

Supplementary Information for

Monocarborane-stabilized iodonium enable for regioselective B12-iodination of [CB₁₁H₁₂][−]

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I General Information

Chemicals

If not otherwise specified, reagents and organic solvents were commercially available from the company Energy (China) and used without further purification. Acetone- d_6 and DMSO- d_6 were purchased from Cambridge Isotope Laboratories. [Cs][1-R-CB₁₁H₁₁] (R = 4-pyridyl, 2-F-4-pyridyl, 2-Cl-4-pyridyl, COOH), [Cs][12-I-CB₁₁H₁₁], [Cs][7,12-2I-CB₁₁H₁₀] and [Cs][7,8,9,10,11,12-6X-CB₁₁H₆] (X=Cl, Br, I) were prepared according to the literature.^[1-5]

Reaction Conditions

Glassware for air-sensitive reactions was dried at 200 °C for at least 6 h and allowed to cool in a vacuum.

Air-sensitive reactions were operated in a glovebox under a nitrogen atmosphere with O₂, H₂O < 1 ppm.

Characterization

1) 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 the temperature indicated. Data are reported as follows: Chemical shift in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, etc.), coupling constant *J* in Hz, integration and interpretation (where applicable). Signals were referenced against solvent peaks (¹H: residual CHD₂C(O)CD₃ = 2.05 ppm, residual CHD₂S(O)CD₃ = 2.50 ppm; ¹³C{¹H}: CD₃C(O)CD₃ = 29.84 ppm, CD₃S(O)CD₃ = 39.52 ppm.). ¹¹B and ¹¹B{¹H} NMR spectra were calibrated against external BF₃·Et₂O = 0 ppm (BF₃·Et₂O capillary in C₆D₆).

Baseline correction for ¹¹B and ¹¹B{¹H} NMR spectra was carried out using the baseline correction function of the software TopSpin 4.3.0.

Additional remark about the NMR spectra:

a) 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. ^[6]

2) Low-resolution ESI-MS data were recorded on an Advion Expression CMS instrument, and high-resolution MS data were recorded using a Shimadzu IT-TOF MS instrument. The plots with a large m/z range demonstrate bulk purity. The zoomed-in plots show the observed isotopic pattern from the HRMS measurements.

3) Elemental analysis was carried out on a Vario MICRO Element Analyzer instrument.

4) Single-crystal X-ray diffraction studies were performed on a Bruker D8 Venture instrument using MoK- α radiation.

II Experimental Section

Preparation of [I(4-RPy)₂][BF₄]¹⁷

A 25 mL glass flask equipped with a magnetic stir bar was charged with AgBF₄ (194.7 mg, 1.0 mmol, 1.0 equiv) and pyridine (2.0 mmol, 2.0 equiv), then sealed with a rubber septum. Dry CH₂Cl₂ (5.0 mL) was added via syringe at room temperature under a nitrogen atmosphere. The resulting mixture was stirred for 10 min until all solids dissolved. Separately, I₂ (254 mg, 1.0 mmol) was dissolved in dry CH₂Cl₂ (5.0 mL) in a sealed vial under nitrogen. This I₂ solution was added to the reaction mixture, which was stirred at 25 °C for 1 h. The resulting turbid solution was filtered into a 50 mL one-necked round-bottom flask, and the solvent was partially removed by rotary evaporation to a final volume of ~2 mL. Dry *n*-hexane (15 mL) was added to precipitate the product. The resulting white solid was collected by filtration through a glass frit and washed three times with a mixture of CH₂Cl₂ (1.0 mL) and *n*-hexane (8.0 mL). The product was dried under vacuum at 25 °C for 24 h to afford [I(4-RPy)₂][BF₄] as a white solid.

General procedure for the preparation of monocarborane-stabilized iodonium salts

A dry 8 mL glass vial, equipped with a magnetic stir bar, was charged with Cesium salt of monocarborane anion (0.05 mmol, 1 equiv). CH₂Cl₂ (2.0 mL) and CH₃CN (0.5 mL) were then added, and the mixture was sonicated until the solid dissolved completely. Separately, [I(4-RPy)₂][BF₄] (0.0525 mmol, 1.05 equiv) was dissolved in CH₂Cl₂ (2.0 mL), and the resulting solution was added to the monocarborane solution. The resulting turbid mixture was stirred at 25 °C for 1 h. After filtration into an 8 mL glass vial, diethyl ether (2.0 mL) was added. Slow evaporation affords colorless crystals of the monocarborane-stabilized iodonium salts in 88-96% yield.

General procedure for the preparation of 1-pyridyl monocarboranes (**7a-7c**)^[1]

A dry 100 mL Schlenk flask equipped with a magnetic stir bar was charged with $[\text{NMe}_3\text{H}][\text{CB}_{11}\text{H}_{12}]$ (203 mg, 1.00 mmol, 1 equiv) and capped with a rubber septum. Anhydrous THF (20 mL) was added, and the resulting solution was stirred at 25 °C for 5 min. A solution of *n*-BuLi (1.60 M in Hexane, 2.0 mL, 3.2 mmol, 3.2 equiv) was added dropwise via a syringe over 5 min. After 1 h of stirring at 25 °C, a yellow solution was obtained. The reaction mixture was cooled to 0 °C in an ice bath, and CuI (209.5 mg, 1.10 mmol, 1.10 equiv) was added to the flask. The ice-bath was then removed, and the reaction was stirred for an additional 1 h at 25 °C to afford a green solution. A solution of $\text{Pd}(\text{OAc})_2$ (22.5 mg, 0.10 mmol, 0.10 equiv), tris(*o*-methoxyphenyl)phosphine (70.5 mg, 0.20 mmol, 0.20 equiv) and iodopyridine (1.30 mmol, 1.30 equiv) in anhydrous THF (8 mL) was added to the reaction mixture at 0 °C. The mixture was stirred at 25 °C for 24 h. Water (5 mL) was slowly added, and THF was removed using a rotary evaporator. The residue was treated with aqueous HCl (1.0 M, 5 mL, 5 mmol) and extracted with diethyl ether (3 x 40 mL). The combined organic extracts were filtered into a 200 mL one-necked round-bottom flask and concentrated using a rotary evaporator. The residue was dissolved in aqueous NaOH solution (1.0 M, 6 mL) and filtered through a pad of celite. The clear, colorless filtrate was acidified with aqueous HCl (1.0 M, 7 mL) to give white precipitate, which was collected by filtration. The solid was transferred to a 20 mL vial, dissolved in aqueous NaOH (1.0 M, 8 mL), and treated with an aqueous CsCl solution (202 mg in 4 mL H_2O). The resulting white precipitates were collected by filtration and dried under vacuum at 60 °C to give compound **7a-7c** in 75-80% yield.

General procedure for the preparation of B(12)-iodine monocarboranes

In a glovebox, A dry 4 mL glass vial, equipped with a magnetic stir bar, was charged with $[\text{Cs}][1\text{-R-CB}_{11}\text{H}_{11}]$ (R=H, 4-pyridyl, 2-F-4-pyridyl, 2-Cl-4-pyridyl, COOH) (0.1 mmol, 1 equiv) and $[\text{I}(4\text{-NMe}_2\text{Py})_2][12\text{-I-CB}_{11}\text{H}_{11}]$ (0.12 mmol, 1.2 equiv). CH_3CN (2.0 mL) was then added, and the resulting solution was stirred at 25 °C. the reaction progress is monitored by mass spectrometry until disappearance of the starting material. In some cases, an additional 0.2 equivalent the iodonium salt was required to achieve full conversion.

Work-up for $[\text{I}(4\text{-NMe}_2\text{Py})_2][12\text{-I-CB}_{11}\text{H}_{11}]$ (**6**):

The resulting light-yellow solution was filtered into an 8 mL glass vial. Water (3 mL) was added and the pH of the aqueous layer was adjusted to approximately 6, Slow evaporation

affords a white solid, which was collected by filtration and dried under vacuum at 60 °C to give compound **6** (80.2 mg, 93% yield).

Work-up for [H][1-R-CB₁₁H₁₀-12-I] (R=4-pyridyl, **8a; 2-F-4-pyridyl, **8b**; 2-Cl-4-pyridyl, **8c**) and [Et₄N][1-COOH-CB₁₁H₁₀-12-I] (**8d**):**

The resulting light-yellow solution was transferred to a 50 mL glass flask, and the CH₃CN was removed using a rotary evaporator. Aqueous HCl solution (0.5 M in H₂O, 10 mL, 5 mmol) was added, and the mixture was extracted with diethyl ether (3 x 30 mL). The combined organic extracts were filtered into a 100 mL one-necked round-bottom flask and concentrated using a rotary evaporator. The residue was treated NaOH solution (0.5 M in H₂O, 5 mL), and the resulting aqueous solution was filtered through a pad of celite. To the clear and colorless filtrate, HCl solution (0.5 M in H₂O, 6 mL) was added (*For **8d**, [Et₄N][Br] (0.2 mmol, 2 equiv) was added to the filtrate prior to the addition of HCl solution*). The resulting white precipitate was collected by filtration and dried under vacuum at 60 °C to give compound **8a-8d** in 92-95% yield.

Stability Tests under Ambient Conditions

Initial stability tests were performed under ambient laboratory conditions without any special protection from light or moisture. Samples were stored in transparent glass vials exposed to air (relative humidity 75–85%, temperature 30–40 °C). Two representative pairs of compounds—[IPy₂][BF₄] and [IPy₂][CB₁₁H₆I₆] (**3a**), as well as [I(4-MePy)₂][BF₄] and [I(4-MePy)₂][CB₁₁H₆I₆] (**3c**)—were selected for comparative NMR stability studies under identical storage conditions. The ¹H and ¹H{¹¹B} NMR spectra of these salts were recorded after 1, 14, and 90 days (Figures S1–S4). The BF₄[−] salts exhibited noticeable decomposition after 3 months, as indicated by new resonances in the ¹H NMR spectra, whereas their monocarborane analogues remained unchanged even after 6 months of air exposure. In contrast, the ¹⁹F NMR spectra of [I(4-MePy)₂][BF₄] and [IPy₂][BF₄] showed no significant changes throughout the monitoring period.

Subsequent control experiments revealed that when the BF₄[−] salts were stored in a desiccator or under refrigeration, no detectable decomposition was observed over a two-week period, indicating that moisture or temperature alone was not responsible for the previously observed changes. Further inspection identified the presence of elemental iodine stored in the same cabinet as the original samples. Given the volatility of iodine, these results suggest that exposure to iodine vapor may contribute to the observed decomposition of the BF₄[−] salts under ambient storage conditions.

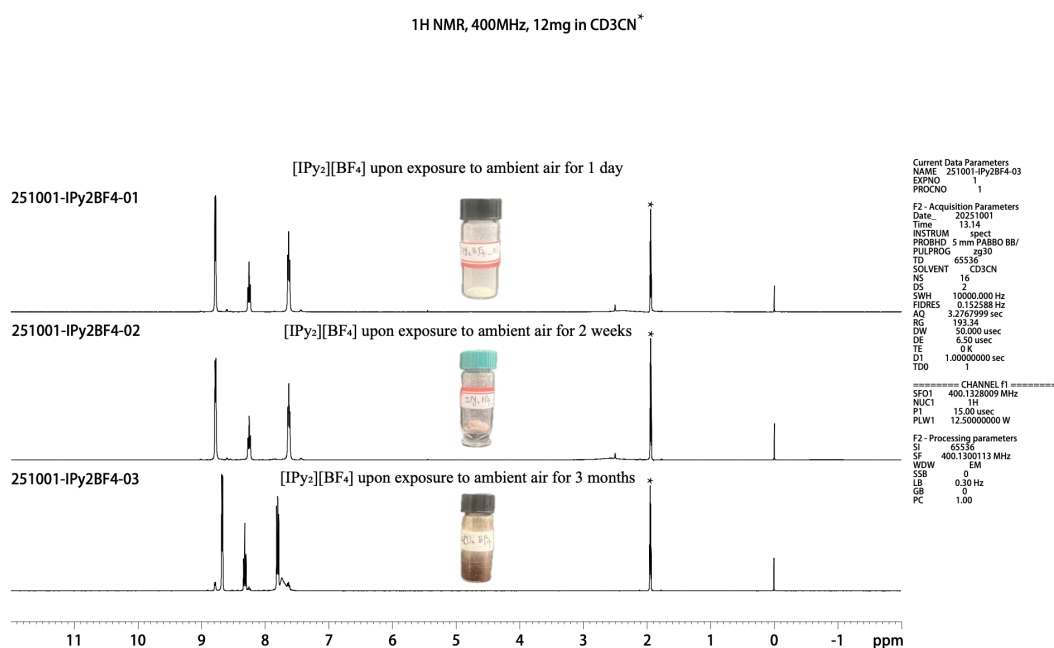


Figure S1. Comparison of the color and ¹H NMR spectra of [IPy₂][BF₄] recorded on day 1, day 14, and day 90.

$^1\text{H}\{^{11}\text{B}\}$ NMR, 400 MHz, 16 mg in Acetone- d_6 *

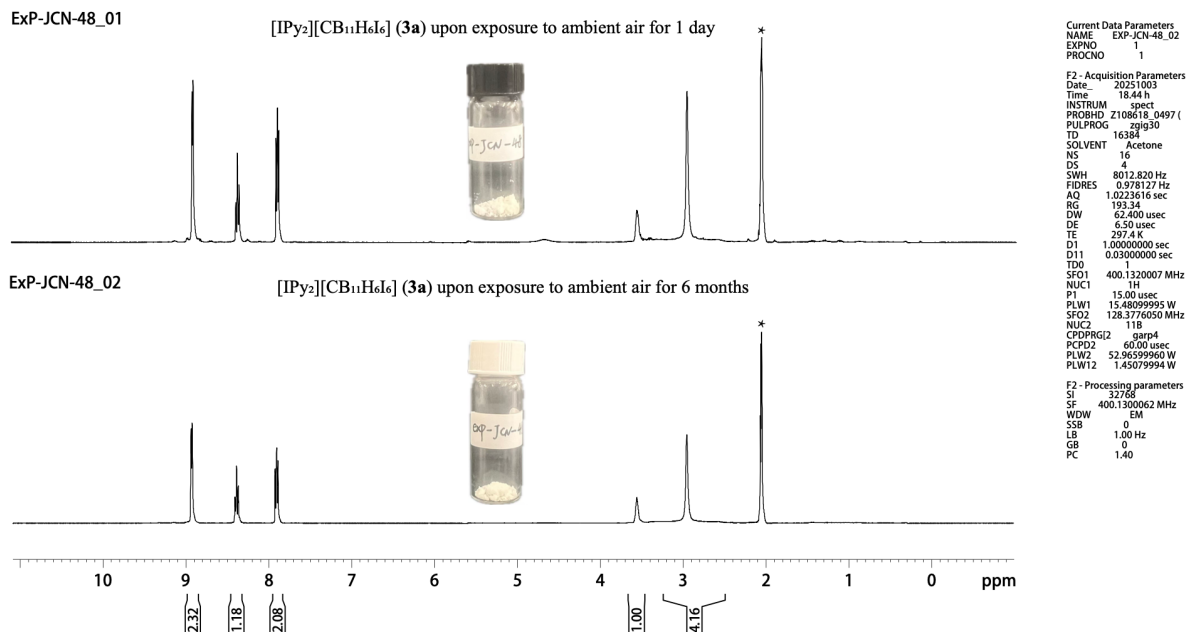


Figure S2. Comparison of the color and $^1\text{H}\{^{11}\text{B}\}$ spectra of $[\text{IPy}_2][\text{CB}_{11}\text{H}_6\text{I}_6]$ (3a) recorded on day 1 and day 180.

^1H NMR, 400MHz, 12mg in CD_3CN *

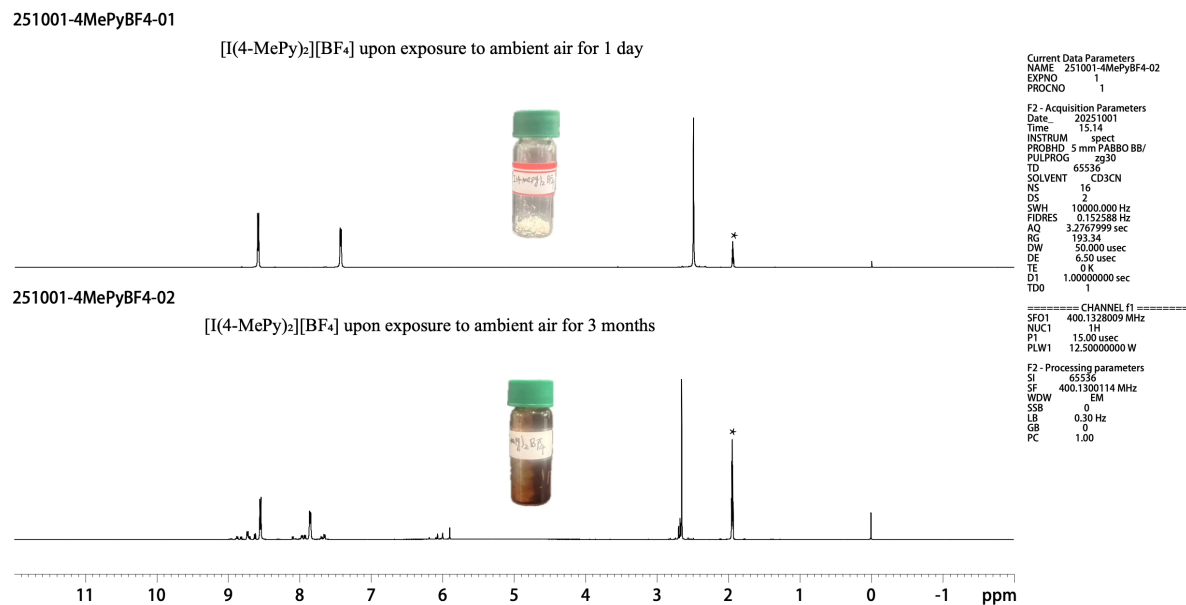


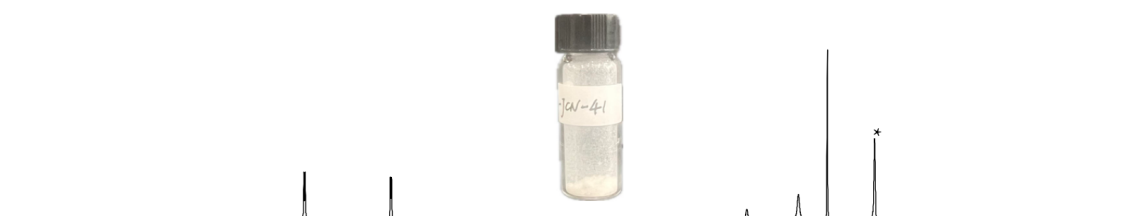
Figure S3. Comparison of the color and ^1H NMR spectra of $[\text{I}(4\text{-MePy})_2][\text{BF}_4]$ recorded on day 1 and day 90.

$^1\text{H}\{^{11}\text{B}\}$ NMR, 100 MHz, 15 mg in Acetone- d_6^*

EXP-JCN-41_01

$[\text{I}(\text{4-MePy})_2][\text{CB}_{11}\text{H}_6\text{I}_6]$ (**3c**) upon exposure to ambient air for 1 day

Current Data Parameters
NAME EXP-JCN-41_01
EXPNO 4
PROCNO 1
F2 - Processing parameters
SI 32768
SF 400.1300071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



EXP-JCN-41_02

$[\text{I}(\text{4-MePy})_2][\text{CB}_{11}\text{H}_6\text{I}_6]$ (**3c**) upon exposure to ambient air for 6 months

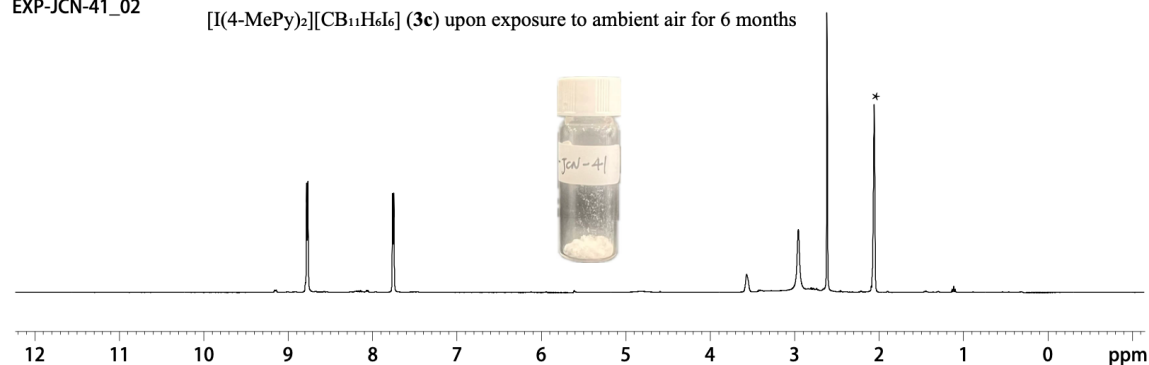
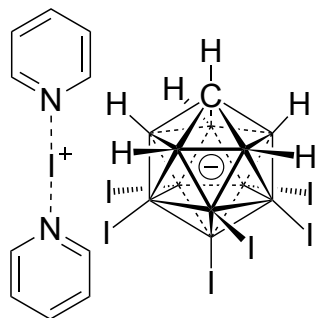


Figure S4. Comparison of the color and $^1\text{H}\{^{11}\text{B}\}$ NMR spectra of $[\text{I}(\text{4-MePy})_2][\text{CB}_{11}\text{H}_6\text{I}_6]$ (**3c**) recorded on day 1 and day 90.

Spectroscopic Data

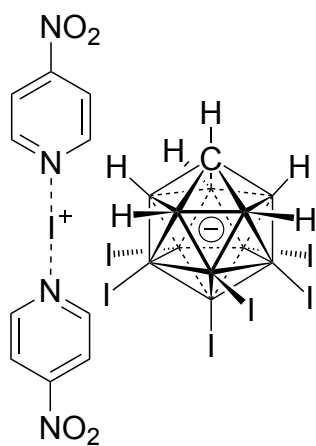


(**3a**, Colorless crystals, 86% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.92 (d, 4H, Ar-H), 8.38 (m, 2H, Ar-H), 7.90 (m, 4H, Ar-H), 3.55 (broad signal, 1H, cage CH), 2.95 (broad signal, 5H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -6.93 (1B), -14.78 (5B), -19.13 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 146.46, 143.31, 126.95 (three pyridyl signals), 56.83 (cage C).

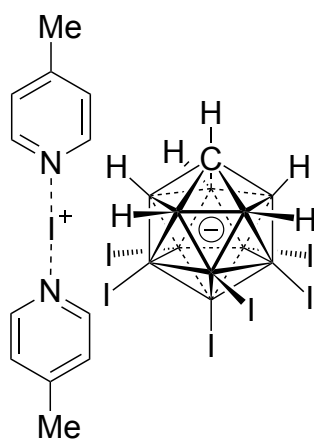


(**3b**, Colorless crystals, 88% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 9.00 (m, 4H, Ar-H), 8.12 (m, 4H, Ar-H), 3.55 (broad signal, 1H, cage CH), 2.95 (broad signal, 5H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -6.89 (1B), -14.77 (5B), -19.13 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 153.05, 142.24, 117.15 (three pyridyl signals), 56.84 (cage C).



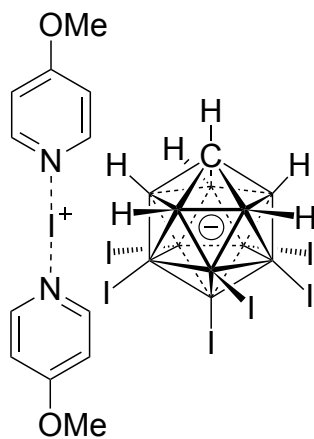
(**3c**, Colorless crystals, 92% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.77 (m, 4H, Ar-H), 7.75 (m, 4H, Ar-H), 3.56 (broad signal, 1H, cage CH), 2.95 (broad signal, 5H, BH), 2.61 (s, 6H, Ar-CH₃).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -6.90 (1B), -14.79 (5B), -19.13 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 156.44, 145.49, 127.59 (three pyridyl signals), 56.83 (cage C), 21.85 (Ar-CH₃).

Elemental analysis: Calc. for C₁₃H₂₀B₁₁I₇N₂: C 12.89%, H 1.66%; found: C 12.86%, H 1.65%.

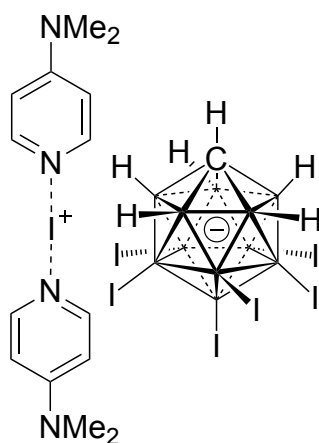


(**3d**, Colorless crystals, 90% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.72 (m, 4H, Ar-H), 7.39 (m, 4H, Ar-H), 4.11 (s, 6H, O-CH₃), 3.57 (broad signal, 1H, cage CH), 2.95 (broad signal, 5H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -6.88 (1B), -14.77 (5B), -19.14 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 170.92, 147.19, 112.73 (three pyridyl signals), 57.46 (Ar-OCH₃), 56.85 (cage C).



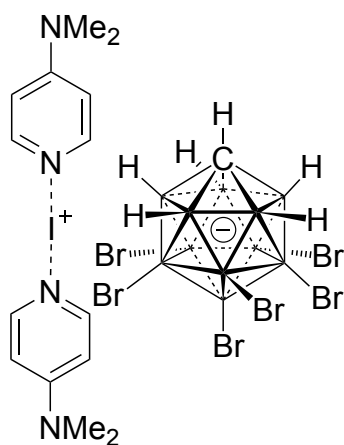
(3e, Colorless crystals, 96% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.24 (d, 4H, Ar-H), 6.78 (d, 4H, Ar-H), 3.56 (broad signal, 1H, cage CH), 3.20 (s, 12H, N-CH₃), 2.95 (broad signal, 5H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -6.87 (1B), -14.77 (5B), -19.12 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 156.70, 148.60, 109.59 (three pyridyl signals), 56.76 (cage C), 39.72 (N-CH₃).

Elemental analysis: Calc. for C₁₅H₂₆B₁₁I₇N₄: C 14.19%, H 2.06%; found: C 14.16%, H 2.05%.

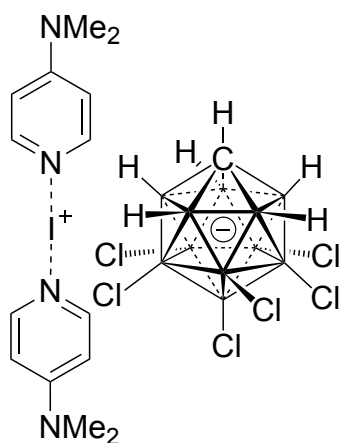


(3f, Colorless crystals, 96% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.28 (m, 4H, Ar-H), 6.94 (m, 4H, Ar-H), 3.24 (s, 12H, N-CH₃), 3.06 (broad signal, 1H, cage CH), 2.32 (broad signal, 5H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -1.64 (1B), -9.72 (5B), -20.20 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 157.59, 143.37, 107.88 (three pyridyl signals), 41.81 (cage C), 39.98 (N-CH₃).

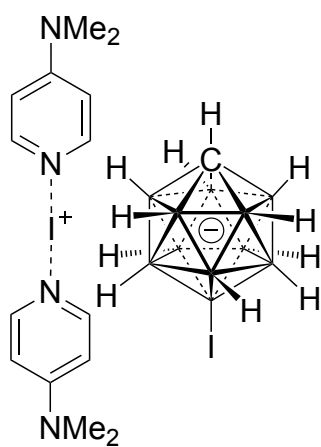


(3g, Colorless crystals, 95% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.27 (d, 4H, Ar-H), 6.94 (d, 4H, Ar-H), 3.23 (s, 12H, N-CH₃), 2.57 (broad signal, 1H, cage CH), 1.92 (broad signal, 5H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ 0.93 (1B), -5.84 (5B), -23.39 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 157.80, 142.70, 107.90 (three pyridyl signals), 40.51 (cage C), 40.04 (N-CH₃).

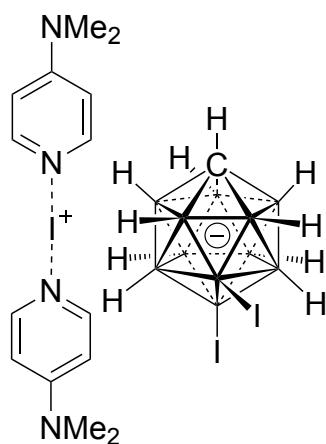


(5a, Colorless crystals, 95% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.26 (m, 4H, Ar-H), 6.91 (m, 4H, Ar-H), 3.22 (s, 12H, N-CH₃), 2.53 (broad signal, 1H, cage CH), 2.02 (broad signal, 5H, BH), 1.69 (broad signal, 5H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -11.69 (5B), -16.17 (5B), -17.86 (1B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 156.66, 148.58, 109.57 (three pyridyl signals), 48.32 (cage C), 39.70 (N-CH₃).

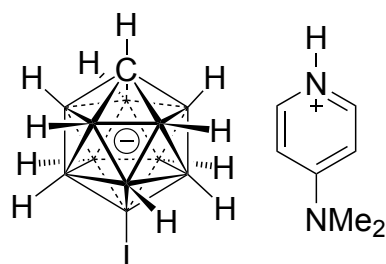


(**5b**, Colorless crystals, 96% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.24 (m, 4H, Ar-H), 6.77 (m, 4H, Ar-H), 3.20 (s, 12H, N-CH₃), 2.73 (broad signal, 1H, cage CH), 2.22-2.12 (overlapping broad signals, 7H, BH), 1.75 (broad signal, 2H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -9.76 (2B), -11.49 (2B), -15.00--17.49 (6B), -22.02 (1B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 156.69, 148.59, 109.58 (three pyridyl signals), 49.76 (cage C), 39.71 (N-CH₃).



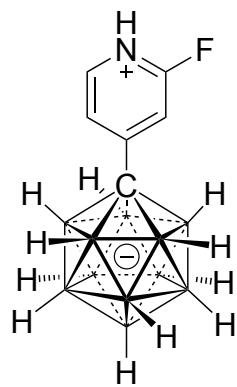
(**6**, white solid, 88-93% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.33 (d, 2H, Ar-H), 7.08 (d, 2H, Ar-H), 3.33 (s, 6H, N-CH₃), 2.53 (broad signal, 1H, cage CH), 2.01 (broad signal, 5H, BH), 1.69 (broad signal, 5H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -11.71 (5B), -16.17 (5B), -17.87 (1B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 158.44, 140.74, 108.05 (three pyridyl signals), 48.33 (cage C), 40.30 (N-CH₃).

HRMS ((-)-ESI): m/z calculated for $[\text{CH}_{11}\text{B}_{11}\text{I}]^-$: 269.1002. Found: 269.1008, $2[\text{CH}_{11}\text{B}_{11}\text{I}]^- + \text{Na}^+$: 561.1908, $2[\text{CH}_{11}\text{B}_{11}\text{I}]^- + \text{Cs}^+$: 671.1062.



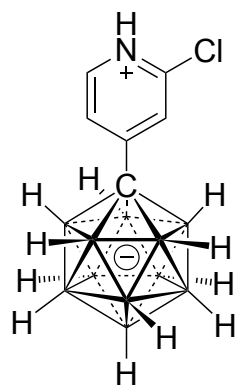
(**7b**, white solid, 75% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.27 (d, 1H, Ar-H), 7.61 (d, 1H, Ar-H), 7.36 (s, 1H, Ar-H), 1.98-1.76 (overlapping broad signals, 11H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -5.93 (1B), -12.05 (5B), -13.21 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 162.58 (Ar-C), 162.44 (d, $^1J_{\text{C,F}} = 248$ Hz, C-F), 144.03 (Ar-C), 123.35 (Ar-C), 111.13 (d, $^2J_{\text{C,F}} = 40$ Hz, Ar-C), 69.74 (cage C).

HRMS ((-)-ESI): m/z calculated for $[\text{C}_6\text{H}_{14}\text{B}_{11}\text{FN}]^-$: 238.2207. Found: 238.2216.



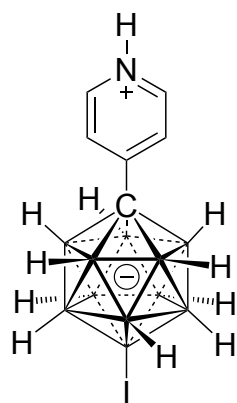
(**7c**, white solid, 80% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.65 (d, 1H, Ar-H), 7.89 (overlapping signals, 2H, Ar-H), 1.98-1.76 (overlapping broad signals, 11H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -5.36 (1B), -11.82 (5B), -13.19 (5B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 162.95, 146.43, 144.95, 127.13, 125.54 (five pyridyl signals), 69.22 (cage C).

HRMS ((-)-ESI): m/z calculated for $[\text{C}_6\text{H}_{14}\text{B}_{11}\text{ClN}]^-$: 254.1911. Found: 254.1922.



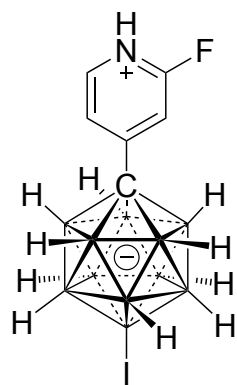
(**8a**, white solid, 94% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, $\text{DMSO-}d_6$, 28 °C): δ 8.36 (d, 2H, Ar-H), 7.27 (d, 2H, Ar-H), 2.03-1.95 (overlapping broad signals, 10H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, $\text{Acetone-}d_6$, 28 °C): δ -10.92 (5B), -13.06 (5B), -16.83 (1B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{Acetone-}d_6$, 28 °C): δ 150.83, 149.83, 123.86 (three pyridyl signals), 68.66 (cage C).

HRMS ((-)-ESI): m/z calculated for $[\text{C}_6\text{H}_{14}\text{B}_{11}\text{IN}]^-$: 347.1231. Found: 347.1248.



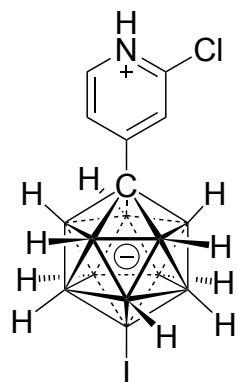
(**8b**, white solid, 95% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, $\text{Acetone-}d_6$, 28 °C): δ 7.99 (d, 1H, Ar-H), 7.29 (d, 1H, Ar-H), 6.96 (m, 1H, Ar-H), 2.18 (broad signals, 5H, BH), 2.02 (overlapping broad signals, 5H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, $\text{Acetone-}d_6$, 28 °C): δ -10.85 (5B), -13.07 (5B), -16.69 (1B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{Acetone-}d_6$, 28 °C): δ 164.41 (d, $^1J_{\text{C,F}} = 234$ Hz, C-F), 157.26 (Ar-C), 147.57 (d, $^3J_{\text{C,F}} = 16$ Hz, Ar-C), 122.25 (Ar-C), 109.26 (d, $^2J_{\text{C,F}} = 40$ Hz, Ar-C), 67.83 (cage C).

HRMS ((-)-ESI): m/z calculated for $[\text{C}_6\text{H}_{13}\text{B}_{11}\text{FIN}]^-$: 364.1173. Found: 364.1187.



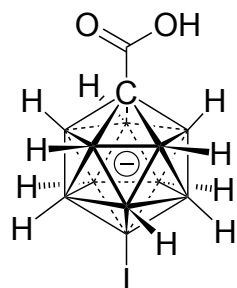
(**8c**, white solid, 94% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 8.17 (d, 1H, Ar-H), 7.35 (s, 2H, Ar-H), 6.96 (m, 1H, Ar-H), 2.18 (broad signals, 5H, BH), 2.00 (overlapping broad signals, 5H, BH).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -10.80 (5B), -13.12 (5B), -16.70 (1B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 154.71, 151.49, 149.84, 124.02, 123.25 (five pyridyl signals), 67.60 (cage C).

HRMS ((-)-ESI): m/z calculated for $[\text{C}_6\text{H}_{13}\text{B}_{11}\text{ClIN}]^-$: 380.0877. Found: 380.0896, $2[\text{C}_6\text{H}_{13}\text{B}_{11}\text{ClIN}]^- + \text{H}^+$: 762.1842, $2[\text{C}_6\text{H}_{13}\text{B}_{11}\text{ClIN}]^- + \text{Na}^+$: 784.1658.



Et_4N^+ (**8d**, white solid, 92% yield)

$^1\text{H}\{^{11}\text{B}\}$ NMR (400 MHz, Acetone- d_6 , 28 °C): δ 3.20 (m, 2H, CH_2 of cation), 1.83 (broad signal, 10H, BH), 1.16 (m, 12H, CH_3 of cation).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, Acetone- d_6 , 28 °C): δ -11.64 (5B), -13.76 (5B), -16.53 (1B).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, Acetone- d_6 , 28 °C): δ 168.89 (C=O), 67.13 (cage C), 53.10 (broad signal, CH_2 of cation), 7.72 (CH_3 of cation).

HRMS ((-)-ESI): m/z calculated for $[\text{C}_2\text{H}_{11}\text{B}_{11}\text{IO}_2]^-$: 313.0900. Found: 313.0908, $2[\text{C}_2\text{H}_{11}\text{B}_{11}\text{IO}_2]^- + \text{Na}^+$: 649.1698.

III X-ray Crystallography

The structures were solved with the dual-space algorithm using *SHELXT*^[8] and were refined by full-matrix least-squares methods on *F*² with *SHELXL-2014*^[9] using the GUI *OLEX2*^[10]. The graphical output was produced with the help of the program *Mercury*^[11]. The hydrogen atoms of the carboranes bound to a boron atom were refined with the AFIX 153 command, fixing the B-H distance to 1.10 Å. Hydrogen atoms of the carboranes bound to a carbon atom were refined with the AFIX 154 command, allowing the C-H distance to vary. If the distances became too short, they were fixed at a minimal distance of 0.96 Å.

Crystal structure of [I(4-MePy)₂][CB₁₁H₆I₆] (3c) (CCDC 2472380)

A dry 8 mL glass vial, equipped with a magnetic stir bar, was charged with compound [Cs][CB₁₁H₆I₆] (51.6 mg, 0.05 mmol, 1 equiv) and [I(4-MePy)₂][BF₄] (21.0 mg, 0.0525 mmol, 1.05 equiv). CH₂Cl₂ (4.0 mL) and CH₃CN (0.4 mL) were then added to the vial, and the resulting solution was stirred at 25 °C for 1 h and then filtered into an 8 mL glass vial and anhydrous ether (2.0 mL) was added. Slow evaporation afforded colorless crystals of the composition [I(4-MePy)₂][CB₁₁H₆I₆] suitable for X-ray diffraction within 6 d at 25 °C.

Table 1 Crystal data and structure refinement for 3c.

Identification code	250404_JCN_34
Empirical formula	C ₁₃ H ₂₀ B ₁₁ I ₇ N ₂
Formula weight	1211.52
Temperature/K	170.00
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	9.8617(4)
b/Å	17.0838(6)
c/Å	18.6279(7)
α/°	90
β/°	96.6910(10)
γ/°	90
Volume/Å ³	3117.0(2)
Z	4
ρ _{calc} /g/cm ³	2.582
μ/mm ⁻¹	37.937
F(000)	2152.0
Crystal size/mm ³	0.13 × 0.06 × 0.04
Radiation	GaKα (λ = 1.34139)
2θ range for data collection/°	7.852 to 121.206
Index ranges	-12 ≤ h ≤ 12, -22 ≤ k ≤ 22, -23 ≤ l ≤ 24
Reflections collected	34927
Independent reflections	7078 [R _{int} = 0.0451, R _{sigma} = 0.0370]
Data/restraints/parameters	7078/0/300
Goodness-of-fit on F ²	1.063
Final R indexes [I > 2σ (I)]	R ₁ = 0.0359, wR ₂ = 0.0903
Final R indexes [all data]	R ₁ = 0.0379, wR ₂ = 0.0915
Largest diff. peak/hole / e Å ⁻³	1.42/-2.15

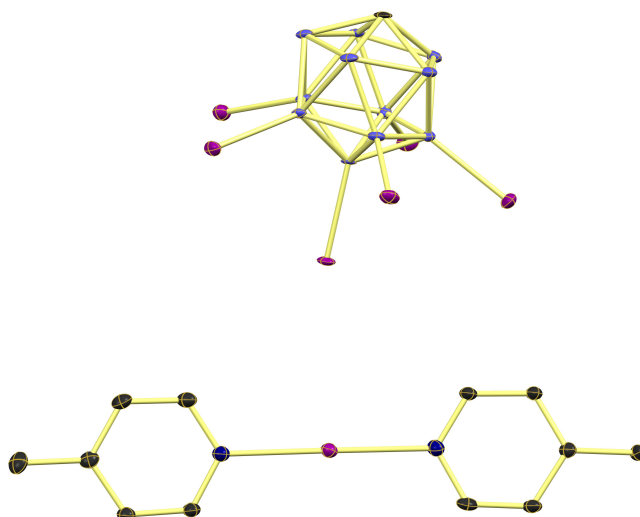


Figure S5. ORTEP representation of **3c**. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

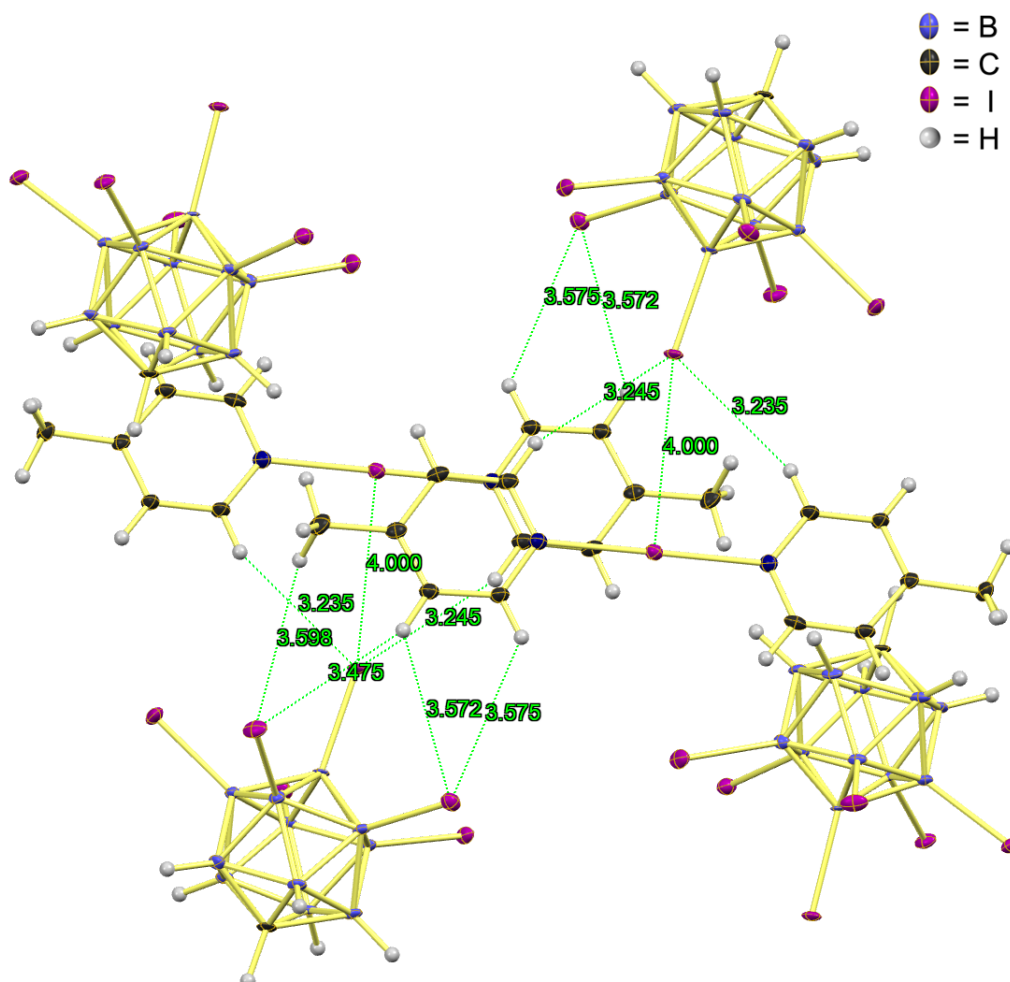


Figure S6. Noncovalent interactions ($\text{B-I}\cdots\text{I}^+$ and $\text{C-H}\cdots\text{I}$) observed in the crystal structure of compound **3c**.

Crystal structure of [I(4-NMe₂Py)₂][CB₁₁H₆I₆] (3e) (CCDC 2472381)

A dry 8 mL glass vial, equipped with a magnetic stir bar, was charged with compound [Cs][CB₁₁H₆I₆] (51.6 mg, 0.05 mmol, 1 equiv) and [I(4-NMe₂Py)₂][BF₄] (24.1 mg, 0.0525 mmol, 1 equiv). CH₂Cl₂ (4.0 mL) and CH₃CN (0.4 mL) were then added to the vial, and the resulting solution was stirred at 25 °C for 1 h and then filtered into an 8 mL glass vial and anhydrous ether (2.0 mL) was added. Slow evaporation afforded colorless crystals of the composition [I(4-NMe₂Py)₂][CB₁₁H₆I₆]•CH₂Cl₂ suitable for X-ray diffraction within 5 d at 25 °C.

Table 2 Crystal data and structure refinement for 3e.

Identification code	241118_ZK_exp_JCN_11
Empirical formula	C ₁₆ H ₂₈ B ₁₁ Cl ₂ I ₇ N ₄
Formula weight	1354.53
Temperature/K	170.00
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	10.2469(6)
b/Å	14.9143(8)
c/Å	24.6138(12)
α/°	90
β/°	93.431(2)
γ/°	90
Volume/Å ³	3754.9(3)
Z	4
ρ _{calc} /g/cm ³	2.396
μ/mm ⁻¹	32.201
F(000)	2448.0
Crystal size/mm ³	0.08 × 0.05 × 0.04
Radiation	GaKα (λ = 1.34139)
2θ range for data collection/°	6.032 to 121.348
Index ranges	-13 ≤ h ≤ 13, -19 ≤ k ≤ 17, -29 ≤ l ≤ 31
Reflections collected	36968
Independent reflections	8620 [R _{int} = 0.0412, R _{sigma} = 0.0394]
Data/restraints/parameters	8620/0/365
Goodness-of-fit on F ²	1.047
Final R indexes [I>2σ (I)]	R ₁ = 0.0280, wR ₂ = 0.0553
Final R indexes [all data]	R ₁ = 0.0364, wR ₂ = 0.0580
Largest diff. peak/hole / e Å ⁻³	1.04/-1.33

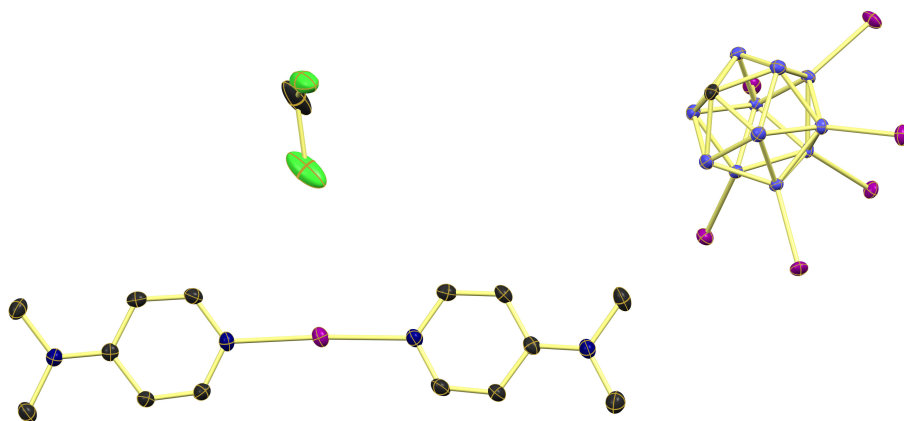


Figure S7. ORTEP representation of **3e**·CH₂Cl₂. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

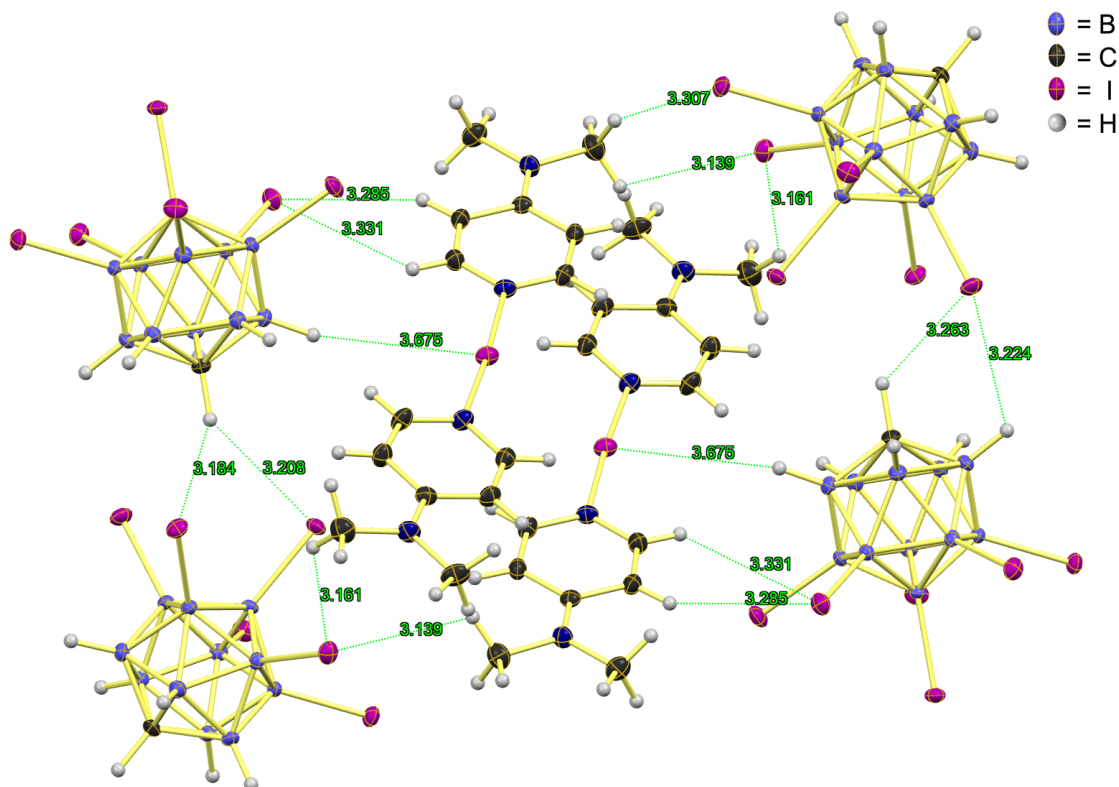


Figure S8. Noncovalent interactions (B–H···I⁺ and B/C–H···I) observed in the crystal structure of **3e**. Solvent molecules are omitted for clarity.

Crystal structure of [I(4-NMe₂Py)₂][CB₁₁H₆Br₆] (3f) (CCDC 2472382)

A dry 8 mL glass vial, equipped with a magnetic stir bar, was charged with compound [Cs][CB₁₁H₆Br₆] (37.5 mg, 0.05 mmol, 1 equiv) and [I(4-NMe₂Py)₂][BF₄] (24.1 mg, 0.0525 mmol, 1.05 equiv). CH₂Cl₂ (4.0 mL) and CH₃CN (0.4 mL) were then added to the vial, and the resulting solution was stirred at 25 °C for 1 h and then filtered into an 8 mL glass vial and anhydrous ether (2.0 mL) was added. Slow evaporation afforded colorless crystals of the composition [I(4-NMe₂Py)₂][CB₁₁H₆Br₆]•CH₂Cl₂ suitable for X-ray diffraction within 7 d at 25 °C.

Table 3 Crystal data and structure refinement for 3f.

Identification code	241206_exp_CLY_15
Empirical formula	C ₁₆ H ₂₈ B ₁₁ Br ₆ Cl ₂ IN ₄
Formula weight	1072.59
Temperature/K	170.00
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	9.7127(3)
b/Å	14.5096(5)
c/Å	24.3406(8)
α/°	90
β/°	90.9220(10)
γ/°	90
Volume/Å ³	3429.81(19)
Z	4
ρ _{calc} /g/cm ³	2.077
μ/mm ⁻¹	11.521
F(000)	2016.0
Crystal size/mm ³	0.09 × 0.06 × 0.04
Radiation	GaKα (λ = 1.34139)
2θ range for data collection/°	6.32 to 121.24
Index ranges	-12 ≤ h ≤ 12, -18 ≤ k ≤ 18, -31 ≤ l ≤ 29
Reflections collected	42040
Independent reflections	7840 [R _{int} = 0.0299, R _{sigma} = 0.0246]
Data/restraints/parameters	7840/6/365
Goodness-of-fit on F ²	1.074
Final R indexes [I > 2σ (I)]	R ₁ = 0.0306, wR ₂ = 0.0801
Final R indexes [all data]	R ₁ = 0.0330, wR ₂ = 0.0812
Largest diff. peak/hole / e Å ⁻³	0.54/-1.65

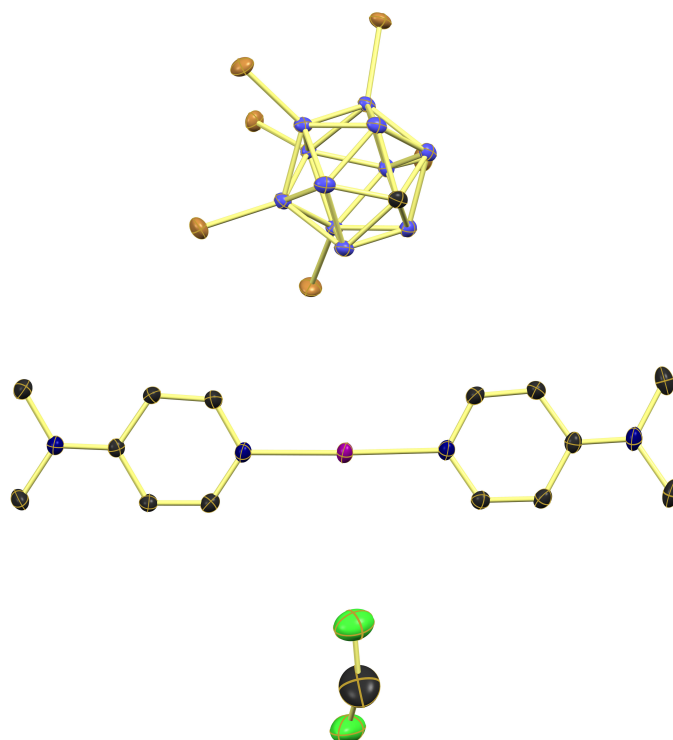


Figure S9. ORTEP representation of **3f**·CH₂Cl₂. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

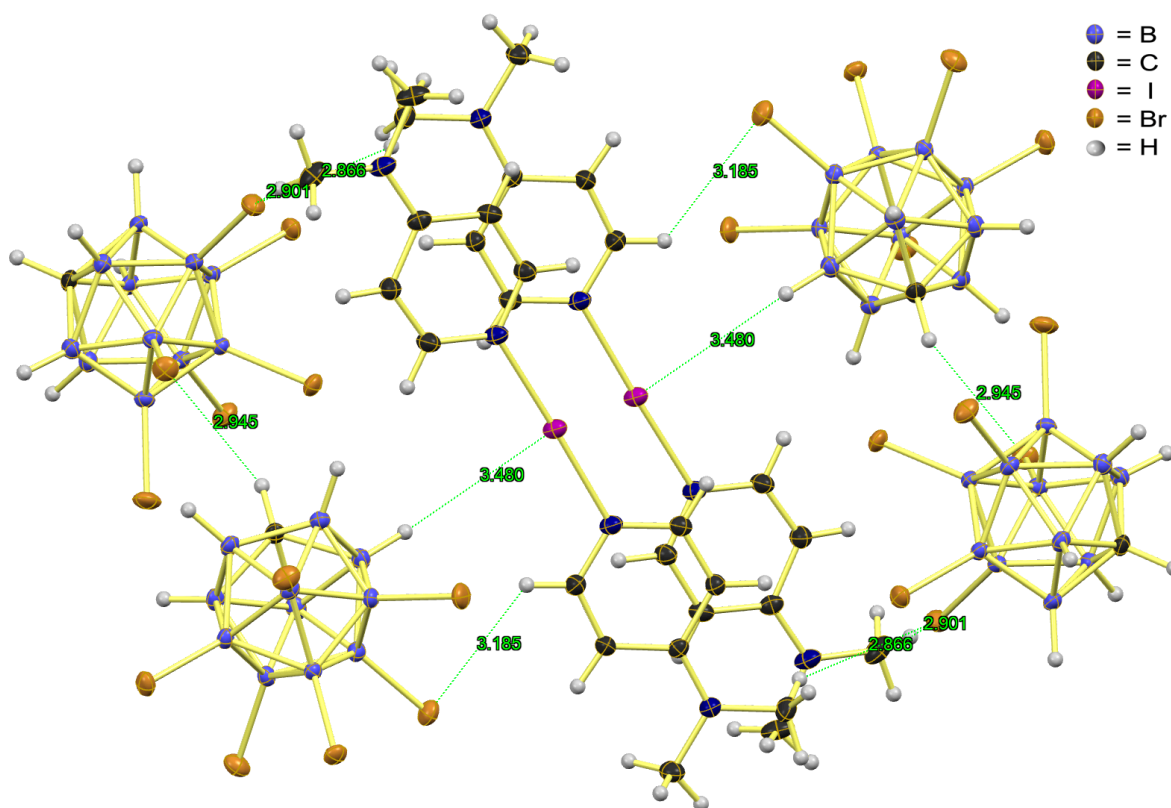


Figure S10. Noncovalent interactions (B-H...I⁺ and B/C-H...Br) observed in the crystal structure of **3f**·CH₂Cl₂. Solvent molecules are omitted for clarity.

Crystal structure of [I(4-NMe₂Py)₂][CB₁₁H₆Cl₆] (3g) (CCDC 2472383)

A dry 8 mL glass vial, equipped with a magnetic stir bar, was charged with compound [Cs][CB₁₁H₆Cl₆] (24.1 mg, 0.05 mmol, 1 equiv) and [I(4-NMe₂Py)₂][BF₄] (24.1 mg, 0.0525 mmol, 1.05 equiv). CH₂Cl₂ (4.0 mL) and CH₃CN (0.4 mL) were then added to the vial, and the resulting solution was stirred at 25 °C for 1 h and then filtered into an 8 mL glass vial and anhydrous ether (2.0 mL) was added. Slow evaporation afforded colorless crystals of the composition [I(4-NMe₂Py)₂][CB₁₁H₆Cl₆] suitable for X-ray diffraction within 7 d at 25 °C.

Table 4 Crystal data and structure refinement for 3g.

Identification code	250404_JCN_39
Empirical formula	C ₁₅ H ₂₆ B ₁₁ Cl ₆ IN ₄
Formula weight	720.91
Temperature/K	170.00
Crystal system	triclinic
Space group	P-1
a/Å	15.3144(8)
b/Å	19.2591(11)
c/Å	32.6030(19)
α/°	92.857(2)
β/°	101.150(2)
γ/°	106.677(2)
Volume/Å ³	8980.7(9)
Z	12
ρ _{calc} /g/cm ³	1.600
μ/mm ⁻¹	9.227
F(000)	4248.0
Crystal size/mm ³	0.06 × 0.04 × 0.04
Radiation	GaKα (λ = 1.34139)
2θ range for data collection/°	4.194 to 121.474
Index ranges	-19 ≤ h ≤ 19, -24 ≤ k ≤ 25, -42 ≤ l ≤ 42
Reflections collected	152420
Independent reflections	40947 [R _{int} = 0.0736, R _{sigma} = 0.1086]
Data/restraints/parameters	40947/2739/2469
Goodness-of-fit on F ²	1.070
Final R indexes [I > 2σ (I)]	R ₁ = 0.0705, wR ₂ = 0.1882
Final R indexes [all data]	R ₁ = 0.1087, wR ₂ = 0.2123
Largest diff. peak/hole / e Å ⁻³	2.11/-1.79

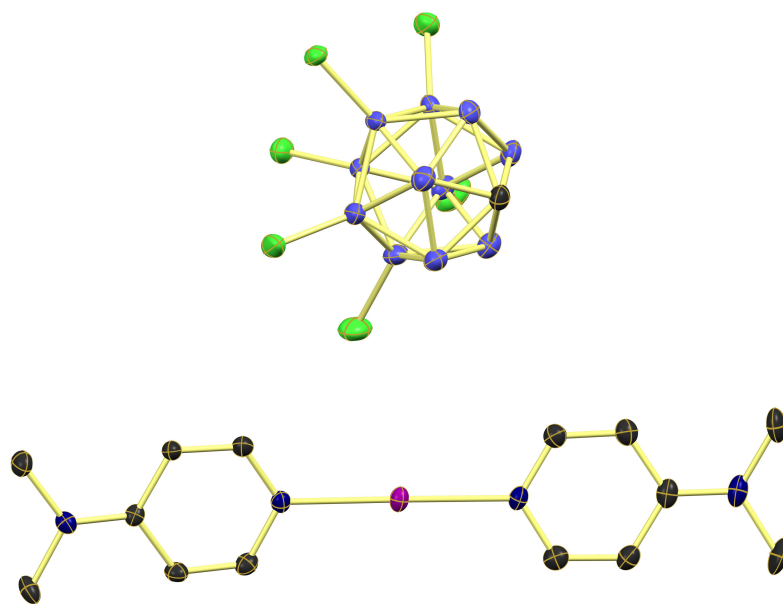


Figure S11. ORTEP representation of **3g**. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

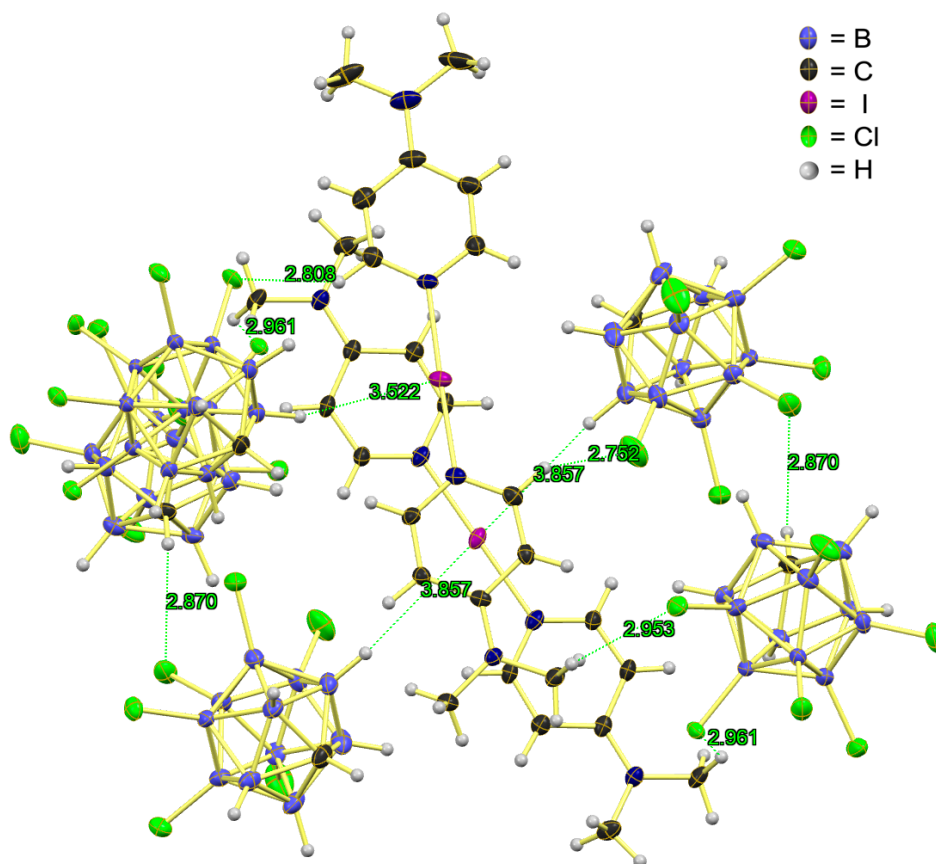


Figure S12. Noncovalent interactions ($\text{B-H}\cdots\text{I}^+$ and $\text{B/C-H}\cdots\text{Cl}$) observed in the crystal structure of **3g**.

Crystal structure of [I(4-NMe₂Py)₂][12-I-CB₁₁H₁₁] (5a) (CCDC 2472384)

A dry 8 mL glass vial, equipped with a magnetic stir bar, was charged with compound [Cs][12-I-CB₁₁H₁₁] (20.1 mg, 0.05 mmol, 1 equiv) and [I(4-NMe₂Py)₂][BF₄] (24.1 mg, 0.0525 mmol, 1.05 equiv). CH₂Cl₂ (4.0 mL) and CH₃CN (0.4 mL) were then added to the vial, and the resulting solution was stirred at 25 °C for 1 h and then filtered into an 8 mL glass vial and anhydrous ether (2.0 mL) was added. Slow evaporation afforded colorless crystals of the composition [I(4-NMe₂Py)₂][12-I-CB₁₁H₁₁] suitable for X-ray diffraction within 7 d at 25 °C.

Table 5 Crystal data and structure refinement for 5a.

Identification code	241118_ZK_exp_CLY_8
Empirical formula	C ₁₅ H ₃₁ B ₁₁ I ₂ N ₄
Formula weight	640.15
Temperature/K	298.00
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	14.9066(6)
b/Å	8.9852(4)
c/Å	21.3656(11)
α/°	90
β/°	106.617(2)
γ/°	90
Volume/Å ³	2742.2(2)
Z	4
ρ _{calc} /g/cm ³	1.551
μ/mm ⁻¹	2.305
F(000)	1240.0
Crystal size/mm ³	0.39 × 0.35 × 0.23
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	3.916 to 56.584
Index ranges	-19 ≤ h ≤ 19, -11 ≤ k ≤ 11, -28 ≤ l ≤ 28
Reflections collected	49167
Independent reflections	6784 [R _{int} = 0.0346, R _{sigma} = 0.0242]
Data/restraints/parameters	6784/0/293
Goodness-of-fit on F ²	1.047
Final R indexes [I > 2σ (I)]	R ₁ = 0.0381, wR ₂ = 0.0820
Final R indexes [all data]	R ₁ = 0.0494, wR ₂ = 0.0942
Largest diff. peak/hole / e Å ⁻³	1.68/-1.50

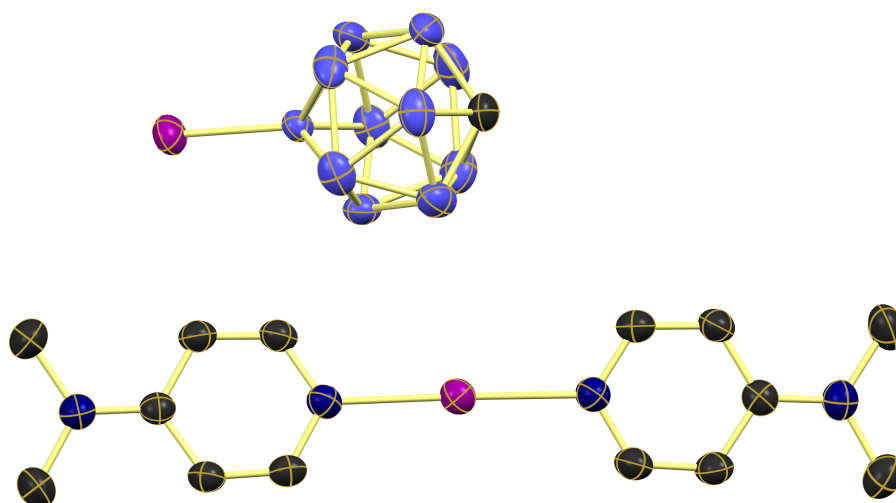


Figure S13. ORTEP representation of **5a**. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

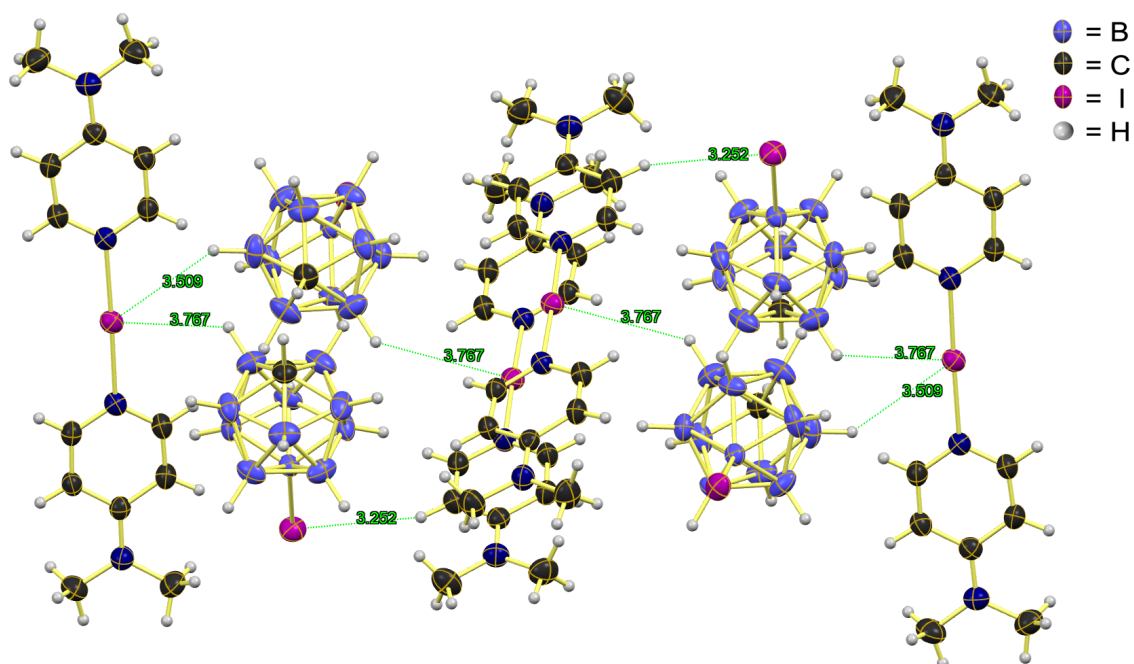


Figure S14. Noncovalent interactions ($\text{B-H}\cdots\text{I}^+$ and $\text{C-H}\cdots\text{I}$) observed in the crystal structure of **5a**.

Crystal structure of [H][1-pyridyl-CB₁₁H₁₀-12-I] (8) (CCDC 2472385)

[H][1-pyridyl-CB₁₁H₁₀-12-I] (10.5 mg) was dissolved in a mixture solution of acetone (1.0 mL) and pyridine (0.2 mL) in a 4mL glass vial. Slow evaporation afforded colorless crystals of the composition [H][1-pyridyl-CB₁₁H₁₀-12-I]•pyridine suitable for X-ray diffraction within 7 d at 25 °C.

Remark: Disorder of the pyridine solvent molecular was observed in the crystal structure.

Table 6 Crystal data and structure refinement for 8.

Identification code	240506_py_1
Empirical formula	C ₂₂ H ₄₁ B ₂₂ IN ₄
Formula weight	726.31
Temperature/K	170.00
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	7.0340(3)
b/Å	16.9143(6)
c/Å	15.5499(5)
α/°	90
β/°	99.8460(10)
γ/°	90
Volume/Å ³	1822.80(12)
Z	2
ρ _{calc} /cm ³	1.323
μ/mm ⁻¹	4.834
F(000)	728.0
Crystal size/mm ³	0.05 × 0.03 × 0.02
Radiation	GaKα (λ = 1.34139)
2θ range for data collection/°	6.772 to 121.48
Index ranges	-9 ≤ h ≤ 9, -21 ≤ k ≤ 20, -17 ≤ l ≤ 20
Reflections collected	19520
Independent reflections	4179 [R _{int} = 0.0382, R _{sigma} = 0.0335]
Data/restraints/parameters	4179/375/251
Goodness-of-fit on F ²	1.079
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0493, wR ₂ = 0.1324
Final R indexes [all data]	R ₁ = 0.0575, wR ₂ = 0.1364
Largest diff. peak/hole / e Å ⁻³	1.10/-0.42

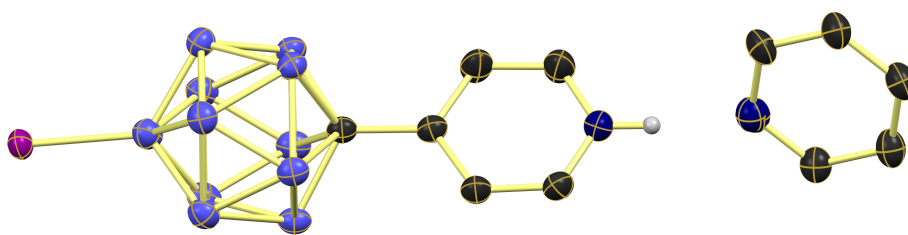


Figure S15. ORTEP representation of **8•pyridine**. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

IV References

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a more recent summary is available online from the Sigma-Aldrich company:
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V NMR spectra

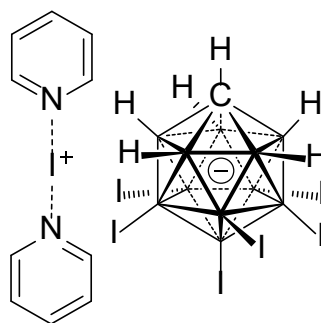
Exp-JCN-48, 16.8 mg in Acetone-d₆^{*}
¹H{¹¹B} NMR, 400 MHz, T= 28 C

8.93
8.92
8.38
7.92
7.90
7.90
7.88

3.55

2.95

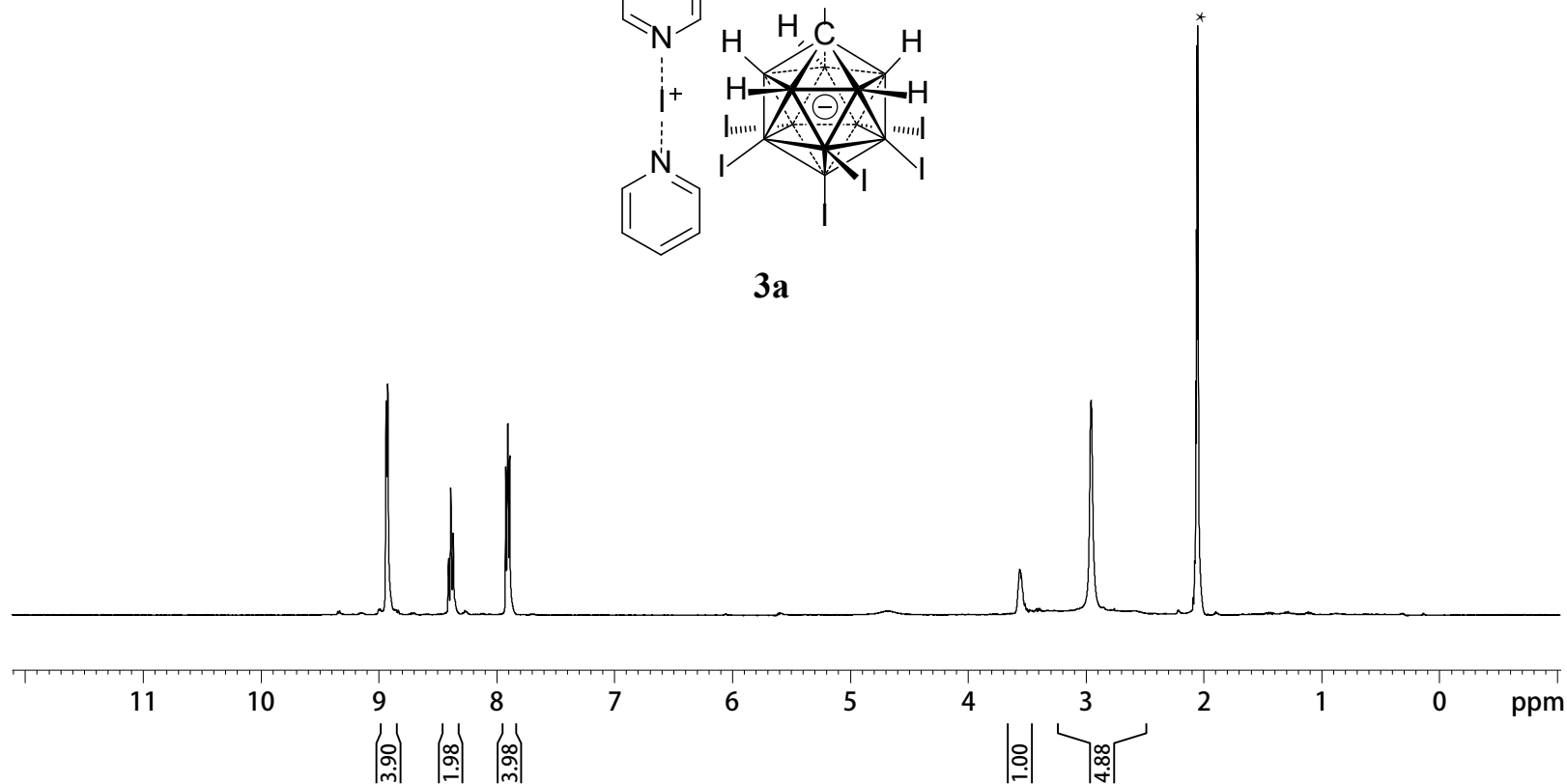
2.05
2.04



3a

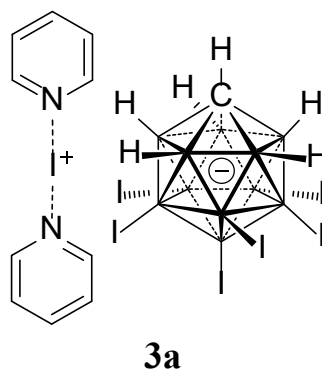
Current Data Parameters
 NAME Exp-JCN-48
 EXPNO 4
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 400.1300074 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40



Exp-JCN-48, 16.8 mg in Acetone-d6
 $^{11}\text{B}\{^1\text{H}\}$ NMR, 128 MHz, T= 28 C

— -6.93
 — -14.78
 — -19.13



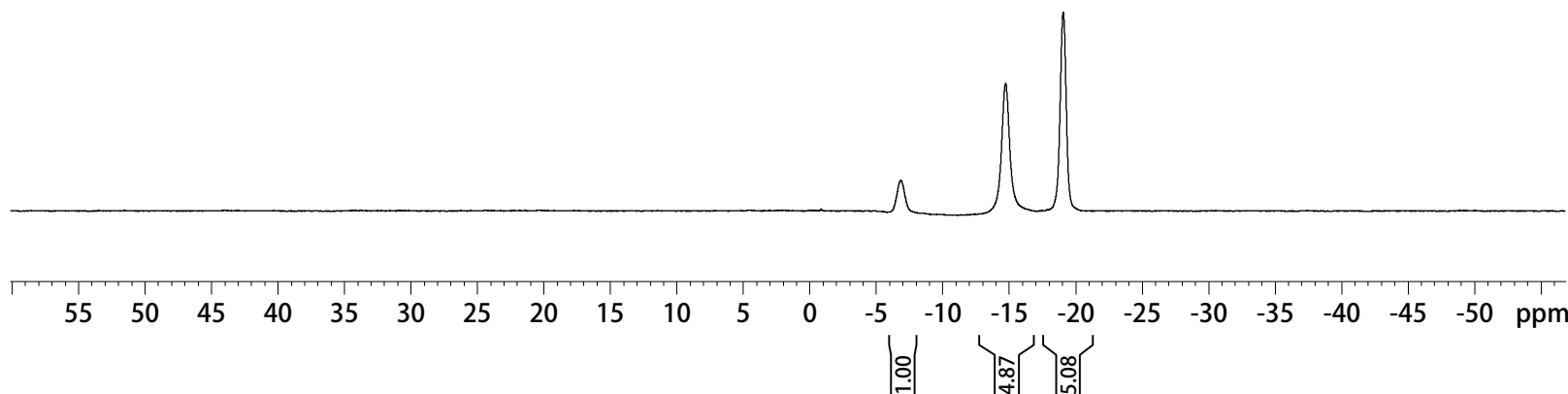
Current Data Parameters
 NAME Exp-JCN-48
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250419
 Time 22.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

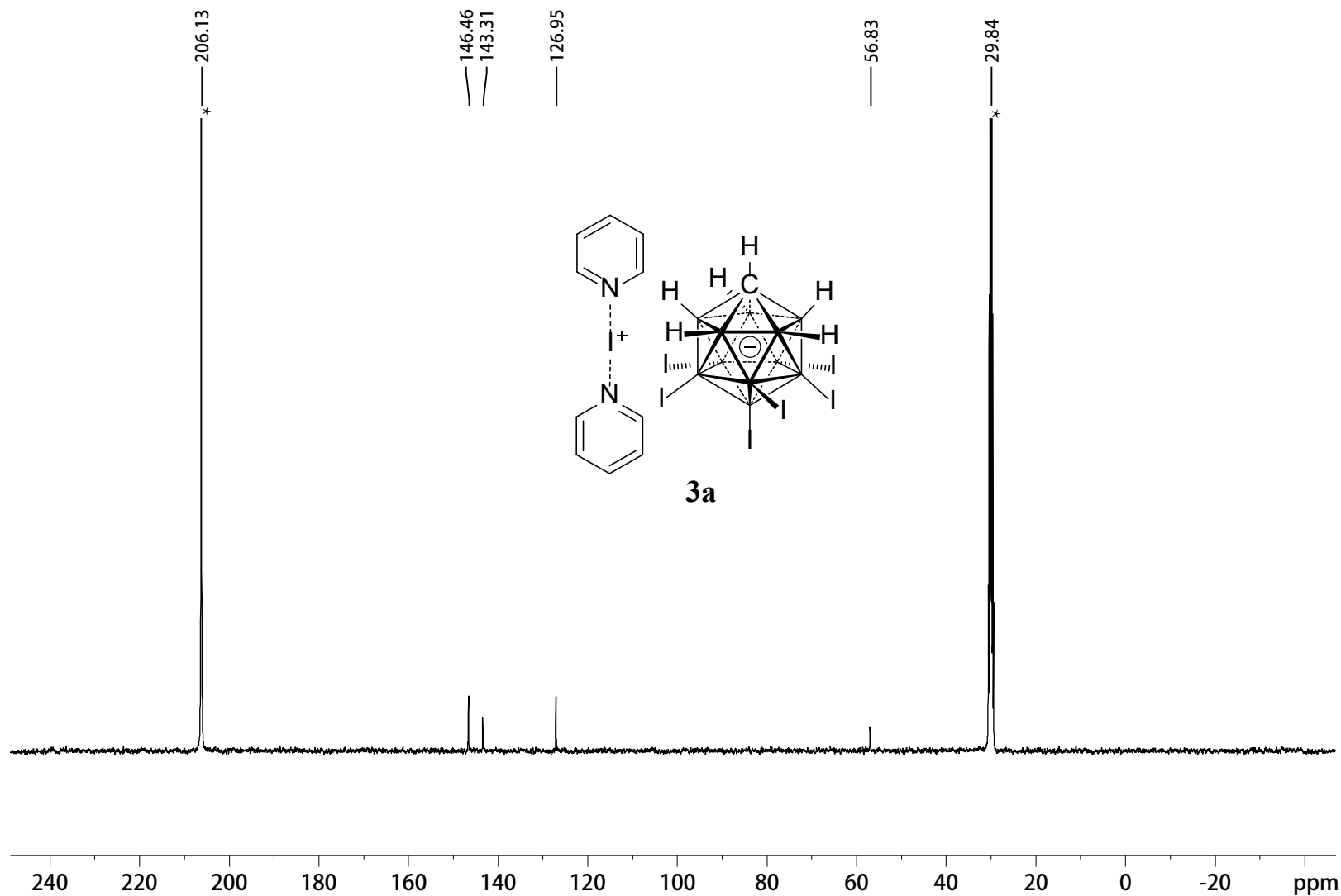
===== CHANNEL f1 =====
 SFO1 128.3776050 MHz
 NUC1 ^{11}B
 P1 9.93 usec
 PLW1 52.96599960 W

===== CHANNEL f2 =====
 SFO2 400.1320007 MHz
 NUC2 ^1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

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



Exp-JCN-48, 16.8 mg in Acetone-d₆^{*}
¹³C{¹H} NMR, 100 MHz, T= 28 C



Current Data Parameters
 NAME Exp-JCN-48
 EXPNO 3
 PROCNO 1

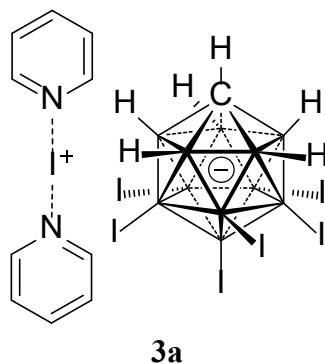
F2 - Acquisition Parameters
 Date_ 20250419
 Time 23.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126800 MHz
 WDW EM
 GB 0

251003-F-01, 10 mg in acetone-d6
¹⁹F NMR, 376 MHz, T=27 C

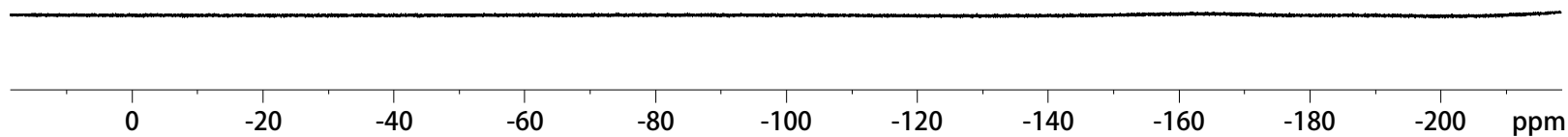


Current Data Parameters
 NAME 251003-F-01
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251003
 Time 18.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 193.34
 DW 5.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 376.4607164 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 376.4983662 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Exp-JCN-47, 18 mg in Acetone-d₆^{*}
¹H{¹¹B} NMR, 400 MHz, T= 27 C

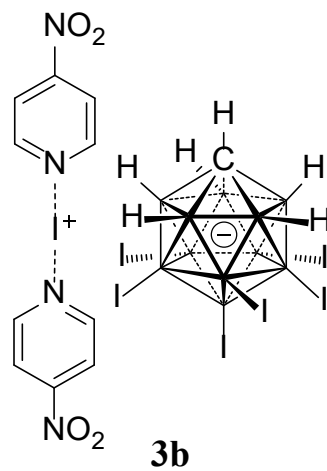
9.00
9.00
8.99

8.13
8.11

3.55

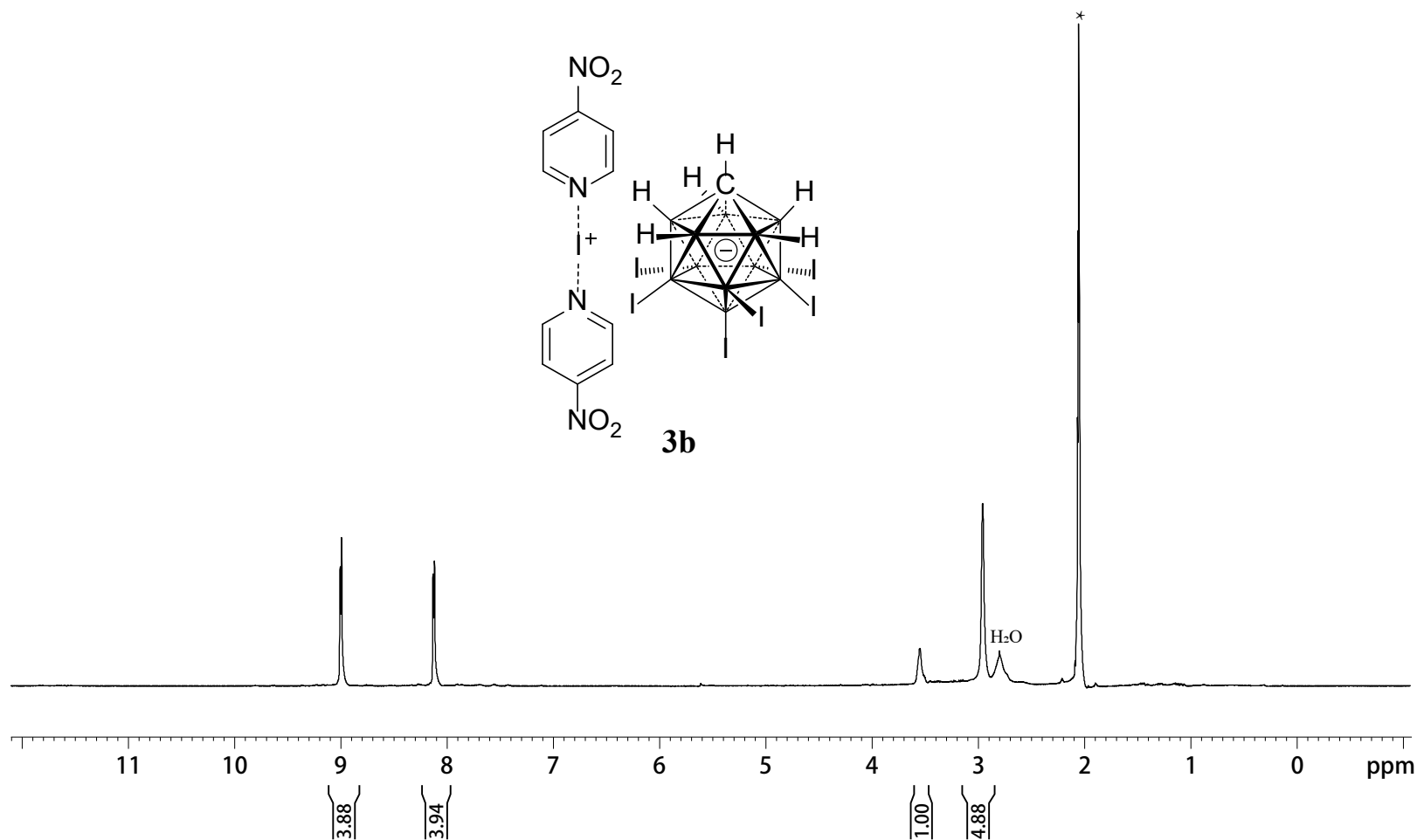
2.95
2.79

2.05
2.04



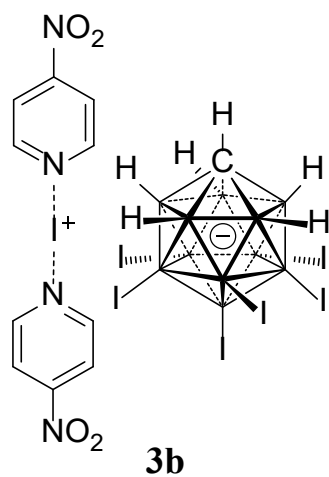
Current Data Parameters
 NAME Exp-JCN-47
 EXPNO 4
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 400.1300079 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40



Exp-JCN-47, 18 mg in Acetone-d₆
¹¹B{¹H} NMR, 128 MHz, T= 27 °C

— -6.89
 — -14.77
 — -19.13



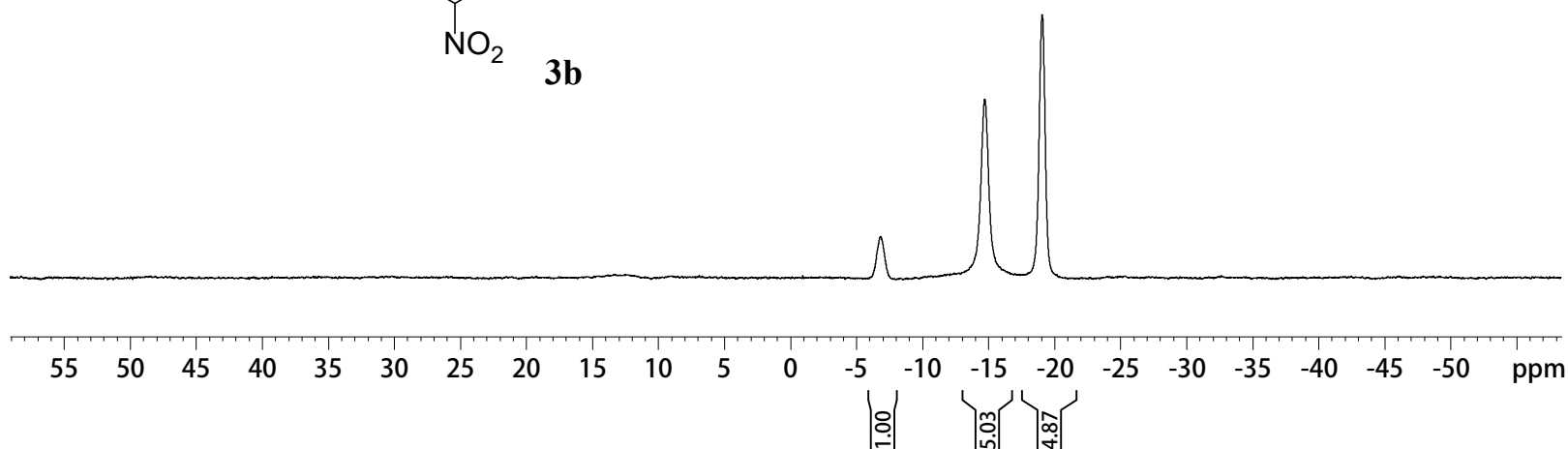
Current Data Parameters
 NAME Exp-JCN-47
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250420
 Time 3.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.0000000 sec
 D11 0.03000000 sec
 TD0 1

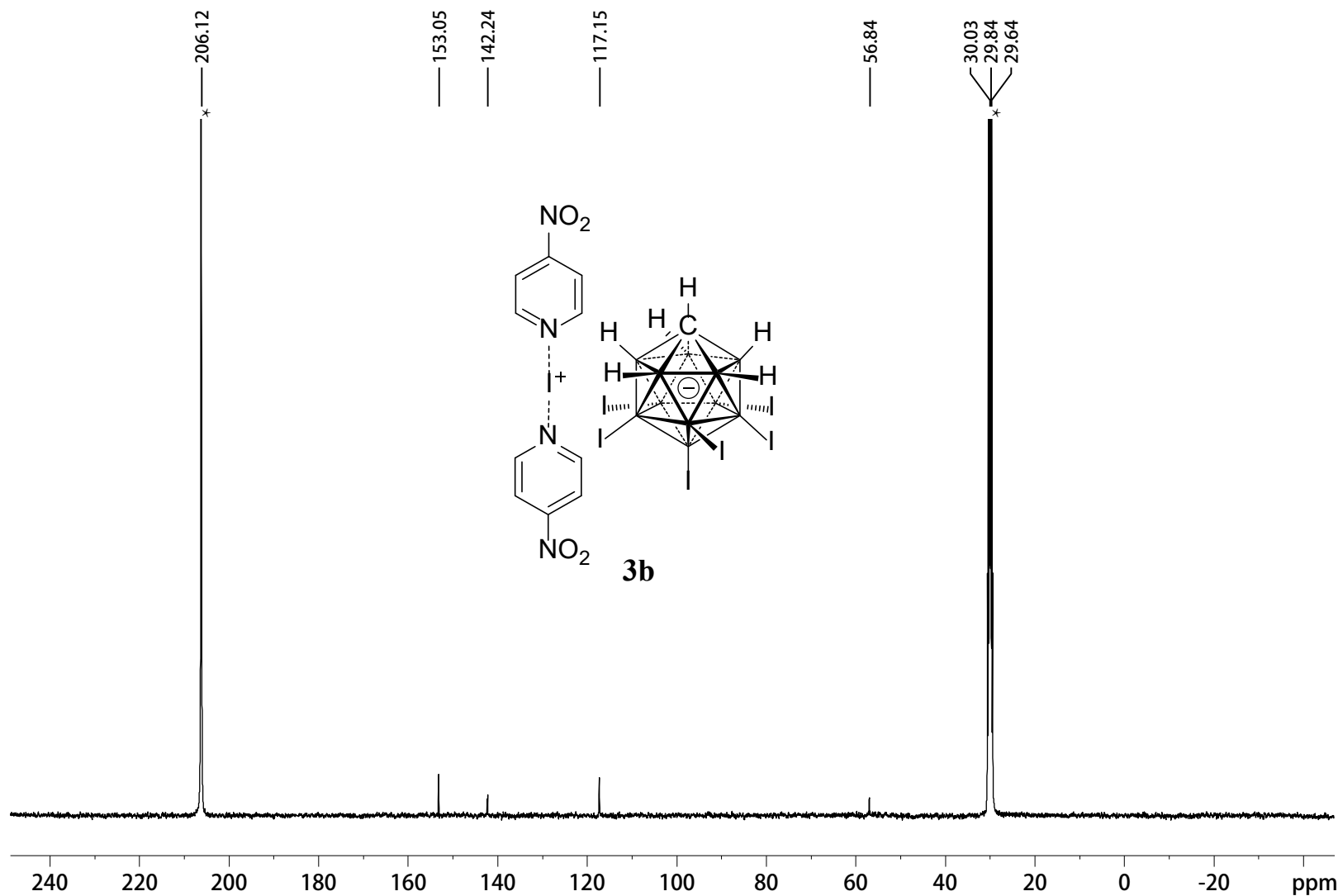
===== CHANNEL f1 =====
 SFO1 128.3776050 MHz
 NUC1 ¹¹B
 P1 9.93 usec
 PLW1 52.96599960 W

===== CHANNEL f2 =====
 SFO2 400.1320007 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

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



Exp-JCN-47, 18 mg in Acetone-d₆^{*}
¹³C{¹H} NMR, 100 MHz, T= 27 C



Current Data Parameters
 NAME Exp-JCN-47
 EXPNO 3
 PROCNO 1

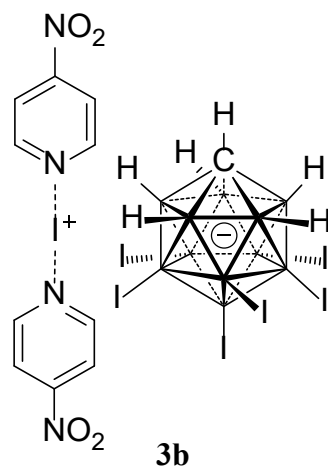
F2 - Acquisition Parameters
 Date_ 20250420
 Time 4.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 2048
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126775 MHz
 WDW EM
 SSB 0

251003-F-02, 12 mg in acetone-d6
¹⁹F NMR, 376 MHz, T=27 C

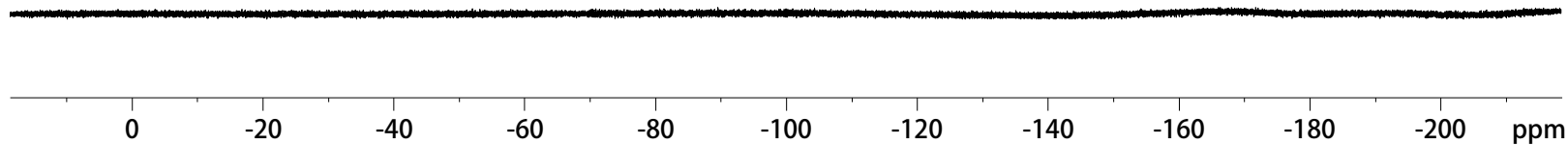


Current Data Parameters
 NAME 251003-F-02
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251003
 Time 18.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 193.34
 DW 5.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 376.4607164 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 376.4983662 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Exp-JCN-41, 17 mg in Acetone-d₆^{*}
¹H{¹¹B} NMR, 100 MHz, T= 27 C

8.78
8.76

7.76
7.74

3.56

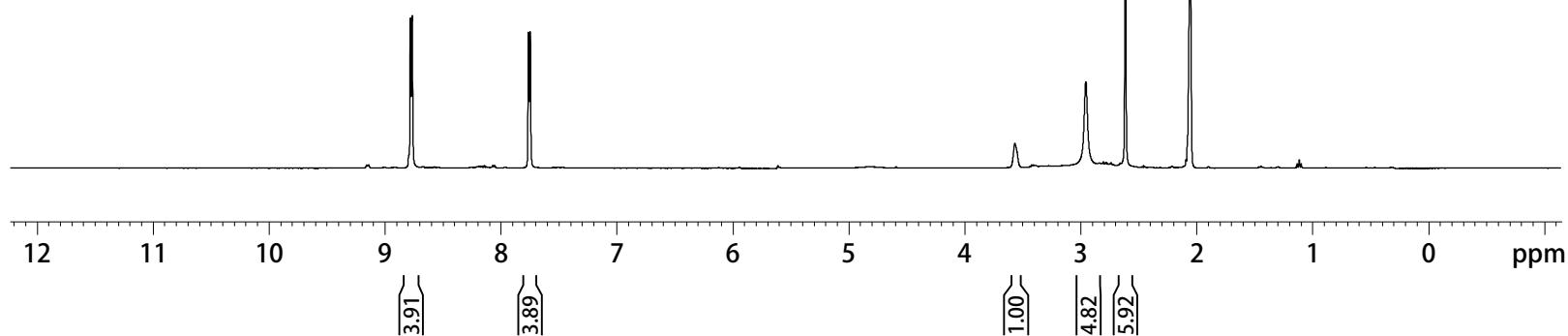
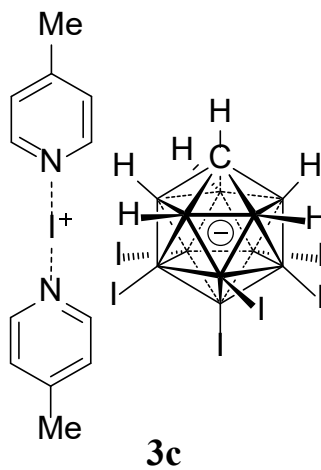
2.95

2.61

2.05

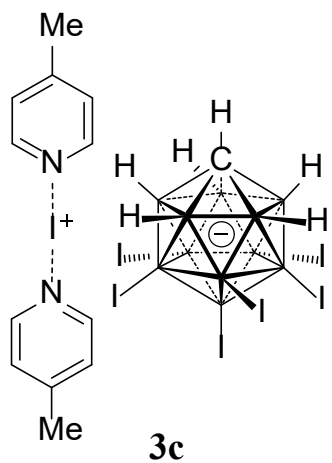
Current Data Parameters
 NAME Exp-JCN-41
 EXPNO 4
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 400.1300071 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40



Exp-JCN-41,17 mg in Acetone-d6
¹¹B{¹H} NMR, 128 MHz, T= 27 C

— -6.90
 — -14.79
 — -19.13



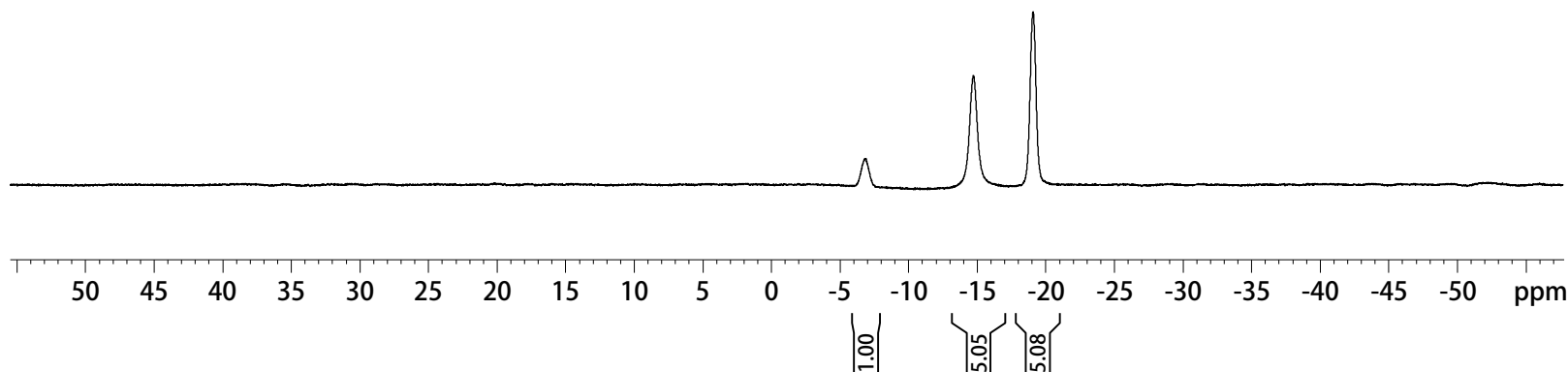
Current Data Parameters
 NAME Exp-JCN-41
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250420
 Time 1.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

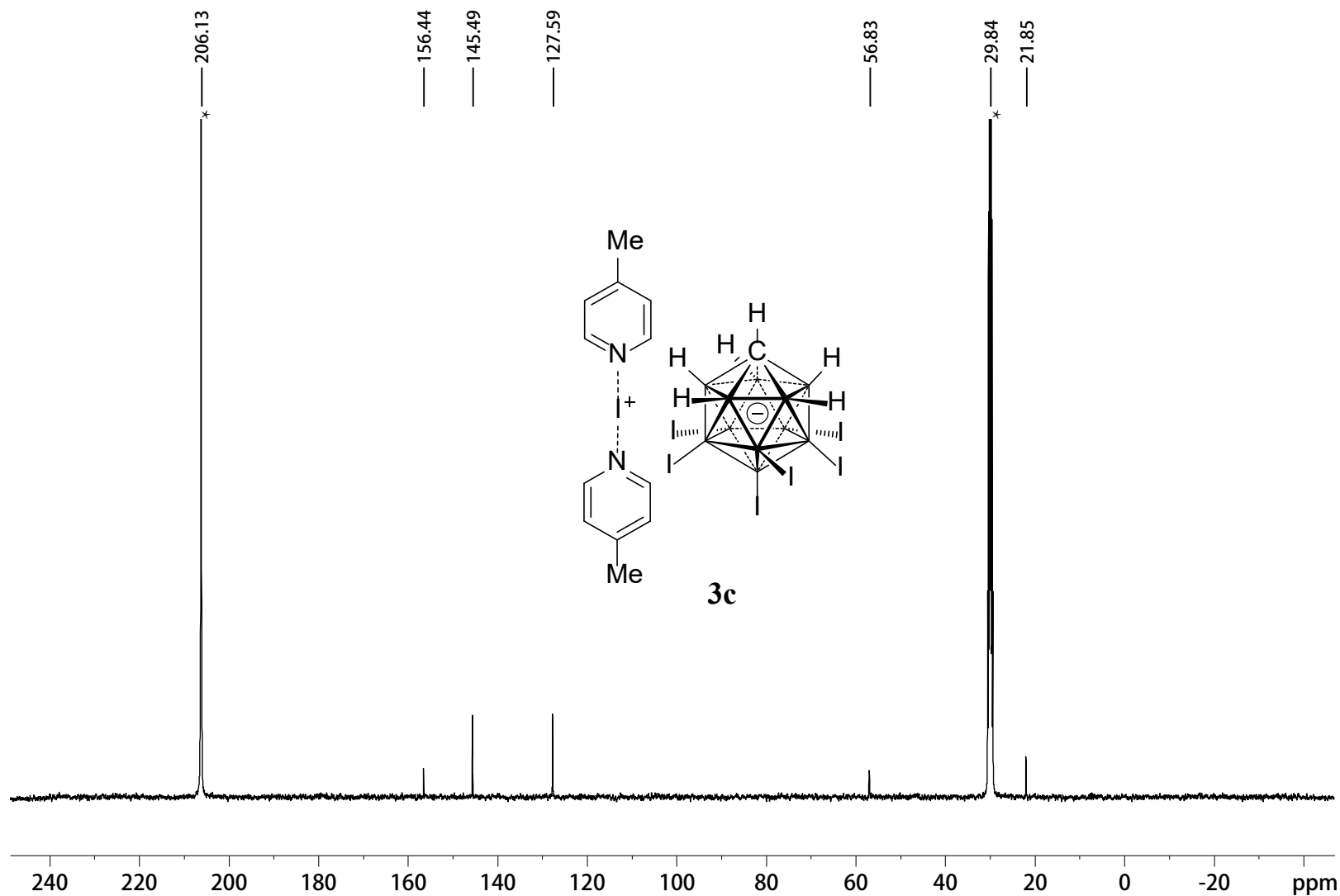
===== CHANNEL f1 =====
 SFO1 128.3776050 MHz
 NUC1 ¹¹B
 P1 9.93 usec
 PLW1 52.96599960 W

===== CHANNEL f2 =====
 SFO2 400.1320007 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

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



Exp-JCN-41,17 mg in Acetone-d6*
 13C{1H} NMR, 100 MHz, T= 27 C



Current Data Parameters
 NAME Exp-JCN-41
 EXPNO 3
 PROCNO 1

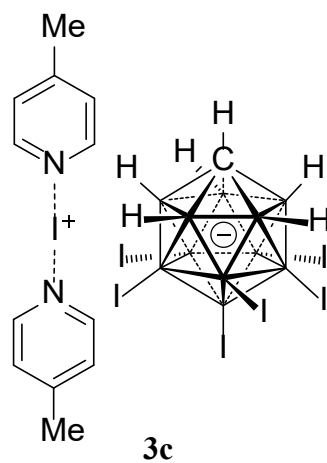
F2 - Acquisition Parameters
 Date_ 20250420
 Time 2.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126800 MHz
 WDW EM
 GB 0

251003-1, 11 mg in acetone-d₆
 19F NMR, 376 MHz, T=27 C

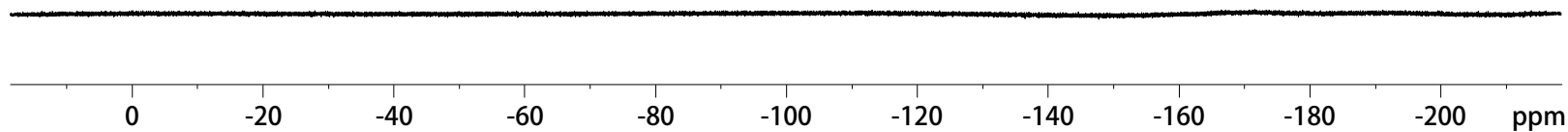


Current Data Parameters
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 EXPNO 3
 PROCNO 1

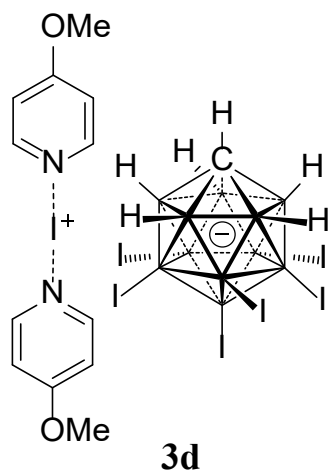
F2 - Acquisition Parameters
 Date_ 20251003
 Time 16.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 193.34
 DW 5.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 376.4607164 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 20.00000000 W

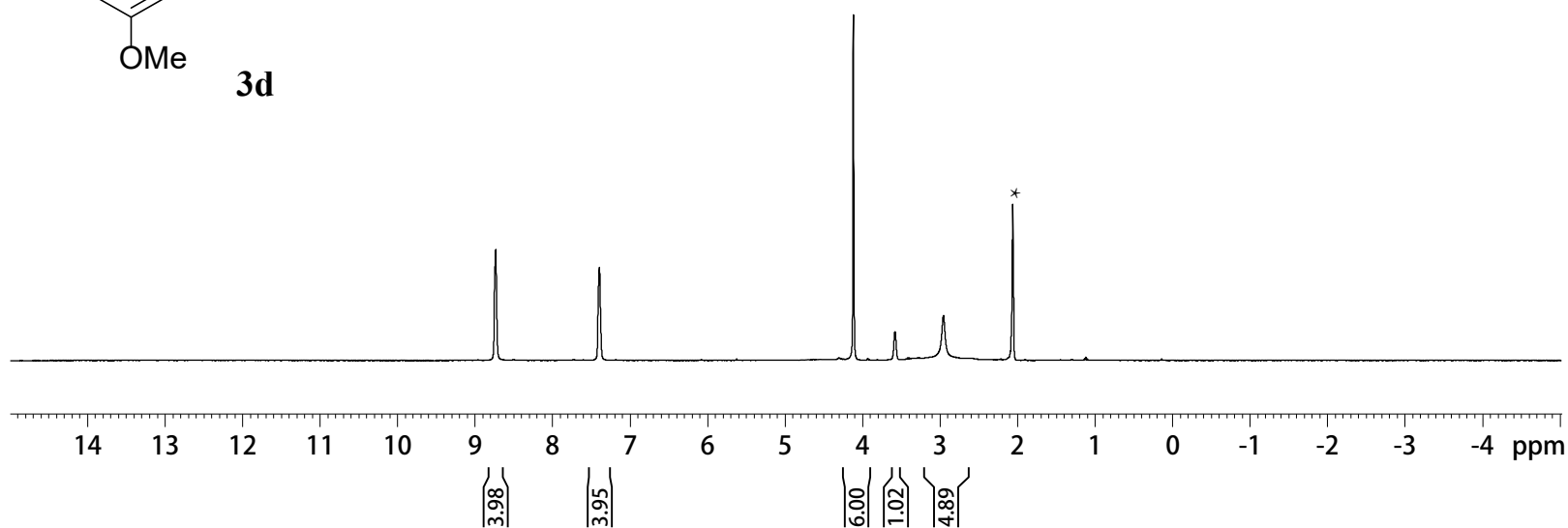
F2 - Processing parameters
 SI 65536
 SF 376.4983662 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



20250716-6I-OMePy, 18 mg in Acetone-d₆^{*}
¹H{¹¹B} NMR, 400 MHz, T= 28 C



8.72
 7.39
 4.11
 3.57
 2.95
 2.05



Current Data Parameters
 NAME 20250716-6I-OMePy
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250716
 Time 14.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgig30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 193.34
 DW 62.400 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

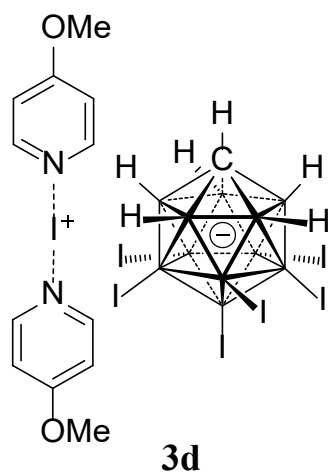
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 SFO1 400.1320007 MHz
 NUC1 ¹H
 P1 15.00 usec
 PLW1 12.50000000 W

===== CHANNEL f2 =====
 SFO2 128.3776050 MHz
 NUC2 ¹¹B
 CPDPRG2 garp4
 PCPD2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.64477998 W

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

20250716-6I-OMePy, 18 mg in Acetone-d6
¹¹B{¹H} NMR, 128 MHz, T= 28 C

— -6.88
 — -14.77
 — -19.14



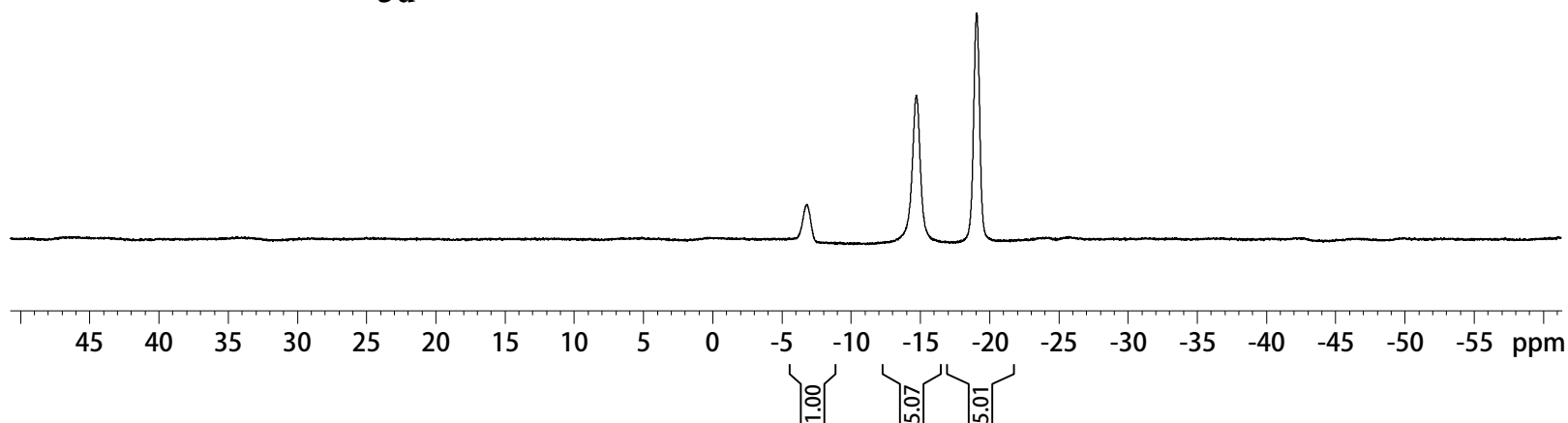
Current Data Parameters
 NAME 20250716-6I-OMePy
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250716
 Time 14.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

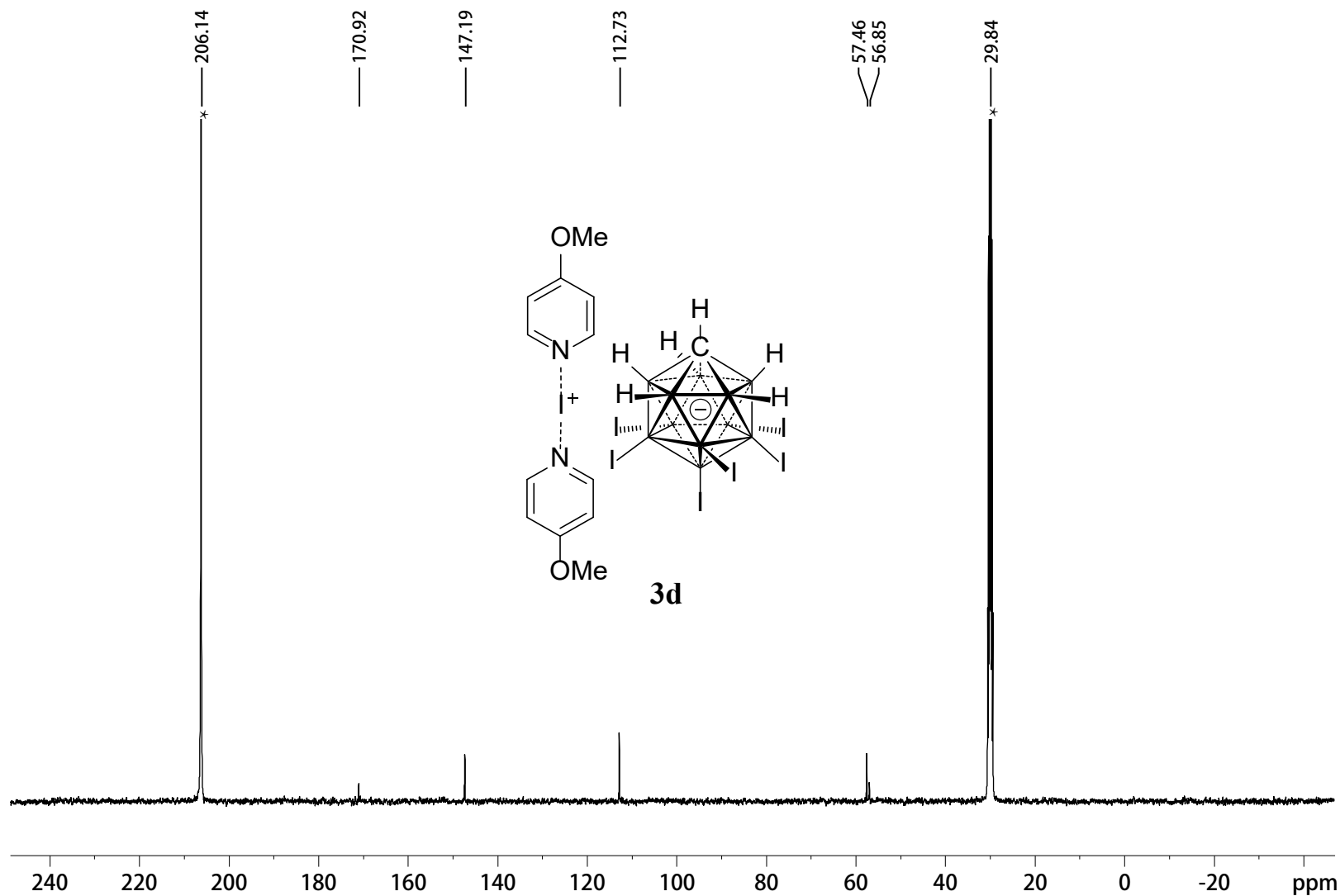
===== CHANNEL f1 =====
 SFO1 128.3776050 MHz
 NUC1 11B
 P1 9.93 usec
 PLW1 52.96599960 W

===== CHANNEL f2 =====
 SFO2 400.1320007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

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



20250716-6I-OMePy, 18 mg in Acetone-d₆^{*}
¹³C{¹H} NMR, 100 MHz, T= 28 C



Current Data Parameters
 NAME 20250716-6I-OMePy
 EXPNO 3
 PROCNO 1

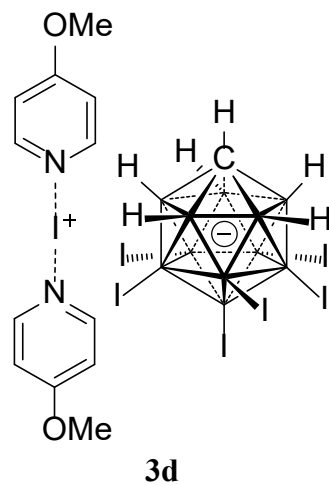
F2 - Acquisition Parameters
 Date_ 20250716
 Time 14.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126799 MHz
 WDW EM
 GB 0

251001-3d, 10 mg in acetone-d₆
¹⁹F NMR, 376 MHz, T=27 °C

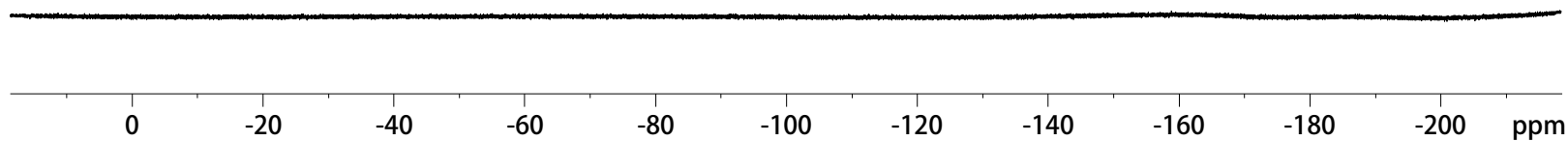


Current Data Parameters
 NAME 251001-3d
 EXPNO 4
 PROCNO 1

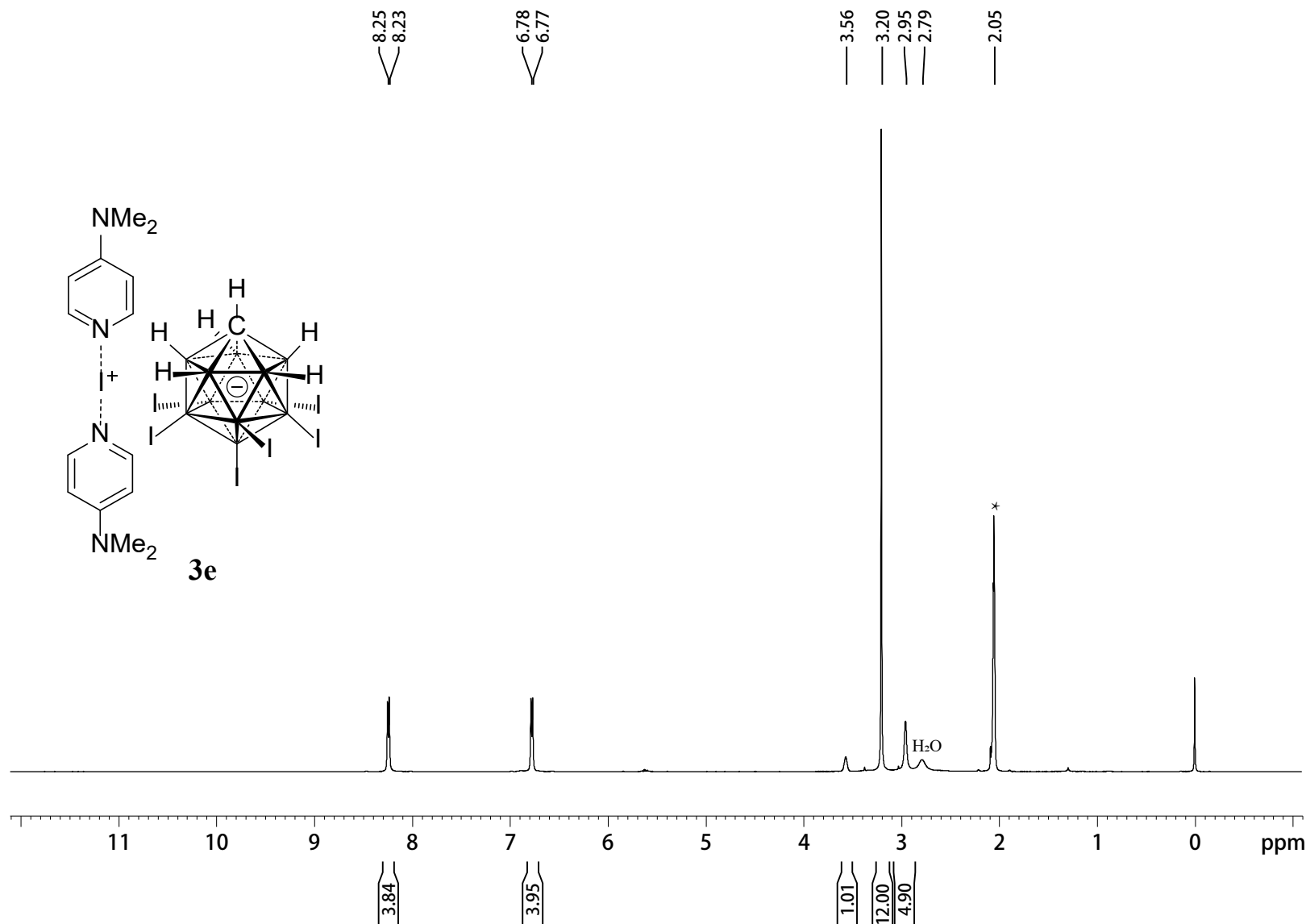
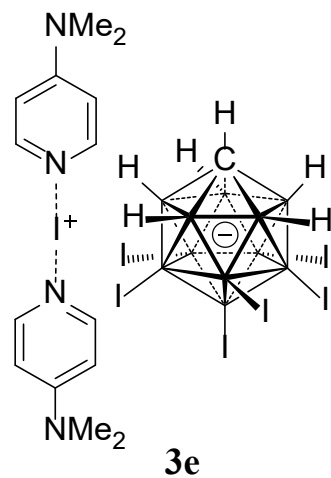
F2 - Acquisition Parameters
 Date_ 20251001
 Time 17.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 193.34
 DW 5.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 376.4607164 MHz
 NUC1 ¹⁹F
 P1 15.00 usec
 PLW1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 376.4983662 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



EXP-CLY-13, 18 mg in Acetone-d₆^{*}
¹H{¹¹B} NMR, 400 MHz, T= 28 C



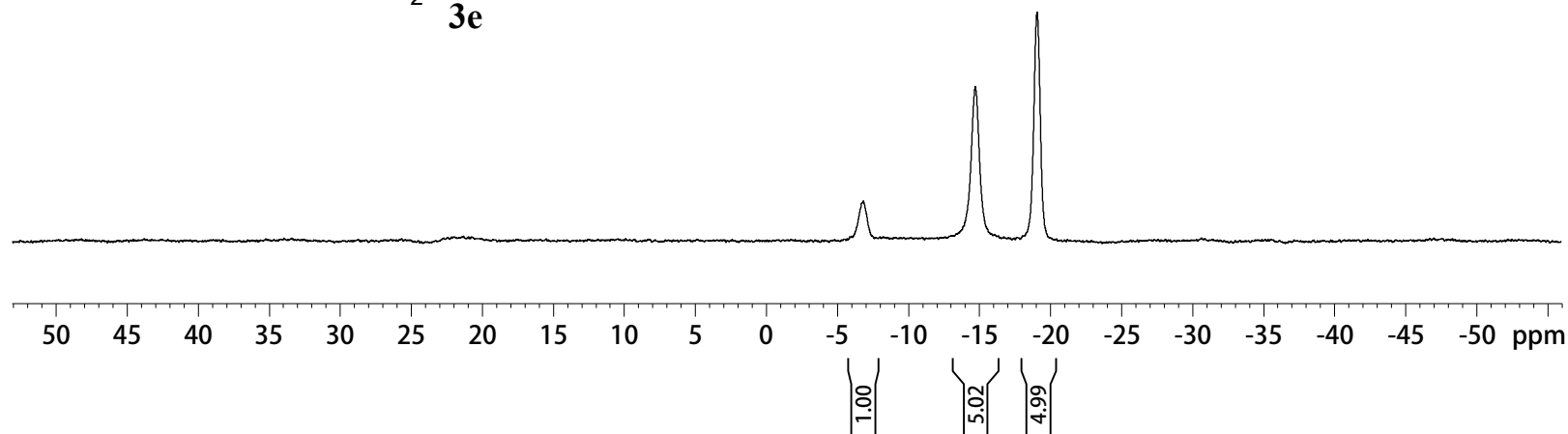
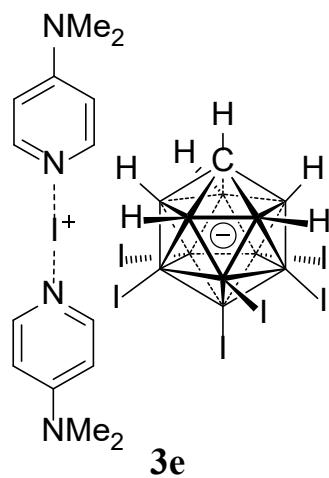
Current Data Parameters
 NAME EXP-CLY-13_2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241219
 Time 15.43 h
 INSTRUM spect
 PROBHD Z108618_0497 (
 PULPROG zgig30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.978127 Hz
 AQ 1.0223616 sec
 RG 193.34
 DW 62.400 usec
 DE 6.50 usec
 TE 297.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 400.1320007 MHz
 NUC1 ¹H
 P1 15.00 usec
 PLW1 15.48099995 W
 SFO2 128.3776050 MHz
 NUC2 ¹¹B
 CPDPRG2 garp4
 PCPD2 60.00 usec
 PLW2 52.96599960 W
 PLW12 1.45079994 W

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

EXP-CLY-13, 18 mg in Acetone-d₆
11B{1H} NMR, 128 MHz, T= 28 C

— -6.87
— -14.77
— -19.12



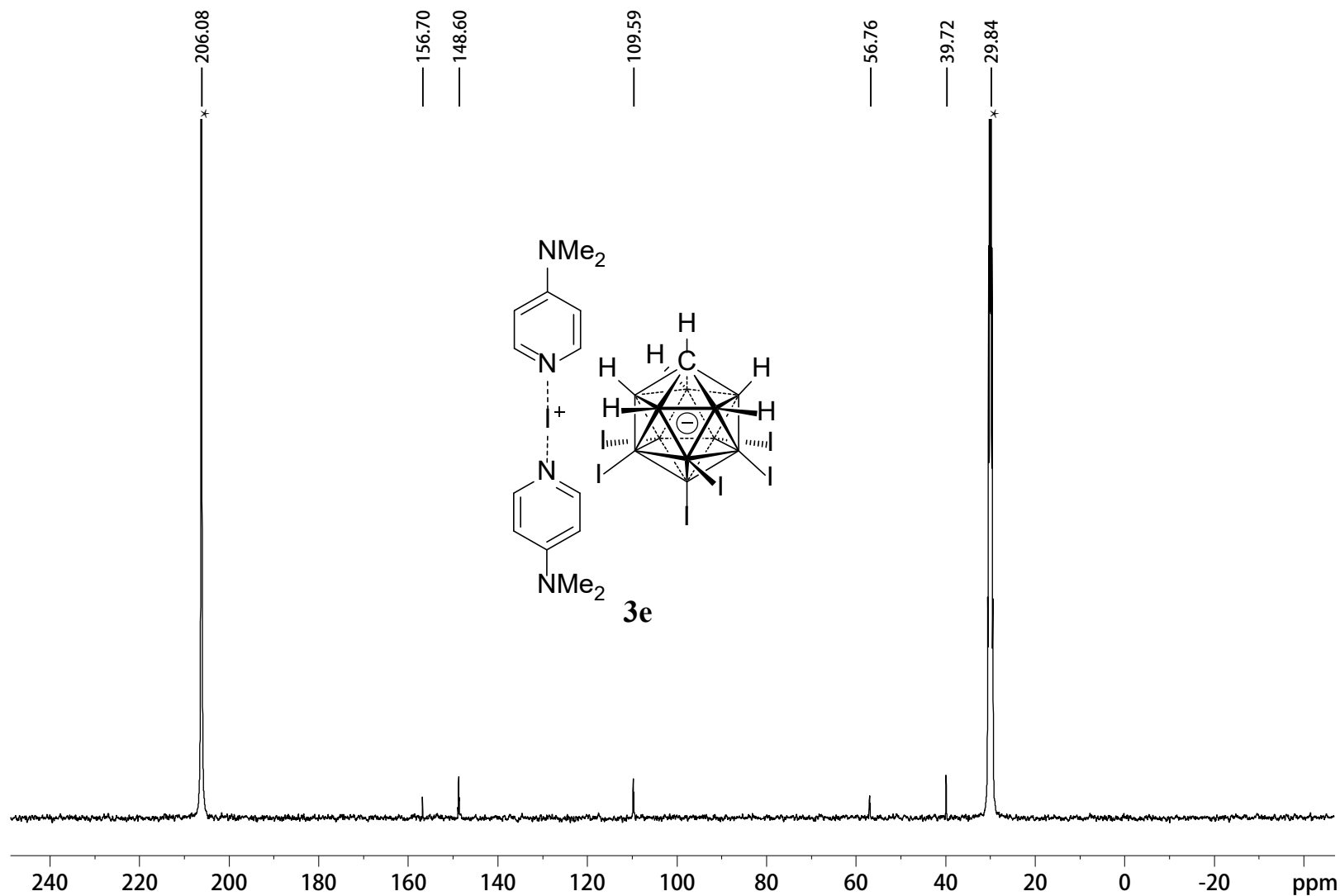
S50

Current Data Parameters
NAME EXP-CLY-13_2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241219
Time 21.23 h
INSTRUM spect
PROBHD Z108618_0497 (
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.778510 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 128.3776050 MHz
NUC1 11B
P1 9.93 usec
PLW1 52.96599960 W
SFO2 400.1320007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.48099995 W
PLW12 0.43002000 W
PLW13 0.21630000 W

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

EXP-CLY-13, 18 mg in Acetone-d₆^{*}
¹³C{¹H} NMR, 100 MHz, T= 28 C

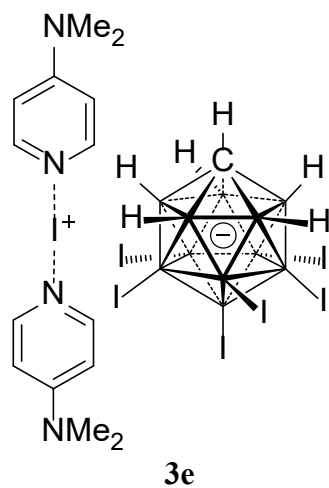


Current Data Parameters
 NAME EXP-CLY-13_2
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241219
 Time 22.10 h
 INSTRUM spect
 PROBHD Z108618_0497 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6228293 MHz
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 66.13099670 W
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 15.48099995 W
 PLW12 0.43002000 W
 PLW13 0.21630000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126772 MHz
 WDW EM
 SSB 0
 LB 10.00 Hz
 GB 0
 PC 1.40

251001-3e, 13 mg in acetone-d6
 19F NMR, 376 MHz, T=27 C

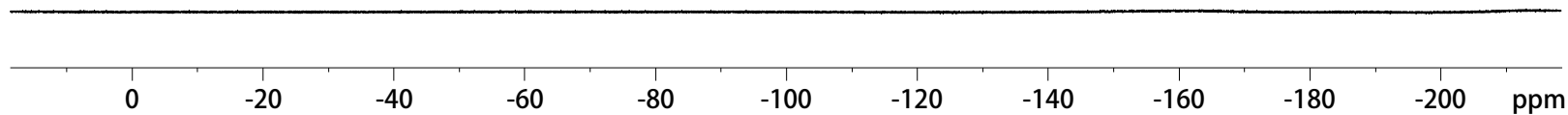


Current Data Parameters
 NAME 251001-3e
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251001
 Time 17.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 193.34
 DW 5.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 376.4607164 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 376.4983662 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



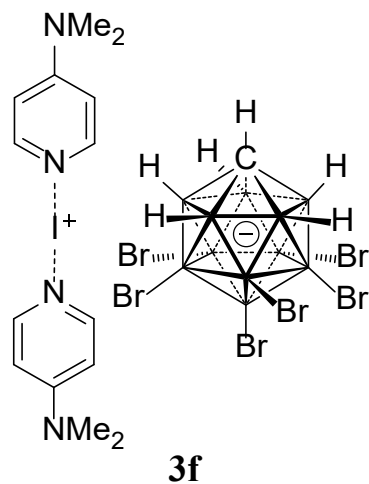
EXP-JCN-15, 16.5 mg in Acetone-d6*
 1H{11B} NMR, 400 MHz, T= 28 C

8.29
8.27

6.95
6.93

3.24
3.06
3.05

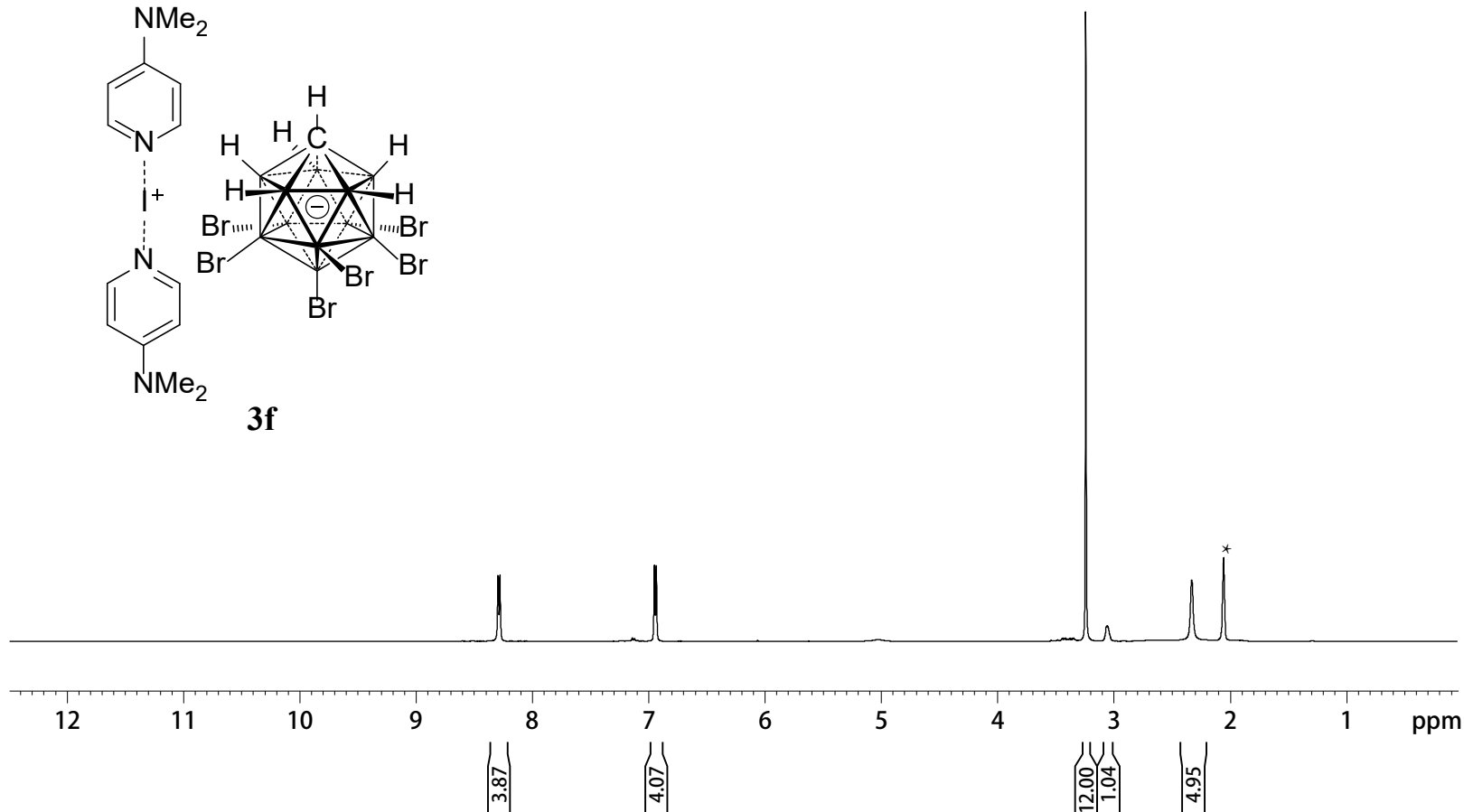
2.32
2.05
2.05
2.05



Current Data Parameters
 NAME EXP-JCN-15
 EXPNO 1
 PROCNO 1

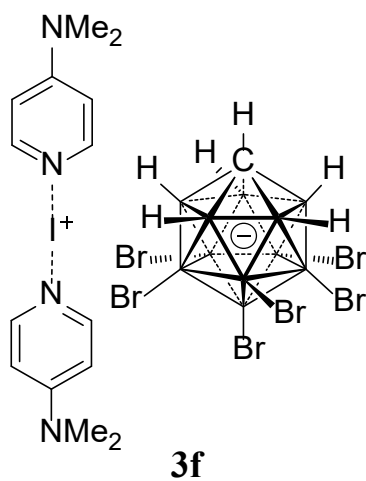
F2 - Acquisition Parameters
 Date_ 20241219
 Time 18.32 h
 INSTRUM spect
 PROBHD Z108618_0497 (
 PULPROG zgig30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.978127 Hz
 AQ 1.0223616 sec
 RG 193.34
 DW 62.400 usec
 DE 6.50 usec
 TE 296.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 400.1320007 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.48099995 W
 SFO2 128.3776050 MHz
 NUC2 11B
 CPDPRG2 garp4
 PCPD2 60.00 usec
 PLW2 52.96599960 W
 PLW12 1.45079994 W

F2 - Processing parameters
 SI 32768
 SF 400.1300075 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



EXP-JCN-15, 16.5 mg in Acetone-d6
¹¹B{¹H} NMR, 128 MHz, T= 28 C

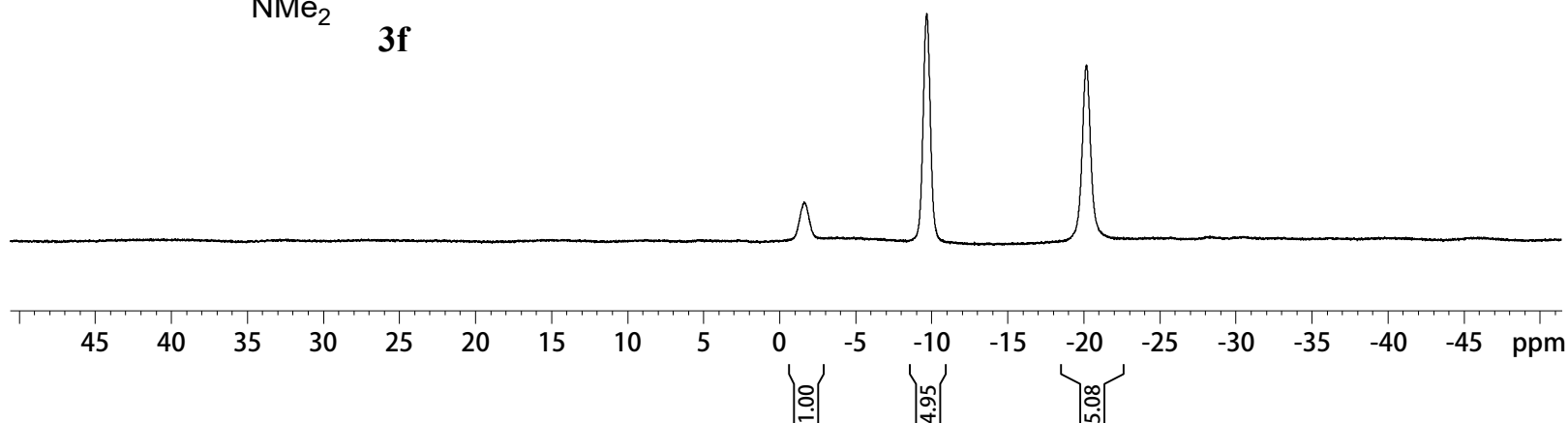
— -1.64 — — -9.72 — — -20.20 —



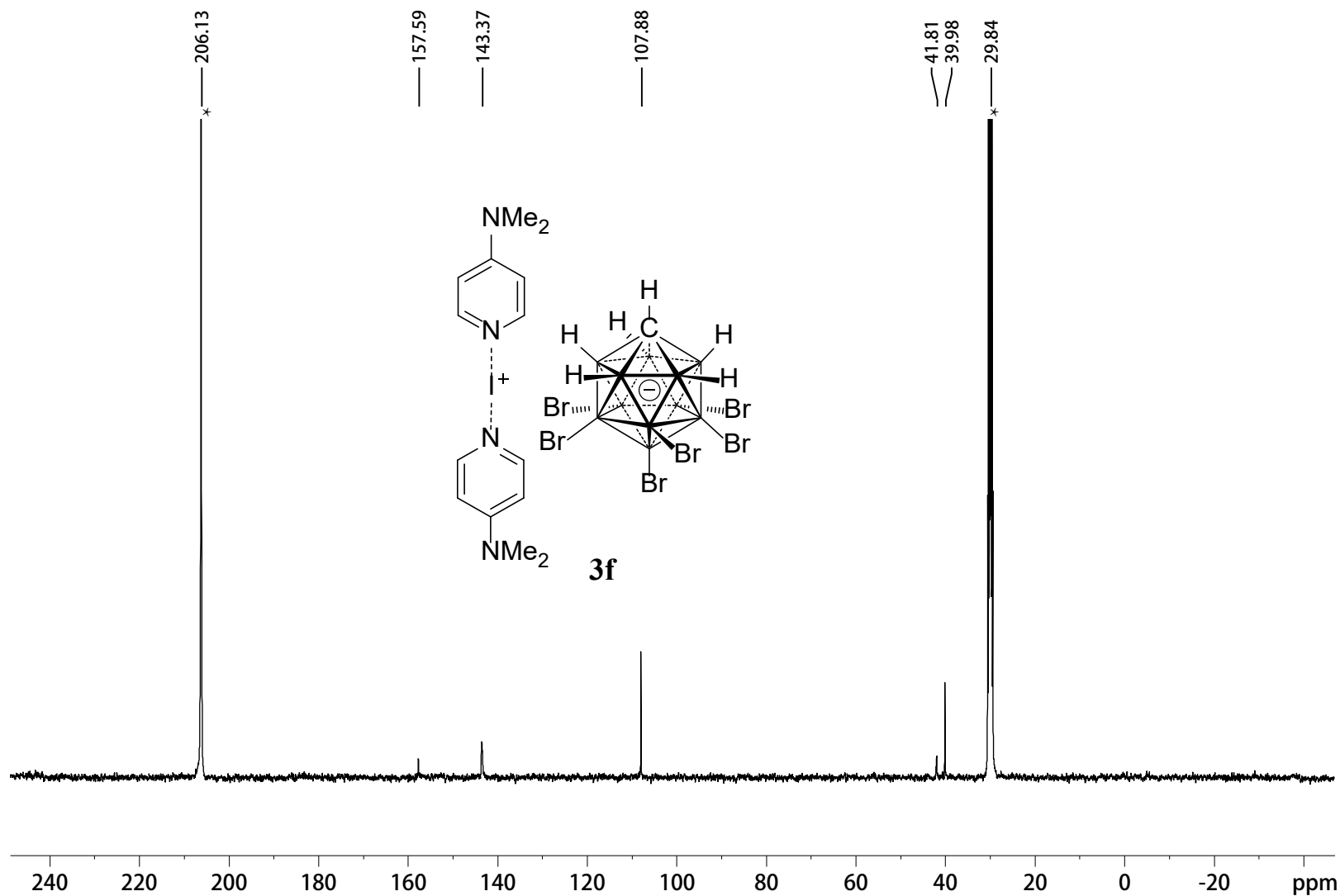
Current Data Parameters
 NAME EXP-JCN-15
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241219
 Time 18.38 h
 INSTRUM spect
 PROBHD Z108618_0497 (
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.778510 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 296.9 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 128.3776050 MHz
 NUC1 ¹¹B
 P1 9.93 usec
 PLW1 52.96599960 W
 SFO2 400.1320007 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 15.48099995 W
 PLW12 0.43002000 W
 PLW13 0.21630000 W

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



EXP-JCN-15, 16.5 mg in Acetone-d₆*
¹³C{¹H} NMR, 100 MHz, T= 28 C

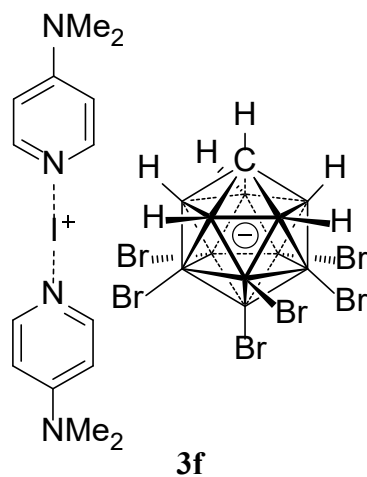


Current Data Parameters
 NAME EXP-JCN-15
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241219
 Time 19.25 h
 INSTRUM spect
 PROBHD Z108618_0497 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6228293 MHz
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 66.13099670 W
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 15.48099995 W
 PLW12 0.43002000 W
 PLW13 0.21630000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126799 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

251001-3f, 12 mg in acetone-d6
 19F NMR, 376 MHz, T=27 C

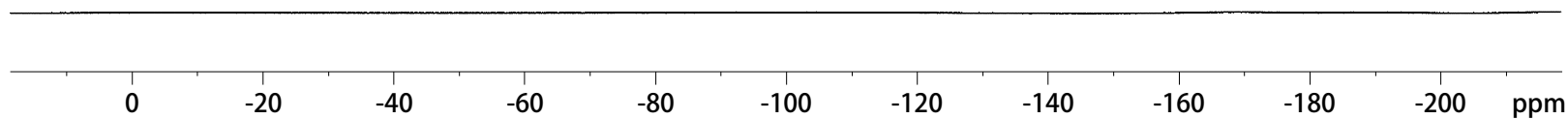


Current Data Parameters
 NAME 251001-3f
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251001
 Time 12.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 193.34
 DW 5.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D0 1

===== CHANNEL f1 =====
 SF01 376.4607164 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 376.4983662 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Exp-JCN-39, 16.5 mg in Acetone-d6*
¹H{¹¹B} NMR, 400 MHz, T= 28 C

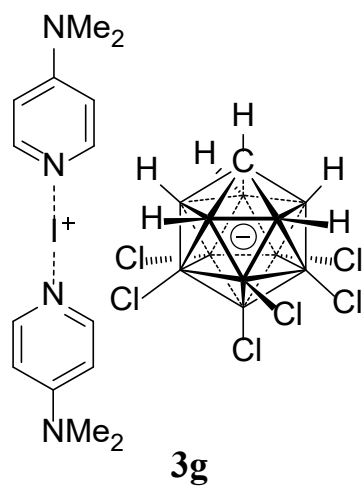
8.28
8.26

6.94
6.93

3.23

2.57

2.05
1.92



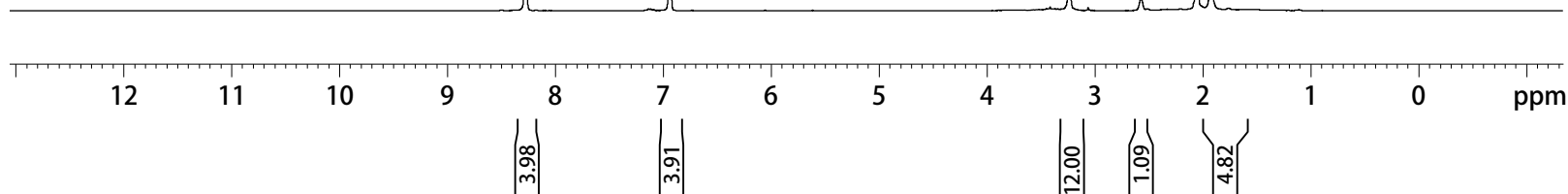
Current Data Parameters
 NAME Exp-JCN-39
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250420
 Time 13.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgig30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 193.34
 DW 62.400 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

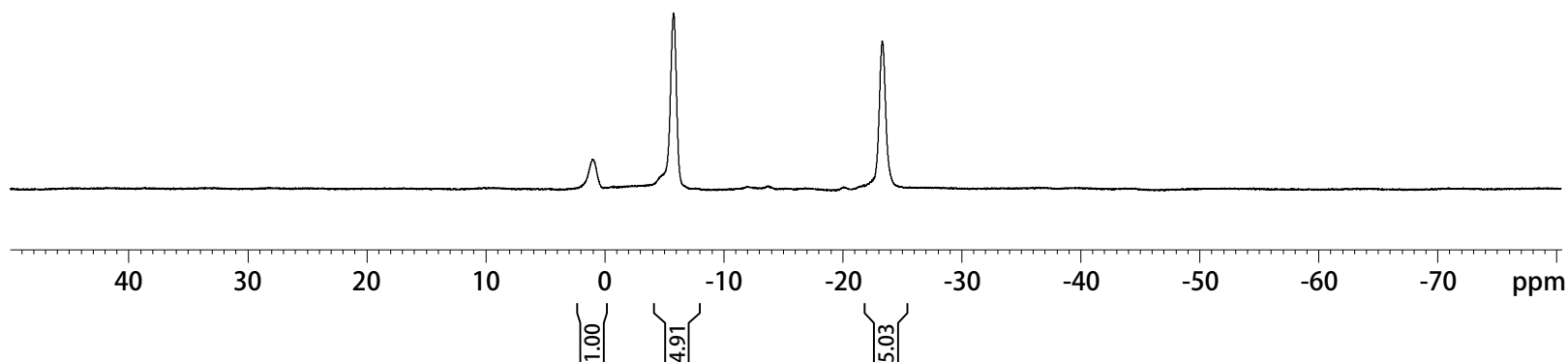
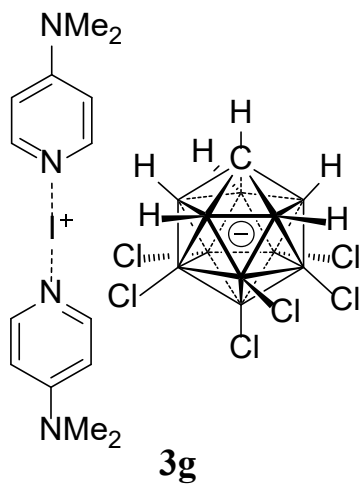
===== CHANNEL f2 =====
 SFO2 128.3776050 MHz
 NUC2 ¹¹B
 CPDPRG2 garp4
 PCPD2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.64477998 W

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



Exp-JCN-39, 16.5 mg in Acetone-d6
 $^{11}\text{B}\{^1\text{H}\}$ NMR, 128 MHz, T= 28 C

0.93
 -5.84
 -23.39



Current Data Parameters
 NAME Exp-JCN-39
 EXPNO 2
 PROCNO 1

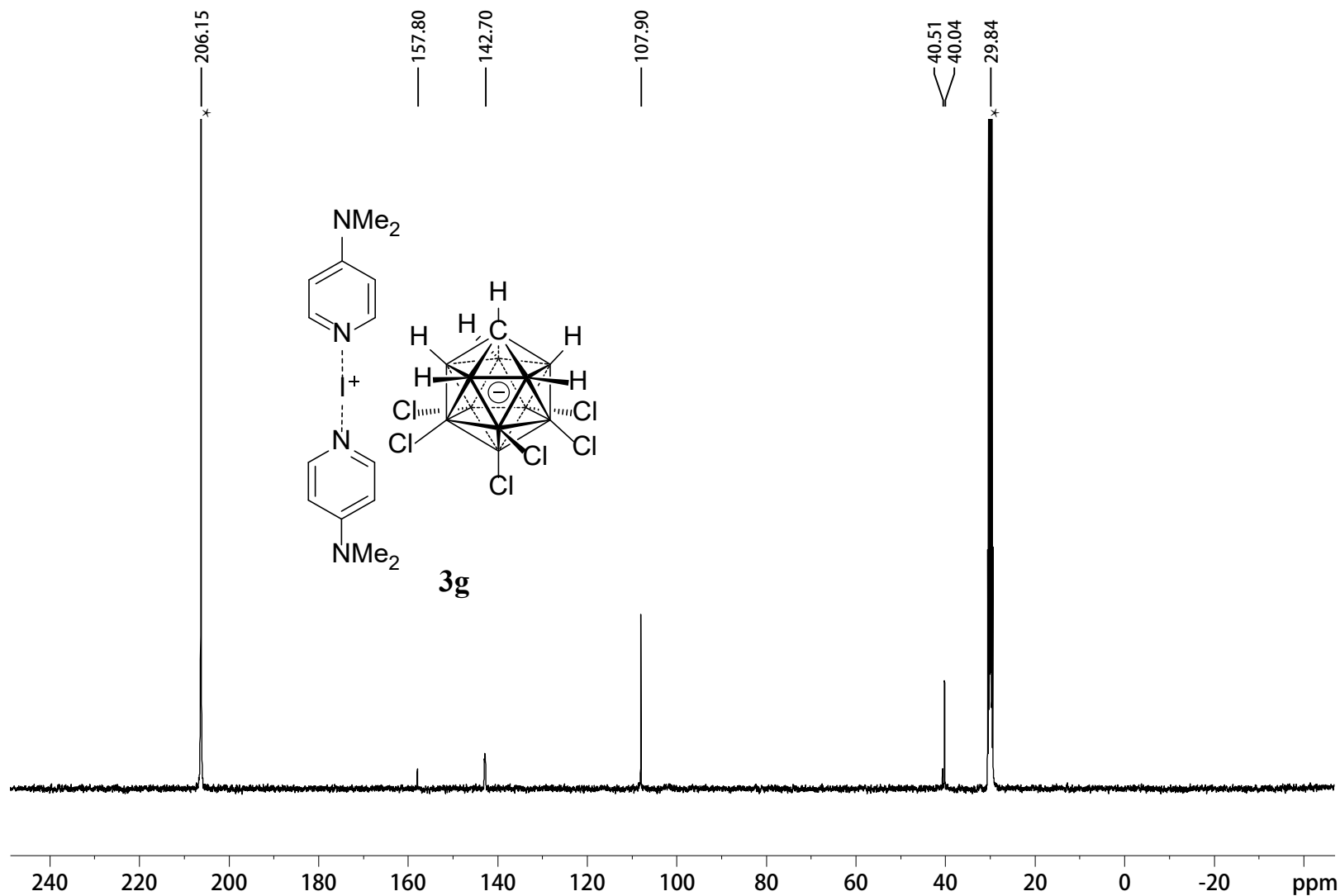
F2 - Acquisition Parameters
 Date_ 20250420
 Time 0.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 SFO2 400.1320007 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

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

Exp-JCN-39, 16.5 mg in Acetone-d6*
¹³C{¹H} NMR, 100 MHz, T= 28 C



Current Data Parameters
 NAME Exp-JCN-39
 EXPNO 3
 PROCNO 1

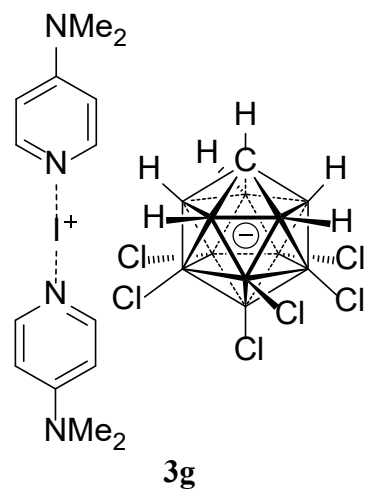
F2 - Acquisition Parameters
 Date_ 20250420
 Time 1.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126800 MHz
 WDW EM
 SSB 0

251003-3g, 13 mg in acetone-d₆
¹⁹F NMR, 376 MHz, T=27 °C

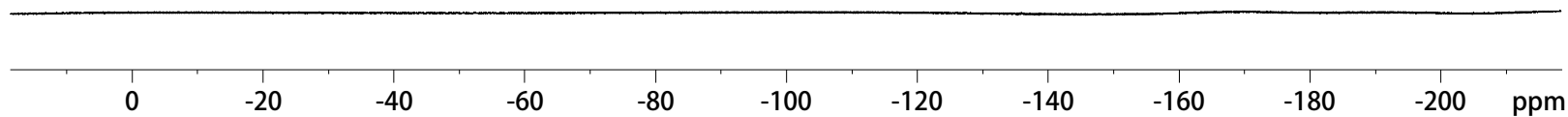


Current Data Parameters
 NAME 251003-3g
 EXPNO 2
 PROCNO 1

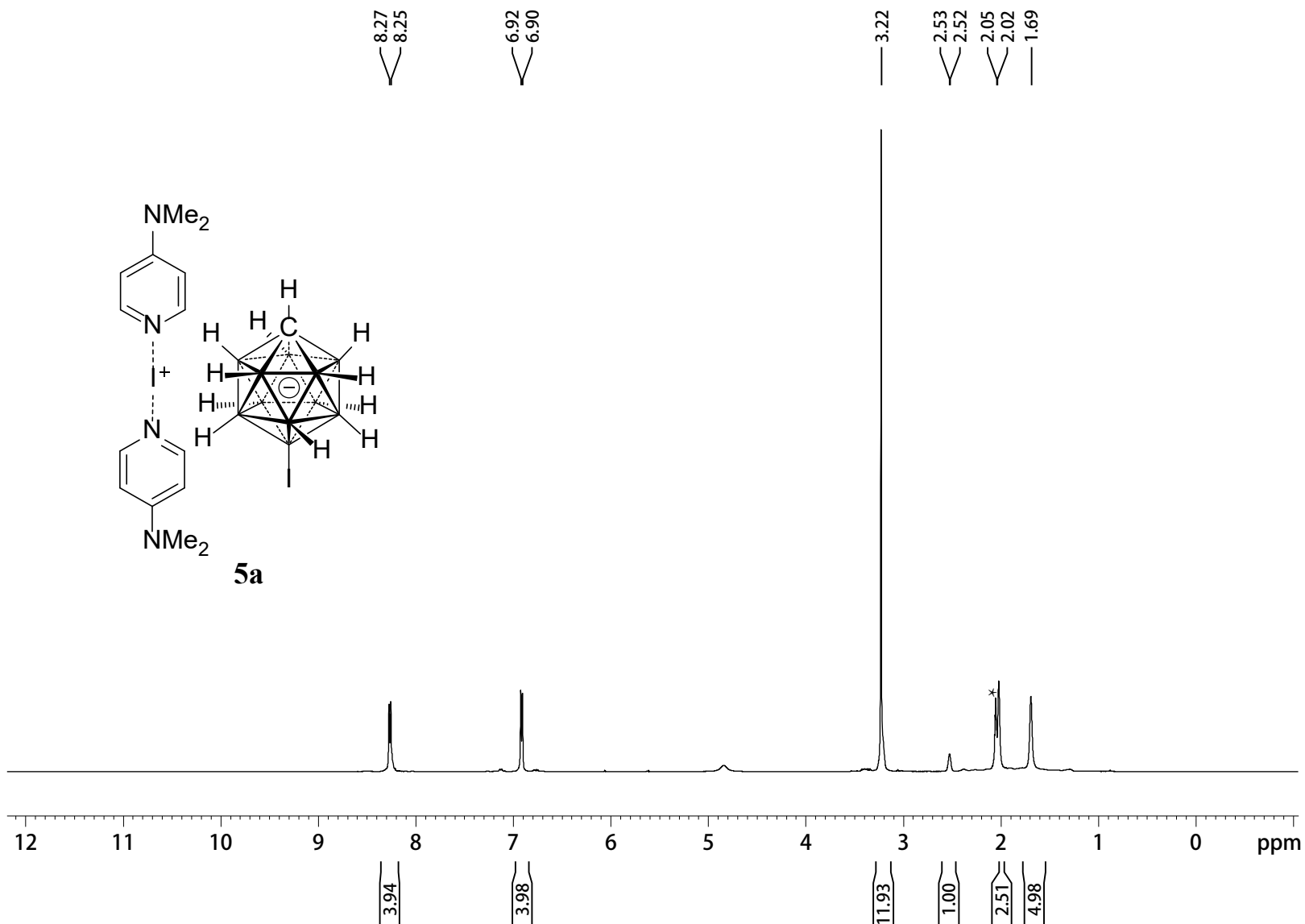
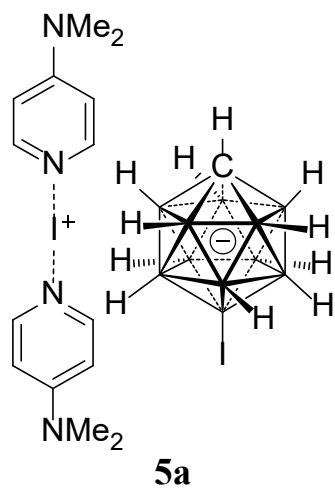
F2 - Acquisition Parameters
 Date_ 20251003
 Time 19.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 193.34
 DW 5.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 376.4607164 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 376.4983662 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



241117-JCNCLY-08, 16.6 mg in Acetone-d₆^{*}
¹H{¹¹B} NMR, 400 MHz, T= 28 C



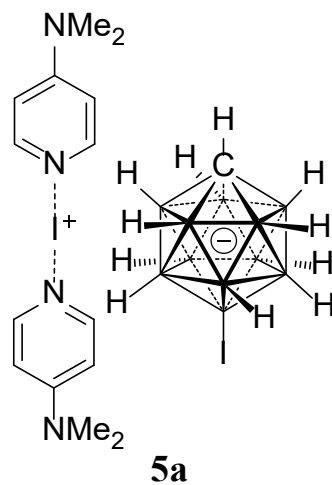
Current Data Parameters
 NAME 241117-JCNCLY-08
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241117
 Time 15.44 h
 INSTRUM spect
 PROBHD Z108618_0497 ()
 PULPROG zgig30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.978127 Hz
 AQ 1.0223616 sec
 RG 170.36
 DW 62.400 usec
 DE 6.50 usec
 TE 299.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 400.1320007 MHz
 NUC1 ¹H
 P1 15.00 usec
 PLW1 15.48099995 W
 SFO2 128.3776050 MHz
 NUC2 ¹¹B
 CPDPRG2 garp4
 PCPD2 60.00 usec
 PLW2 52.96599960 W
 PLW12 1.45079994 W

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

241117-JCNCLY-08, 16.6 mg in Acetone-d6
¹¹B{¹H} NMR, 400 MHz, T= 28 C

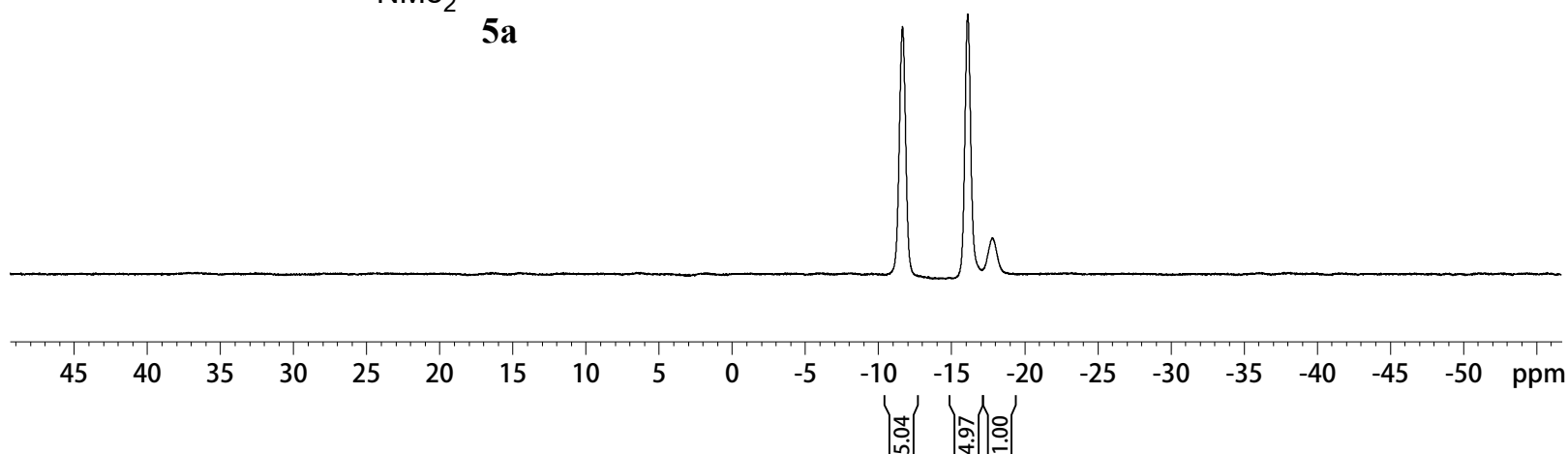
— 11.69
 — 16.17
 — 17.86



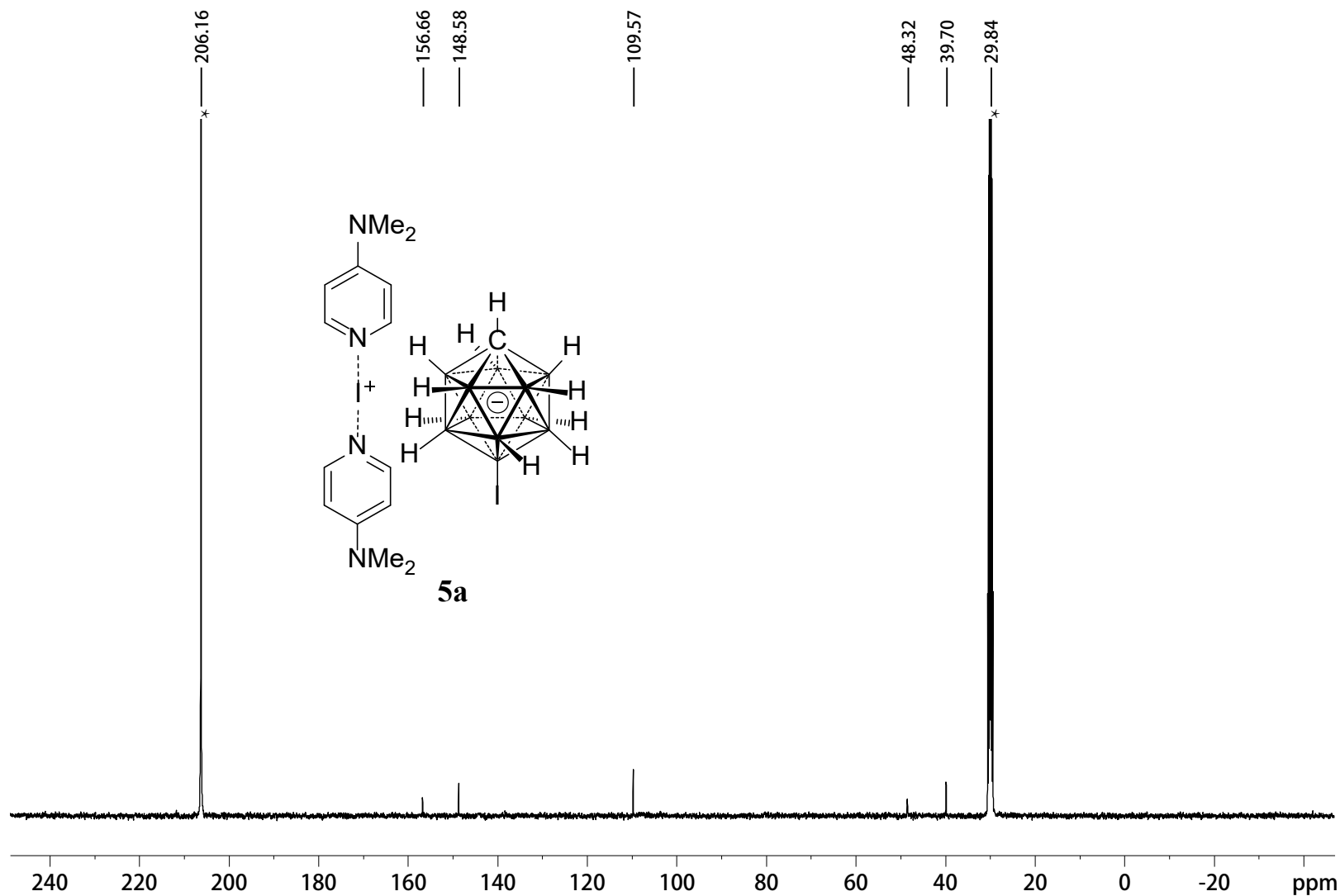
Current Data Parameters
 NAME 241117-JCNCLY-08
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241117
 Time 15.50 h
 INSTRUM spect
 PROBHD Z108618_0497 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.778510 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 300.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 128.3776050 MHz
 NUC1 ¹¹B
 P1 9.93 usec
 PLW1 52.96599960 W
 SFO2 400.1320007 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 15.48099995 W
 PLW12 0.43002000 W
 PLW13 0.21630000 W

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



241117-JCNCLY-08, 16.6 mg in Acetone-d₆
¹³C{¹H} NMR, 100 MHz, T= 28 C



Current Data Parameters
 NAME 241117-JCNCLY-08
 EXPNO 1
 PROCNO 1

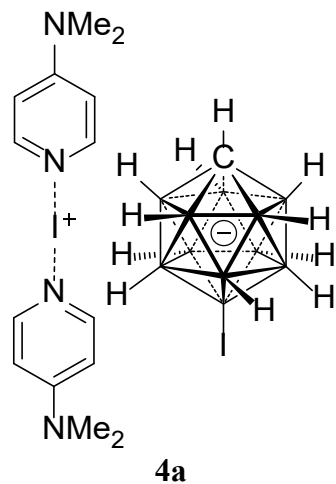
F2 - Acquisition Parameters
 Date_ 20241117
 Time 13.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126790 MHz
 WDW EM
 GB 0

251003-4a, 12 mg in acetone-d6
 19F NMR, 376 MHz, T=28 C

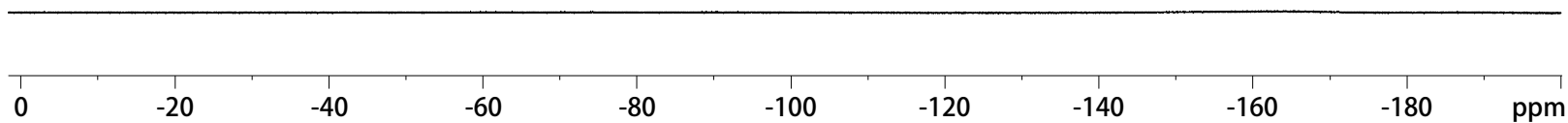


Current Data Parameters
 NAME 251003-4a
 EXPNO 1
 PROCNO 1

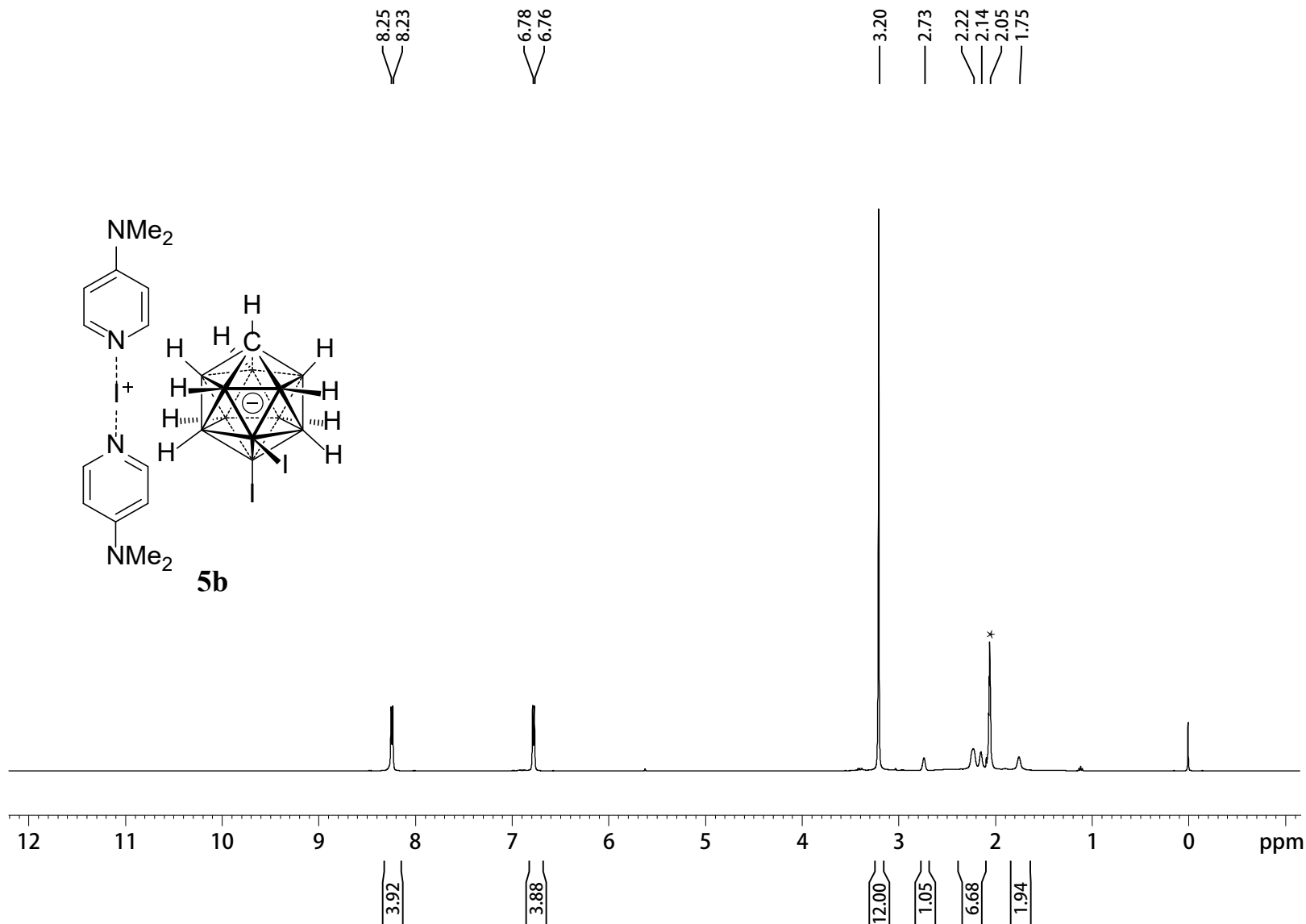
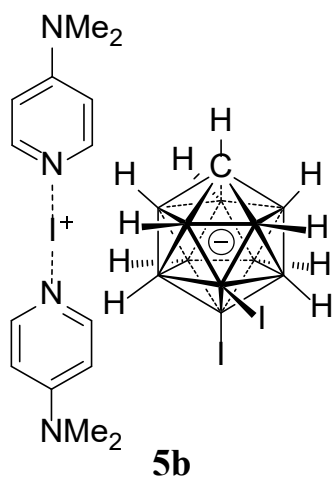
F2 - Acquisition Parameters
 Date_ 20251003
 Time 18.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 193.34
 DW 5.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 376.4607164 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 376.4983662 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



EXP-CLY-16, 15.5 mg in Acetone-d₆^{*}
¹H{¹¹B} NMR, 400 MHz, T= 28 C



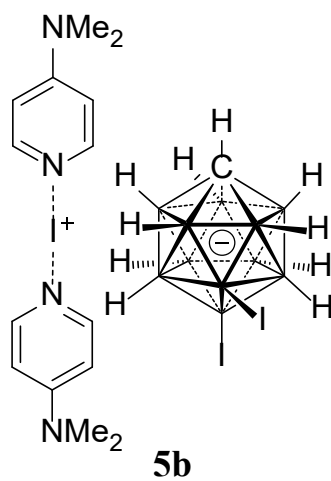
Current Data Parameters
 NAME EXP-CLY-16
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241219
 Time 20.21 h
 INSTRUM spect
 PROBHD Z108618_0497 (
 PULPROG zgig30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.978127 Hz
 AQ 1.0223616 sec
 RG 193.34
 DW 62.400 usec
 DE 6.50 usec
 TE 297.4 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 400.1320007 MHz
 NUC1 ¹H
 P1 15.00 usec
 PLW1 15.48099995 W
 SFO2 128.3776050 MHz
 NUC2 ¹¹B
 CPDPRG2 garp4
 PCPD2 60.00 usec
 PLW2 52.96599960 W
 PLW12 1.45079994 W

F2 - Processing parameters
 SI 32768
 SF 400.1300062 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

EXP-CLY-16, 15.5 mg in Acetone-d6
¹¹B{¹H} NMR, 128 MHz, T= 28 C

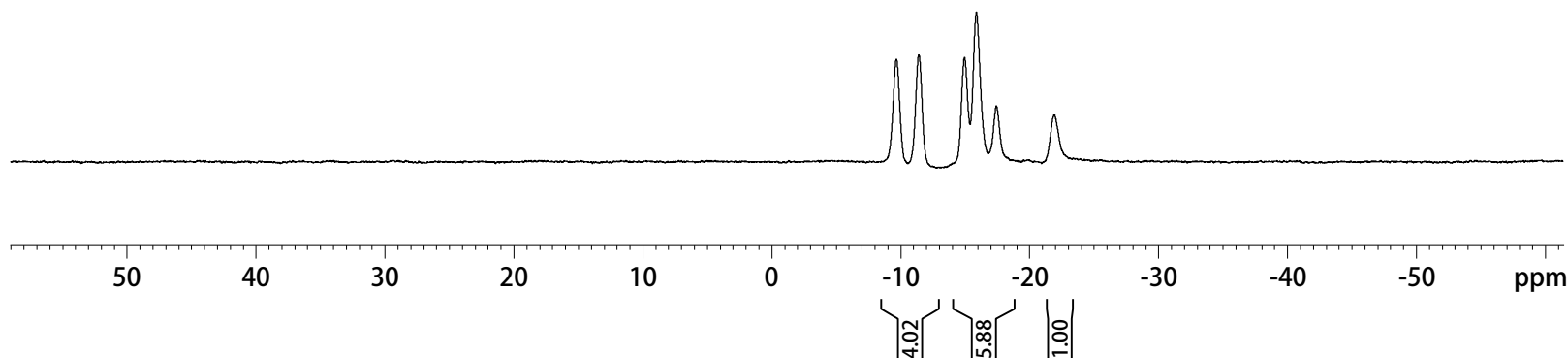
-9.76
 -11.49
 -15.00
 -15.95
 -17.49
 -22.02



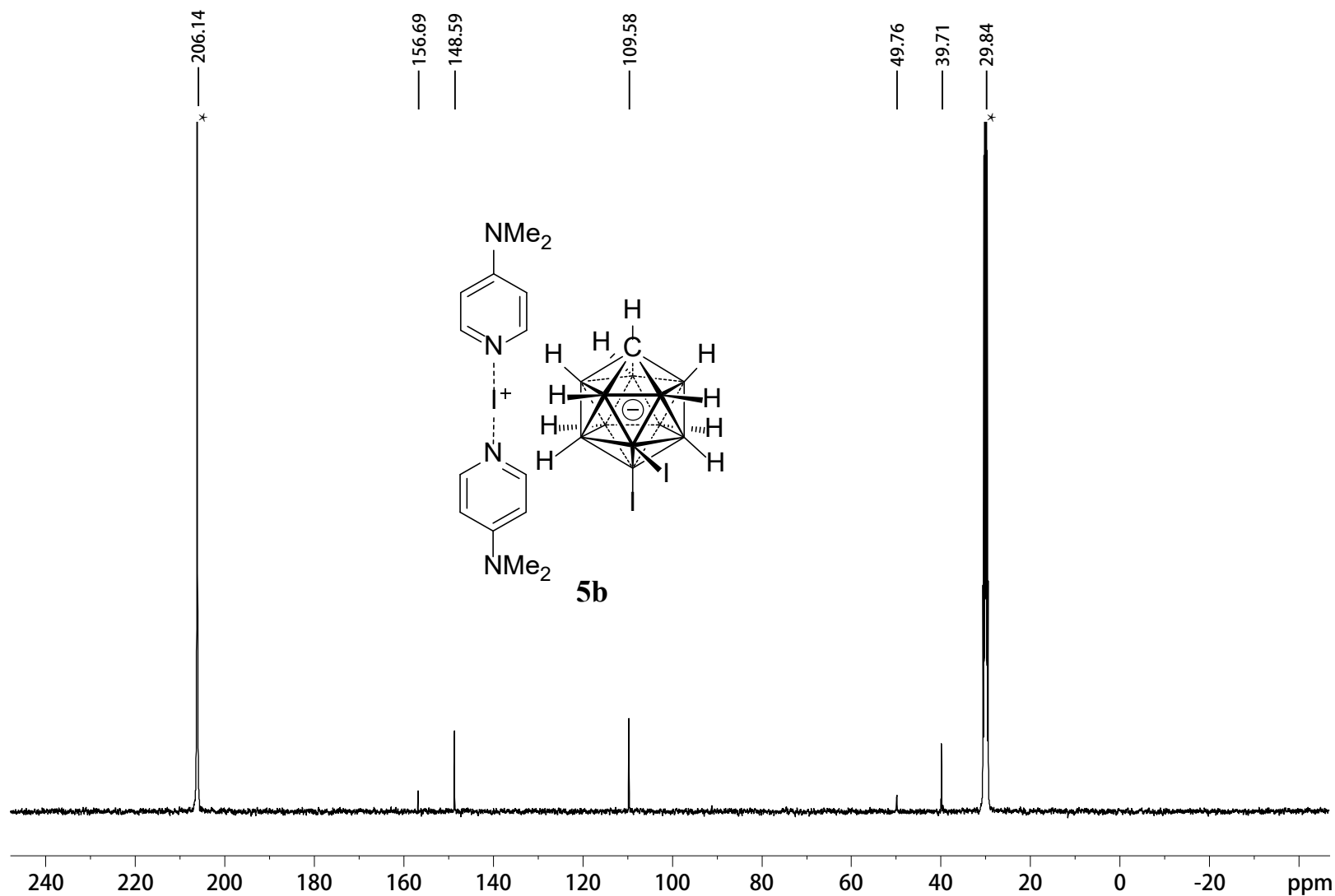
Current Data Parameters
 NAME EXP-CLY-16
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241219
 Time 20.27 h
 INSTRUM spect
 PROBHD Z108618_0497 (
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.778510 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 128.3776050 MHz
 NUC1 ¹¹B
 P1 9.93 usec
 PLW1 52.96599960 W
 SFO2 400.1320007 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 15.48099995 W
 PLW12 0.43002000 W
 PLW13 0.21630000 W

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



EXP-CLY-16, 15.5 mg in Acetone-d₆^{*}
¹³C{¹H} NMR, 100 MHz, T= 28 C

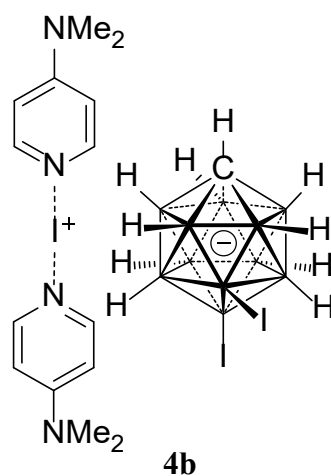


Current Data Parameters
 NAME EXP-CLY-16
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241219
 Time 21.14 h
 INSTRUM spect
 PROBHD Z108618_0497 (
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6228293 MHz
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 66.13099670 W
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 15.48099995 W
 PLW12 0.43002000 W
 PLW13 0.21630000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126777 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

251003-4b, 13 mg in acetone-d₆
¹⁹F NMR, 376 MHz, T=26 C

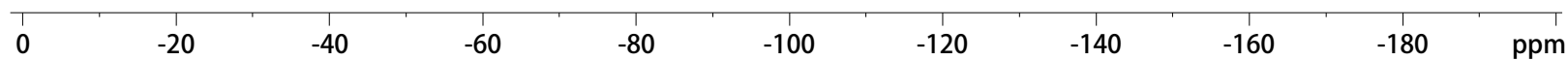


Current Data Parameters
 NAME 251003-4b
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251003
 Time 18.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 193.34
 DW 5.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 TD0 1

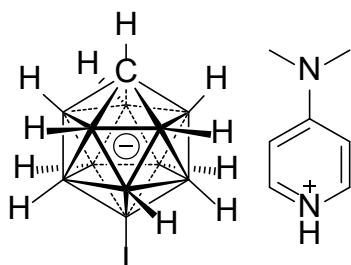
===== CHANNEL f1 =====
 SF01 376.4607164 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 376.4983662 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

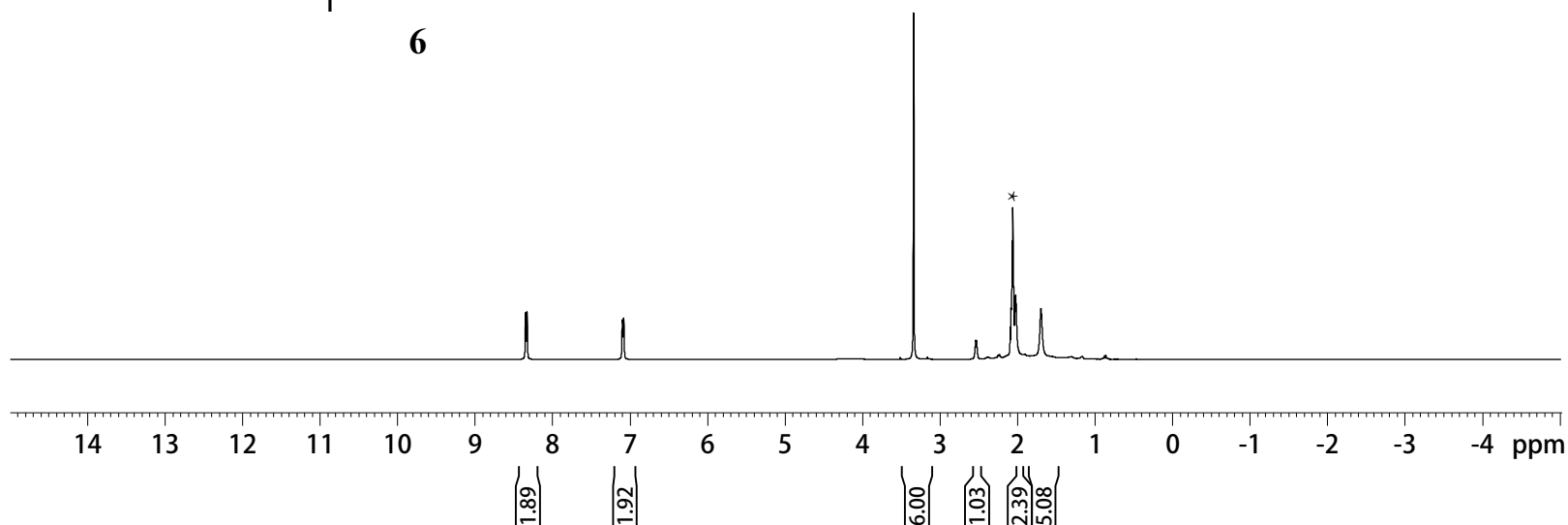


py-01, 16.6 mg in Acetone-d6*
¹H{¹¹B} NMR, 400 MHz, T= 27 C

8.34
8.32
7.09
7.07
3.33
2.53
2.52
2.05
2.01
1.69



6



Current Data Parameters
 NAME py-01
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250703
 Time 21.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgig30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 193.34
 DW 62.400 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

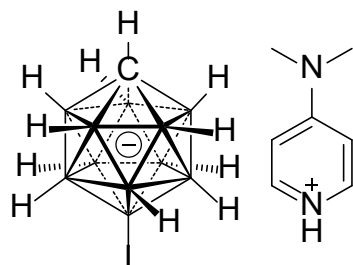
===== CHANNEL f1 =====
 SFO1 400.1320007 MHz
 NUC1 ¹H
 P1 15.00 usec
 PLW1 12.50000000 W

===== CHANNEL f2 =====
 SFO2 128.3776050 MHz
 NUC2 ¹¹B
 CPDPRG2 garp4
 PCPD2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.64477998 W

F2 - Processing parameters
 SI 32768
 SF 400.1300070 MHz
 WDW EM
 SSB 0
 GB 0

py-01, 16.6 mg in Acetone-d6
¹¹B{¹H} NMR, 128 MHz, T= 27 C

11.71
 16.17
 17.87



6

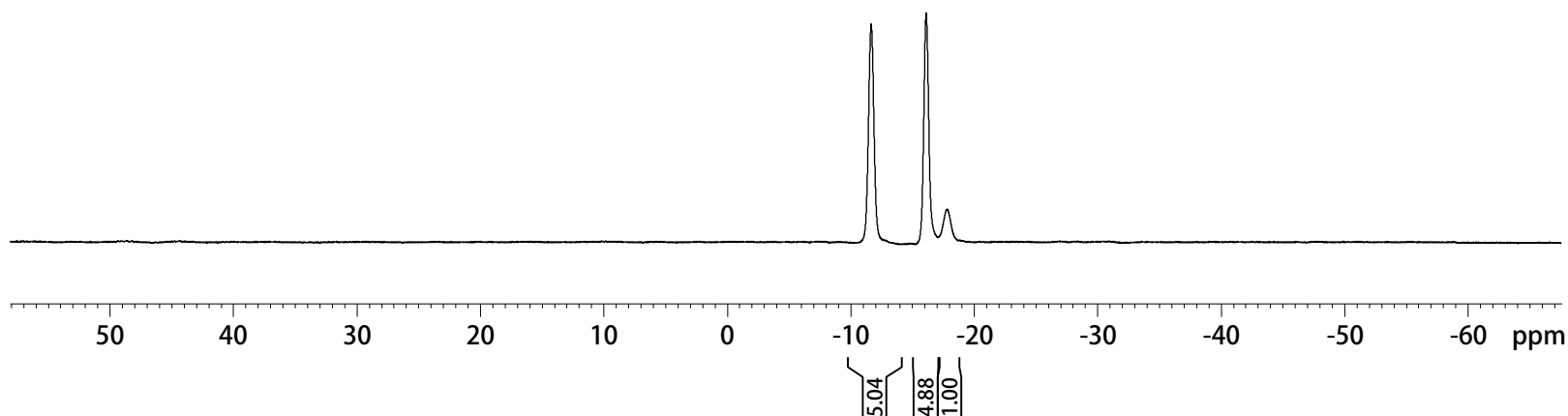
Current Data Parameters
 NAME py-01
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250703
 Time 21.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

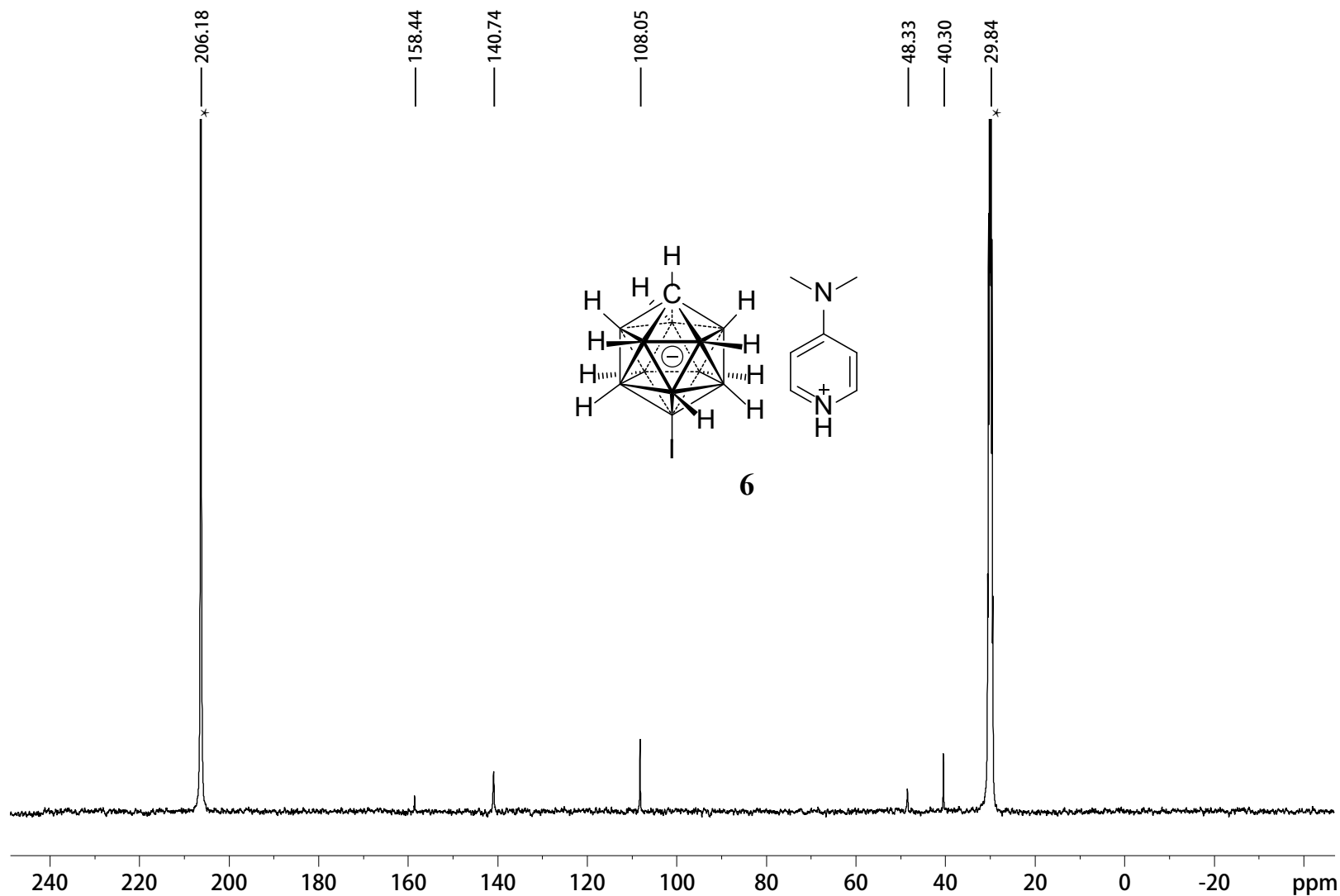
===== CHANNEL f1 =====
 SFO1 128.3776050 MHz
 NUC1 ¹¹B
 P1 9.93 usec
 PLW1 52.96599960 W

===== CHANNEL f2 =====
 SFO2 400.1320007 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

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



py-01, 16.6 mg in Acetone-d₆^{*}
¹³C{¹H} NMR, 100 MHz, T= 27 C



Current Data Parameters
 NAME py-01
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250703
 Time 21:57
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

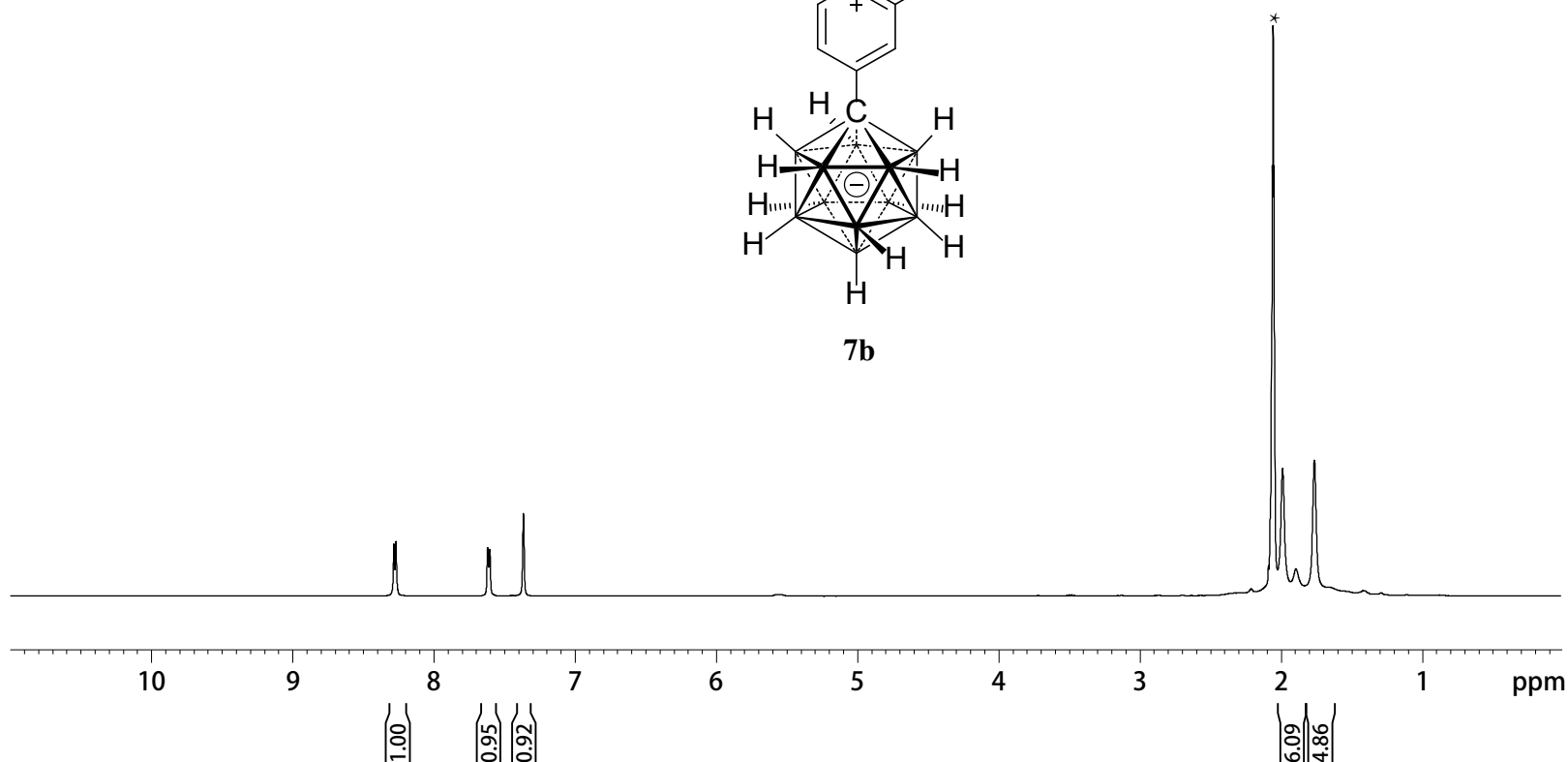
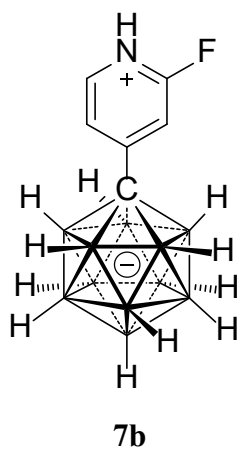
F2 - Processing parameters
 SI 32768
 SF 100.6126794 MHz
 WDW EM
 GB 0

20230916-zk-Py-F-H, 19 mg in Acetone-d₆^{*}
¹H{¹¹B} NMR, 400MHz, T= 28 C

8.28
8.26

7.61
7.60
7.36

2.05
1.98
1.89
1.89
1.76



Current Data Parameters
NAME 20230916-zk-Py-F-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230916
Time 17.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgig30
TD 16384
SOLVENT Acetone
NS 16
DS 4
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 107.6
DW 62.400 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

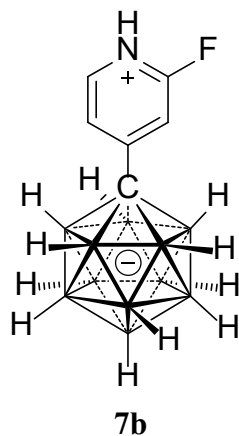
===== CHANNEL f1 =====
NUC1 ¹H
P1 15.00 usec
PLW1 15.48099995 W
SFO1 400.1320007 MHz

===== CHANNEL f2 =====
CPDPRG2 garp4
NUC2 ¹¹B
PCPD2 90.00 usec
PLW2 52.96599960 W
PLW12 0.64477998 W
SFO2 128.3776050 MHz

F2 - Processing parameters
SI 32768
SF 400.1300069 MHz
WDW EM
SSB 0
GB 0

20230916-zk-Py-F-H, 19 mg in Acetone-d6
 $^{11}\text{B}\{^1\text{H}\}$ NMR, 128MHz, T= 28 C

— -5.93
 \ -12.05
 / -13.21



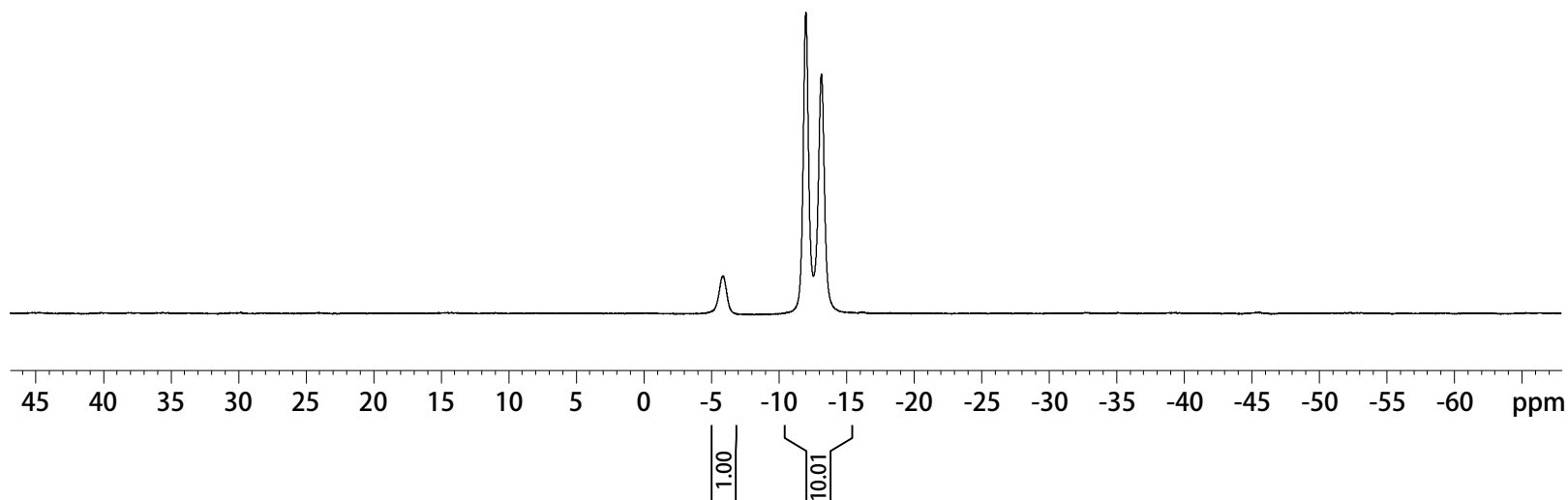
Current Data Parameters
 NAME 20230916-zk-Py-F-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230916
 Time 17.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

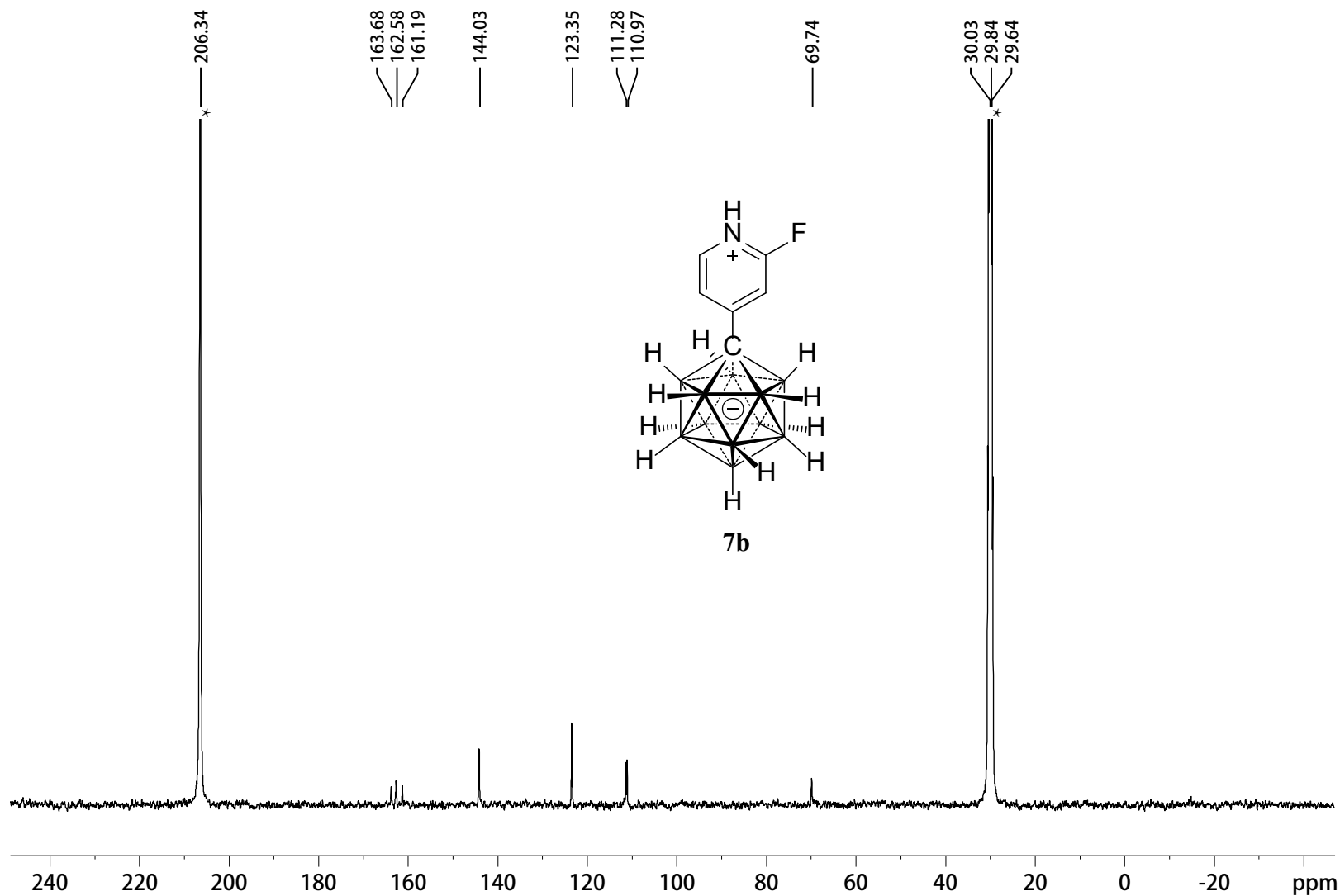
===== CHANNEL f1 =====
 NUC1 ^{11}B
 P1 9.93 usec
 PLW1 52.96599960 W
 SFO1 128.3776050 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ^1H
 PCPD2 80.00 usec
 PLW2 15.48099995 W
 PLW12 0.54425001 W
 PLW13 0.34832001 W
 SFO2 400.1320007 MHz

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



20230916-zk-Py-F-H, 19 mg in Acetone-d₆^{*}
¹³C{¹H} NMR, 100MHz, T= 28 C



Current Data Parameters
 NAME 20230916-zk-Py-F-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230916
 Time 20.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 301.8 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 66.13099670 W
 SFO1 100.6228293 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 15.48099995 W
 PLW12 0.54425001 W
 PLW13 0.34832001 W
 SFO2 400.1316005 MHz

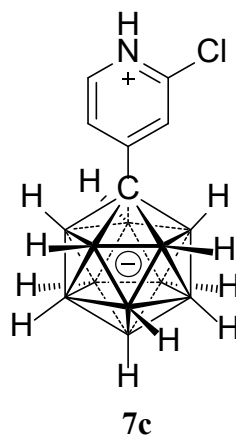
F2 - Processing parameters
 SI 32768
 SF 100.6126788 MHz
 WDW EM
 SFO 100.6126788 MHz

20230916-zk-Py-Cl, 17 mg in Acetone-d6*
¹H{¹¹B} NMR, 400MHz, T= 28 C

8.65
8.64

7.89
7.88

2.05
1.98
1.78



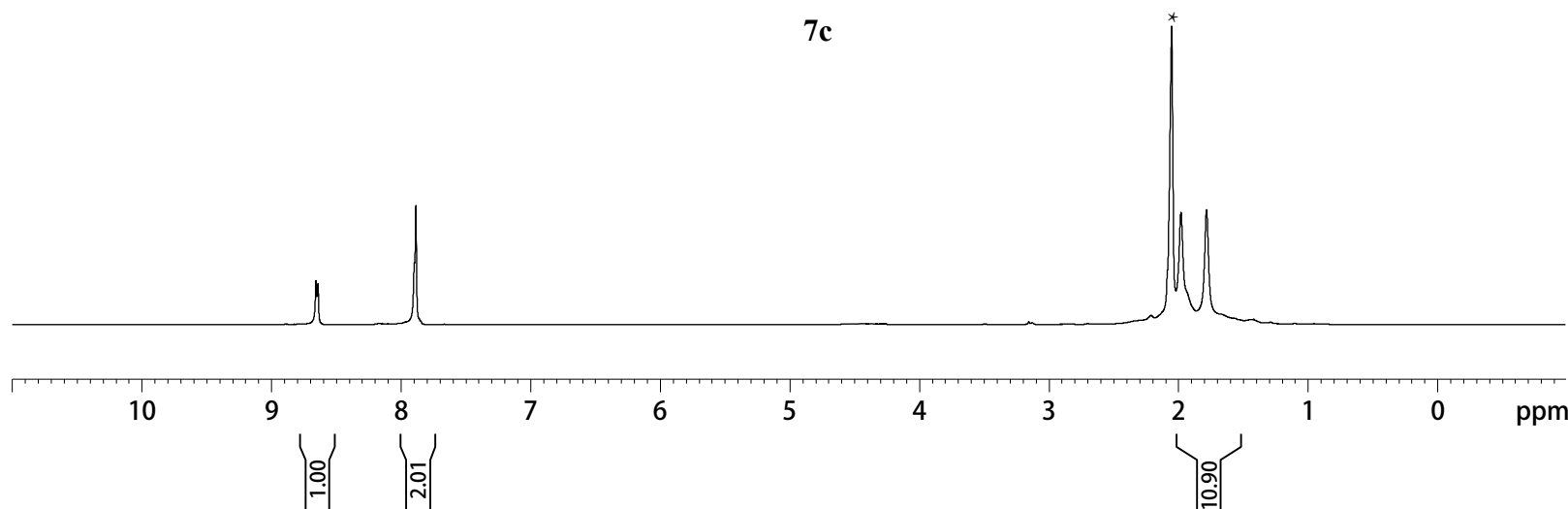
Current Data Parameters
 NAME 20230916-zk-Py-Cl
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230916
 Time 17.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgig30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 107.6
 DW 62.400 usec
 DE 6.50 usec
 TE 300.3 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

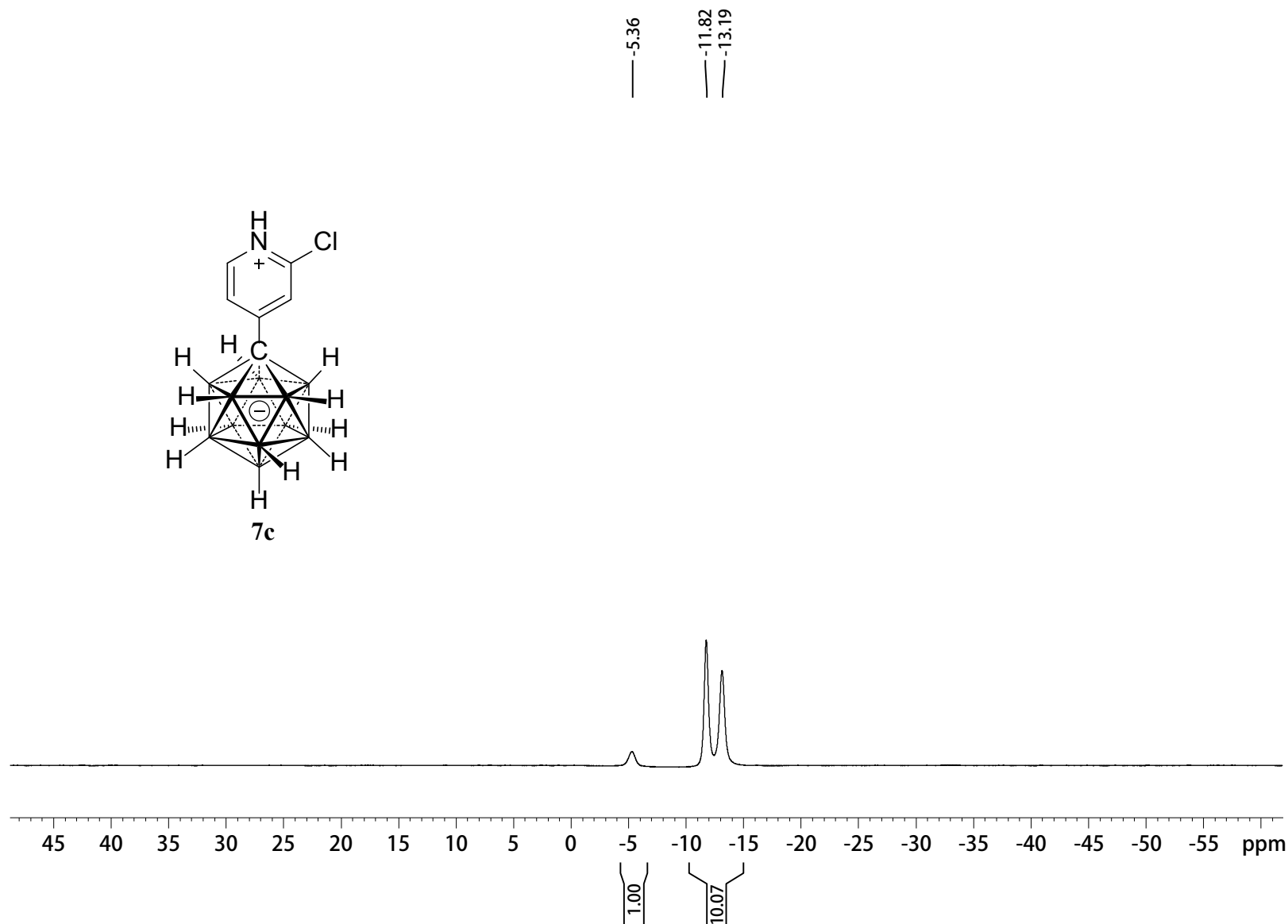
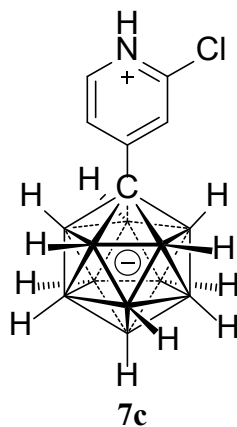
===== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.00 usec
 PLW1 15.48099995 W
 SFO1 400.1320007 MHz

===== CHANNEL f2 =====
 CPDPRG2 garp4
 NUC2 ¹¹B
 PCPD2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.64477998 W
 SFO2 128.3776050 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300074 MHz
 WDW EM
 SSB 0
 GB 0



20230916-zk-Py-Cl, 17 mg in Acetone-d6
¹¹B{¹H} NMR, 128 MHz, T= 28 C



Current Data Parameters
 NAME 20230916-zk-Py-Cl
 EXPNO 2
 PROCNO 1

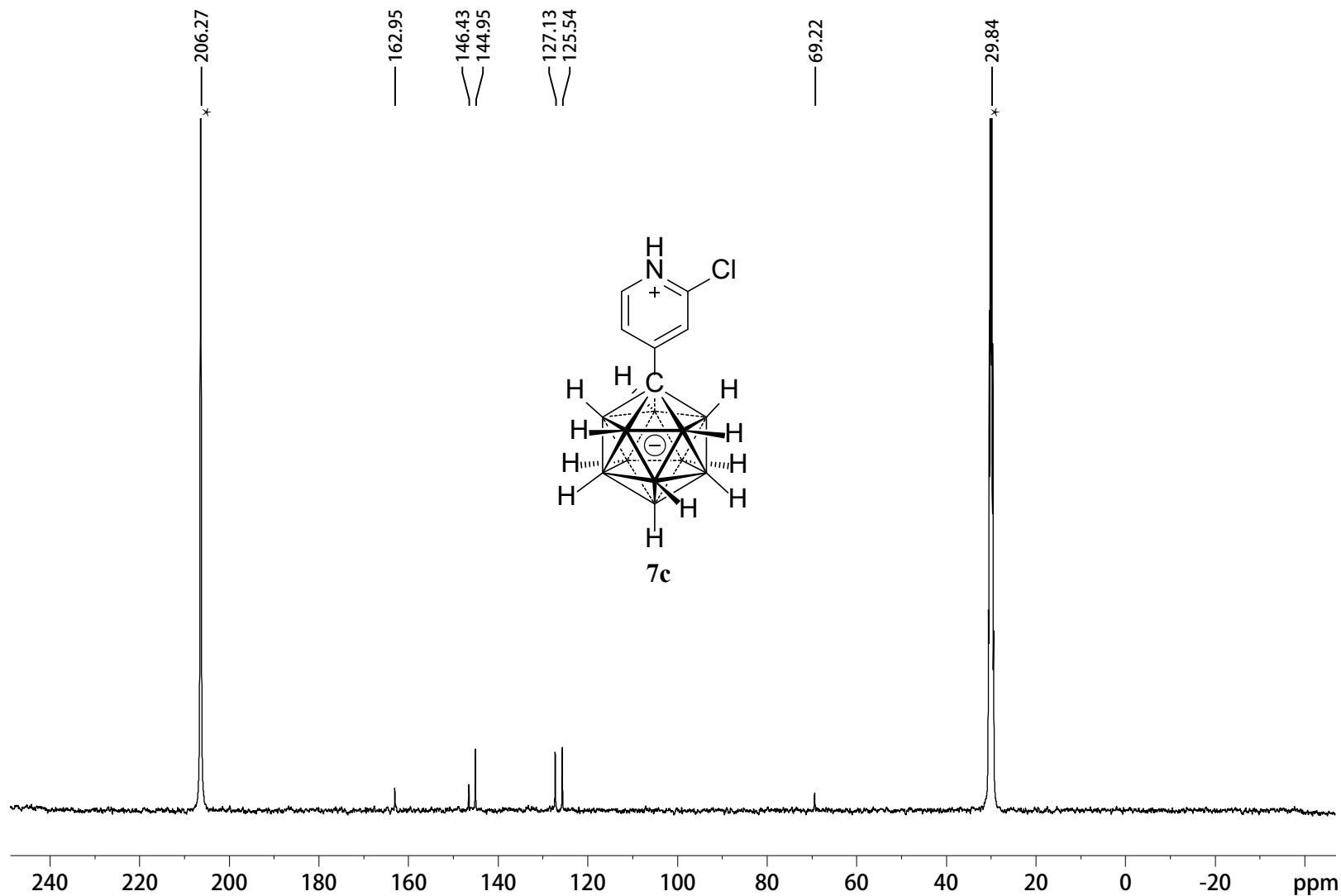
F2 - Acquisition Parameters
 Date_ 20230916
 Time 17.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 301.4 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 15.48099995 W
 PLW12 0.54425001 W
 PLW13 0.34832001 W
 SFO2 400.1320007 MHz

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

20230916-zk-Py-Cl, 17 mg in Acetone-d6*
¹³C{¹H} NMR, 100 MHz, T= 28 C



Current Data Parameters
 NAME 20230916-zk-Py-Cl
 EXPNO 4
 PROCNO 1

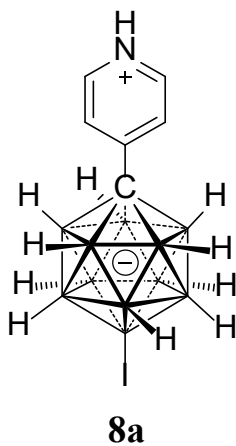
F2 - Acquisition Parameters
 Date_ 20230916
 Time 21.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 302.0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 66.13099670 W
 SFO1 100.6228293 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PLW2 15.48099995 W
 PLW12 0.54425001 W
 PLW13 0.34832001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126776 MHz
 WDW EM
 SSB 0

241117-4Py-12-I, 17.5 mg in DMSO-d₆^{*}
¹H{¹¹B} NMR, 400MHz, T= 27 C

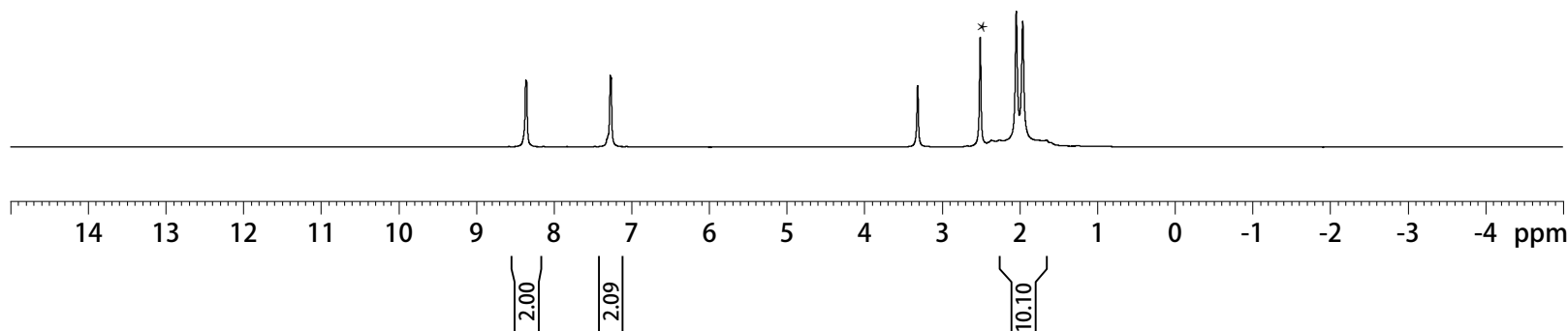


8.36
8.35
7.27
7.26
3.31
2.50
2.03
1.95

Current Data Parameters
NAME 241117-4Py-12-I-DMSO
EXPNO 1
PROCNO 1

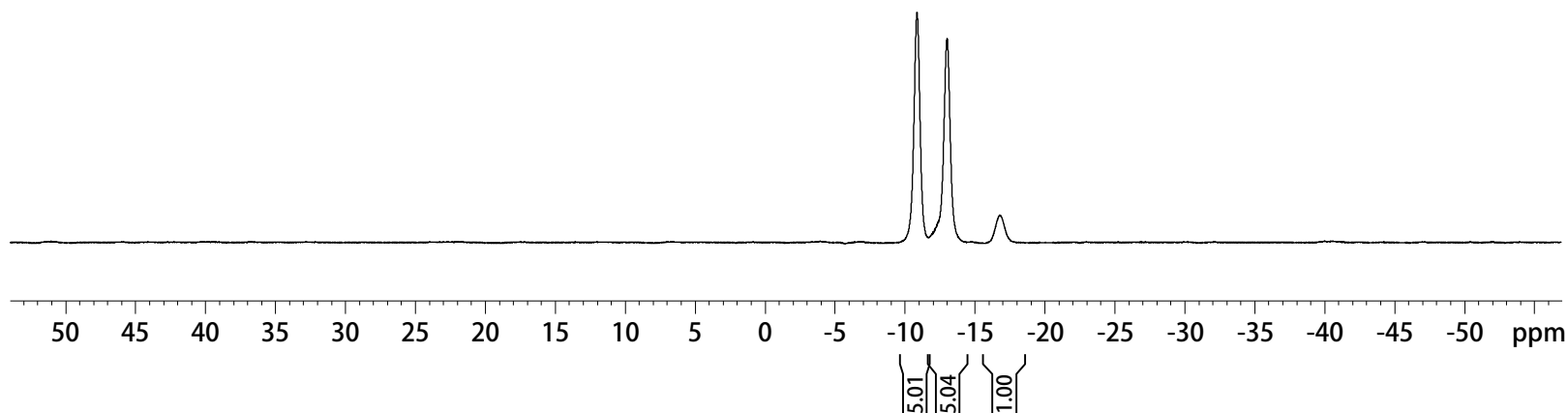
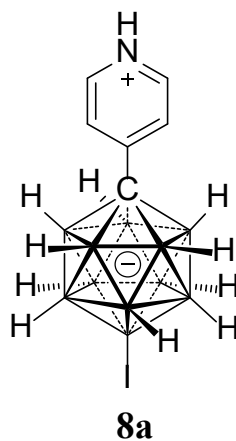
F2 - Acquisition Parameters
Date_ 20241117
Time 19.02 h
INSTRUM spect
PROBHD Z108618_0497 (
PULPROG zgig30
TD 16384
SOLVENT DMSO
NS 16
DS 4
SWH 8012.820 Hz
FIDRES 0.978127 Hz
AQ 1.0223616 sec
RG 193.34
DW 62.400 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 400.1320007 MHz
NUC1 ¹H
P1 15.00 usec
PLW1 15.48099995 W
SFO2 128.3776050 MHz
NUC2 ¹¹B
CPDPRG2 garp4
PCPD2 60.00 usec
PLW2 52.96599960 W
PLW12 1.45079994 W

F2 - Processing parameters
SI 32768
SF 400.1300039 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



241117-4Py-12-I, 17.6 mg in Acetone-d6
¹¹B{¹H} NMR, 128 MHz, T= 27 C

10.92
 13.06
 16.83

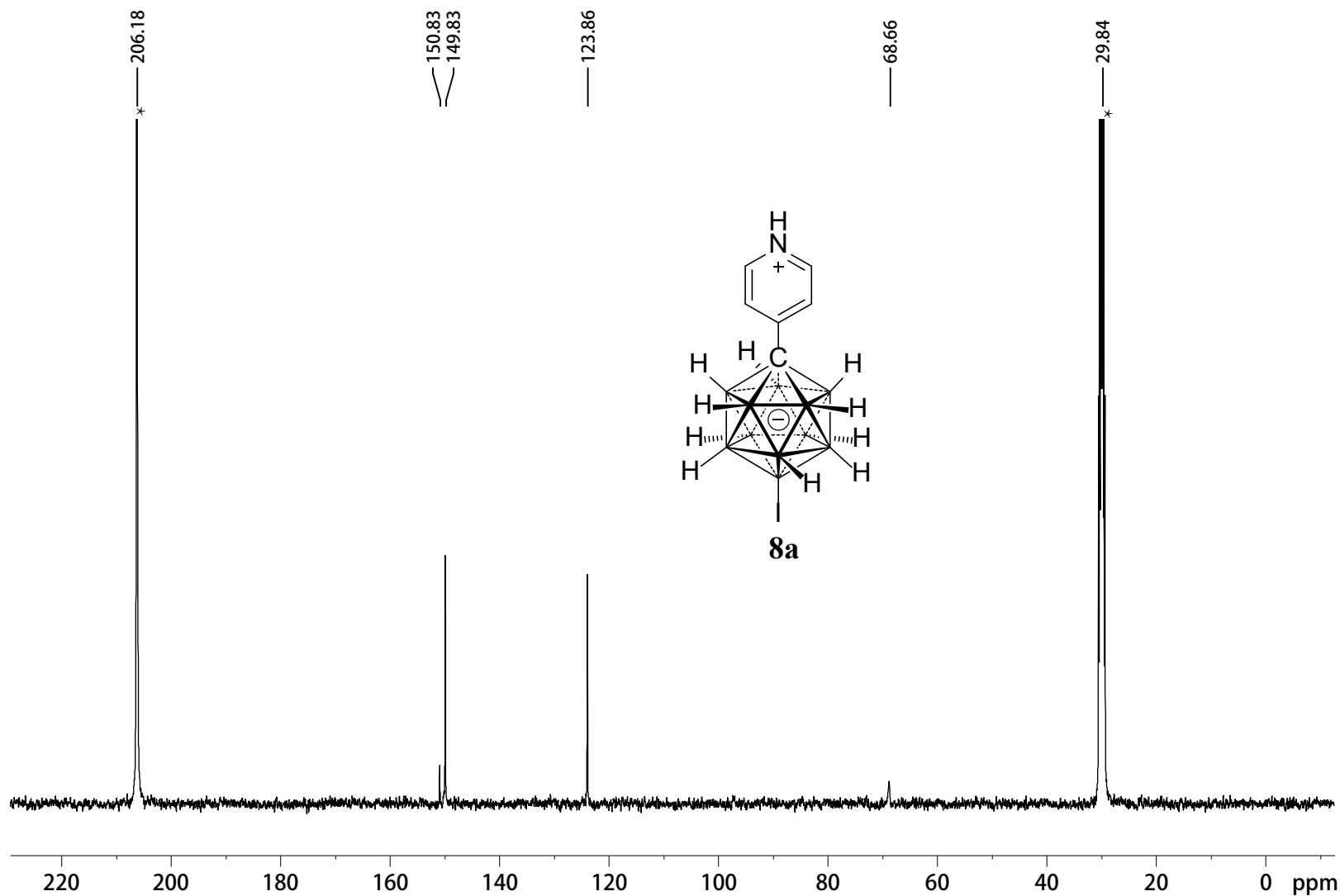


Current Data Parameters
 NAME 241117-4Py-12-I
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241117
 Time 14.51 h
 INSTRUM spect
 PROBHD Z108618_0497 (
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.778510 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 299.9 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 128.3776050 MHz
 NUC1 11B
 P1 9.93 usec
 PLW1 52.96599960 W
 SFO2 400.1320007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 15.48099995 W
 PLW12 0.43002000 W
 PLW13 0.21630000 W

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

241117-4Py-12-I, 17.6 mg in Acetone-d6*
¹³C{¹H} NMR, 100 MHz, T= 27 C



Current Data Parameters
 NAME 241117-4Py-12-I
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241117
 Time 15.38 h
 INSTRUM spect
 PROBHD Z108618_0497 (
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 300.3 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6228293 MHz
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 66.13099670 W
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 15.48099995 W
 PLW12 0.43002000 W
 PLW13 0.21630000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126799 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

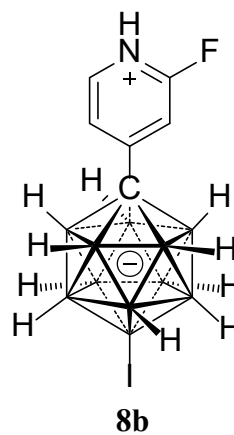
251001-Py-F-12-I, 18 mg in Acetone-d₆^{*}
¹H{¹¹B} NMR, 400 MHz, T= 28 C

7.99
7.98

7.29
7.28
6.96

2.83

2.18
2.05
2.02



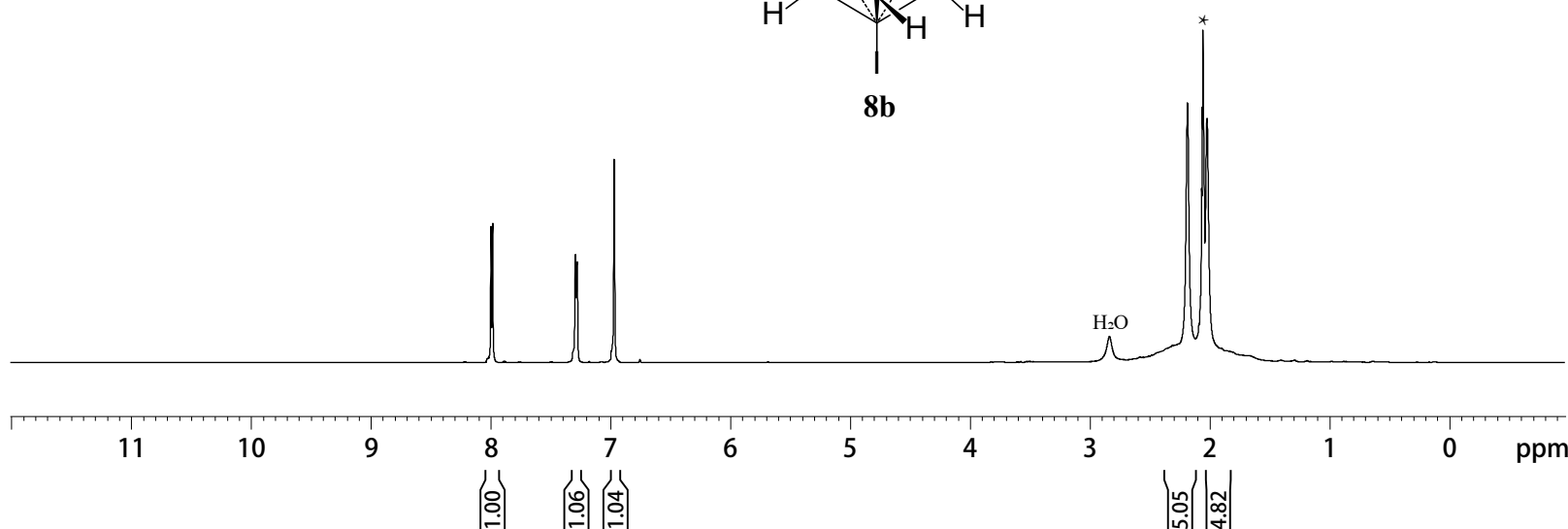
Current Data Parameters
 NAME 251001-Py-F-12-I
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251001
 Time 13.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgig30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 193.34
 DW 62.400 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

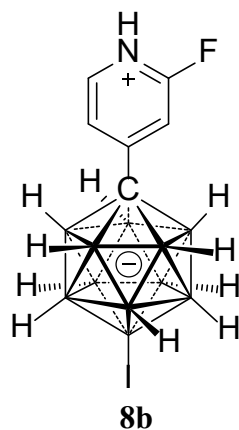
===== CHANNEL f2 =====
 SFO2 128.3776050 MHz
 NUC2 ¹¹B
 CPDPRG2 garp4
 PCPD2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.64477998 W

F2 - Processing parameters
 SI 32768
 SF 400.1300069 MHz
 WDW EM
 SSB 0
 GB 1.000000



251001-Py-F-12-I, 18 mg in Acetone-d6
¹¹B{¹H} NMR, 128 MHz, T= 28 C

— 10.85
 — 13.07
 — 16.69



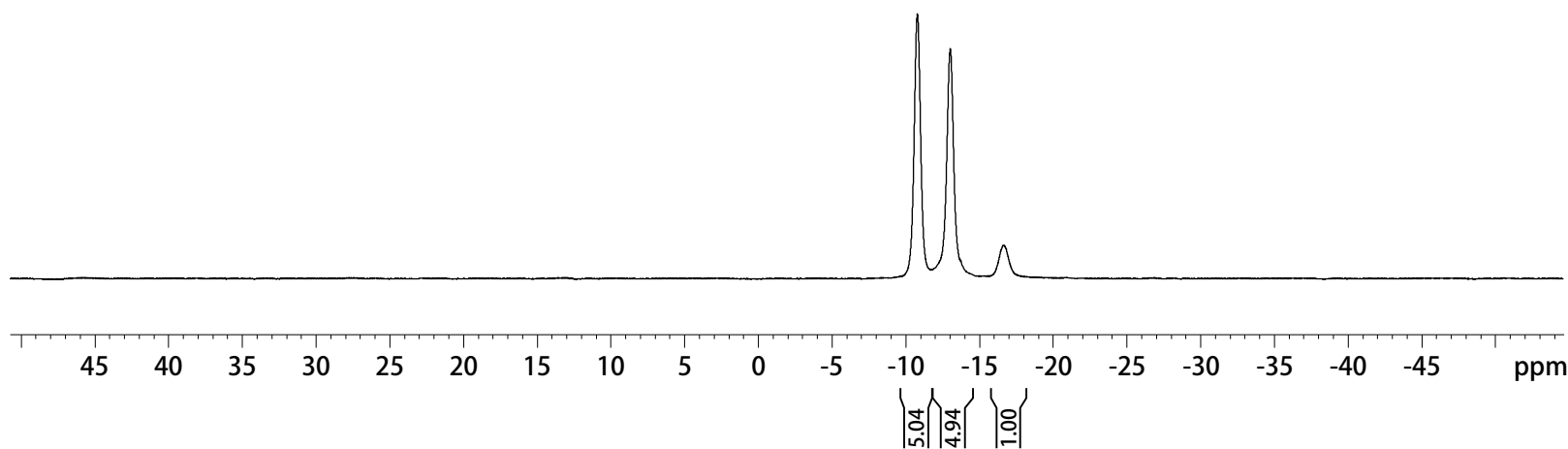
Current Data Parameters
 NAME 251001-Py-F-12-I
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251001
 Time 13.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

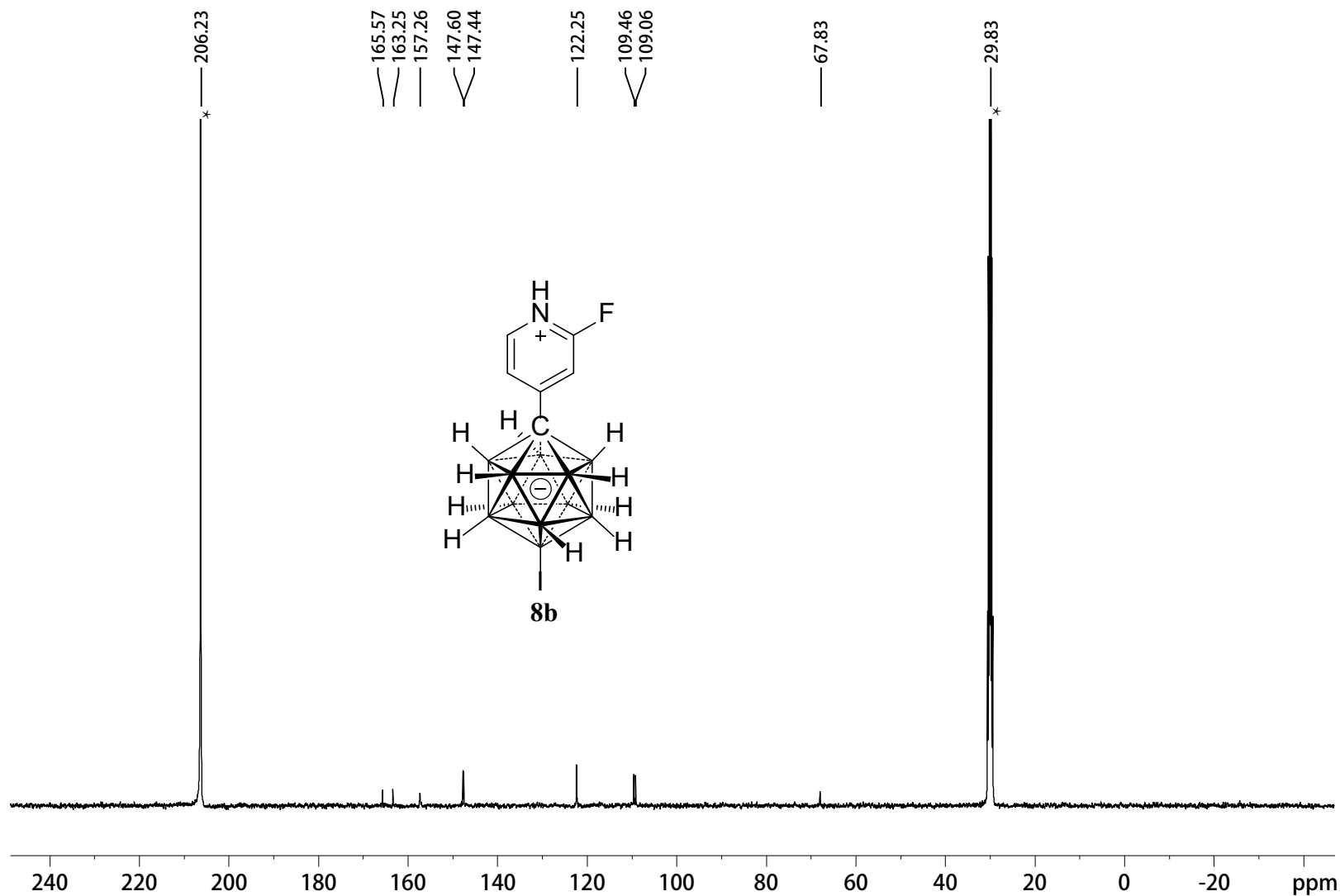
===== CHANNEL f1 =====
 SFO1 128.3776050 MHz
 NUC1 ¹¹B
 P1 9.93 usec
 PLW1 52.96599960 W

===== CHANNEL f2 =====
 SFO2 400.1320007 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

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



251001-Py-F-12-I, 18 mg in Acetone-d₆
¹³C{¹H} NMR, 100 MHz, T= 28 C



Current Data Parameters
 NAME 251001-Py-F-12-I
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251001
 Time 14.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126817 MHz
 WDW EM
 SSB 0

251001-Py-Cl-12-I, 20 mg in Acetone-d₆^{*}
¹H{¹¹B} NMR, 400 MHz, T= 28 C

8.17
8.16

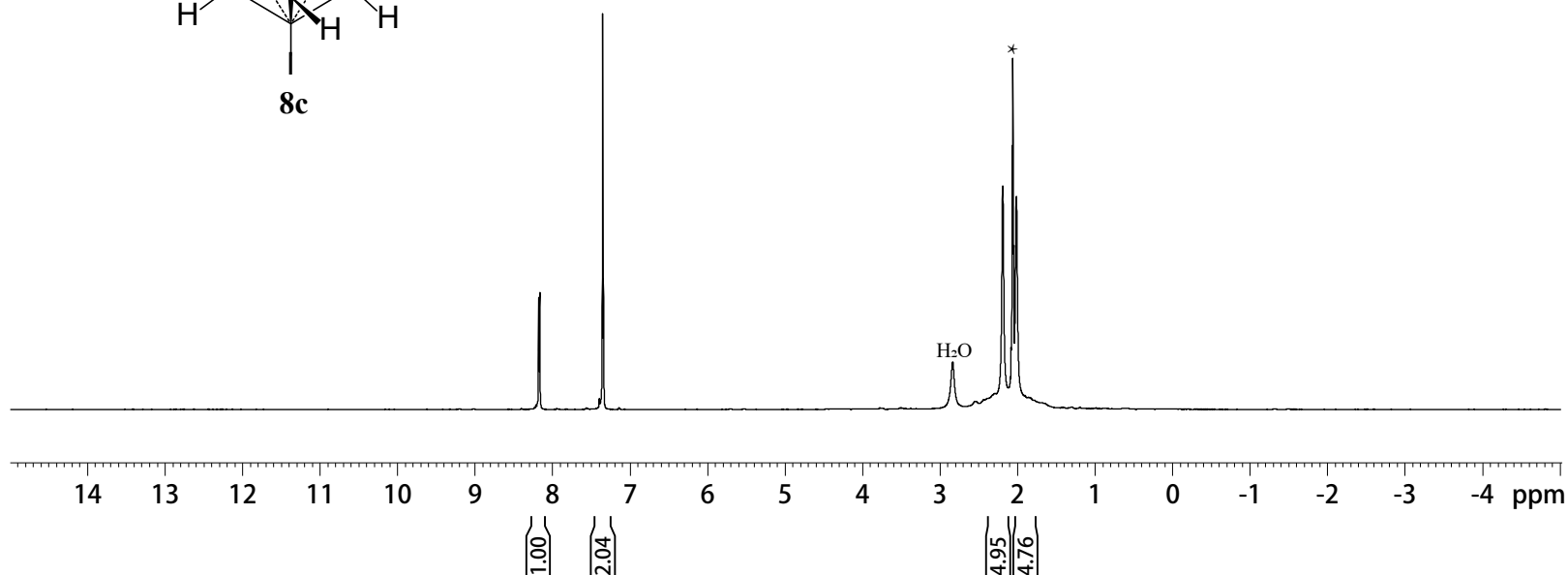
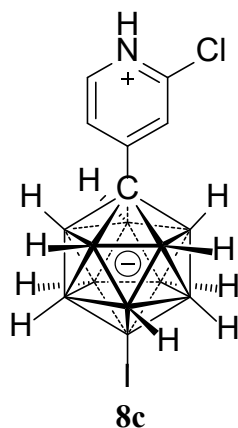
7.35

2.83

2.18

2.05

2.00



Current Data Parameters
 NAME 251001-Py-Cl-12-I
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251001
 Time 14.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 16384
 SOLVENT Acetone
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 193.34
 DW 62.400 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

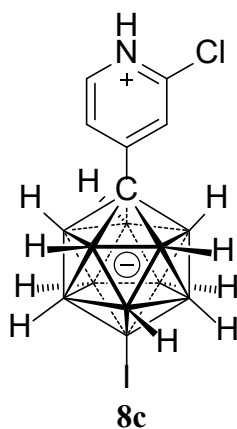
===== CHANNEL f1 =====
 SFO1 400.132007 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 12.50000000 W

===== CHANNEL f2 =====
 SFO2 128.3776050 MHz
 NUC2 11B
 CPDPRG2 garp4
 PCPD2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.64477998 W

F2 - Processing parameters
 SI 32768
 SF 400.1300071 MHz
 WDW EM
 SSB 0
 GB 1.000000

251001-Py-Cl-12-I, 18 mg in Acetone-d6
 $^{11}\text{B}\{^1\text{H}\}$ NMR, 128 MHz, T= 28 C

— 10.80
 — 13.12
 — 16.70



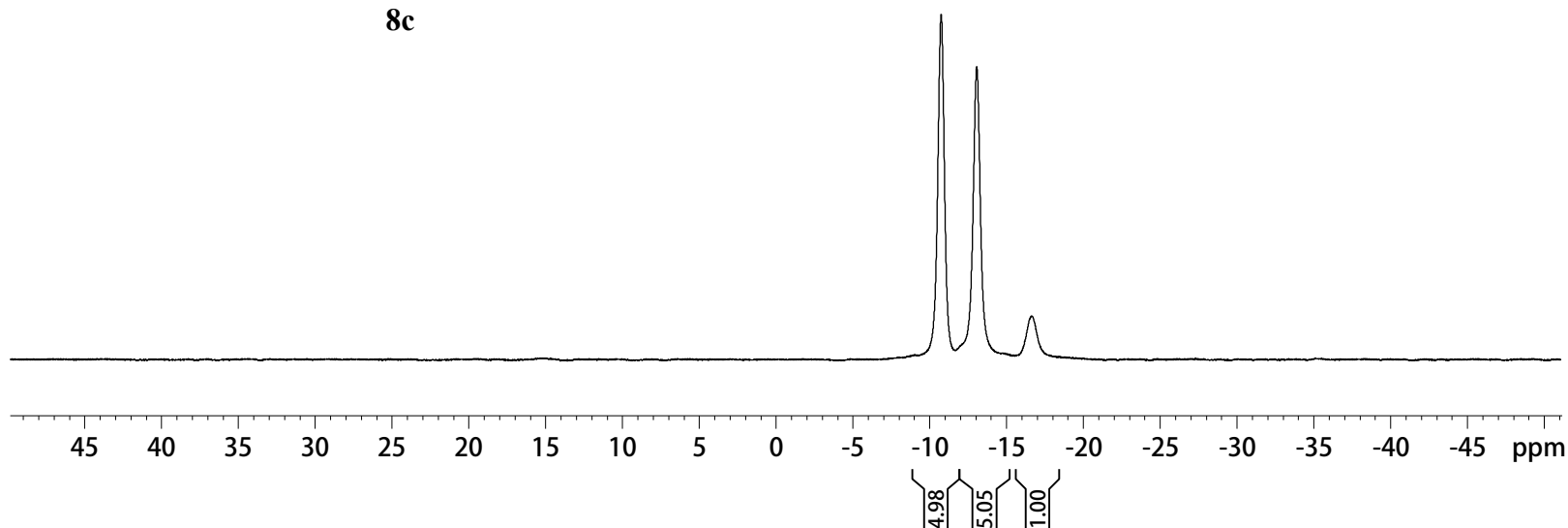
Current Data Parameters
 NAME 251001-Py-Cl-12-I
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251001
 Time 14.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

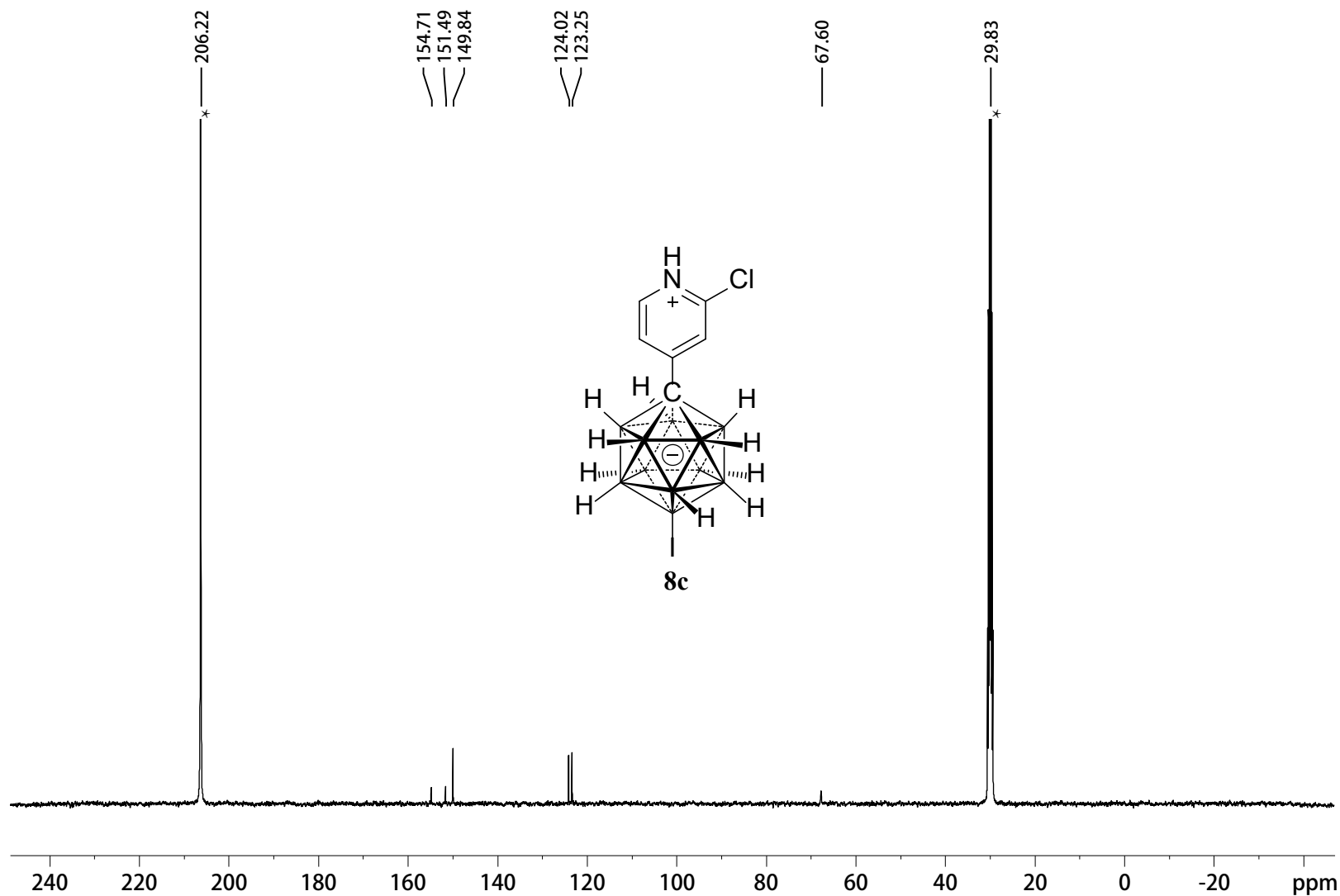
===== CHANNEL f1 =====
 SFO1 128.3776050 MHz
 NUC1 ^{11}B
 P1 9.93 usec
 PLW1 52.96599960 W

===== CHANNEL f2 =====
 SFO2 400.1320007 MHz
 NUC2 ^1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

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



251001-Py-Cl-12-I, 18 mg in Acetone-d₆^{*}
¹³C{¹H} NMR, 100 MHz, T= 28 C



Current Data Parameters
 NAME 251001-Py-Cl-12-I
 EXPNO 3
 PROCNO 1

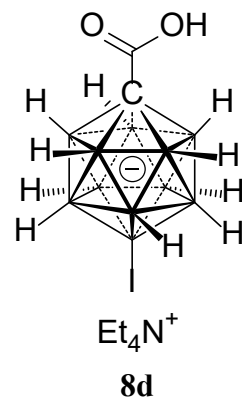
F2 - Acquisition Parameters
 Date_ 20251001
 Time 15.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

F2 - Processing parameters
 SI 32768
 SF 100.6126809 MHz
 WDW EM
 SSB 0

251003-1-COOH-12-I-DMSO, 18 mg in DMSO-d₆^{*}
¹H{¹¹B} NMR, 400 MHz, T= 28 C



3.31
3.21
3.19
2.50
1.83
1.16
1.16
1.16

H₂O

*

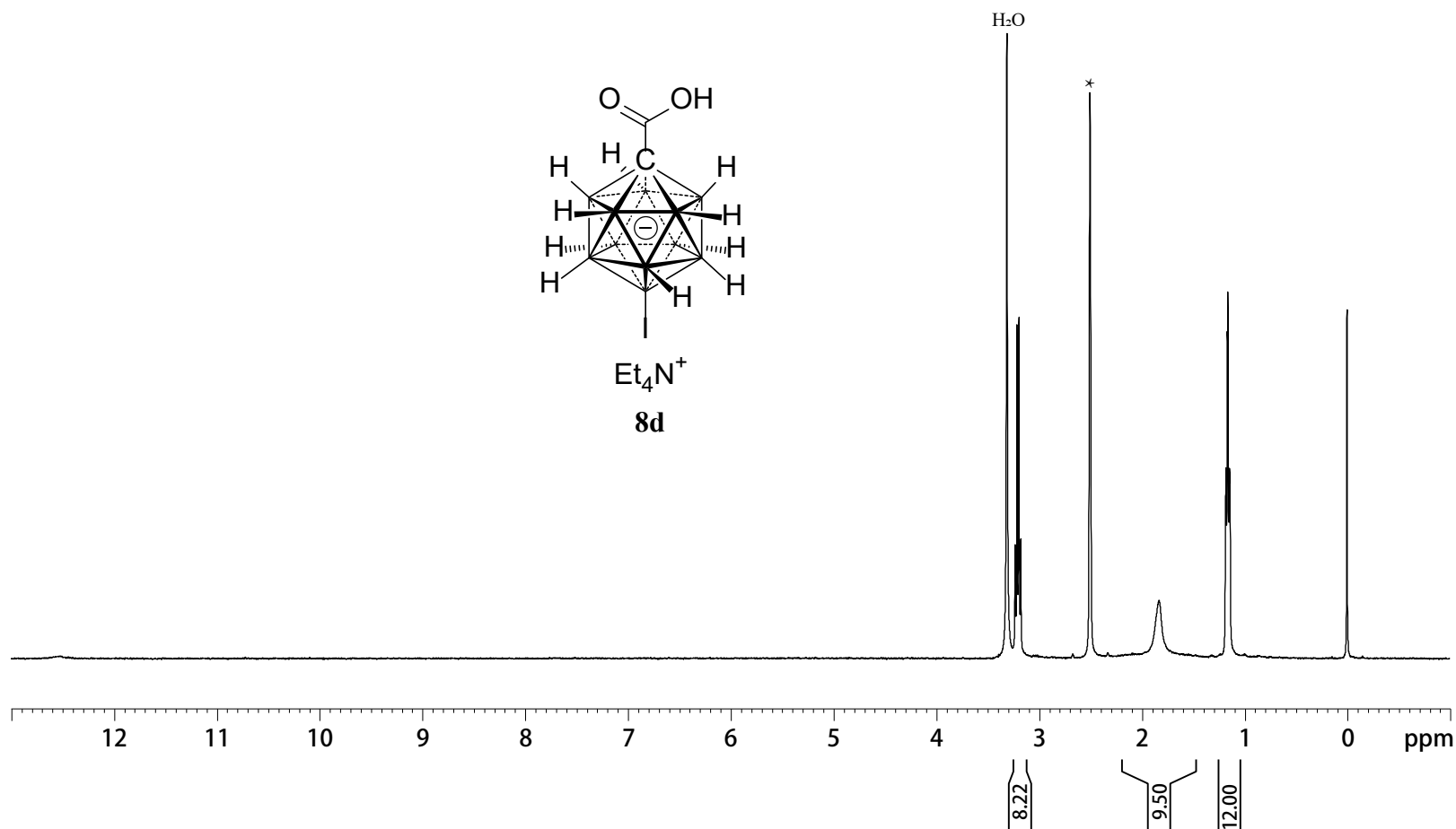
Current Data Parameters
 NAME 251003-1-COOH-12-I-DMSO
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251003
 Time 18.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgig30
 TD 16384
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 193.34
 DW 62.400 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

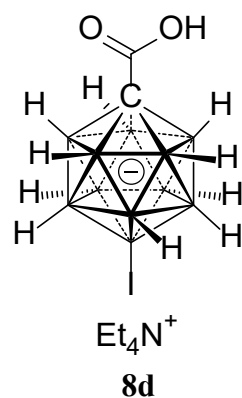
===== CHANNEL f2 =====
 SFO2 128.3776050 MHz
 NUC2 ¹¹B
 CPDPRG2 garp4
 PCPD2 90.00 usec
 PLW2 52.96599960 W
 PLW12 0.64477998 W

F2 - Processing parameters
 SI 32768
 SF 400.1300034 MHz
 WDW EM
 SSB 0
 GB 0



251003-1-COOH-12-I-Acetone, 18 mg in Acetone-d6
¹¹B{¹H} NMR, 400 MHz, T= 28 C

— -11.64
 — -13.76
 — -16.53



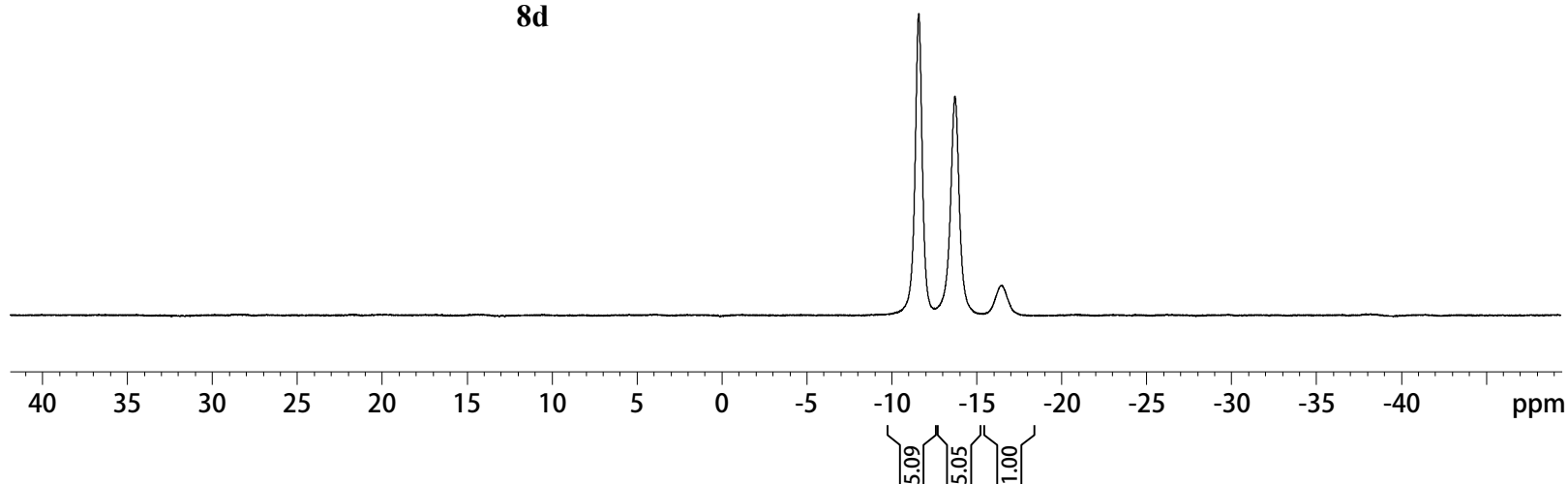
Current Data Parameters
 NAME 251003-1-COOH-12-I-Acetone
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251003
 Time 16.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845056 sec
 RG 193.34
 DW 19.600 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

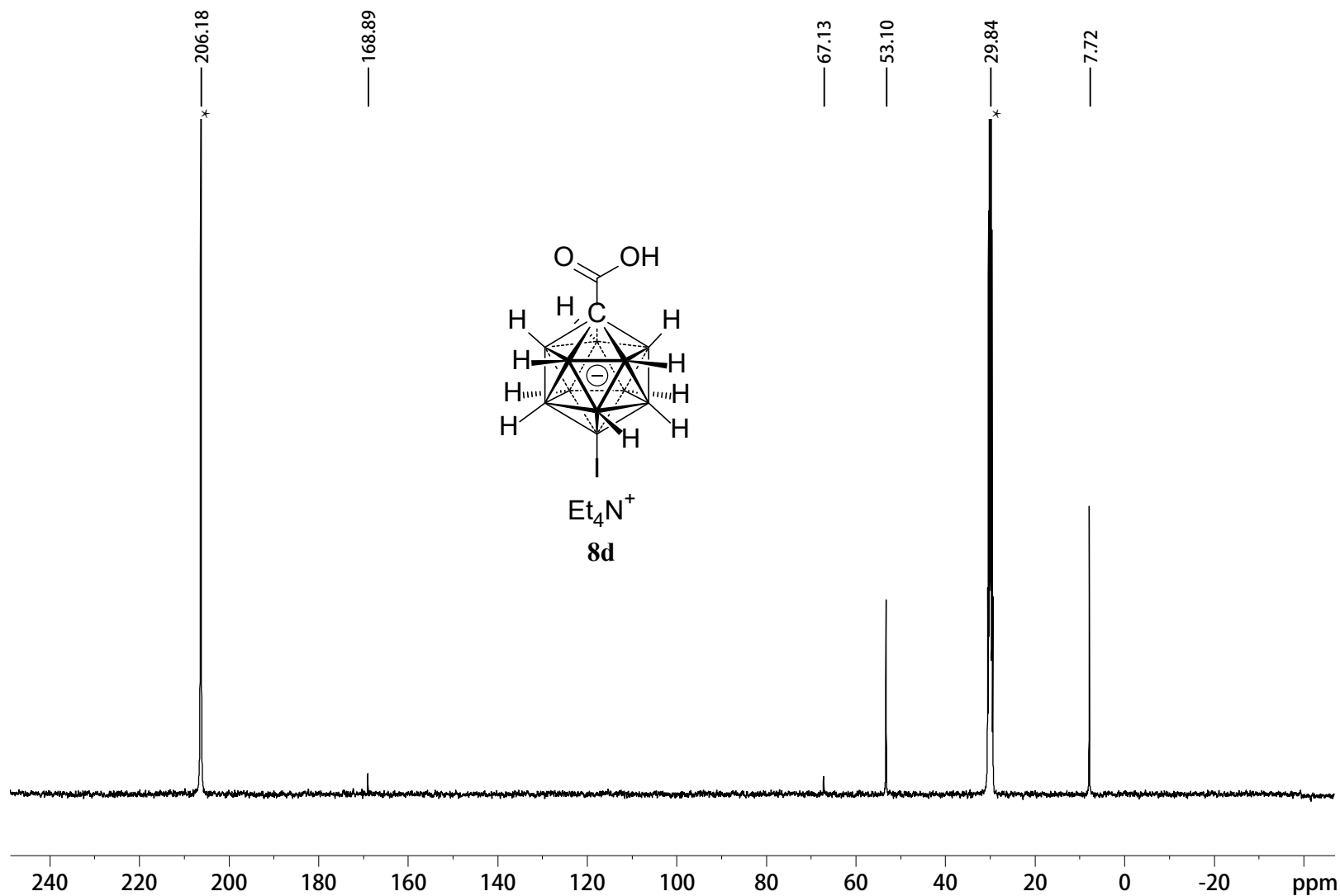
===== CHANNEL f2 =====
 SFO2 400.1320007 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

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



S88

251003-1-COOH-12-I-Acetone, 18 mg in Acetone-d₆
¹³C{¹H} NMR, 100 MHz, T= 28 C



Current Data Parameters
 NAME 251003-1-COOH-12-I-Acetone
 EXPNO 4
 PROCNO 1

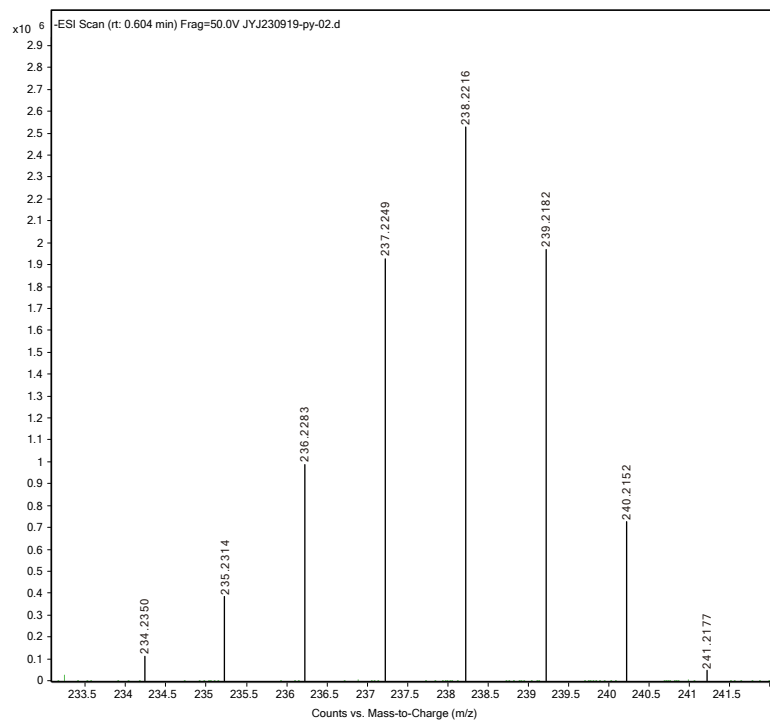
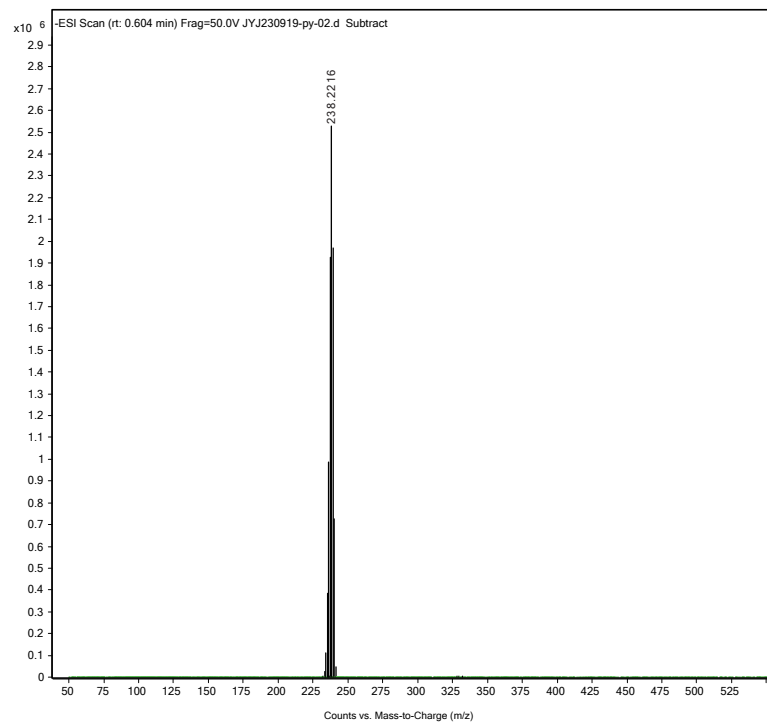
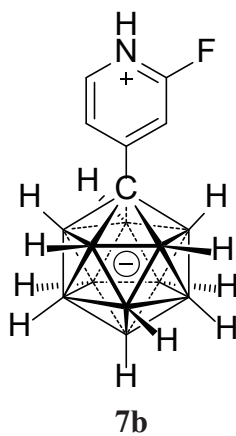
F2 - Acquisition Parameters
 Date_ 20251003
 Time 17.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 193.34
 DW 16.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

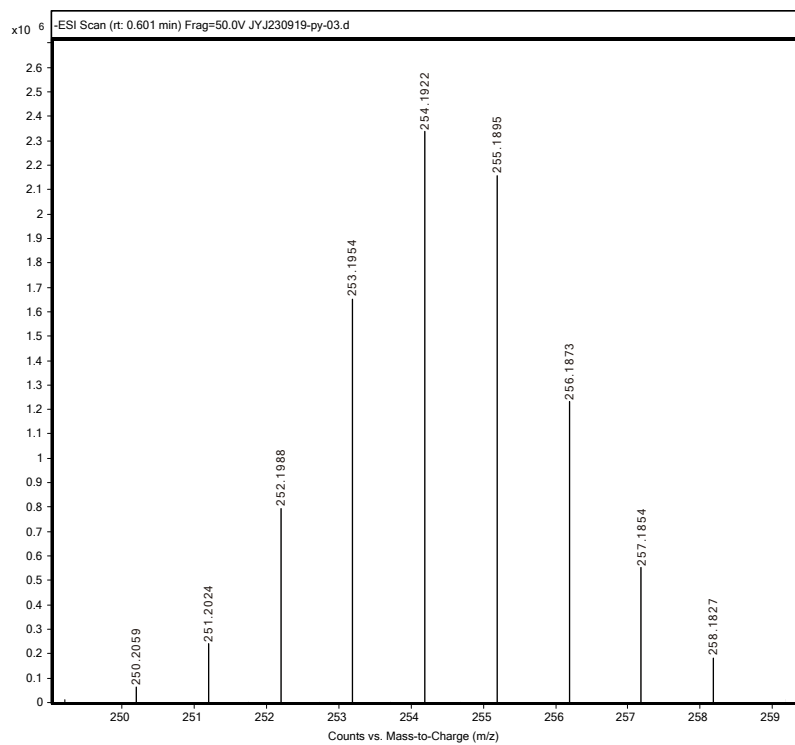
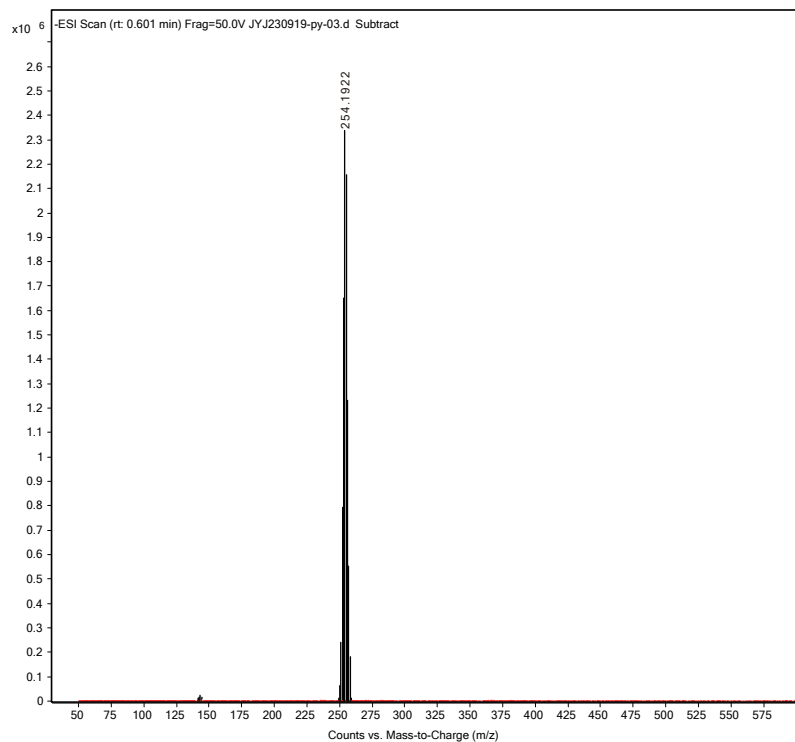
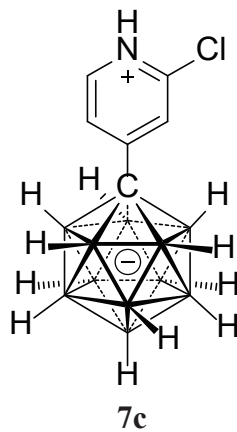
===== CHANNEL f1 =====
 SFO1 100.6228293 MHz
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 53.00000000 W

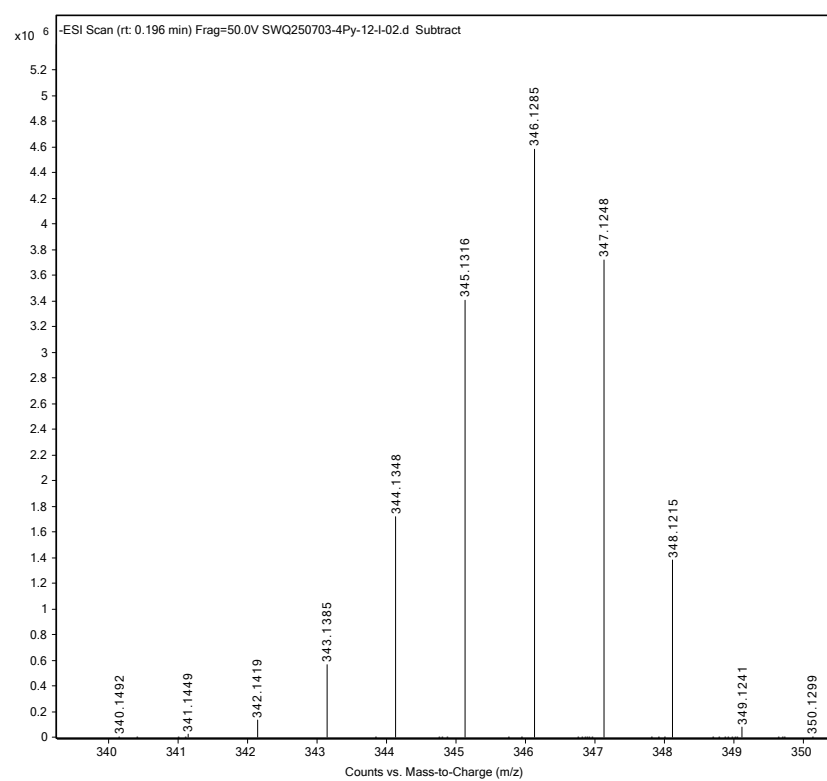
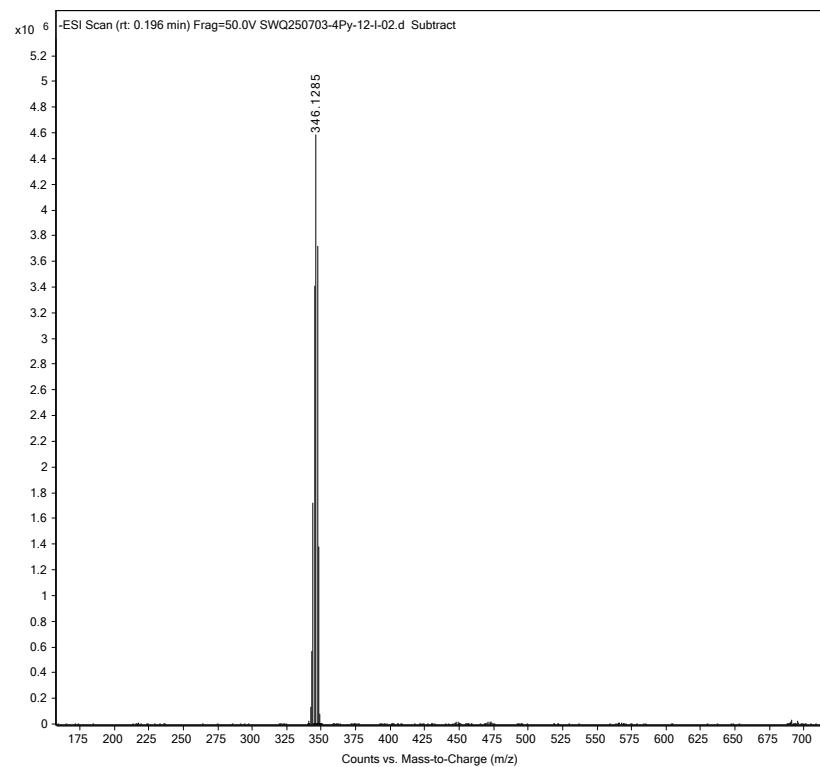
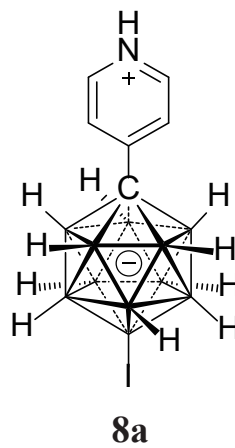
===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.50000000 W
 PLW12 0.34722000 W
 PLW13 0.17465000 W

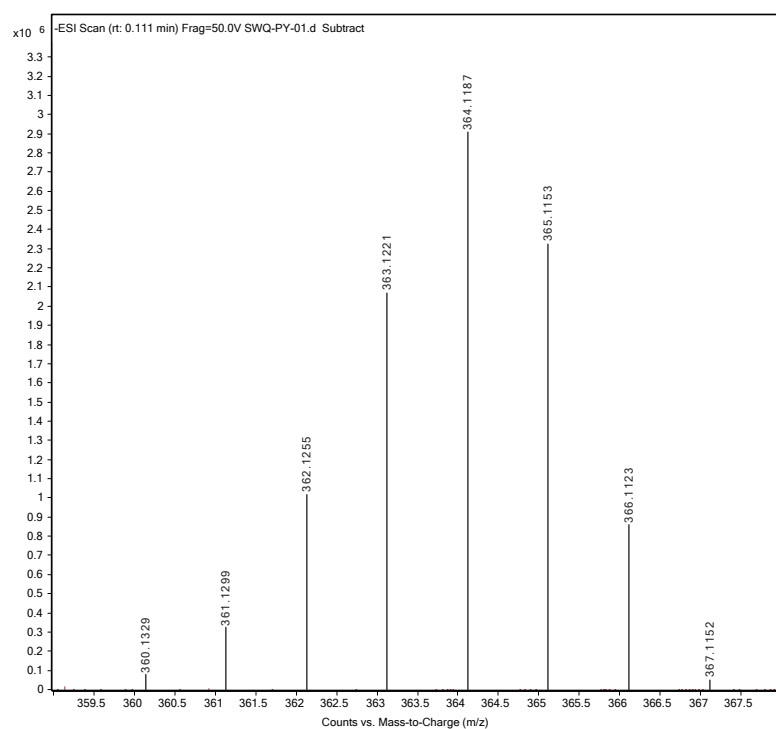
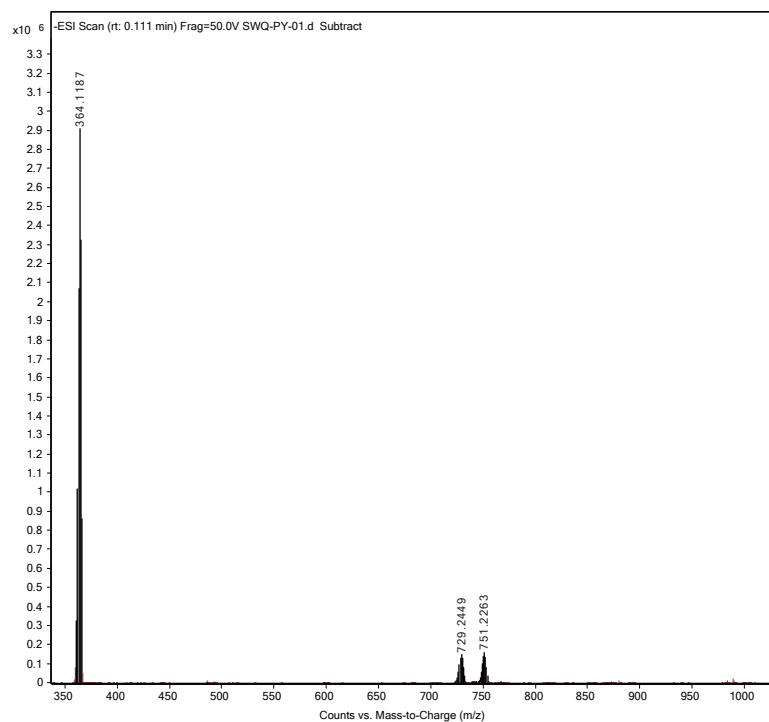
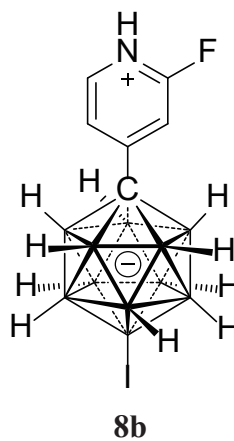
F2 - Processing parameters
 SI 32768
 SF 100.6126799 MHz
 WDW EM
 SSB 0

VI Mass spectra









HRMS((-)-ESI)

