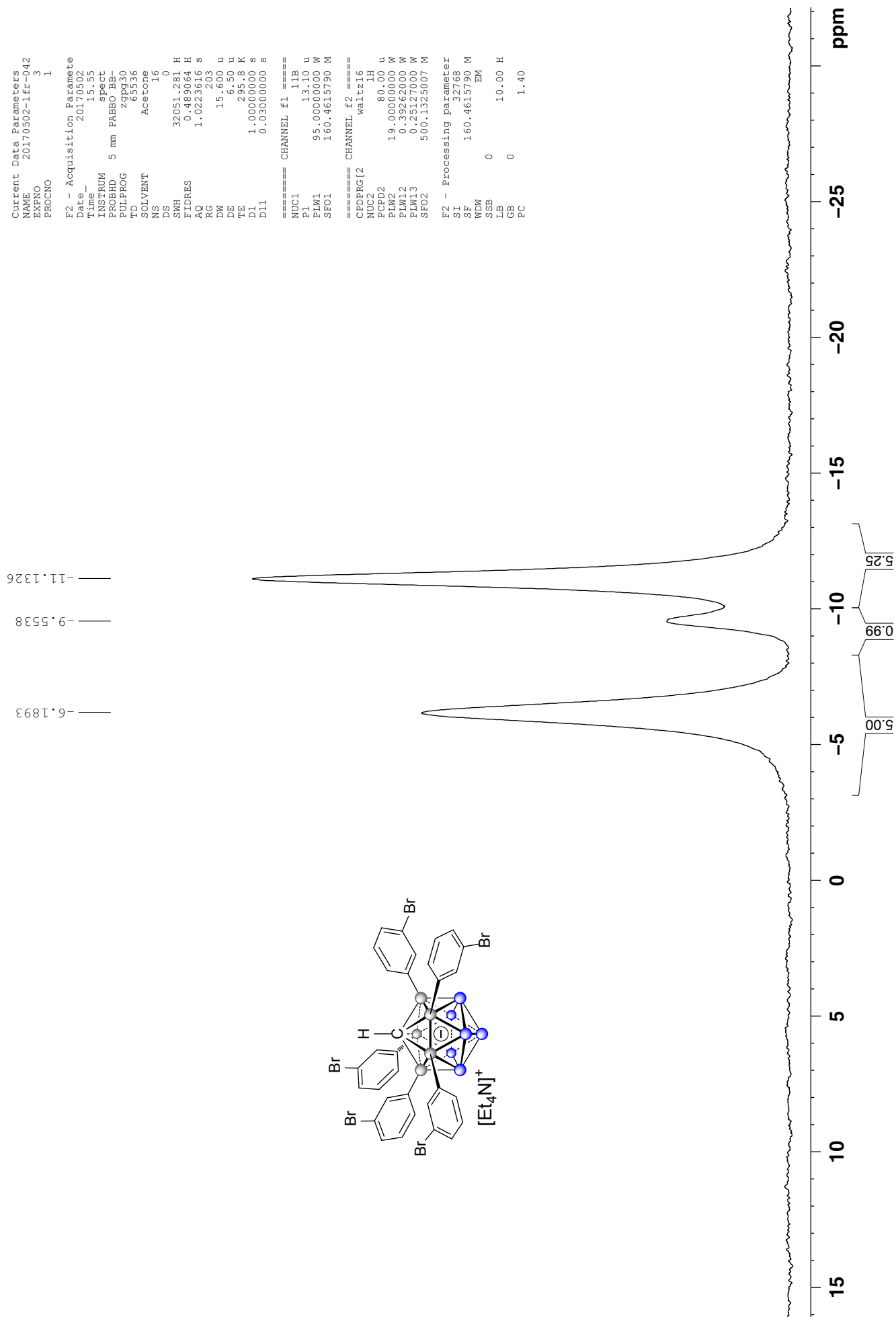
20170501-lfr-0427 [NEt₄][H-CB₁₁H₆-(C₆H₄-m-Br)₅]
500 MHz, ¹H{¹B} NMR, 30 mg dissolved in acetone-d₆*



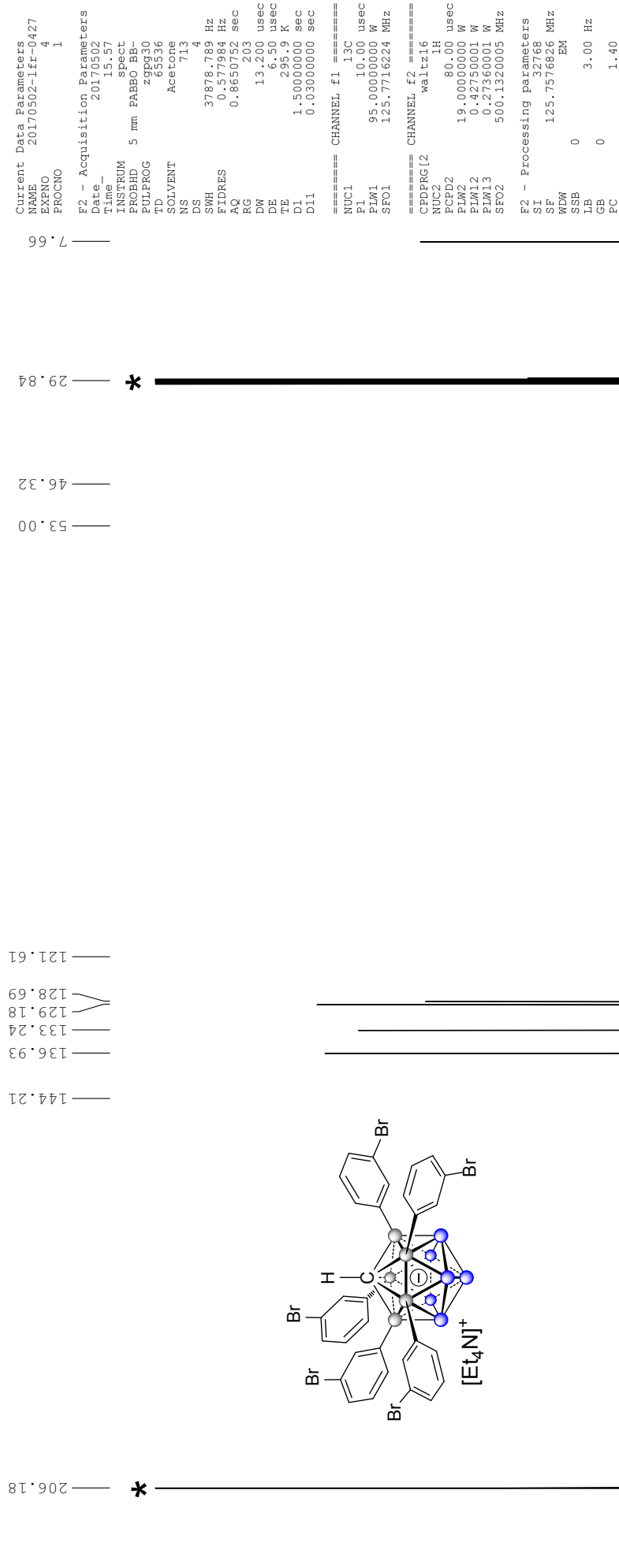
20170501-lfr-0427 [NEt₄][H-CB₁₁H₆-(C₆H₄-m-Br)₅]
 160 MHz, ¹¹B NMR, 30 mg dissolved in acetone-d₆



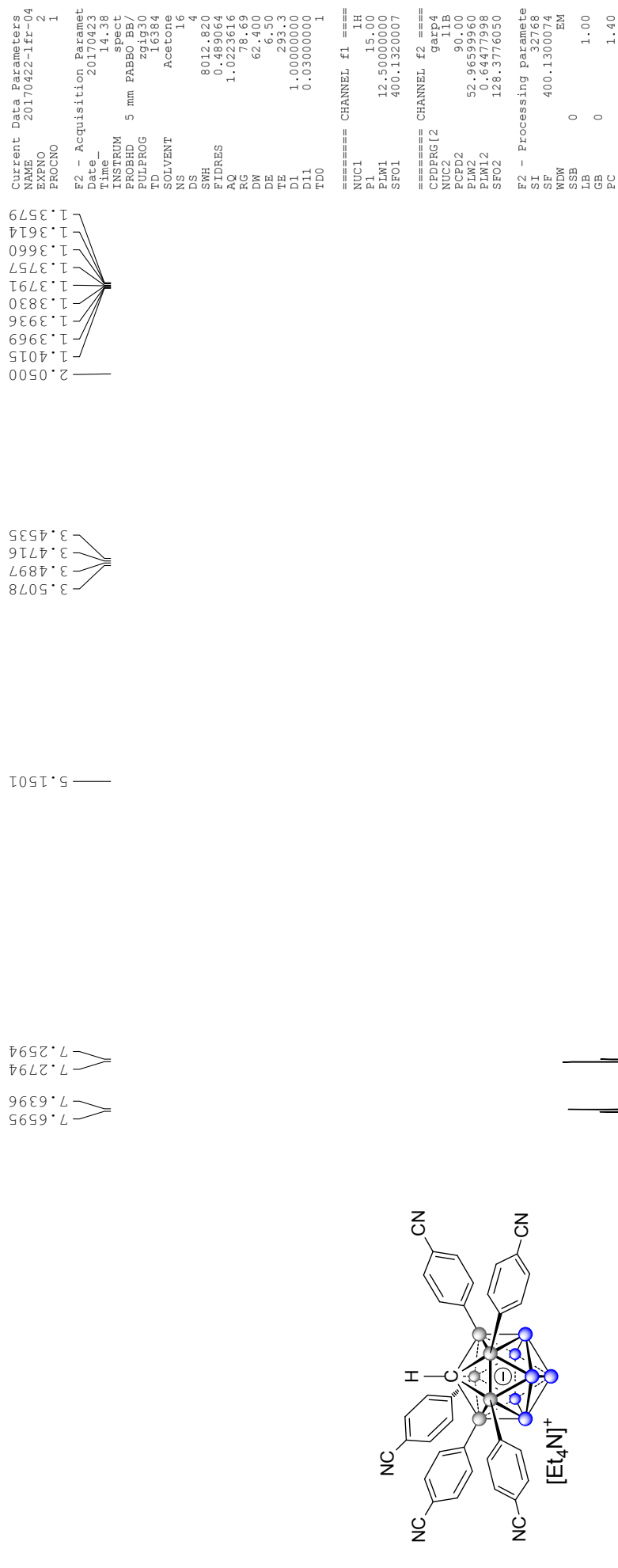
20170501-lfr-0427 [NEt₄][H-CB₁₁H₆-(C₆H₄-m-Br)₅]
 160 MHz, ¹B{¹H} NMR, 30 mg dissolved in acetone-d₆



20170501-lfr-0427 [NEt₄][H-CB₁₁H₆-(C₆H₄-m-Br)₅]
 126 MHz, ¹³C{¹H} NMR, 30 mg dissolved in acetone-d₆*



20170422-lfr-0420 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-CN)₅]
 400 MHz, ¹H{¹B} NMR, 30 mg dissolved in acetone-d₆*



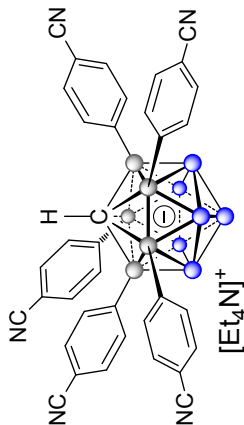
20170422-lfr-0420 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-CN)₅]
 128 MHz, ¹¹B NMR, 30 mg dissolved in acetone-d₆

Current Data Parameters
 NAME 20170422-lfr-042
 EXPNO 3
 PROCNO 1

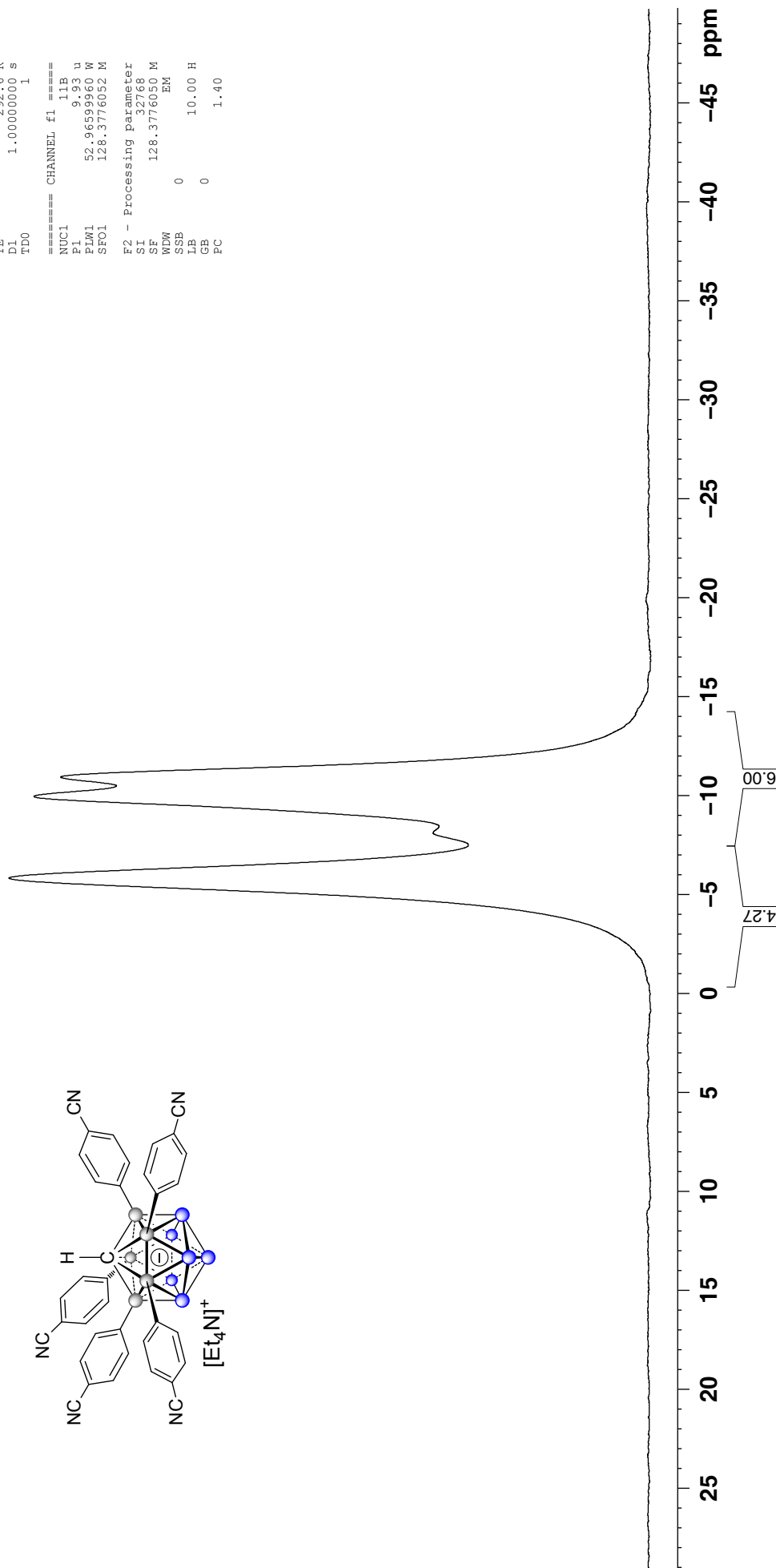
F2 - Acquisition Parameters
 Date_ 20170423
 Time 14.50
 INSTRUM spect
 PROBHD 5 mm PABBO BE/
 PULPROG zg
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 H
 FIDRES 0.389255 H
 AQ 1.2845056 s
 RG 193.34
 DW 19.600 u
 DE 6.50 u
 TE 292.6 K
 D1 1.00000000 s
 TD0 1

===== CHANNEL f1 =====
 NUC1 11B
 P1 9.93 u
 PLW1 52.9659960 W
 SFO1 128.3776052 M

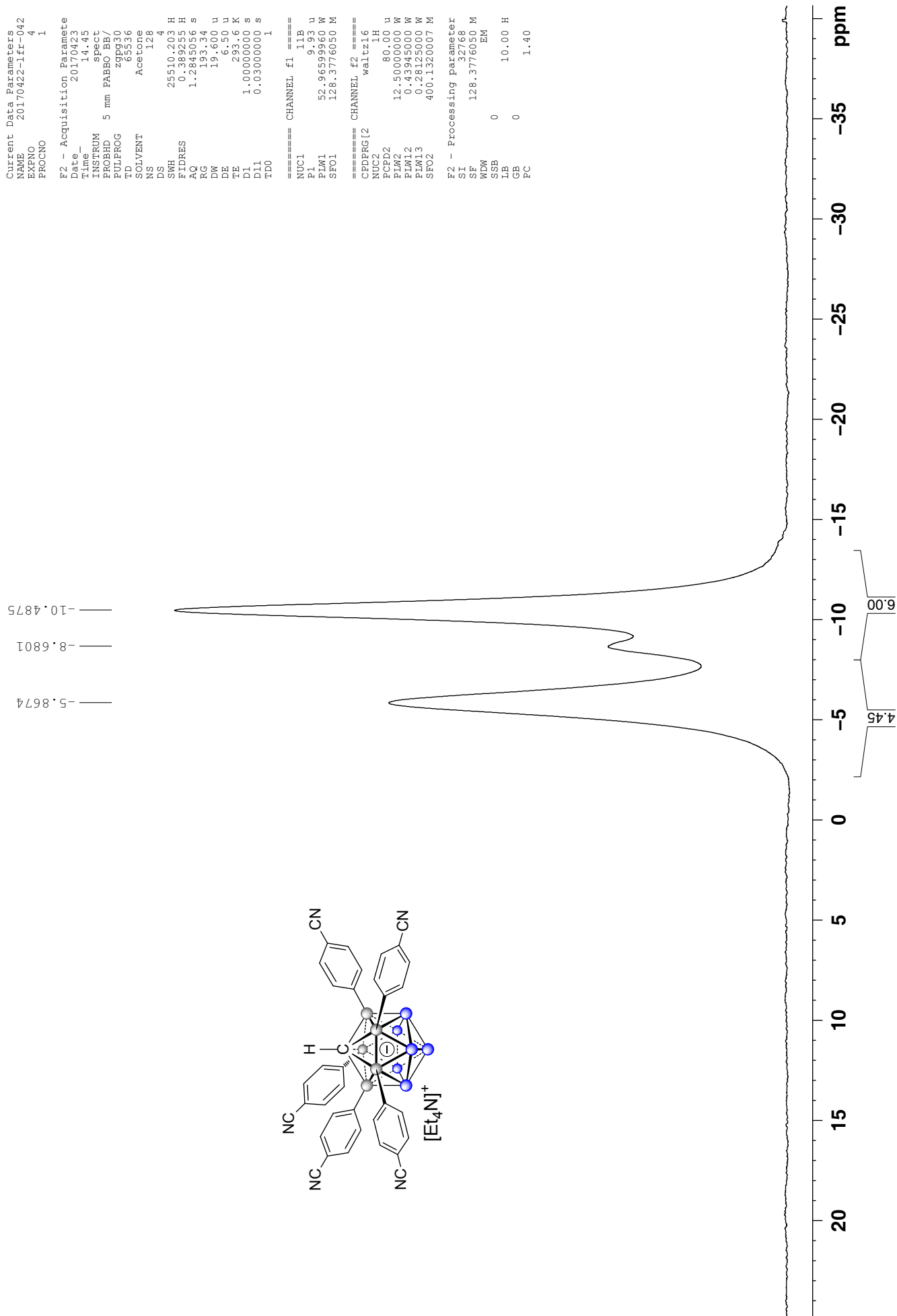
F2 - Processing parameters
 SI 32768
 SF 128.3776050 M
 WDW EM
 SSB 0
 LB 10.00 H
 GB 0
 PC 1.40



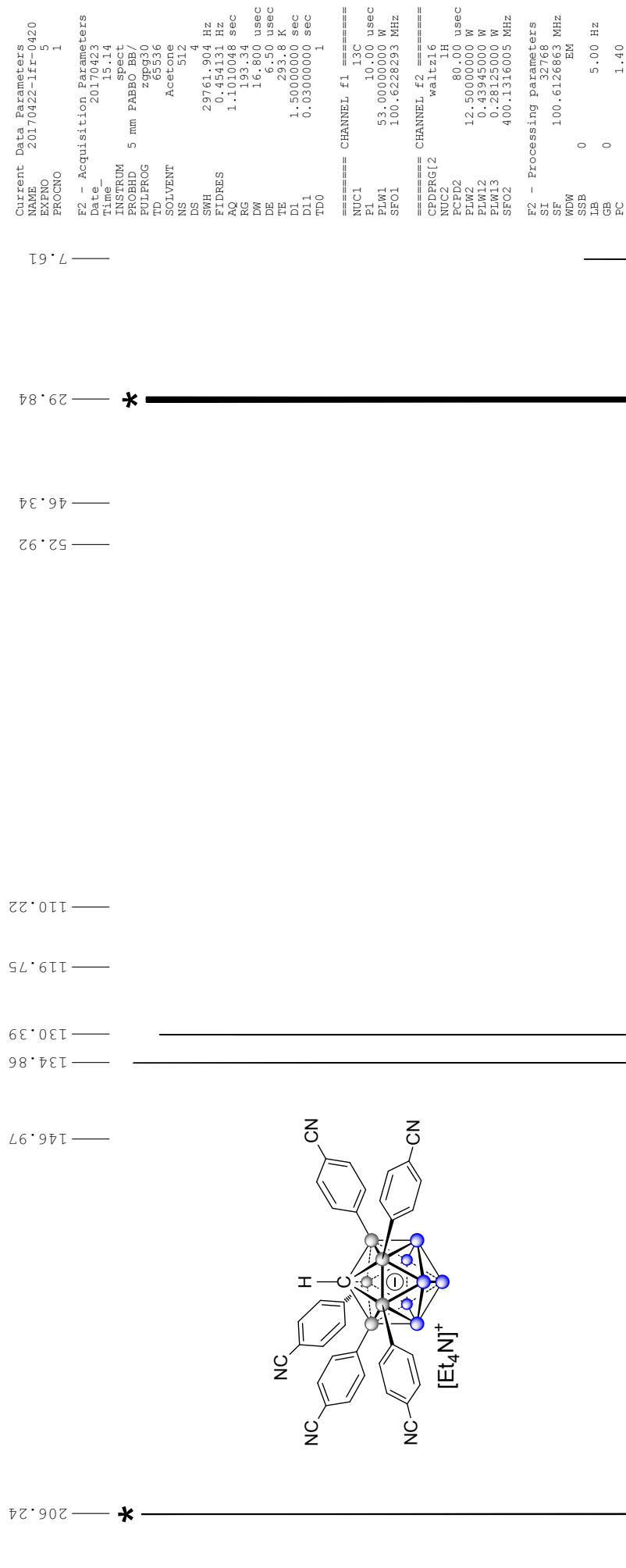
Chemical shift values (ppm):
 -5.8607
 -8.1018
 -9.9784
 -10.9358



20170422-lfr-0420 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-CN)₅]
128 MHz, ¹B{¹H} NMR, 30 mg dissolved in acetone-d₆



20170422-lfr-0420 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-CN)₅]
101 MHz, ¹³C{¹H} NMR, 30 mg dissolved in acetone-d₆*



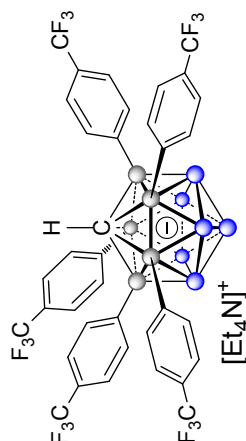
20170425-lfr-0422 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-CF₃)₅]
 500 MHz, ¹H{¹B} NMR, 35 mg dissolved in acetone-d₆*

7.7264
7.7105
7.2017
7.1857

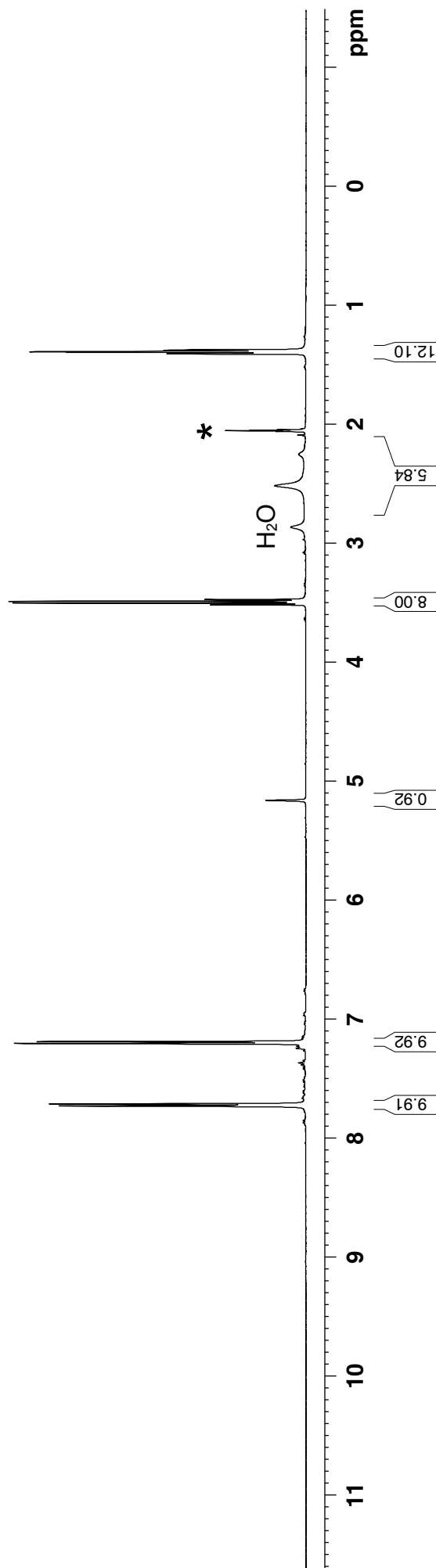
5.1579

3.5138
3.4993
3.4847
3.4702

2.0500
1.4061
1.4030
1.3994
1.3918
1.3885
1.3848
1.3773
1.3740
1.3703

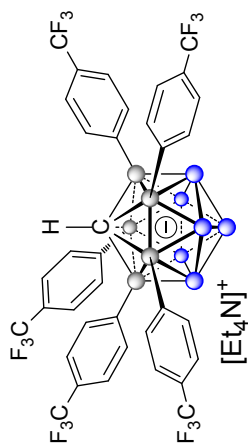


Current Data Parameters
 NAME 20170425-lfr-0422
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20170425
 Time 16.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 0
 SWH 20000.000 H
 FIDRES 0.305176 H
 AQ 1.6384000 S
 RG 64
 DW 25.000 u
 DE 6.50 u
 TE 295.6 K
 D1 5.0000000 S
 D11 0.0300000 S
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 11.50 u
 PLW1 19.00000000 W
 SFO1 500.1300000 M
 ===== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 11B
 PCPD2 100.00 u
 PLW2 95.00000000 W
 PLW12 1.63030005 W
 SFO2 160.4615690 M
 F2 - Processing parameters
 SI 65536
 SF 500.1300100 M
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

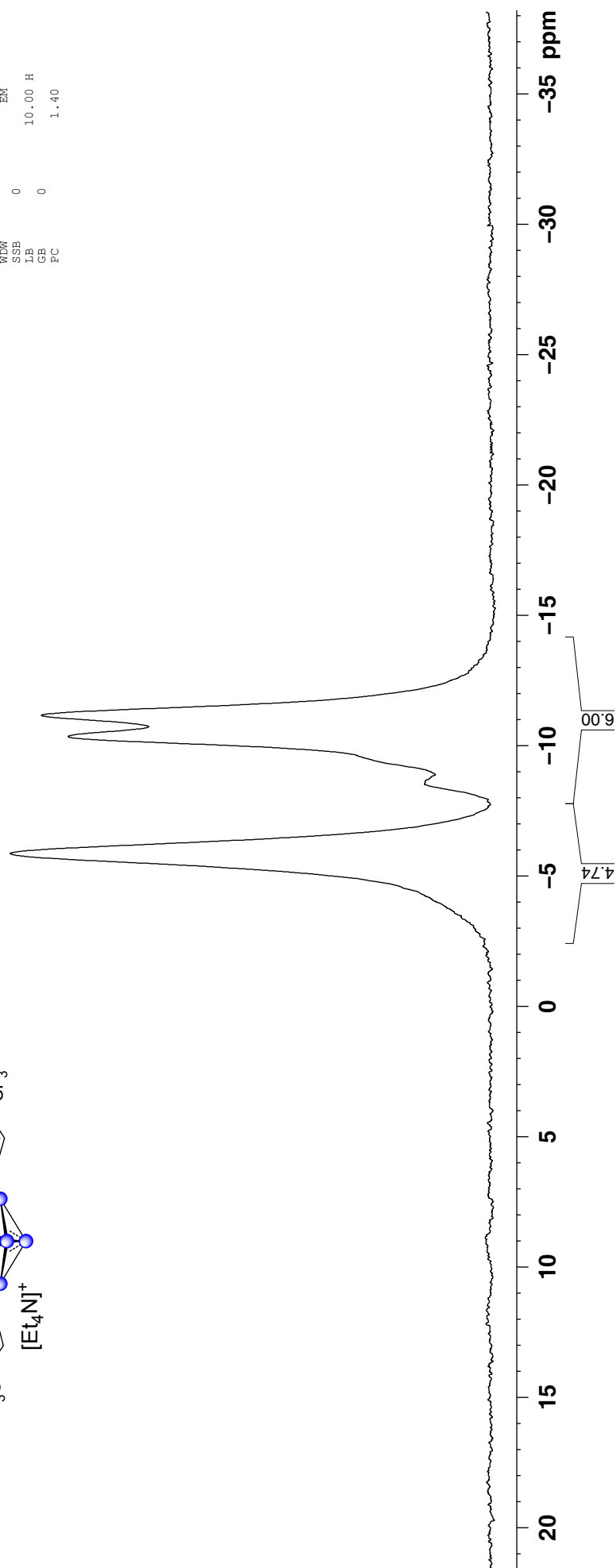


20170425-lfr-0422 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-CF₃)₅]
160 MHz, ¹¹B NMR, 35 mg dissolved in acetone-d₆

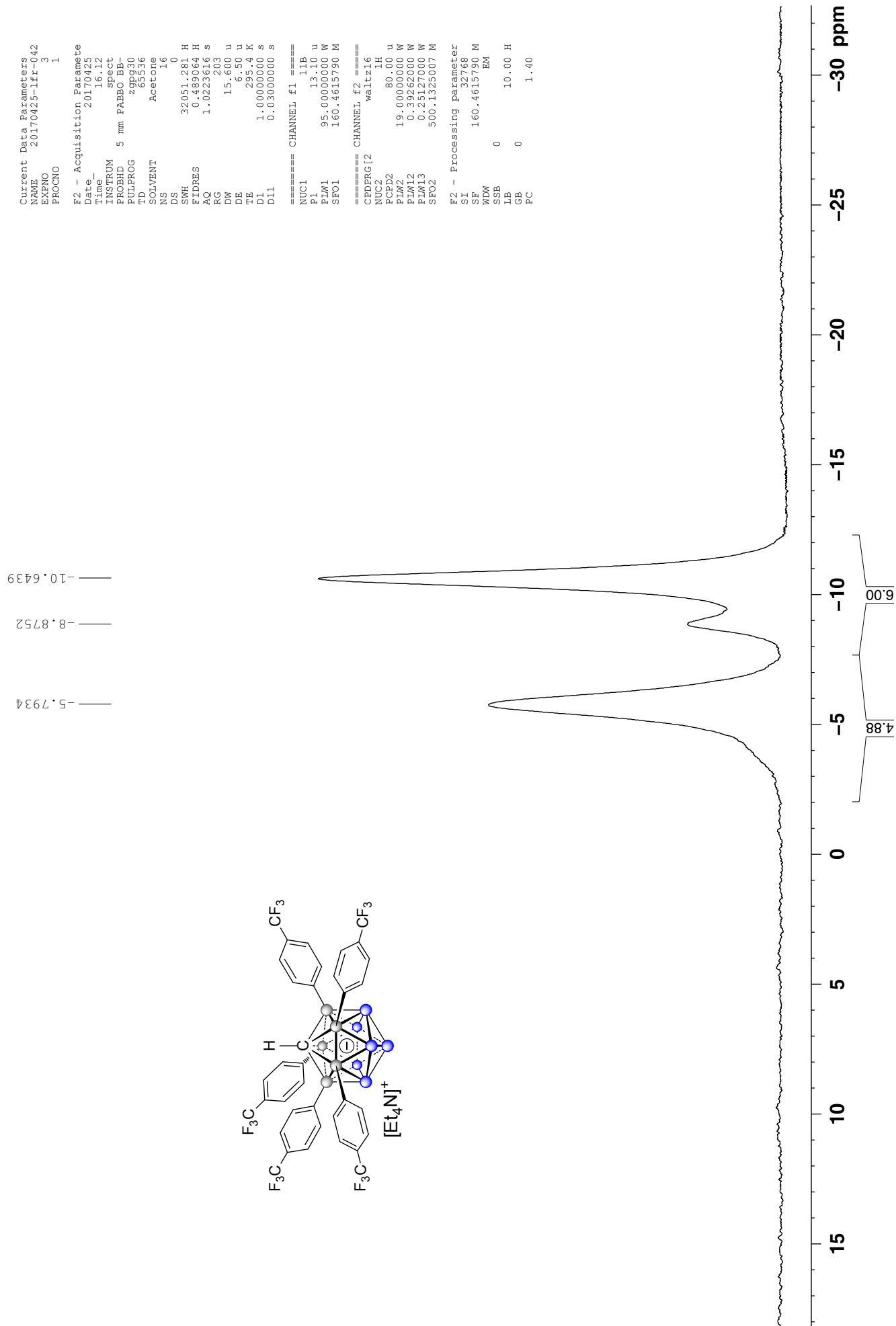
— -5.9006
— -8.5640
— -10.3905
— -11.2012



Current Data Parameters
NAME 20170425-lfr-042
EXPNO 2
PROCNO 1
F2 - Acquisition Parameter
Date_ 20170425
Time_ 16.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 64098
SOLVENT Acetone
NS 32
DS 0
SWH 32051.281 H
FIDRES 0.500036 H
AQ 0.9999288 s
RG 203
DW 15.600 u
DE 6.50 u
TE 295.4 K
D1 1.0000000 s
===== CHANNEL f1 =====
NUC1 11B
P1 13.10 u
PLW1 95.0000000 W
SFO1 160.4615792 M
F2 - Processing parameter
SI 32768
SF 160.4615986 M
WDW EM
SSB 0
LB 10.00 H
GB 0
PC 1.40



20170425-lfr-0422 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-CF₃)₅]
 160 MHz, ¹¹B{¹H} NMR, 35 mg dissolved in acetone-d₆



20170425-lfr-0422 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-CF₃)₅]
 126 MHz, ¹³C{¹H} NMR, 35 mg dissolved in acetone-d₆*

146.19
134.78
128.96
128.34
128.09
127.84
127.59
127.59
126.81
124.65
123.37
123.34
123.31
123.28
122.50

53.01

46.64

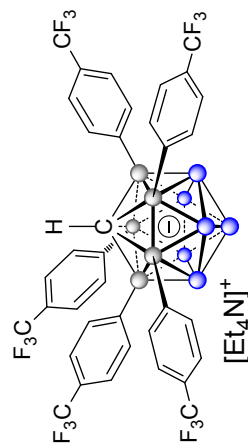
29.84

7.63

*

*

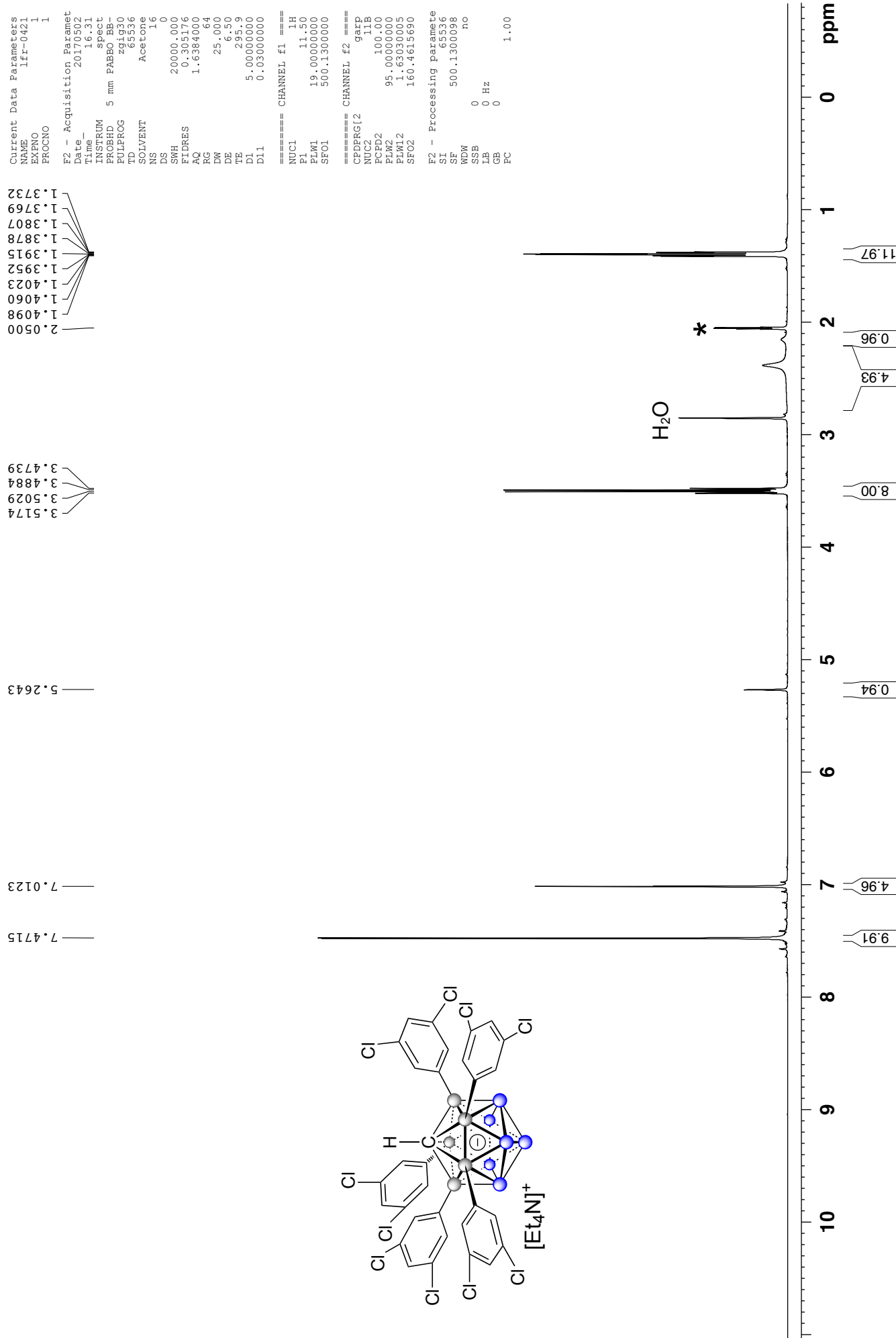
128.96
128.34
128.09
127.84
127.59
126.81
124.65
123.37
123.34
123.31
123.28
122.50



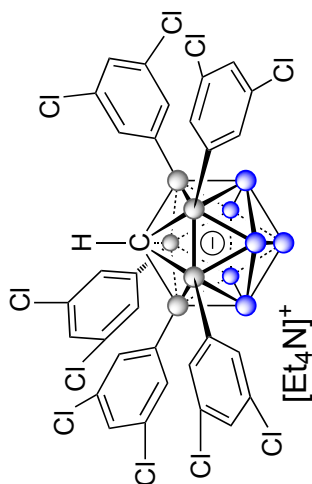
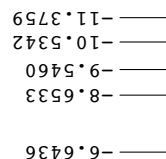
Current Data Parameters
 NAME 20170425-lfr-0422
 EXPNO 4
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20170425
 Time 16.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 877
 DS 4
 SWH 37878.789 Hz
 FIDRES 0.577984 Hz
 AQ 0.8650752 sec
 RG 203
 DW 13.200 usec
 DE 6.50 usec
 TE 296.0 K
 D1 1.5000000 sec
 D11 0.0300000 sec
 ===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 95.0000000 W
 SFO1 125.7716224 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 P2 80.00 usec
 PL2 19.0000000 W
 PLW2 0.42750001 W
 PLW3 0.27360001 W
 SFO2 500.1320005 MHz
 F2 - Processing parameters
 SI 32768
 SF 125.7576782 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

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

20170501-lfr-0421 [NEt₄][H-CB₁₁H₆-(C₆H₃-3,5-Cl₂)₅]
500 MHz, ¹H{¹¹B} NMR, 30 mg dissolved in acetone-d₆*



20170501-lfr-0421 [NEt₄][H-CB₁₁H₆-(C₆H₃-3,5-Cl₂)₅]
160 MHz, ¹¹B NMR, 30 mg dissolved in acetone-d₆



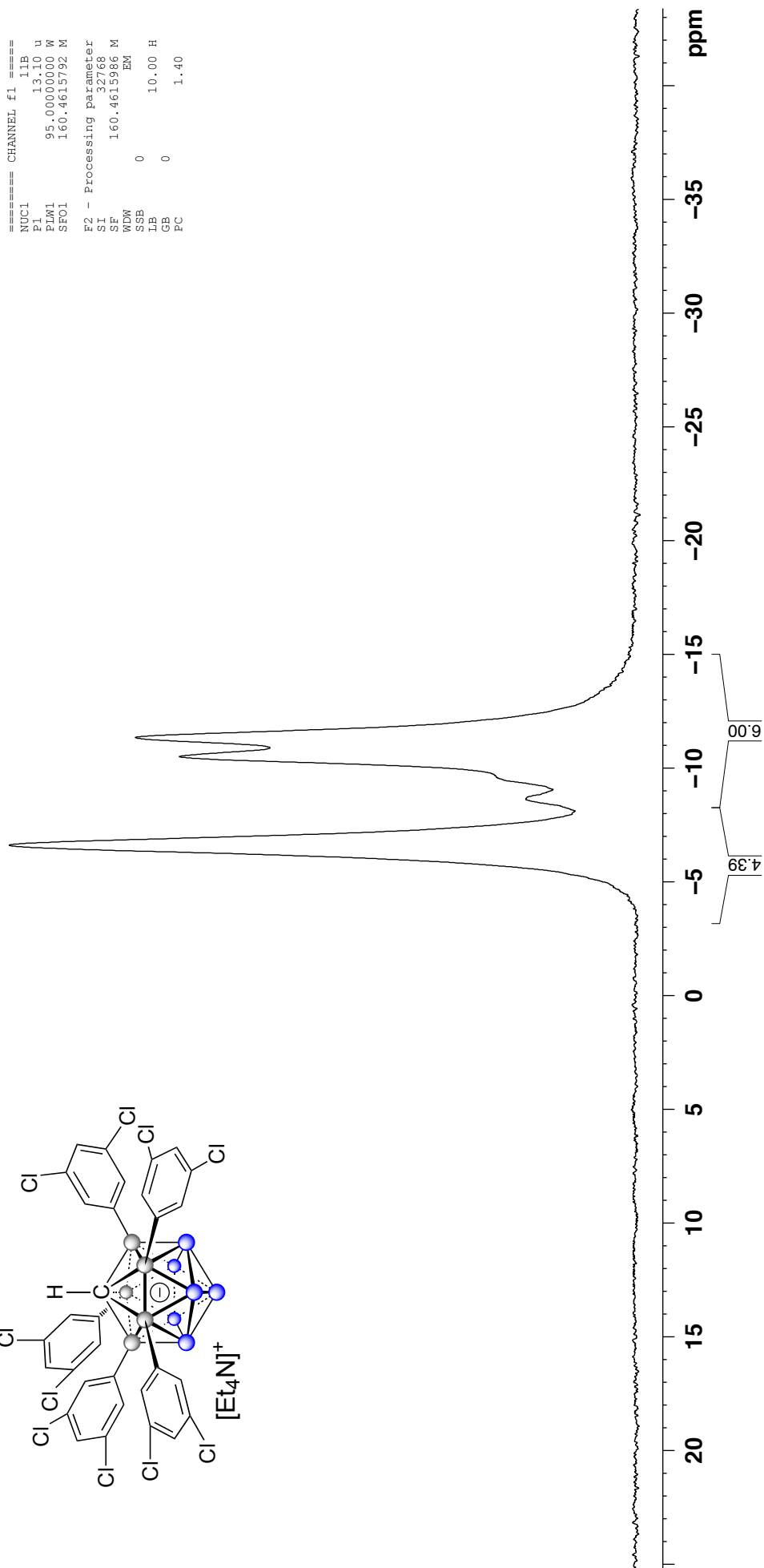
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Current Data Parameters
NAME      20170501-lfr-042
EXPNO     2
PROCNO    1

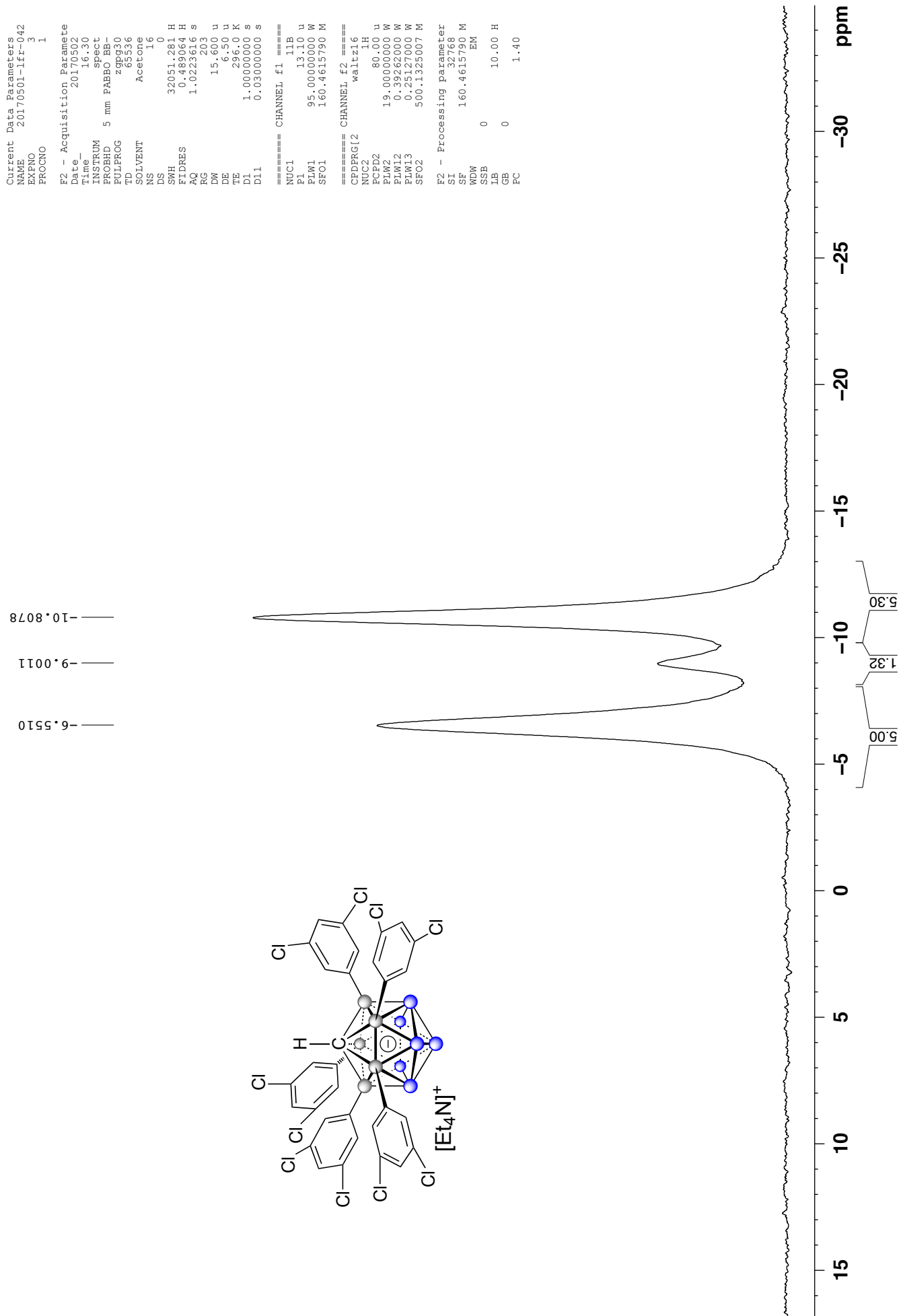
F2 - Acquisition Parameter
Date_     20170502
Time      16.28
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        64098
SOLVENT   Acetone
NS         32
DS         0
SWH        32051.281 H
FIDRES     0.500036 H
AQ         0.9999288 s
RG         203
DW         15.600 u
DE         6.50 u
TE         296.0 K
D1         1.00000000 s

===== CHANNEL f1 =====
NUC1       11B
P1         13.10 u
PLA1       95.00000000 W
SFO1       160.4615792 M

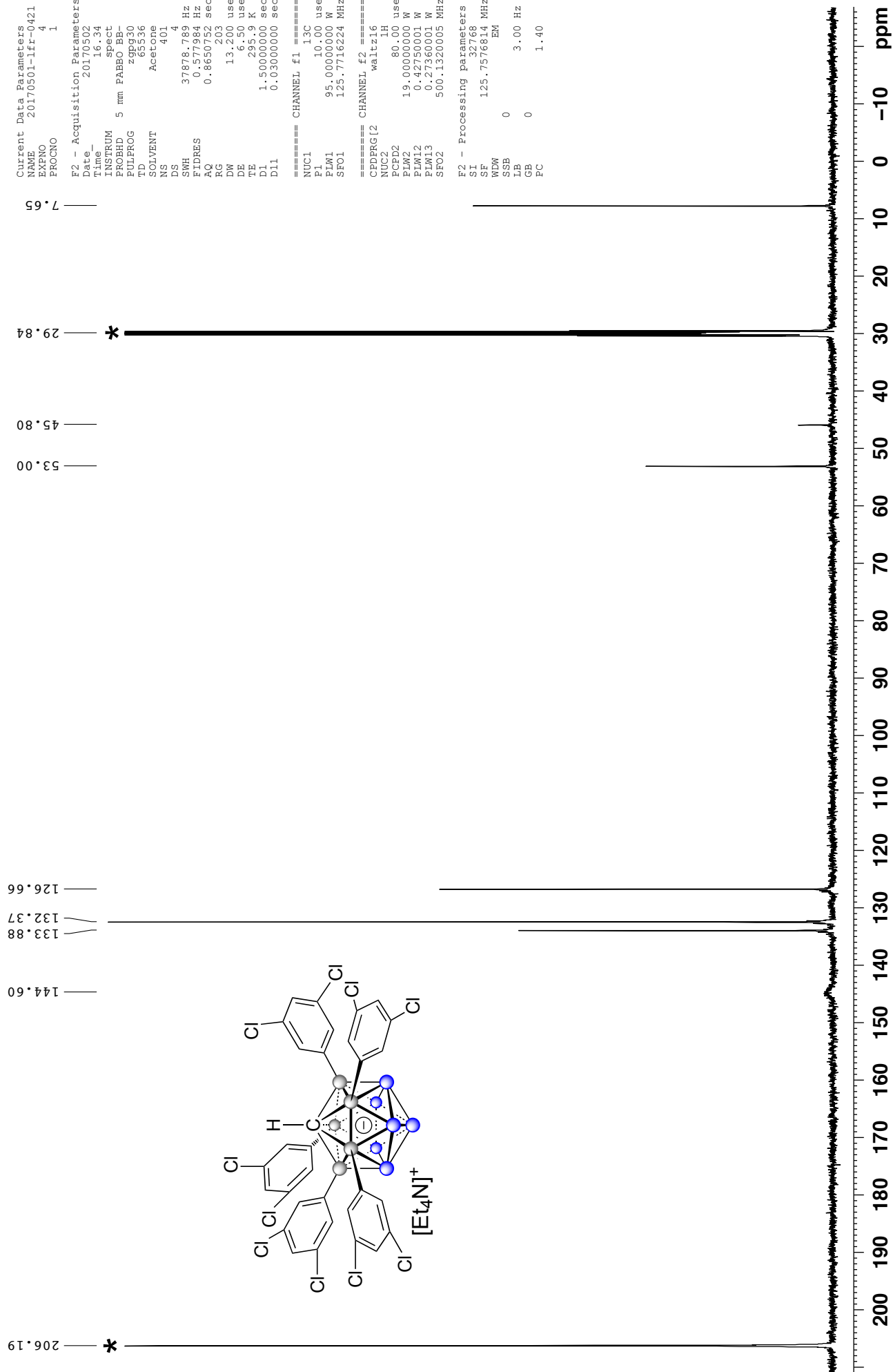
F2 - Processing parameter
SI         32768
SF         160.4615986 M
WDW        EM
SSB        0
LB         10.00 H
GB         0
PC         1.40
  
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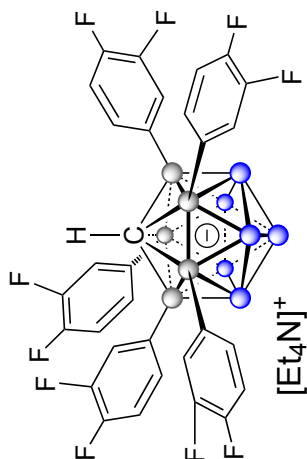
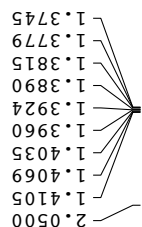
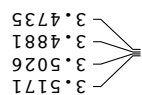
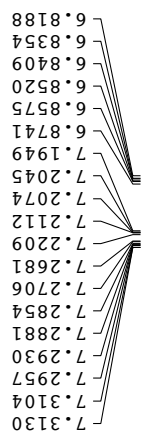
20170501-lfr-0421 [NEt₄][H-CB₁₁H₆-(C₆H₃-3,5-Cl₂)₅]
 160 MHz, ¹¹B{¹H} NMR, 30 mg dissolved in acetone-d₆



20170501-lfr-0421 [NEt₄][H-CB₁₁H₆-(C₆H₃-3,5-Cl₂)₅]
 126 MHz, ¹³C{¹H} NMR, 30 mg dissolved in acetone-d₆*



20170511-lfr-0431 [NEt₄][H-CB₁₁H₆-(C₆H₃-3,4-F₂)₅]
500 MHz, ¹H{¹B} NMR, 30 mg dissolved in acetone-d₆*



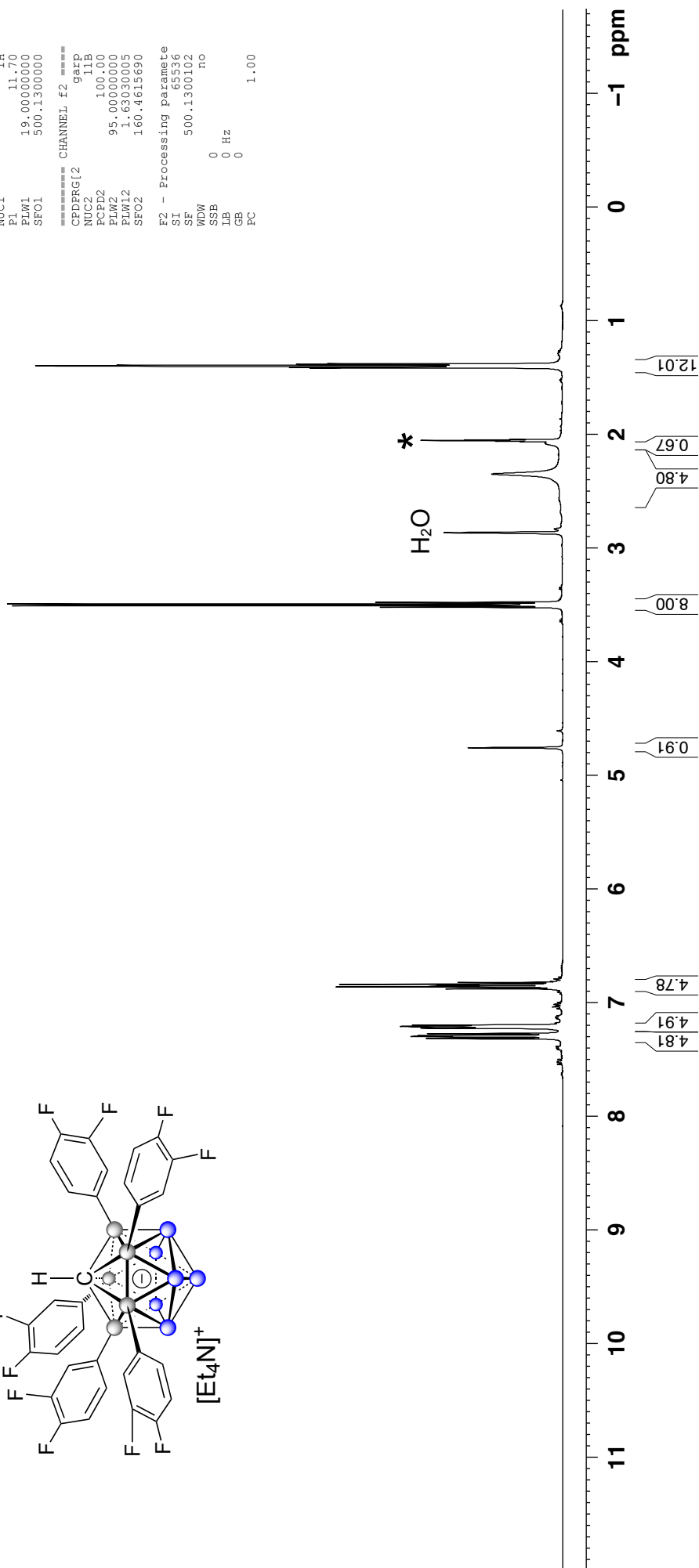
Current Data Parameters
NAME 20170511-lfr-04
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170511
Time_ 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgig30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 20000.000
FIDRES 0.305176
AQ 1.6384000
RG 64
DW 25.000
DE 6.50
TE 295.6
D1 5.00000000
D11 0.03000000

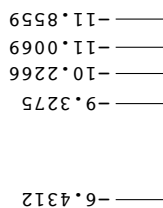
==== CHANNEL f1 ====
NUC1 1H
P1 11.70
PL1 19.00000000
SFO1 500.1300000

==== CHANNEL f2 ====
CPDPRG2 garp
NUC2 11B
PCPD2 100.00
PLW2 95.00000000
PLW12 1.63030005
SFO2 160.4615690

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

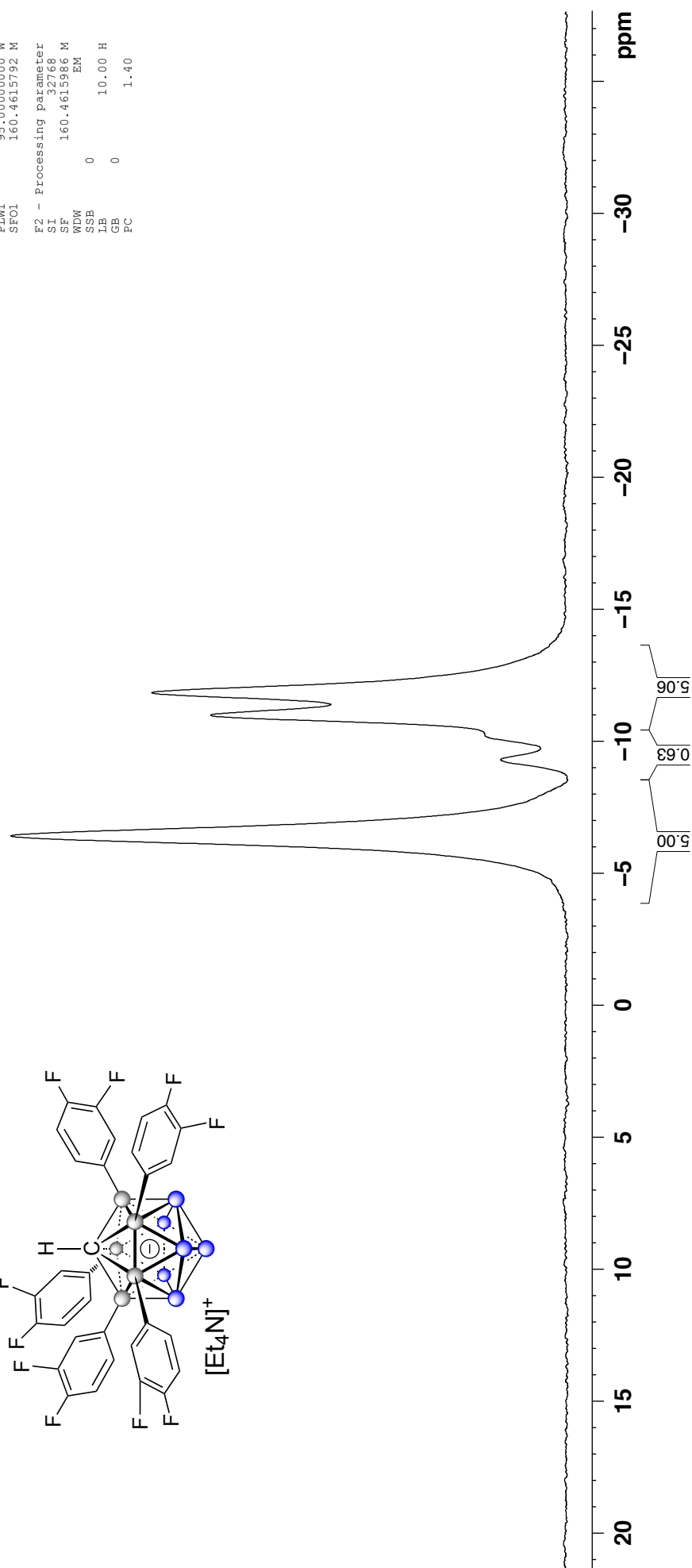
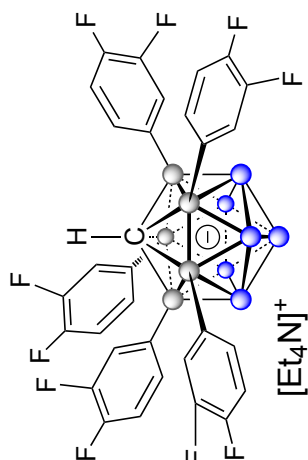


20170511-lfr-0431 [NEt₄][H-CB₁₁H₆-(C₆H₃-3,4-F₂)₅]
 160 MHz, ¹¹B NMR, 30 mg dissolved in acetone-d₆



Current Data Parameters
 NAME 20170511-lfr-0431
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20170511
 Time_ 15:53
 INSTRUM spect
 PROHD 5 mm PABBO BB-
 PULPROG zg30
 TD 64098
 SOLVENT Acetone
 NS 32
 DS 0
 SWH 32051.281 H
 FIDRES 0.500036 H
 AQ 0.9999288 s
 RG 203
 DW 15.600 u
 DE 6.50 u
 TE 295.5 K
 D1 1.0000000 s

===== CHANNEL f1 =====
 NUC1 ¹¹B
 P1 13.10 u
 PL1 95.0000000 W
 SF01 160.4615792 M
 F2 - Processing parameters
 SI 32768
 SF 160.4615986 M
 WDW EM
 SSB 0
 LB 10.00 H
 GB 0
 PC 1.40



20170511-lfr-0431 [NEt₄][H-CB₁₁H₆-(C₆H₃-3,4-F₂)₅]
160 MHz, ¹H{¹H} NMR, 30 mg dissolved in acetone-d₆

```

Current Data Parameters
NAME      20170511-lfr-043
EXPNO     3
PROCNO    1

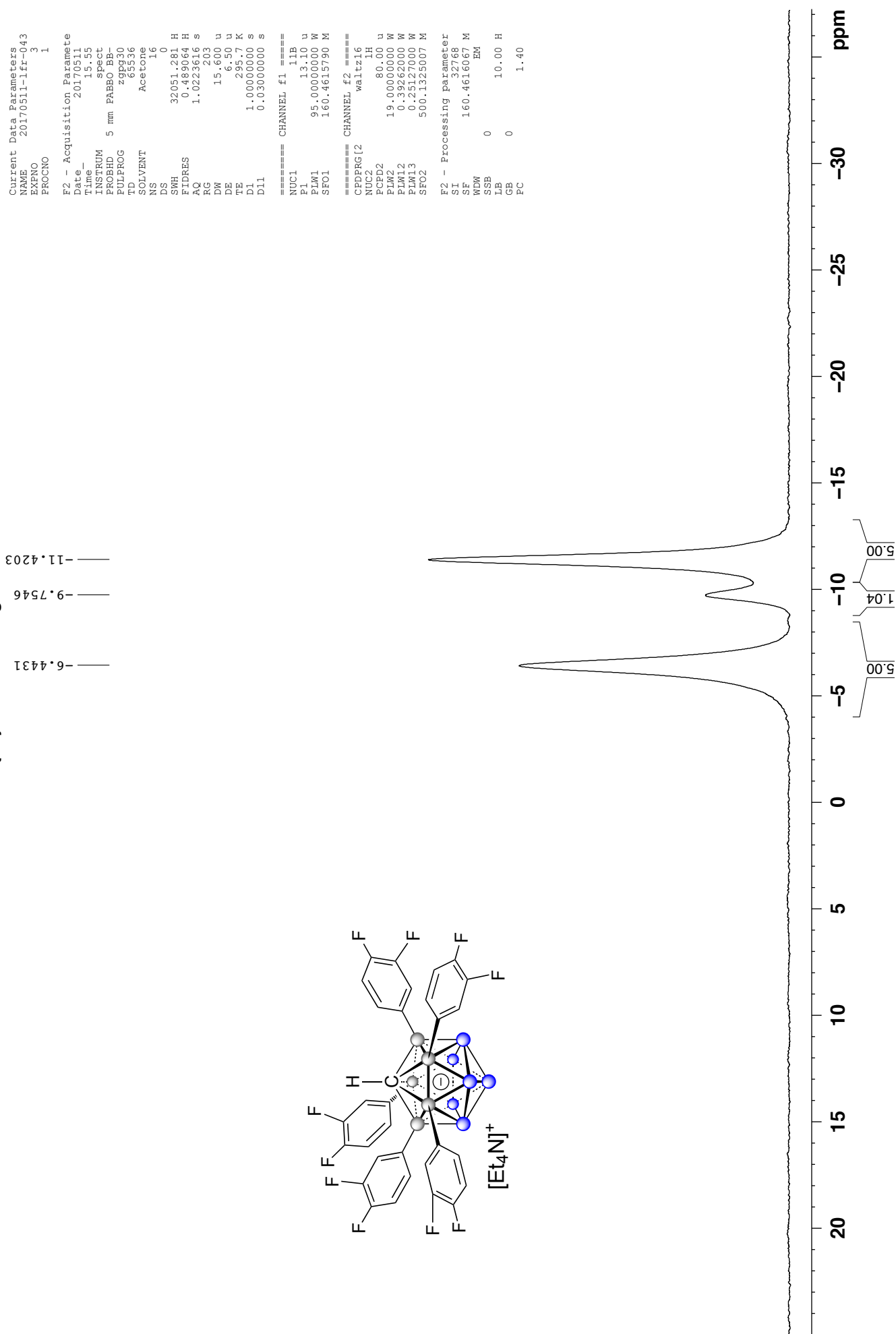
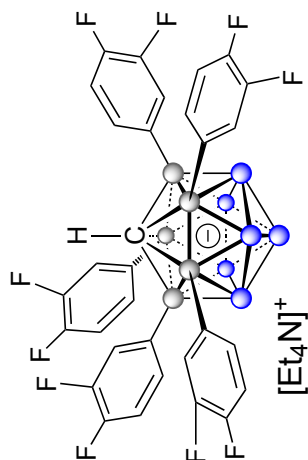
F2 - Acquisition Parameters
Date_     20170511
Time      15:55
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   Acetone
NS         16
DS         0
SFOH      32051.281 H
FIDRES    0.489064 H
AQ         1.0223616 S
RG         15.600 U
DW         6.50 U
DE         295.7 K
TE         1.0000000 S
D1         0.0300000 S
D11        0.0300000 S

===== CHANNEL f1 =====
NUC1       11B
P1         13.10 U
PL1        95.0000000 W
SFO1       160.4615790 M

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       80.00 U
PLW2        19.0000000 W
PLW12       0.3926200 W
PLW13       0.2512700 W
SFO2        500.1325007 M

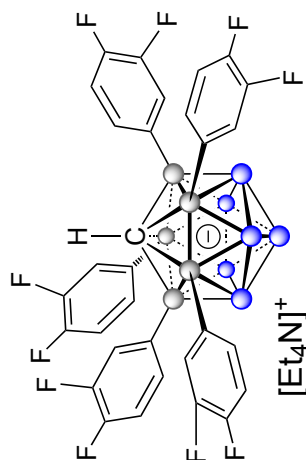
F2 - Processing parameters
SI          32768
SF          160.4616067 M
WDW         EM
SSB         0
LB          10.00 H
GB          0
PC          1.40

```



20170511-lfr-0431 [NEt₄][H-CB₁₁H₆-(C₆H₃-3,4-F₂)₅]
 101 MHz, ¹³C{¹H} NMR, 30 mg dissolved in acetone-d₆*

150.94
 150.82
 148.52
 148.40
 138.61
 130.88
 130.85
 130.83
 130.79
 122.43
 122.28
 115.98
 115.83



206.24

150.94
 150.82
 148.52
 148.40
 138.61
 130.88
 130.85
 130.83
 130.79
 122.43
 122.28
 115.98
 115.83

52.96
 47.90

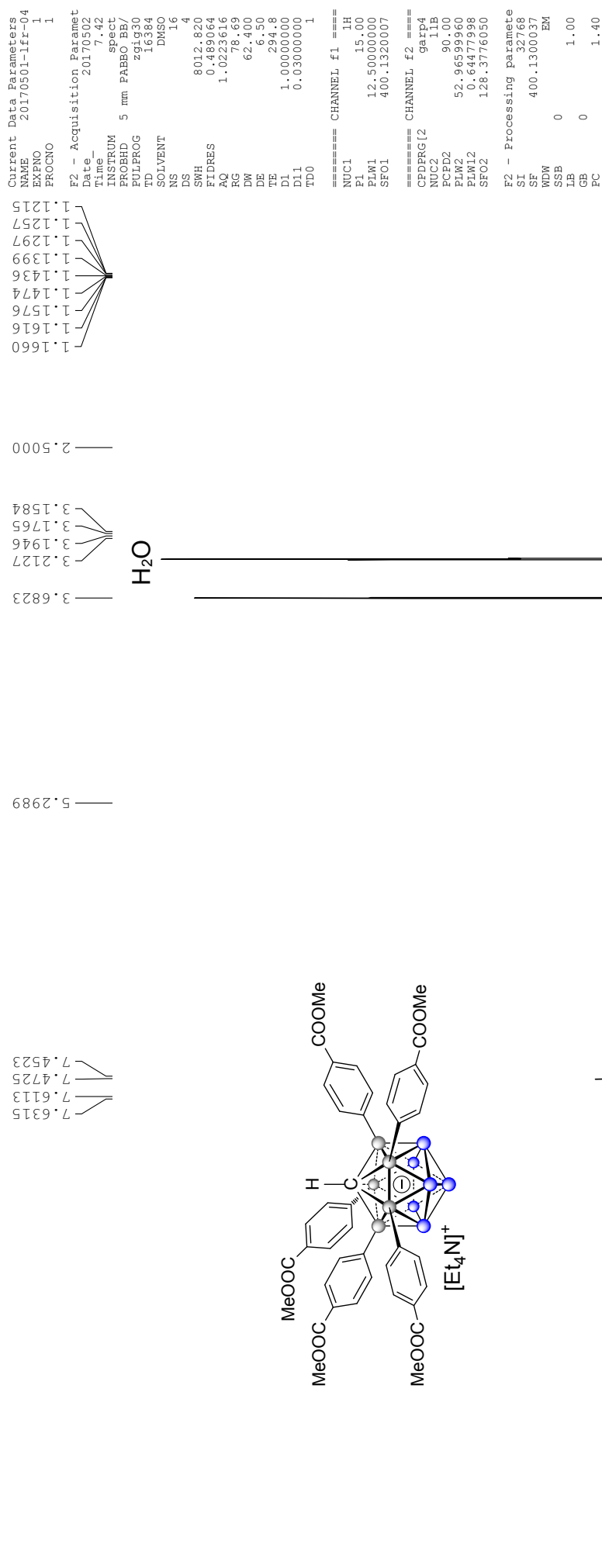
29.84

7.63

Current Data Parameters
 NAME 20170511-lfr-0431
 EXPNO 4
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20170512
 Time_ 5:19
 INSTRUM spect
 PROBHD 5 mm PABBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 use
 DE 6.50 use
 TE 293.2 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 ID0 1
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 use
 PLW1 53.00000000 W
 SFO1 100.6228293 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 use
 PLW2 12.50000000 W
 PLW12 0.43945000 W
 PLW13 0.28125000 W
 SFO2 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6128811 MHz
 EM
 WDW 0
 SSB 0
 LB 3.00 Hz
 GB 0
 FC 1.40

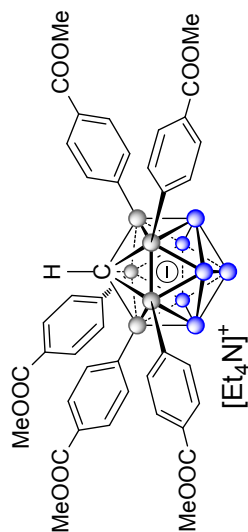
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

20170501-lfr-0425 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-COOMe)₅]
 400 MHz, ¹H{¹B} NMR, 24 mg dissolved in 0.55 mL dmsO-d6*



20170501-lfr-0425 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-COOMe)₅]
 128 MHz, ¹¹B NMR, 24 mg dissolved in 0.55 mL dmsO-d₆

— -11.0019



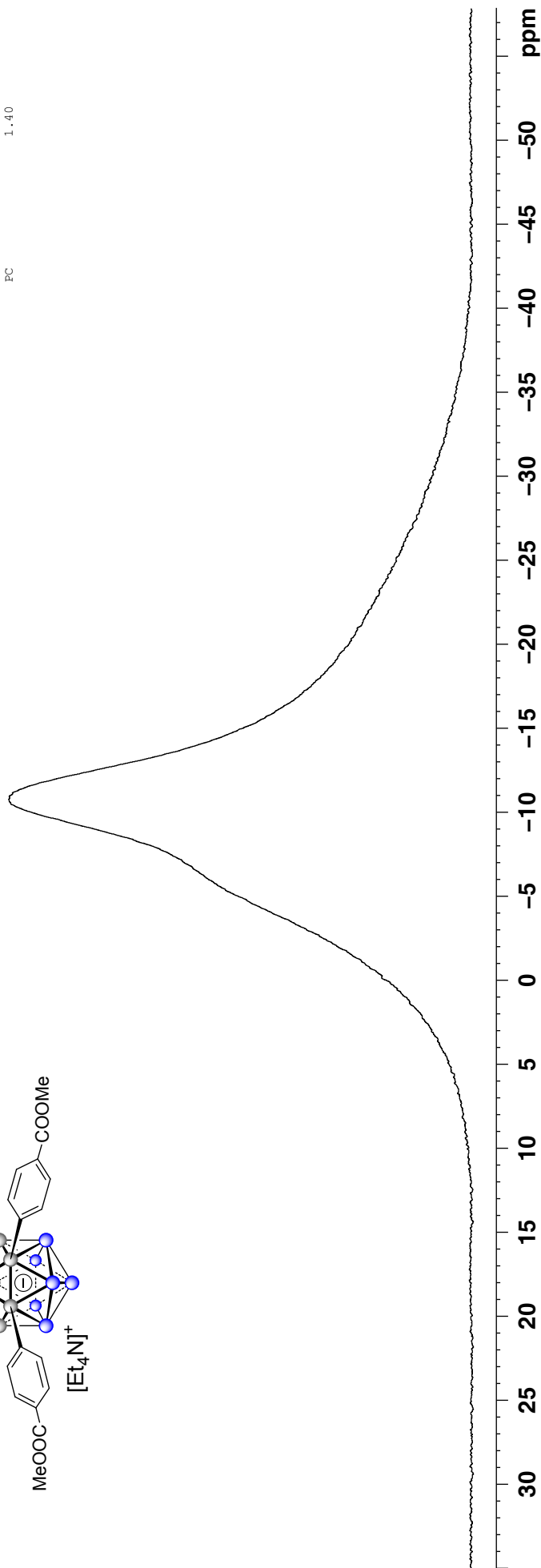
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Current Data Parameters
NAME      20170501-lfr-042
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20170502
Time      7.47
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg
TD         65536
SOLVENT   DMSO
NS         128
DS         4
SWH        25510.203 H
FIDRES     0.389255 H
AQ         1.2886056 s
RG         133.34
DW         15.00 u
DE         64.50 u
TE         294.8 K
D1         1.00000000 s
TD0        1

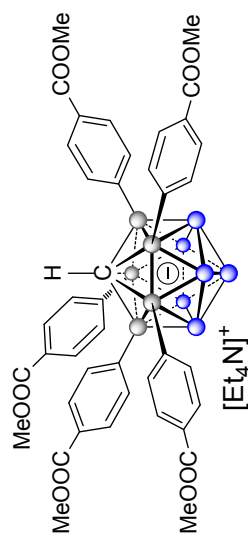
===== CHANNEL f1 =====
NUC1       11B
P1         9.93 u
PLW1       52.9659960 W
SF01       128.3776052 M

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



20170501-lfr-0425 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-COOMe)₅]
 128 MHz, ¹B{¹H} NMR, 24 mg dissolved in 0.55 mL dmsO-d6

10.8921



```
Current Data Parameters
NAME      20170501-lfr-042
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20170502
Time      7.54
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         128
DS         4
SWH        25510.203 H
FIDRES     0.389255 H
AQ         1.2845056 s
RG         193.34
DW         19.600 u
DE         6.50 u
TE         294.9 K
D1         1.00000000 s
D11        0.03000000 s
TD0        1

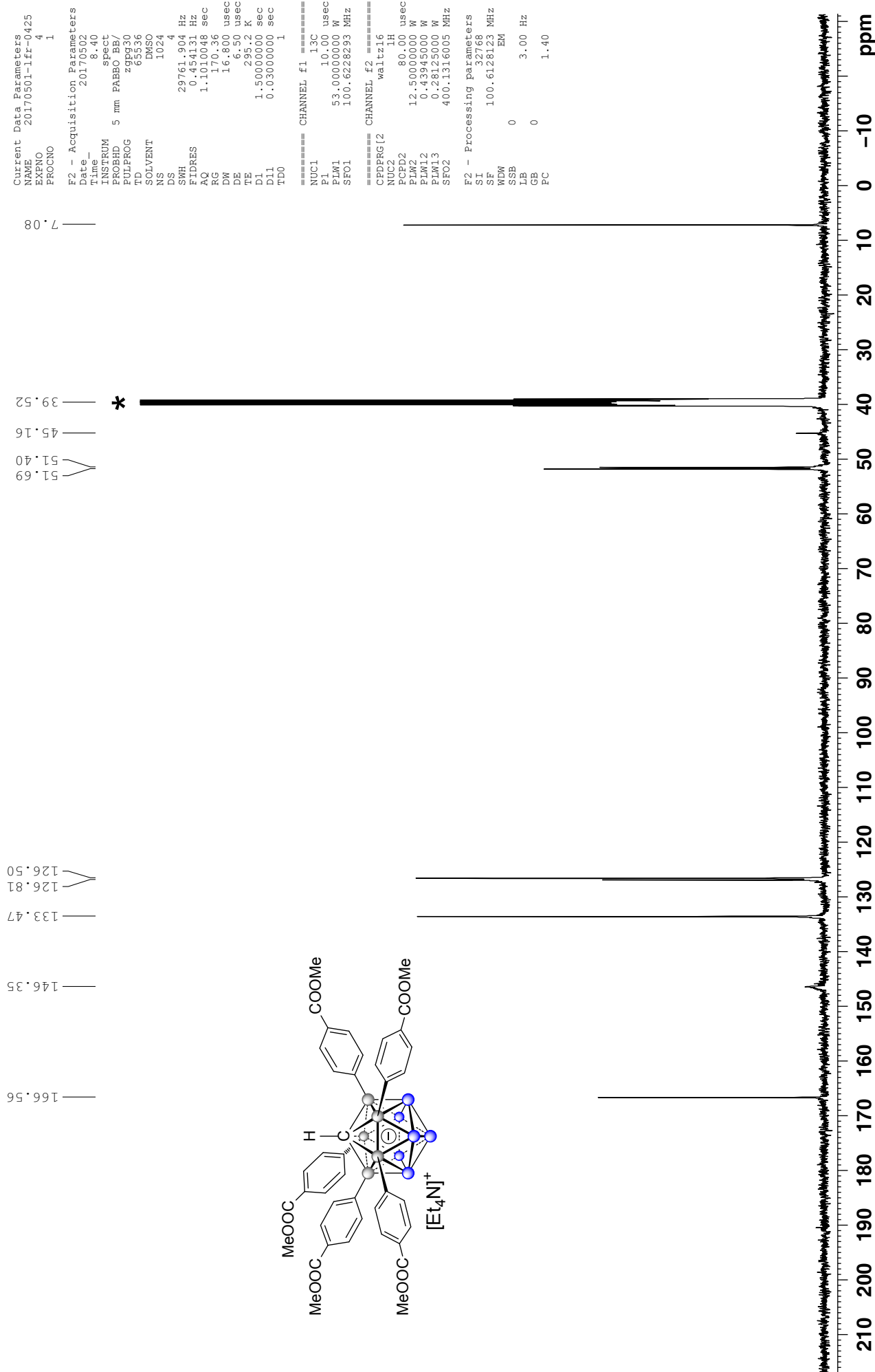
===== CHANNEL f1 =====
NUC1       11B
P1         9.93 u
PLM1       52.9659960 M
SFO1       128.3776050 M

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 u
PCPD2      12.50000000 M
PLM2       0.43945000 M
PLM3       0.28135000 M
SFO2       400.1320007 M

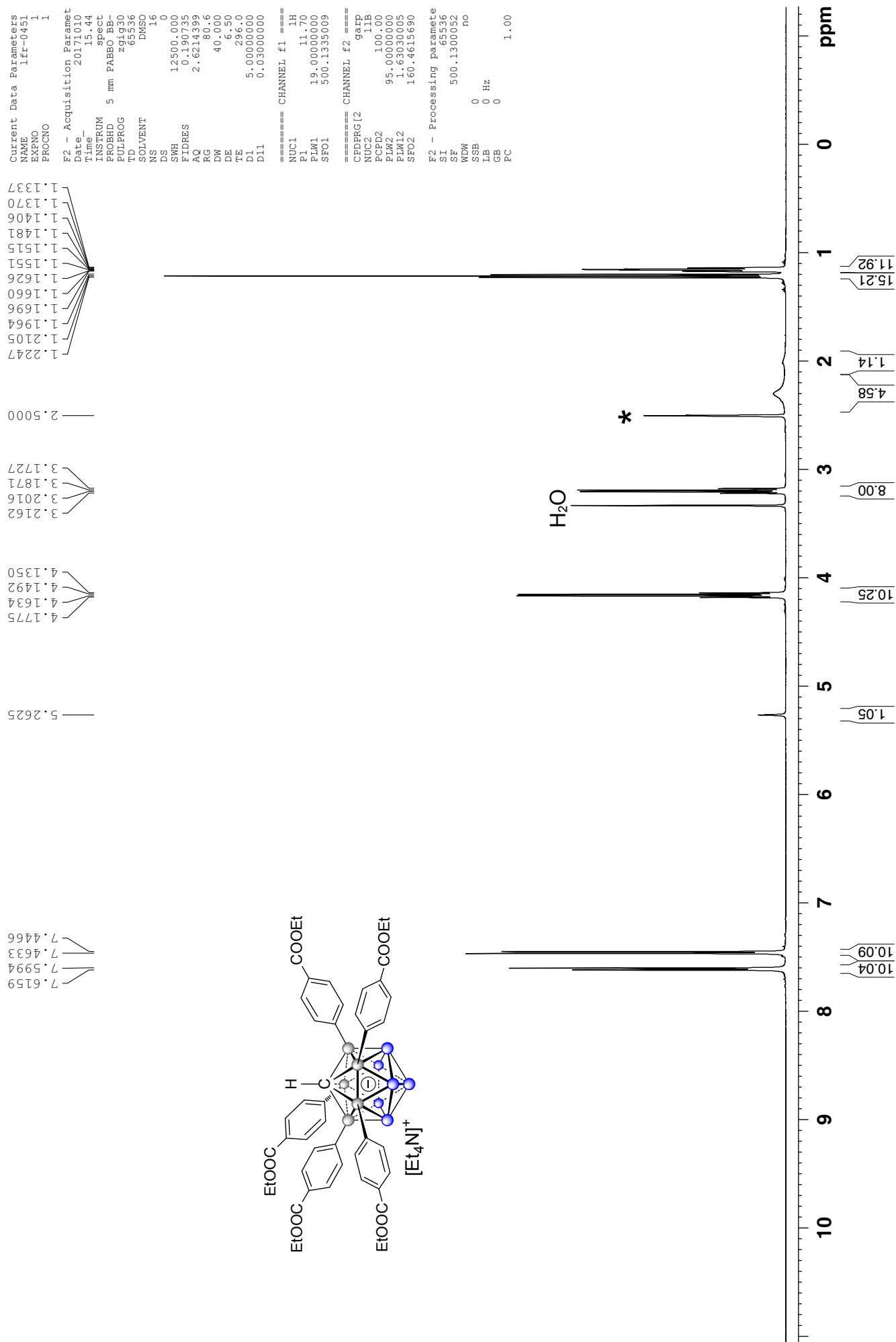
F2 - Processing parameters
SI         32768
SF         128.3776050 M
RG         EM
WDW         0
SSB         0
LB         10.00 H
GB         0
PC         1.40
```

35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 ppm

20170501-lfr-0425 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-COOMe)₆]
 101 MHz, ¹³C{¹H} NMR, 24 mg dissolved in 0.55 mL dmso-d₆*

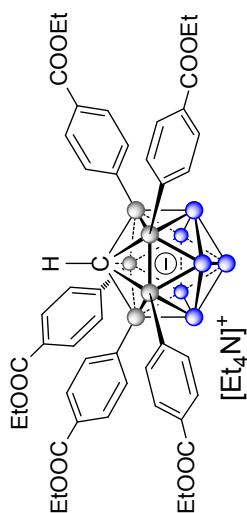


20171010-lfr-0451 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-COOEt)₅]
 500 MHz, ¹H{¹B} NMR, 10 mg dissolved in 0.55 mL dmsO-d6*



20171010-lfr-0451 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-COOEt)₅]
 160 MHz, ¹B NMR, 32 mg dissolved in 0.55 mL dmsO-d6*

— 5.9204
 — 10.8151

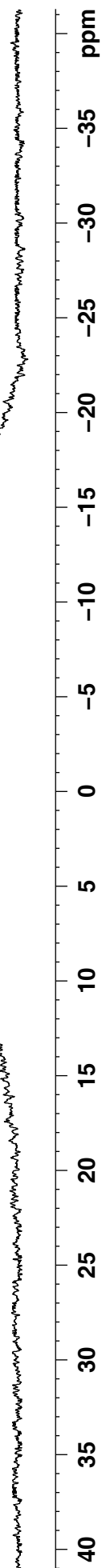


```
Current Data Parameters
NAME      lfr-0451
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20171010
Time      15.57
INSTRUM   spect
PROBHD    5 mm FAPBO BB-
PULPROG   zg30
TD        64098
SOLVENT   DMSO
NS        32
DS        0
SWH       32051.281 H
FIDRES    0.500036 H
AQ         0.9999288 s
RG         203
DW        15.600 u
DE         6.50 u
TE        295.9 K
D1         1.00000000 s

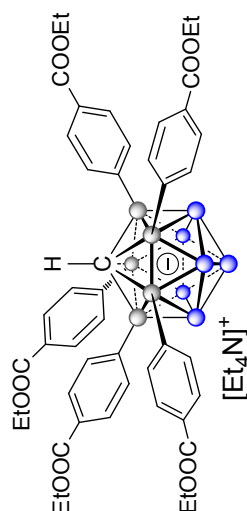
===== CHANNEL f1 =====
NUC1      11B
P1        13.10 u
PLW1      95.00000000 W
SFO1      160.4615792 M

F2 - Processing parameters
SI        32768
SF        160.4615986 M
WDW       EM
SSB       0
LB        10.00 H
GB        0
PC        1.40
```



20171010-lfr-0451 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-COOEt)₅]
 160 MHz, ¹¹B{¹H} NMR, 32 mg dissolved in 0.55 mL dmsO-d6

— 10.6312
 — 6.2490



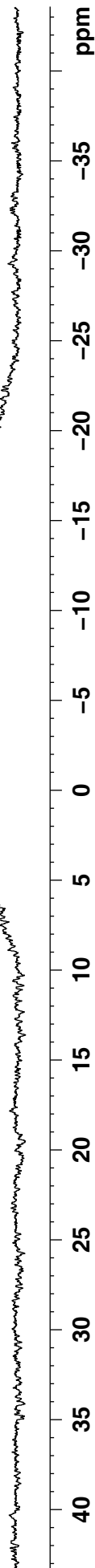
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Current Data Parameters
NAME      lfr-0451
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20171010
Time      15.58
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        16
DS        0
SWH       32051.281 H
FIDRES    0.489064 H
AQ         1.0223616 s
RG         203
DW         15.600 u
DE         6.50 u
TE        296.1 K
D1         1.00000000 s
D11        0.03000000 s

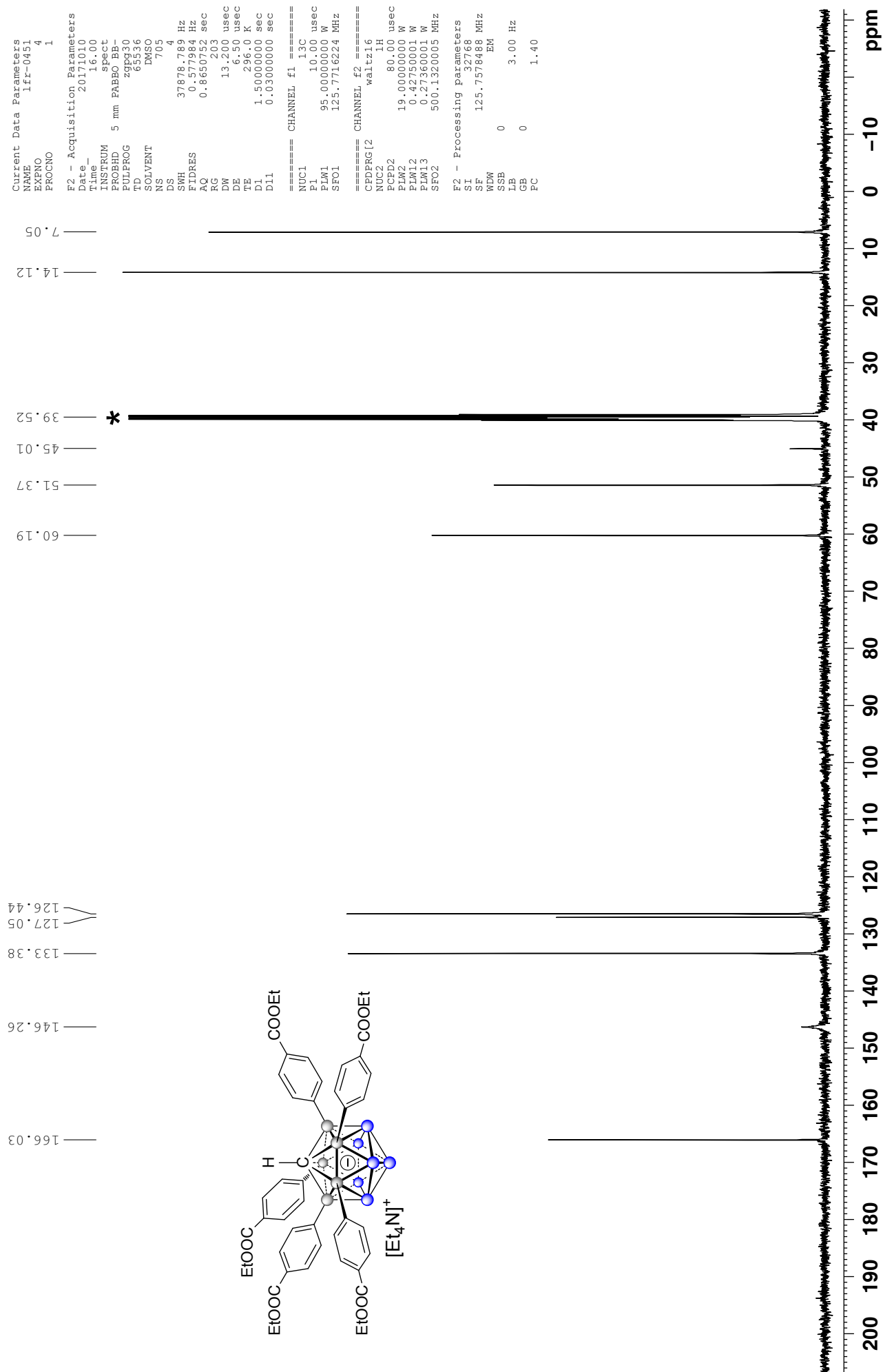
===== CHANNEL f1 =====
NUC1       11B
P1         13.10 u
PLW1       95.00000000 W
SFO1       160.4615790 M

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 u
PLW2       19.00000000 W
PLW12      0.39262000 W
PLW13      0.25127000 W
SFO2       500.1325007 M

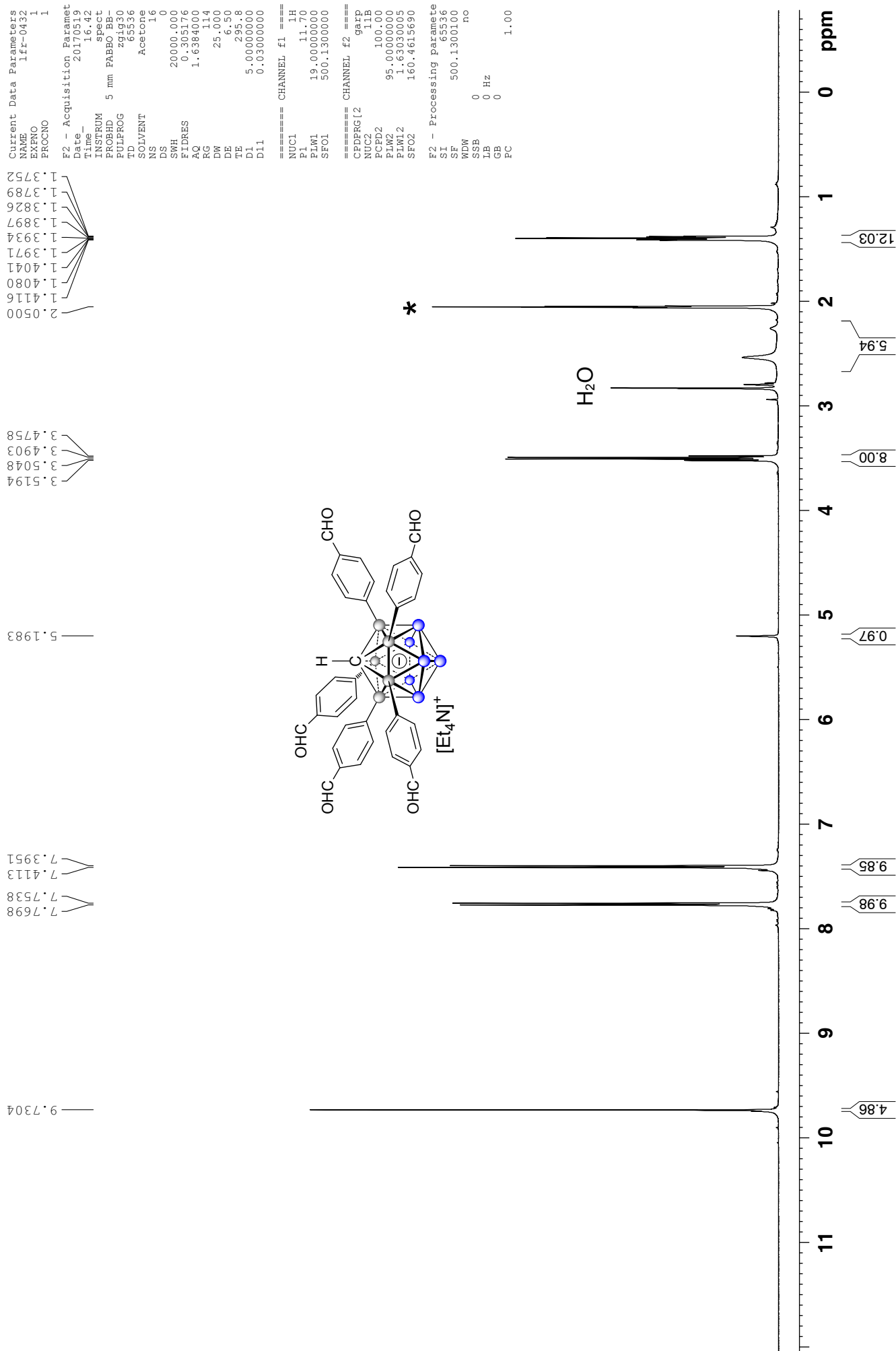
F2 - Processing parameters
SI         32768
SF         160.4615790 M
WDW        EM
SSB        0
LB         10.00 H
GB         0
PC         1.40
```



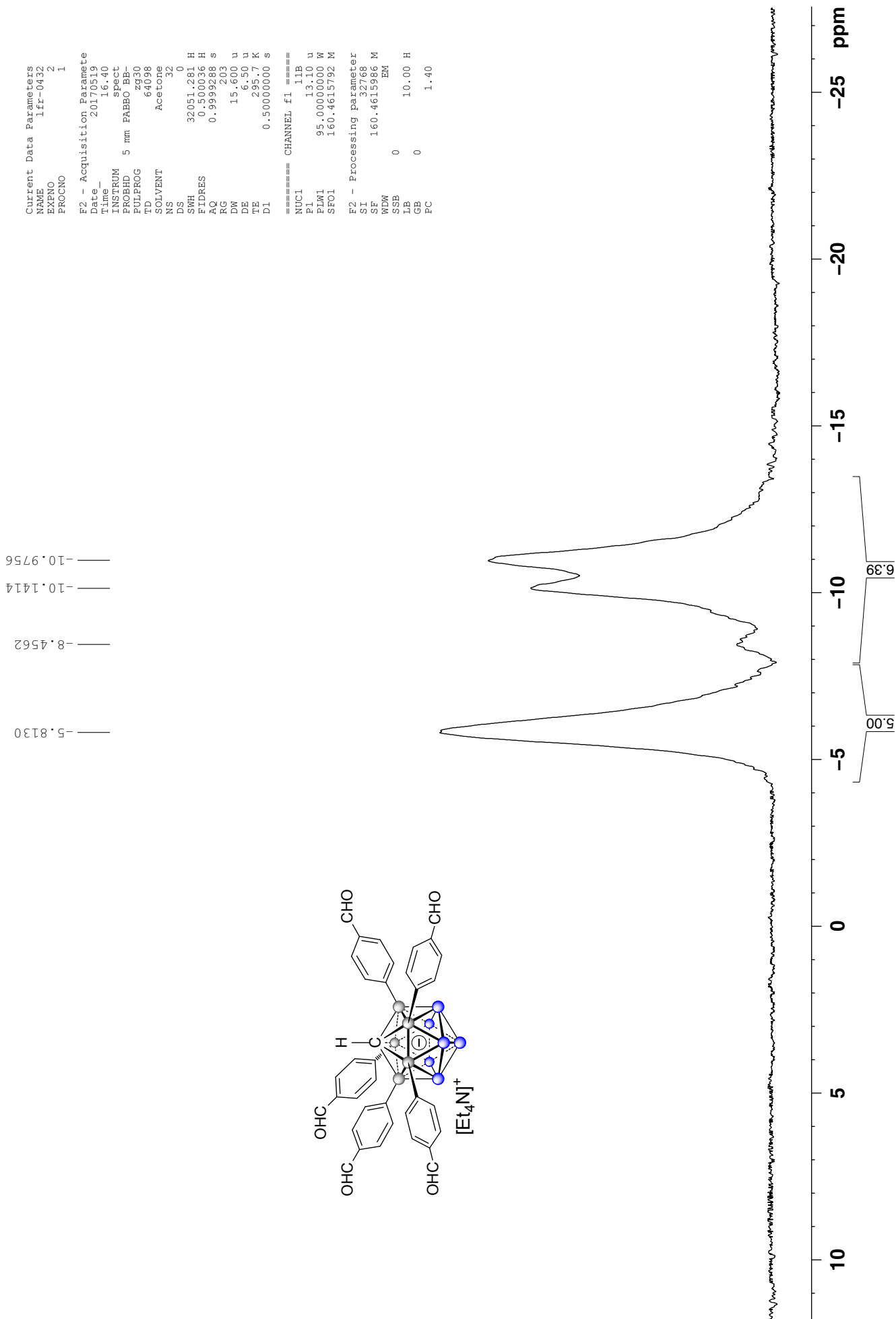
20171010-lfr-0451 [NEt₄][H-CB₁₁H₆-(C₆H₄-p-COOEt)₅]
 126 MHz, ¹³C{¹H} NMR, 32 mg dissolved in 0.55 mL dmsO-d₆*



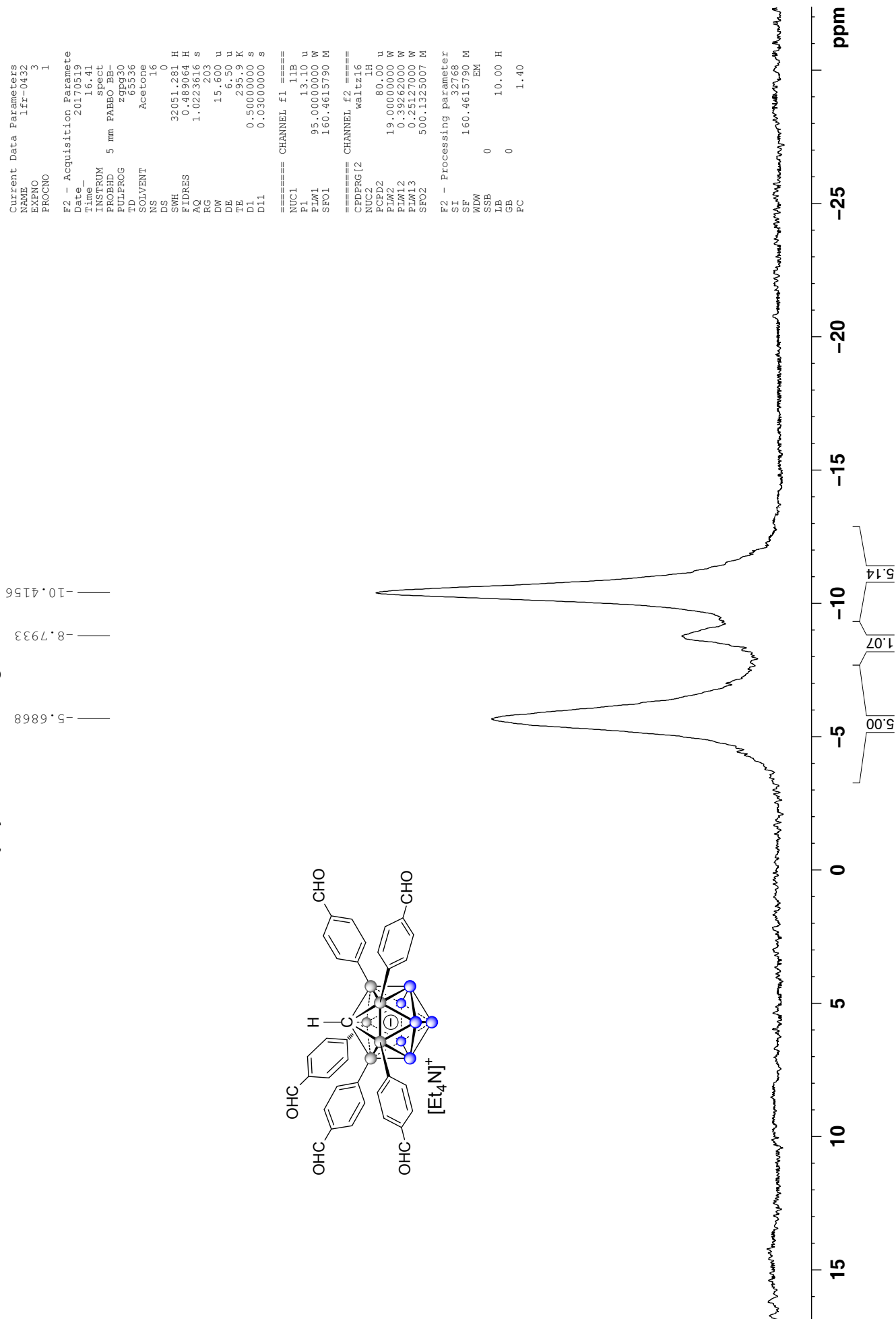
20170519-lfr-0432 [NEt₄][H-CB₁₁H₆-(4-CHO-C₆H₄)₅]
 500 MHz, ¹H{¹B} NMR, ca. 5 mg dissolved in 0.55 mL acetone-d₆*



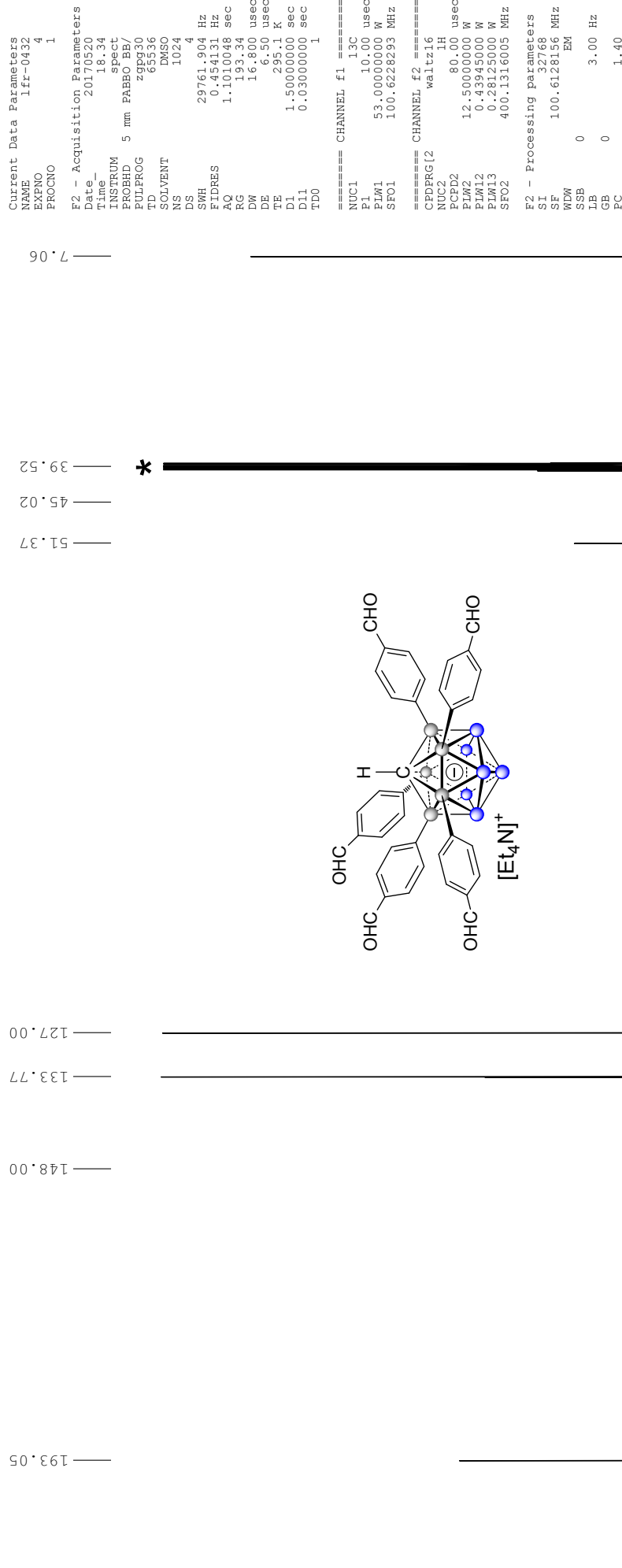
20170519-lfr-0432 [NEt₄][H-CB₁₁H₆-(4-CHO-C₆H₄)₅]
 160 MHz, ¹¹B NMR, ca. 5 mg dissolved in 0.55 mL acetone-d₆



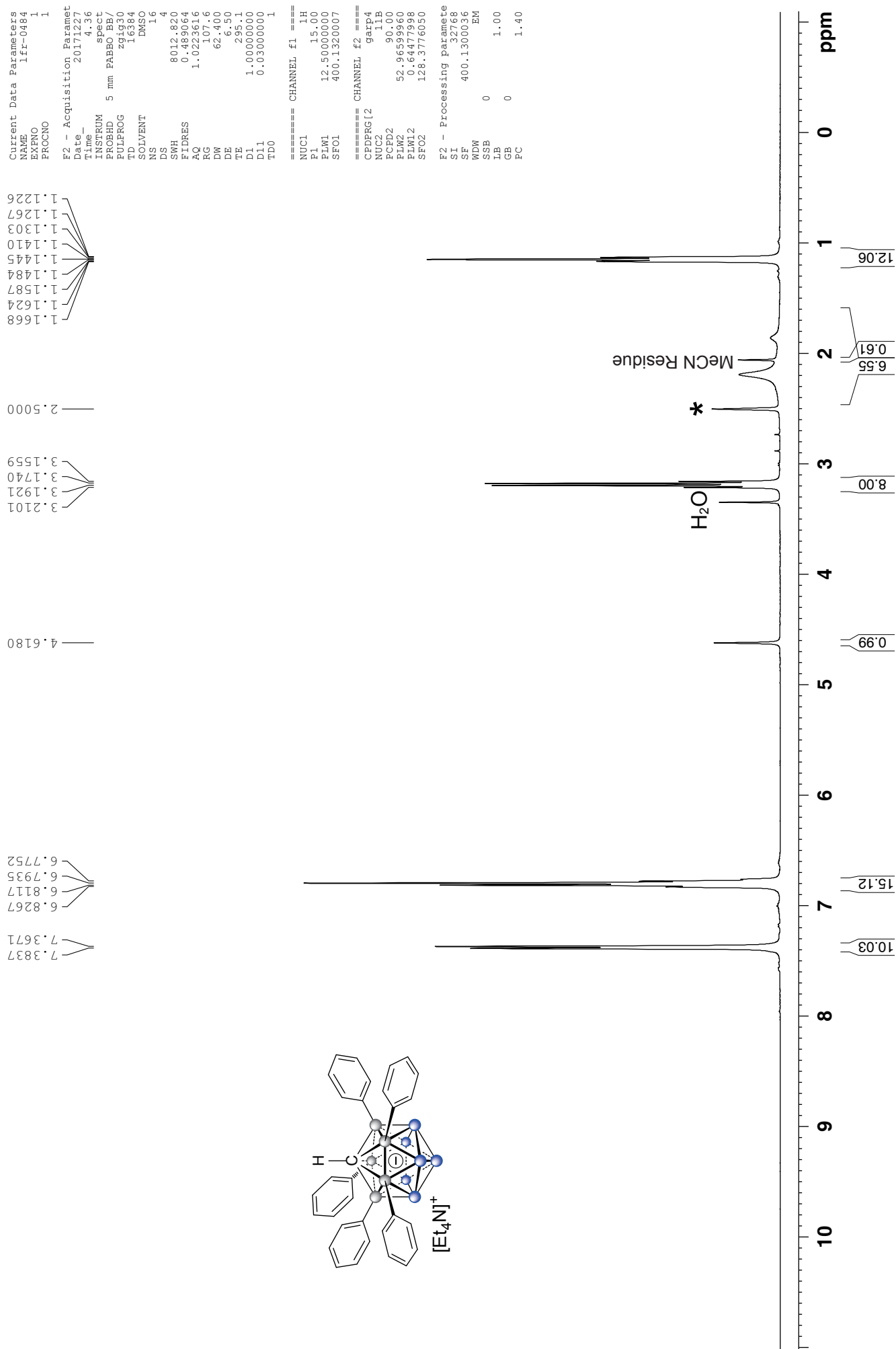
20170519-lfr-0432 [NEt₄][H-CB₁₁H₆-(4-CHO-C₆H₄)₅]
 160 MHz, ¹¹B{¹H} NMR, ca. 5 mg dissolved in 0.55 mL acetone-d₆



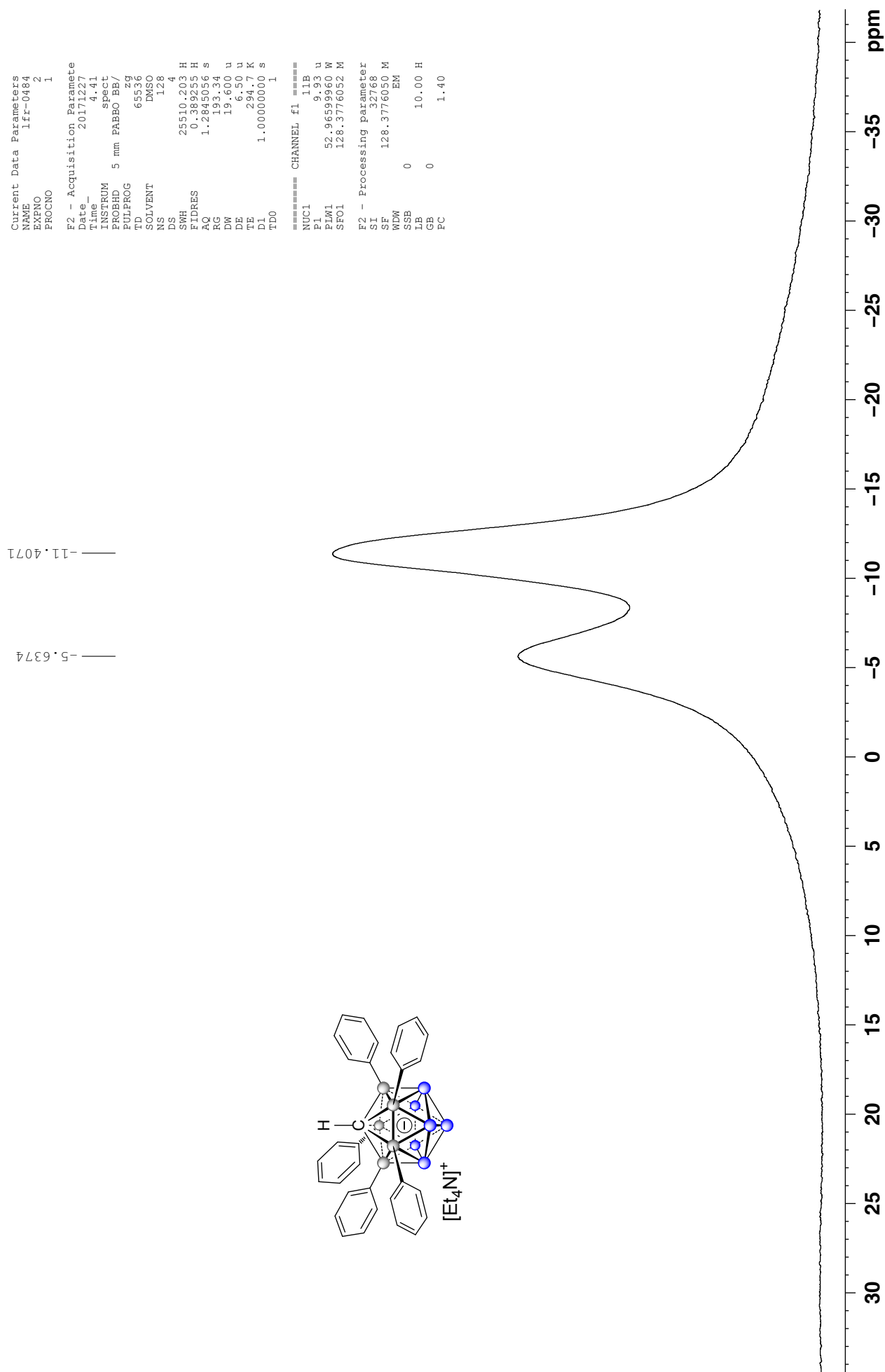
20170519-lfr-0432 [NEt₄][H-CB₁₁H₆-(4-CHO-C₆H₄)₅]
 101 MHz, ¹H{¹B} NMR, ca. 15 mg dissolved in 0.55 mL dmsO-d₆*



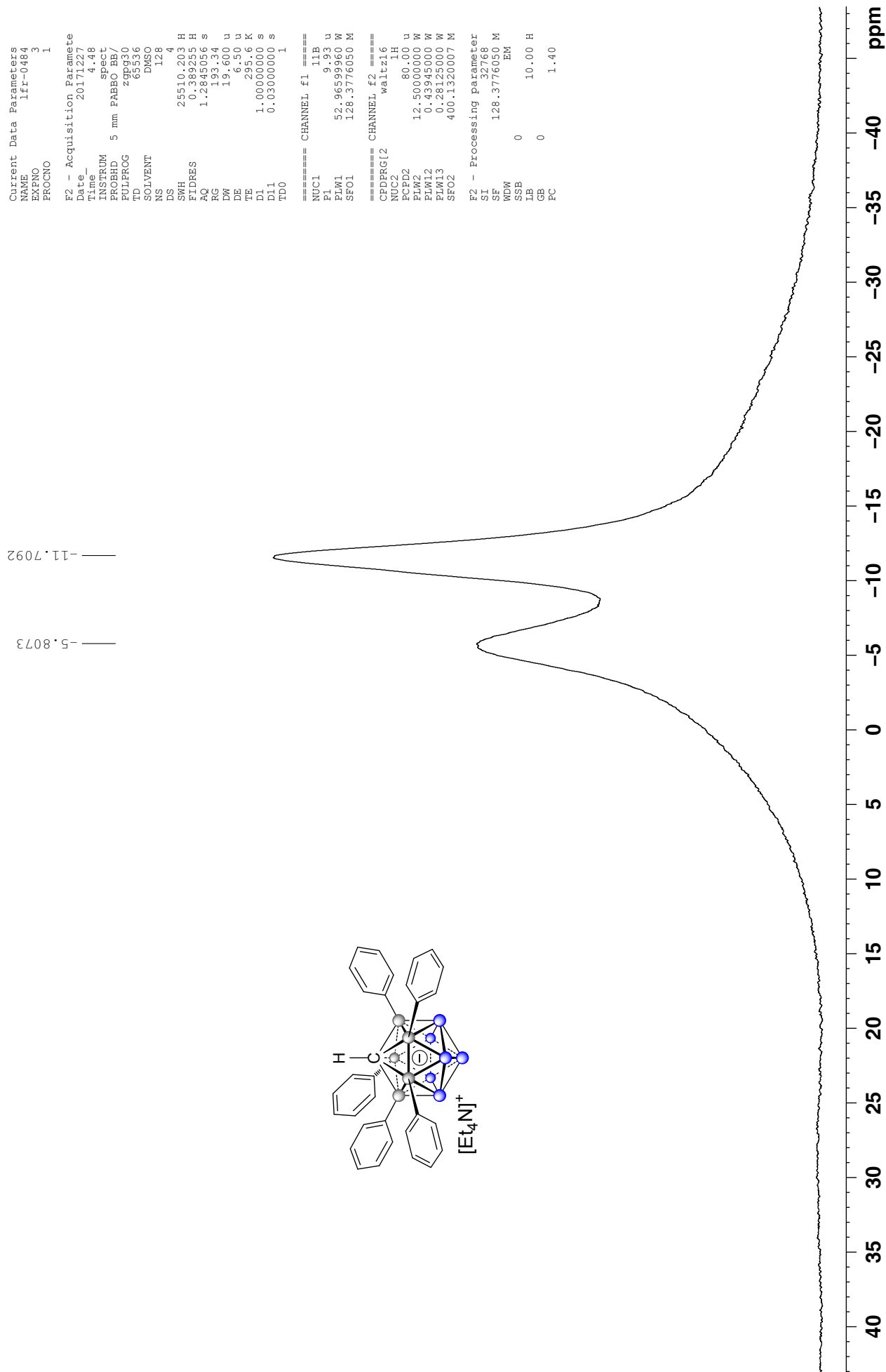
20171225-lfr-0484 [NEt₄][H-CB₁₁H₆-(Ph)₅]
 400 MHz, ¹H{¹B} NMR, ca. 15 mg dissolved in 0.55 mL dmsO-d₆*



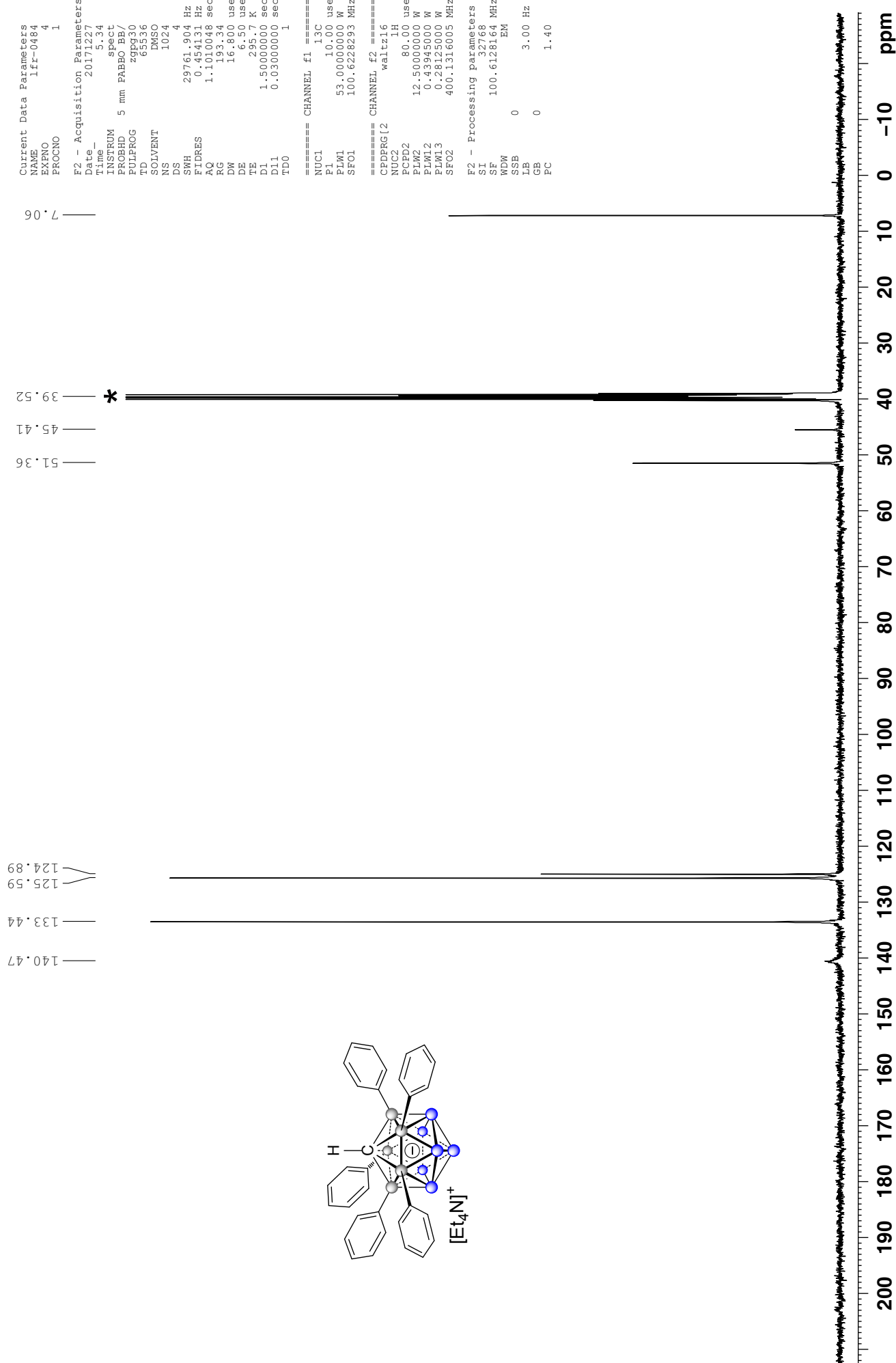
20171225-lfr-0484 [NEt₄][H-CB₁₁H₆-(Ph)₅]
 128 MHz, ¹¹B NMR, ca. 15 mg dissolved in 0.55 mL dmsO-d6*



20171225-lfr-0484 [NEt₄][H-CB₁₁H₆-(Ph)₅]
 128 MHz, ¹B{¹H} NMR, ca. 15 mg dissolved in 0.55 mL dmsO-d6*



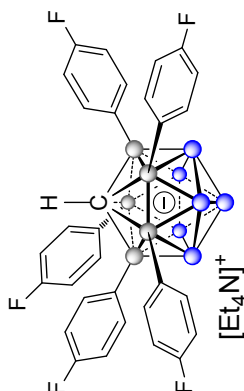
20171225-lfr-0484 [NEt₄][H-CB₁₁H₆-(Ph)₅]
 101 MHz, ¹³C{¹H} NMR, ca. 15 mg dissolved in 0.55 mL dmsO-d6*



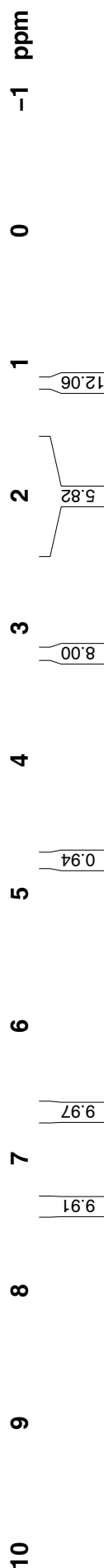
20171121-lfr-0487 [NEt₄][H-CB₁₁H₆-(4-F-C₆H₄)₅]
500 MHz, ¹H{¹B} NMR, ca. 10 mg dissolved in 0.55 mL dmsO-d6*



H₂O

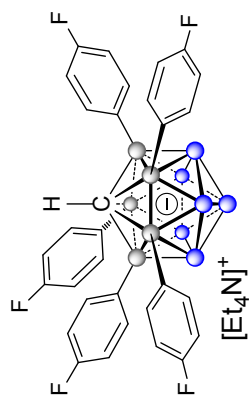


Current Data Parameters
NAME lfr-0487
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171128
Time_ 17.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 12500.000
FIDRES 0.190735
AQ 2.621499
RG 40.000
DE 1.4
TE 65.3
D1 673.1
D11 5.0000000
===== CHANNEL f1 =====
NUC1 1H
P1 11.50
PLW1 19.00000000
SFO1 500.1335009
===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 11B
PCPD2 100.00
PLW2 95.00000000
PLW12 1.63030005
SFO2 160.4615690
F2 - Processing parameters
SI 65536
SF 500.1297804
WDW no
SSB 0 Hz
LB 0
GB 0
PC 1.00



20171121-lfr-0487 [NEt₄][H-CB₁₁H₆-(4-F-C₆H₄)₅]
 160 MHz, ¹¹B NMR, ca. 10 mg dissolved in 0.55 mL dmsO-d₆

— -6.0440
 — -11.9361

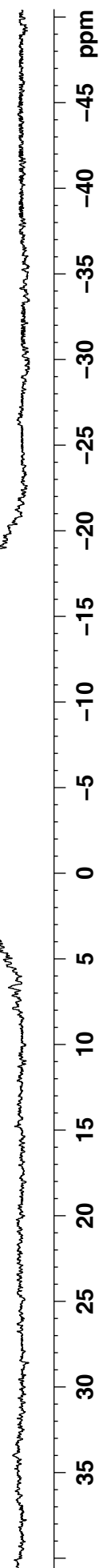


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Current Data Parameters
NAME      lfr-0487
EXPNO     2
PROCNO    1

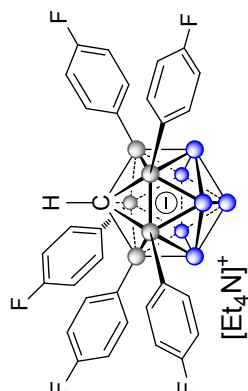
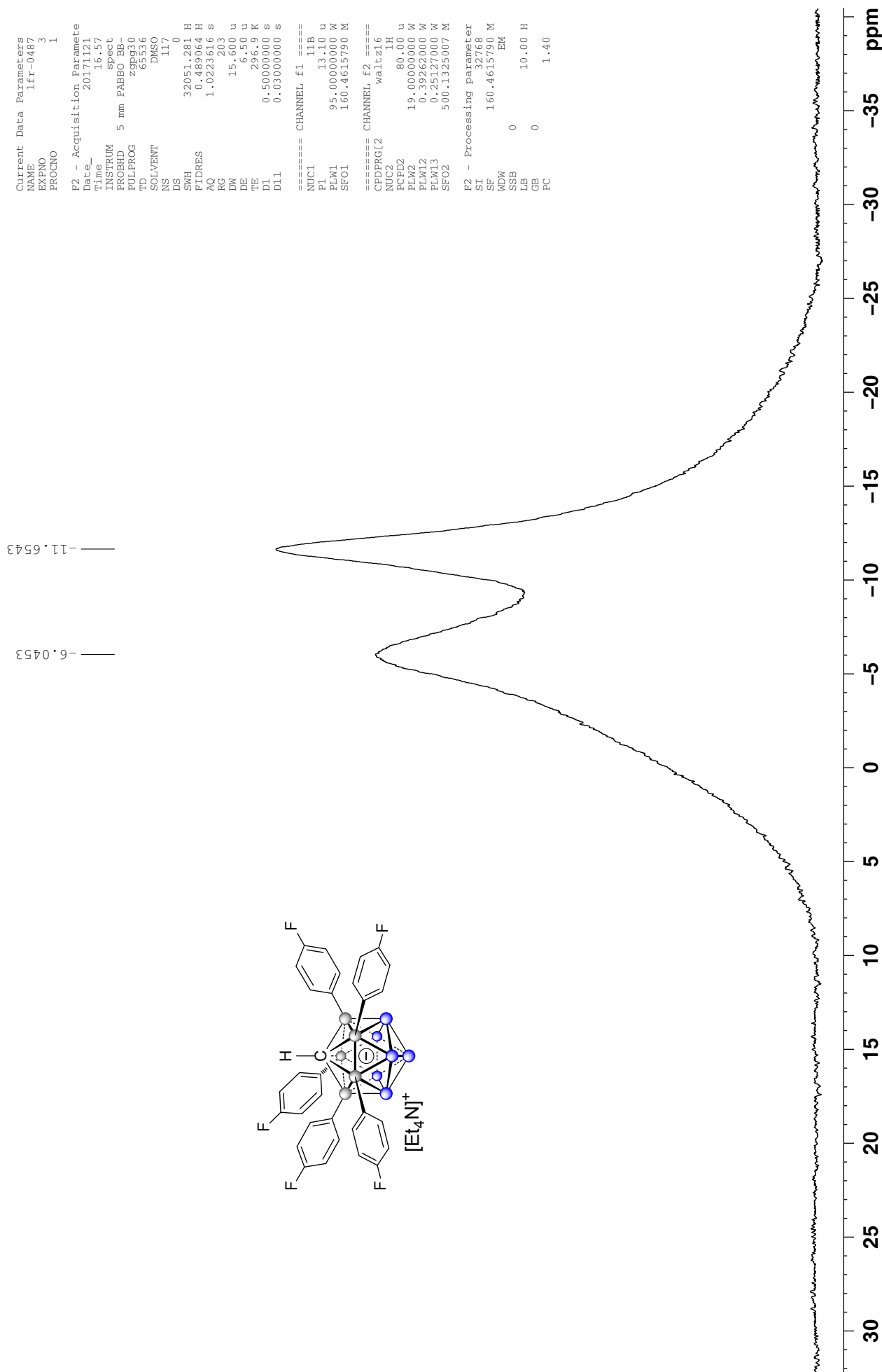
F2 - Acquisition Parameters
Date_     20171121
Time      16.49
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   zg30
TD        65536
SOLVENT   DMSO
NS         227
DS         2
SWH        32051.281 H
FIDRES     0.489064 H
AQ         1.0223616 s
RG         203
DW         15.600 u
DE         6.50 u
TE         296.9 K
D1         0.50000000 s

===== CHANNEL f1 =====
NUC1       11B
P1         10.00 u
PLW1       75.00000000 W
SFO1       160.4615792 M

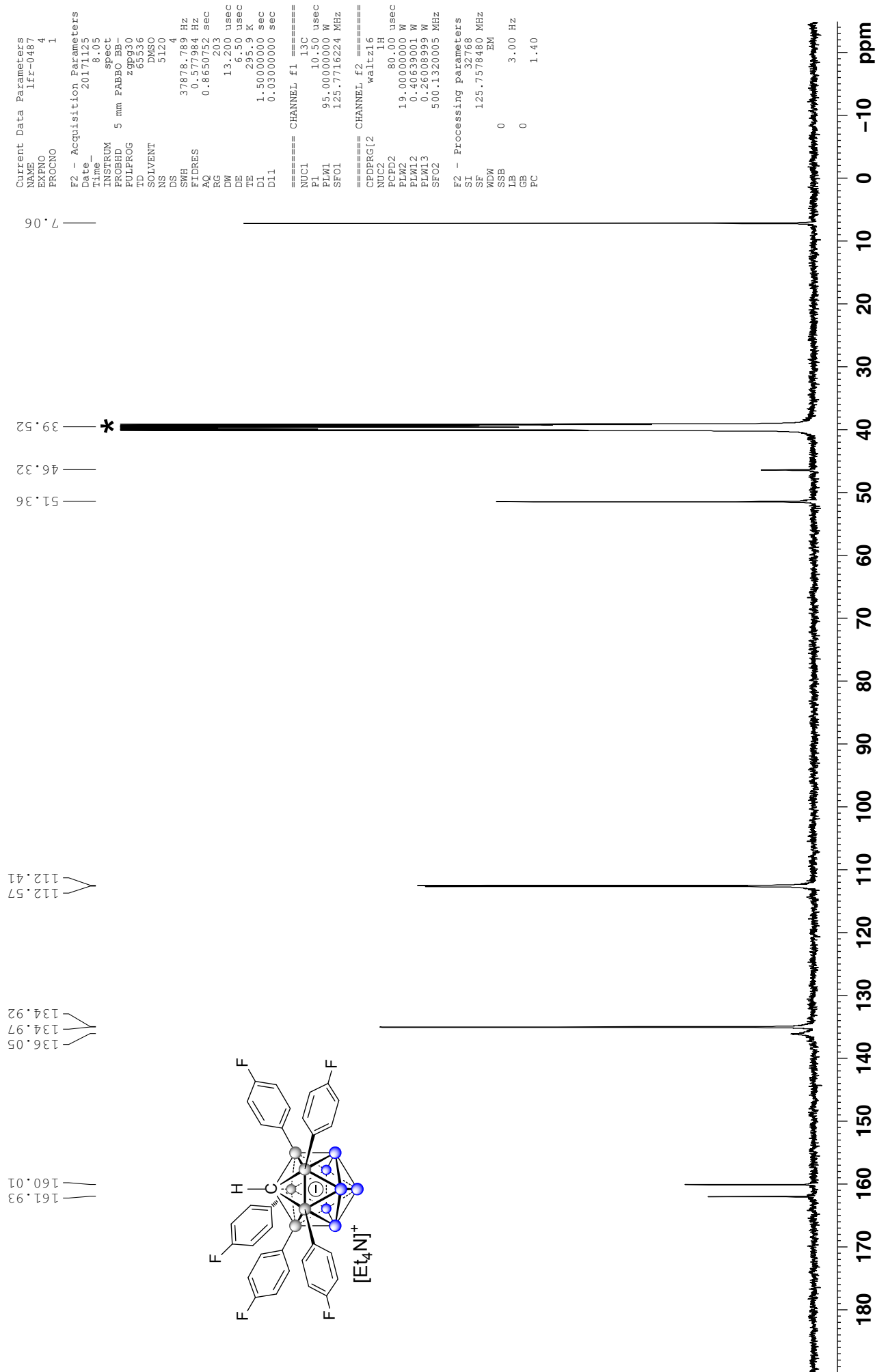
F2 - Processing parameters
SI         32768
SF         160.4615790 M
WDW        EM
SSB        0
LB         0
GB         0
PC         1.40
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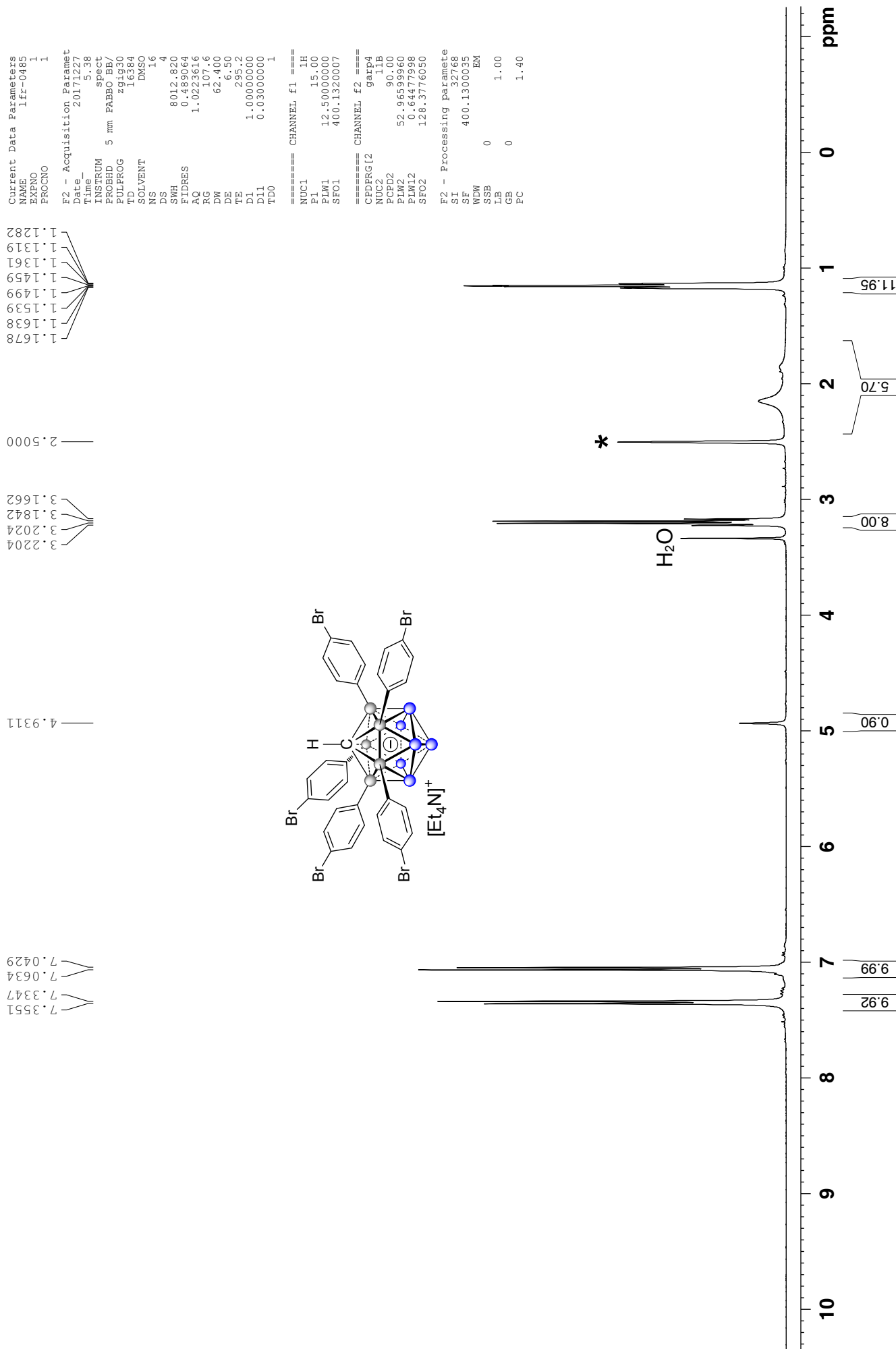
20171121-lfr-0487 [NEt₄][H-CB₁₁H₆-(4-F-C₆H₄)₅]
 160 MHz, ¹B{¹H} NMR, ca. 10 mg dissolved in 0.55 mL dmsO-d₆



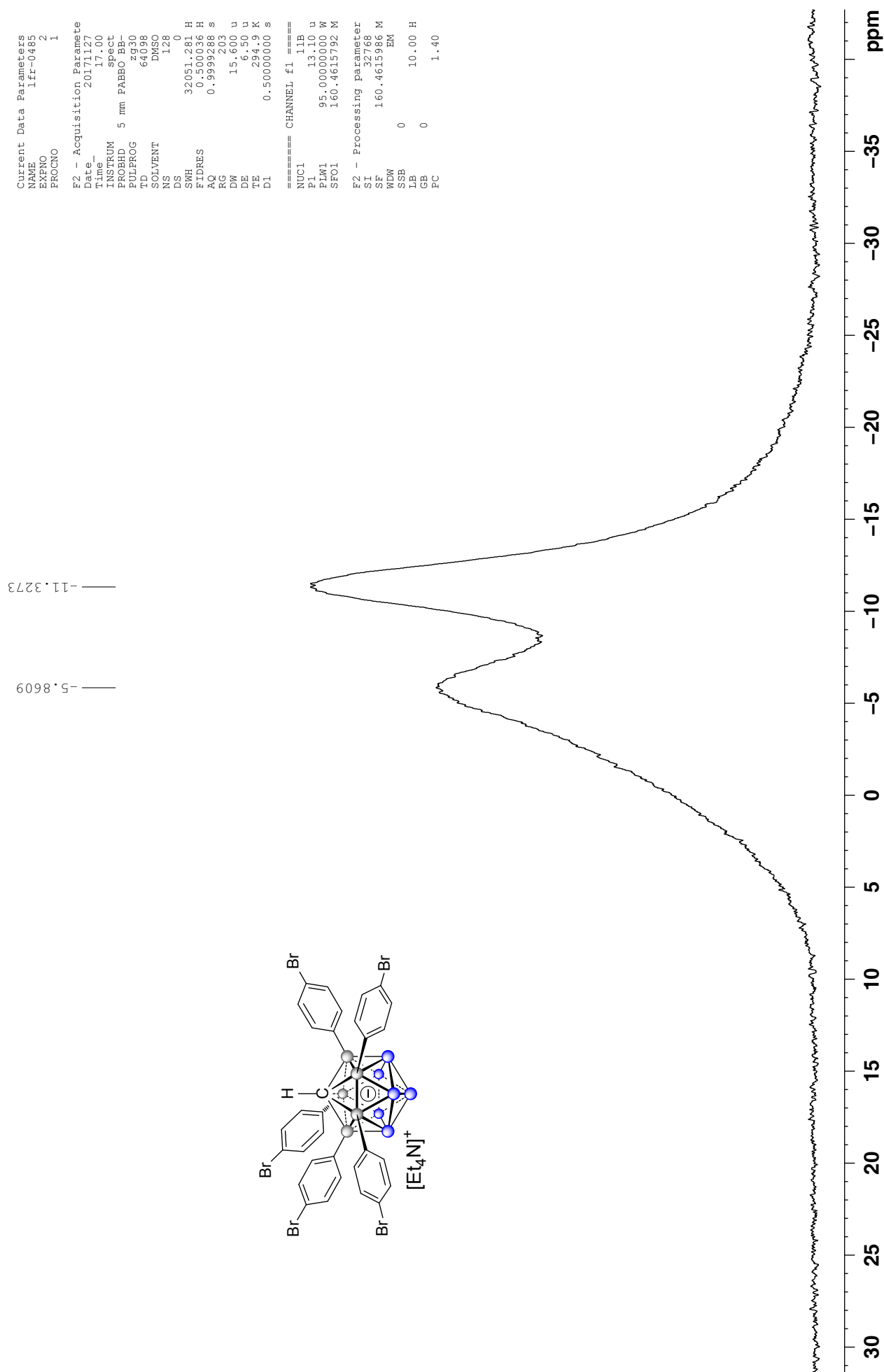
20171121-lfr-0487 [NEt₄][H-CB₁₁H₆-(4-F-C₆H₄)₅]
 126 MHz, ¹³C{¹H} NMR, ca. 10 mg dissolved in 0.55 mL dmsO-d₆*



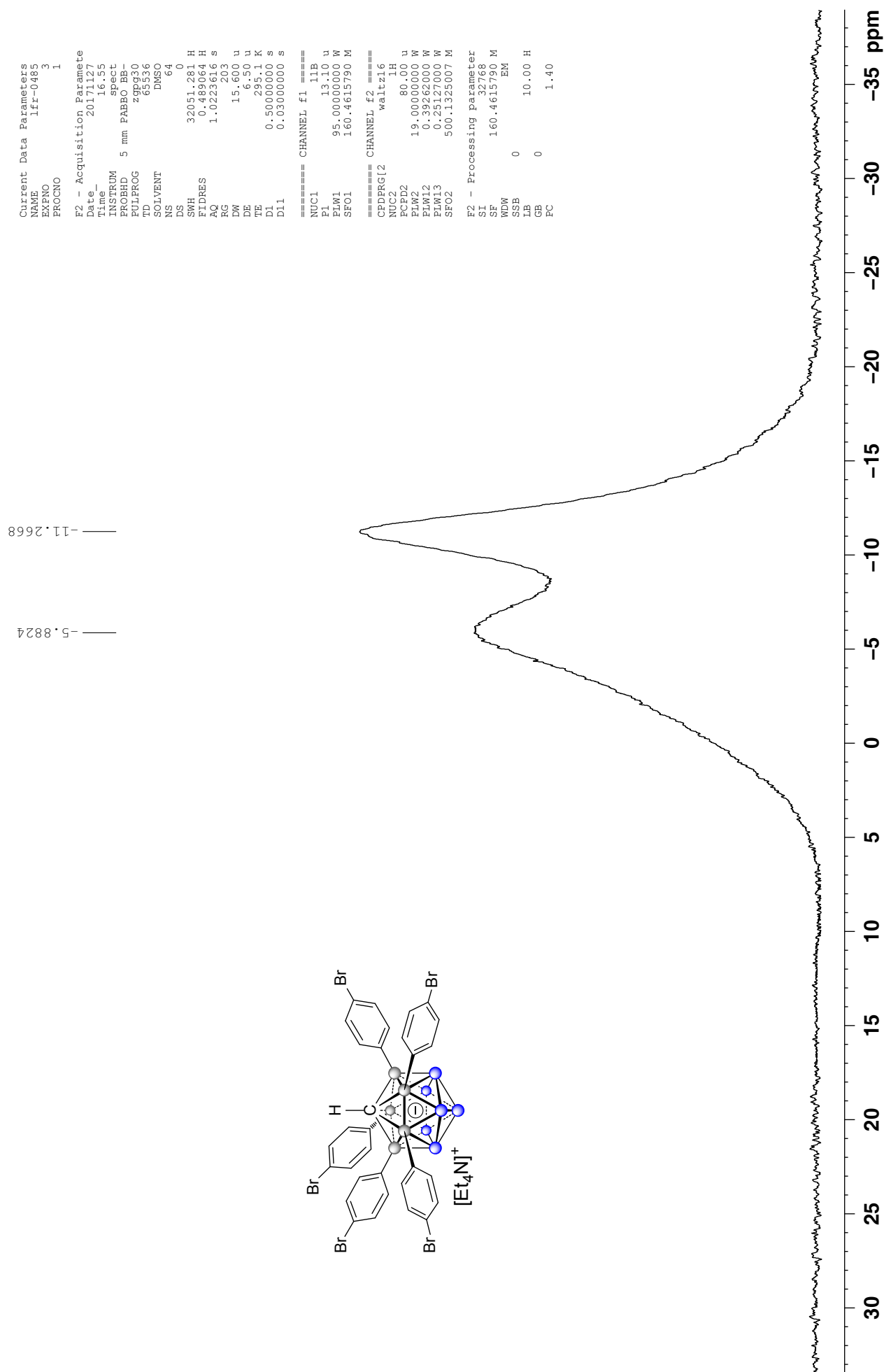
20171225-lfr-0485 [NEt₄][H-CB₁₁H₆⁻(4-Br-C₆H₄)₅]
 400 MHz, ¹H{¹B} NMR, ca. 9 mg dissolved in 0.55 mL dmsO-d6*



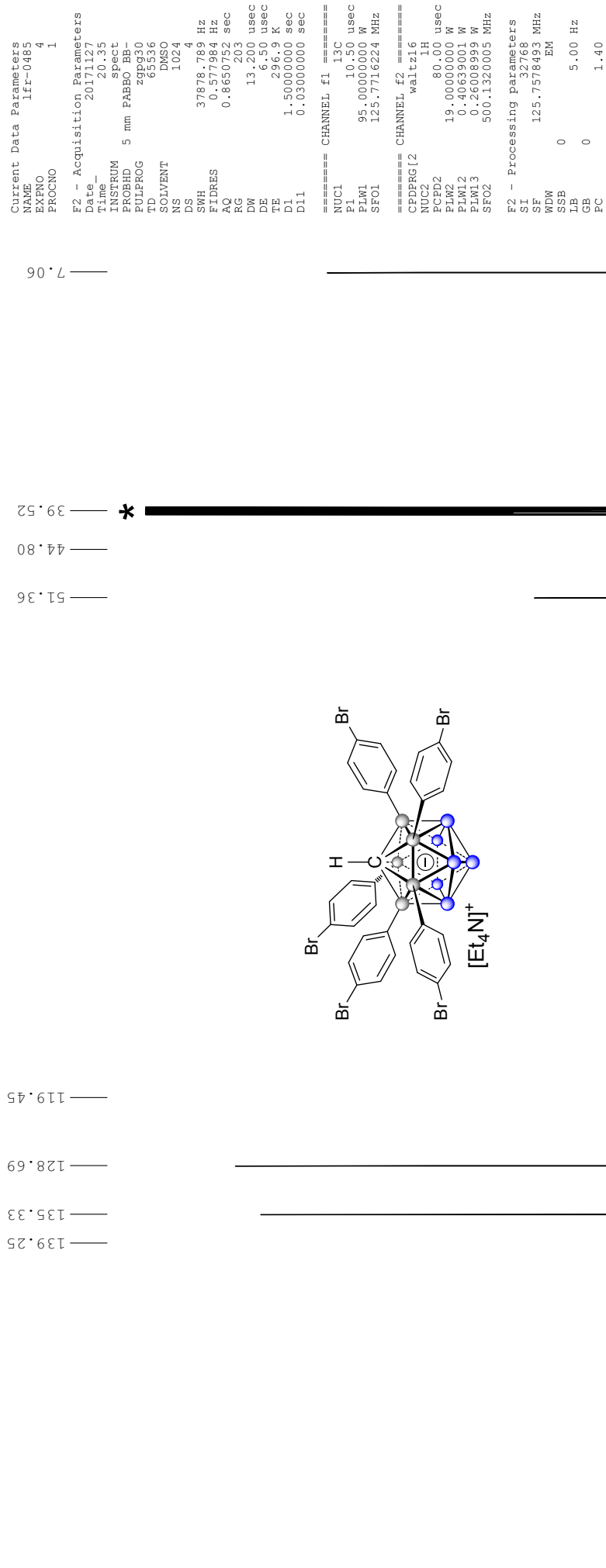
20171127-lfr-0485 [NEt₄][H-CB₁₁H₆-(4-Br-C₆H₄)₅]
 160 MHz, ¹¹B NMR, ca. 17 mg dissolved in 0.55 mL dmsO-d₆



20171127-lfr-0485 [NEt₄][H-CB₁₁H₆-(4-Br-C₆H₄)₅]
 160 MHz, ¹B{¹H} NMR, ca. 17 mg dissolved in 0.55 mL dmsO-d6



20171127-lfr-0485 [NEt₄][H-CB₁₁H₆-(4-Br-C₆H₄)₅]
 126 MHz, ¹³C{¹H} NMR, ca. 17 mg dissolved in 0.55 mL dmsO-d₆*



20171121-lfr-0488 [NEt₄][H-CB₁₁H₆-(4-Et-C₆H₄)₅]
500 MHz, ¹H{¹B} NMR, ca. 10 mg dissolved in 0.55 mL dms₂-d₆*

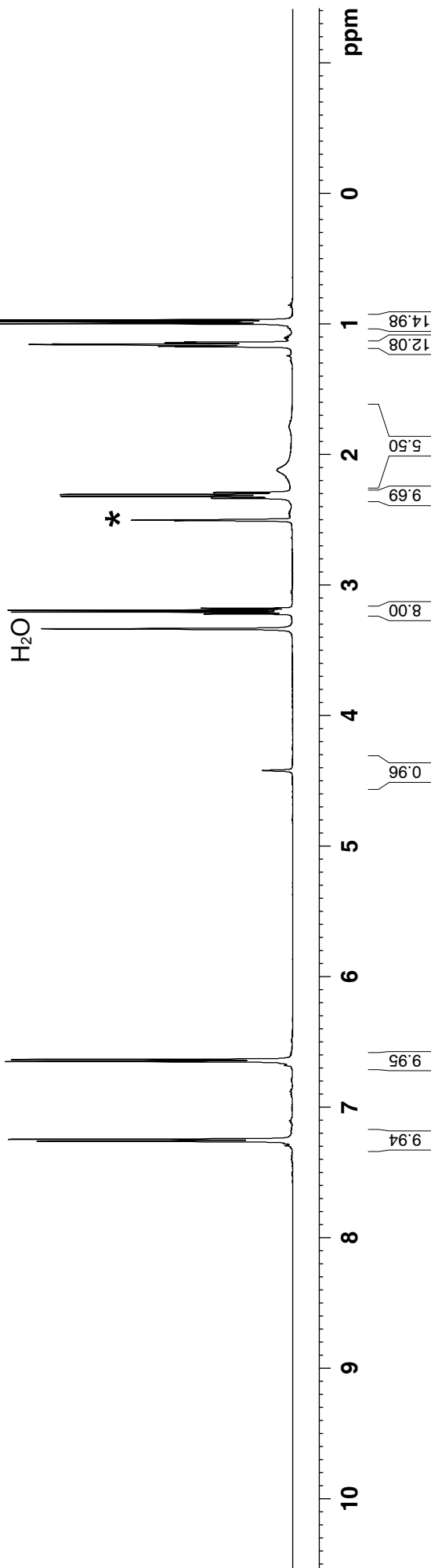
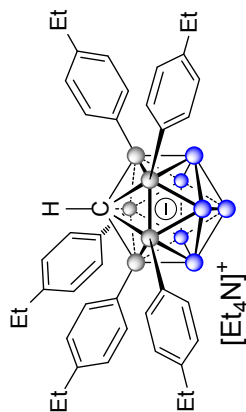
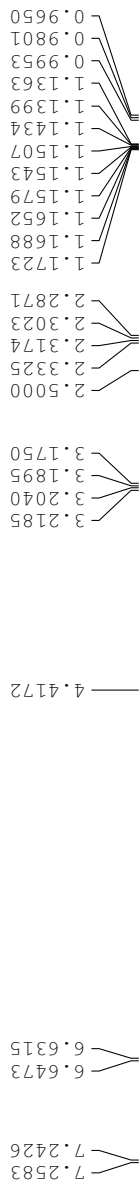
Current Data Parameters
NAME lfr-0488
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171128
Time_ 17.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 12500.000
FIDRES 0.190735
AQ 2.6214399
RG 114
DM 40.000
DE 6.50
TE 300.2
D1 5.00000000
D11 0.03000000

===== CHANNEL f1 =====
NUC1 ¹H
P1 11.50
PLW1 19.00000000
SFO1 500.1335009

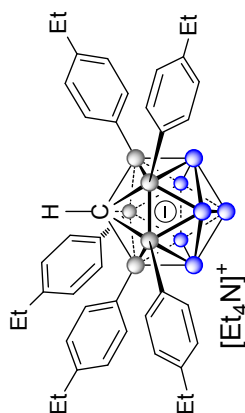
===== CHANNEL f2 =====
CPDPRG[2] garp
NUC2 ¹¹B
P2 11.50
PLW2 95.00000000
SFO2 160.4615690

F2 - Processing parameters
SI 65536
SF 500.1297805
WDW no
SSB 0 Hz
LB 0
GB 0
PC 1.00



20171121-lfr-0488 [NEt₄][H-CB₁₁H₆-(4-Et-C₆H₄)₅]
 160 MHz, ¹¹B NMR, ca. 10 mg dissolved in 0.55 mL dmsO-d₆

— -5.7788
 — -12.3265

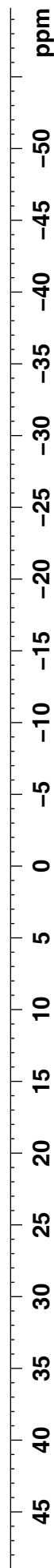


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Current Data Parameters
NAME      lfr-0488
EXPNO     2
PROCNO    1

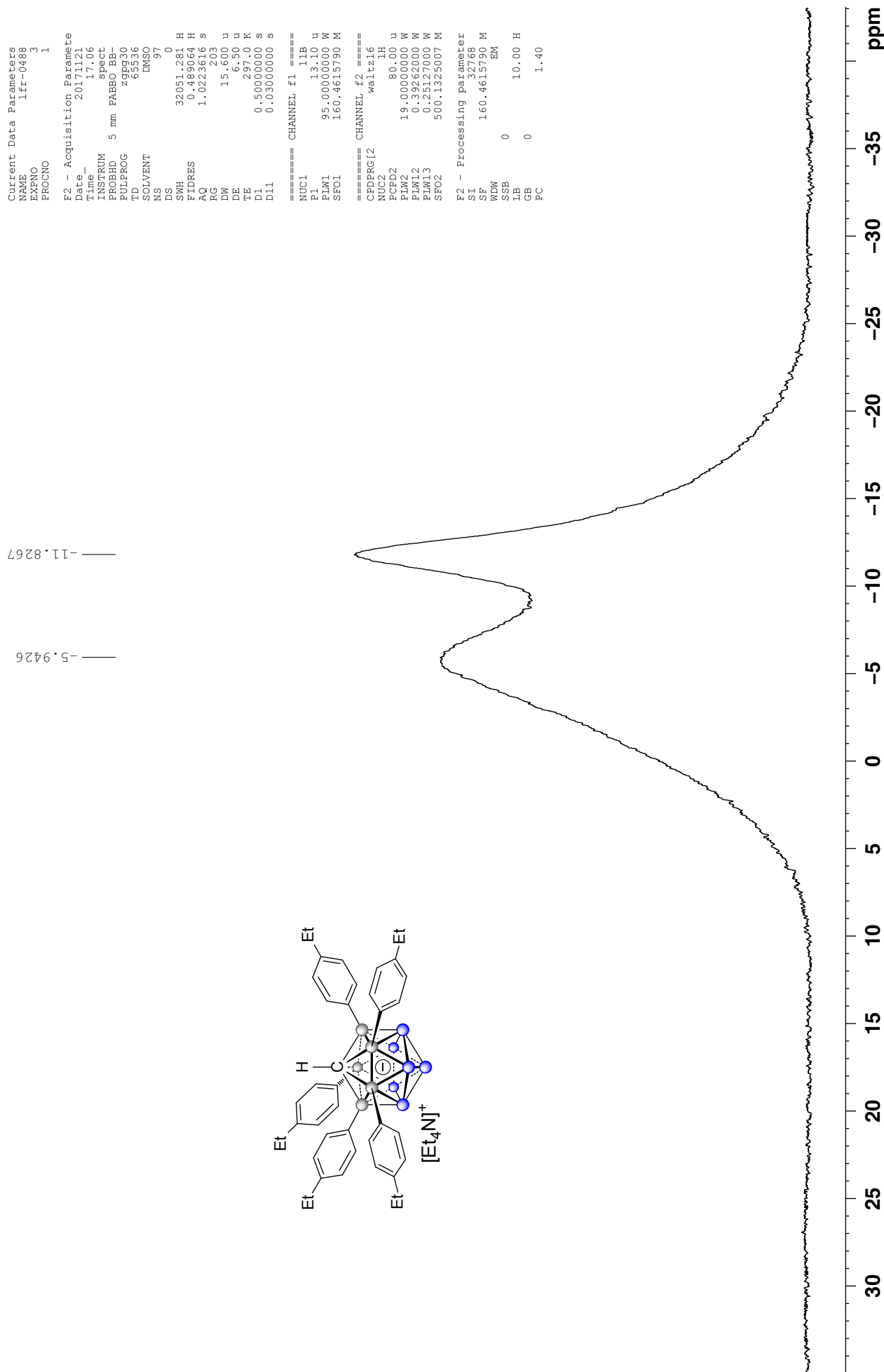
F2 - Acquisition Parameters
Date_     20171121
Time      17.03
INSTRUM   spect
PROBHD    5 mm PABBO-BB-
PULPROG   zg30
TD         64098
SOLVENT   DMSO
NS         146
DS         0
SWH        32051.281 H
FIDRES     0.50036 H
AQ          0.9999288 s
RG          15.203
DE          15.600 u
TE          296.9 K
D1          0.50000000 s

===== CHANNEL f1 =====
NUC1       11B
P1         13.10 u
PLW1       95.0000000 W
SF01       160.4615792 M

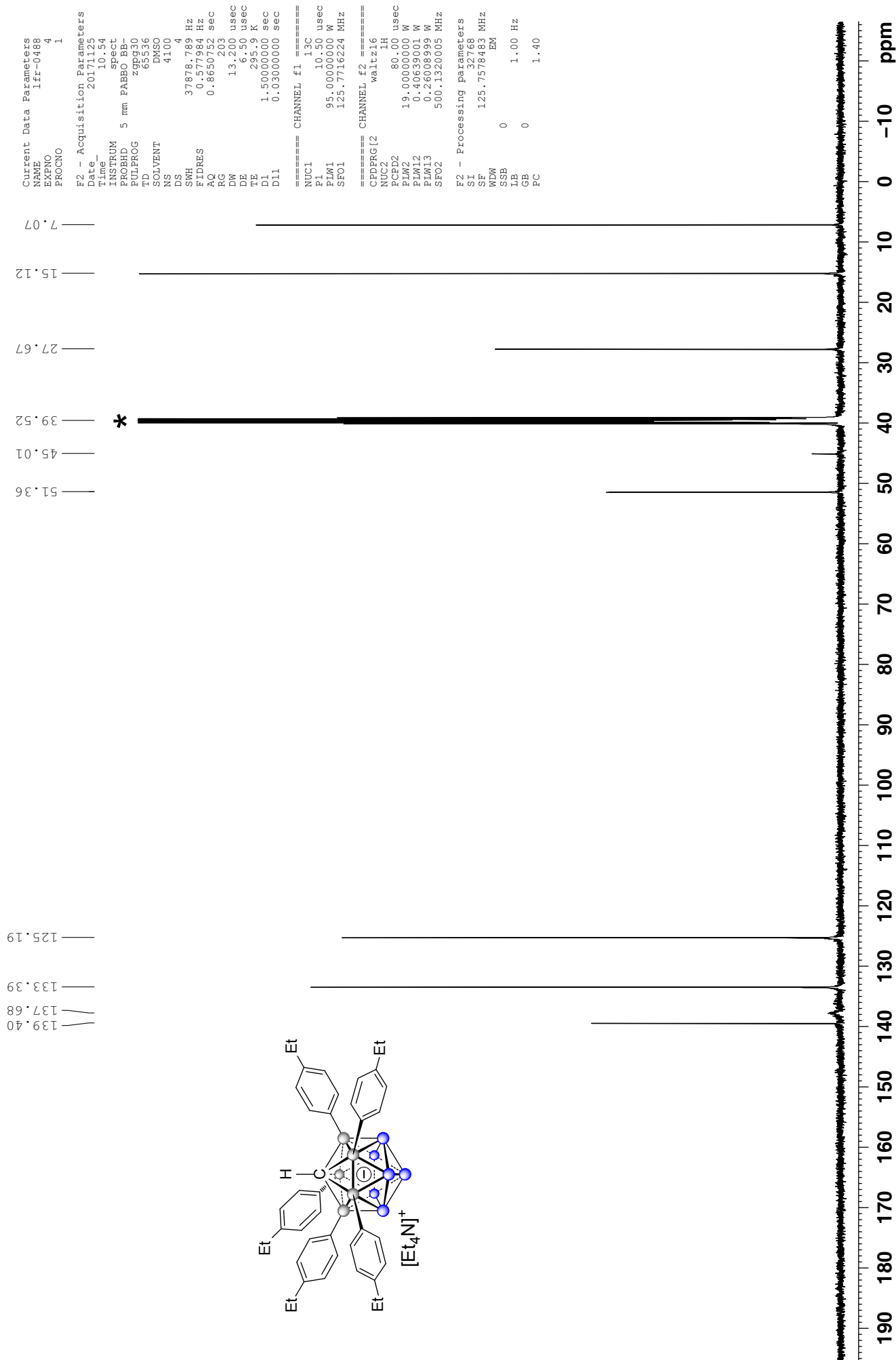
F2 - Processing parameters
SI         32768
SF         160.4615986 M
WDW        EM
SSB        0
LB         10.00 H
GB         0
PC         1.40
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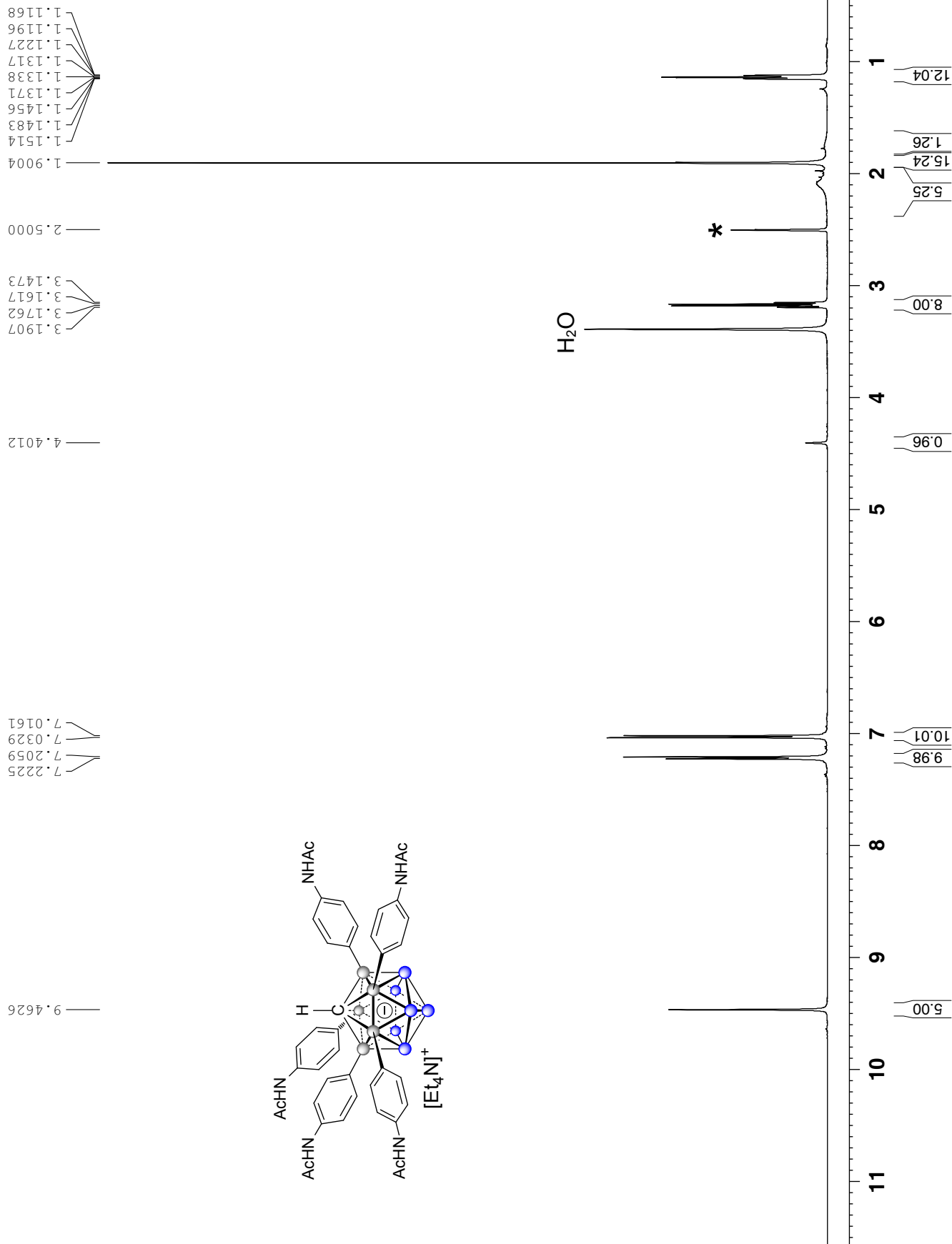
20171121-lfr-0488 [NEt₄][H-CB₁₁H₆-(4-Et-C₆H₄)₅]
 160 MHz, ¹¹B{¹H} NMR, ca. 10 mg dissolved in 0.55 mL dmsO-d₆



20171121-lfr-0488 [NEt₄][H-CB₁₁H₆-(4-Et-C₆H₄)₅]
 126 MHz, ¹³C{¹H} NMR, ca. 10 mg dissolved in 0.55 mL dmsO-d₆*

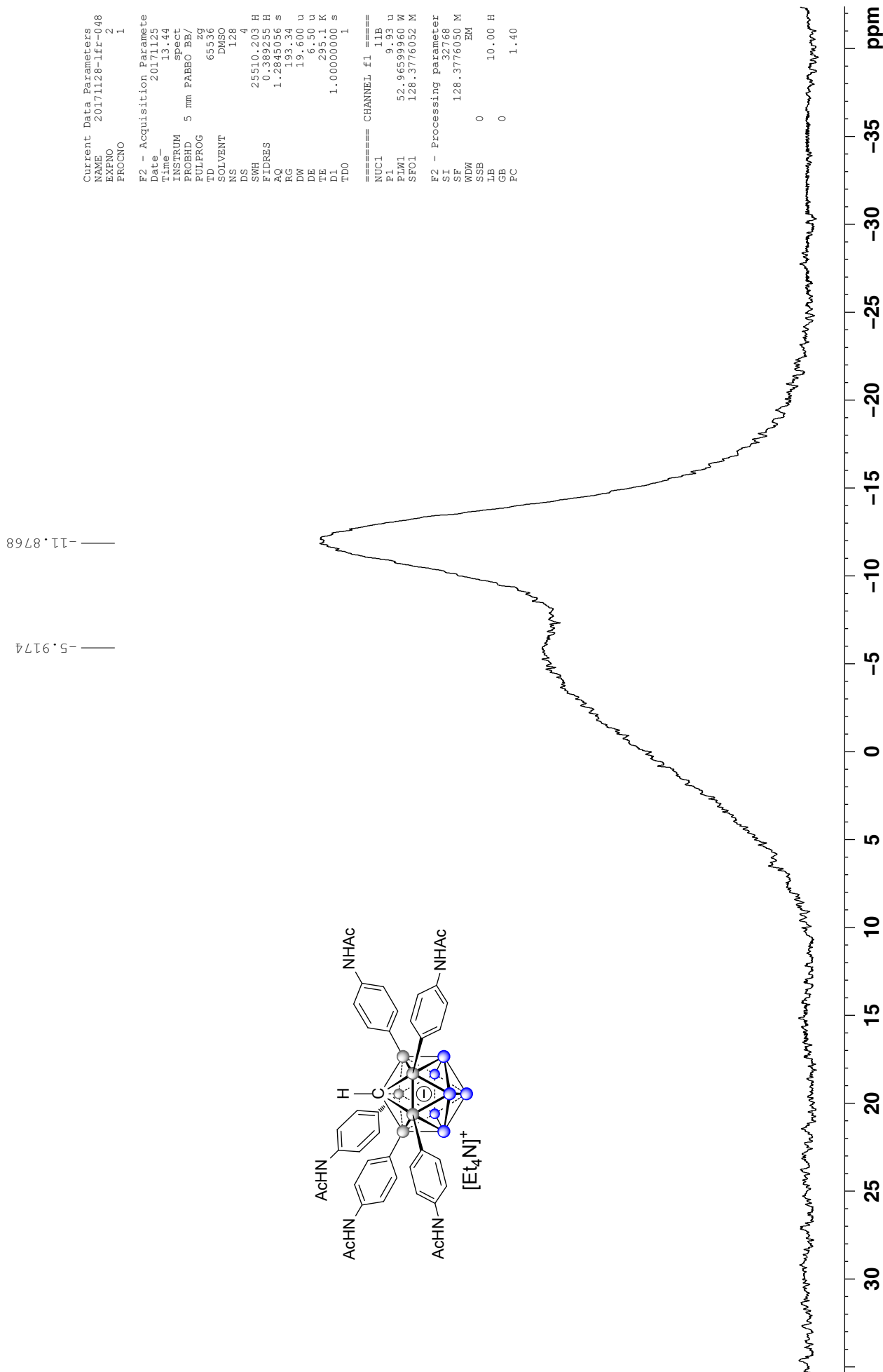


20171128-lfr-0488 [NEt₄][H-CB₁₁H₆-(4-NHAc-C₆H₄)₅]
500 MHz, ¹H{¹¹B} NMR, ca. 20 mg dissolved in 0.55 mL dmsO-d₆*

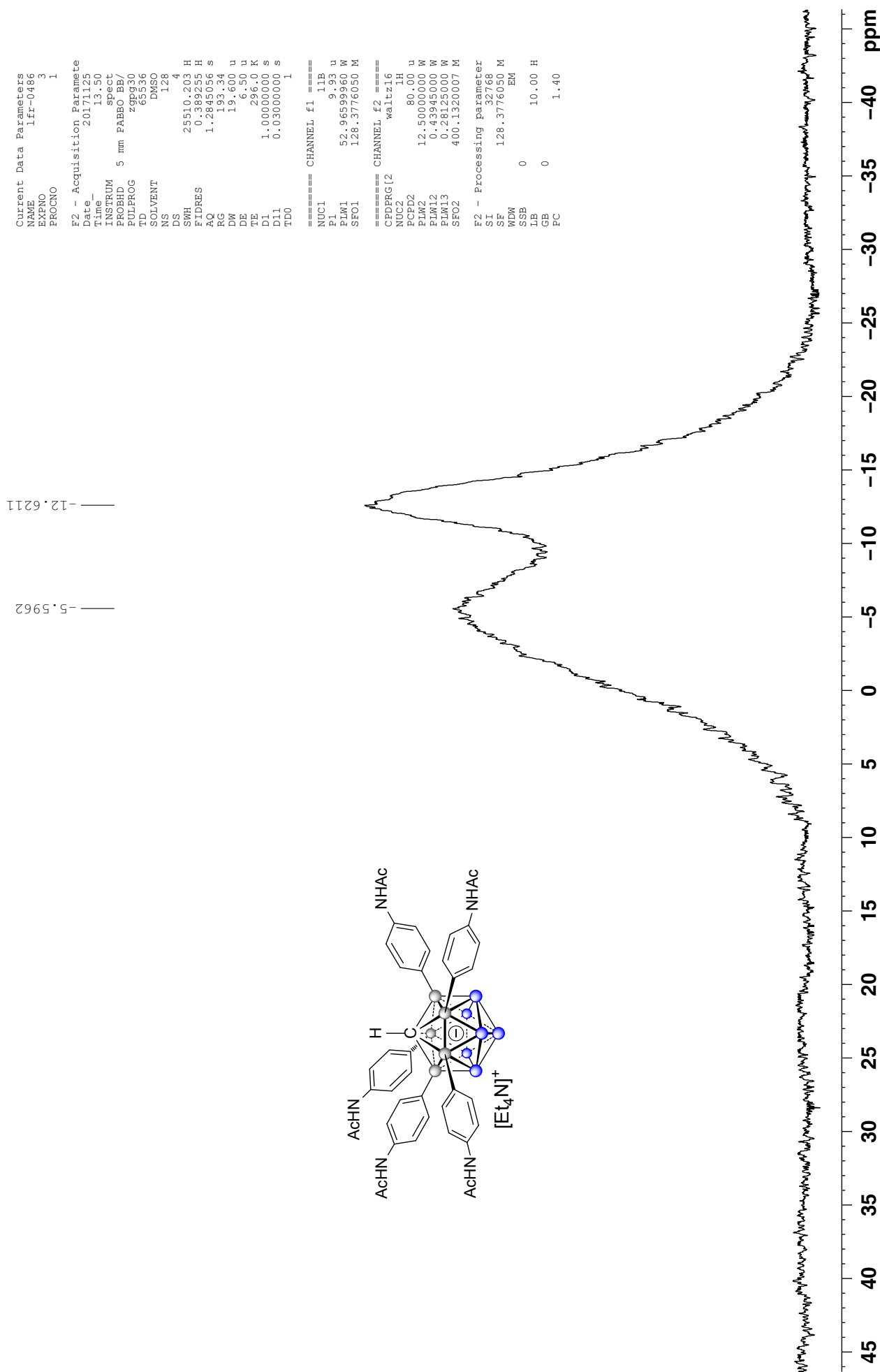


Current Data Parameters
NAME lfr-0486
EXNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171128
Time_ 17.39
INSTRUM spect
PROBHD 5 mm FAPBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 12500.000
FIDRES 0.190735
AQ 2.6214399
RG 114
DW 40.000
DE 6.50
TE 673.1
D1 5.00000000
D11 0.03000000
===== CHANNEL f1 =====
NUC1 1H
P1 11.50
PLW1 19.00000000
SFO1 500.1335009
===== CHANNEL f2 =====
CPDPRG [2
NUC2 11B
PCPD2 100.00
PLW2 95.00000000
PLW12 1.63030005
SFO2 160.4615690
F2 - Processing parameters
SI 65536
SF 500.1297805
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

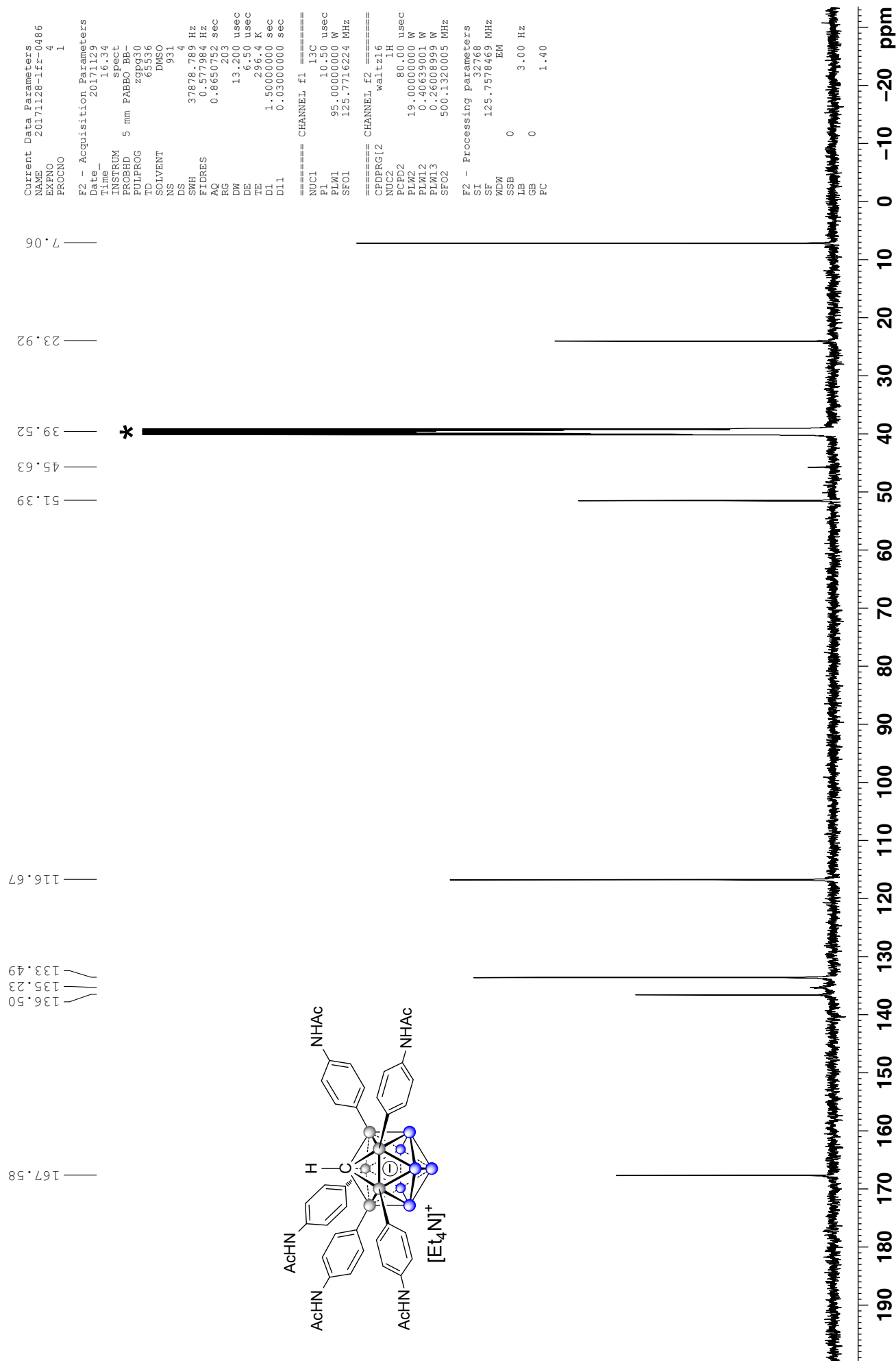
20171128-lfr-0488 [NEt₄][H-CB₁₁H₆-(4-NHAc-C₆H₄)₅]
 160 MHz, ¹¹B NMR, ca. 20 mg dissolved in 0.55 mL dmsO-d₆



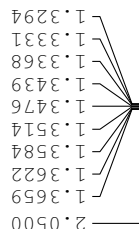
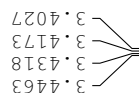
20171128--lfr-0488 [NEt₄][H-CB₁₁H₆-(4-NHAc-C₆H₄)₅]
 160 MHz, ¹H{¹H} NMR, ca. 20 mg dissolved in 0.55 mL dmsO-d₆



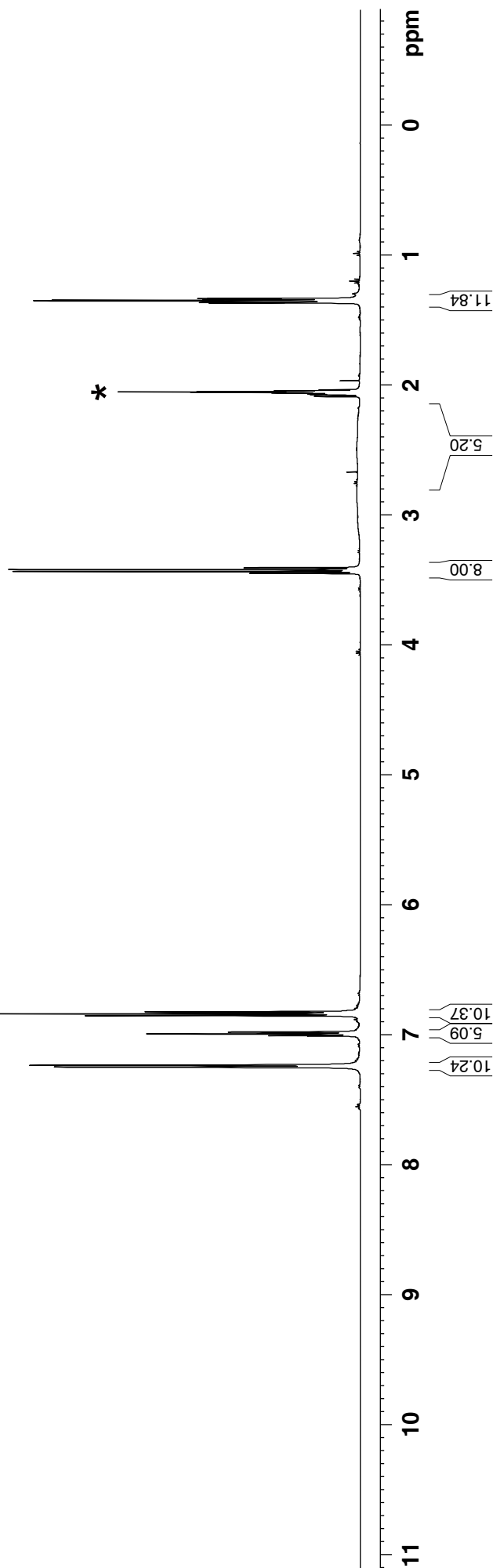
20171128-lfr-0488 [NEt₄][H-CB₁₁H₆-(4-NHAc-C₆H₄)₅]
 126 MHz, ¹³C{¹H} NMR, ca. 20 mg dissolved in 0.55 mL dmsO-d₆*



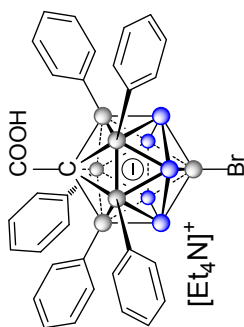
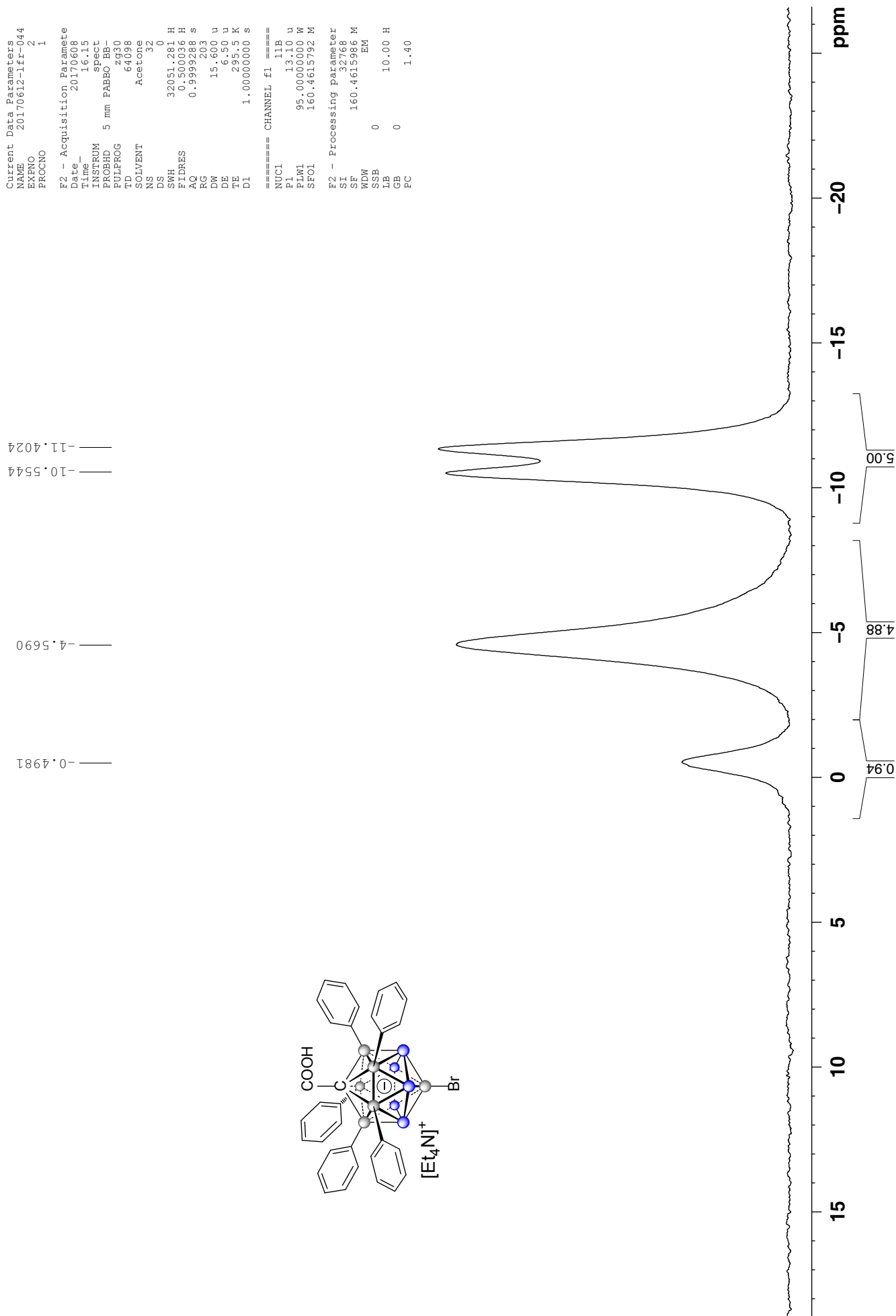
2017608-lfr-0447 [NEt₄][COOH-CB₁₁H₅-(4-CN-C₆H₄)₅-12Br]
500 MHz, ¹H NMR, ca. 26 mg dissolved in 0.55 mL acetone-d₆*



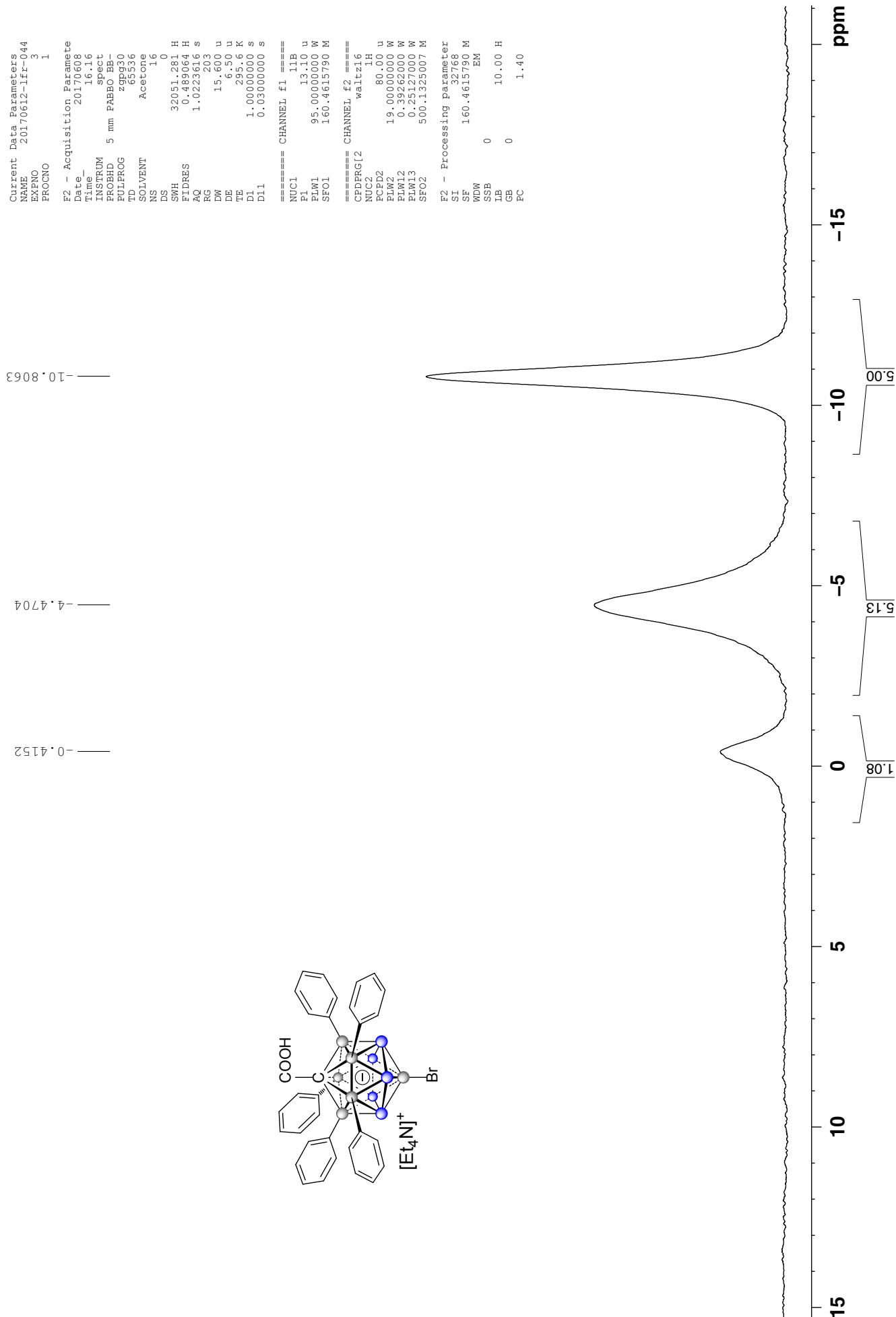
Current Data Parameters
NAME 20170612-lfr-04
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170613
Time_ 2.38
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zg30
TD 65536
SOLVENT acetone
NS 16
DS 2
SWH 15000.000
FIDRES 0.228892
AQ 2.184334
RG 50.8
DE 33.333
TE 296.8
D1 1.00000000
===== CHANNEL f1 =====
NUC1 1H
P1 11.70
PLW1 19.00000000
SFO1 500.1340010
F2 - Processing parameters
SI 65536
SF 500.1300100
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00



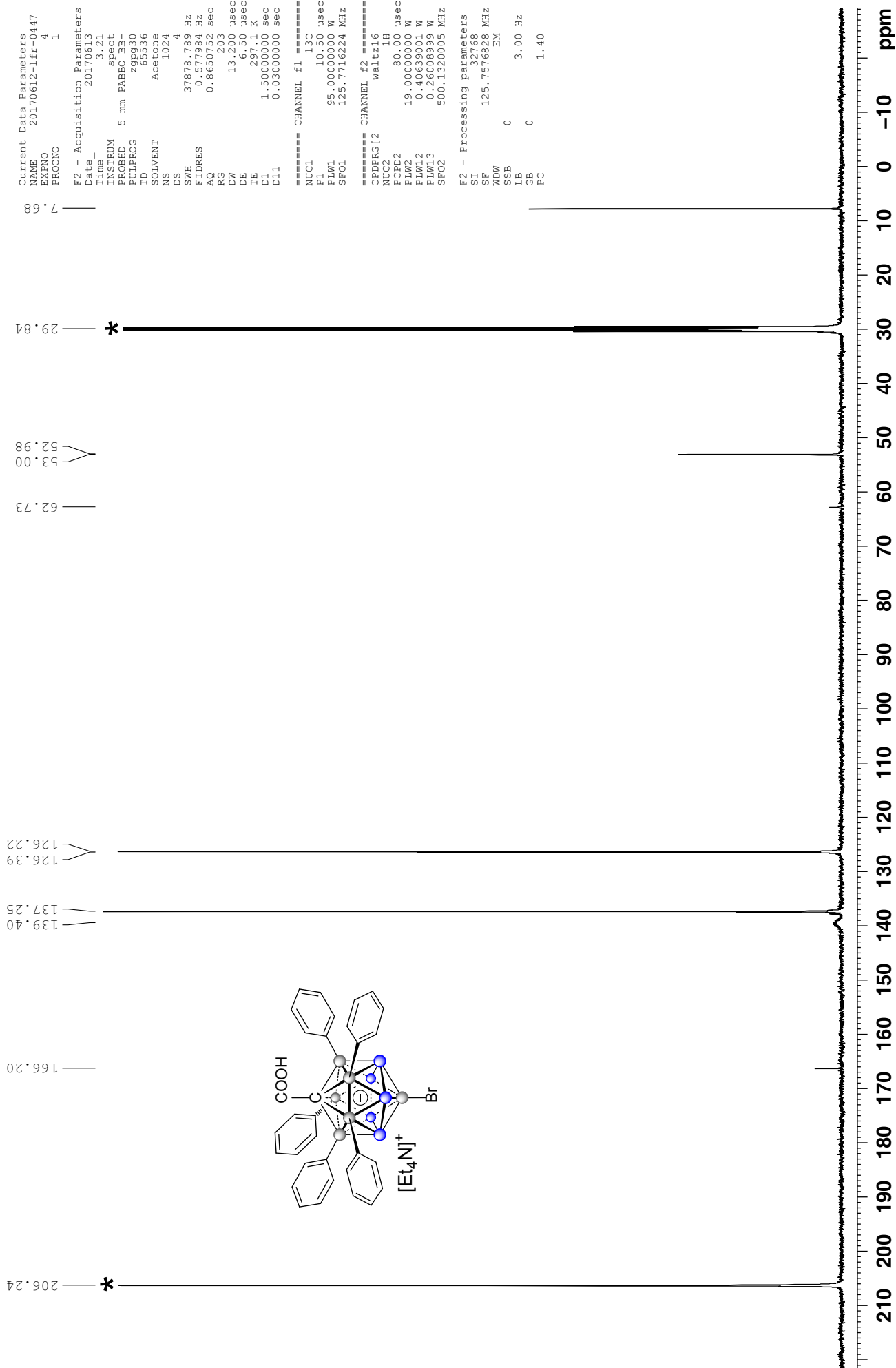
2017608-lfr-0447 [NEt₄][COOH-CB₁₁H₅-(4-CN-C₆H₄)₅-12Br]
160 MHz, ¹¹B NMR, ca. 26 mg dissolved in 0.55 mL acetone-d₆



2017608-lfr-0447 [NEt₄][COOH-CB₁₁H₅-(4-CN-C₆H₄)₅-12Br]
 160 MHz, ¹B{¹H} NMR, ca. 26 mg dissolved in 0.55 mL acetone-d₆



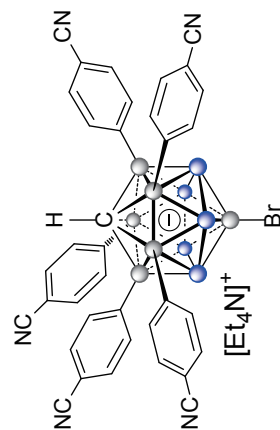
2017608-lfr-0447 [NEt₄][COOH-CB₁₁H₅-(4-CN-C₆H₄)₅-12Br]
 126 MHz, ¹³C{¹H} NMR, ca. 26 mg dissolved in 0.55 mL acetone-d₆*



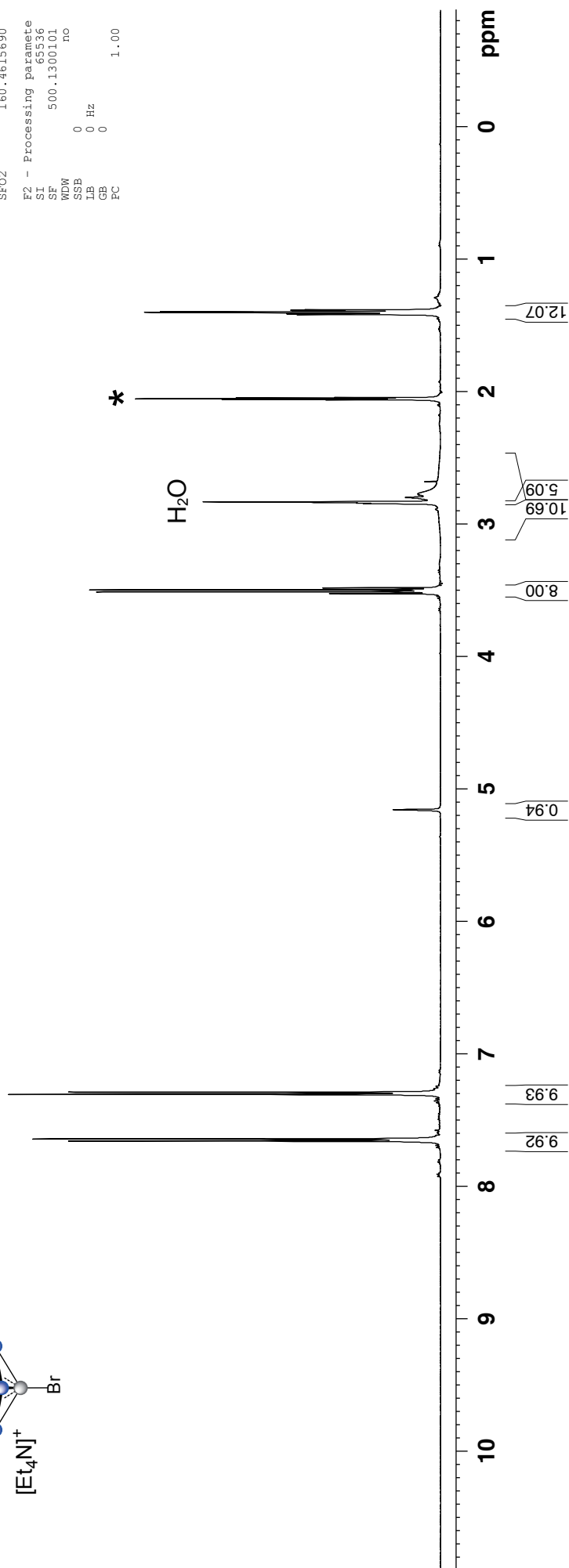
2017608-lfr-0445 [NEt₄][H-CB₁₁H₅-(4-CN-C₆H₄)₅-12Br]
 500 MHz, ¹H{¹B} NMR, ca. 10 mg dissolved in 0.55 mL acetone-d₆*



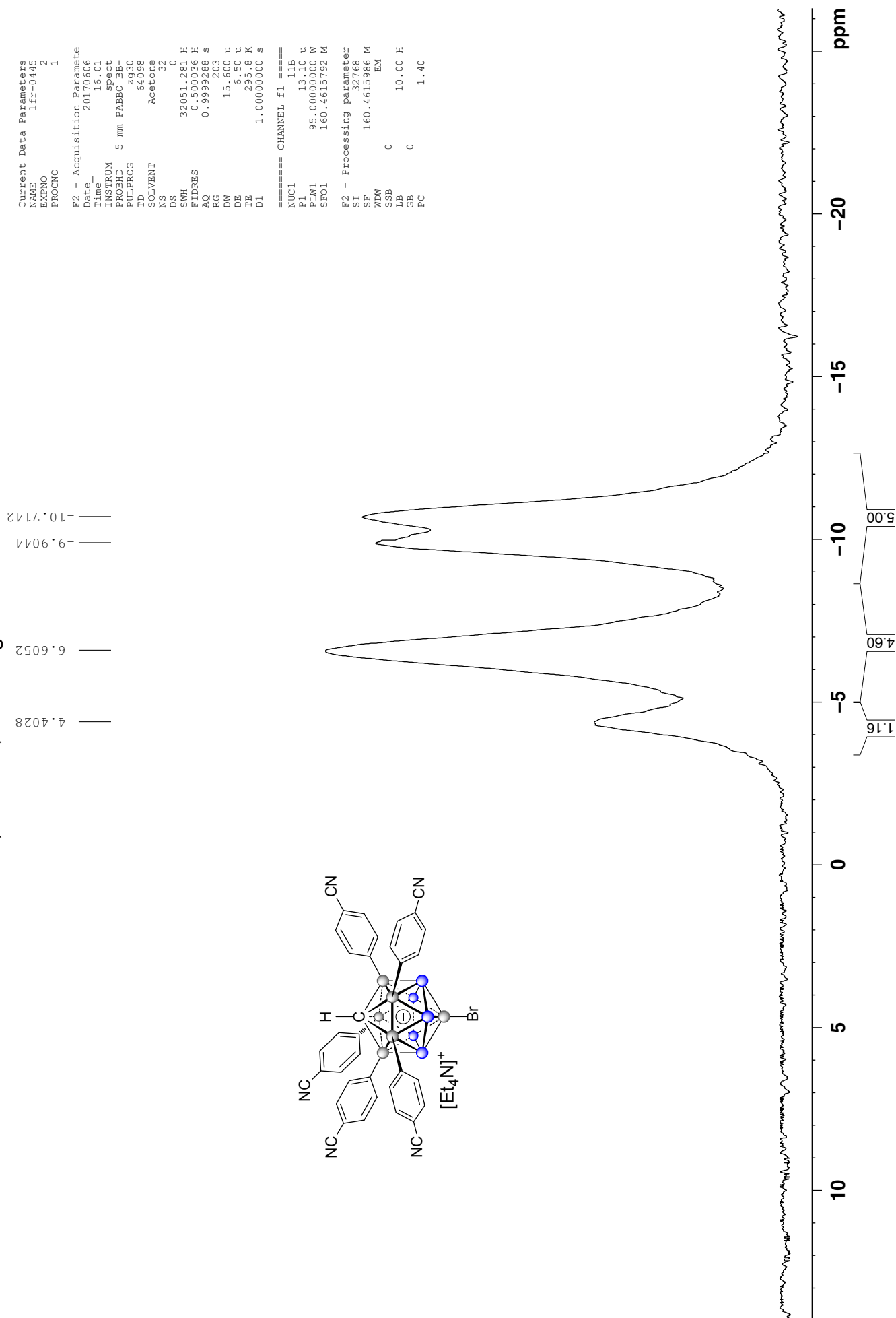
Current Data Parameters
 NAME lfr-0445
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Paramet
 Date_ 20170608
 Time_ 16.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 0
 SWH 14097.744
 FIDRES 0.215115
 AQ 2.3243434
 RG 101
 DW 35.467
 DE 6.50
 TE 295.6
 D1 5.00000000
 D11 0.03000000



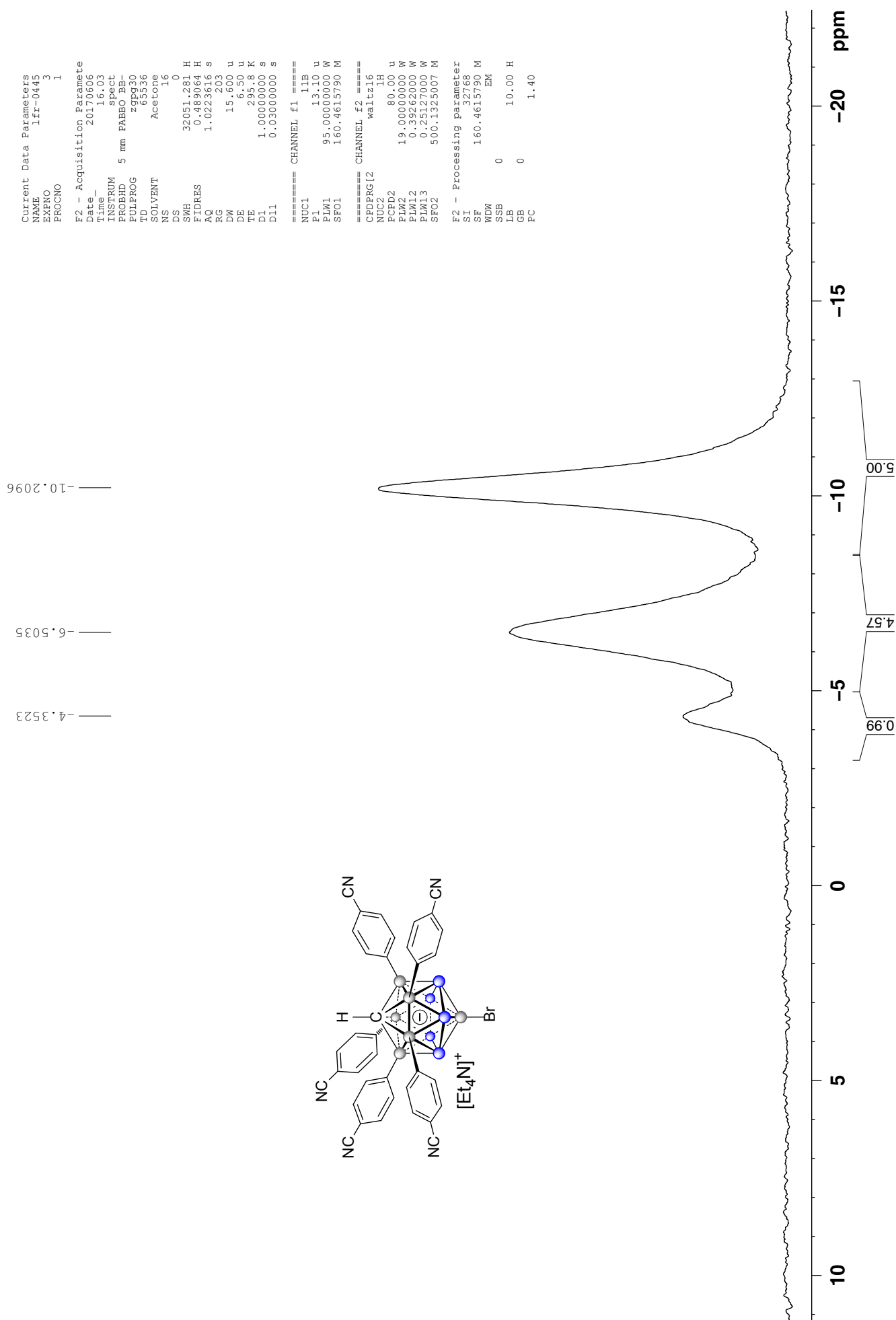
S306



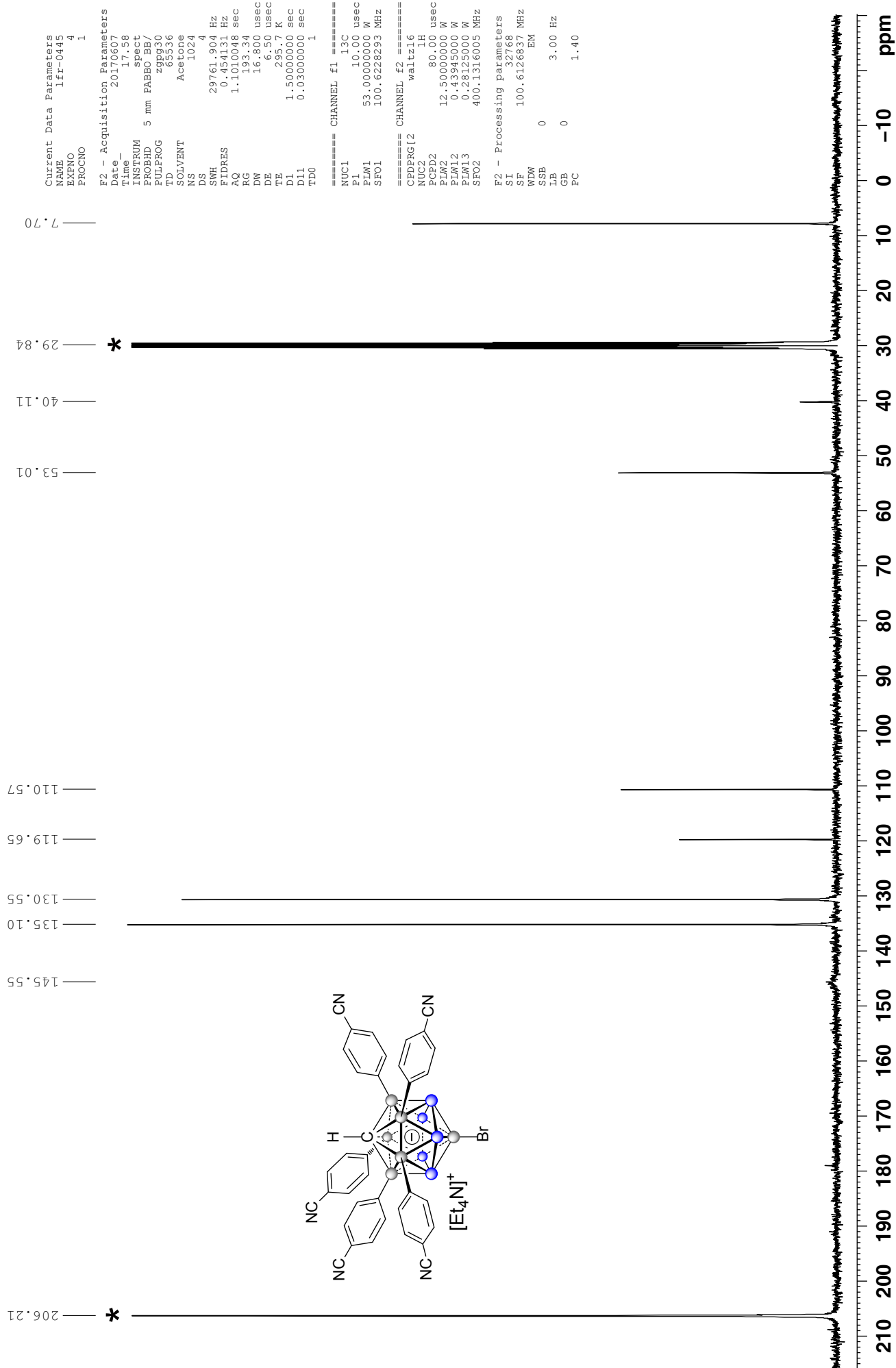
2017608-lfr-0445 [NEt₄][H-CB₁₁H₆-(4-CN-C₆H₄)₅-12Br]
 160 MHz, ¹¹B NMR, ca. 10 mg dissolved in 0.55 mL acetone-d₆



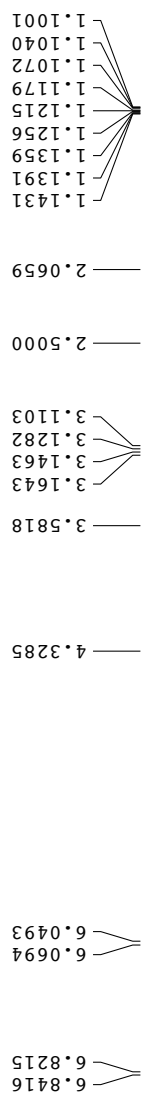
2017608--lfr-0445 [NEt₄][H-CB₁₁H₆-(4-CN-C₆H₄)₅-12Br]
 160 MHz, ¹¹B{¹H} NMR, ca. 10 mg dissolved in 0.55 mL acetone-d₆



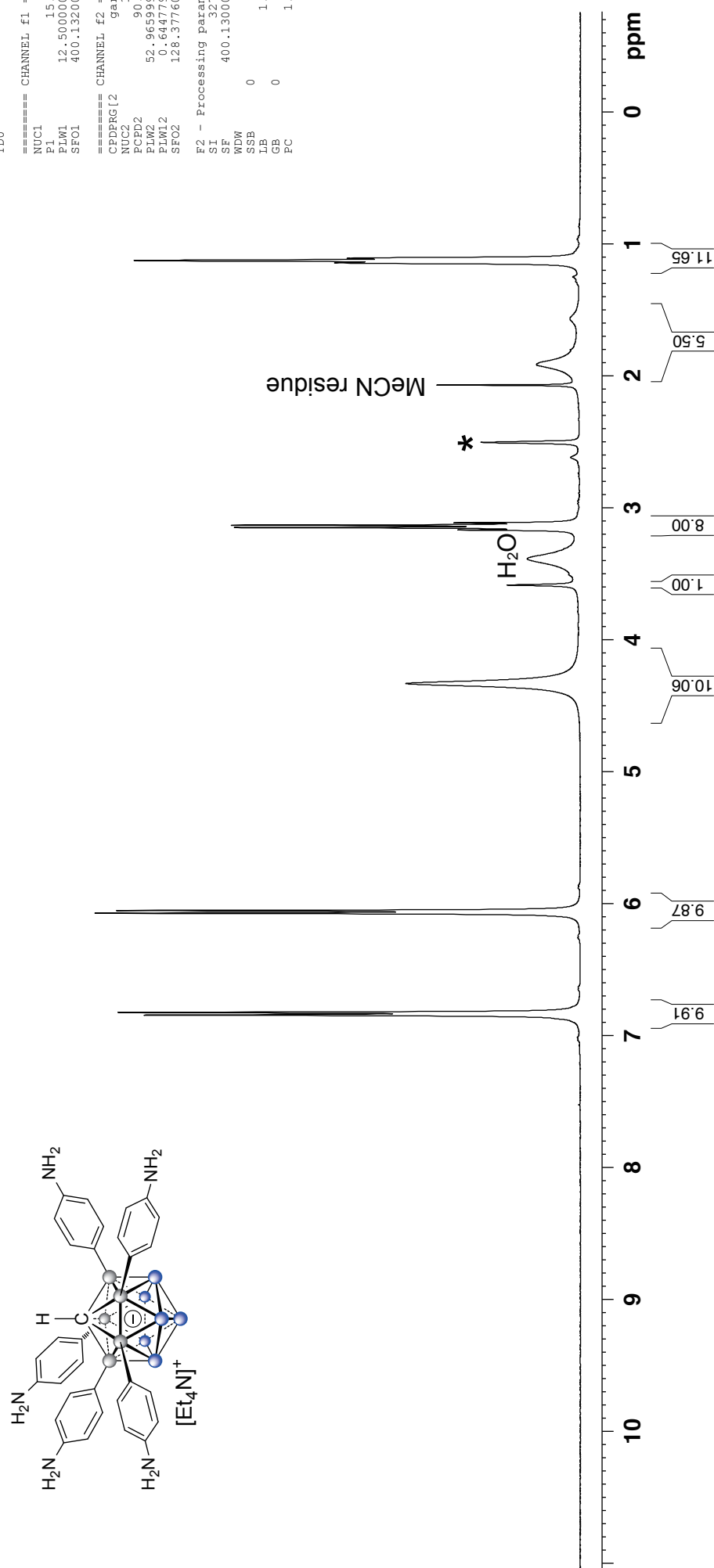
2017608-lfr-0445 [NEt₄][H-CB₁₁H₆-(4-CN-C₆H₄)₅-12Br]
 101 MHz, ¹³C{¹H} NMR, ca. 10 mg dissolved in 0.55 mL acetone-d₆*



20171228-lfr-0500 [NEt₄][H-CB₁₁H₆-(4-NH₂-C₆H₄)₅]
 400 MHz, ¹H{¹B} NMR, ca. 17 mg dissolved in 0.55 mL dms^o-d₆*

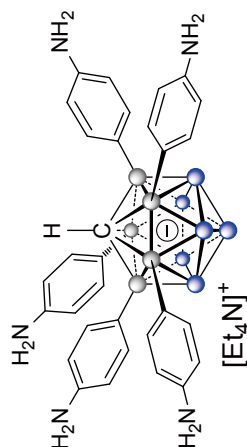


Current Data Parameters
 NAME lfr-0500
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20171229
 Time 10.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgig30
 TD 16384
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 8012.820
 FIDRES 0.489064
 AQ 1.0223616
 RG 107.6
 DW 62.400
 DE 6.50
 TE 294.5
 D1 1.00000000
 D11 0.03000000
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00
 PLW1 12.50000000
 SFO1 400.1320007
 ===== CHANNEL f2 =====
 CPDPRG2 garp4
 NUC2 11B
 P1 90.00
 PLW2 52.96599960
 PLW12 0.64477998
 SFO2 128.3776050
 F2 - Processing parameters
 SI 32768
 SF 400.1300037
 WDW EM
 SSB 0
 LB 1.00
 GB 0
 PC 1.40



20171228-lfr-0500 [NEt₄][H-CB₁₁H₆-(4-NH₂-C₆H₄)₅]
 128 MHz, ¹¹B NMR, ca. 17 mg dissolved in 0.55 mL dmsd-d₆

— -4.9781
 — -13.0627

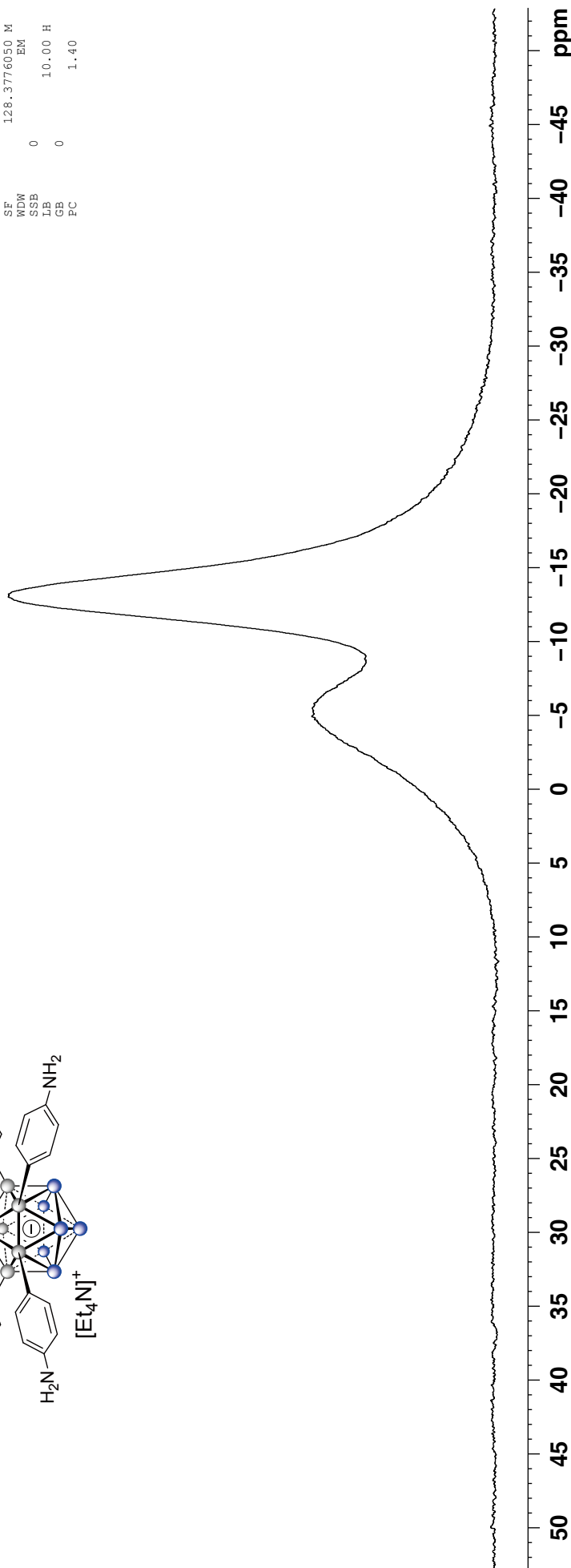


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Current Data Parameters
NAME      lfr-0500
EXPNO     2
PROCNO    1

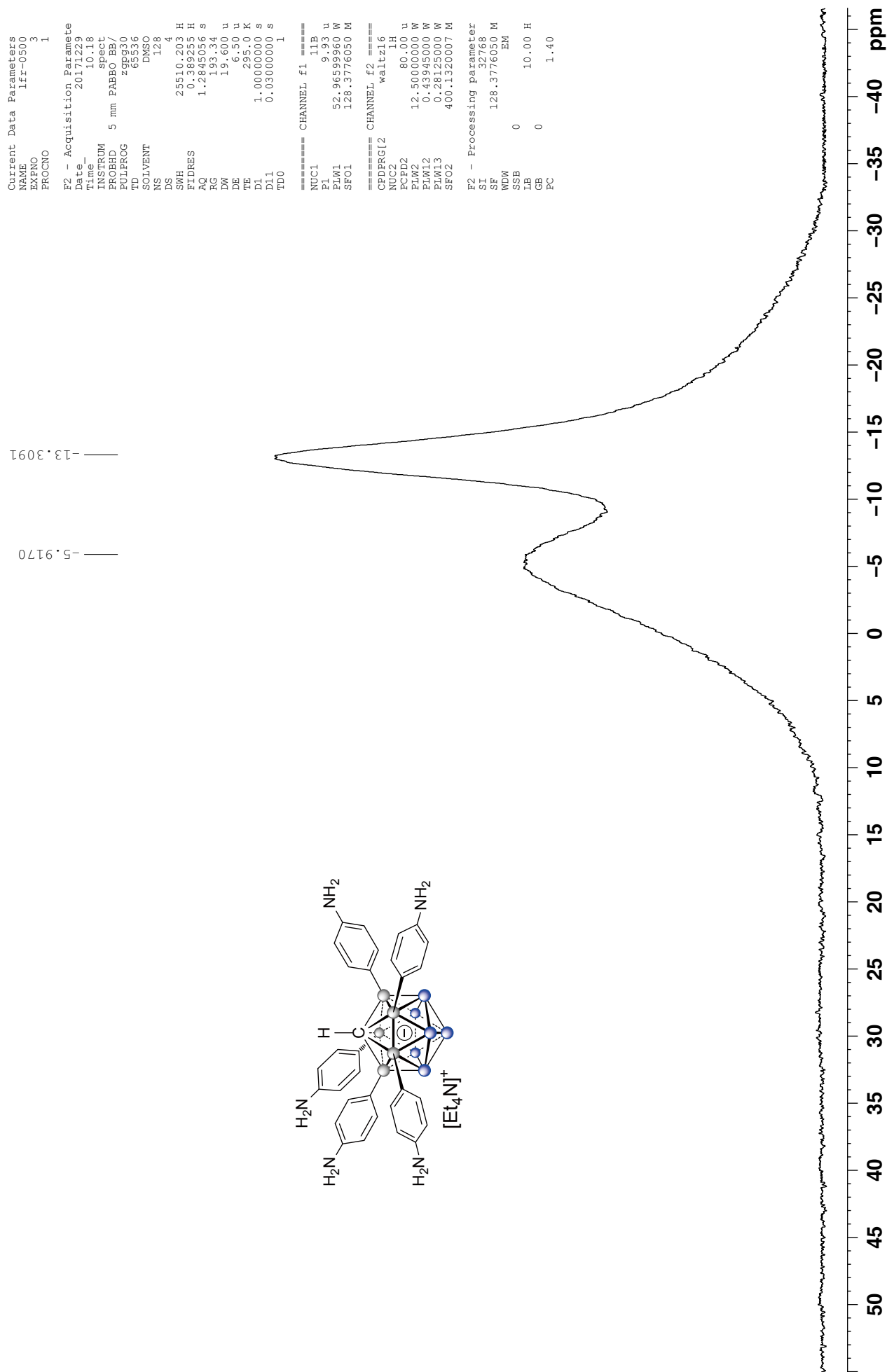
F2 - Acquisition Parameters
Date_     20171229
Time      10.12
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg
TD         65536
SOLVENT   DMSO
NS         128
DS         4
SWH        25510.203 H
FIDRES     0.389255 H
AQ         1.285056 S
RG         193.34
DW         13.600 u
DE         6.50 u
TE         294.2 K
D1         1.0000000 s
TD0        1

===== CHANNEL f1 =====
NUC1       11B
FL1        9.93 u
FLW1       52.9659960 W
SFO1       128.3776052 M

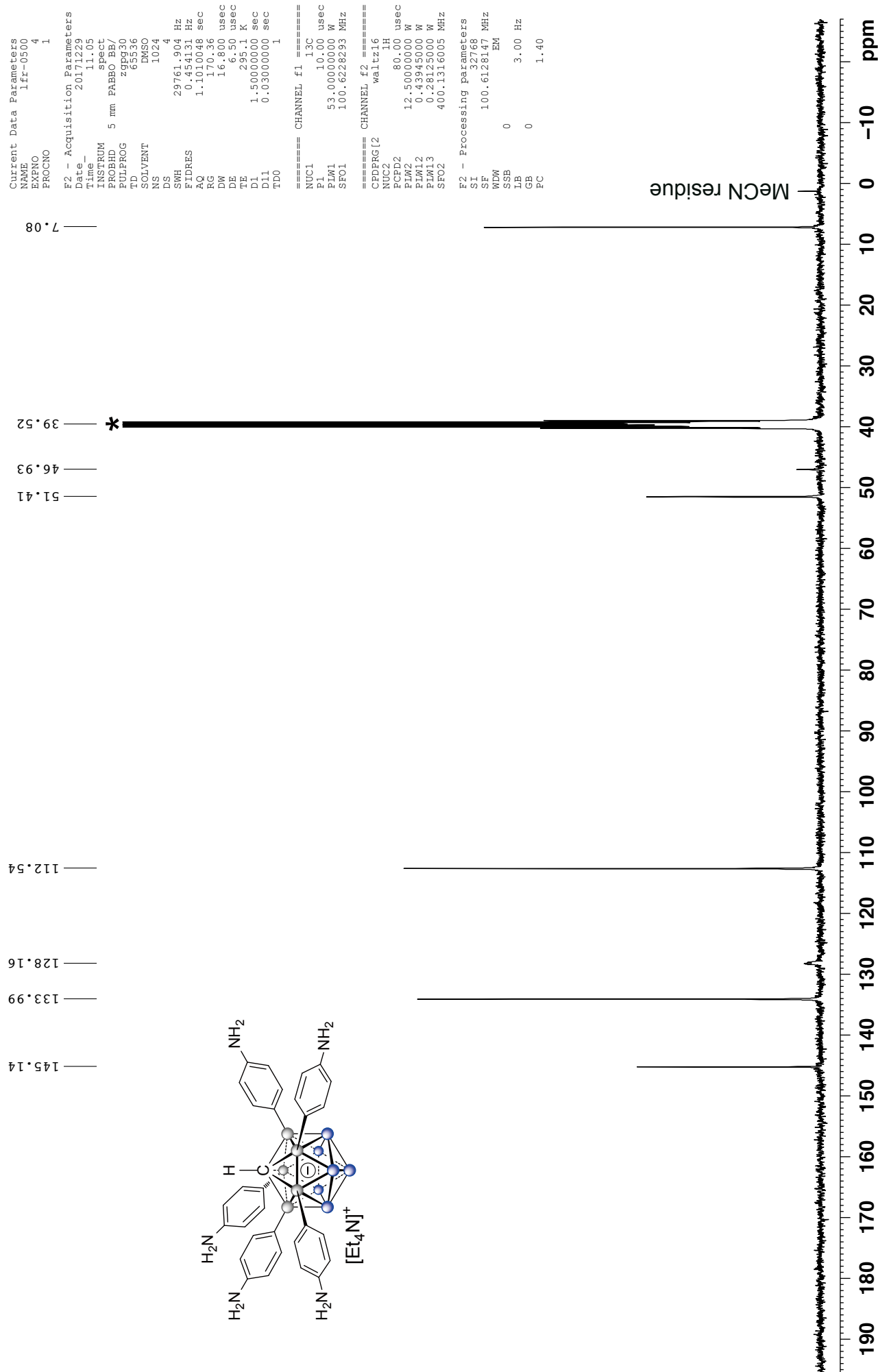
F2 - Processing parameters
SI         32768
SF         128.3776050 M
WDW        EM
SSB        0
LB         0
GB         0
PC         1.40
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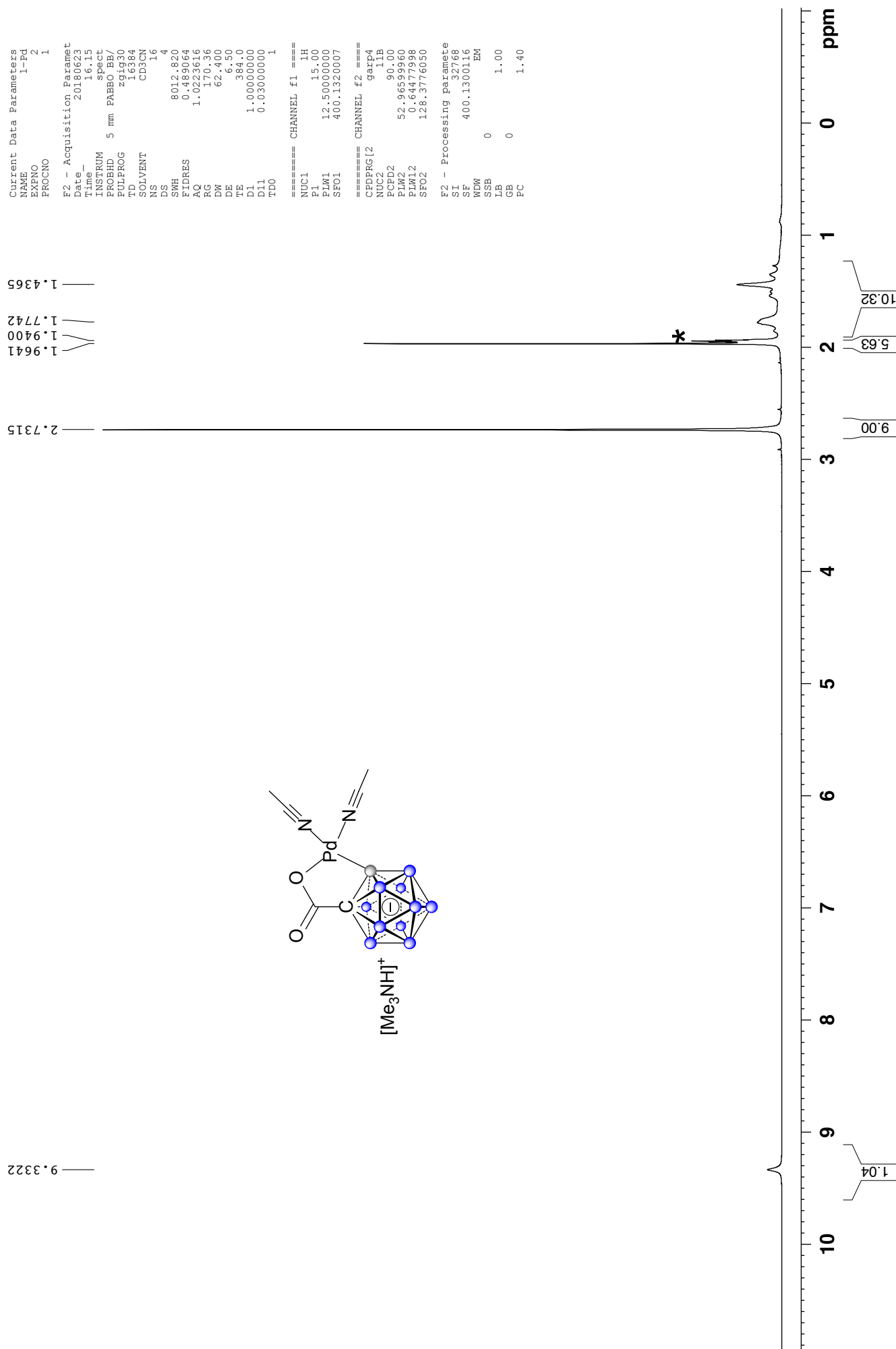
20171228-lfr-0500 [NEt₄][H-CB₁₁H₆-(4-NH₂-C₆H₄)₅]
 128 MHz, ¹H{¹H} NMR, ca. 17 mg dissolved in 0.55 mL dmsO-d6



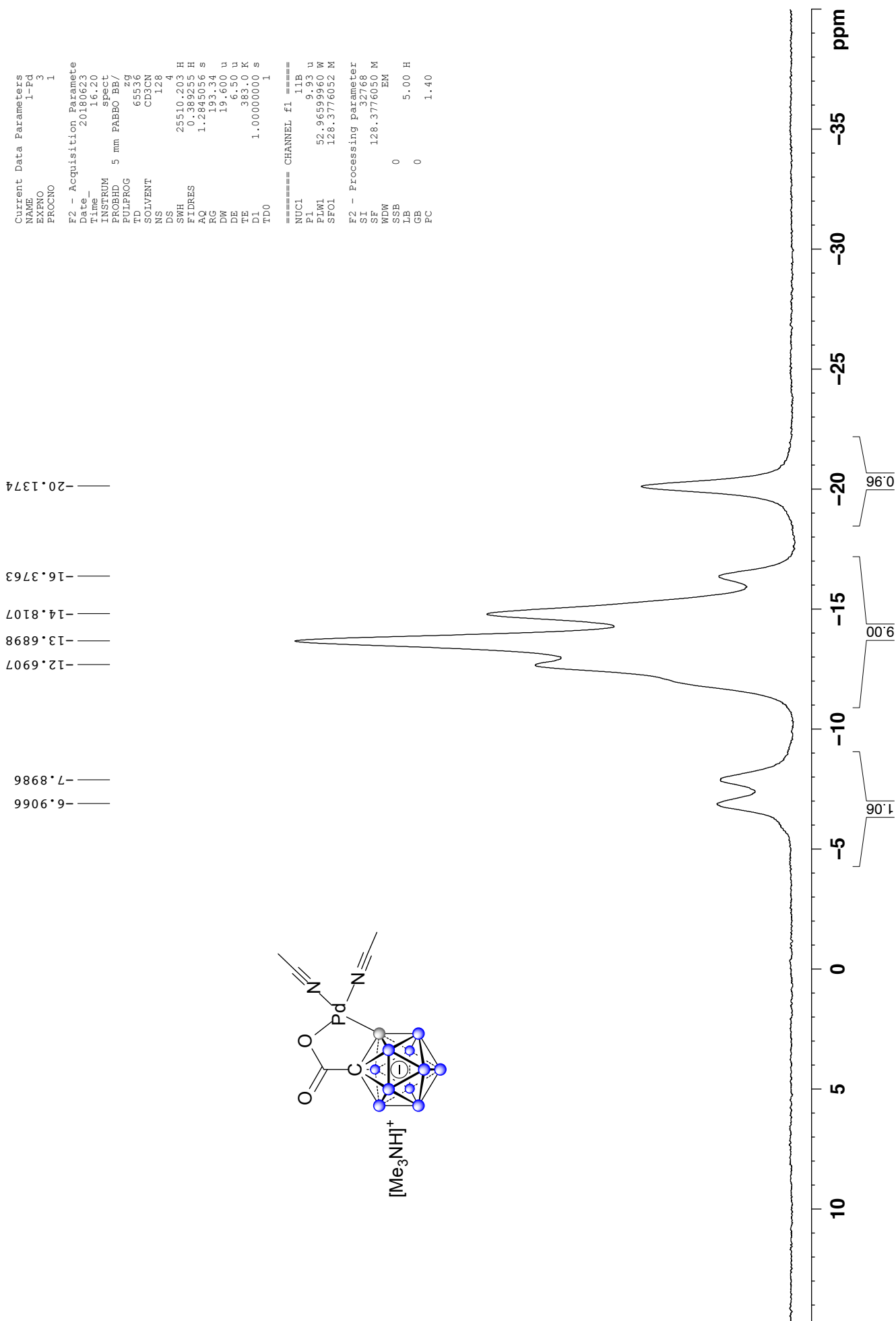
20171228-lfr-0500 [NEt₄][H-CB₁₁H₆-(4-NH₂-C₆H₄)₅]
 101 MHz, ¹³C{¹H} NMR, ca. 17 mg dissolved in 0.55 mL dmsO-d₆*



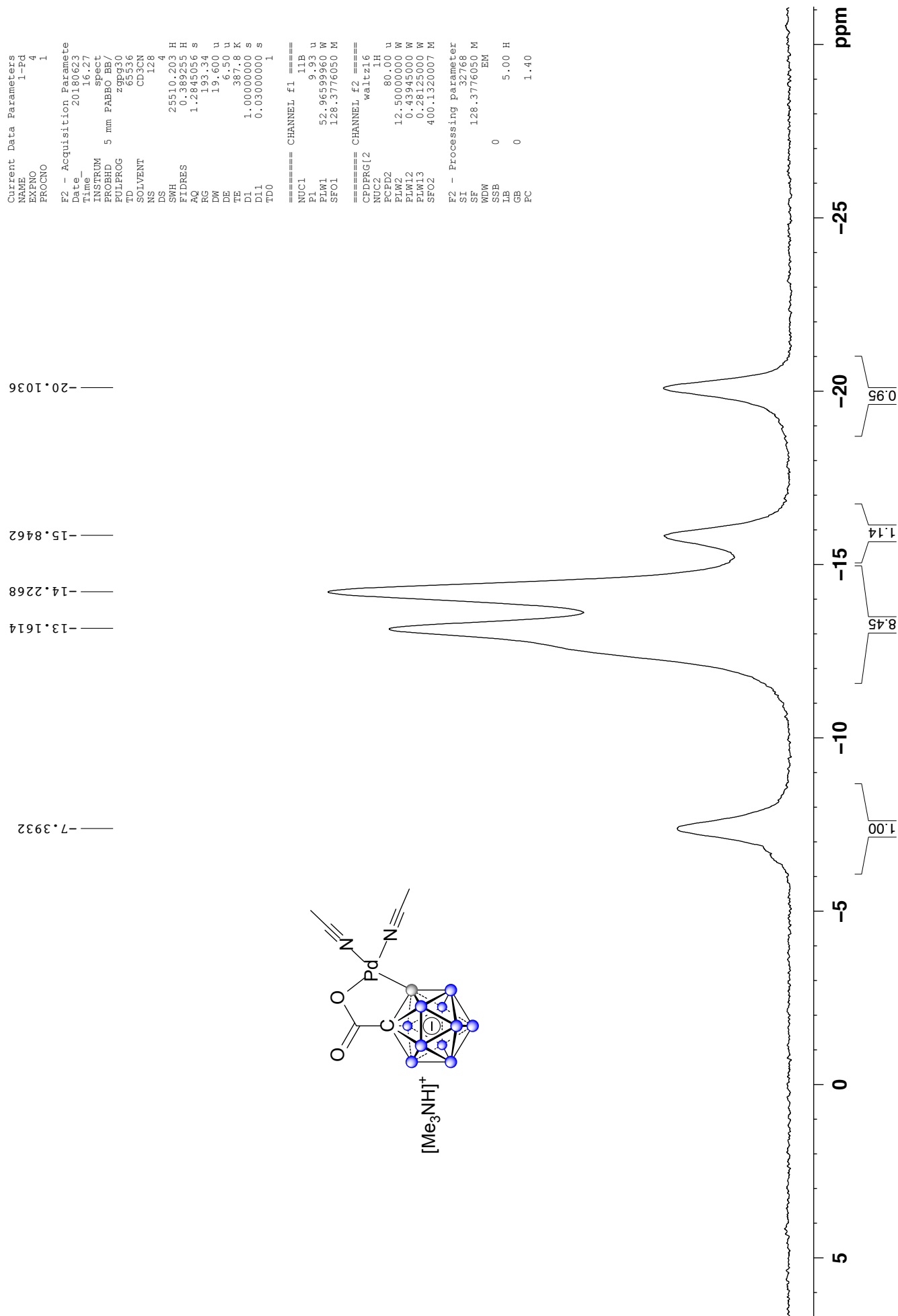
20180622-1-Pd, NMe₃H⁺[COOPdCB₁₁H₁₀]
 400 MHz, ¹H{¹B} NMR, ca. 30 mg dissolved in 0.6 mL acetonitrile-d₃*



20180622-1-Pd, NMe₃H⁺[COOPdCB₁₁H₁₀]
 128 MHz, ¹¹B NMR, ca. 30 mg dissolved in 0.6 mL acetonitrile-d₃



20180622-1-Pd, NMe₃H⁺[COOPdCB₁₁H₁₀]
 128 MHz, ¹B{¹H} NMR, ca. 30 mg dissolved in 0.6 mL acetonitrile-d₃



20180622-1-Pd, NMe₃H⁺[COOPdCB₁₁H₁₀]
 101 MHz, ¹³C{¹H} NMR, ca. 30 mg dissolved in 0.6 mL acetonitrile-d₃*

