

Supporting Information

Regioselective Insertion of Carborynes into Ethereal C–H Bonds: Facile Synthesis of α -Carboranylated Ethers

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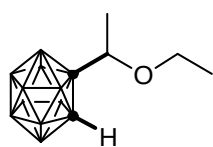
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Experimental Section

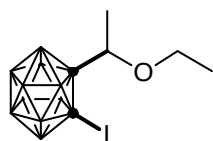
General Information. All reactions were carried out in flame-dried glassware under an atmosphere of dry N₂ using standard Schlenk techniques unless otherwise specified. All organic solvents were freshly distilled from Na-K alloy immediately prior to use. All other chemicals were purchased from either Aldrich or Acros Chemical Co. and used as received unless otherwise noted. ¹H NMR spectra were recorded on a Bruker DPX 400 spectrometer at 400 MHz. ¹³C NMR spectra were recorded on a Bruker DPX 300 spectrometer at 75 MHz or a Bruker DPX 400 spectrometer at 100 MHz. ¹¹B NMR spectra were recorded on a Bruker DPX 300 spectrometer at 96 MHz or a Varian Inova 400 spectrometer at 128 MHz. All signals were reported in ppm with reference to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, and to external BF₃·OEt₂ (0.00 ppm) for boron chemical shifts. The data were reported as (s = singlet, d = doublet, t = triplet, q = quadruplet, m = multiplet or unresolved, br = broad, coupling constant(s) in Hz, integration). Mass spectra were obtained on a Thermo Finnigan MAT 95 XL spectrometer or Waters Micromass GCT Premier. UV-visible spectra were obtained on a Cary 1E UV-visible spectrophotometer.

Reaction of *o*-Carboryne with Diethyl Ether under Fluorescent Light Irradiation. To a diethyl ether solution (10 mL) of 1,2-Li₂-*o*-C₂B₁₀H₁₀ (1.0 mmol), prepared in situ from the reaction of ⁿBuLi (1.25 mL, 1.6 M in hexane, 2.0 mmol) with *o*-carborane (144.2 mg, 1.0 mmol) in an ice-water bath, was added iodine (253.8 mg, 1.0 mmol). After stirring for another 0.5 h at 0 °C, iodine was completely disappeared and a colorless, clear solution was obtained. The resulting mixture was stirred at room temperature for 24 h and quenched by wet *n*-hexane. The solution was quickly passed through a short column of silica gel to remove the inorganic salt and washed with ether. The organic portions were combined. After removal of the solvents, the residue was purified by flash column chromatography on silica gel (230-400 mesh) using *n*-hexane/ether (*n*-hexane/ether = 80/1 in v/v) as eluent to give product **6aa** (172.7 mg, 80%).



6aa: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 4.09 (br, 1H) (cage CH), 3.88 (q, $J = 6.4$ Hz, 1H) (OCH), 3.63 (m, 1H), 3.38 (m, 1H) (OCHH), 1.32 (d, $J = 6.0$ Hz, 3H), 1.17 (t, $J = 7.2$ Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 78.1 (cage C), 75.3 (cage C), 66.0, 58.6, 19.8, 15.1. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.9 (1B), -4.8 (1B), -9.4 (2B), -12.2 (3B), -13.5 (1B), -14.7 (br, 2B). HRMS (EI) calcd for $\text{C}_6\text{H}_{18}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$ ($[\text{M}-2\text{H}]^+$): 214.2355. Found: 214.2348.

Reaction of *o*-Carboryne with Diethyl Ether in the Dark. To a diethyl ether solution (10 mL) of 1,2- Li_2 -*o*- $\text{C}_2\text{B}_{10}\text{H}_{10}$ (1.0 mmol) in the dark (covered with aluminum foil), prepared in situ from the reaction of $n\text{BuLi}$ (1.25 mL, 1.6 M in hexane, 2.0 mmol) with *o*-carborane (144.2 mg, 1.0 mmol) in an ice-water bath, was added iodine (253.8 mg, 1.0 mmol). After stirring for another 0.5 h at 0 $^\circ\text{C}$, iodine was completely disappeared and a colorless, clear solution was obtained. The resulting mixture was stirred at room temperature for 24 h and quenched by wet *n*-hexane in the dark. The solution was quickly passed through a short column of silica gel to remove the inorganic salt and washed with ether. The organic portions were combined. After removal of the solvents, the residue was purified by flash column chromatography on silica gel (230-400 mesh) using *n*-hexane/ether (*n*-hexane/ether = 80/1 in v/v) as eluent to give a mixture of product **6aa** (25.7 mg, 12%) and **7aa** (6.8 mg, 2%).



7aa: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 3.74 (m, 1H) (OCH), 3.71 (m, 1H), 3.57 (m, 1H) (OCHH), 1.45 (d, $J = 6.0$ Hz, 3H), 1.24 (t, $J = 7.2$ Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 82.6 (cage C), 78.4, 65.8, 20.5, 15.8 (cage C), 15.2. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -2.9 (1B), -3.6 (1B), -7.2 (1B), -8.4 (br, 4B), -9.5 (1B), -11.3 (1B), -12.4 (1B). HRMS (EI) calcd for $\text{C}_6\text{H}_{19}^{11}\text{B}_8^{10}\text{B}_2\text{OI}^+$: 342.1481. Found: 342.1468.

UV-visible Absorption Spectrum of the Reaction Solution of 2a in Diethyl Ether. To a diethyl ether solution (10 mL) of 1,2- Li_2 -*o*- $\text{C}_2\text{B}_{10}\text{H}_{10}$ (1.0 mmol) in the dark (covered with aluminum foil),

prepared in situ from the reaction of $n\text{BuLi}$ (1.25 ml, 1.6 M in hexane, 2.0 mmol) with *o*-carborane (144.2 mg, 1.0 mmol) in an ice-water bath, was added iodine (253.8 mg, 1.0 mmol). The resulting solution was diluted by 100 times to obtain a solution of ca. 1.0 mM for examination. All these operations were carefully and quickly conducted in the dark. The resultant UV-vis spectrum was shown in Figure S1.

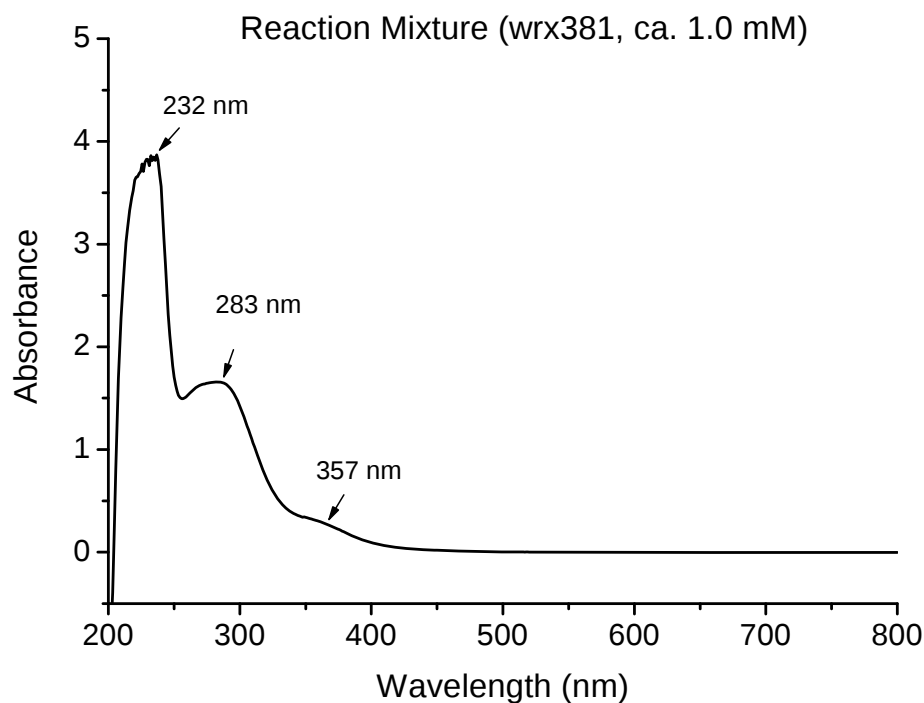
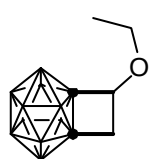


Figure S1. UV-visible Absorption Spectrum of the Reaction Solution

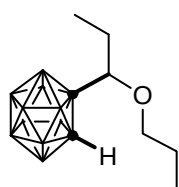
Reaction of 1-Br-2-Li-1,2- $\text{C}_2\text{B}_{10}\text{H}_{10}$ with Diethyl Ether under Heating. To a diethyl ether solution (10 mL) of 1,2- Li_2 -*o*- $\text{C}_2\text{B}_{10}\text{H}_{10}$ (1.0 mmol), prepared in situ from the reaction of $n\text{BuLi}$ (1.25 ml, 1.6 M in hexane, 2.0 mmol) with *o*-carborane (144.2 mg, 1.0 mmol) in an ice-water bath, was added bromine (160.0 mg, 1.0 mmol). After stirring for another 0.5 h at 0 °C, bromine was completely disappeared and a colorless, clear solution was obtained. The resulting solution was refluxed for 24 h and quenched by wet *n*-hexane. The solution was quickly passed through a short column of silica gel to

remove the inorganic salt and washed with ether. The organic portions were combined. After removal of the solvents, the residue was purified by flash column chromatography on silica gel (230-400 mesh) using *n*-hexane/ether (*n*-hexane/ether = 80/1 in v/v) as eluent to give product **6aa** (17.5 mg, 8%) and a four-membered ring product **6aa-S** (17.1 mg, 8%). *The results were interestingly different from those of the iodo analog. However, the bromo anion 1-Br-2-Li-1,2-C₂B₁₀H₁₀ was stable at room temperature either under fluorescent light or UV-light irradiation.*

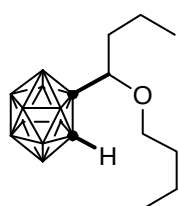


1aa-S: Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 4.57 (dd, *J* = 6.0, 2.8 Hz, 1H) (OCH), 3.62 (m, 1H), 3.43 (m, 1H) (OCHH), 2.99 (dd, *J* = 12.4, 6.0 Hz, 1H), 2.69 (dd, *J* = 12.0, 2.4 Hz, 1H) (CHH), 1.23 (t, *J* = 7.2 Hz, 3H) (CH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 79.4, 65.5, 44.1, 14.9, the cage carbons were not observed. ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -2.8 (1B), -4.1 (1B), -7.2 (1B), -8.7 (2B), -9.7 (4B), -11.8 (1B). HRMS (EI) calcd for C₆H₁₈¹¹B₈¹⁰B₂O⁺: 214.2358. Found: 214.2357.

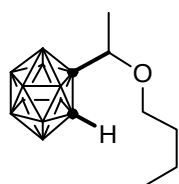
General Procedures for Reactions of *o*-Carborynes with Ethers under UV-light Irradiation (365 nm). A Representative Reaction of *o*-Carboryne with Diethyl Ether. To a diethyl ether solution (10 mL) of 1,2-Li₂-*o*-C₂B₁₀H₁₀ (1.0 mmol) in the dark, prepared in situ from the reaction of ⁿBuLi (1.25 ml, 1.6 M in hexane, 2.0 mmol) with *o*-carborane (144.2 mg, 1.0 mmol) in an ice-water bath, was added iodine (253.8 mg, 1.0 mmol). After stirring for another 0.5 h at 0 °C, iodine was completely disappeared and a colorless, clear solution was obtained. The resulting mixture was stirred at room temperature for 24 h under a handheld UV lamp irradiation (365 nm) and quenched by wet *n*-hexane. The solution was quickly passed through a short column of silica gel to remove the inorganic salt and washed with ether. The organic portions were combined. After removal of the solvents, the residue was purified by flash column chromatography on silica gel (230-400 mesh) using *n*-hexane/ether (*n*-hexane/ether = 80/1 in v/v) as eluent to give product **6aa** (183.5 mg, 85%).



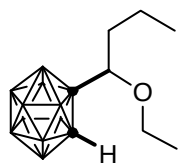
6ab: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 3.96 (br, 1H) (cage CH), 3.61 (dd, J = 9.2, 4.0 Hz, 1H) (OCH), 3.50 (t, J = 6.8 Hz, 2H) (OCH_2), 1.75 (m, 1H), 1.57 (m, 3H) (CH_2), 1.00 (t, J = 7.2 Hz, 3H), 0.92 (t, J = 7.2 Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 81.6 (cage C), 78.6 (cage C), 75.5, 58.6, 29.1, 23.1, 10.6, 10.5. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.6 (1B), -4.4 (1B), -9.1 (2B), -11.9 (3B), -13.2 (1B), -14.2 (2B). HRMS (EI) calcd for $\text{C}_8\text{H}_{23}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$ ($[\text{M}-\text{H}]^+$): 243.2751. Found: 243.2750.



6ac: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 3.95 (br, 1H) (cage CH), 3.67 (dd, J = 8.8, 4.0 Hz, 1H) (OCH), 3.52 (m, 2H) (OCH_2), 1.57 (m, 5H), 1.34 (m, 3H) (CH_2), 0.92 (m, 6H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 80.1 (cage C), 78.7 (cage C), 73.5, 58.7, 38.2, 31.9, 19.3, 19.2, 13.9, 13.8. $^{11}\text{B}\{^1\text{H}\}$ NMR (96 MHz, CDCl_3): δ -3.9 (m, 2B), -9.4 (2B), -12.2 (2B), -14.3 (m, 4B). HRMS (EI) calcd for $\text{C}_{10}\text{H}_{26}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$ ($[\text{M}-2\text{H}]^+$): 270.2981. Found: 270.2977.

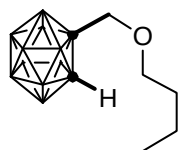


6ad: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 4.07 (br, 1H) (cage CH), 3.86 (d, J = 6.4 Hz, 1H) (OCH), 3.55 (m, 1H), 3.31 (m, 1H) (OCHH), 1.52 (m, 2H), 1.33 (m, 2H) (CH_2), 1.31 (d, J = 6.4 Hz, 3H), 0.92 (t, J = 7.2 Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 78.2 (cage C), 75.5 (cage C), 70.3, 58.5, 31.7, 19.7, 19.3, 13.8. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.7 (1B), -4.6 (1B), -9.2 (2B), -12.0 (3B), -13.3 (1B), -14.1 (m, 2B). HRMS (EI) calcd for $\text{C}_8\text{H}_{24}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$: 244.2829. Found: 244.2822.

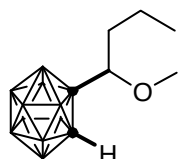


6ad': Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 3.95 (br, 1H) (cage CH), 3.68 (dd, J = 8.8, 4.0 Hz, 1H) (OCH), 3.60 (m, 2H) (OCH_2), 1.61 (m, 1H), 1.53 (m, 2H), 1.34 (m, 1H) (CH_2), 1.19 (t, J = 7.2 Hz, 3H), 0.94 (t, J = 7.2 Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 80.3 (cage C), 78.7 (cage C), 69.2, 58.8, 38.3, 19.4, 15.2, 13.8. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 80.3 (cage C), 78.7 (cage C), 69.2, 58.8, 38.3, 19.4, 15.2, 13.8.

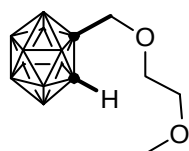
MHz, CDCl₃): δ -3.6 (1B), -4.5 (1B), -9.1 (2B), -11.9 (3B), -13.3 (1B), -14.1 (2B). HRMS (EI) calcd for C₈H₂₄¹¹B₈¹⁰B₂O⁺: 244.2829. Found: 244.2826.



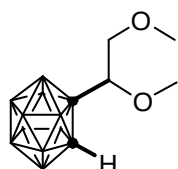
6ae: Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 3.95 (br, 1H) (cage CH), 3.83 (s, 2H) (OCH₂), 3.45 (t, *J* = 6.4 Hz, 2H) (OCH₂CH₃), 1.54 (m, 2H), 1.34 (m, 2H) (CH₂), 0.91 (t, *J* = 7.2 Hz, 3H) (CH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 72.7 (cage C), 71.9, 71.6 (cage C), 57.5, 31.3, 19.1, 13.8. ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -3.2 (1B), -5.0 (1B), -9.2 (1B), -10.3 (1B), -11.7 (2B), -13.4 (m, 4B). HRMS (EI) calcd for C₇H₂₂¹¹B₁₀O⁺: 232.2609. Found: 232.2601.



6ae': Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 3.97 (br, 1H) (cage CH), 3.59 (dd, *J* = 9.2, 3.6 Hz, 1H) (OCH), 3.46 (s, 3H) (OCH₃), 1.63 (m, 1H), 1.55 (m, 2H), 1.37 (m, 1H) (CH₂), 0.95 (t, *J* = 7.2 Hz, 3H) (CH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 82.0 (cage C), 78.4 (cage C), 61.3, 58.7, 38.0, 19.3, 13.8. ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -3.9 (1B), -4.6 (1B), -9.3 (2B), -12.2 (3B), -13.5 (1B), -14.4 (2B). HRMS (EI) calcd for C₇H₂₂¹¹B₈¹⁰B₂O⁺: 230.2673. Found: 230.2674.



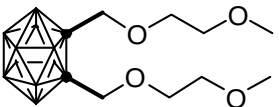
6af: Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 4.01 (br, 1H) (cage CH), 3.94 (s, 2H) (OCH₂), 3.64 (m, 2H), 3.50 (m, 2H) (OCH₂CH₂O), 3.36 (s, 3H) (OCH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 72.8 (cage C), 72.4 (cage C), 71.7, 71.4, 59.0, 57.6. ¹¹B{¹H} NMR (96 MHz, CDCl₃): δ -3.3 (1B), -5.1 (1B), -9.3 (2B), -11.9 (2B), -13.4 (4B). HRMS (EI) calcd for C₆H₂₀¹¹B₈¹⁰B₂O₂⁺: 232.2461. Found: 232.2462.

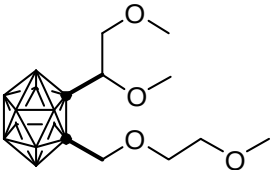


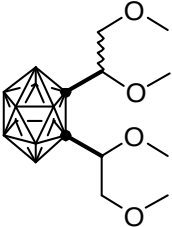
6af': Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 4.06 (br, 1H) (cage CH), 3.77 (dd, *J* = 6.4, 4.0 Hz, 1H) (OCH), 3.60 (dd, *J* = 10.4, 4.0 Hz, 1H) (OCHH), 3.51 (s, 3H)

(OCH₃), 3.42 (dd, *J* = 10.4, 6.4 Hz, 1H) (OCHH), 3.36 (s, 3H) (OCH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 79.7 (cage C), 75.1 (cage C), 74.4, 61.0, 59.2, 58.3. ¹¹B{¹H} NMR (96 MHz, CDCl₃): δ -3.6 (2B), -9.3 (2B), -12.0 (3B), -13.4 (1B), -14.1 (2B). HRMS (EI) calcd for C₆H₂₀¹¹B₈¹⁰B₂O₂⁺: 232.2461. Found: 232.2453.

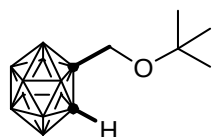
8af were obtained in a total yield of 15% with the isolated yields for each isomer reported as follows:

 (*l,l*)-**8af**: 1% yield. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 4.06 (s, 4H) (OCH₂), 3.66 (m, 4H), 3.52 (m, 4H) (OCH₂CH₂O), 3.37 (s, 6H) (OCH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 71.8, 71.5, 71.2, 59.1, the cage carbons were not observed. ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -3.8 (2B), -11.4 (8B). HRMS (EI) calcd for C₁₀H₂₈¹¹B₈¹⁰B₂O₄⁺: 320.2991. Found: 320.2992.

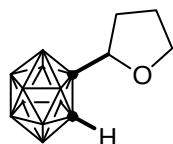
 (*b,l*)-**8af**: 6% yield. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 4.14 (d, *J* = 12.8 Hz, 1H), 4.08 (d, *J* = 12.4 Hz, 1H) (OCHH), 3.85 (dd, *J* = 7.2, 4.0 Hz, 1H) (OCH), 3.66 (m, 3H), 3.52 (m, 3H + 3H) (OCH₂ + OCH₃), 3.38 (s, 3H), 3.36 (s, 3H) (OCH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 78.8, 78.5 (cage C), 75.2, 71.9, 71.8, 71.1, 60.3, 59.0 (2 × OCH₃), another cage carbon was not observed. ¹¹B{¹H} NMR (96 MHz, CDCl₃): δ -2.7 (1B), -4.2 (1B), -11.2 (8B). HRMS (EI) calcd for C₁₀H₂₆¹¹B₈¹⁰B₂O₄⁺ ([M-2H]⁺): 318.2829. Found: 318.2819.

 (*b,b*)-**8af**: 8% yield, dr = 53:47. Colorless oil. Two diastereoisomers were inseparable. ¹H NMR (400 MHz, CDCl₃): δ 4.01 (dd, *J* = 7.2, 4.0 Hz, 2H) (isomer **A**), 3.94 (dd, *J* = 6.8, 3.6 Hz, 2H) (isomer **B**) (OCH), 3.68 (m, 4H) (OCHH), 3.53 (s, 6H) (OCH₃), 3.51 (m, 4H) (OCHH), 3.38 (s, 3H), 3.37 (s, 3H) (OCH₃). ¹³C{¹H} NMR (100 MHz,

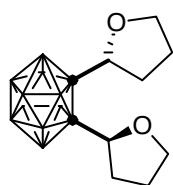
CDCl₃): isomer **A**: δ 81.0 (cage C), 79.3, 75.1, 60.1, 59.0; isomer **B**: δ 81.6 (cage C), 79.0, 75.0, 59.9, 59.0. ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -3.4 (2 × 2B), -10.6 (8B), -12.1 (8B). HRMS (EI) calcd for C₁₀H₂₇¹¹B₈¹⁰B₂O₄⁺ ([M-H]⁺) (isomers **A** + **B**): 319.2912. Found: 319.2919.



6ag: Colorless crystals. ¹H NMR (400 MHz, CDCl₃): δ 3.98 (br, 1H) (cage CH), 3.77 (s, 2H) (OCH₂), 1.16 (s, 9H) (C(CH₃)₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 75.0, 73.2 (cage C), 63.6, 57.2 (cage C), 27.2. ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -3.7 (1B), -5.5 (1B), -9.5 (2B), -11.8 (2B), -13.1 (2B), -13.7 (2B). HRMS (EI) calcd for C₇H₂₁¹¹B₈¹⁰B₂O⁺ ([M-H]⁺): 229.2590. Found: 229.2592.



6aj: Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 4.27 (t, *J* = 6.8 Hz, 1H) (OCH), 4.04 (br, 1H) (cage CH), 3.88 (m, 1H), 3.80 (m, 1H) (OCHH), 2.15 (m, 1H), 1.95 (m, 3H) (CH₂). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 79.1 (cage C), 77.8 (cage C), 69.6, 59.3, 32.8, 26.0. ¹¹B{¹H} NMR (96 MHz, CDCl₃): δ -3.5 (1B), -4.7 (1B), -9.2 (2B), -12.2 (3B), -13.2 (1B), -13.8 (m, 2B). HRMS (EI) calcd for C₆H₁₇¹¹B₈¹⁰B₂O⁺ ([M-H]⁺): 213.2277. Found: 213.2273.



meso-**8aj**: Colorless crystals. ¹H NMR (400 MHz, CDCl₃): δ 4.41 (t, *J* = 6.8 Hz, 2H) (OCH), 3.93 (m, 2H), 3.85 (m, 2H) (OCHH), 2.10 (m, 6H), 1.90 (m, 2H) (CH₂). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 83.1 (cage C), 77.6, 69.4, 33.4, 25.9. ¹¹B{¹H} NMR (96 MHz, CDCl₃): δ -3.7 (2B), -11.4 (m, 8B). HRMS (EI) calcd for C₁₀H₂₃¹¹B₈¹⁰B₂O₂⁺ ([M-H]⁺): 283.2696. Found: 283.2700.

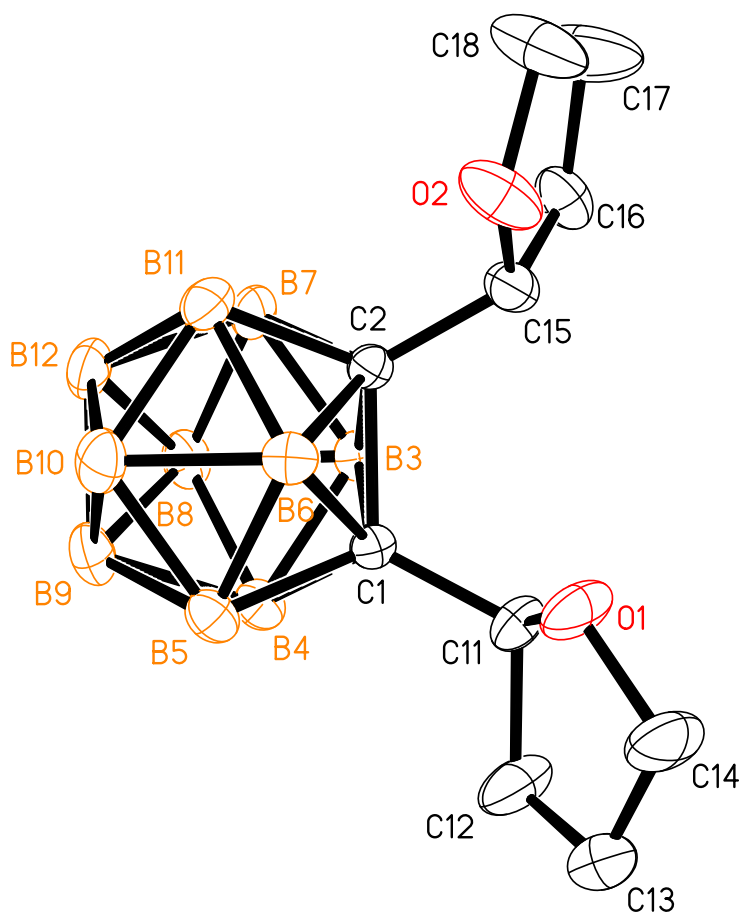
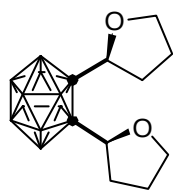
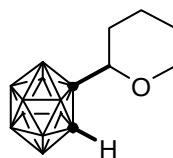


Figure S2. Molecular Structure of *meso*-**8aj**

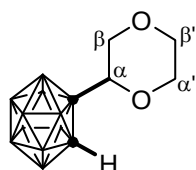


rac-8aj: White solid. ^1H NMR (400 MHz, CDCl_3): δ 4.51 (t, $J = 7.2$ Hz, 2H) (OCH), 3.87 (m, 4H) (OCH_2), 2.21 (m, 2H), 2.02 (m, 4H), 1.89 (m, 2H) (CH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 82.9 (cage C), 77.5, 69.3, 33.4, 26.0. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.4 (2B), -11.8 (m, 8B). HRMS (EI) calcd for $\text{C}_{10}\text{H}_{23}^{11}\text{B}_8^{10}\text{B}_2\text{O}_2^+$ ($[\text{M}-\text{H}]^+$): 283.2696. Found: 283.2684.

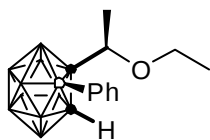


6ak: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 4.14 (br, 1H) (cage CH), 4.00 (dd, $J = 12.4, 2.0$ Hz, 1H) (OCH), 3.69 (dd, $J = 11.2, 2.0$ Hz, 1H), 3.40 (m, 1H) (OCHH), 1.91 (m, 1H), 1.82 (m, 1H), 1.42 (m, 4H) (CH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 77.1

(cage C), 69.7, 58.0, 31.7, 24.9, 23.1, another cage carbon was not observed. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -4.3 (1B), -4.7 (1B), -10.0 (2B), -11.7 (1B), -12.8 (2B), -13.5 (1B), -14.7 (2B). HRMS (EI) calcd for $\text{C}_7\text{H}_{20}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$: 228.2515. Found: 228.2513.



6al: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 4.09 (br, 1H) (cage CH), 3.95 (dd, J = 10.0, 2.4 Hz, 1H) (OC_αH), 3.88 (dd, J = 11.6, 2.4 Hz, 1H), 3.84 (dd, J = 11.6, 2.4 Hz, 1H) ($\text{OC}_\alpha'\text{HH}$), 3.72 (m, 2H) (OC_βHH , $\text{OC}_\beta'\text{HH}$), 3.52 (m, 1H) ($\text{OC}_\beta'\text{HH}$), 3.34 (dd, J = 11.6, 10.0 Hz, 1H) (OC_βHH). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 77.2 (cage C), 73.6, 70.3, 67.8, 65.7, 57.5 (cage C). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -4.1 (2B), -9.6 (1B), -10.0 (1B), -11.8 (1B), -13.5 (3B), -14.7 (2B). HRMS (EI) calcd for $\text{C}_6\text{H}_{18}^{11}\text{B}_8^{10}\text{B}_2\text{O}_2^+$: 230.2308. Found: 230.2312.



(R,R)-6ba: Colorless crystals. ^1H NMR (400 MHz, CDCl_3): δ 7.58 (m, 2H), 7.36 (m, 3H) (C_6H_5), 4.35 (br, 1H) (cage CH), 3.80 (q, J = 6.4 Hz, 1H) (OCH), 3.39 (m, 1H), 3.26 (m, 1H) (OCHH), 1.09 (t, J = 7.2 Hz, 3H), 0.93 (d, J = 6.4 Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 134.1, 129.2, 127.8, 76.1 (cage C), 65.8, 57.8, 18.2, 15.0, another cage carbon was not observed. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -2.8 (1B), -3.5 (2B), -6.9 (1B), -10.4 (5B), -13.7 (1B). HRMS (EI) calcd for $\text{C}_{12}\text{H}_{24}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$: 292.2825. Found: 298.2830.

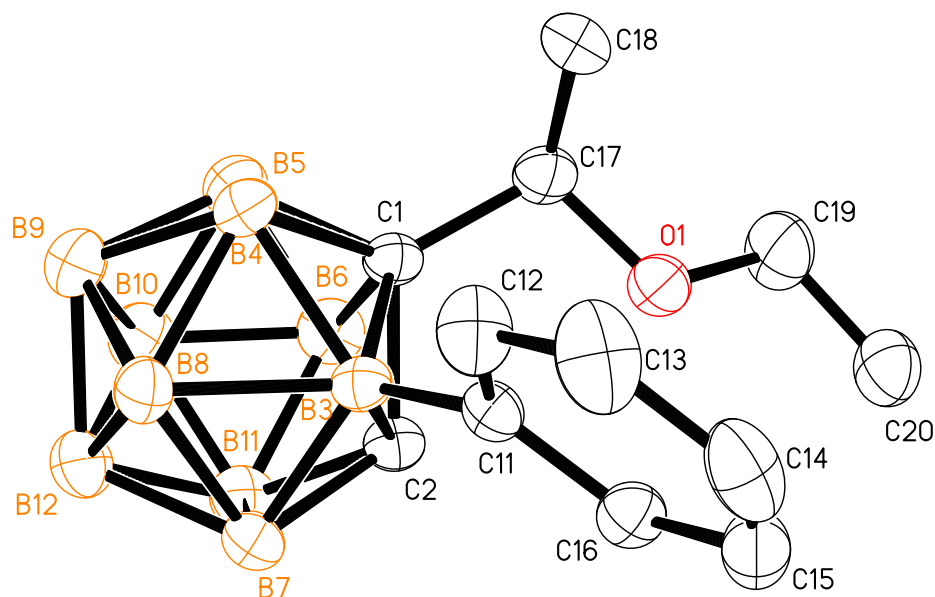
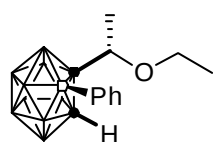
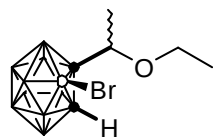


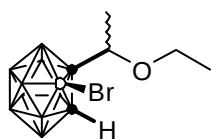
Figure S3. Molecular Structure of (*R,R*)-**6ba**



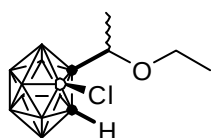
(*R,S*)-**6ba**: White solid. ^1H NMR (400 MHz, CDCl_3): δ 7.57 (m, 2H), 7.39 (m, 3H) (C_6H_5), 4.41 (br, 1H) (cage CH), 3.38 (q, $J = 6.4$ Hz, 1H) (OCH), 3.20 (m, 1H), 2.24 (m, 1H) (OCHH), 1.24 (d, $J = 6.4$ Hz, 3H), 0.91 (t, $J = 7.2$ Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 133.8, 129.6, 128.1, 72.1 (cage C), 64.6, 58.2, 19.0, 14.8, another cage carbon was not observed. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -2.6 (1B), -4.2 (1B), -7.0 (1B), -10.9 (2B), -12.2 (3B), -13.1 (2B). HRMS (EI) calcd for $\text{C}_{12}\text{H}_{24}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$: 292.2825. Found: 298.2823.



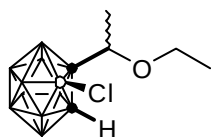
6ca: Colorless oil. The relative configuration was not determined. ^1H NMR (400 MHz, CDCl_3): δ 4.22 (br, 1H) (cage CH), 4.10 (q, $J = 6.4$ Hz, 1H) (OCH), 3.67 (m, 1H), 3.44 (m, 1H) (OCHH), 1.40 (d, $J = 6.0$ Hz, 3H), 1.18 (t, $J = 7.2$ Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 78.0 (cage C), 73.2 (cage C), 65.3, 61.9, 19.5, 15.2. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.1 (2B), -6.6 (1B), -8.8 (1B), -10.5 (2B), -11.6 (3B), -12.7 (1B). HRMS (EI) calcd for $\text{C}_6\text{H}_{19}^{11}\text{B}_8^{10}\text{B}_2\text{OBr}^+$: 295.1606. Found: 295.1597.



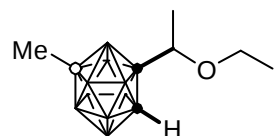
6ca': Colorless oil. The relative configuration was not determined. ^1H NMR (400 MHz, CDCl_3): δ 4.10 (br, 1H) (cage CH), 4.06 (q, $J = 6.4$ Hz, 1H) (OCH), 3.65 (m, 1H), 3.50 (m, 1H) (OCHH), 1.42 (d, $J = 6.8$ Hz, 3H), 1.21 (t, $J = 7.2$ Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 77.6 (cage C), 76.4 (cage C), 66.5, 61.8, 18.6, 15.1. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -2.9 (2B), -6.5 (1B), -9.3 (1B), -10.7 (5B), -13.1 (1B). HRMS (EI) calcd for $\text{C}_6\text{H}_{19}^{11}\text{B}_8^{10}\text{B}_2\text{OBr}^+$: 295.1606. Found: 295.1595.



6da: Colorless oil. The relative configuration was not determined. ^1H NMR (400 MHz, CDCl_3): δ 4.18 (br, 1H) (cage CH), 4.06 (q, $J = 6.4$ Hz, 1H) (OCH), 3.66 (m, 1H), 3.41 (m, 1H) (OCHH), 1.40 (d, $J = 6.4$ Hz, 3H), 1.17 (t, $J = 7.2$ Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 78.3 (cage C), 72.2 (cage C), 65.4, 61.5, 19.3, 15.2. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -4.2 (1B), -5.0 (2B), -8.7 (1B), -12.3 (2B), -13.4 (1B), -14.4 (4B). HRMS (EI) calcd for $\text{C}_6\text{H}_{19}^{11}\text{B}_8^{10}\text{B}_2\text{OCl}^+$ ($[\text{M}-\text{H}]^+$): 250.2020. Found: 250.2016.

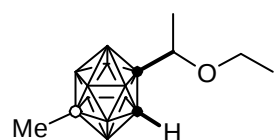
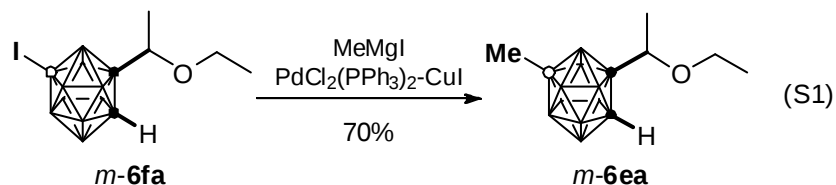


6da': Colorless oil. The relative configuration was not determined. ^1H NMR (400 MHz, CDCl_3): δ 4.14 (br, 1H) (cage CH), 4.05 (q, $J = 6.4$ Hz, 1H) (OCH), 3.65 (m, 1H), 3.48 (m, 1H) (OCHH), 1.41 (d, $J = 6.4$ Hz, 3H), 1.21 (t, $J = 7.2$ Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 77.8 (cage C), 76.0 (cage C), 66.4, 61.4, 18.5, 15.1. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -4.9 (2B), -5.6 (1B), -8.5 (1B), -11.0 (1B), -12.1 (3B), -13.8 (1B), -15.1 (1B). HRMS (EI) calcd for $\text{C}_6\text{H}_{19}^{11}\text{B}_8^{10}\text{B}_2\text{OCl}^+$ ($[\text{M}-\text{H}]^+$): 250.2020. Found: 250.2026.

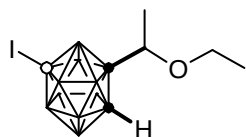


***m*-6ea**: Pure *m*-6ea was obtained from the transformation of pure *m*-6fa (eq S1).¹ Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 3.91 (br, 1H) (cage CH), 3.85 (q, $J = 6.4$ Hz, 1H) (OCH), 3.62 (m, 1H), 3.38 (m, 1H) (OCHH), 1.30 (d, $J = 6.0$ Hz, 3H), 1.17 (t, $J = 7.2$ Hz, 3H) (CH_3), 0.21 (br, 3H) ($\text{B}-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 75.4 (cage C),

66.0, 51.5, 19.8, 15.2, another cage carbon and the B-CH₃ were not observed. ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ 6.1 (1B), -3.7 (1B), -8.2 (1B), -11.7 (m, 3B), -14.0 (1B), -14.8 (2B). HRMS (EI) calcd for C₇H₂₂¹¹B₈¹⁰B₂O⁺: 230.2672. Found: 230.2667.



p-6ea: Data were only collected from a mixture of *m-6ea* and *p-6ea*. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 4.03 (br, 1H) (cage CH), 3.91 (q, *J* = 6.4 Hz, 1H) (OCH), 3.62 (m, 1H), 3.38 (m, 1H) (OCHH), 1.31 (d, *J* = 6.4 Hz, 3H), 1.17 (t, *J* = 7.2 Hz, 3H) (CH₃), 0.22 (br, 3H) (B-CH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 74.9 (cage C), 66.0, 58.0, 20.0, 15.2, another cage carbon and the B-CH₃ were not observed. HRMS (EI) calcd for C₇H₂₂¹¹B₈¹⁰B₂O⁺ (*m-6ea* + *p-6ea*): 230.2672. Found: 230.2670.



m-6fa: Colorless crystals. ¹H NMR (400 MHz, CDCl₃): δ 4.37 (br, 1H) (cage CH), 3.89 (q, *J* = 6.4 Hz, 1H) (OCH), 3.63 (m, 1H), 3.38 (m, 1H) (OCHH), 1.35 (d, *J* = 6.4 Hz, 3H), 1.17 (t, *J* = 7.2 Hz, 3H) (CH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 79.0 (cage C), 75.1 (cage C), 66.1, 54.9, 19.8, 15.1. ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -2.0 (1B), -6.4 (2B), -10.2 (3B), -12.0 (1B), -12.8 (m, 2B), -16.3 (1B). HRMS (EI) calcd for C₆H₁₉¹¹B₈¹⁰B₂OI⁺: 342.1481. Found: 342.1476.

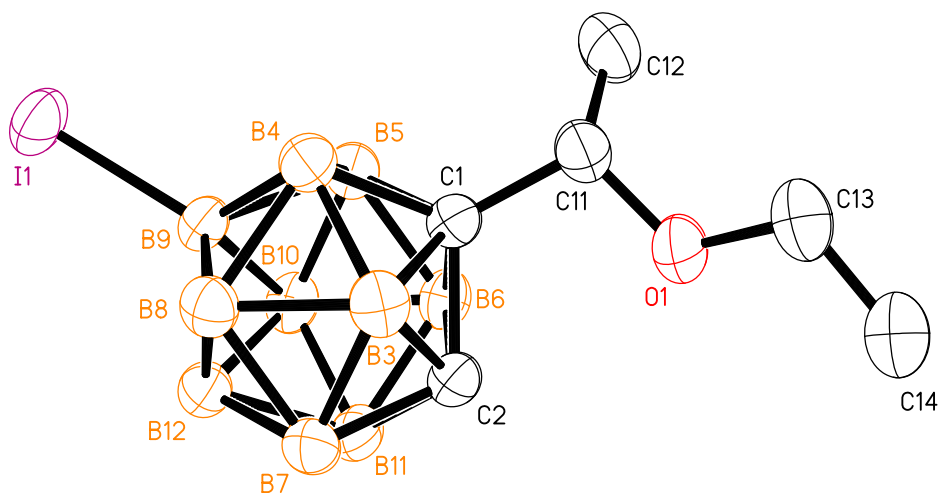
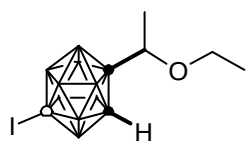
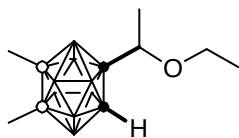


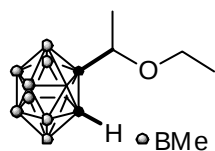
Figure S4. Molecular Structure of *m*-**6fa**



***p*-6fa:** Colorless crystals. ^1H NMR (400 MHz, CDCl_3): δ 4.18 (br, 1H) (cage CH), 3.81 (q, $J = 6.4$ Hz, 1H) (OCH), 3.62 (m, 1H), 3.36 (m, 1H) (OCHH), 1.29 (d, $J = 6.0$ Hz, 3H), 1.17 (t, $J = 7.2$ Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 75.4 (cage C), 66.0, 59.5, 19.7, 15.1, the other cage carbon was not observed. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -1.1 (1B), -6.4 (2B), -10.8 (4B), -12.1 (1B), -13.3 (1B), -16.3 (1B). HRMS (EI) calcd for $\text{C}_6\text{H}_{19}^{11}\text{B}_8^{10}\text{B}_2\text{OI}^+$: 342.1481. Found: 342.1483.



***6ga*:** Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 3.89 (m, 2H) (cage CH + OCH), 3.61 (m, 1H), 3.37 (m, 1H) (OCHH), 1.31 (d, $J = 6.4$ Hz, 3H), 1.17 (t, $J = 6.8$ Hz, 3H) (CH_3), 0.17 (br, 6H) (B- CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 75.0 (cage C), 66.0, 51.9, 20.0, 15.2, the other cage carbon and the two B- CH_3 were not observed. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 6.1 (1B), 5.3 (1B), -7.2 (2B), -12.0 (m, 2B), -13.3 (2B), -14.1 (2B), -16.0 (1B). HRMS (EI) calcd for $\text{C}_8\text{H}_{24}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$: 244.2829. Found: 244.2823.



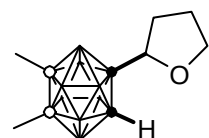
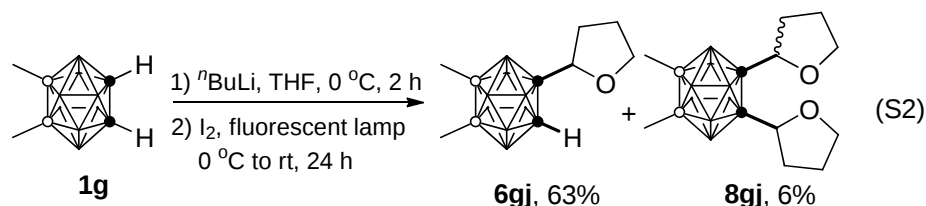
6ha: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 3.80 (q, $J = 6.4$ Hz, 1H) (OCH), 3.60 (m, 1H) (OCHH), 3.41 (m, 2H) (cage CH + OCHH), 1.27 (d, $J = 6.4$ Hz, 3H), 1.17 (t, $J = 7.2$ Hz, 3H) (CH_3), 0.12 (br, 3H), 0.11 (br, 3H), 0.09 (br, 3H), 0.04 (br, 3H), -0.02 (br, 3H), -0.05 (br, 3H), -0.25 (br, 6H) (B- CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 72.6 (cage C), 62.8 (cage C), 66.2, 53.6, 20.2, 15.2, -4.4 (br). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 7.5 (1B), 6.3 (1B), -1.3 (2B), -5.9 (1B), -7.1 (m, 3B), -13.2 (2B), -14.5 (1B). HRMS (EI) calcd for $\text{C}_{14}\text{H}_{36}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$: 328.3764. Found: 328.3760.

Reaction of 2a with Diethyl Ether in the Presence of TEMPO. To an in situ prepared diethyl ether solution (10 mL) of 1-iodo-2-Li-*o*- $\text{C}_2\text{B}_{10}\text{H}_{10}$ (1.0 mmol) in the dark in an ice-water bath, was added TEMPO (171.6 mg, 1.1 mmol). The resulting solution was then stirred for 24 h at room temperature under UV-light irradiation (365 nm) and then quenched by wet *n*-hexane. The resolution was quickly passed through a short column of silica gel to remove the inorganic salt and washed with ether. The organic portions were combined. After removal of the solvents, the crude product was then analyzed by ^1H NMR and GC-MS. The results showed that most of the crude product was 1-iodo-*o*-carborane, which was generated from the protonation of **2a**, with a trace contaminant of *o*-carborane and 1,2-diiodo-*o*-carborane, and no C-H bond insertion product **6aa** or any TEMPO-coupled product was observed.

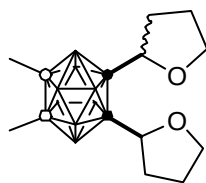
The Kinetic Isotope Effect Experiments

(1) Reaction of 9,12-Dimethyl-*o*-Carboryne with THF under Fluorescent Light Irradiation. To a THF solution (5 mL) of 1,2-Li₂-9,12-Me₂-*o*- $\text{C}_2\text{B}_{10}\text{H}_8$ (0.4 mmol), prepared in situ from the reaction of $n\text{BuLi}$ (0.5 mL, 1.6 M in hexane, 0.8 mmol) with 9,12-Me₂-*o*- $\text{C}_2\text{B}_{10}\text{H}_{10}$ (68.8 mg, 0.4 mmol) in THF in an ice-water bath, was added iodine (101.6 mg, 0.4 mmol). After stirring for another 0.5 h at 0 °C, iodine was completely disappeared and a colorless, clear solution was obtained. The resulting mixture

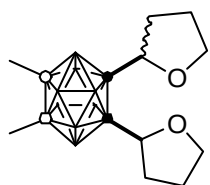
was stirred at room temperature for 24 h and then quenched by wet *n*-hexane. The solution was quickly passed through a short column of silica gel to remove the inorganic salt and washed with ether. The organic portions were combined. After removal of the solvents, the residue was purified by flash column chromatography on silica gel (230-400 mesh) using *n*-hexane/ether (*n*-hexane/ether = 70/1 in v/v) as eluent to give product **6gj** (61.0 mg, 63%) and products **8gj** (6.1 mg, 6%) with an isomeric ratio of 44/56. See eq S2.



6gj: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 4.29 (t, $J = 6.8$ Hz, 1H) (OCH), 3.89 (m, 1H) (OCHH), 3.78 (m, 2H) (cage CH + OCHH), 2.15 (m, 1H), 1.93 (m, 3H) (CH_2), 0.17 (br, 6H) (B- CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 79.0 (cage C), 70.8 (cage C), 69.5, 52.5, 32.9, 26.1, the two B- CH_3 were not observed. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 6.2 (1B), 5.0 (1B), -7.4 (1B), -7.7 (1B), -12.6 (2B), -13.4 (2B), -14.1 (1B), -16.1 (1B). HRMS (EI) calcd for $\text{C}_8\text{H}_{22}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$: 242.2672. Found: 242.2671.



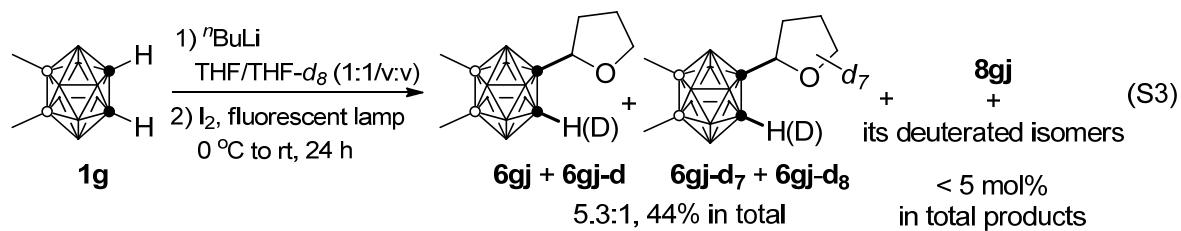
8gj: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 4.52 (t, $J = 6.8$ Hz, 2H) (OCH), 3.85 (m, 4H) (OCH_2), 2.21 (m, 2H), 2.01 (m, 4H), 1.87 (m, 2H) (CH_2), 0.19 (br, 6H) (B- CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ 77.4, 69.1, 33.7, 26.0, the cage carbons and the B- CH_3 were not observed (noted that the CDCl_3 carbon signal was overlapped with one of the carbons in THF motif, whereas that of C_6D_6 did not show any overlapping with THF). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 6.6 (2B), -9.7 (m, 3B), -11.5 (2B), -12.2 (3B). HRMS (EI) calcd for $\text{C}_{12}\text{H}_{28}^{11}\text{B}_8^{10}\text{B}_2\text{O}_2^+$: 312.3093. Found: 312.3094.



8gj': Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 4.41 (t, $J = 6.8$ Hz, 2H) (OCH), 3.92 (m, 2H), 3.83 (m, 2H) (OCHH), 2.16 (m, 2H), 2.10 (m, 2H), 2.03 (m, 2H), 1.88 (m, 2H) (CH_2), 0.19 (br, 6H) (B- CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ 77.6, 68.9,

33.5, 26.0, the cage carbons and the B- CH_3 were not observed. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 6.1 (2B), -8.4 (1B), -9.5 (1B), -11.5 (2B), -12.3 (br, 4B). HRMS (EI) calcd for $\text{C}_{12}\text{H}_{28}^{11}\text{B}_8^{10}\text{B}_2\text{O}_2^+$: 312.3093. Found: 312.3080.

(2) Reaction of 9,12-Dimethyl-*o*-Carboryne with THF/THF- d_8 under Fluorescent Light Irradiation. To a THF/THF- d_8 (1:1 in v/v) solution (3+3 mL) of 1,2-Li₂-9,12-Me₂-*o*-C₂B₁₀H₈ (0.4 mmol), prepared in situ from the reaction of $n\text{-BuLi}$ (0.5 mL, 1.6 M in hexane, 0.8 mmol) with 9,12-Me₂-*o*-C₂B₁₀H₁₀ (68.8 mg, 0.4 mmol) in an ice-water bath, was added iodine (101.6 mg, 0.4 mmol). After stirring for another 0.5 h at 0 °C, iodine was completely disappeared and a colorless clear solution was obtained. The resulting mixture was stirred at room temperature for 24 h and quenched by wet *n*-hexane. The solution was quickly passed through a short column of silica gel to remove the inorganic salt and washed with ether. The organic portions were combined. After removal of the solvents, the residue was purified by flash column chromatography on silica gel (230-400 mesh) using *n*-hexane/ether (*n*-hexane/ether = 70/1 in v/v) as eluent to give product **6gj** and its deuterated isomers (43.0 mg, 44%). A trace amount of products **8gj** and its deuterated isomers (less than 5 mol% in total products) were observed in the ^1H NMR spectrum of the crude product, which may induce little but negligible inaccuracy in the *KIE* value. See eq S3.



Calculations based on the ^1H NMR spectrum (with a duration of 10 seconds) of the isolated mixture of the product **6gj** and its deuterated isomers showed a k_H/k_D value of 5.3 (Fig S5 and Fig S6.). Furthermore, the ^2H NMR spectrum of the same mixture showed that ca. 43% of total cage C-H was deuterated (Fig S7.).

Fig 5. ^1H NMR spectrum of **6gj** ($d_1 = 10$ seconds) (For reference)

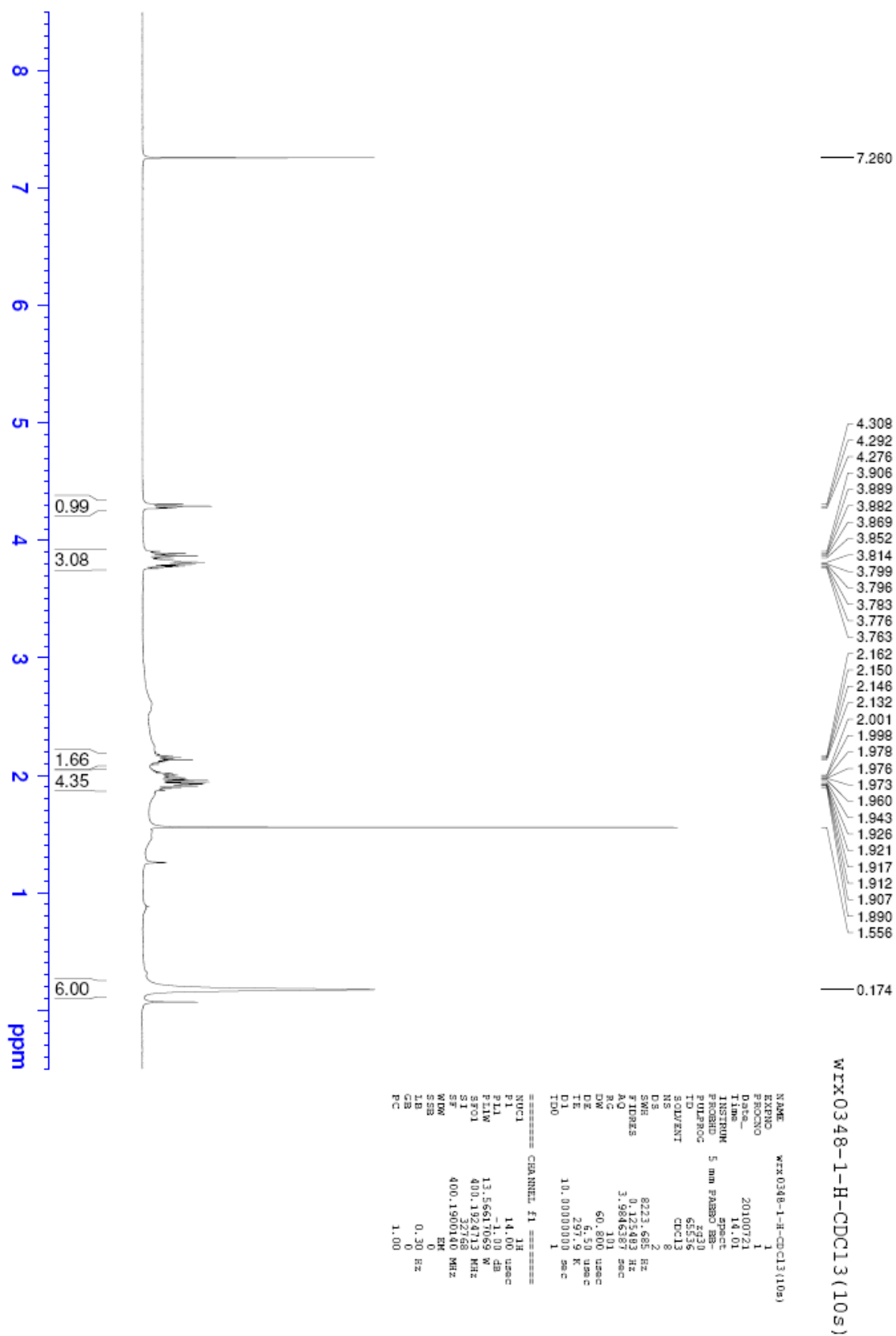


Fig 6. ^1H NMR spectrum for Determination of *KIE* value ($d_1 = 10$ seconds)

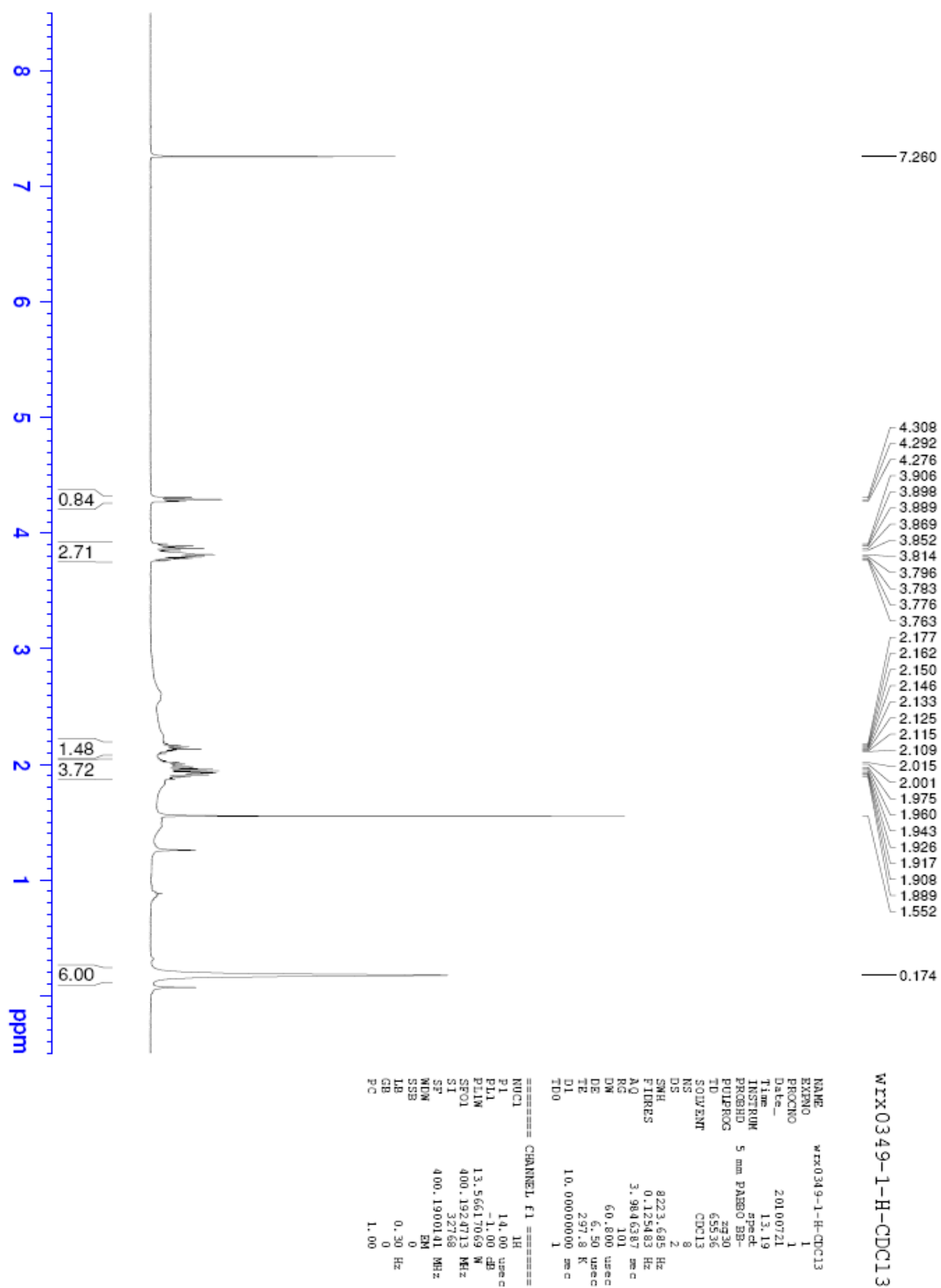
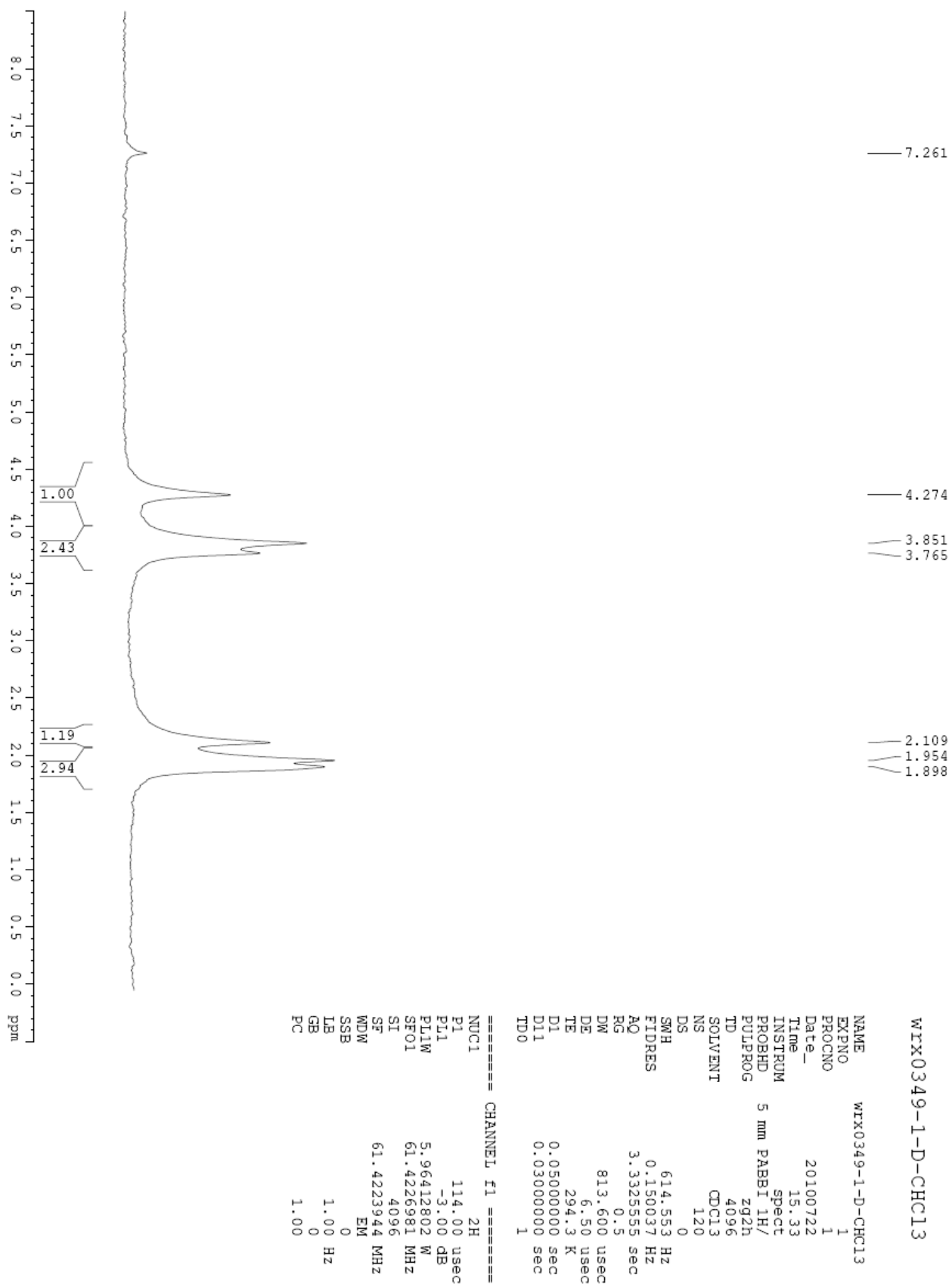
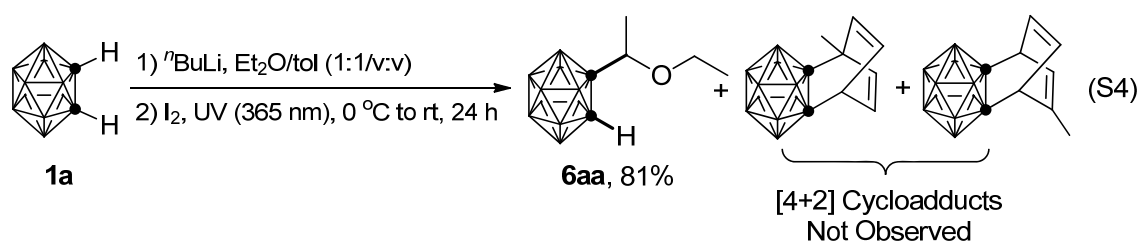


Fig 7. ^2H NMR spectrum of the Mixture of 6gj and Its Deuterated Isomers

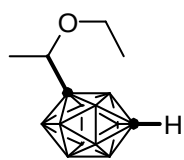


Competitive Reaction between Diethyl Ether and Toluene with *o*-Carboryne. To a diethyl ether/toluene (1:1/v:v) solution (5+5 mL) of 1,2-Li₂-*o*-C₂B₁₀H₁₀ (1.0 mmol), prepared in situ from the reaction of ⁿBuLi (1.25 ml, 1.6 M in hexane, 2.0 mmol) with *o*-carborane (144.2 mg, 1.0 mmol) in an ice-water bath, was added iodine (253.8 mg, 1.0 mmol). After stirring for another 0.5 h at 0 °C, iodine was completely disappeared and a colorless, clear solution was obtained. The resulting mixture was stirred at room temperature for 24 h under UV light irradiation (365 nm) and quenched by wet *n*-hexane. The solution was quickly passed through a short column of silica gel to remove the inorganic salt and washed with ether. The organic portions were combined. After removal of the solvents, the residue was purified by flash column chromatography on silica gel (230-400 mesh) using *n*-hexane/ether (*n*-hexane/ether = 80/1 in v/v) as eluent to give product **6aa** (174.2 mg, 81%). No [4+2] cycloadducts between *o*-carboryne and toluene were observed in the ¹H NMR spectrum of the crude product. See eq S4.



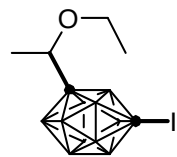
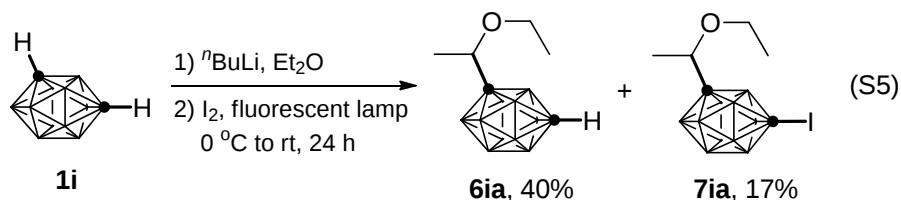
Reaction of *m*-Carboryne with Diethyl Ethers under UV-light Irradiation (365 nm). To a diethyl ether solution (10 mL) of 1,7-Li₂-*m*-C₂B₁₀H₁₀ (0.8 mmol), prepared in situ from the reaction of ⁿBuLi (1.0 ml, 1.6 M in hexane, 1.6 mmol) with *m*-carborane (115.2 mg, 0.8 mmol) in an ice-water bath, was added iodine (203.4 mg, 0.8 mmol). After stirring for another 0.5 h at 0 °C, iodine was completely disappeared and a colorless, clear solution was obtained. The resulting mixture was stirred at room temperature for 24 h under a handheld UV lamp irradiation (365 nm) and quenched by wet *n*-hexane. The solution was quickly passed through a short column of silica gel to remove the inorganic salt and washed with ether. The organic portions were combined. After removal of the solvents, the

residue was purified by flash column chromatography on silica gel (230-400 mesh) using *n*-hexane/ether (*n*-hexane/ether = 80/1 in v/v) as eluent to give product **6ia** (133.0 mg, 77%).



6ia: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 3.53 (m, 2H) (OCH + OCHH), 3.45 (m, 1H) (OCHH), 2.88 (br, 1H) (cage CH), 1.18 (m, 6H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 81.5 (cage C), 76.1, 66.3, 54.2 (cage C), 21.1, 15.1, 15.2. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -4.1 (1B), -7.9 (1B), -10.5 (3B), -11.5 (1B), -12.9 (2B), -15.0 (1B), -15.4 (1B). HRMS (EI) calcd for $\text{C}_6\text{H}_{20}^{11}\text{B}_8^{10}\text{B}_2\text{O}^+$: 216.2515. Found: 216.2519.

The same reaction did not proceed to completion in 24h under fluorescent light irradiation. See eq S5.



7ia: Colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 3.54 (m, 2H) (OCH + OCHH), 3.45 (m, 1H) (OCHH), 1.18 (m, 6H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 84.1 (cage C), 76.0, 66.4, 21.0, 15.1, 3.5 (cage C). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -4.3 (1B), -7.4 (1B), -9.2 (2B), -10.8 (2B), -11.6 (1B), -12.3 (m, 3B). HRMS (EI) calcd for $\text{C}_6\text{H}_{19}^{11}\text{B}_8^{10}\text{B}_2\text{OI}^+$: 342.1481. Found: 342.1493.

X-ray Structure Determination. All data were collected at 293 K on a Bruker SMART 1000 CCD diffractometer using Mo-K α radiation. An empirical absorption correction was applied using the SADABS program.² All structures were solved by direct methods and subsequent Fourier difference techniques and refined anisotropically for all non-hydrogen atoms by full-matrix least squares calculations on F^2 using the SHELXTL program package.³ All hydrogen atoms were geometrically fixed using the riding model. Crystal data and details of data collection and structure refinements are given in Table S1.

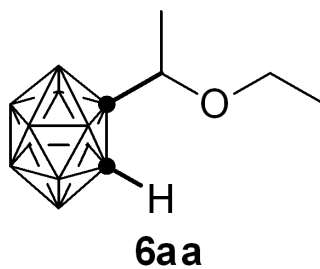
References

- (1) Zheng, Z. J.; Jiang, W.; Zinn, A. A.;Knobler, C. B.; Hawthorne, M. F. *Inorg. Chem.* **1995**, *34*, 2095.
- (2) Sheldrick, G. M. SADABS: Program for Empirical Absorption Correction of Area Detector Data. University of Göttingen: Germany, **1996**.
- (3) Sheldrick, G. M. SHELXTL 5.10 for Windows NT: Structure Determination Software Programs. Bruker Analytical X-ray Systems, Inc., Madison, Wisconsin, USA, **1997**.

Table S1. Crystal Data and Summary of Data Collection and Refinement

	<i>(R,R)</i> -6ba	<i>m</i> -6fa	<i>meso</i> -8aj
formula	C ₁₂ H ₂₄ B ₁₀ O	C ₆ H ₁₉ B ₁₀ OI	C ₁₀ H ₂₄ B ₁₀ O ₂
crystal size (mm)	0.50×0.40×0.30	0.50×0.40×0.30	0.50×0.30×0.20
fw	292.41	342.21	284.39
crystal system	orthorhombic	orthorhombic	monoclinic
space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>C</i> 2/c
<i>a</i> , Å	7.582 (1)	7.198 (1)	28.060 (2)
<i>b</i> , Å	10.124 (1)	9.186 (1)	7.378 (1)
<i>c</i> , Å	3.702 (2)	22.876 (1)	17.176 (1)
α , deg	90	90	90
β , deg	90	90	112.13 (1)
γ , deg	90	90	90
<i>V</i> , Å ³	1819.4 (3)	1512.4 (1)	3293.8 (4)
<i>Z</i>	4	4	8
<i>D</i> _{calcd} , Mg/m ³	1.068	1.503	1.147
radiation (λ), Å	0.71073	0.71073	0.71073
2 θ range, deg	3.44 to 50.50	4.78 to 50.50	3.14 to 50.50
μ , mm ⁻¹	0.055	2.092	0.063
<i>F</i> (000)	616	664	1200
no. of obsd rflns	3284	2732	2987
no. of params refnd	208	164	199
goodness of fit	1.057	1.141	1.053
R1	0.053	0.017	0.078
wR2	0.133	0.045	0.212

7.260



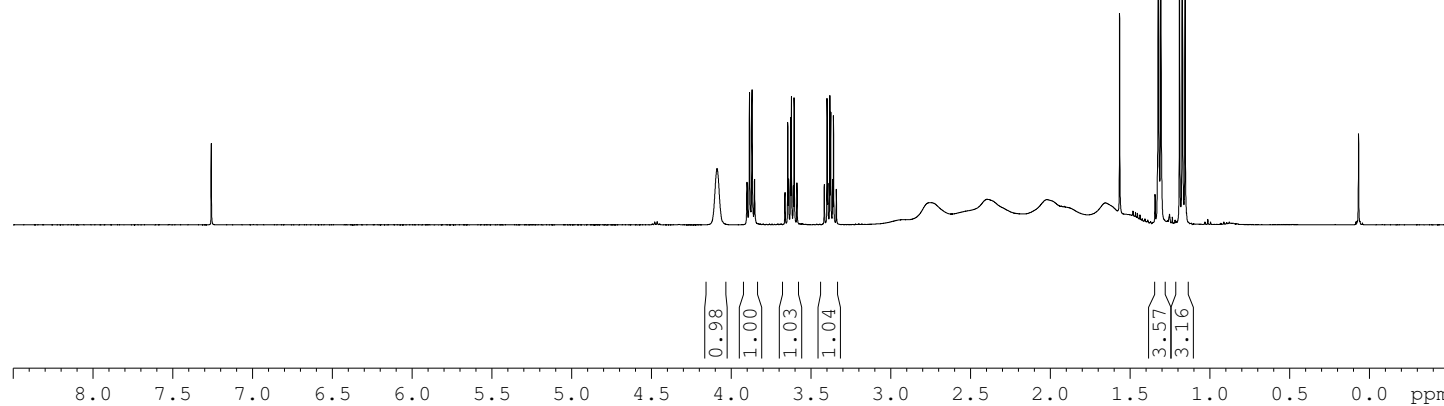
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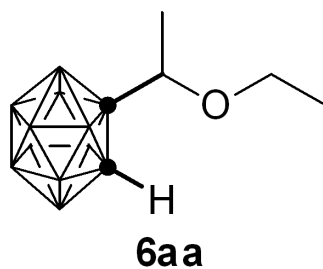
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PROCNO 1
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SOLVENT CDC13
NS 2
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
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RG 64
DW 50.000 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1

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SI 65536
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





78.10
77.32
77.00
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75.30
— 66.01
— 58.61

— 19.81
— 15.13

wrx-CB+Et2O-C-CDCl3

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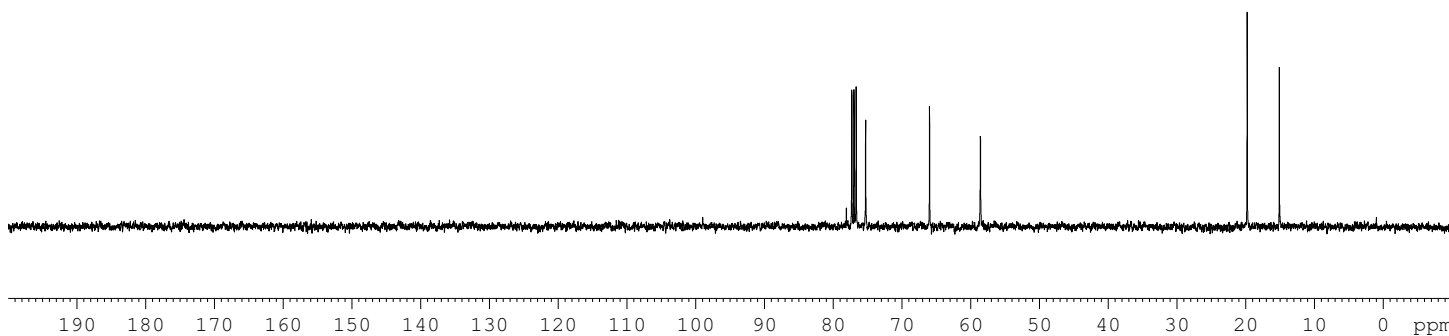
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PL2         0.00 dB
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PL12W       0.22585411 W
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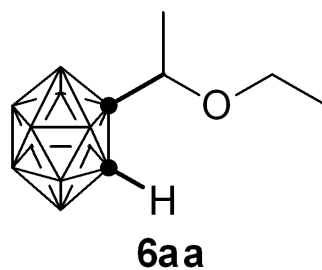
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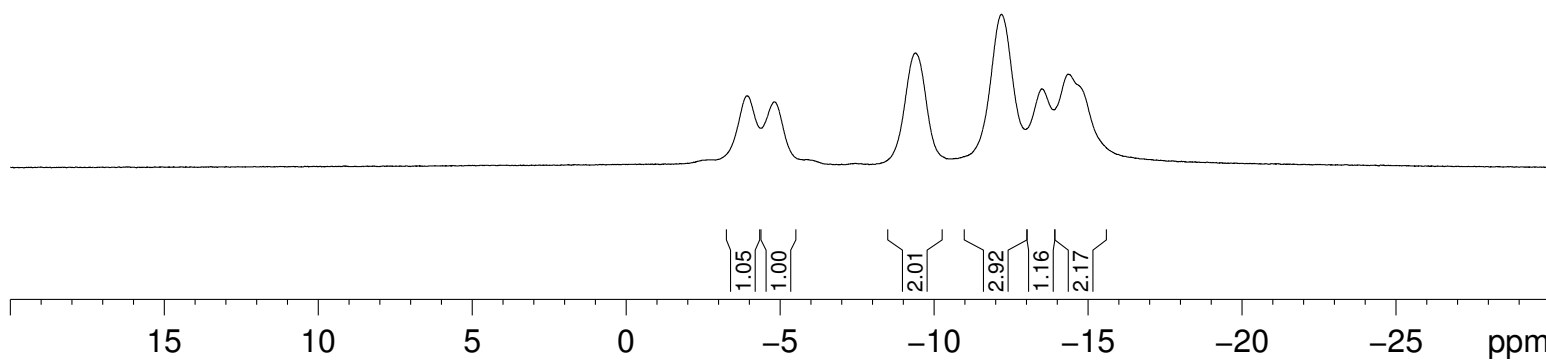


wrx-CB+Et2O-B-CDCl3

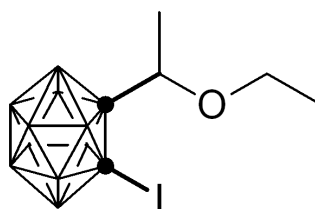
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— 7.260

**7aa**

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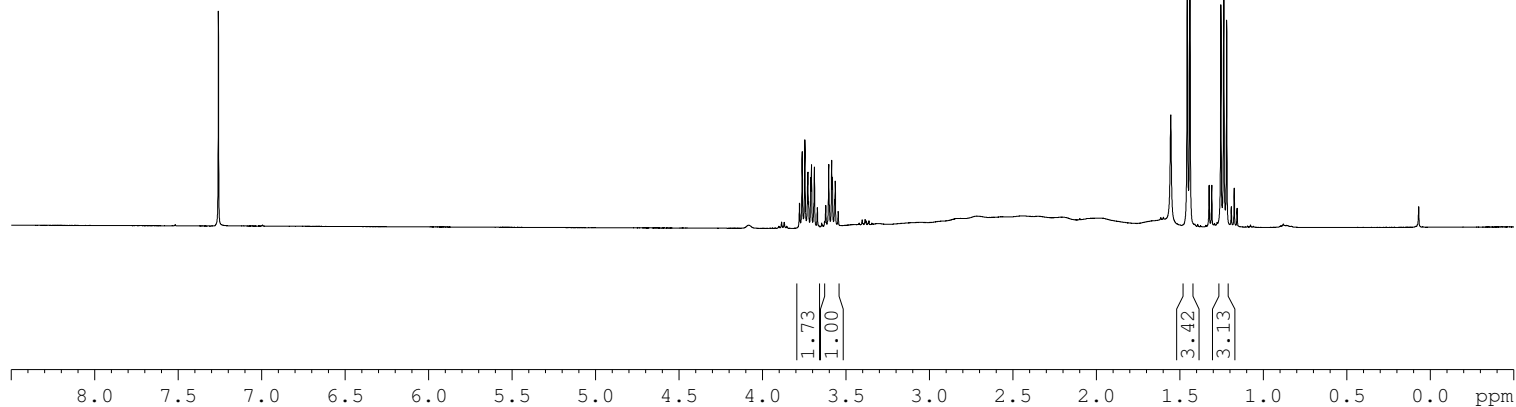
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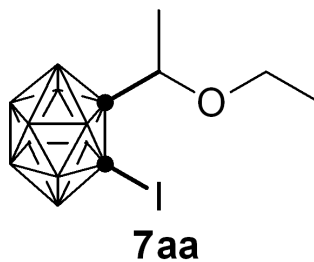
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RG          144
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D1          1.00000000 sec
TD0         1
  
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WDW          EM
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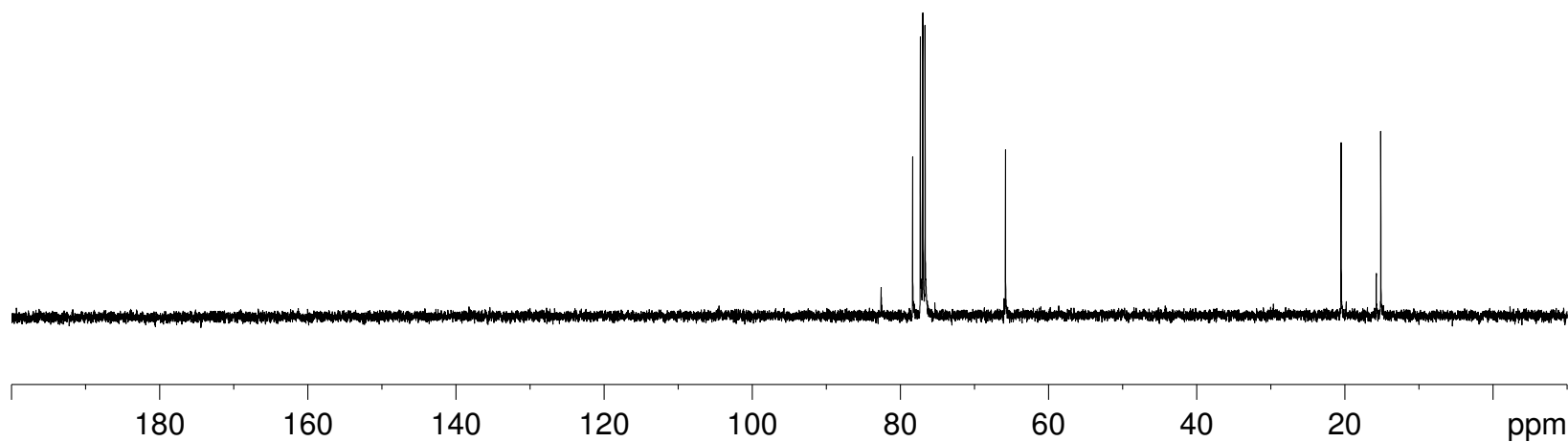
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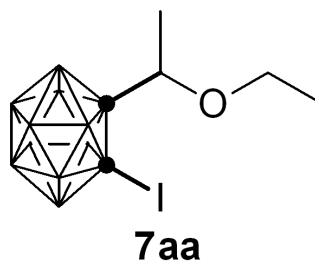
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PL13 18.62 dB
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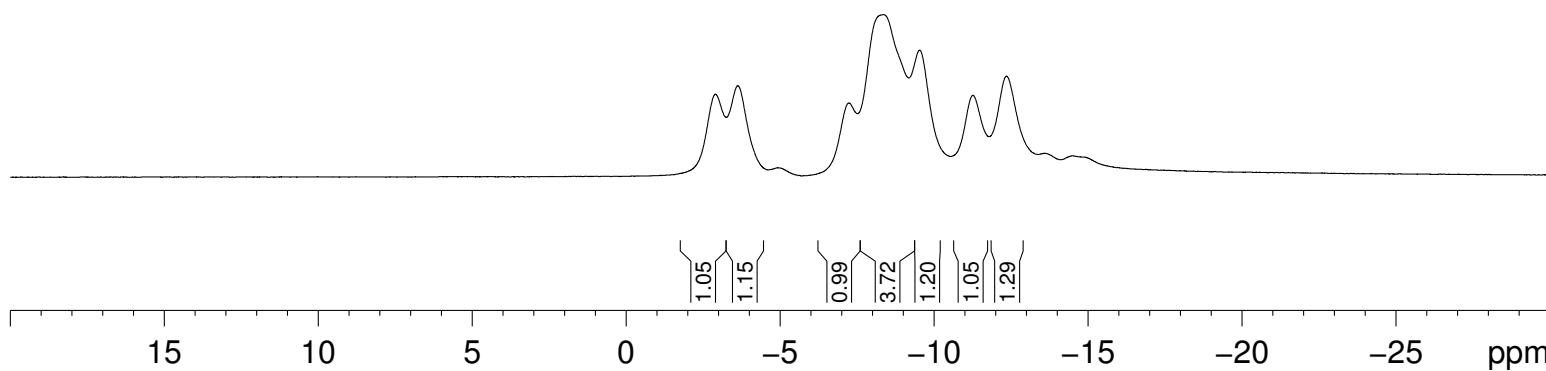
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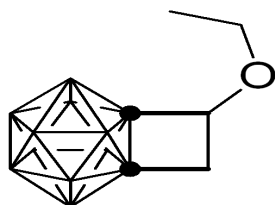
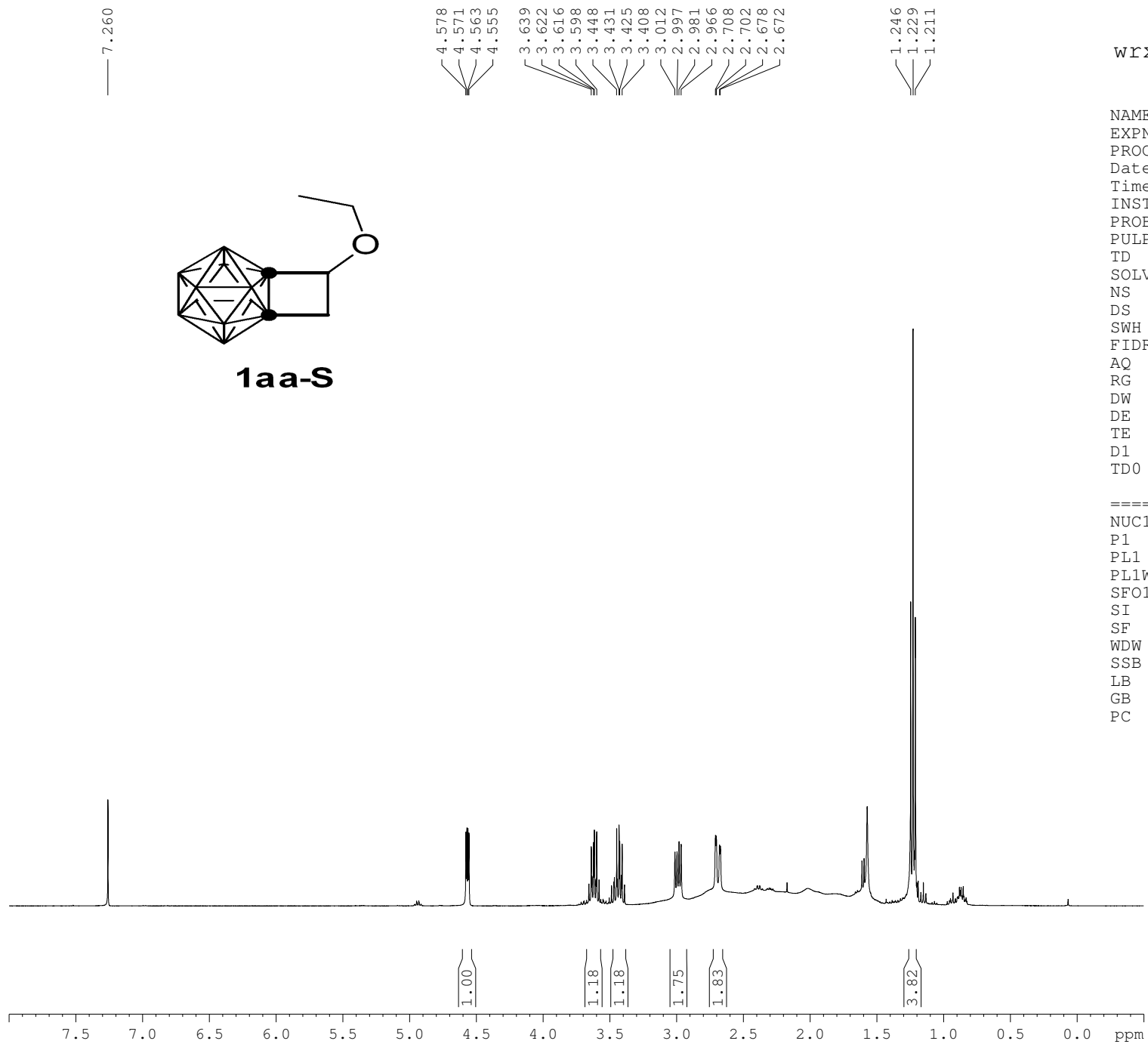
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EXPNO 1
PROCNO 1
Date_ 20100827
Time 9.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 65536
SOLVENT CDC13
NS 12
DS 0
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 181
DW 19.600 usec
DE 6.50 usec
TE 303.3 K
D1 5.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 7.60 usec
PL1 -3.00 dB
PL1W 55.13059616 W
SFO1 128.3968556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
SFO2 400.1916008 MHz
SI 32768
SF 128.3969002 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



— 7.260

**1aa-S**

4.578
4.571
4.563
4.555

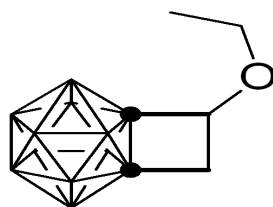
3.639
3.622
3.616
3.598
3.448
3.431
3.425
3.408
3.012
2.997
2.981
2.966
2.708
2.702
2.678
2.672

1.246
1.229
1.211

wrx0281-3a-H-CDCl3

NAME wrx0281-3a-H-CDCl3
 EXPNO 1
 PROCNO 1
 Date_ 20100324
 Time 10.18
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zg
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 128
 DW 62.400 usec
 DE 6.50 usec
 TE 295.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PL1 0.00 dB
 PL1W 8.31434441 W
 SFO1 400.1316005 MHz
 SI 65536
 SF 400.1300053 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

**1aa-S**

79.359
77.318
77.001
76.683

65.533

44.136

14.856

wrx0281-3a-C-CDCl₃

```

NAME      wrx0281-3a-C-CDCl3
EXPNO      1
PROCNO     1
Date_      20100325
Time       20.49
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgdc
TD          131072
SOLVENT    CDCl3
NS          625
DS          0
SWH         29761.904 Hz
FIDRES      0.227065 Hz
AQ          2.2020595 sec
RG          203
DW          16.800 usec
DE          6.50 usec
TE          295.2 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0         1

```

```

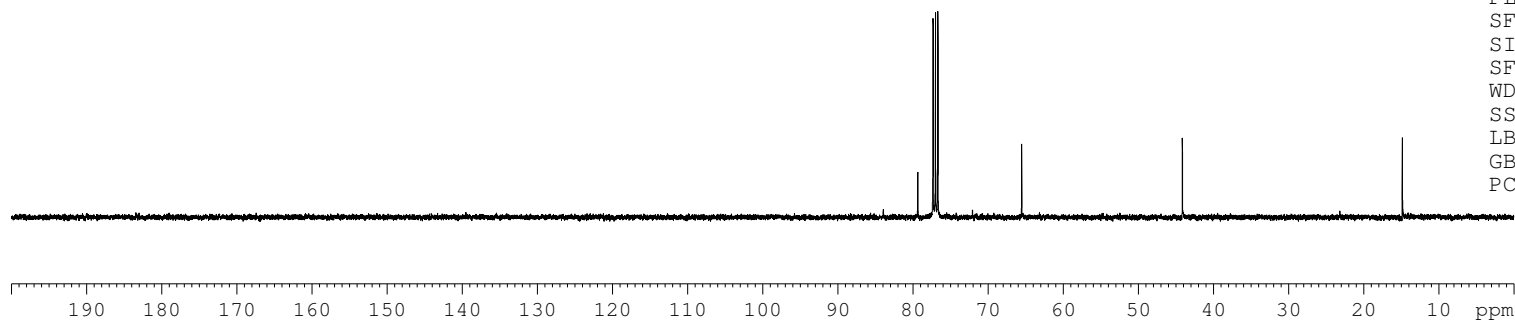
===== CHANNEL f1 =====
NUC1        13C
P1           3.50 usec
PL1          -0.60 dB
PL1W         41.24164963 W
SFO1         100.6227690 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2        90.00 usec
PL2           0.00 dB
PL12         16.10 dB
PL2W         8.31434441 W
PL12W        0.20409293 W
SFO2         400.1320007 MHz
SI           131072
SF           100.6127707 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

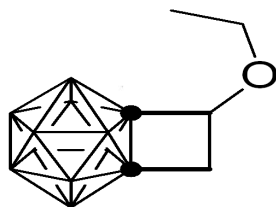


wrx0281-3a-B-CDC13

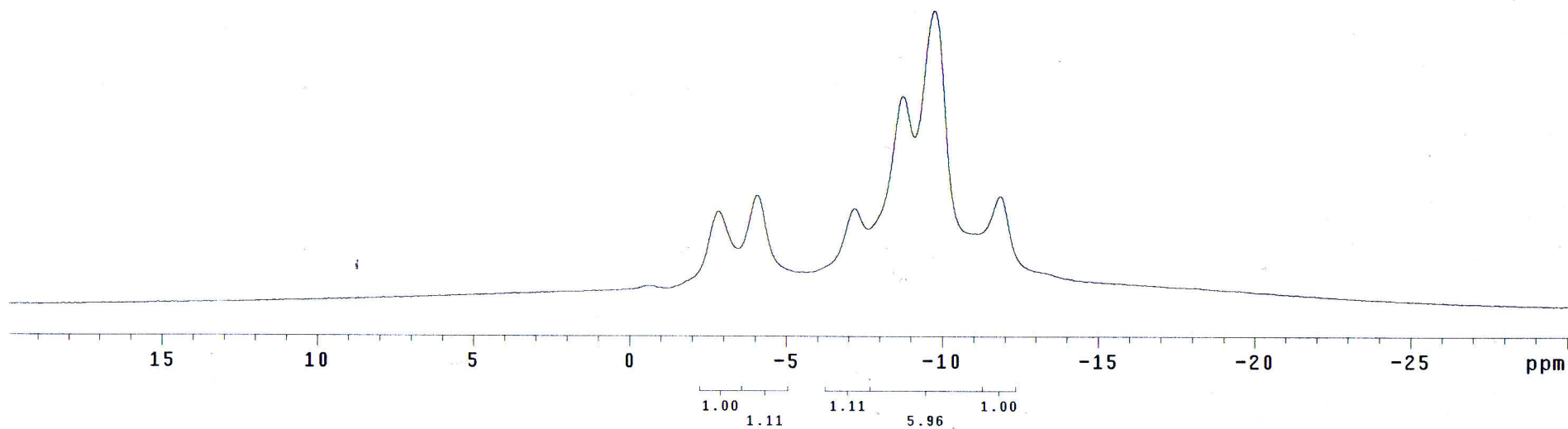
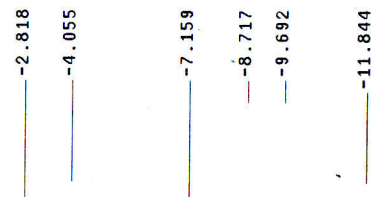
S35

exp1 s2pu1

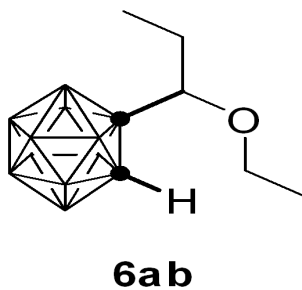
SAMPLE		DEC. & VT	
date	Mar 23 2010	dfrq	399.951
solvent	CDC13	dn	H1
file	/export/home/~	dpwr	40
wrx/wrx0281-3a-B-C~		dof	0
	DC13.fid	dm	yyy
ACQUISITION		dmm	g
sfrq	128.317	dmf	11765
tn	B11	PROCESSING	
at	0.655	lb	3.00
np	65536	wtfile	
sw	50000.0	proc	ft
fb	28000	fn	not used
bs	4		
tpwr	52	werr	
pw	7.0	wexp	
d1	1.000	wbs	
tof	0	wnt	
nt	200		
ct	0		
alock	n		
gain	40		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-3871.3		
wp	6428.7		
vs	178		
sc	0		
wc	250		
hzmm	25.71		
is	500.00		
rfl	26821.2		
rfp	0		
th	6		
ins	6.000		
ai	ph		



1aa-S



— 7.260

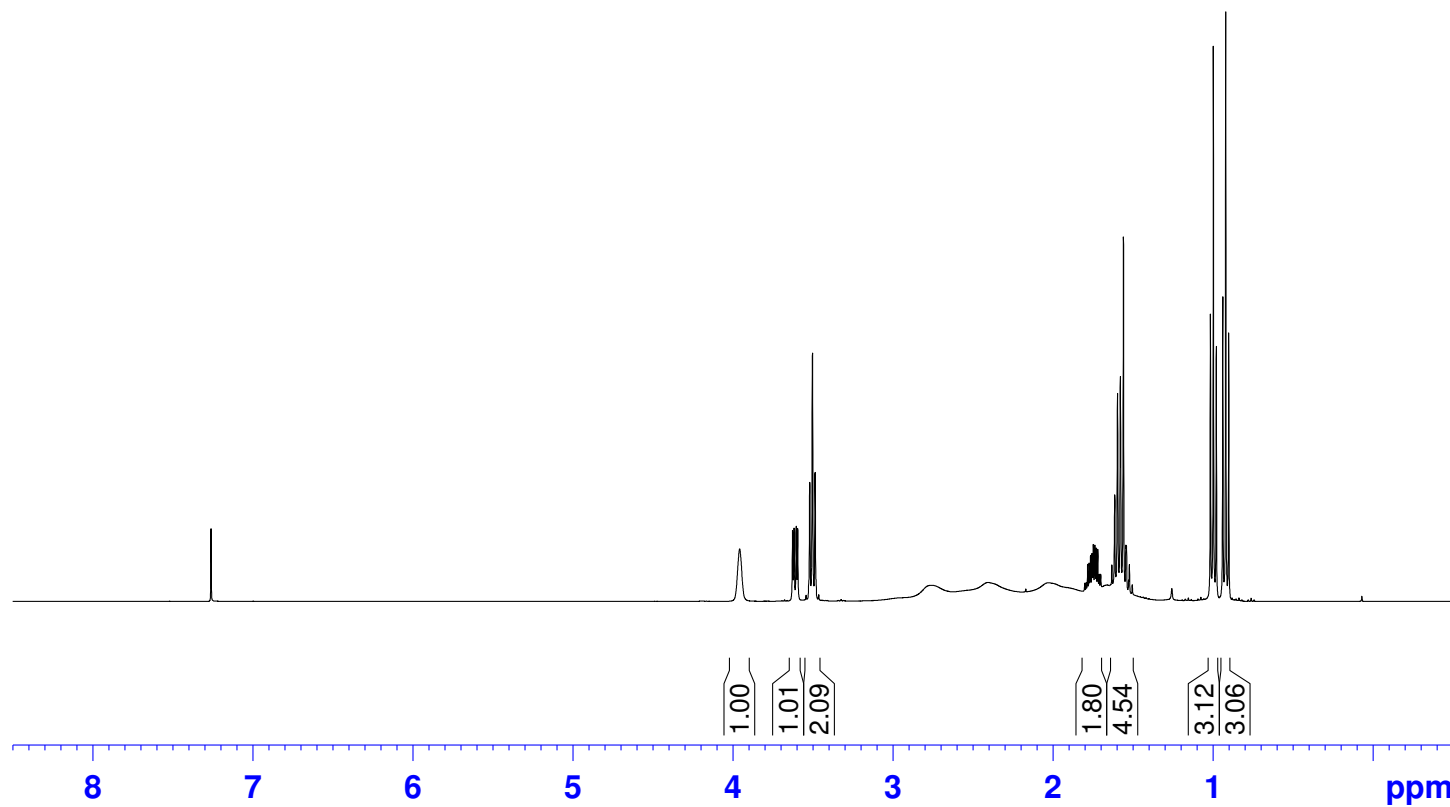


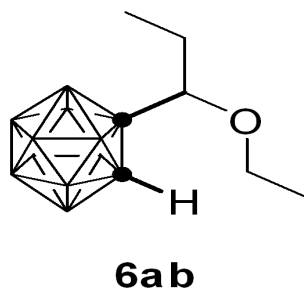
3.956
3.626
3.616
3.603
3.594
3.518
3.501
3.485
1.802
1.783
1.774
1.748
1.739
1.730
1.702
1.632
1.597
1.579
1.560
1.527
1.522
1.504
1.016
0.998
0.979
0.939
0.920
0.902

wrx0343-1-H-CDC13

NAME wrx0343-1-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100701
Time 14.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 45.2
DW 60.800 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -1.00 dB
PL1W 13.56617069 W
SFO1 400.1924713 MHz
SI 32768
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





81.58
78.64
77.32
77.00
76.68
75.48

— 58.59

— 29.10

— 23.12

10.61
10.51

wrx0343-1-C-CDCl3

```

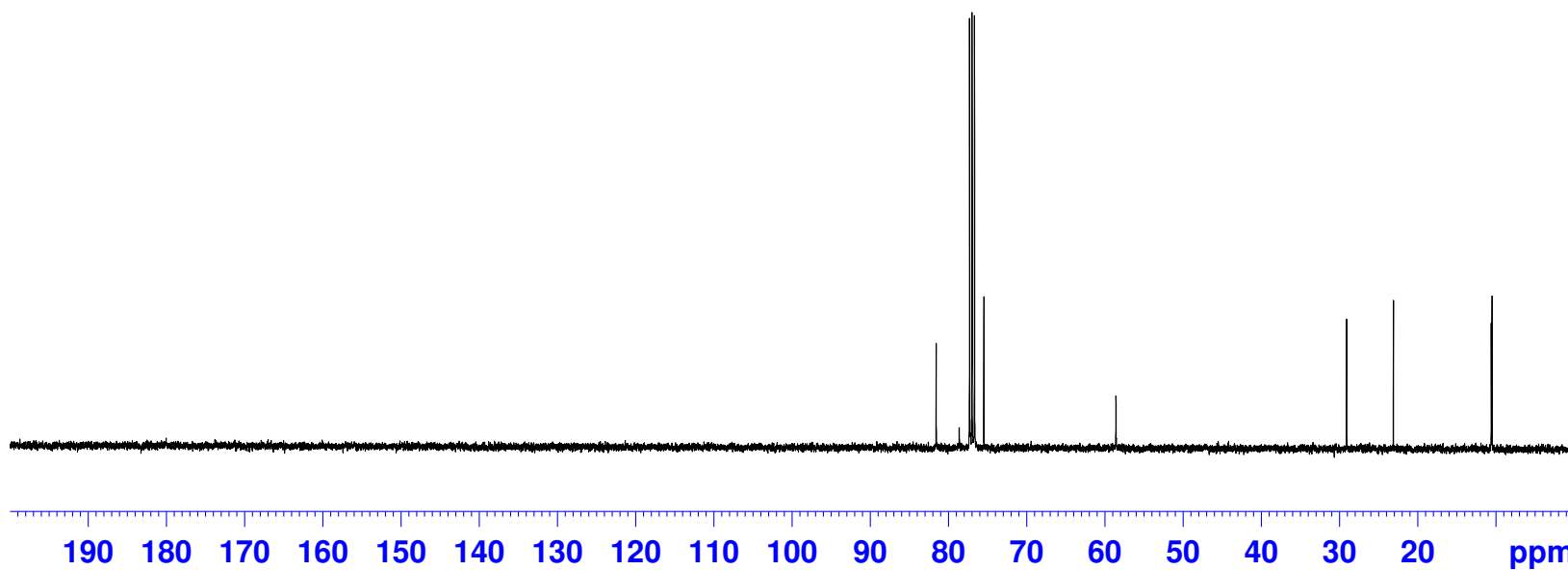
NAME      wrx0343-1-C-CDCl3
EXPNO     1
PROCNO    1
Date_     20100701
Time      14.31
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         144
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG          181
DW          20.800 usec
DE          6.50 usec
TE         299.4 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1
  
```

```

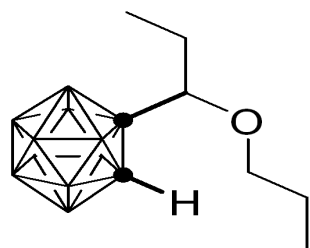
===== CHANNEL f1 =====
NUC1      13C
P1         9.90 usec
PL1        -2.00 dB
PL1W       55.33689499 W
SFO1      100.6379183 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      90.00 usec
PL2         -1.00 dB
PL12        15.16 dB
PL13        18.62 dB
PL2W       13.56617069 W
PL12W       0.32844096 W
PL13W       0.14806664 W
SFO2      400.1916008 MHz
SI         32768
SF         100.6278588 MHz
WDW         EM
SSB          0
LB          1.00 Hz
GB           0
PC           1.40
  
```



wrx0343-1-B-CDC13

**6a**

— -3.61
— -4.42

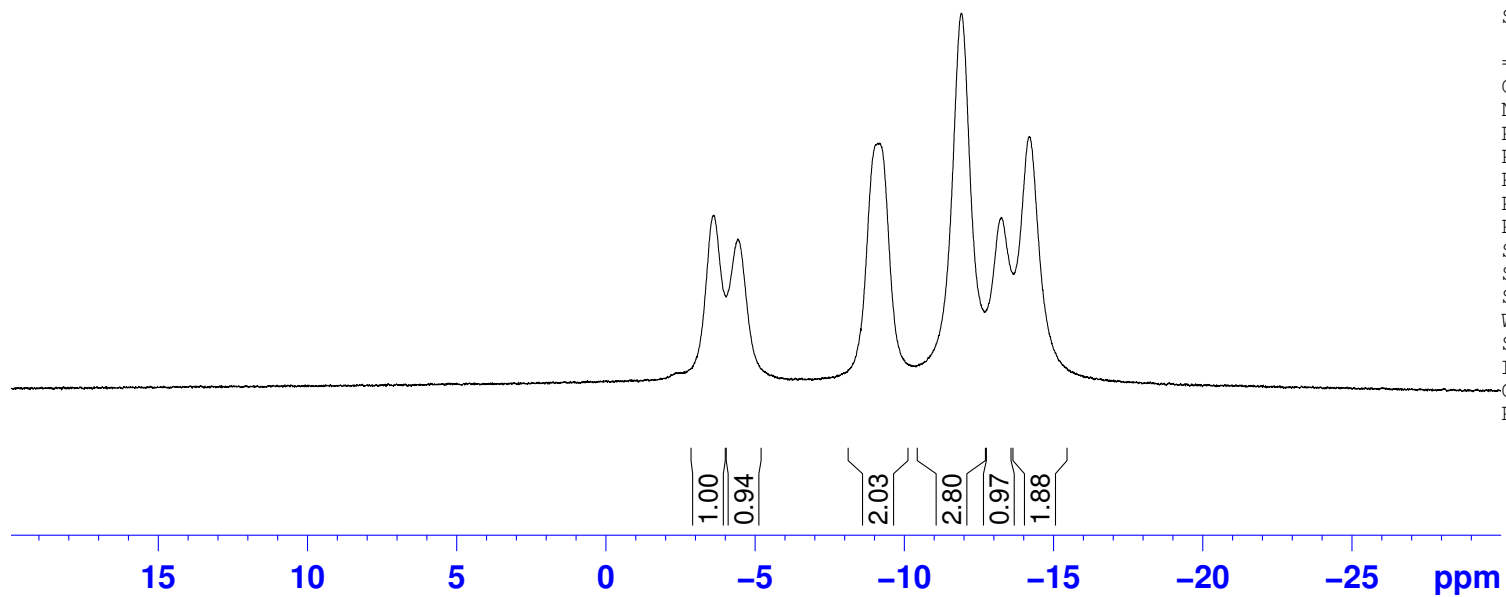
— -9.10

— -11.91
— -13.25
— -14.18

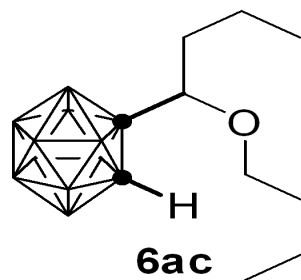
NAME wrx0343-1-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100701
Time 14.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 65536
SOLVENT CDC13
NS 7
DS 0
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 287
DW 19.600 usec
DE 6.50 usec
TE 299.3 K
D1 5.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 7.60 usec
PL1 -3.00 dB
PL1W 55.13059616 W
SFO1 128.3968556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
SFO2 400.1916008 MHz
SI 32768
SF 128.3968560 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



— 7.260



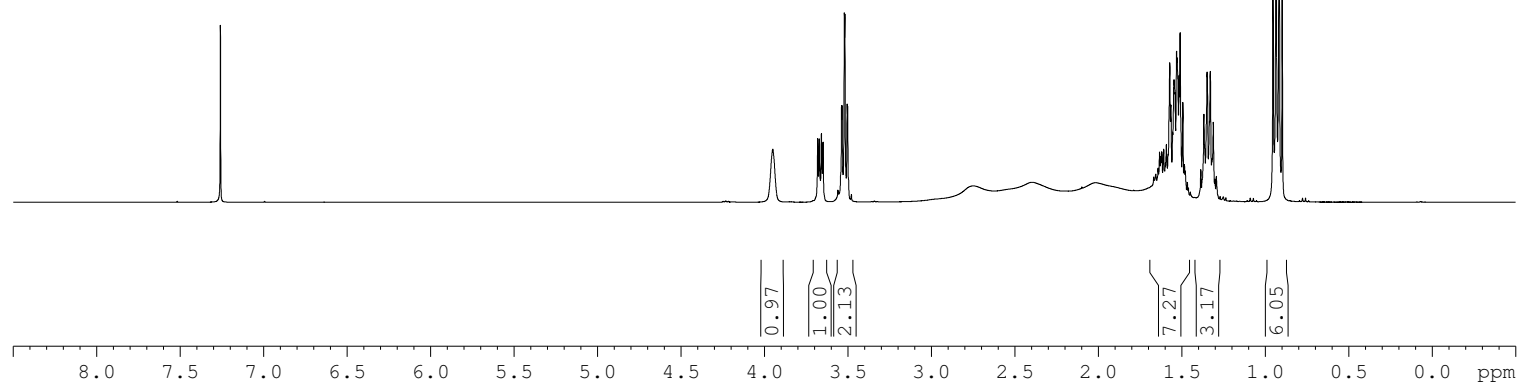
3.951
3.681
3.672
3.660
3.650
3.539
3.535
3.522
3.519
3.506
3.503

1.669
1.634
1.609
1.573
1.547
1.511
1.494
1.387
1.368
1.349
1.335
1.330
1.312
1.294
0.954
0.936
0.917
0.899

wrx0367-1-H-CDC13

NAME wrx0367-1-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100813
Time 19.34
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

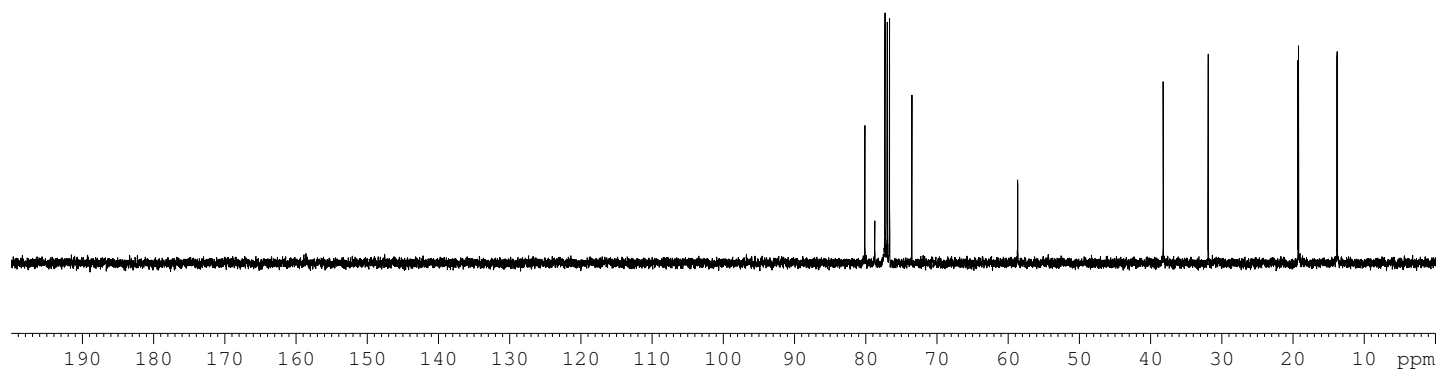
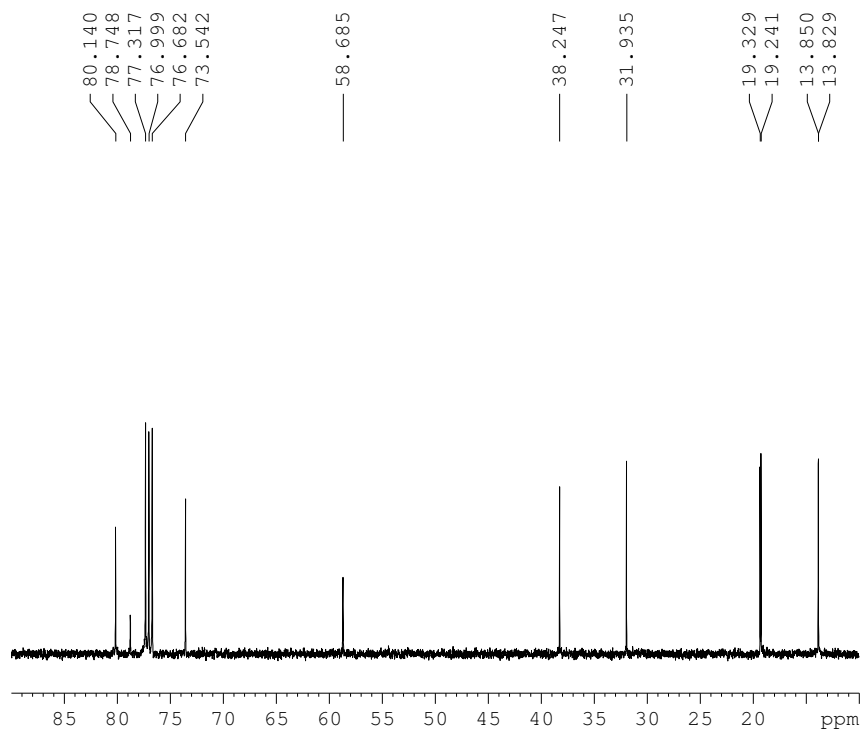
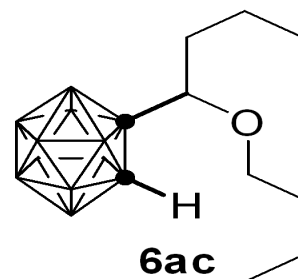


wrx0367-1-C-CDC13

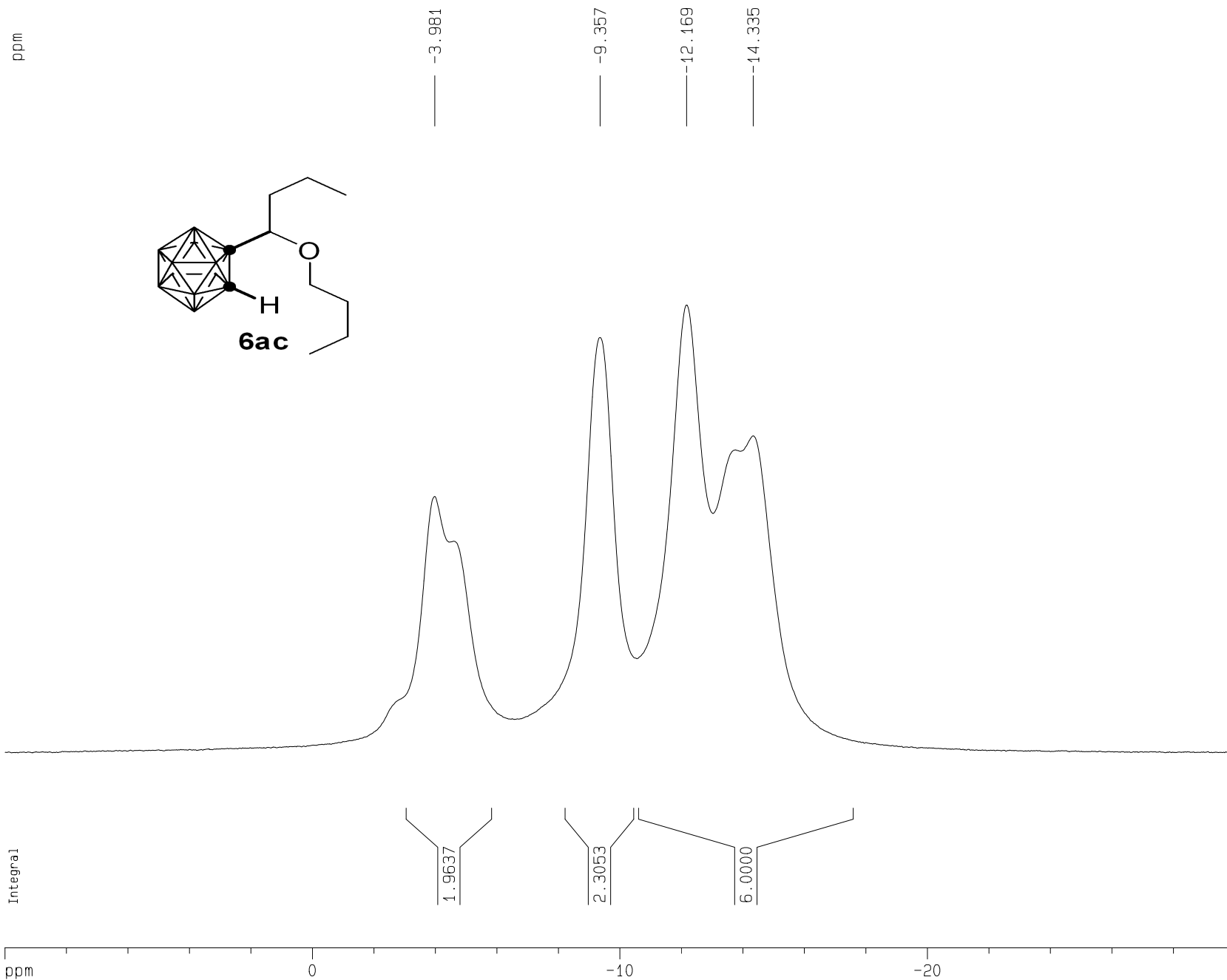
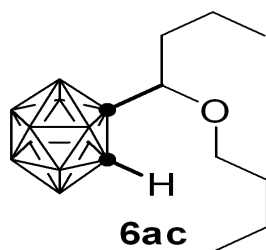
NAME wrx0367-1-C-CDC13
 EXPNO 1
 PROCNO 1
 Date_ 20100813
 Time 20.23
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 80
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 294.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 14.50 usec
 PL1 -4.00 dB
 PL1W 90.22689819 W
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 18.80 dB
 PL13 18.80 dB
 PL2W 13.17734718 W
 PL12W 0.10960442 W
 PL13W 0.10960442 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127720 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



wrx0122-3-B-CDC13



Current Data Parameters
 NAME wrx0122-3-B-CDC13
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090830
 Time 22.38
 INSTRUM dpx300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgdc
 TD 65536
 SOLVENT CDC13
 NS 32
 DS 0
 SWH 57803.469 Hz
 FIDRES 0.882011 Hz
 AQ 0.5669364 sec
 RG 32
 DW 8.650 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

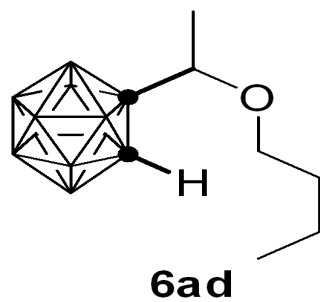
===== CHANNEL f1 =====
 NUC1 11B
 P1 3.00 usec
 PL1 -6.00 dB
 SF01 96.2966310 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 300.1310908 MHz

F2 - Processing parameters
 SI 65536
 SF 96.2936551 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
 F1P 10.000 ppm
 F1 962.94 Hz
 F2P -30.000 ppm
 F2 -2888.81 Hz
 PPMCM 1.81818 ppm/cm
 HZCM 175.07938 Hz/cm

— 7.260

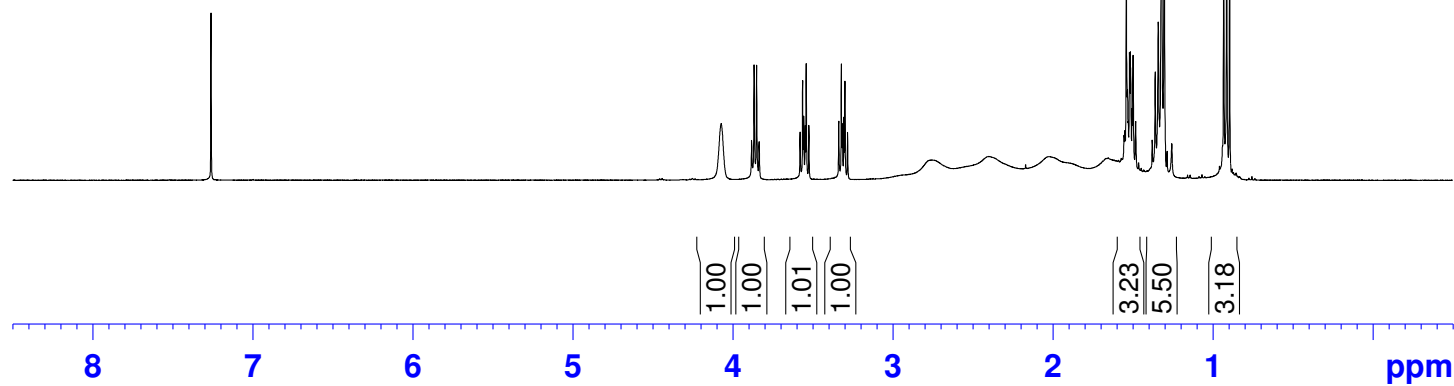


4.074
3.883
3.868
3.852
3.836
3.580
3.564
3.558
3.548
3.542
3.526
3.339
3.323
3.316
3.306
3.300
3.284
1.542
1.535
1.522
1.517
1.506
1.500
1.483
1.380
1.342
1.321
1.305
1.287
0.933
0.915
0.896

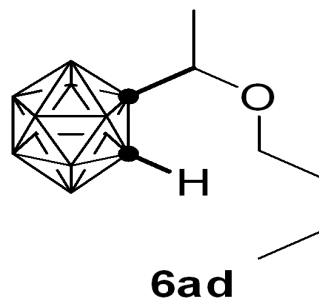
wrx0344-1-H-CDC13

NAME wrx0344-1-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100702
Time 15.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 45.2
DW 60.800 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -1.00 dB
PL1W 13.56617069 W
SFO1 400.1924713 MHz
SI 32768
SF 400.1900141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S43



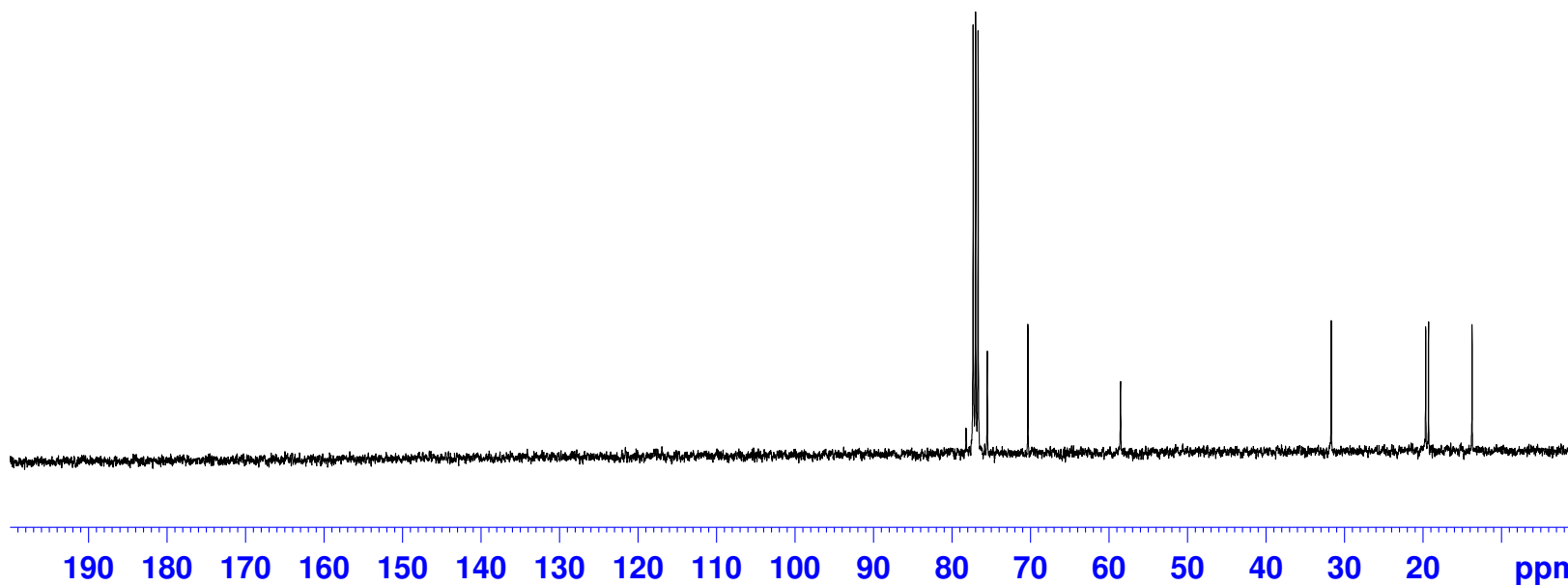
78.22
77.32
77.00
76.68
75.51
70.34
— 58.54
— 31.69
19.66
19.30
— 13.75

wrx0344-1-C-CDC13

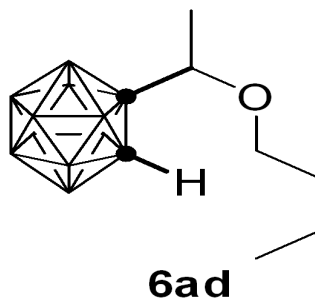
NAME wrx0344-1-C-CDC13
EXPNO 1
PROCNO 1
Date_ 20100701
Time 21.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 140
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6379183 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL13 18.62 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
PL13W 0.14806664 W
SFO2 400.1916008 MHz
SI 32768
SF 100.6278581 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



wrx0344-1-B-CDCl3



— -3.72
— -4.58

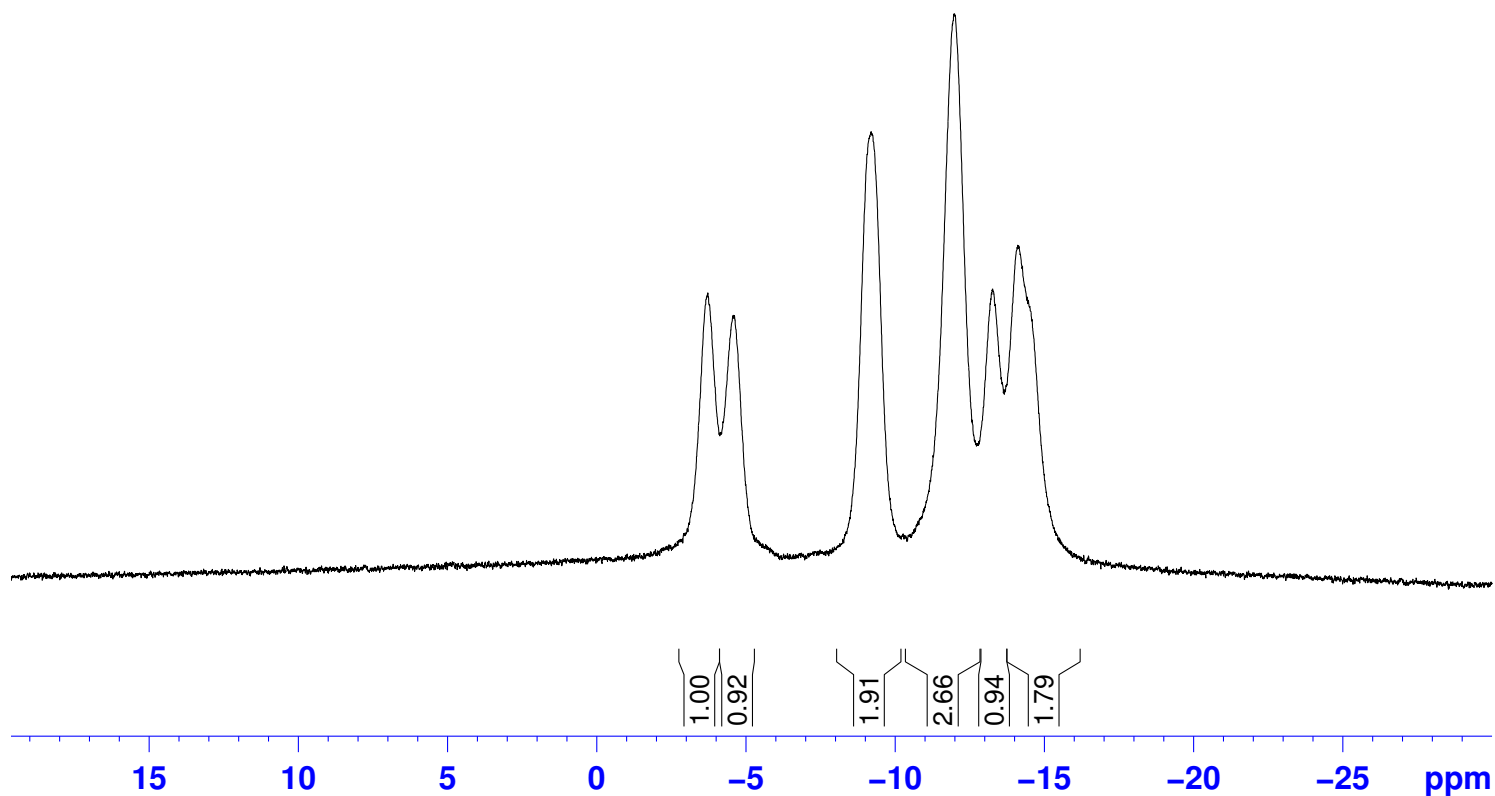
— -9.19

— -11.99
— -13.26
— -14.10

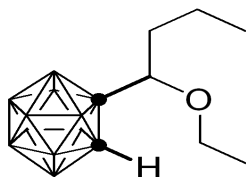
NAME wrx0344-1-B-CDCl3
EXPNO 1
PROCNO 1
Date_ 20100702
Time 15.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 7
DS 0
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 287
DW 19.600 usec
DE 6.50 usec
TE 299.0 K
D1 5.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 7.60 usec
PL1 -3.00 dB
PL1W 55.13059616 W
SFO1 128.3968556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
SFO2 400.1916008 MHz
SI 32768
SF 128.3968560 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



— 7.260

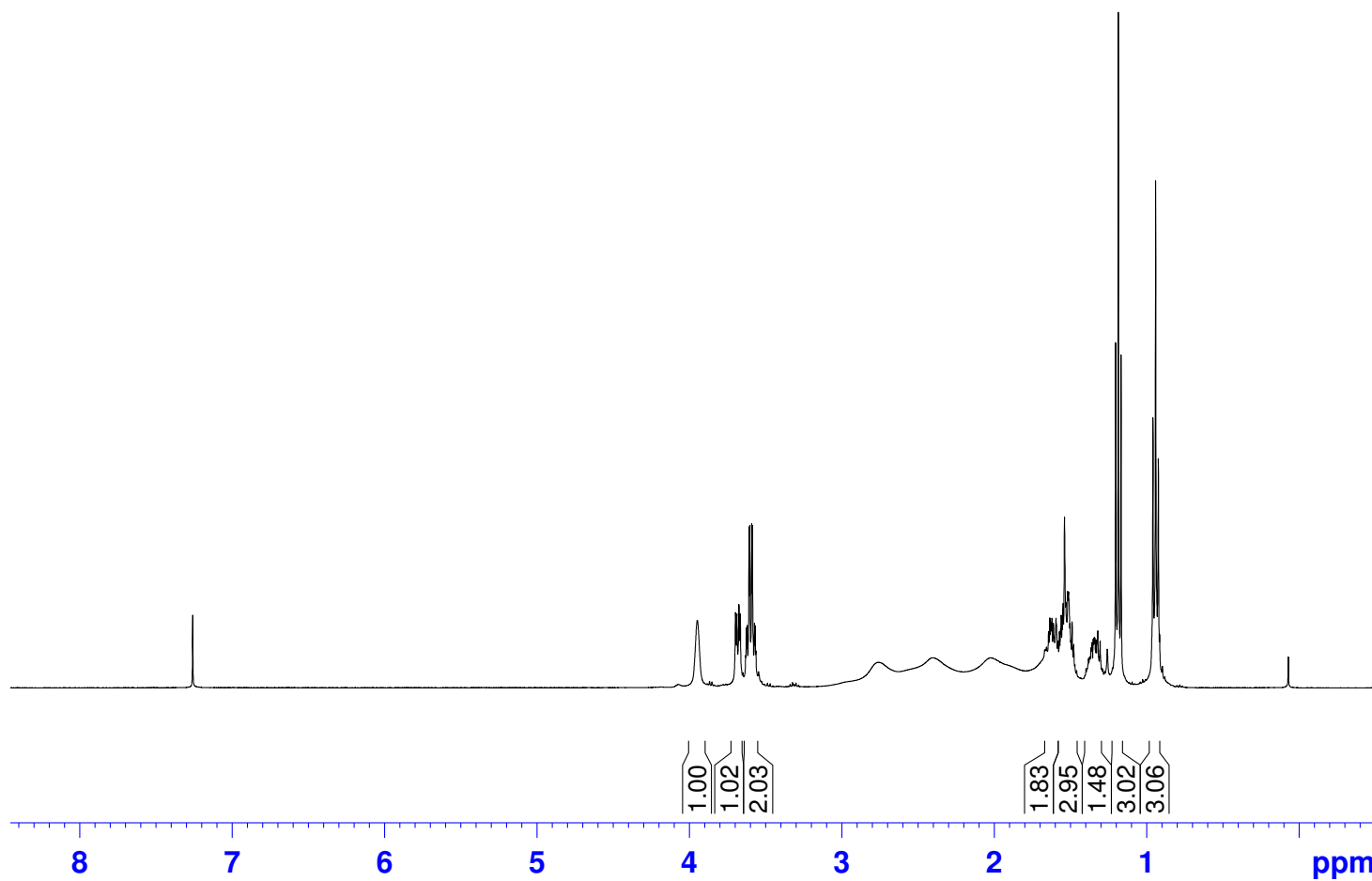
**6ad'**

3.949
3.699
3.689
3.676
3.667
3.627
3.622
3.610
3.604
3.592
3.587
3.575
3.569
1.636
1.622
1.612
1.595
1.561
1.540
1.519
1.513
1.489
1.479
1.399
1.359
1.351
1.345
1.341
1.333
1.326
1.321
1.306
1.204
1.186
1.169
0.960
0.942
0.924

wrx0344-2-H-CDC13

NAME wrx0344-2-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100701
Time 21.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 45.2
DW 60.800 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -1.00 dB
PL1W 13.56617069 W
SFO1 400.1924713 MHz
SI 32768
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S46

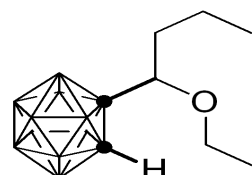
80.27
78.70
77.32
77.00
76.68
69.22

58.76

38.30

19.38
15.23
13.82

wrx0344-2-C-CDCl3

**6ad'**

NAME wrx0344-2-C-CDCl3
EXPNO 1
PROCNO 1
Date_ 20100701
Time 21.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 52
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6379183 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL13 18.62 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
PL13W 0.14806664 W
SFO2 400.1916008 MHz
SI 32768
SF 100.6278588 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

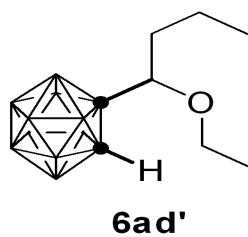


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

— -3.60
— -4.46

— -9.08

— -11.88
— -13.30
— -14.12

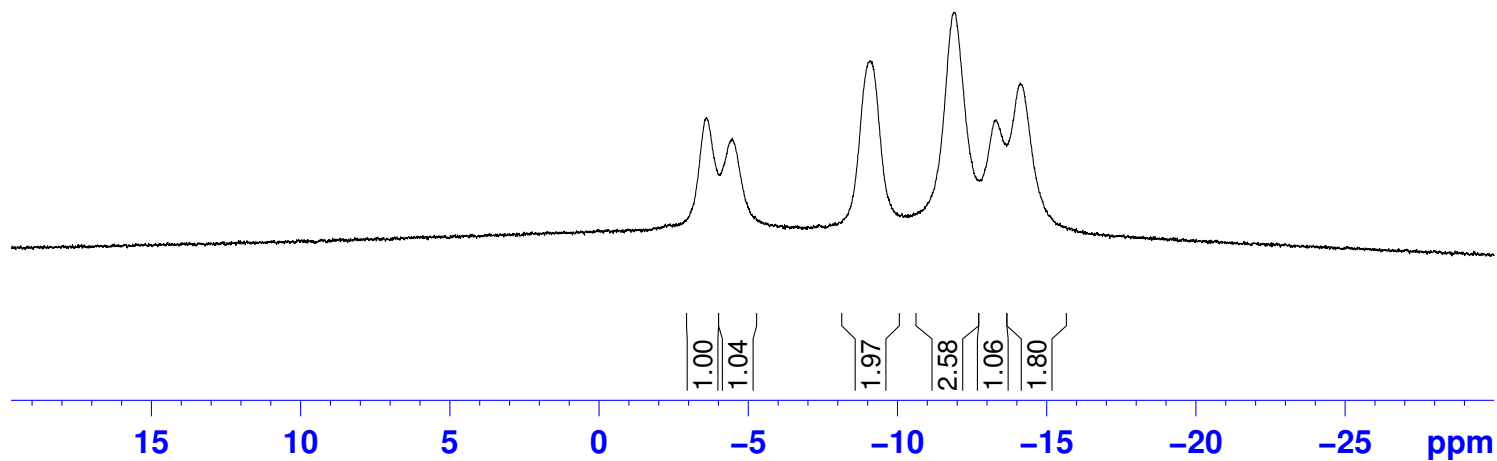


wrx0344-2-B-CDC13

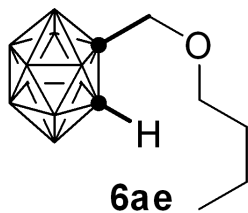
NAME wrx0344-2-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100702
Time 15.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 287
DW 19.600 usec
DE 6.50 usec
TE 299.0 K
D1 5.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 7.60 usec
PL1 -3.00 dB
PL1W 55.13059616 W
SFO1 128.3968556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
SFO2 400.1916008 MHz
SI 32768
SF 128.3968560 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



— 7.260



3.950
3.831
3.467
3.451
3.435

1.569
1.561
1.544
1.537
1.527
1.507
1.491
1.367
1.348
1.329
1.310
0.930
0.912
0.894

wrx0331-1-H-CDC13

```

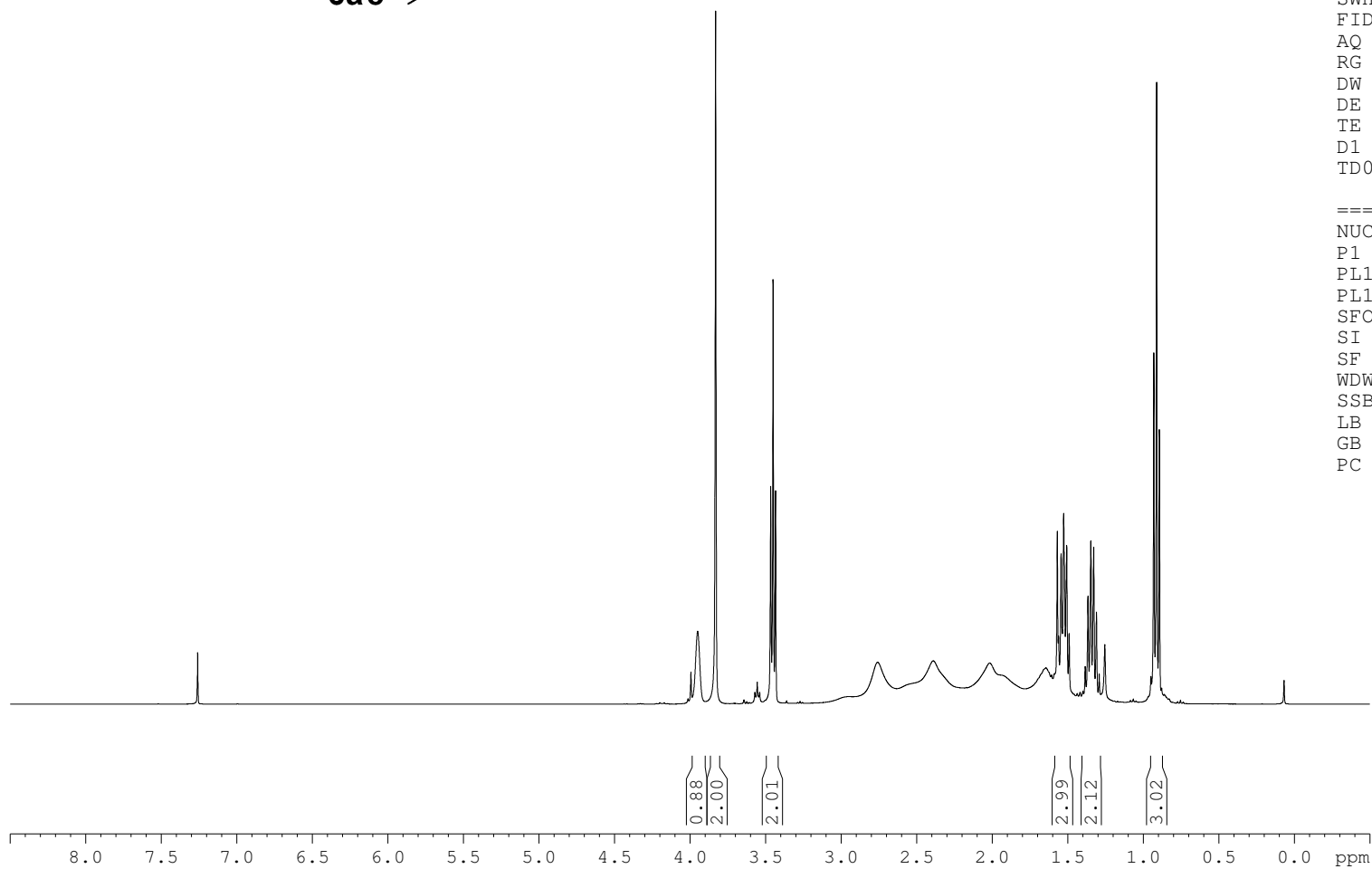
NAME      wrx0331-1-H-CDC13
EXPNO      1
PROCNO     1
Date_      20100603
Time       21.04
INSTRUM    spect
PROBHD     5 mm PABBI 1H/
PULPROG    zg
TD          65536
SOLVENT     CDC13
NS          8
DS          0
SWH         8012.820 Hz
FIDRES      0.122266 Hz
AQ          4.0894966 sec
RG          28.5
DW          62.400 usec
DE          6.50 usec
TE          294.5 K
D1          1.00000000 sec
TD0         1

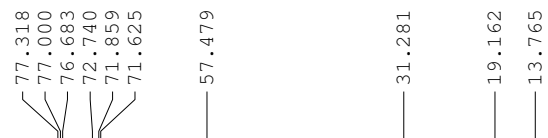
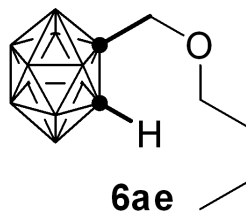
```

```

===== CHANNEL f1 =====
NUC1        1H
P1           7.10 usec
PL1         -2.00 dB
PL1W        13.17734718 W
SFO1        400.1316005 MHz
SI           65536
SF          400.1300057 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00

```





wrx0331-1-C-CDCl3

```

NAME      wrx0331-1-C-CDCl3
EXPNO      1
PROCNO     1
Date_      20100604
Time       19.22
INSTRUM    spect
PROBHD     5 mm PABBI 1H/
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         137
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         294.9 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

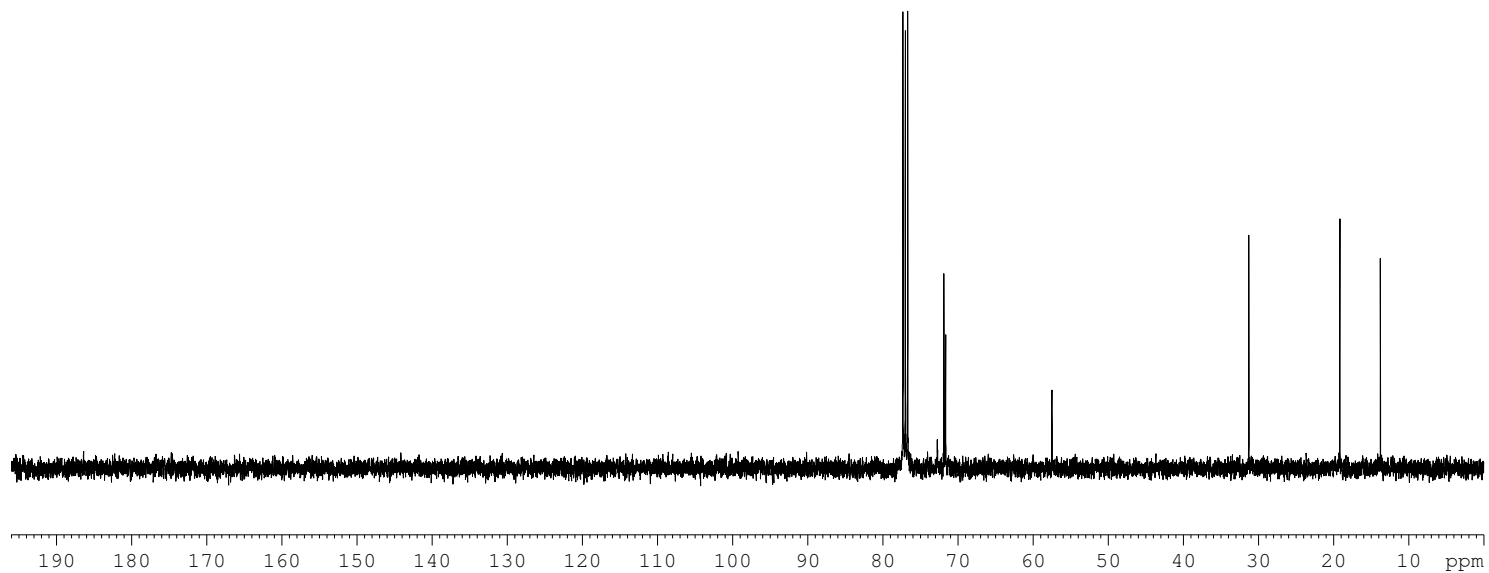
===== CHANNEL f1 =====
NUC1       13C
P1         14.50 usec
PL1        -4.00 dB
PL1W       90.22689819 W
SFO1       100.6228298 MHz

```

```

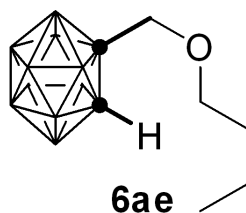
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -2.00 dB
PL12       18.80 dB
PL13       18.80 dB
PL2W       13.17734718 W
PL12W      0.10960442 W
PL13W      0.10960442 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127710 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



S50

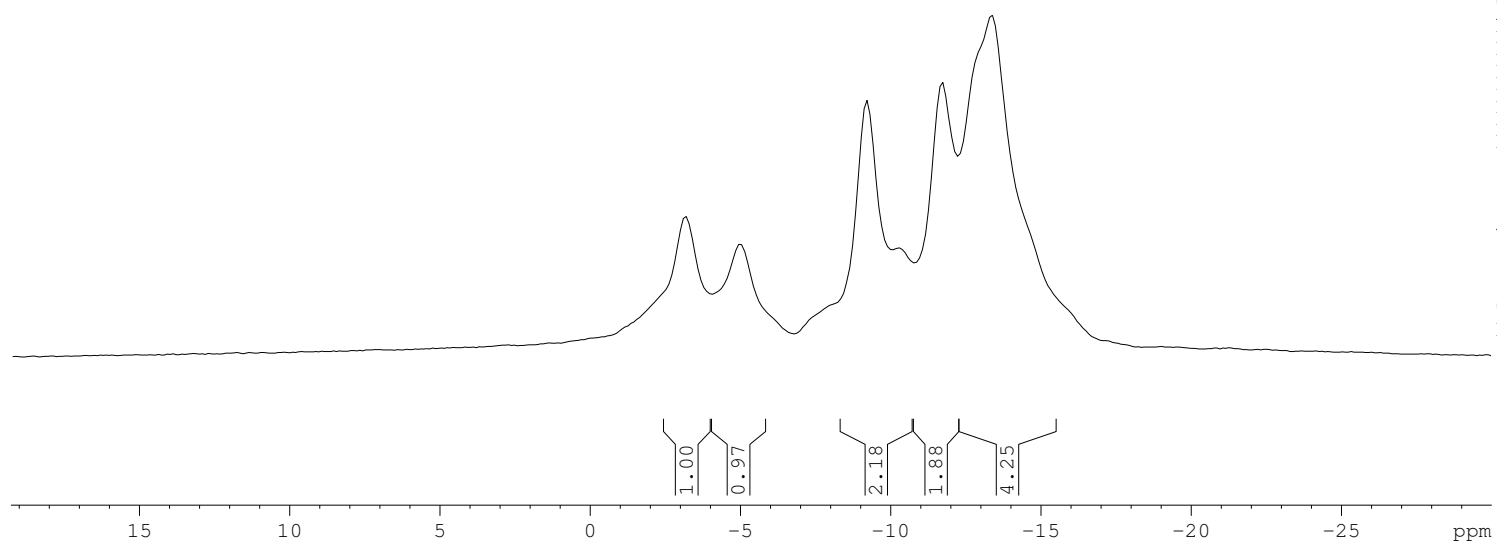
wrx0331-1-B-CDC13



NAME wrx0331-1-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100604
Time 12.04
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgdc
TD 4000
SOLVENT C6D6
NS 62
DS 4
SWH 25510.203 Hz
FIDRES 6.377551 Hz
AQ 0.0784500 sec
RG 203
DW 19.600 usec
DE 6.50 usec
TE 294.8 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 14.50 usec
PL1 -4.00 dB
SFO1 128.3776076 MHz

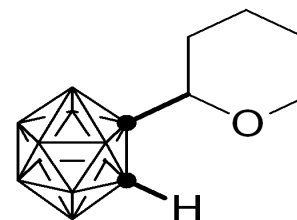
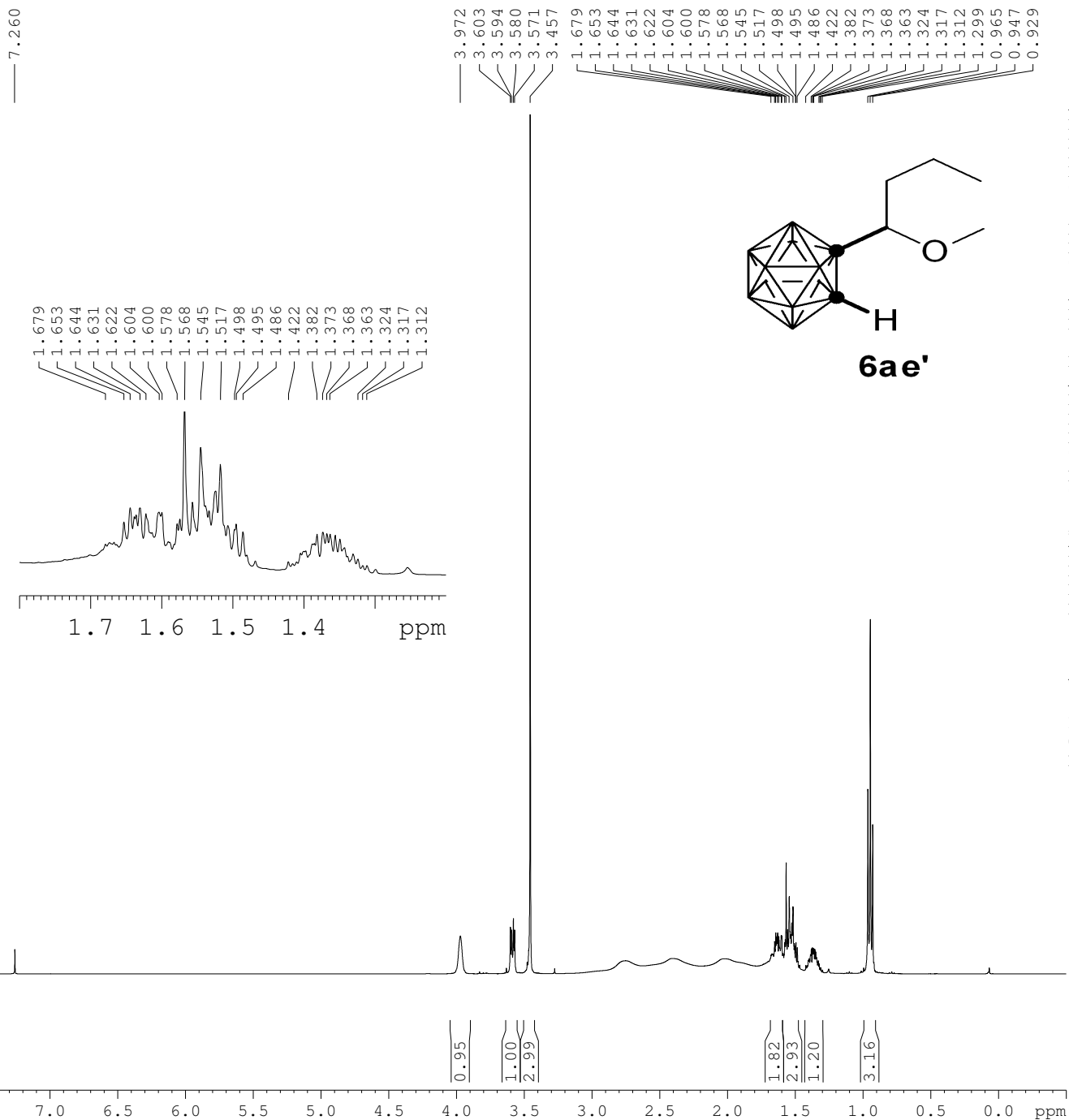
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.80 dB
PL2W 13.17734718 W
PL12W 0.10960442 W
SFO2 400.1316005 MHz
SI 2048
SF 128.3776263 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

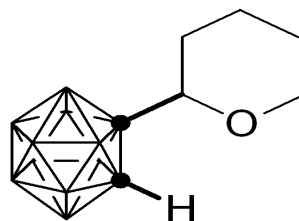


wrx0331-2-H-CDC13

NAME wrx0331-2-H-CDC13
 EXPNO 1
 PROCNO 1
 Date_ 20100603
 Time 21.09
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 28.5
 DW 62.400 usec
 DE 6.50 usec
 TE 294.5 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 -2.00 dB
 PL1W 13.17734718 W
 SFO1 400.1316005 MHz
 SI 65536
 SF 400.1300053 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

**6ae'**

**6ae'**

81.971
78.392
77.316
76.998
76.681

61.288
58.690

38.023

19.301
13.823

wrx0331-2-C-CDC13

```

NAME      wrx0331-2-C-CDC13
EXPNO      1
PROCNO     1
Date_      20100604
Time       19.13
INSTRUM    spect
PROBHD     5 mm PABBI 1H/
PULPROG    zgpg30
TD         65536
SOLVENT    CDC13
NS         68
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         294.7 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

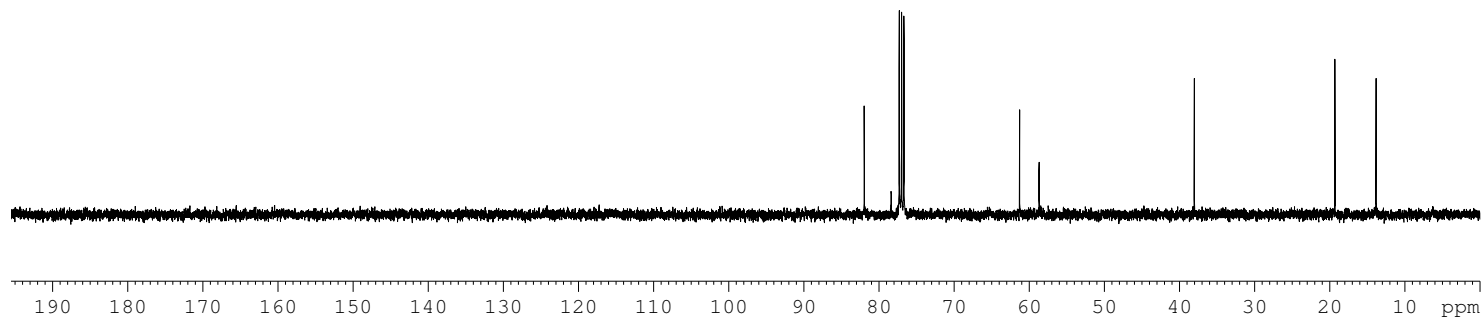
===== CHANNEL f1 =====
NUC1      13C
P1        14.50 usec
PL1       -4.00 dB
PL1W      90.22689819 W
SFO1      100.6228298 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12      18.80 dB
PL13      18.80 dB
PL2W      13.17734718 W
PL12W     0.10960442 W
PL13W     0.10960442 W
SFO2      400.1316005 MHz
SI        32768
SF        100.6127719 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```



S53

— -3.881
— -4.609

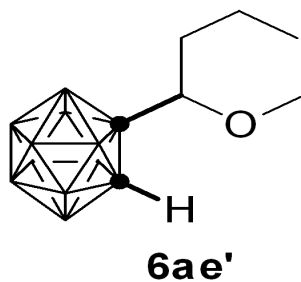
— -9.315

— -12.194

— -13.473

— -14.420

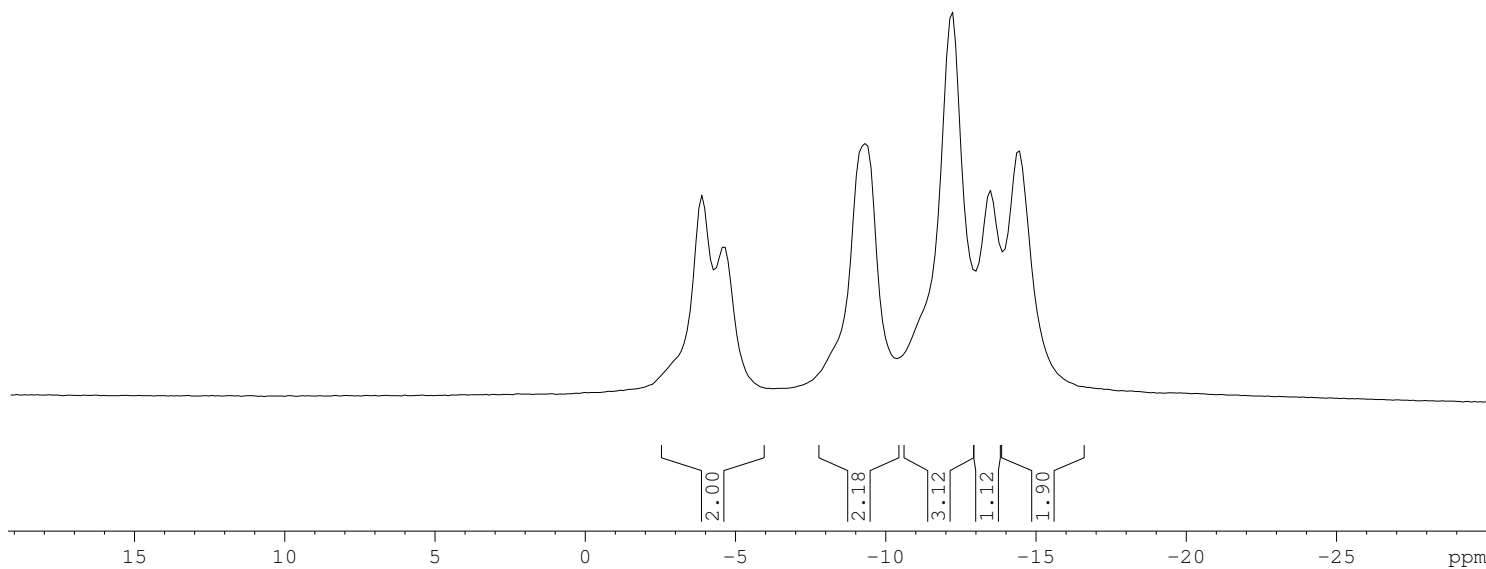
wrx0331-2-B-CDC13

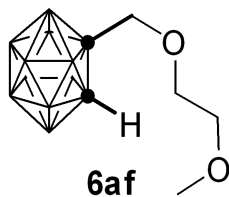


NAME wrx0331-2-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100603
Time 14.00
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgdc
TD 4000
SOLVENT CDC13
NS 42
DS 4
SWH 25510.203 Hz
FIDRES 6.377551 Hz
AQ 0.0784500 sec
RG 181
DW 19.600 usec
DE 6.50 usec
TE 294.7 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 14.50 usec
PL1 -4.00 dB
SFO1 128.3776076 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.80 dB
PL2W 13.17734718 W
PL12W 0.10960442 W
SFO2 400.1316005 MHz
SI 2048
SF 128.3776263 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40





4.011
3.944
3.650
3.643
3.640
3.634
3.628
3.515
3.508
3.503
3.500
3.493
3.359

— 1.607

— 1.250

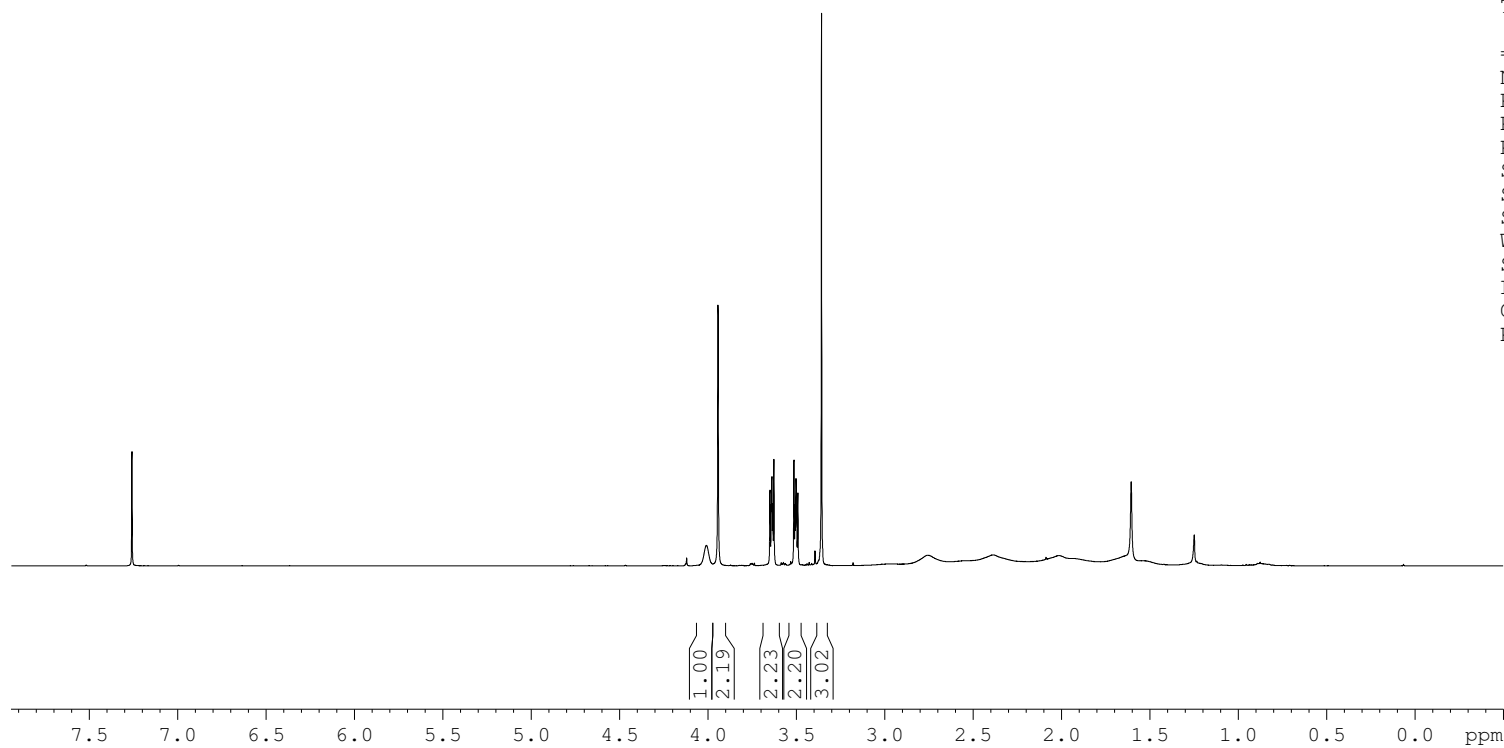
wrx0119-22-H-CDCl₃

```

NAME      wrx0119-22-H-CDCl3
EXPNO      1
PROCNO     1
Date_      20090828
Time       20.35
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zg
TD          65536
SOLVENT    CDCl3
NS          4
DS          0
SWH         8012.820 Hz
FIDRES      0.122266 Hz
AQ          4.0894966 sec
RG          161
DW          62.400 usec
DE          6.50 usec
TE          294.8 K
D1          1.00000000 sec
TD0         1
  
```

```

===== CHANNEL f1 =====
NUC1       1H
P1         14.83 usec
PL1        0.00 dB
PL1W       8.31434441 W
SFO1       400.1316005 MHz
SI         65536
SF         400.1300052 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

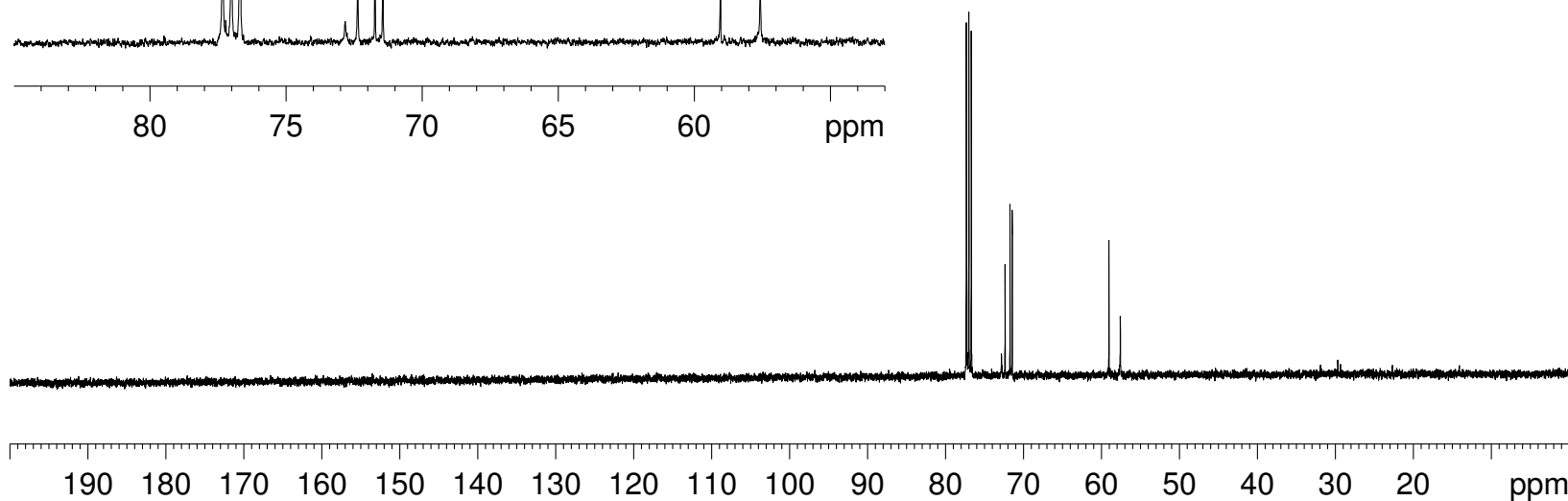
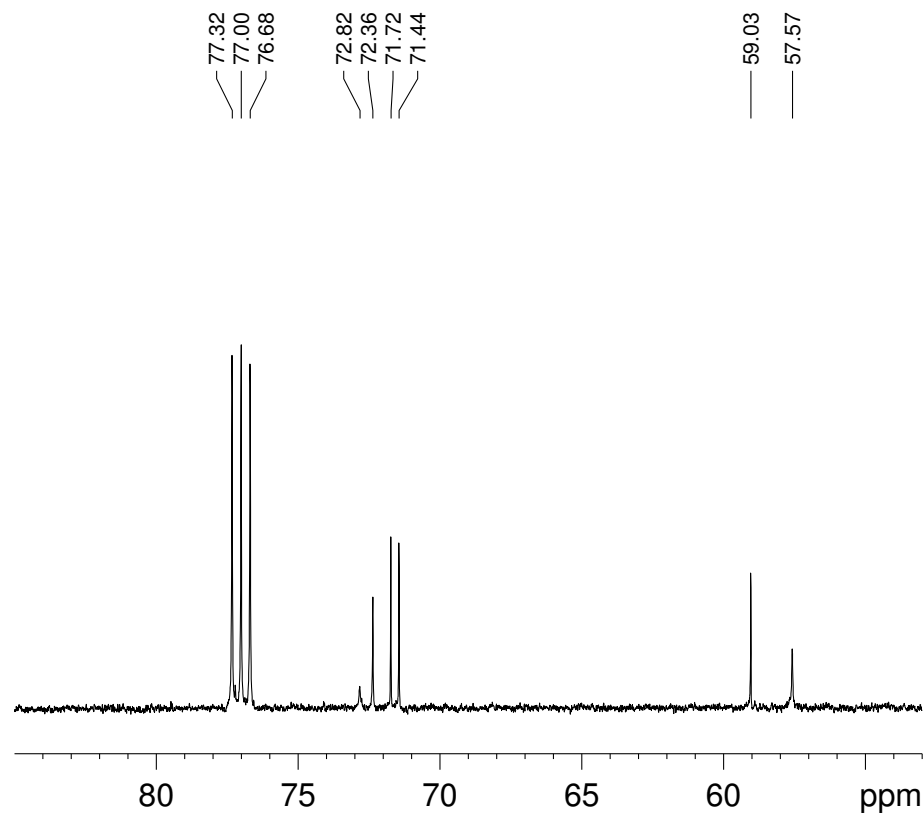
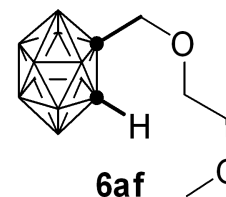


wrx0407-3-C-CDC13

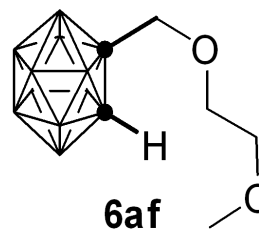
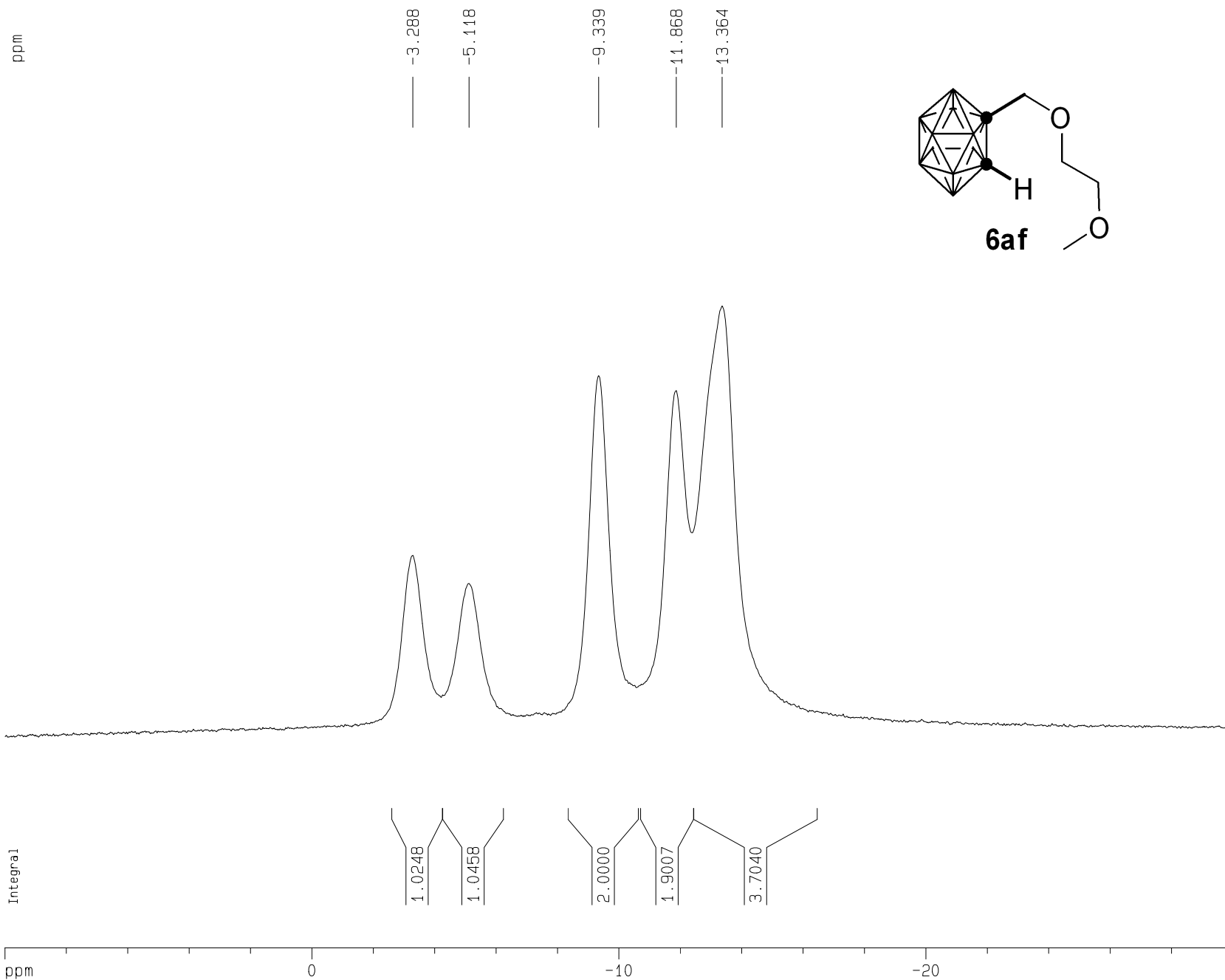
NAME wrx0407-3-C-CDC13
 EXPNO 1
 PROCNO 1
 Date_ 20100902
 Time 16.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 120
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 181
 DW 20.800 usec
 DE 6.50 usec
 TE 298.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.90 usec
 PL1 -2.00 dB
 PL1W 55.33689499 W
 SFO1 100.6379183 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -1.00 dB
 PL12 15.16 dB
 PL13 18.62 dB
 PL2W 13.56617069 W
 PL12W 0.32844096 W
 PL13W 0.14806664 W
 SFO2 400.1916008 MHz
 SI 32768
 SF 100.6278595 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



wrx0119-22-B-CDC13



Current Data Parameters
 NAME wrx0119-22-B-CDC13
 EXPNO 1
 PROCNO 1

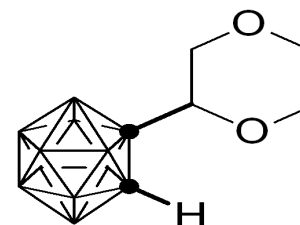
F2 - Acquisition Parameters
 Date_ 20090828
 Time 21.18
 INSTRUM dpx300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgdc
 TD 65536
 SOLVENT CDC13
 NS 67
 DS 0
 SWH 57803.469 Hz
 FIDRES 0.882011 Hz
 AQ 0.5669364 sec
 RG 32
 DW 8.650 usec
 DE 6.00 usec
 TE 294.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 11B
 P1 3.00 usec
 PL1 -6.00 dB
 SF01 96.2966310 MHz

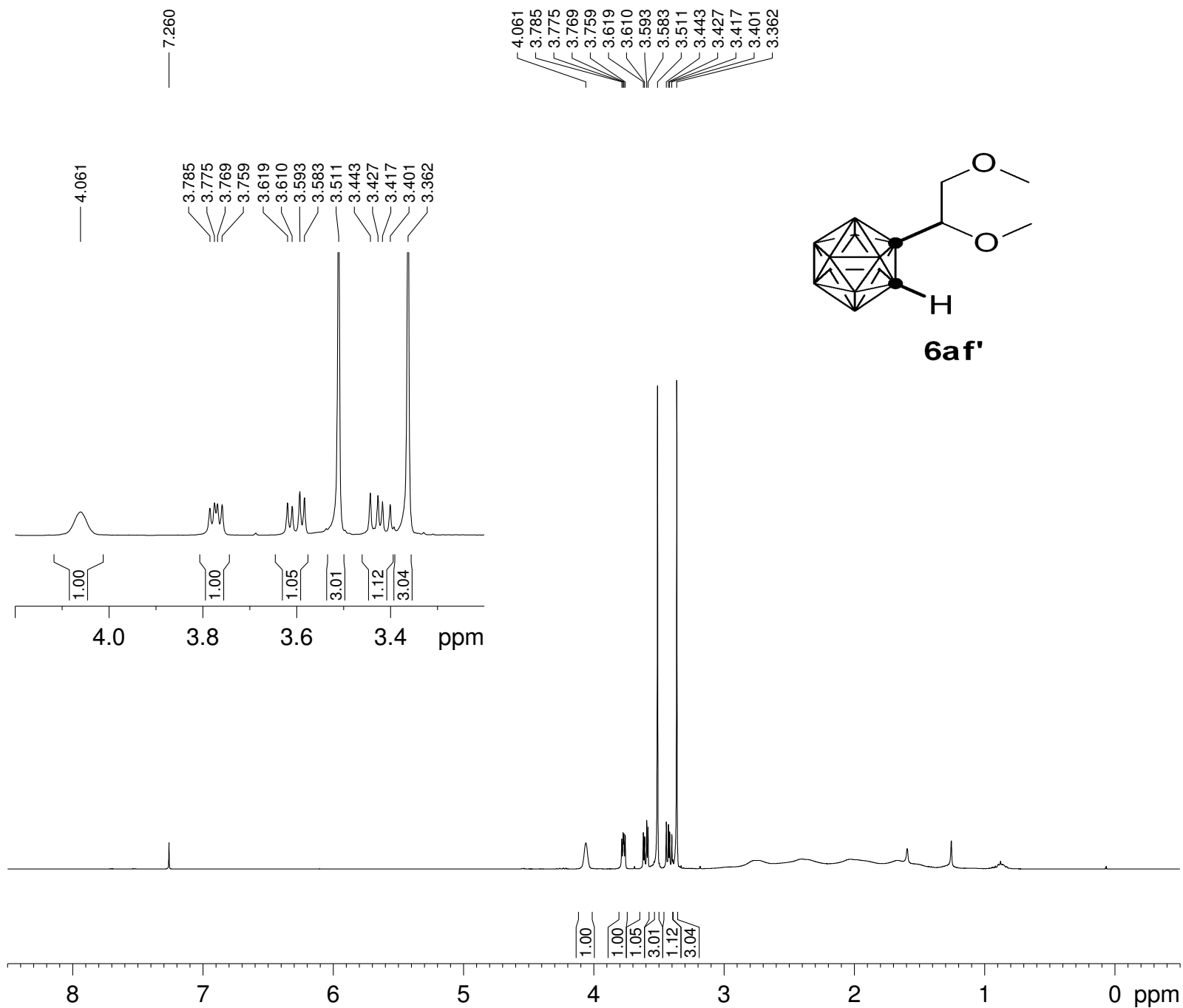
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 300.1310908 MHz

F2 - Processing parameters
 SI 65536
 SF 96.2936551 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
 F1P 10.000 ppm
 F1 962.94 Hz
 F2P -30.000 ppm
 F2 -2888.81 Hz
 PPMCM 1.81818 ppm/cm
 HZCM 175.07938 Hz/cm

**6af'**

wrx0407-2-H-CDC13



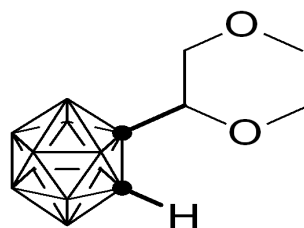
NAME wrx0407-2-H-CDC13
 EXPNO 1
 PROCNO 1
 Date_ 20100829
 Time 23.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 32
 DW 60.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 -1.00 dB
 PL1W 13.56617069 W
 SFO1 400.1924713 MHz
 SI 32768
 SF 400.1900136 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S58

79.74
77.32
77.00
76.68
75.08
74.38
60.96
59.18
58.32

wrx0407-2-C-CDC13

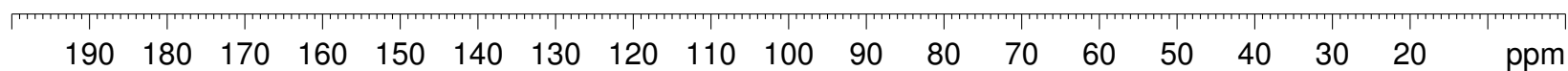


6af'

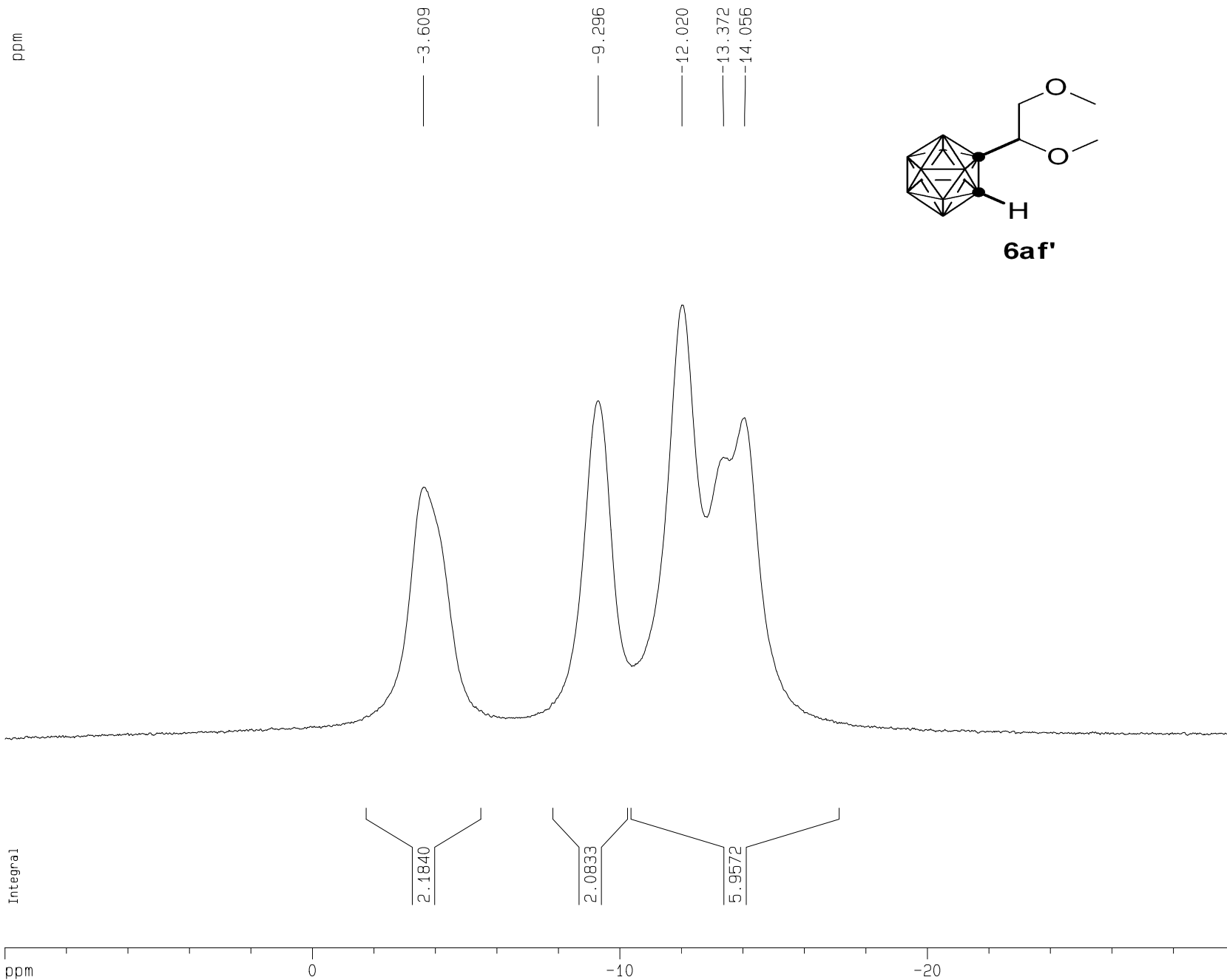
```
NAME      wrx0407-2-C-CDC13
EXPNO     1
PROCNO    1
Date_     20100829
Time      23.25
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   CDC13
NS        60
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        181
DW        20.800 usec
DE        6.50 usec
TE        298.5 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
```

```
===== CHANNEL f1 =====
NUC1      13C
P1        9.90 usec
PL1       -2.00 dB
PL1W      55.33689499 W
SFO1      100.6379183 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -1.00 dB
PL12      15.16 dB
PL13      18.62 dB
PL2W      13.56617069 W
PL12W     0.32844096 W
PL13W     0.14806664 W
SFO2      400.1916008 MHz
SI        32768
SF        100.6278603 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```



wrx0119-14-B-CDC13



Current Data Parameters
NAME wrx0119-14-B-CDC13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090828
Time 21.08
INSTRUM dpx300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDC13
NS 59
DS 0
SWH 57803.469 Hz
FIDRES 0.882011 Hz
AQ 0.5669364 sec
RG 32
DW 8.650 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

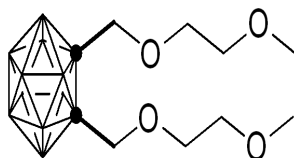
===== CHANNEL f1 =====
NUC1 11B
P1 3.00 usec
PL1 -6.00 dB
SF01 96.2966310 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 19.00 dB
SF02 300.1310908 MHz

F2 - Processing parameters
SI 65536
SF 96.2936551 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 962.94 Hz
F2P -30.000 ppm
F2 -2888.81 Hz
PPMCM 1.81818 ppm/cm
HZCM 175.07938 Hz/cm

— 7.260

**(1,1)-8af**

4.057
3.668
3.660
3.657
3.652
3.645
3.530
3.523
3.518
3.515
3.507
3.366

— 1.600

— 1.249

wrx0407-6-H-CDCl₃

```

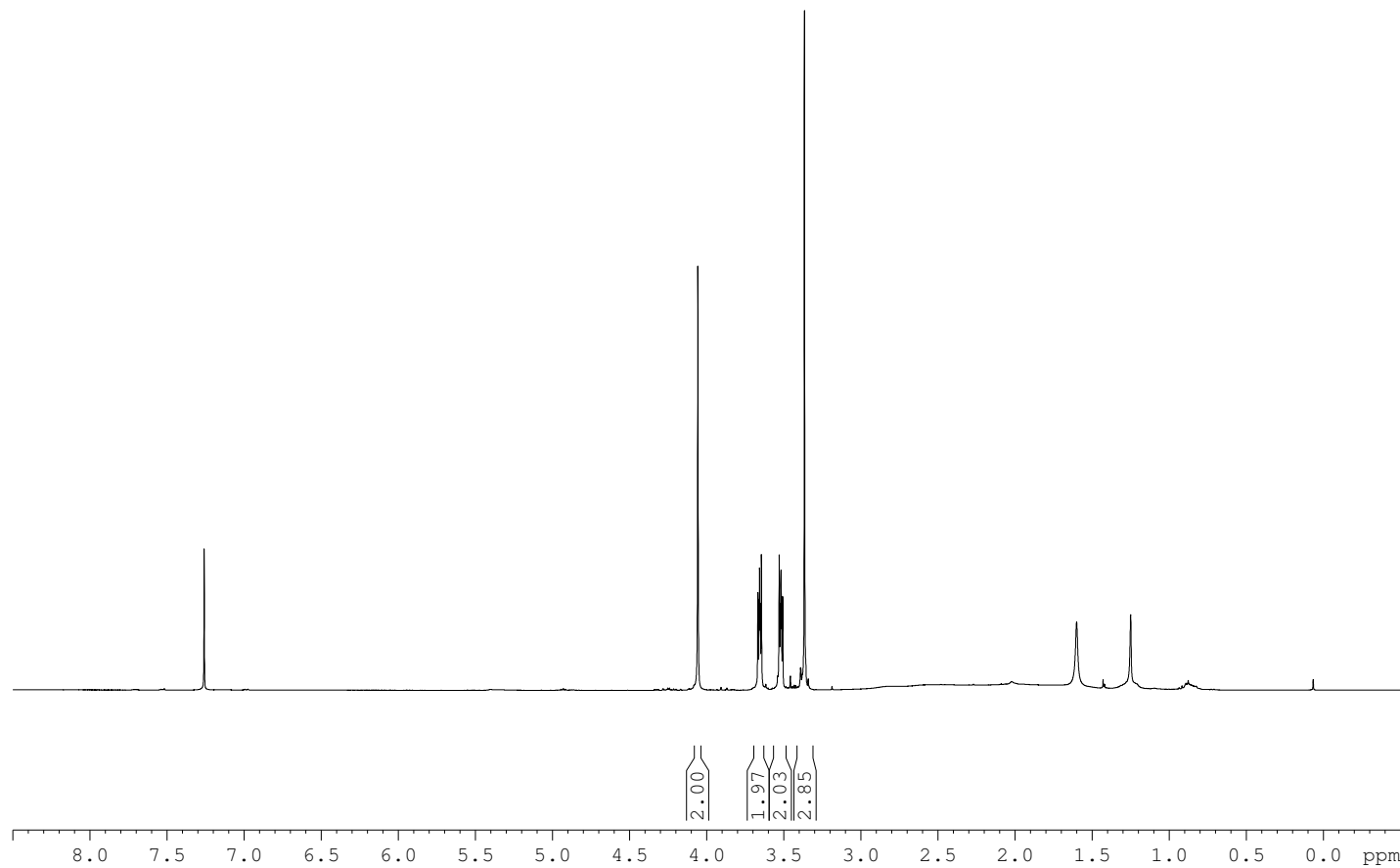
NAME      wrx0407-6-H-CDCl3
EXPNO      1
PROCNO     1
Date_      20100930
Time       19.50
INSTRUM    spect
PROBHD     5 mm PABBI 1H/
PULPROG    zg
TD          65536
SOLVENT    CDCl3
NS          8
DS          0
SWH         10000.000 Hz
FIDRES     0.152588 Hz
AQ          3.2768500 sec
RG          128
DW          50.000 usec
DE          6.50 usec
TE          294.3 K
D1          1.00000000 sec
TD0         1

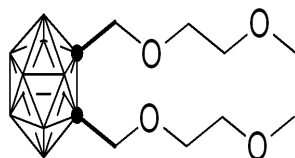
```

```

===== CHANNEL f1 =====
NUC1        1H
P1           7.10 usec
PL1          -2.00 dB
PL1W        13.17734718 W
SFO1        400.1318000 MHz
SI           65536
SF          400.1300053 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00

```





(1,1)-8af

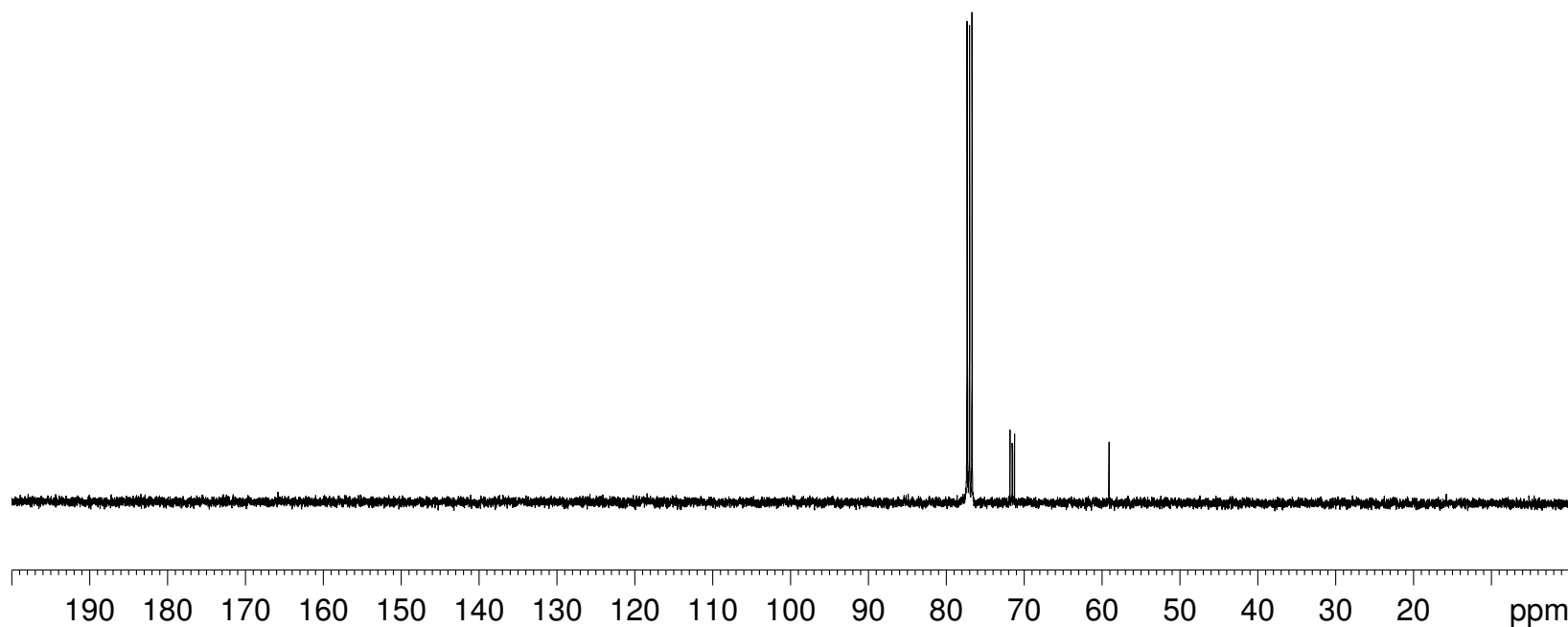
77.31
77.00
76.68
71.81
71.52
71.24
59.08

wrx0407-6-C-CDC13

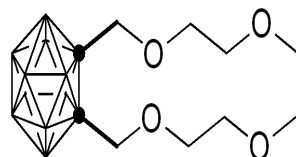
NAME wrx0407-6-C-CDC13
EXPNO 1
PROCNO 1
Date_ 20100831
Time 9.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 160
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6379183 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL13 18.62 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
PL13W 0.14806664 W
SFO2 400.1916008 MHz
SI 32768
SF 100.6278588 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



wrx0407-6-B-CDCl3

**(1,1)-8af**

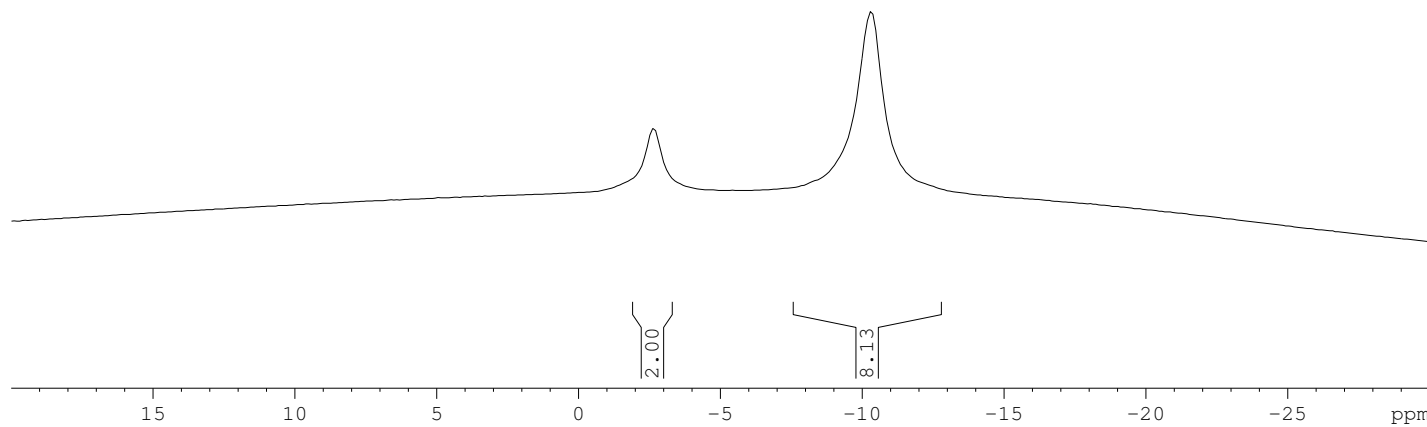
— -2.644

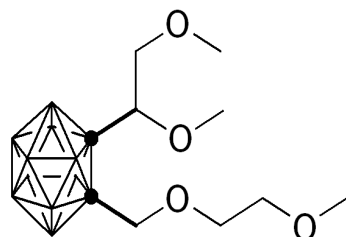
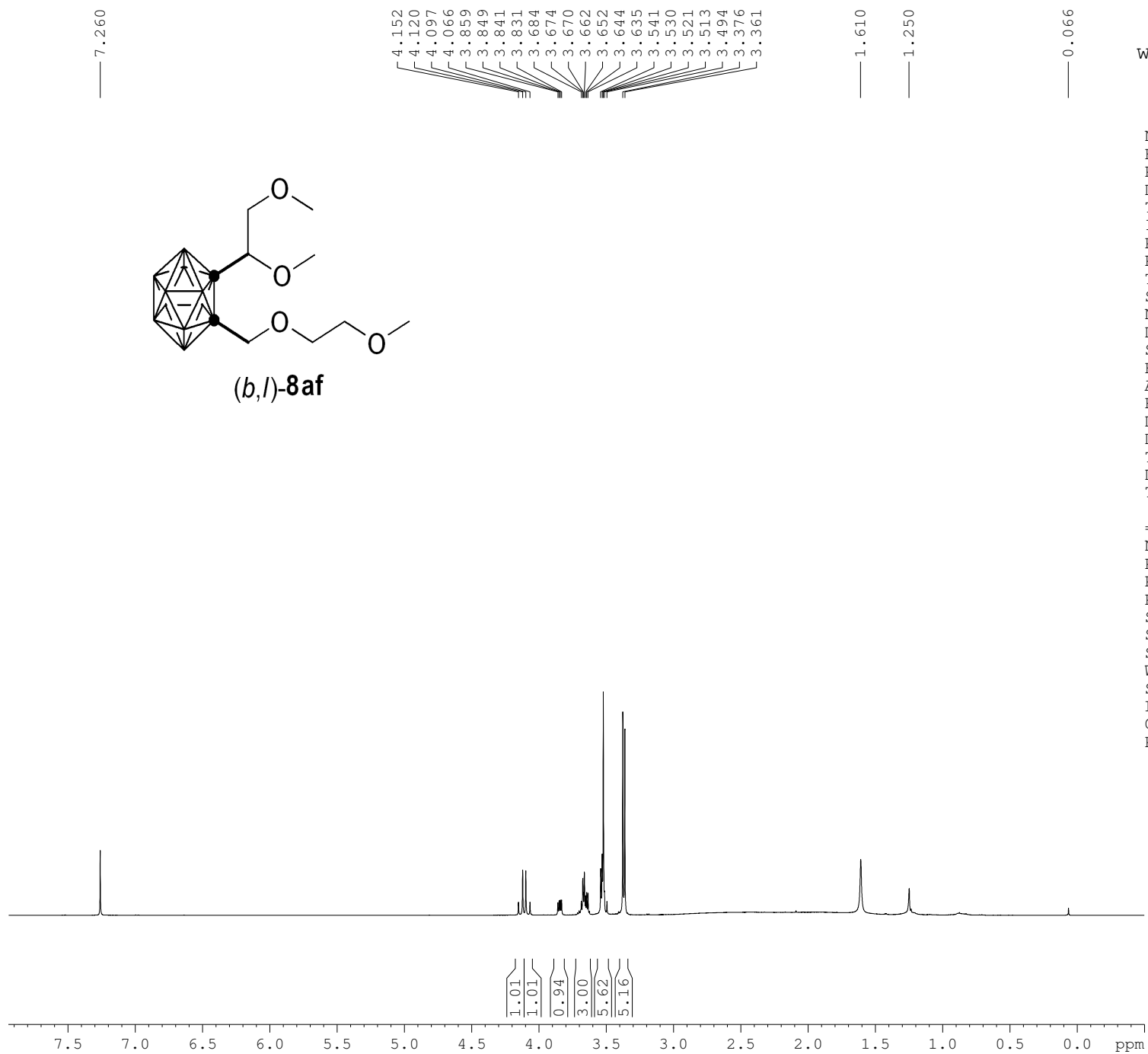
— -10.310

NAME wrx0407-6-B-CDCl3
EXPNO 1
PROCNO 1
Date_ 20100930
Time 23.47
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgdc
TD 4000
SOLVENT CDCl3
NS 307
DS 4
SWH 25510.203 Hz
FIDRES 6.377551 Hz
AQ 0.0784500 sec
RG 114
DW 19.600 usec
DE 6.50 usec
TE 294.7 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 10.00 usec
PL1 -4.00 dB
PL1W 63.09573364 W
SFO1 128.3776076 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.80 dB
PL2W 13.17734718 W
PL12W 0.10960442 W
SFO2 400.1316005 MHz
SI 2048
SF 128.3775017 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



**(b,l)-8af**

wrx0119-30-H-CDCl3

```

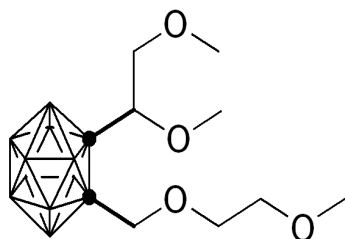
NAME      wrx0119-30-H-CDCl3
EXPNO      1
PROCNO     1
Date_      20090829
Time       15.28
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zg
TD          65536
SOLVENT    CDCl3
NS          4
DS          0
SWH         10000.000 Hz
FIDRES      0.152588 Hz
AQ          3.2768500 sec
RG          161
DW          50.000 usec
DE          6.50 usec
TE          295.0 K
D1          1.00000000 sec
TD0         1

```

```

===== CHANNEL f1 =====
NUC1       1H
P1          14.83 usec
PL1         0.00 dB
PL1W        8.31434441 W
SFO1       400.1318000 MHz
SI          65536
SF          400.1300054 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

```



(b,l)-8af

— 4.152
— 4.120
— 4.097
— 4.066

3.859
3.849
3.841
3.831

3.684
3.674
3.670
3.662
3.652
3.644
3.635

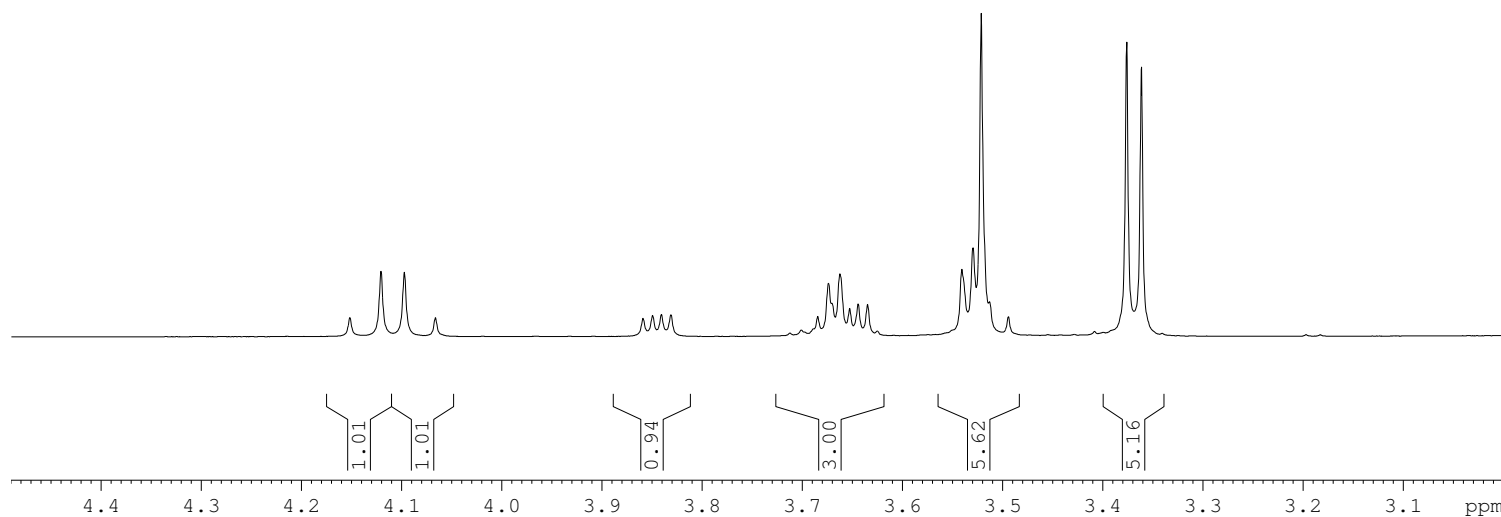
3.541
3.530
3.521
3.513
3.494

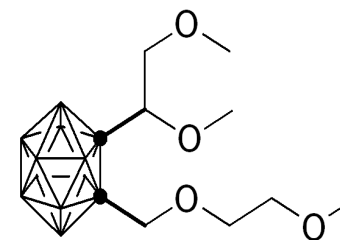
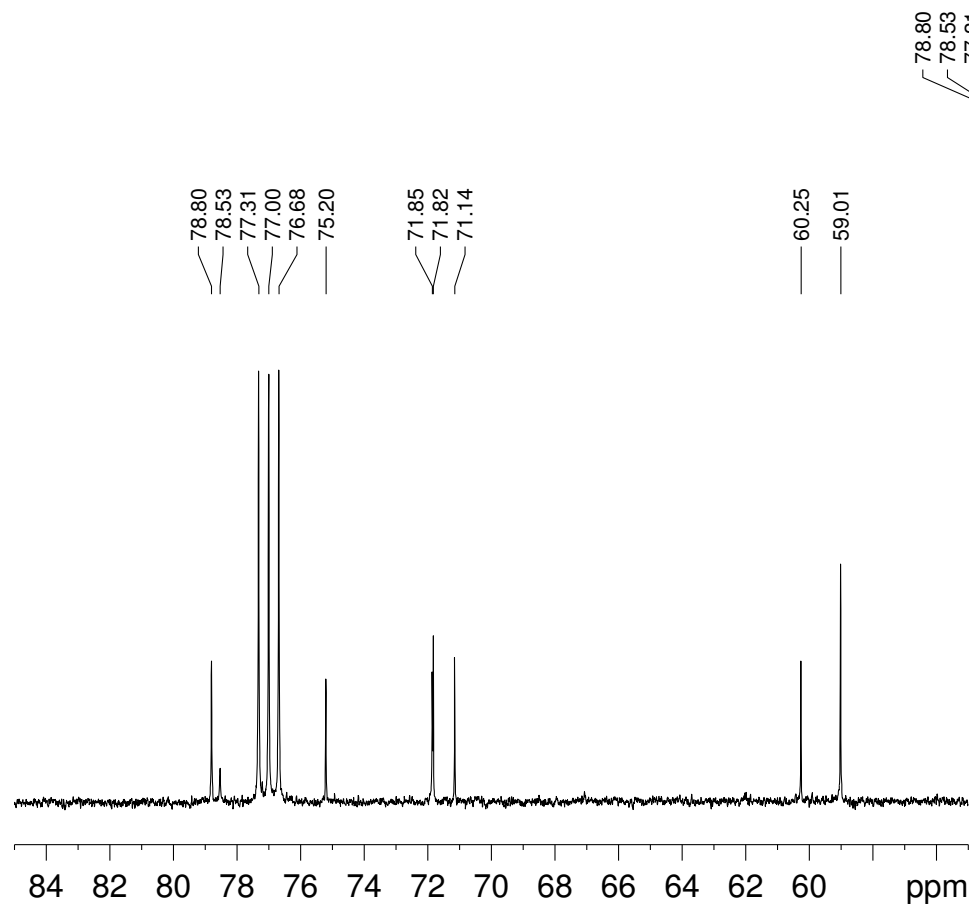
3.376
3.361

wrx0119-30-H-CDC13

NAME wrx0119-30-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20090829
Time 15.28
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 161
DW 50.000 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PL1 0.00 dB
PL1W 8.31434441 W
SFO1 400.1318000 MHz
SI 65536
SF 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



**(b,l)-8af**

wrx0407-5-C-CDCl3

```

NAME      wrx0407-5-C-CDCl3
EXPNO     1
PROCNO    1
Date_     20100830
Time      11.37
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        100
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        181
DW        20.800 usec
DE        6.50 usec
TE        298.4 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

```

```

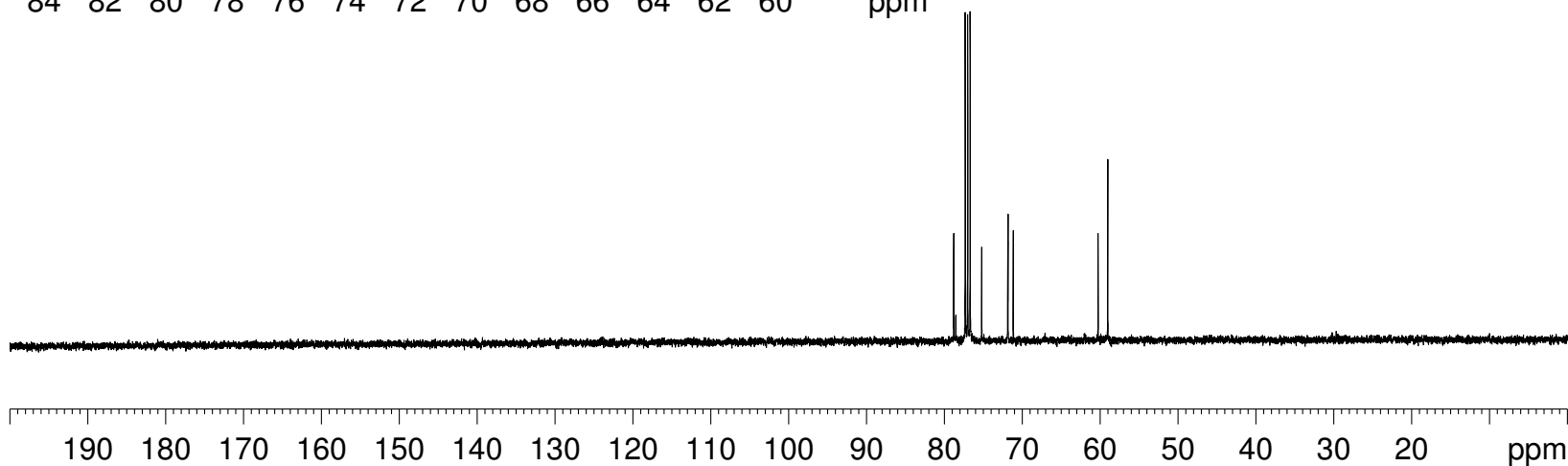
===== CHANNEL f1 =====
NUC1      13C
P1        9.90 usec
PL1       -2.00 dB
PL1W      55.33689499 W
SFO1      100.6379183 MHz

```

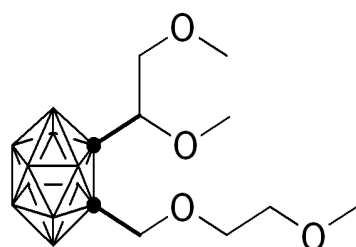
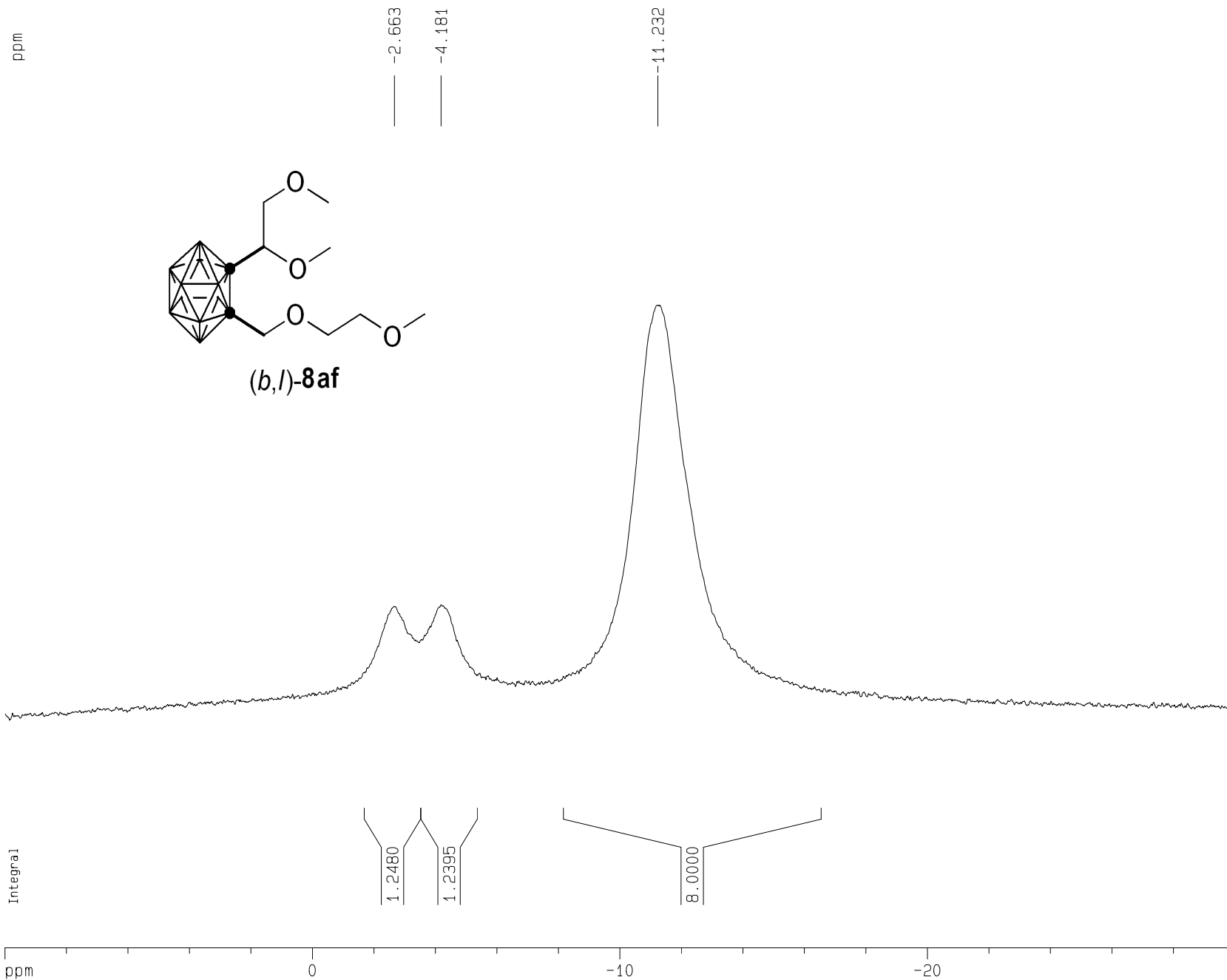
```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2        -1.00 dB
PL12       15.16 dB
PL13       18.62 dB
PL2W       13.56617069 W
PL12W      0.32844096 W
PL13W      0.14806664 W
SFO2      400.1916008 MHz
SI         32768
SF        100.6278602 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



wrx0119-30-B-CDC13

**(b,l)-8af**

Current Data Parameters
 NAME wrx0119-30-B-CDC13
 EXPNO 1
 PROCNO 1

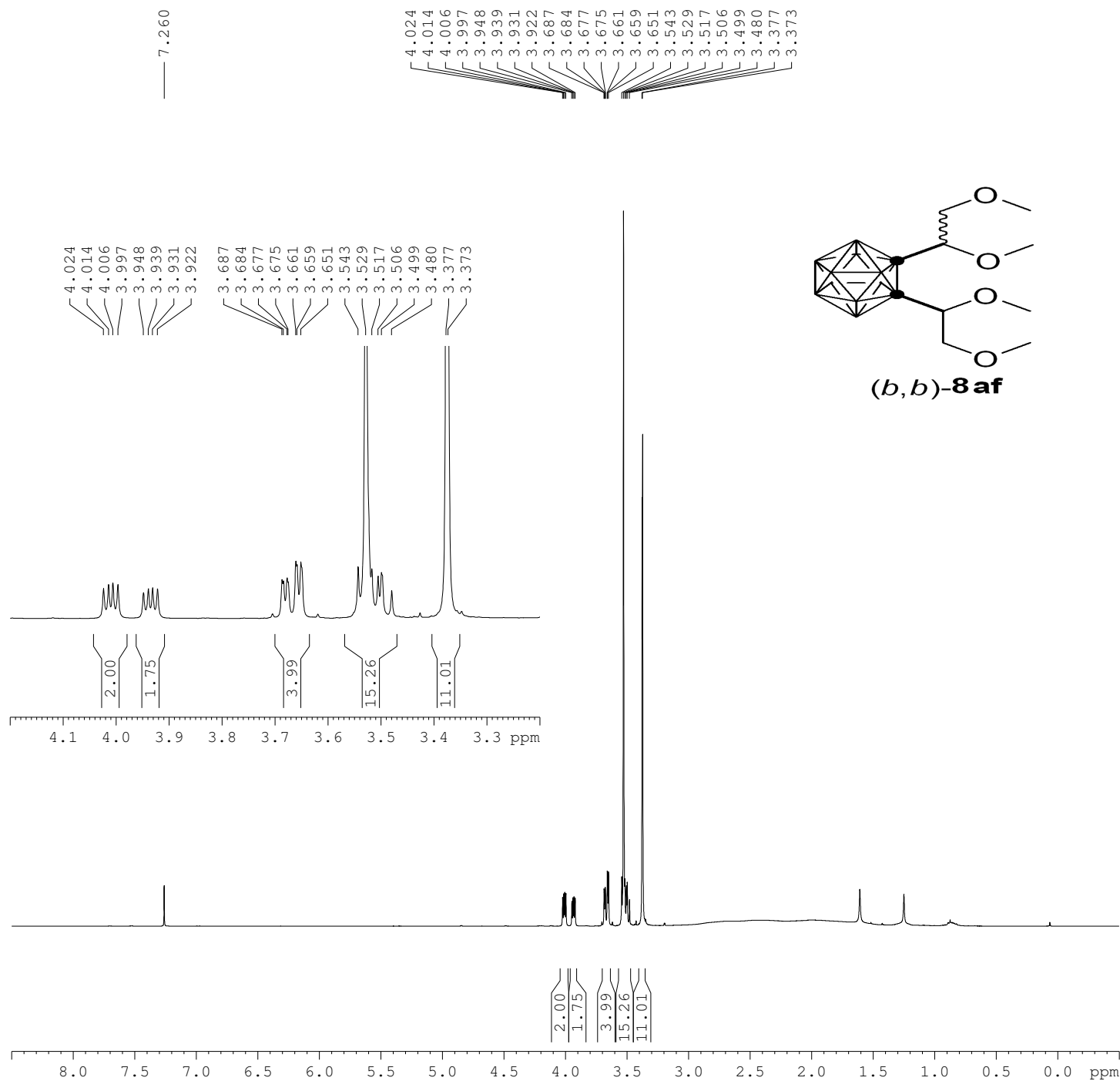
F2 - Acquisition Parameters
 Date_ 20090829
 Time 21.03
 INSTRUM dpx300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgdc
 TD 65536
 SOLVENT CDC13
 NS 100
 DS 0
 SWH 57803.469 Hz
 FIDRES 0.882011 Hz
 AQ 0.5669364 sec
 RG 32
 DW 8.650 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 11B
 P1 3.00 usec
 PL1 -6.00 dB
 SF01 96.2966310 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 300.1310908 MHz

F2 - Processing parameters
 SI 65536
 SF 96.2936560 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

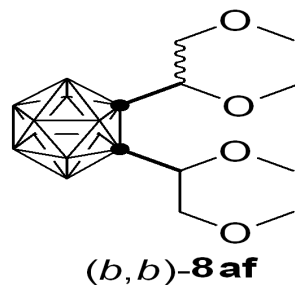
1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
 F1P 10.000 ppm
 F1 962.94 Hz
 F2P -30.000 ppm
 F2 -2888.81 Hz
 PPMCM 1.81818 ppm/cm
 HZCM 175.07938 Hz/cm



wrx0407-4-H-CDCl3

NAME wrx0407-4-H-CDCl3
 EXPNO 1
 PROCNO 1
 Date_ 20101003
 Time 14.29
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2768500 sec
 RG 25.4
 DW 50.000 usec
 DE 6.50 usec
 TE 294.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 -2.00 dB
 PL1W 13.17734718 W
 SFO1 400.1318000 MHz
 SI 65536
 SF 400.1300051 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



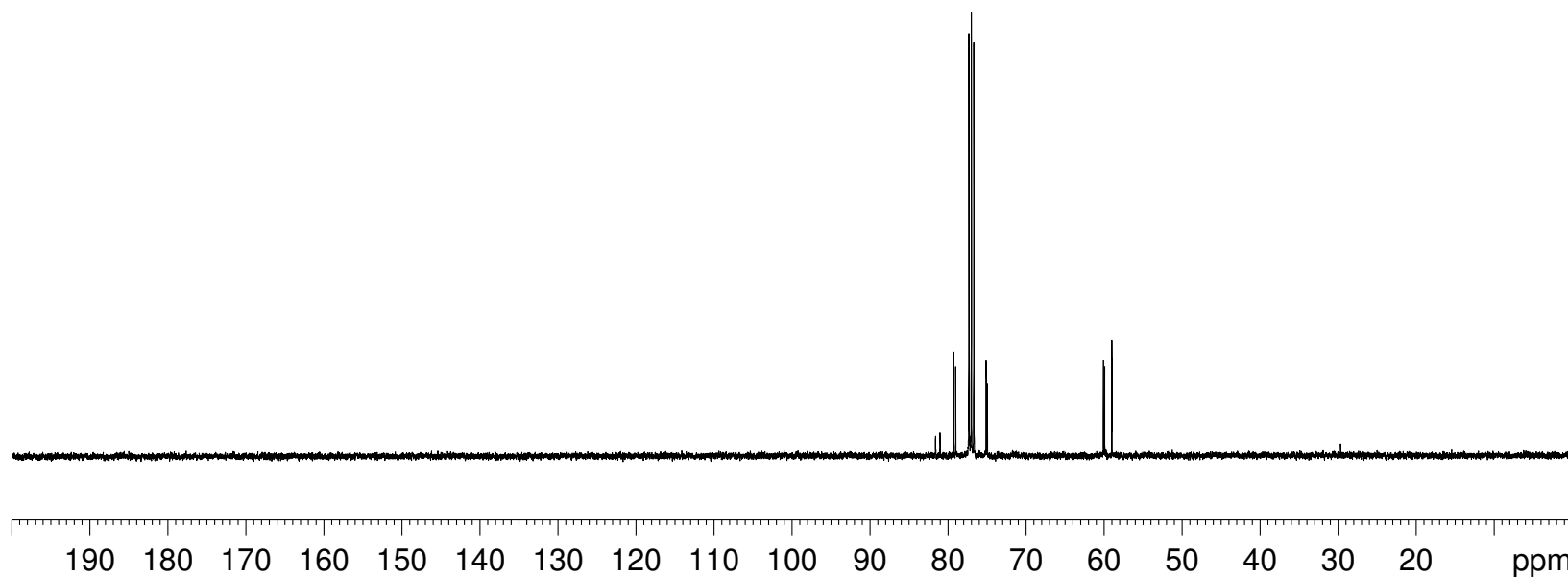
81.59
81.02
79.30
79.01
77.32
77.20
77.00
76.68
75.10
74.96
60.08
59.91
59.02
58.99

wrx0407-4-C-CDC13

NAME wrx0407-4-C-CDC13
EXPNO 1
PROCNO 1
Date_ 20100902
Time 14.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 160
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6379183 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL13 18.62 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
PL13W 0.14806664 W
SFO2 400.1916008 MHz
SI 32768
SF 100.6278588 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

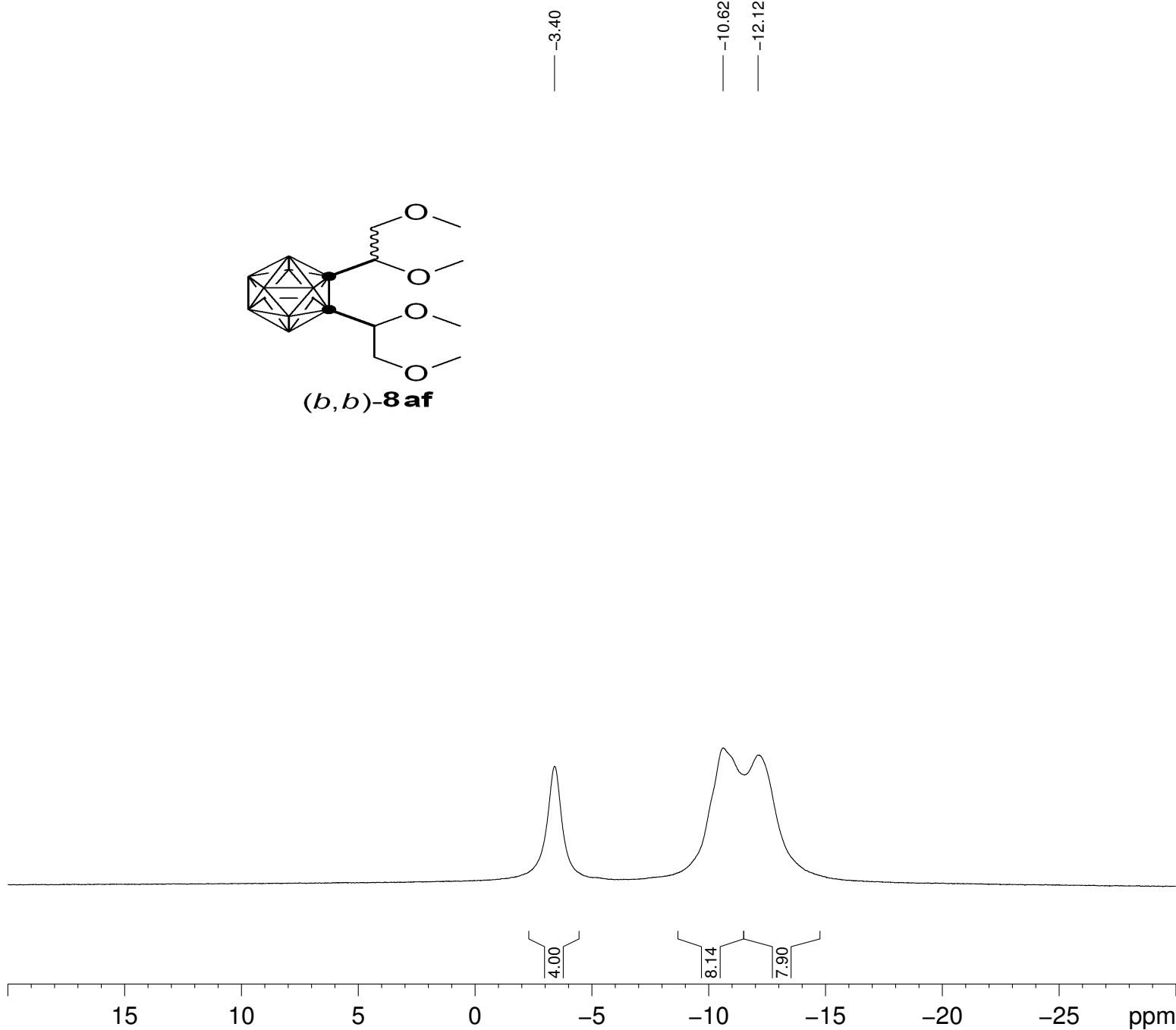
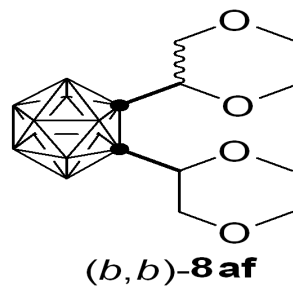


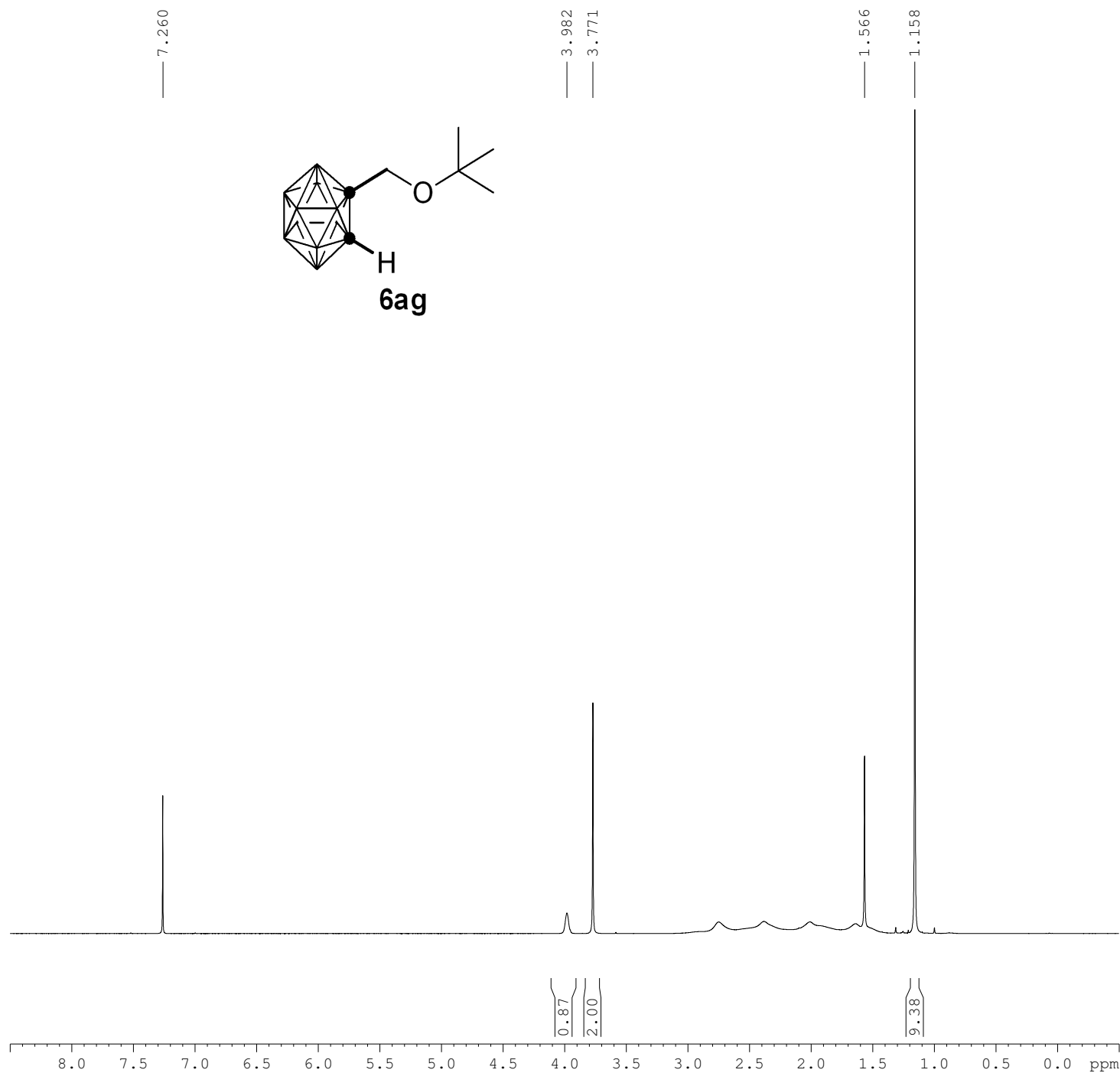
wrx0407-4-B-CDC13

NAME wrx0407-4-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100831
Time 9.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 228
DW 19.600 usec
DE 6.50 usec
TE 298.6 K
D1 5.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 7.60 usec
PL1 -3.00 dB
PL1W 55.13059616 W
SFO1 128.3968556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
SFO2 400.1916008 MHz
SI 32768
SF 128.3969002 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



wrx0387-1p-H-CDCl₃

NAME wrx0387-1p-H-CDCl₃
EXPNO 1
PROCNO 1
Date_ 20100911
Time 13.29
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg
TD 65536
SOLVENT CDCl₃
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 144
DW 50.000 usec
DE 6.50 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1

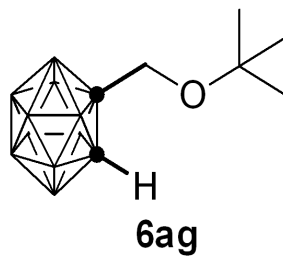
===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1318000 MHz
SI 65536
SF 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S71

77.317
77.000
76.682
75.037
73.185
63.606
57.194

27.205

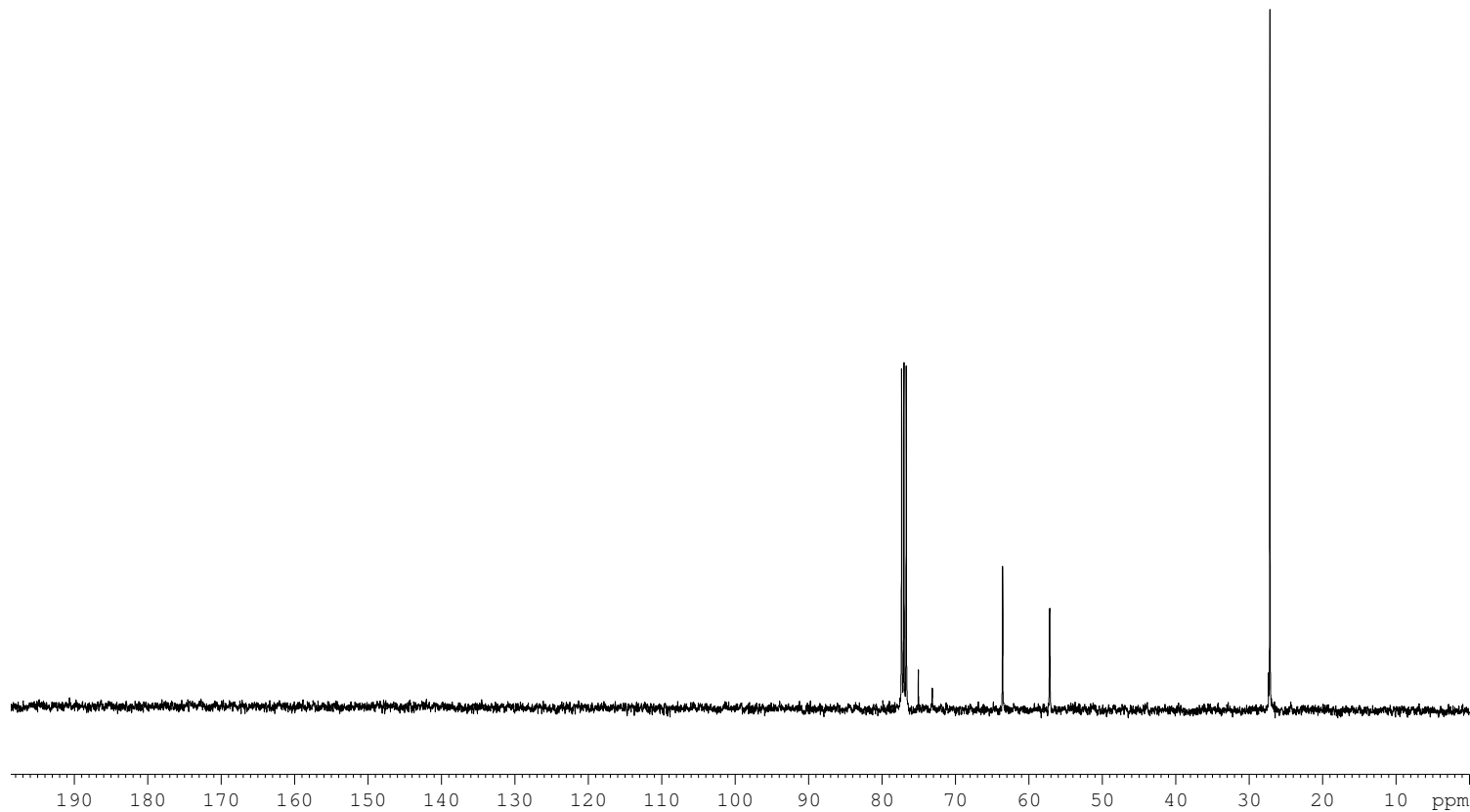
wrx0118-2-6-C13-CDC13



NAME wrx0118-2-6-C13-CDC1
EXPNO 1
PROCNO 1
Date_ 20090828
Time 13.36
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgdc
TD 131072
SOLVENT CDC13
NS 413
DS 0
SWH 29761.904 Hz
FIDRES 0.227065 Hz
AQ 2.2020595 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

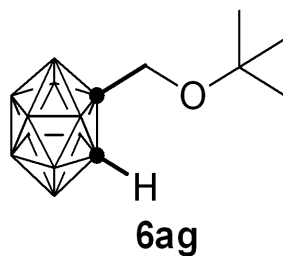
===== CHANNEL f1 =====
NUC1 13C
P1 9.68 usec
PL1 -0.60 dB
PL1W 41.24164963 W
SFO1 100.6227690 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 15.66 dB
PL2W 8.31434441 W
PL12W 0.22585411 W
SFO2 400.1320007 MHz
SI 131072
SF 100.6127708 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



S72

— -3.70
— -5.45
— -9.45
— -11.82
— -13.12
— -13.70

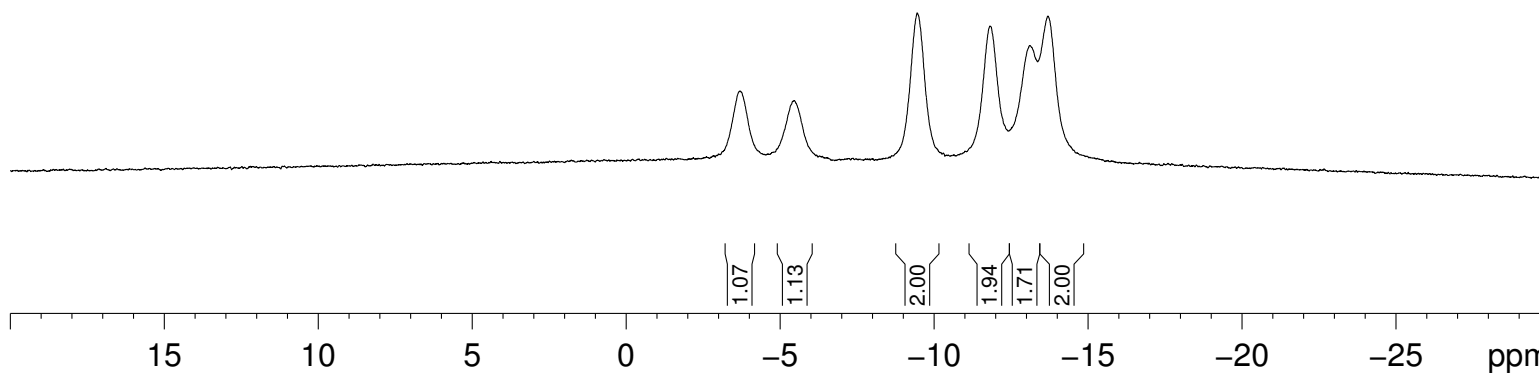


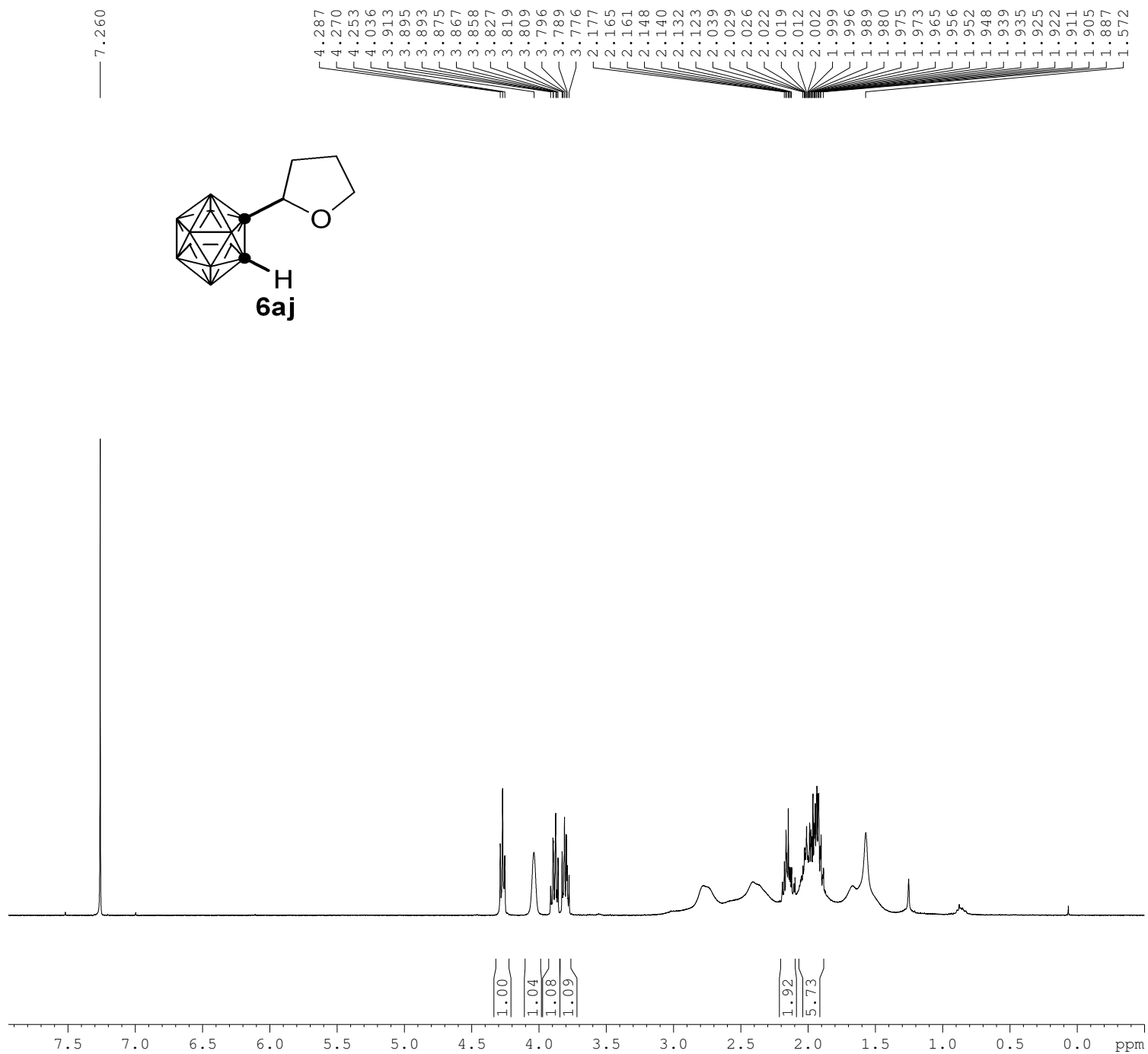
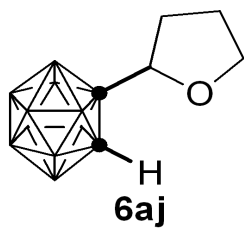
wrx0387-1-1p-B-CDC13

NAME wrx0387-1-1p-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100911
Time 13.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 65536
SOLVENT CDC13
NS 12
DS 0
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 406
DW 19.600 usec
DE 6.50 usec
TE 298.2 K
D1 5.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 7.60 usec
PL1 -3.00 dB
PL1W 55.13059616 W
SFO1 128.3968556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
SFO2 400.1916008 MHz
SI 32768
SF 128.3969002 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40





wrx0108-1-H-CDCl3

```

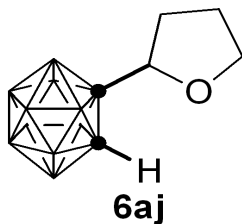
NAME      wrx0108-1-H-CDCl3
EXPNO     1
PROCNO    1
Date_     20090813
Time      9.22
INSTRUM   spect
PROBHD    5 mm PADUL 13C
PULPROG   zg
TD         65536
SOLVENT   CDCl3
NS         4
DS         0
SWH        10000.000 Hz
FIDRES     0.152588 Hz
AQ         3.2768500 sec
RG         203
DW         50.000 use
DE         6.50 use
TE         294.8 K
D1         1.00000000 sec
TD0        1

```

```

===== CHANNEL f1 =====
NUC1       1H
P1         14.83 use
PL1        0.00 dB
PL1W       8.31434441 W
SFO1       400.1318000 MHz
SI         65536
SF         400.1300052 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```



79.088
77.805
77.318
77.000
76.683

69.590

59.292

32.814

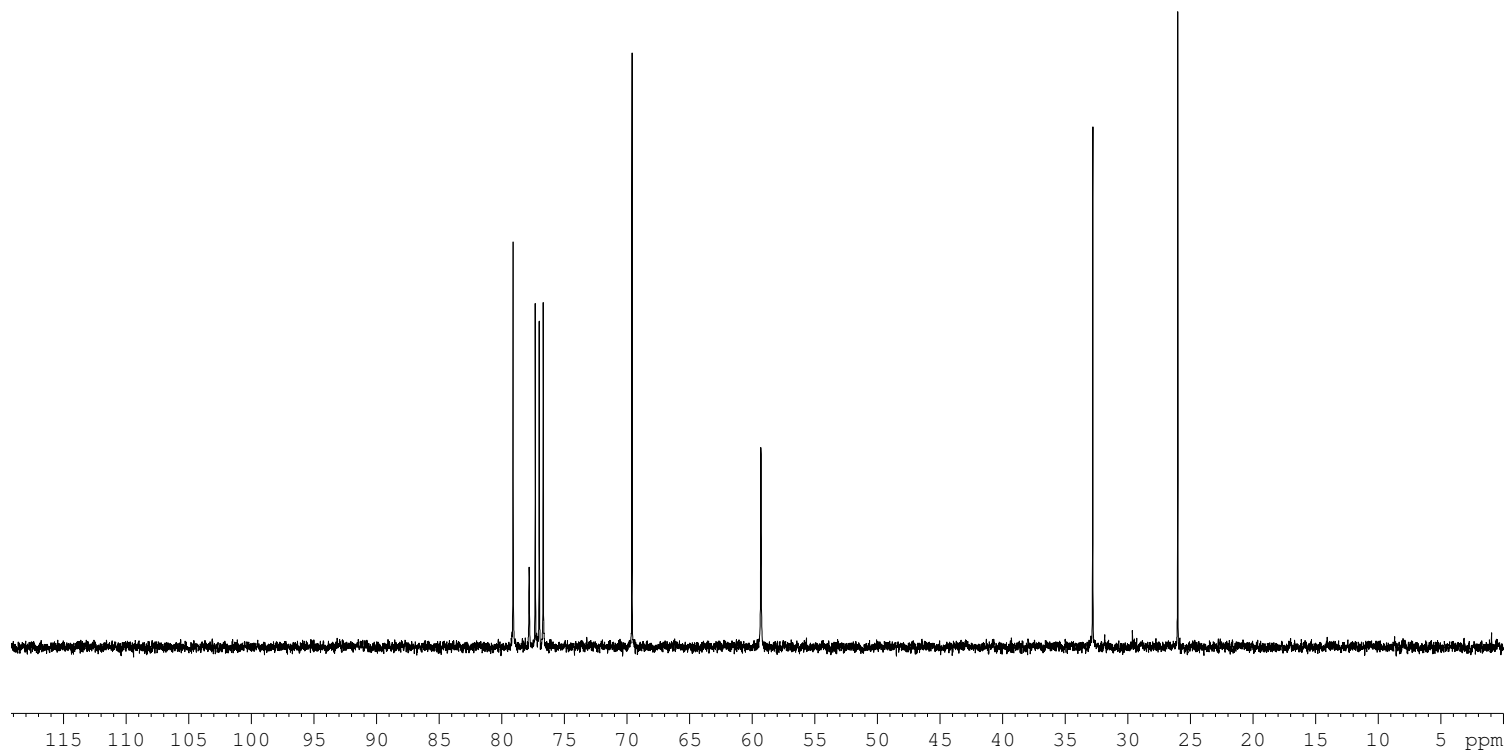
26.025

wrx0108-1-C-CDCl₃

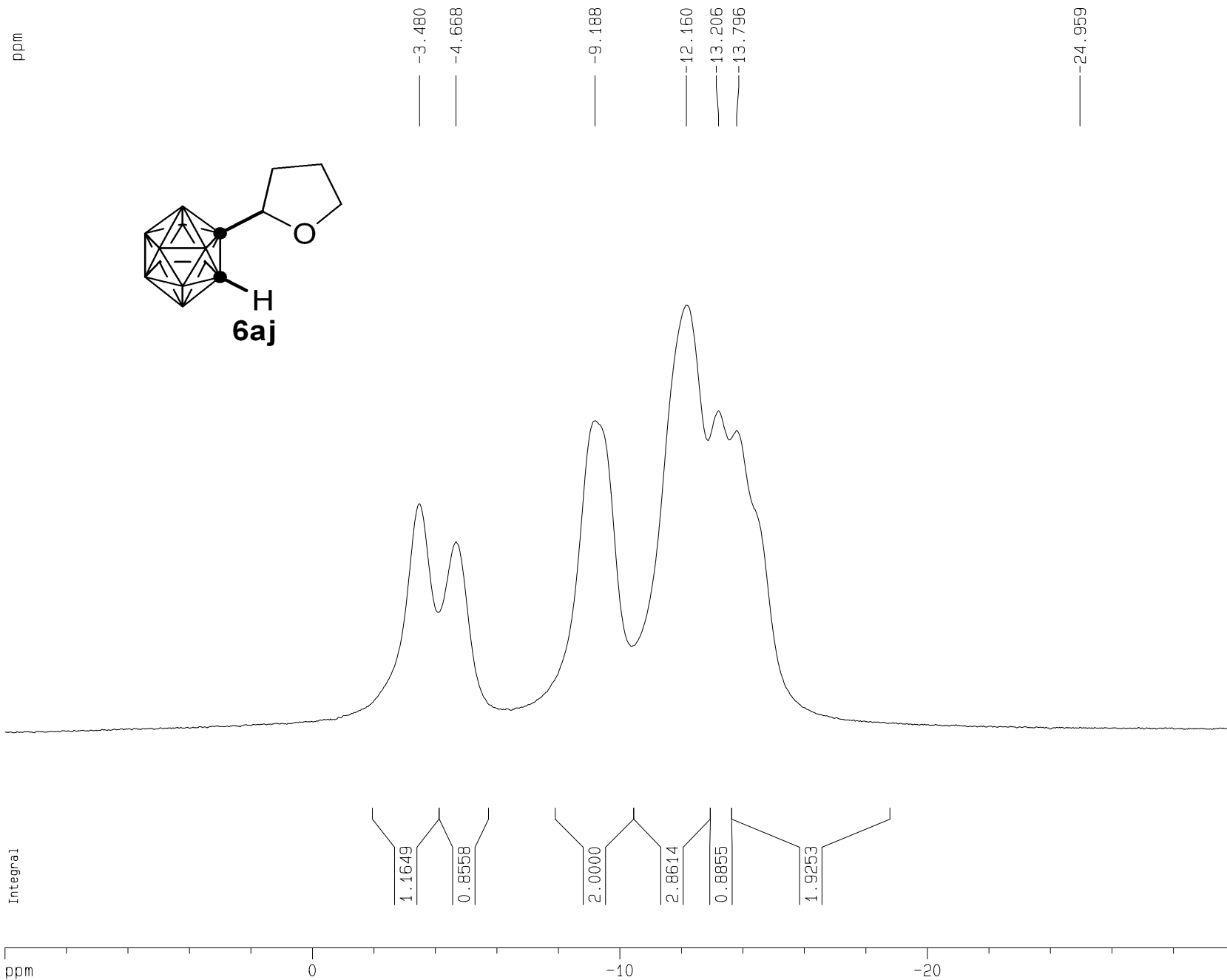
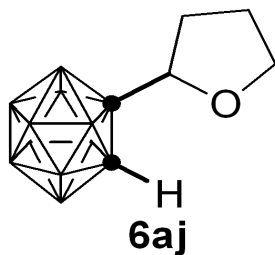
NAME wrx0108-1-C-CDCl₃
EXPNO 1
PROCNO 1
Date_ 20090813
Time 9.38
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 49
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 use
DE 6.50 use
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.68 use
PL1 -0.60 dB
PL1W 41.24164963 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 use
PL2 0.00 dB
PL12 15.66 dB
PL13 15.92 dB
PL2W 8.31434441 W
PL12W 0.22585411 W
PL13W 0.21272963 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127762 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



wrx-CB+THF-B-CDC13-300M



Current Data Parameters
 NAME wrx-CB+THF-B-CDC13-300M
 EXPNO 1
 PROCNO 1

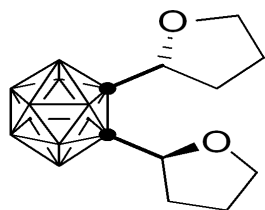
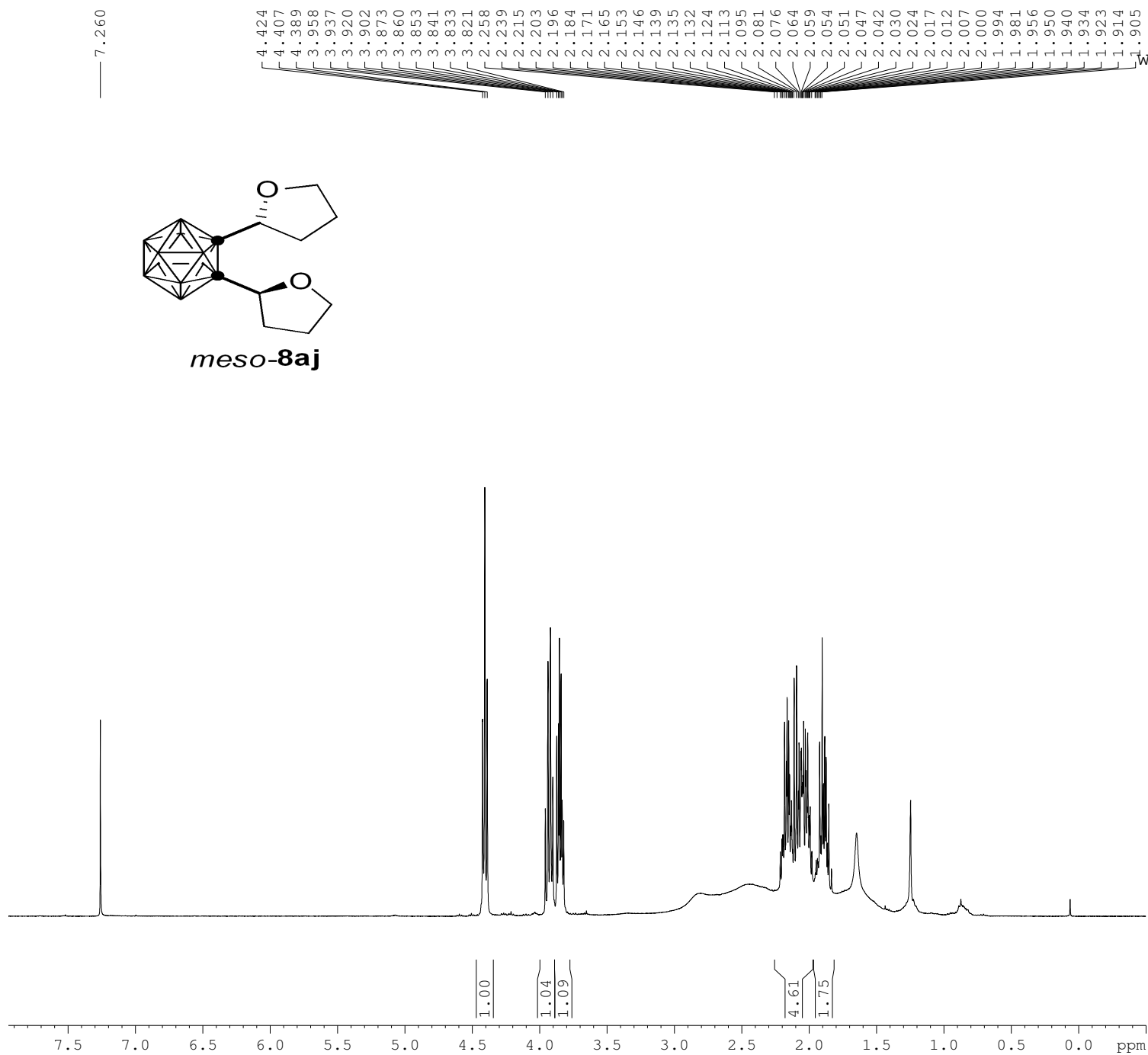
F2 - Acquisition Parameters
 Date_ 20090816
 Time 12.18
 INSTRUM dpx300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgdc
 TD 65536
 SOLVENT CDC13
 NS 200
 DS 0
 SWH 57803.469 Hz
 FIDRES 0.882011 Hz
 AQ 0.5669364 sec
 RG 32
 DW 8.650 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 3.00 usec
 PL1 -6.00 dB
 SF01 96.2966310 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 300.1310908 MHz

F2 - Processing parameters
 SI 65536
 SF 96.2936560 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
 F1P 10.000 ppm
 F1 962.94 Hz
 F2P -30.000 ppm
 F2 -2888.81 Hz
 PPMCM 1.81818 ppm/cm
 HZCM 175.07938 Hz/cm

*meso-8aj*

wrx0108-2-H-CDCl3

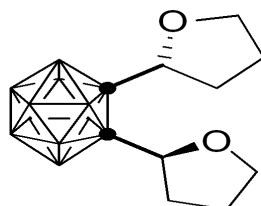
NAME wrx0108-2-H-CDCl3
 EXPNO 1
 PROCNO 1
 Date_ 20090814
 Time 13.10
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zg
 TD 65536
 SOLVENT CDCl3
 NS 4
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2768500 sec
 RG 64
 DW 50.000 use
 DE 6.50 use
 TE 294.7 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 use
 PL1 0.00 dB
 PL1W 8.31434441 W
 SFO1 400.1318000 MHz
 SI 65536
 SF 400.1300052 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

83.121
77.560
77.317
77.000
76.682
69.416

33.395
29.678
25.945

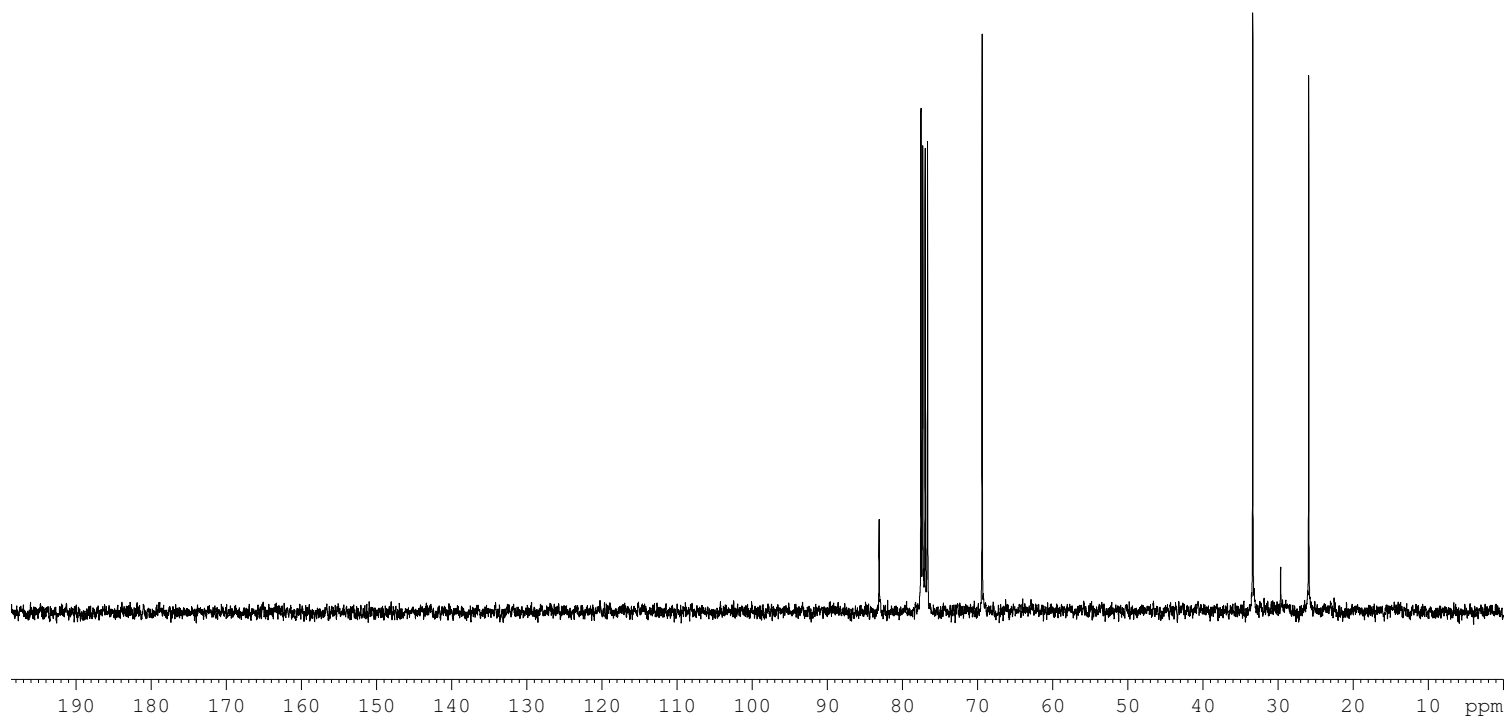
wrx0108-2-C-CDC13

*meso-8aj*

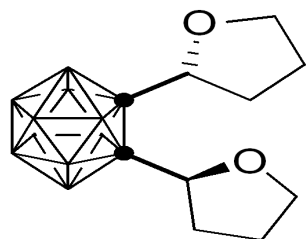
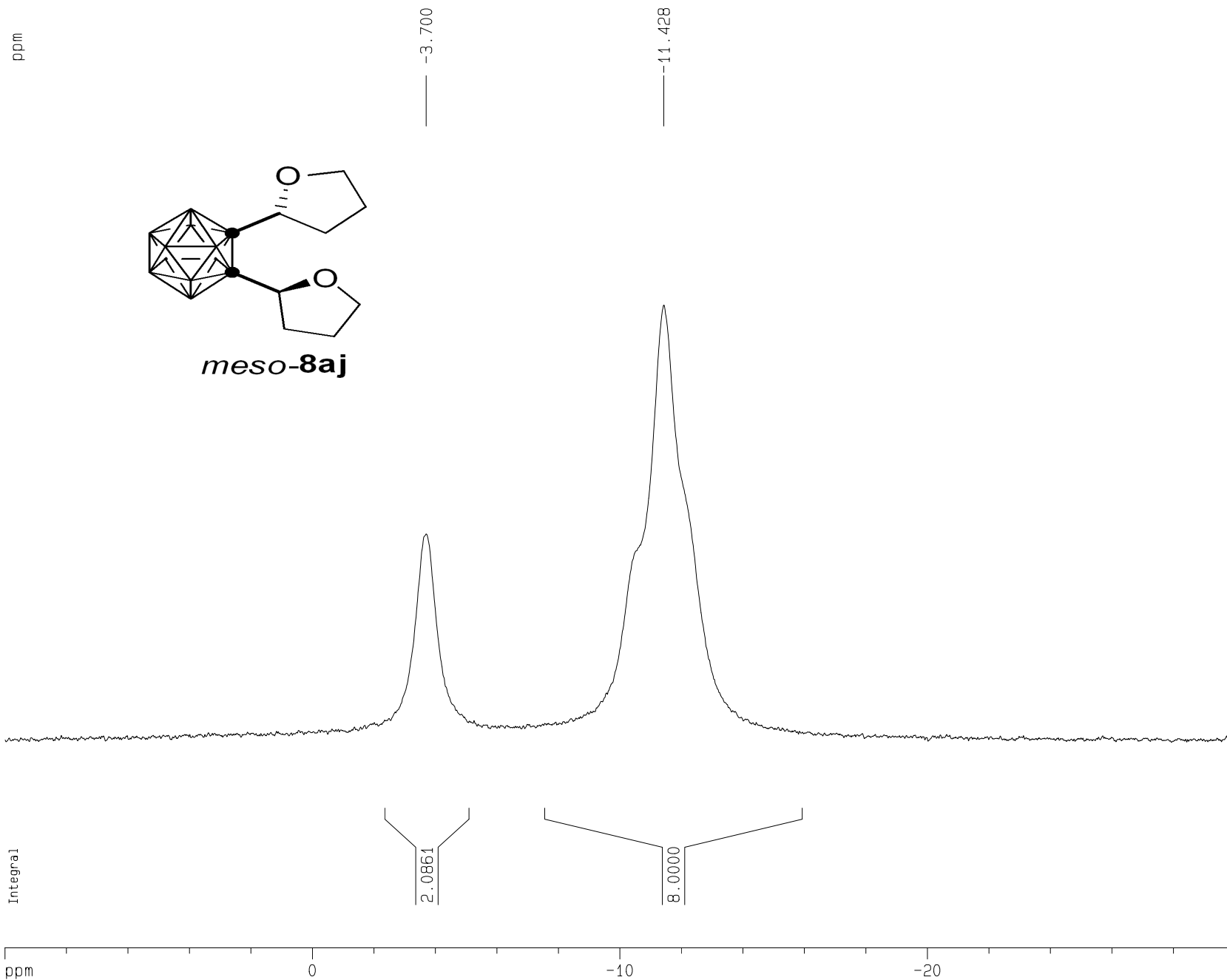
NAME wrx0108-2-C-CDC13
EXPNO 1
PROCNO 1
Date_ 20090814
Time 13.42
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgdc
TD 131072
SOLVENT CDC13
NS 329
DS 0
SWH 29761.904 Hz
FIDRES 0.227065 Hz
AQ 2.2020595 sec
RG 203
DW 16.800 use
DE 6.50 use
TE 295.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.68 use
PL1 -0.60 dB
PL1W 41.24164963 W
SFO1 100.6227690 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 use
PL2 0.00 dB
PL12 15.66 dB
PL2W 8.31434441 W
PL12W 0.22585411 W
SFO2 400.1320007 MHz
SI 131072
SF 100.6127718 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



wrx0108-2-all-2-B-CDC13

*meso*-8aj

Current Data Parameters
NAME wrx0108-2-all-2-B-CDC13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090827
Time 12.56
INSTRUM dpx300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 57803.469 Hz
FIDRES 0.882011 Hz
AQ 0.5669364 sec
RG 32
DW 8.650 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

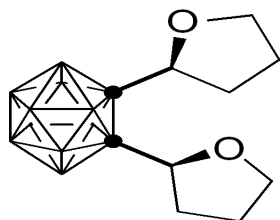
===== CHANNEL f1 =====
NUC1 11B
P1 3.00 usec
PL1 -6.00 dB
SF01 96.2966310 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 19.00 dB
SF02 300.1310908 MHz

F2 - Processing parameters
SI 65536
SF 96.2936551 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 962.94 Hz
F2P -30.000 ppm
F2 -2888.81 Hz
PPMCM 1.81818 ppm/cm
HZCM 175.07938 Hz/cm

— 7.260

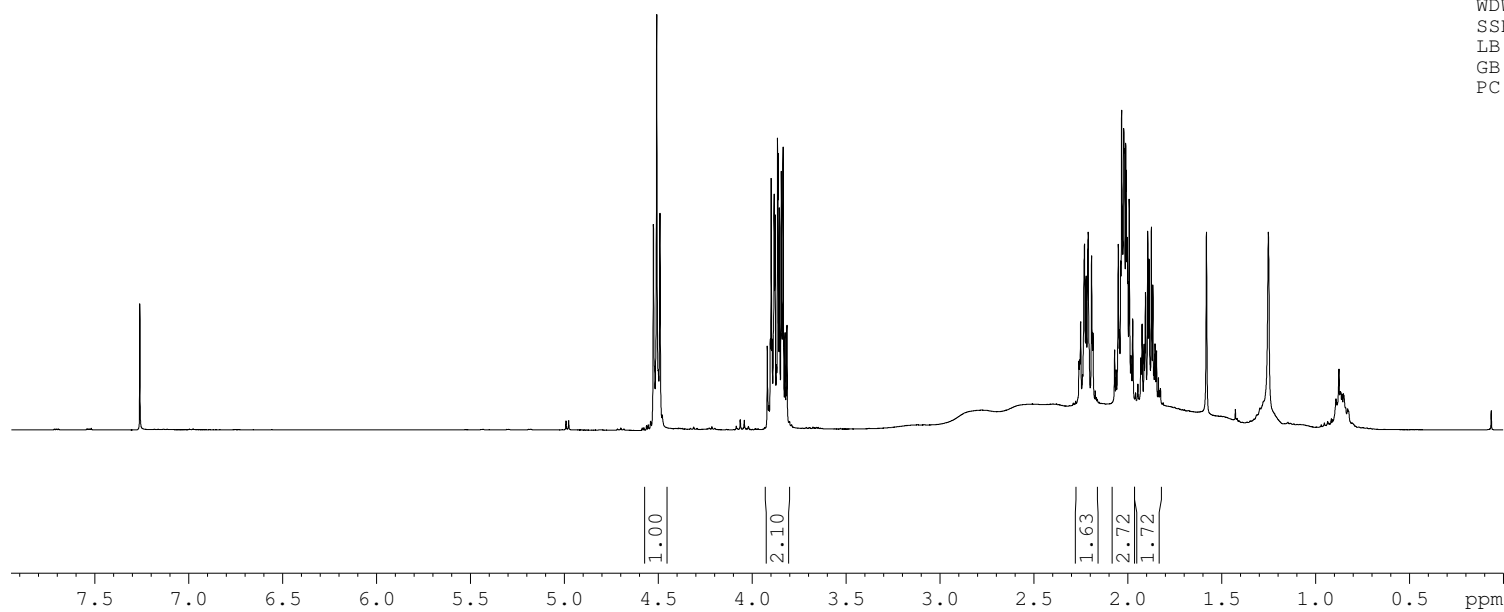
*rac-8aj*

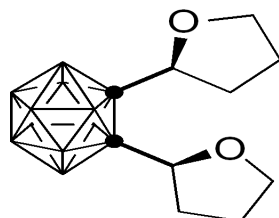
4.525
4.508
4.490
3.919
3.903
3.898
3.893
3.882
3.877
3.865
3.862
3.854
3.845
3.835
3.825
3.814
2.251
2.230
2.221
2.210
2.192
2.185
2.069
2.050
2.043
2.038
2.032
2.026
2.021
2.020
2.018
2.010
2.008
2.003
2.000
1.999
1.992
1.983
1.973
1.923
1.913
1.906
1.893
1.886
1.874
1.866
1.856

wrx0108-2-all-1-H-CDC13

NAME wrx0108-2-all-1-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20090915
Time 22.38
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PL1 0.00 dB
PL1W 8.31434441 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



*rac-8aj*

82.930
77.534
77.318
77.000
76.683
69.276

33.434
25.963

wrx0108-2-all-1-C-CDCl₃

```

NAME      wrx0108-2-all-1-C-CDCl
EXPNO      1
PROCNO     1
Date_      20090816
Time       20.41
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         79
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         295.6 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

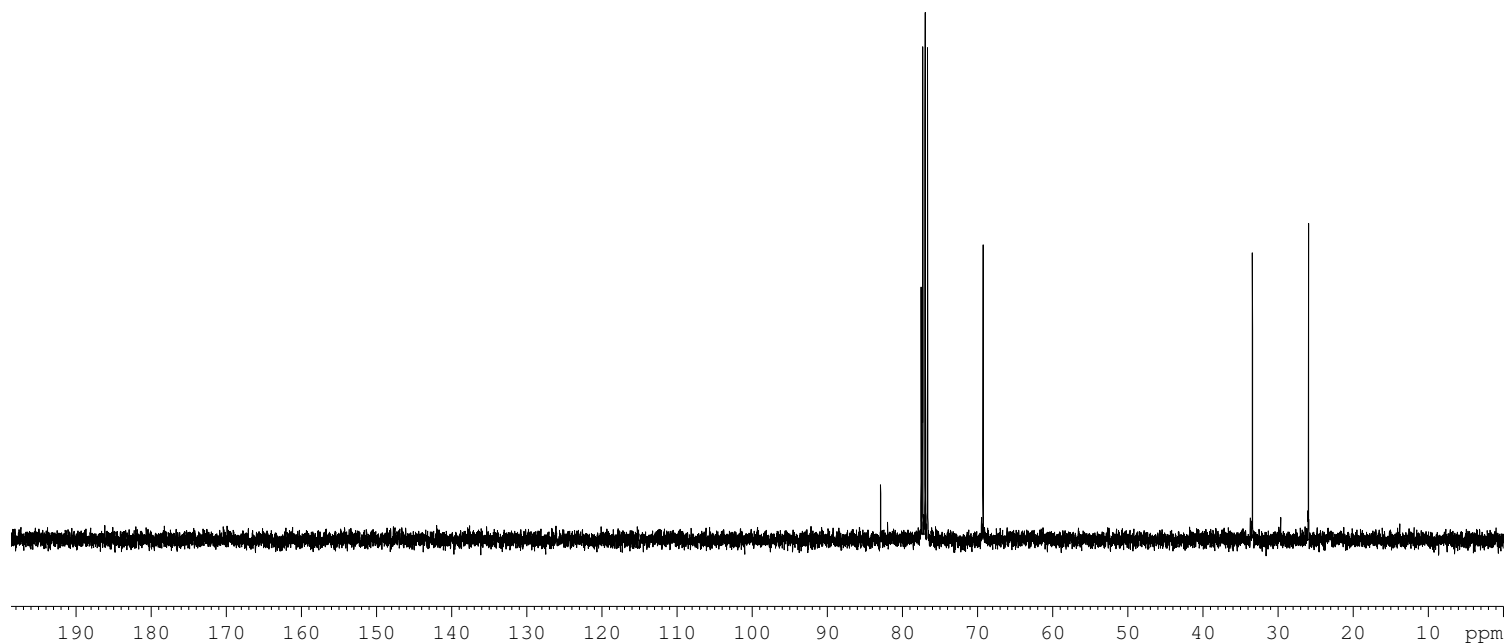
===== CHANNEL f1 =====
NUC1       13C
P1         9.68 usec
PL1        -0.60 dB
PL1W       41.24164963 W
SFO1       100.6228298 MHz

```

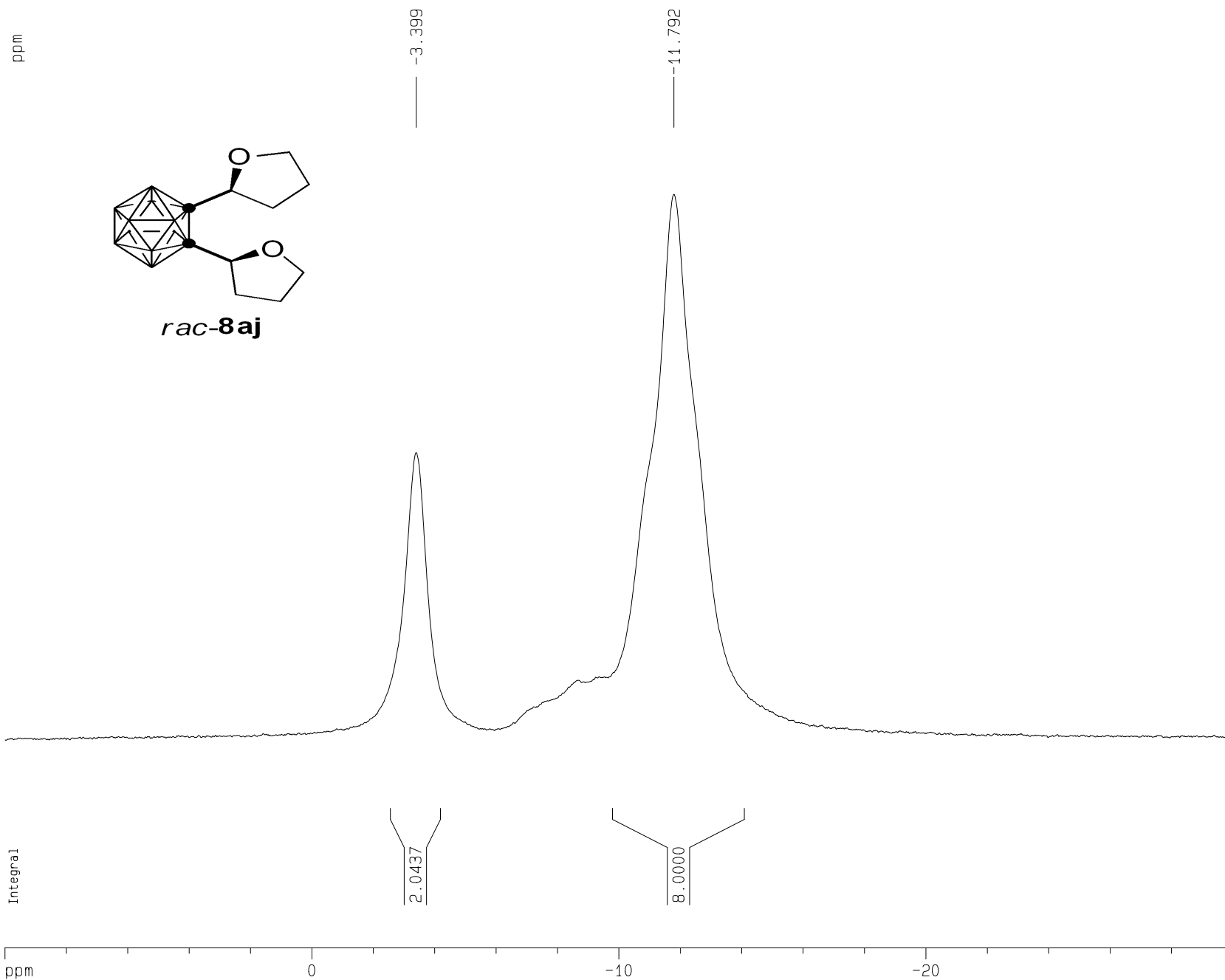
```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2         0.00 dB
PL12       15.66 dB
PL13       15.92 dB
PL2W       8.31434441 W
PL12W      0.22585411 W
PL13W      0.21272963 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127714 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



wrx0108-2-all-1-B-CDC13-300M



Current Data Parameters
 NAME wrx0108-2-all-1-B-CDC13-300M
 EXPNO 1
 PROCNO 1

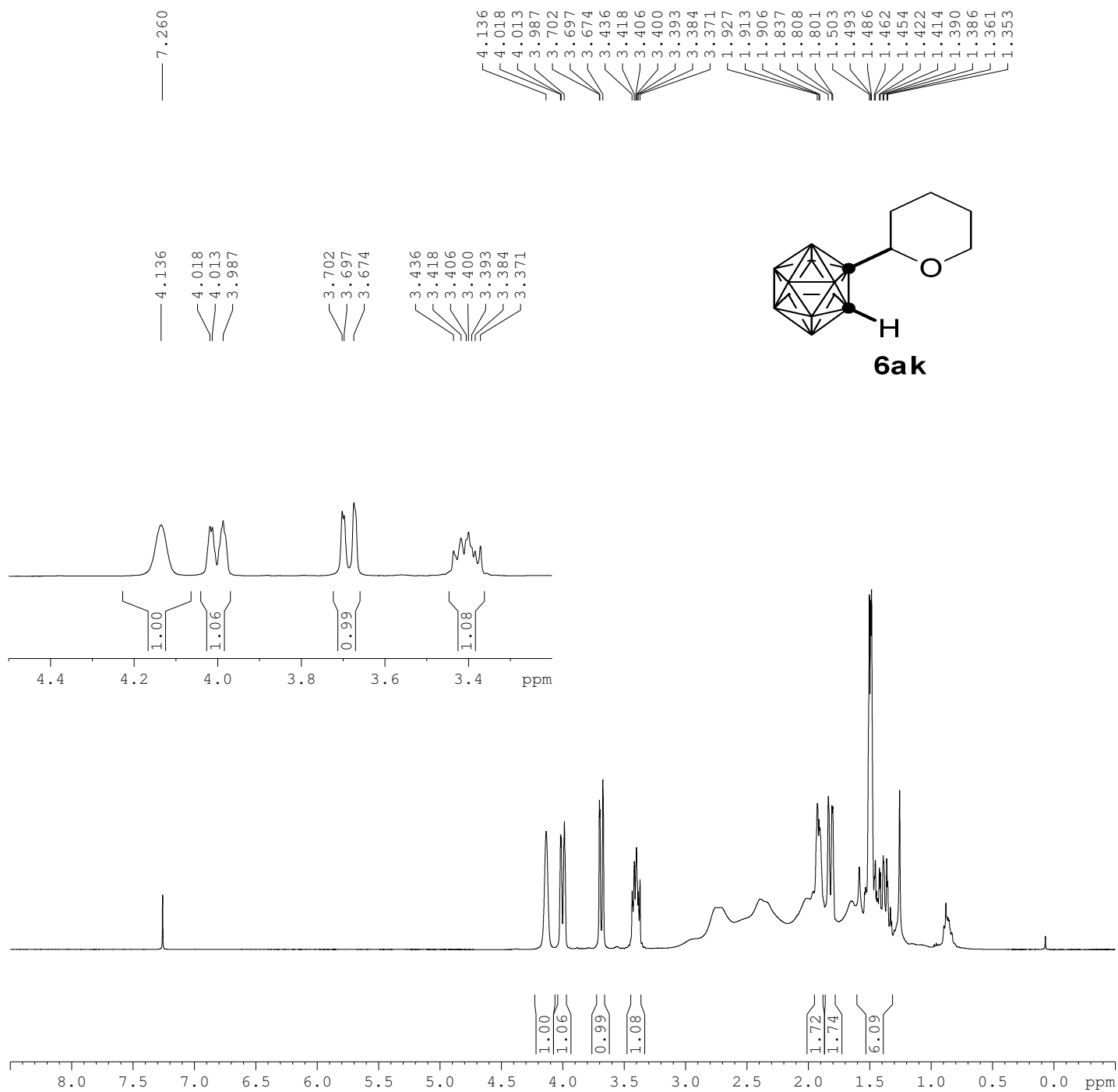
F2 - Acquisition Parameters
 Date_ 20090816
 Time 10.12
 INSTRUM dpv300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgdc
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 57803.469 Hz
 FIDRES 0.882011 Hz
 AQ 0.5669364 sec
 RG 32
 DW 8.650 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWAK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 11B
 P1 3.00 usec
 PL1 -6.00 dB
 SF01 96.2966310 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SF02 300.1310908 MHz

F2 - Processing parameters
 SI 65536
 SF 96.2936551 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 22.00 cm
 CY 10.00 cm
 F1P 10.000 ppm
 F1 962.94 Hz
 F2P -30.000 ppm
 F2 -2888.81 Hz
 PPMCM 1.81818 ppm/cm
 HZCM 175.07938 Hz/cm



wrx0394-1-H-CDCl3

NAME wrx0394-1-H-CDCl3
 EXPNO 1
 PROCNO 1
 Date_ 20100916
 Time 21.33
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 18
 DW 62.400 usec
 DE 6.50 usec
 TE 294.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 -2.00 dB
 PL1W 13.17734718 W
 SFO1 400.1316005 MHz
 SI 65536
 SF 400.1300056 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S83

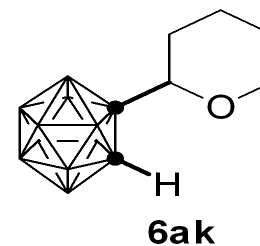
77.32
77.06
77.00
76.68
69.69
58.02
31.73
24.93
23.12

wrx0394-1-C-CDCl3

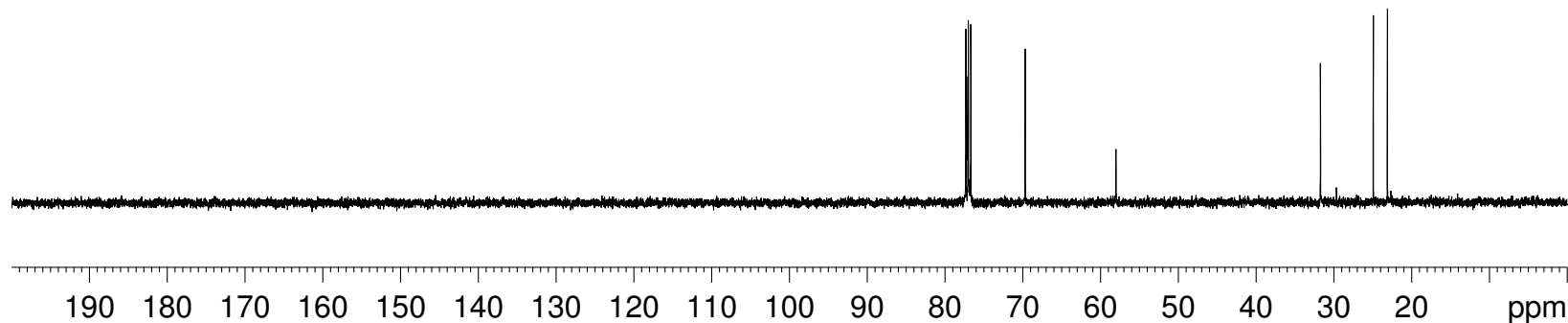
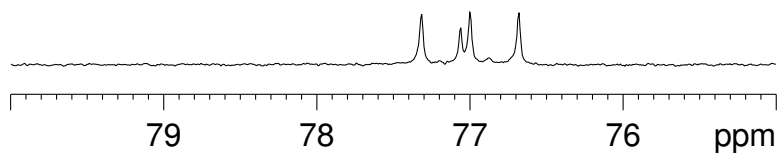
NAME wrx0394-1-C-CDCl3
EXPNO 1
PROCNO 1
Date_ 20100917
Time 10.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 20
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

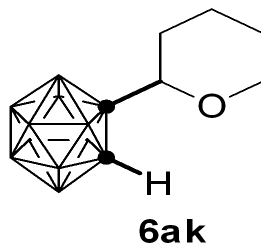
===== CHANNEL f1 =====
NUC1 13C
P1 9.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6379183 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL13 18.62 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
PL13W 0.14806664 W
SFO2 400.1916008 MHz
SI 32768
SF 100.6278610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



77.32
77.06
77.00
76.68





—4.28
—4.73

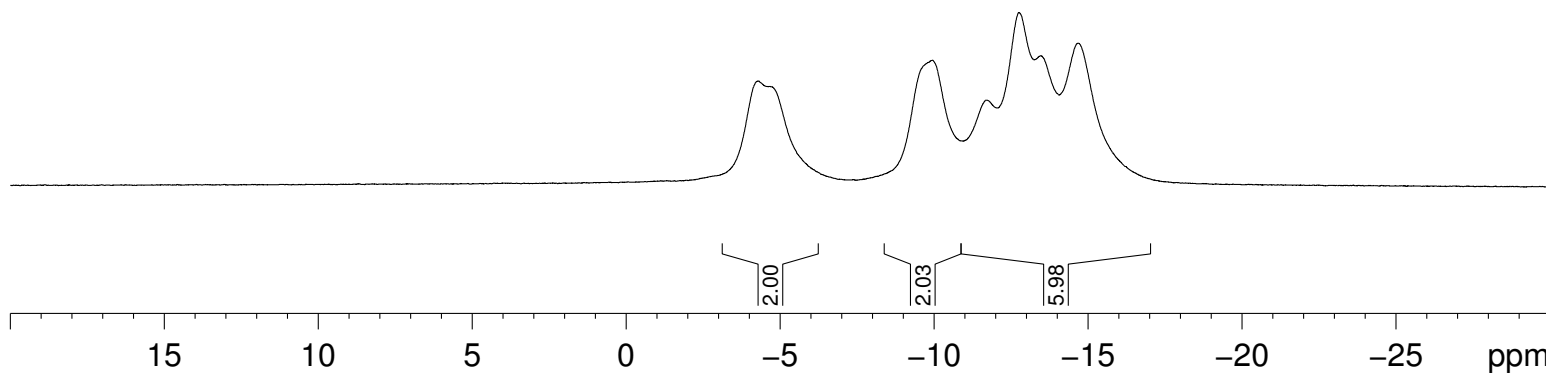
—9.95
—11.73
—12.77
—13.47
—14.67

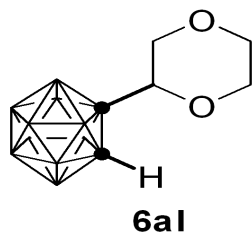
wrx0394-1-B-CDC13

NAME wrx0394-1-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100917
Time 9.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 144
DW 19.600 usec
DE 6.50 usec
TE 298.6 K
D1 5.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 7.60 usec
PL1 -3.00 dB
PL1W 55.13059616 W
SFO1 128.3968556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
SFO2 400.1916008 MHz
SI 32768
SF 128.3969002 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40





77.318
77.204
77.001
76.683
73.630
70.255
67.825
65.712
— 57.473

wrx0297-2-C-CDC13

```

NAME      wrx0297-2-C-CDC13
EXPNO     1
PROCNO    1
Date_     20100527
Time      22.28
INSTRUM    spect
PROBHD     5 mm PABBI 1H/
PULPROG    zgpg30
TD         65536
SOLVENT    CDC13
NS         10715
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         294.6 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

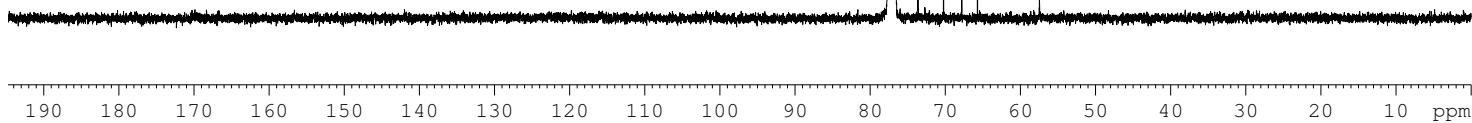
===== CHANNEL f1 =====
NUC1       13C
P1         14.50 usec
PL1        -4.00 dB
PL1W       90.22689819 W
SFO1       100.6228298 MHz

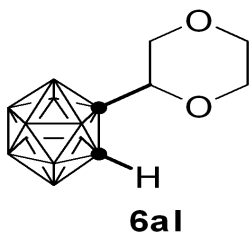
```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -2.00 dB
PL12       18.80 dB
PL13       18.80 dB
PL2W       13.17734718 W
PL12W      0.10960442 W
PL13W      0.10960442 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127703 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```





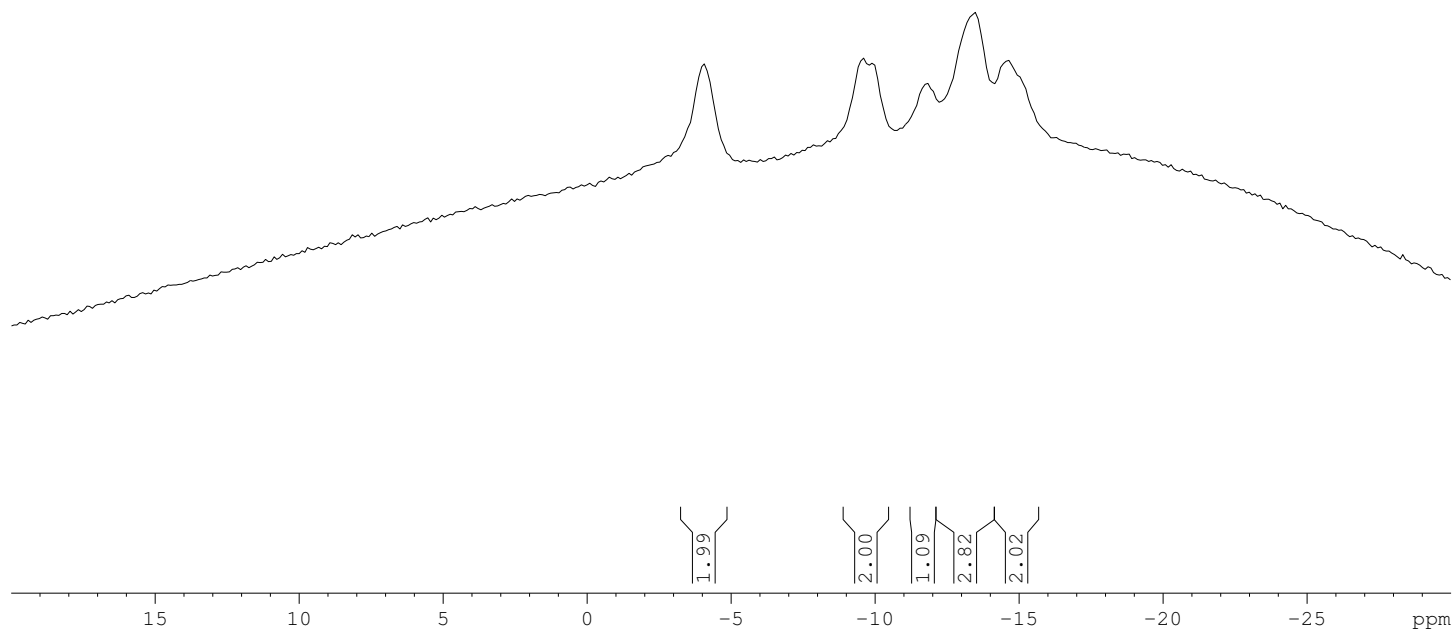
— -4.054
 \ -9.590
 / -9.970
 — -11.792
 — -13.462
 — -14.687

wrx0297-2-B-CDC13

NAME wrx0297-2-B-CDC13
 EXPNO 1
 PROCNO 1
 Date_ 20100427
 Time 17.11
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zgdc
 TD 4000
 SOLVENT Acetone
 NS 132
 DS 4
 SWH 25510.203 Hz
 FIDRES 6.377551 Hz
 AQ 0.0784500 sec
 RG 203
 DW 19.600 usec
 DE 6.50 usec
 TE 294.4 K
 D1 0.10000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 11B
 P1 14.50 usec
 PL1 -4.00 dB
 SFO1 128.3776076 MHz

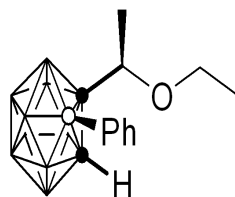
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 18.80 dB
 PL2W 13.17734718 W
 PL12W 0.10960442 W
 SFO2 400.1316005 MHz
 SI 2048
 SF 128.3775390 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40



7.595
7.579
7.576
7.402
7.383
7.376
7.369
7.365
7.361
7.351
7.348
7.336
7.333
7.316
7.311
7.260

4.355
3.820
3.804
3.788
3.772
3.427
3.409
3.405
3.392
3.387
3.382
3.374
3.370
3.352
3.292
3.275
3.270
3.257
3.252
3.240
3.235

1.551
1.109
1.091
1.074
0.941
0.925

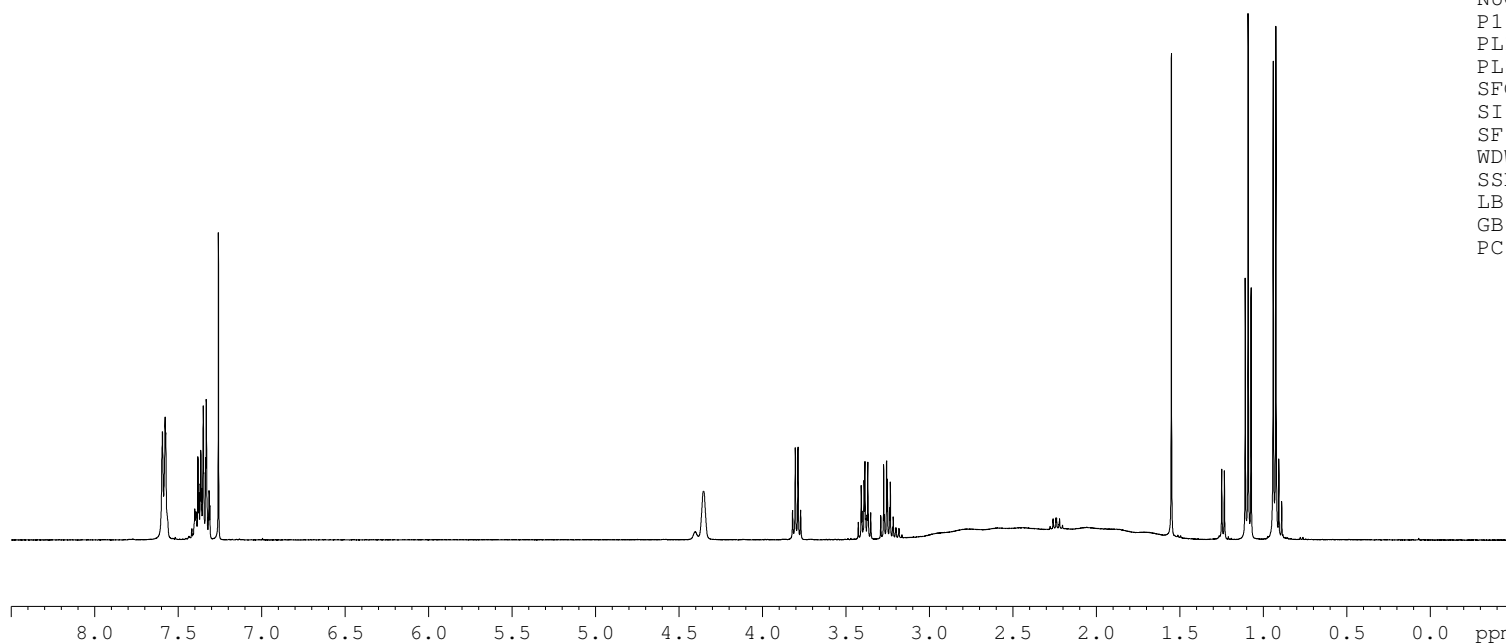


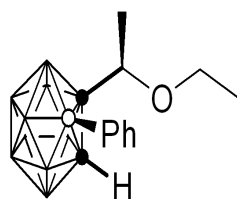
(R,R)-6ba

wrx0264-1-re-H-CDCl₃

NAME wrx0264-1-re-H-CDCl₃
EXPNO 1
PROCNO 1
Date_ 20100305
Time 16.10
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDCl₃
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PL1 0.00 dB
PL1W 8.31434441 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



**(R,R)-6ba**

134.120
129.152
127.776

77.317
77.000
76.683
76.137
65.773
57.829

18.150
15.022

wrx0260-P2-C-CDCl₃

```

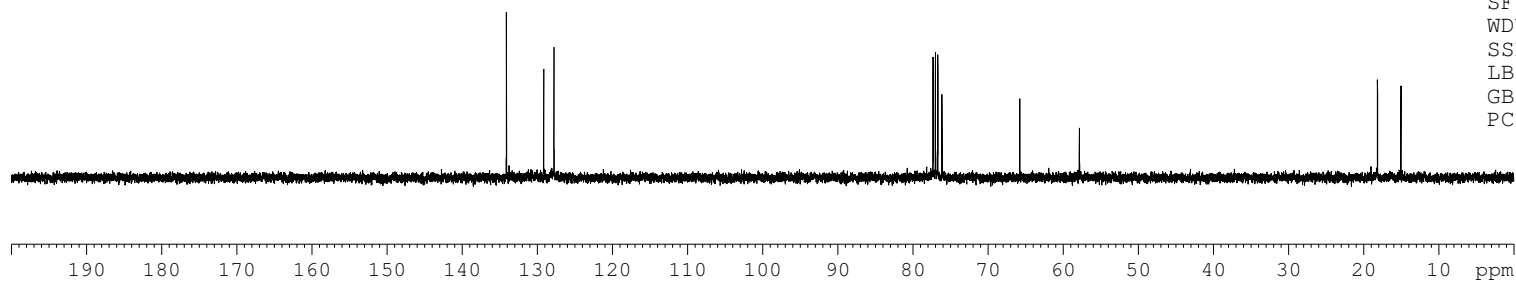
NAME      wrx0260-P2-C-CDCl3
EXPNO      1
PROCNO     1
Date_      20100302
Time       23.35
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgdc
TD         131072
SOLVENT    CDCl3
NS         36
DS         0
SWH        29761.904 Hz
FIDRES     0.227065 Hz
AQ         2.2020595 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE         295.7 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1       13C
P1         9.68 usec
PL1        -0.60 dB
PL1W       41.24164963 W
SFO1       100.6227690 MHz
  
```

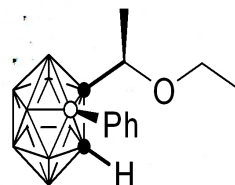
```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        0.00 dB
PL12       15.66 dB
PL2W       8.31434441 W
PL12W      0.22585411 W
SFO2       400.1320007 MHz
SI         131072
SF         100.6127718 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



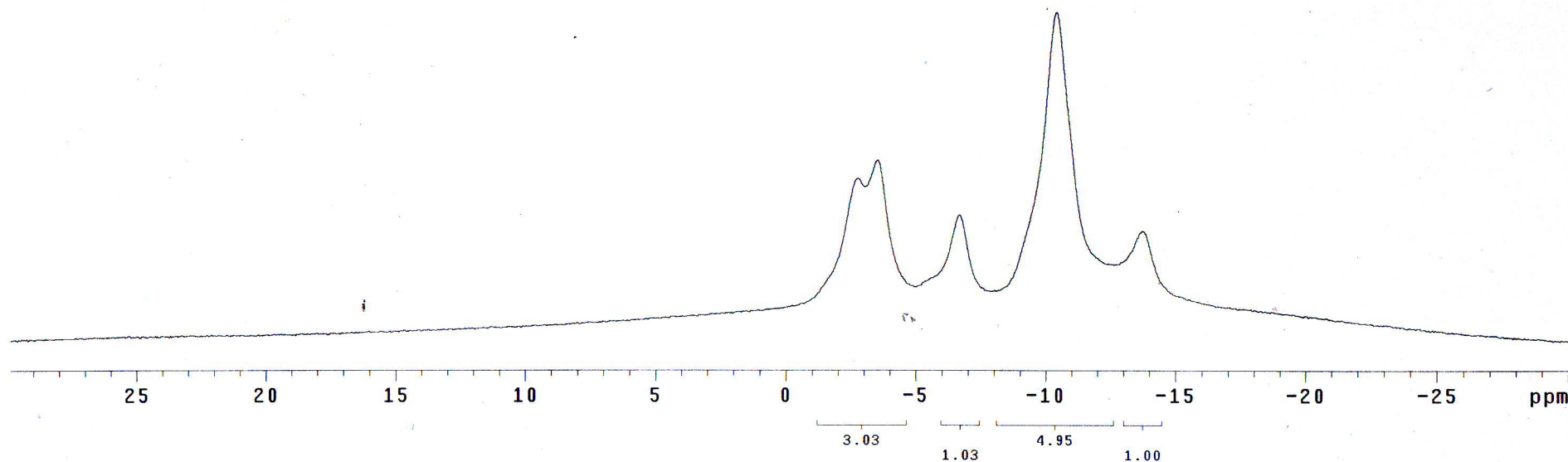
exp1 s2pul

SAMPLE		DEC. & VT	
date	Mar 6 2010	dfrq	399.951
solvent	CDC13	dn	H1
file	exp	dpwr	40
ACQUISITION		PROCESSING	
sfrq	128.317	dm	yyv
tn	B11	dmm	g
at	0.655	dmf	11765
np	65536	lb	3.00
sw	50000.0	wtfile	
fb	28000	proc	ft
bs	52	fn	not used
tpwr	7.0		
pw	1.000	werr	
d1	0	wexp	
tof	200	wbs	
nt	0	wnt	
ct	0		
alock	n		
gain	40		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-3888.1		
wp	7725.8		
vs	386		
sc	0		
wc	250		
hzmm	30.90		
is	500.00		
rfl	26821.2		
rfp	0		
th	6		
ins	1.000		
ai	ph		



(R,R)-6ba

-2.759
-3.544
-6.683
-10.370
-13.735



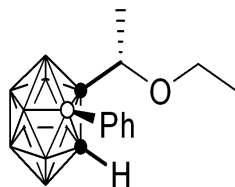
7.585
7.569
7.421
7.413
7.404
7.396
7.378
7.361
7.356
7.260

4.407

3.401
3.385
3.369
3.354
3.223
3.205
3.201
3.184

2.282
2.264
2.246
2.243
2.225
2.208

1.563
1.251
1.235
0.926
0.909
0.891

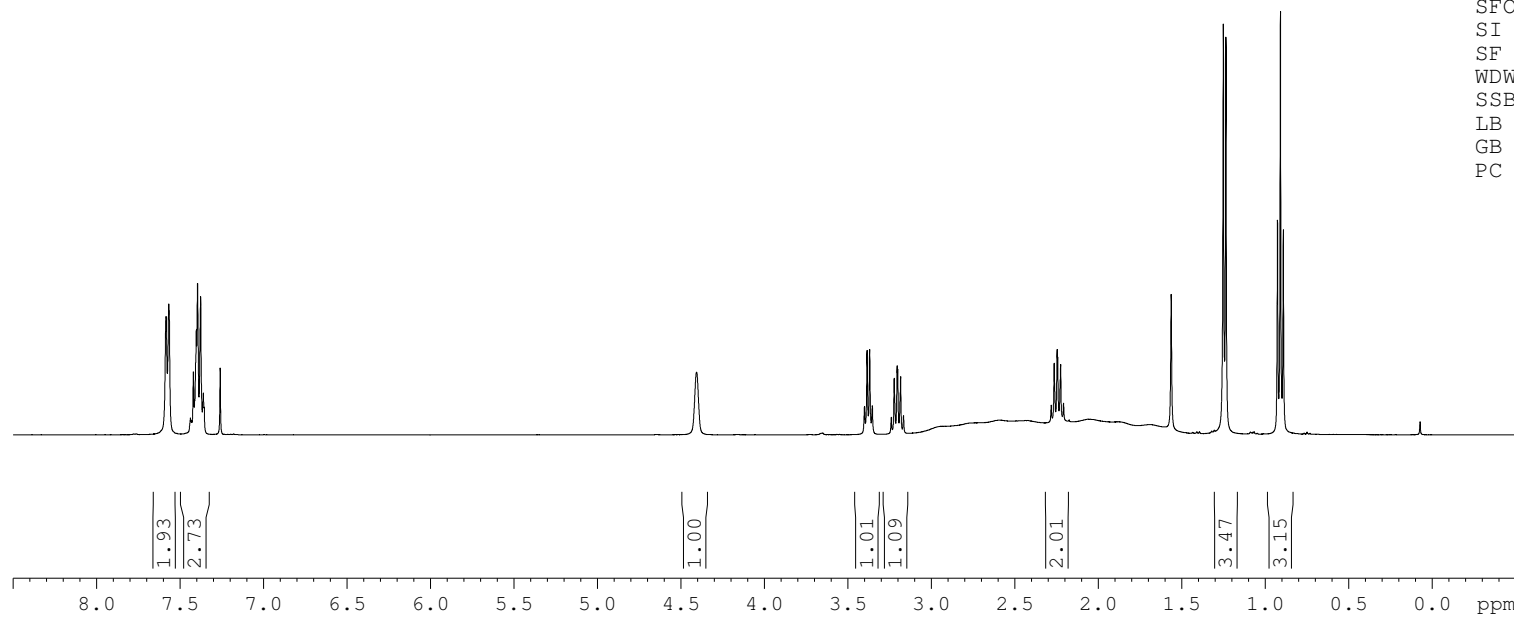


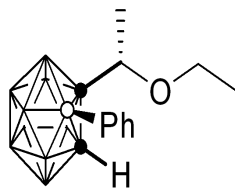
(R,S)-6ba

wrx0260-P1-H-CDC13

NAME wrx0260-P1-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100303
Time 0.00
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PL1 0.00 dB
PL1W 8.31434441 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



**(R,S)-6ba**

— 133.772
— 129.584
— 128.081

77.319
77.001
76.682
72.078
— 64.551
— 58.235

— 19.025
— 14.843

wrx0260-P1-C-CDCl₃

```

NAME      wrx0260-P1-C-CDCl3
EXPNO      1
PROCNO     1
Date_      20100302
Time       23.43
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgdc
TD         131072
SOLVENT    CDCl3
NS         60
DS         0
SWH        29761.904 Hz
FIDRES     0.227065 Hz
AQ         2.2020595 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE         295.6 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

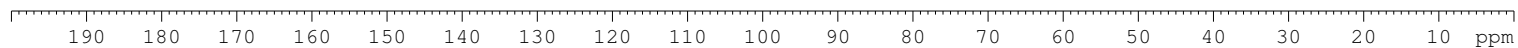
===== CHANNEL f1 =====
NUC1       13C
P1         9.68 usec
PL1        -0.60 dB
PL1W       41.24164963 W
SFO1       100.6227690 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        0.00 dB
PL12       15.66 dB
PL2W       8.31434441 W
PL12W      0.22585411 W
SFO2       400.1320007 MHz
SI         131072
SF         100.6127707 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

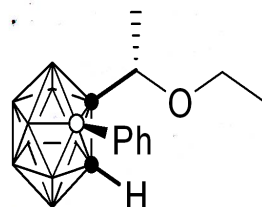
```



wrx0260-P1-B-CDC13

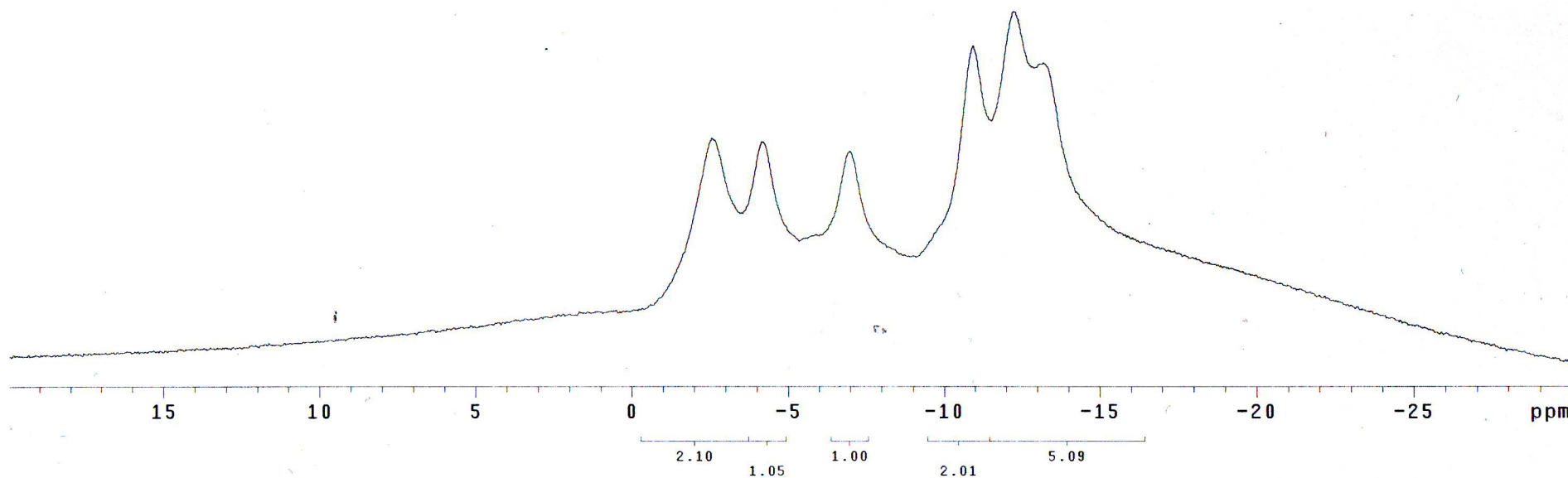
exp1 s2pu1

SAMPLE		DEC. & VT	
date	Mar 3 2010	dfrq	399.951
solvent	CDC13	dn	H1
file	exp	dpwr	40
ACQUISITION			
sfrq	128.317	dof	0
tn	B11	dm	yyy
at	0.655	dmm	g
np	65536	dmf	11765
sw	50000.0	PROCESSING	
fb	28000	lb	3.00
bs	4	wtfile	
tpwr	52	proc	ft
pw	7.0	fn	not used
d1	1.000	werr	
tof	0	wexp	
nt	200	wbs	
ct	0	wnt	
alock	n		
gain	40		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-3871.3		
wp	6433.3		
vs	1412		
sc	0		
wc	250		
hzmm	25.73		
is	500.00		
rfl	26821.2		
rfp	0		
th	8		
ins	1.000		
ai	ph		

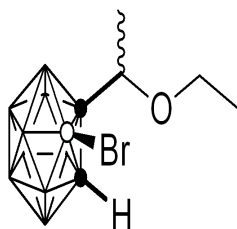


(R,S)-6ba

-2.557
-4.150
-6.969
-10.893
-12.201
-13.164



— 7.260

**6ca**

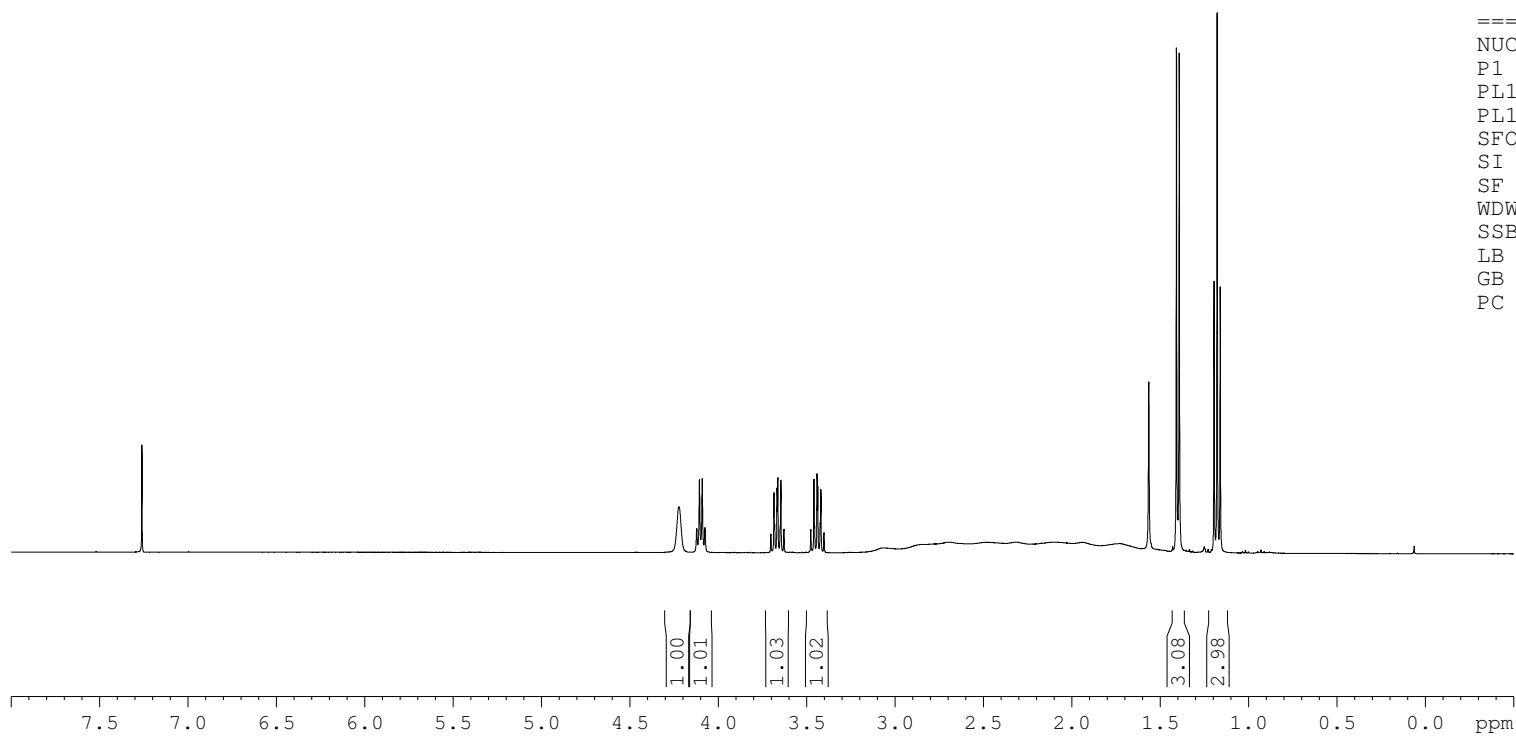
4.224
4.123
4.107
4.092
4.076
3.703
3.686
3.681
3.668
3.664
3.651
3.647
3.629
3.477
3.459
3.455
3.442
3.438
3.424
3.420
3.403

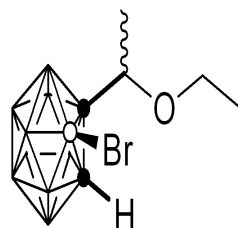
1.565
1.408
1.393
1.196
1.178
1.161

wrx0266-1-1-H-CDC13

NAME wrx0266-1-1-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100307
Time 15.27
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





6ca

78.027
77.316
76.999
76.681
73.183
65.299
61.880

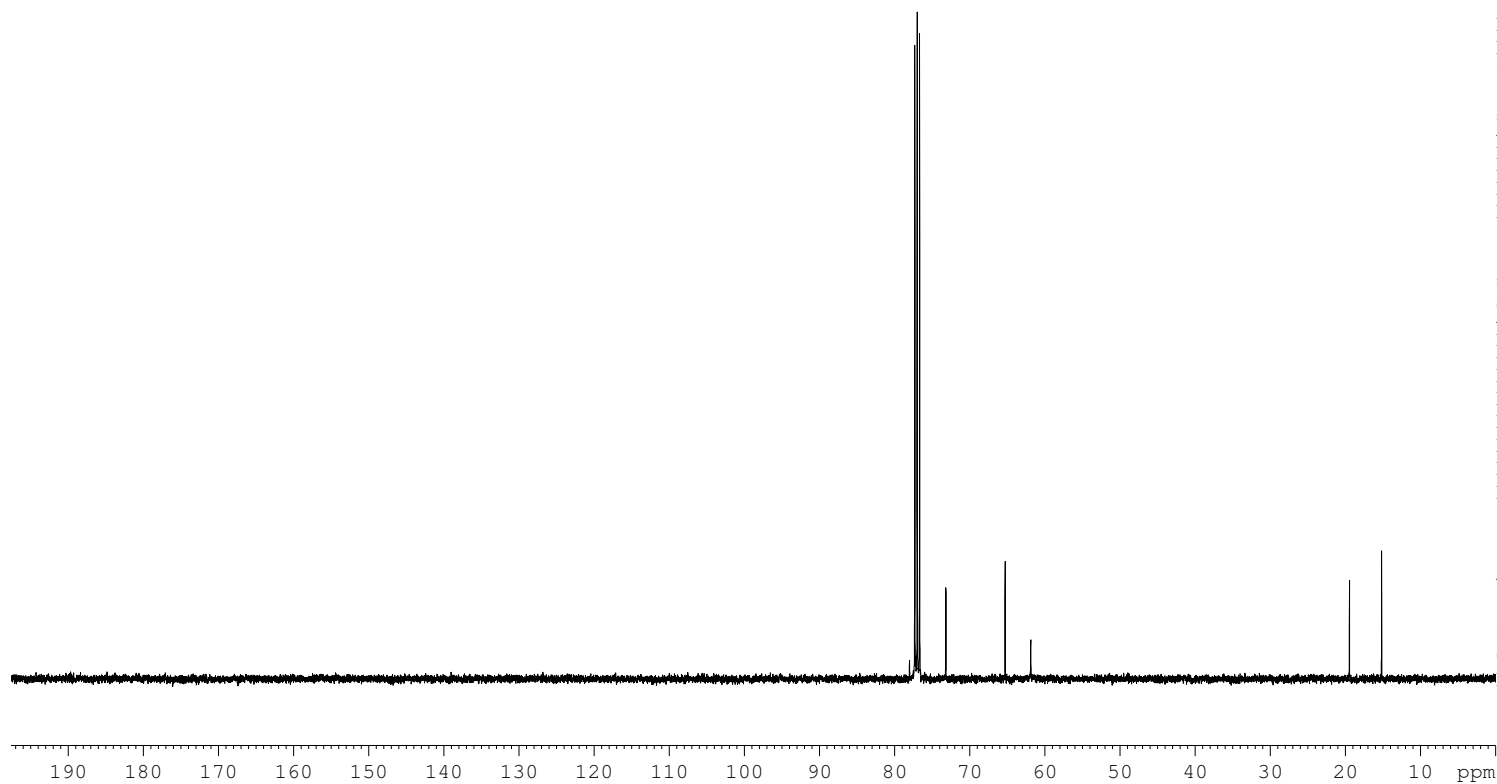
19.453
15.178

wrx0266-1-1-C-CDC13

NAME wrx0266-1-1-C-CDC13
EXPNO 1
PROCNO 1
Date_ 20100307
Time 15.30
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 390
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

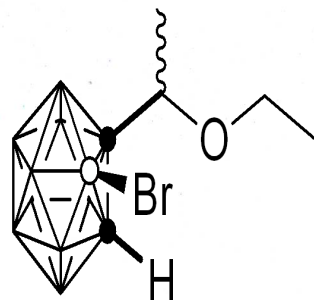
===== CHANNEL f1 =====
NUC1 13C
P1 9.68 usec
PL1 -0.60 dB
PL1W 41.24164963 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 15.66 dB
PL13 15.92 dB
PL2W 8.31434441 W
PL12W 0.22585411 W
PL13W 0.21272963 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127707 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



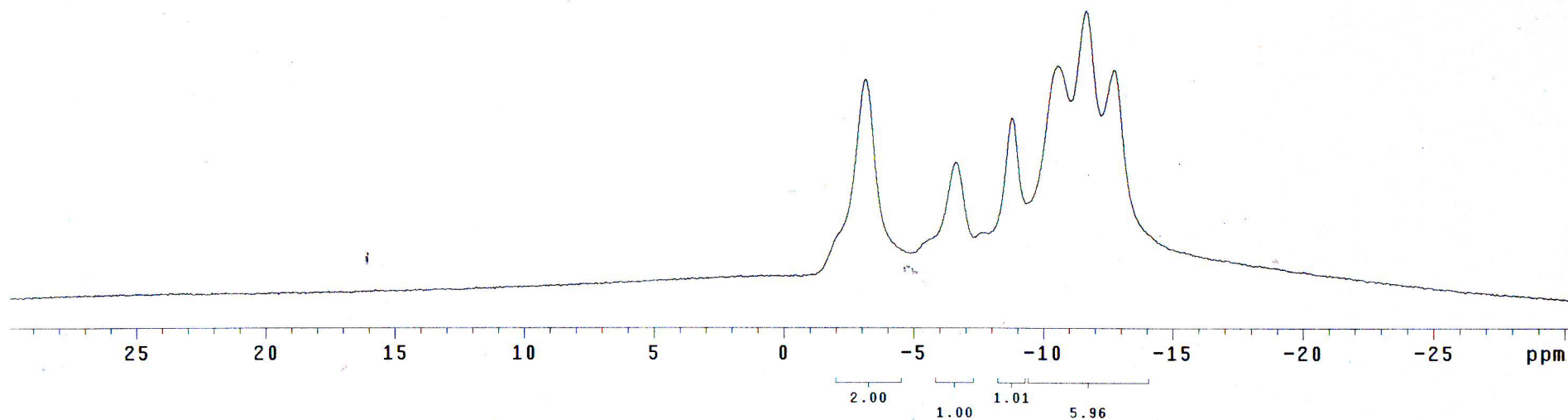
exp1 s2pul

SAMPLE		DEC. & VT	
date	Mar 6 2010	dfrq	399.951
solvent	CDC13	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	128.317	dm	yyy
tn	811	dmm	g
at	0.655	dmf	11765
np	65536	PROCESSING	
sw	50000.0	lb	3.00
fb	28000	wtfile	
bs	4	proc	ft
tpwr	52	fn	not used
pw	7.0		
d1	1.000	werr	
tof	0	wexp	
nt	200	wbs	
ct	0	wnt	
alock	n		
gain	40		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-3888.1		
wp	7725.8		
vs	323		
sc	0		
wc	250		
hzmm	30.90		
is	500.00		
rfl	26821.2		
rfp	0		
th	20		
ins	1.000		
ai	ph		

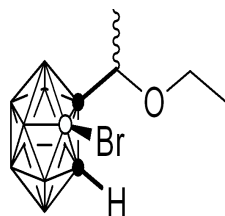


6ca

-3.128
-6.600
-8.764
-10.524
-11.618
-12.700



— 7.260

**6ca'**

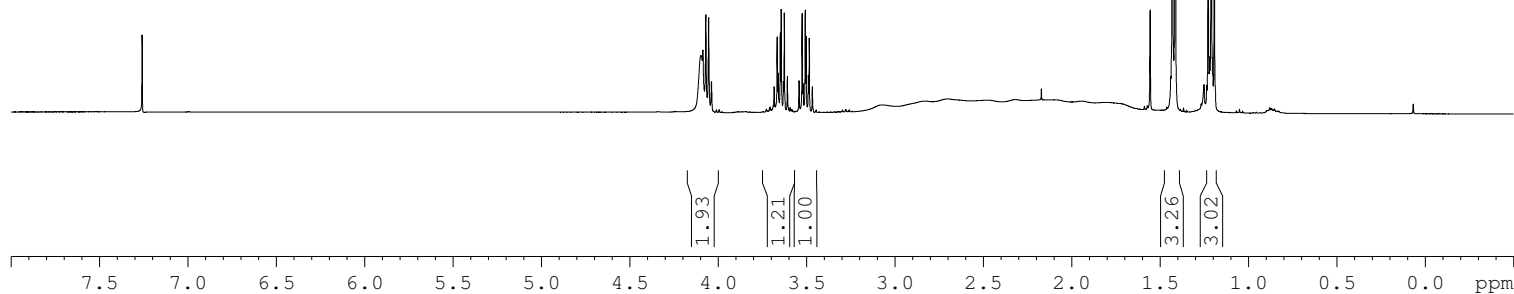
4.098
4.087
4.071
4.055
4.039
3.684
3.667
3.662
3.649
3.644
3.632
3.627
3.609
3.543
3.526
3.521
3.508
3.503
3.491
3.485
3.468

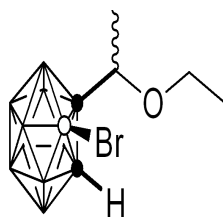
1.557
1.431
1.414
1.229
1.211
1.194

wrx0266-2-H-CDC13

NAME wrx0266-2-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100306
Time 17.06
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





6ca'

77.567
77.318
77.000
76.683
76.403
— 66.485
— 61.759

— 18.592
— 15.081

wrx0266-2-C-CDC13

```

NAME      wrx0266-2-C-CDC13
EXPNO     1
PROCNO    1
Date_     20100306
Time      17.14
INSTRUM   spect
PROBHD    5 mm PADUL 13C
PULPROG   zgdc
TD         131072
SOLVENT   CDC13
NS         217
DS         0
SWH        29761.904 Hz
FIDRES     0.227065 Hz
AQ         2.2020595 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE         295.5 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

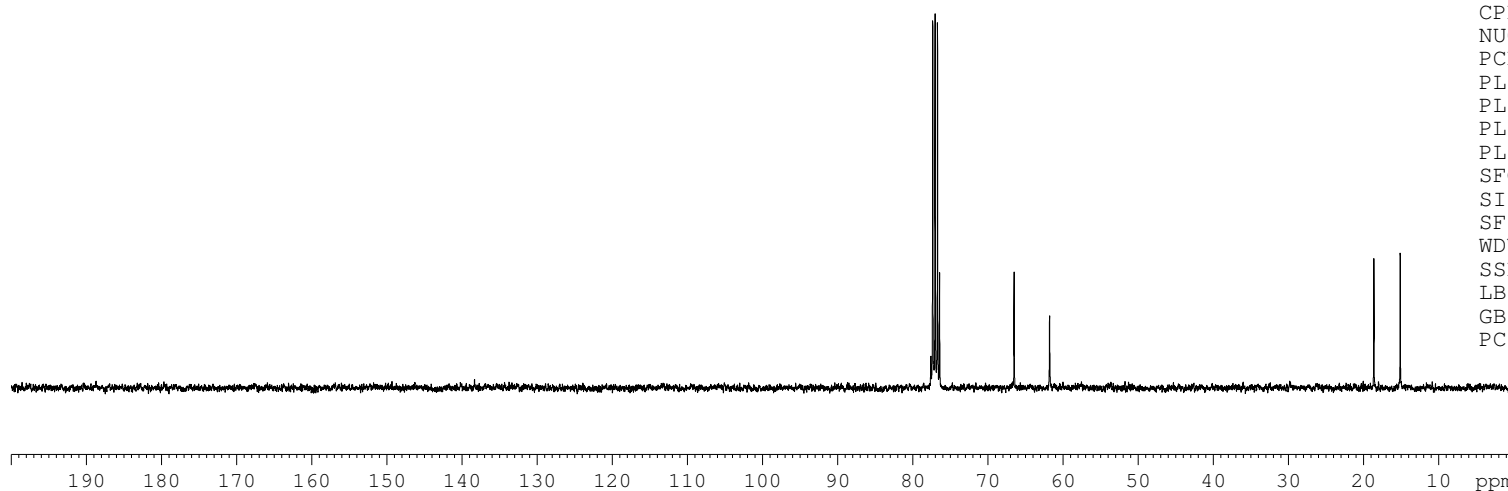
===== CHANNEL f1 =====
NUC1      13C
P1         3.50 usec
PL1        -0.60 dB
PL1W       41.24164963 W
SFO1      100.6227690 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      90.00 usec
PL2         0.00 dB
PL12        16.10 dB
PL2W       8.31434441 W
PL12W      0.20409293 W
SFO2      400.1320007 MHz
SI         131072
SF         100.6127711 MHz
WDW        EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40

```

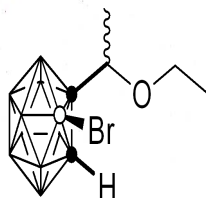


wrx0266-2-B-CDC13

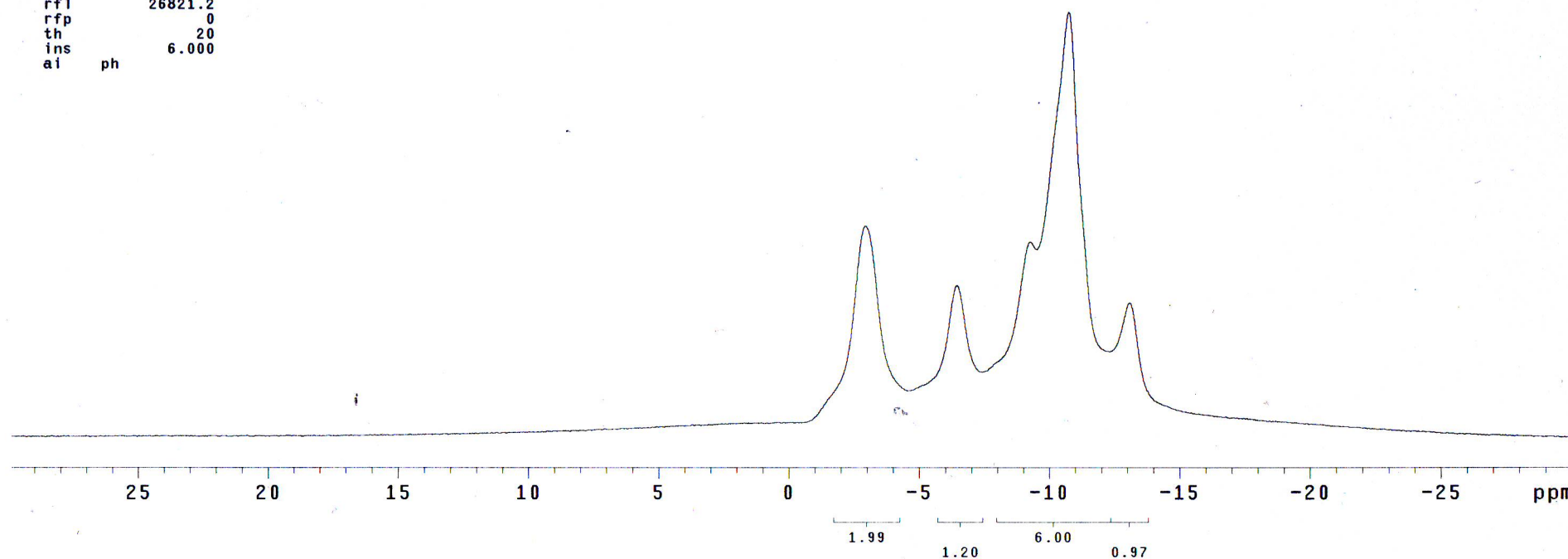
S99

exp1 s2pu1

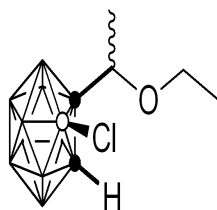
SAMPLE		DEC. & VT	
date	Mar 6 2010	dfrq	399.951
solvent	CDC13	dn	H1
file	/export/home/~	dpwr	40
wrx/wrx0266-2-B-CD~		dof	0
C13.fid		dm	yyy
ACQUISITION		dmm	g
sfrq	128.317	dmf	11765
tn	811	PROCESSING	
at	0.655	lb	3.00
np	65536	wtfile	
sw	50000.0	proc	ft
fb	28000	fn	not used
bs	4		
tpwr	52	werr	
pw	7.0	wexp	
d1	1.000	wbs	
tof	0	wnt	
nt	200		
ct	0		
alock	n		
gain	40		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-3888.1		
wp	7725.8		
vs	196		
sc	0		
wc	250		
hzmm	30.90		
is	500.00		
rfl	26821.2		
rfp	0		
th	20		
ins	6.000		
ai	ph		



6ca'



— 7.260

**6da**

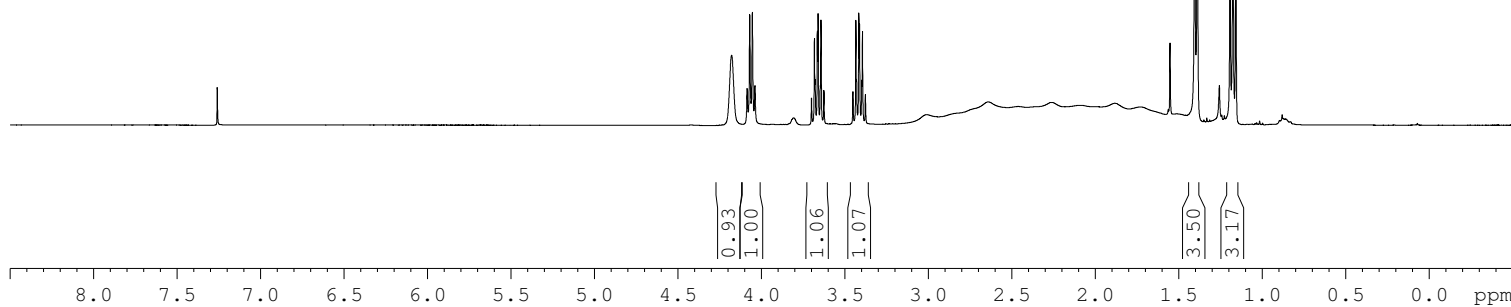
4.178
4.086
4.070
4.054
4.039
3.700
3.683
3.678
3.665
3.661
3.648
3.643
3.626
3.452
3.434
3.430
3.417
3.412
3.399
3.395
3.377

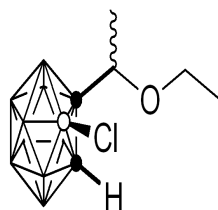
1.405
1.389
1.193
1.175
1.158

wrx0319-1-H-CDC13

NAME wrx0319-1-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100509
Time 14.49
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 25.4
DW 62.400 usec
DE 6.50 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





6da

78.352
77.318
77.001
76.683
72.168
65.377
61.459

19.327
15.160

wrx0319-1-C-CDC13

```

NAME      wrx0319-1-C-CDC13
EXPNO     1
PROCNO    1
Date_     20100509
Time      15.27
INSTRUM   spect
PROBHD    5 mm PABBI 1H/
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         120
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         295.1 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

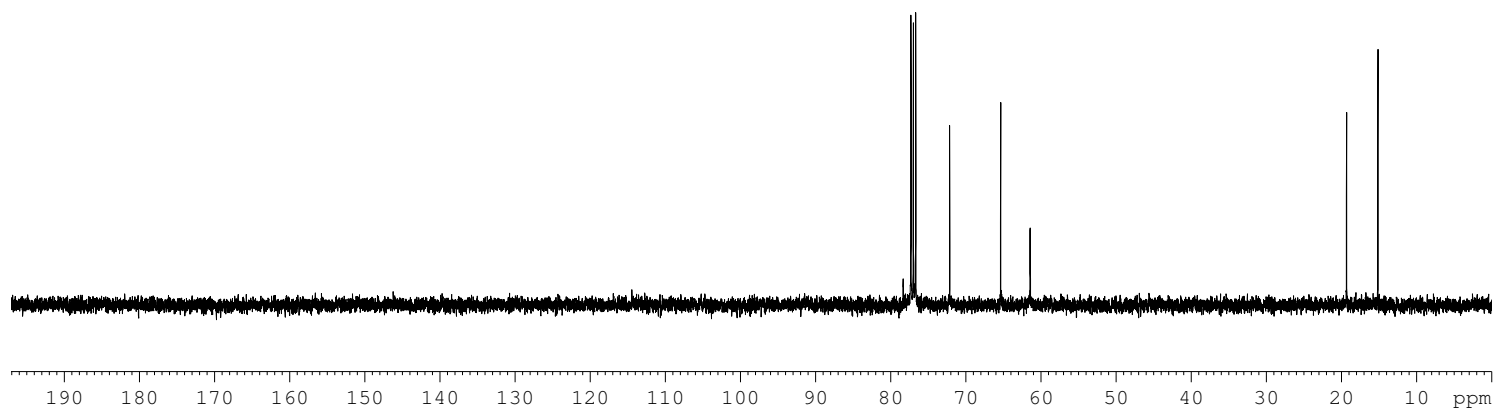
===== CHANNEL f1 =====
NUC1       13C
P1         14.50 usec
PL1        -4.00 dB
PL1W       90.22689819 W
SFO1       100.6228298 MHz

```

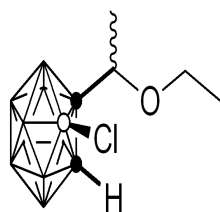
```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -2.00 dB
PL12       18.80 dB
PL13       18.80 dB
PL2W       13.17734718 W
PL12W      0.10960442 W
PL13W      0.10960442 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127711 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



S102



6da

— -4.237
— -4.990

— -8.723

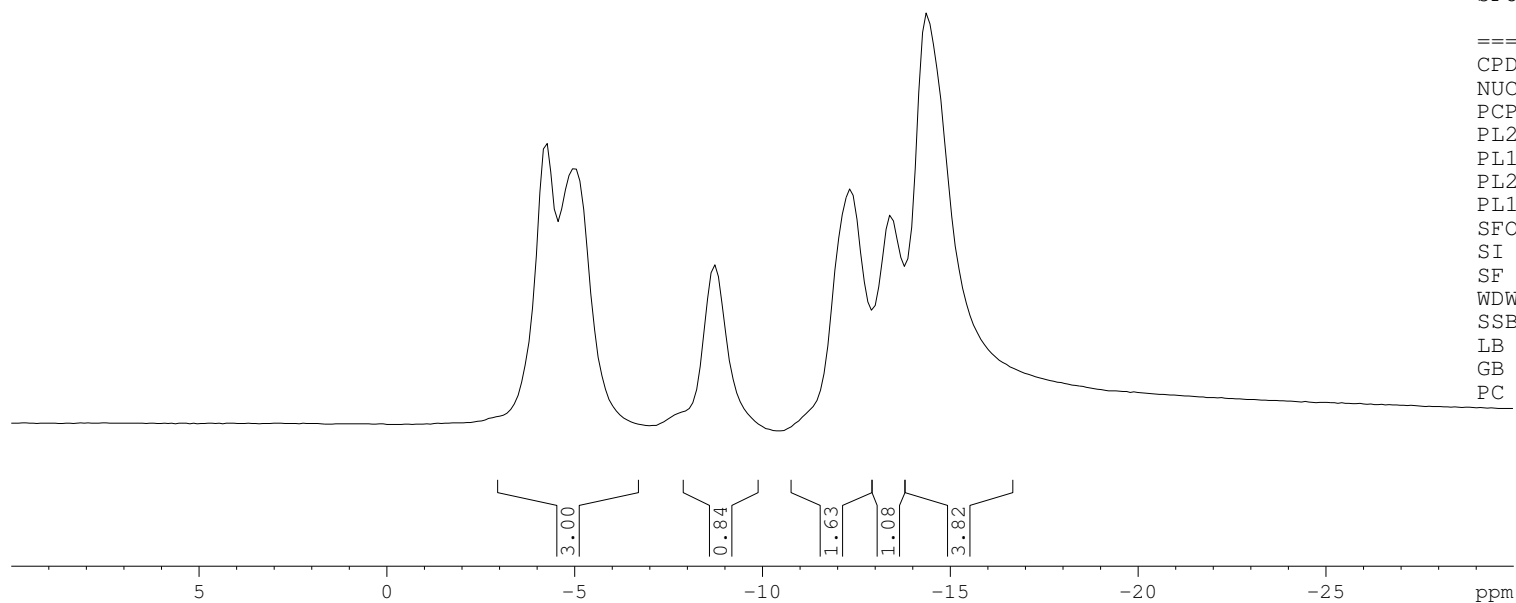
— -12.329
— -13.411
— -14.374

wrx0319-1-B-CDC13

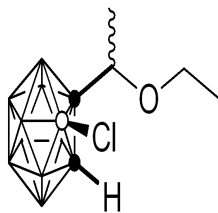
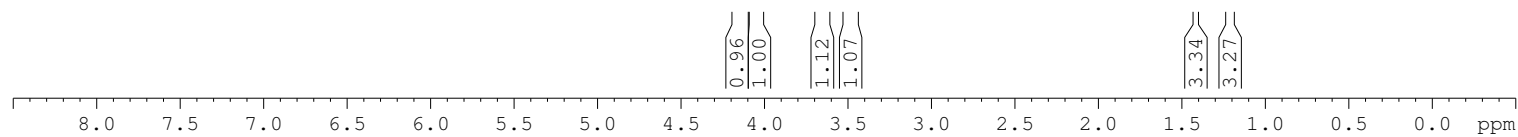
NAME wrx0319-1-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100510
Time 12.03
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgdc
TD 4000
SOLVENT CDC13
NS 62
DS 4
SWH 25510.203 Hz
FIDRES 6.377551 Hz
AQ 0.0784500 sec
RG 203
DW 19.600 usec
DE 6.50 usec
TE 294.3 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 14.50 usec
PL1 -4.00 dB
SFO1 128.3776076 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.80 dB
PL2W 13.17734718 W
PL12W 0.10960442 W
SFO2 400.1316005 MHz
SI 2048
SF 128.3776263 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



— 7.260

**6da'**

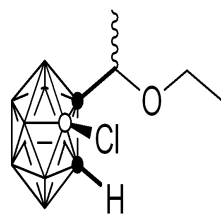
4.139
4.072
4.055
4.039
4.023
3.690
3.672
3.667
3.655
3.650
3.637
3.632
3.615
3.521
3.503
3.499
3.486
3.481
3.469
3.463
3.446

1.421
1.405
1.228
1.210
1.193

wrx0319-2-H-CDC13

NAME wrx0319-2-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100509
Time 15.21
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 9
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300057 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



6da'

77.783
77.319
77.001
76.684
76.037
— 66.449
— 61.419

— 18.470
— 15.081

wrx0319-2-C-CDC13

```

NAME      wrx0319-2-C-CDC13
EXPNO      1
PROCNO     1
Date_      20100509
Time       15.18
INSTRUM    spect
PROBHD     5 mm PABBI 1H/
PULPROG    zgpg30
TD         65536
SOLVENT    CDC13
NS         48
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         294.9 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

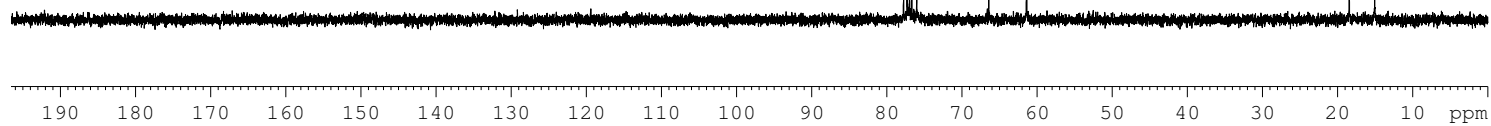
===== CHANNEL f1 =====
NUC1       13C
P1         14.50 usec
PL1        -4.00 dB
PL1W       90.22689819 W
SFO1       100.6228298 MHz

```

```

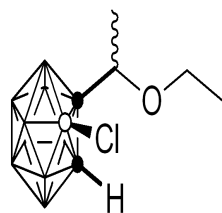
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -2.00 dB
PL12       18.80 dB
PL13       18.80 dB
PL2W       13.17734718 W
PL12W      0.10960442 W
PL13W      0.10960442 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127729 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



S105

wrx0319-2-B-CDC13

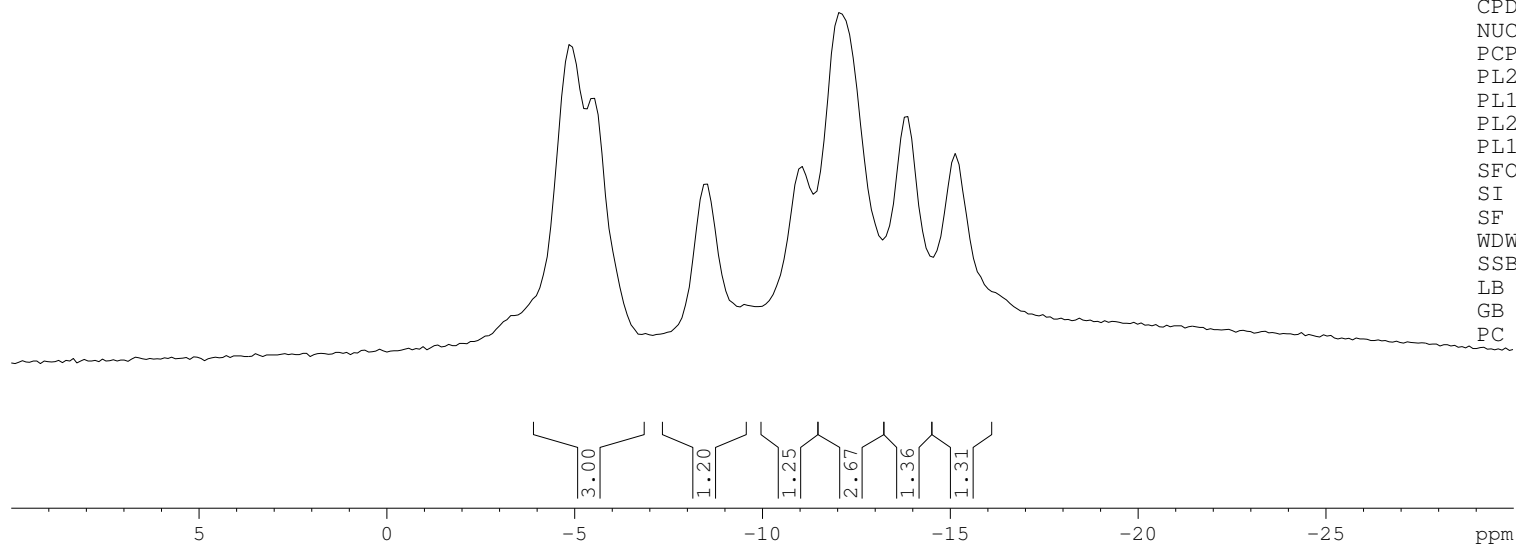
**6da'**

— -4.887
— -8.492
— -11.036
— -12.070
— -13.830
— -15.132

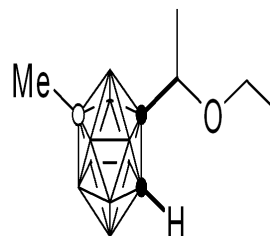
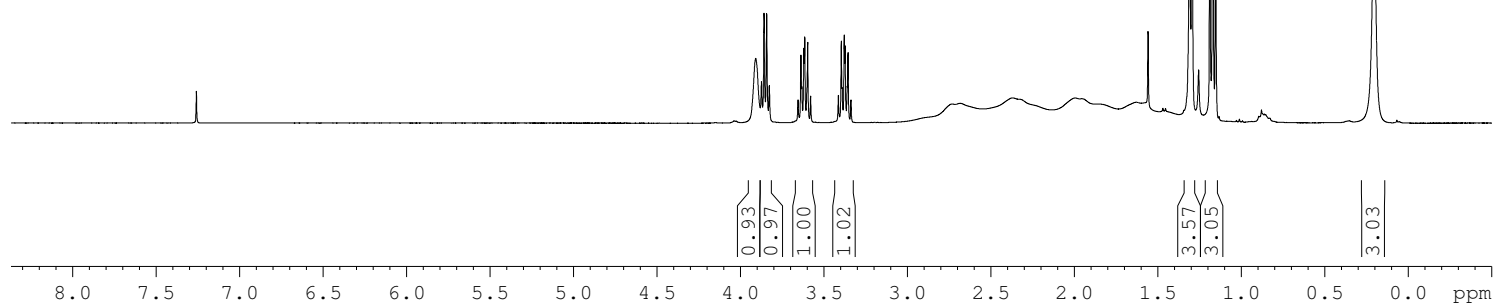
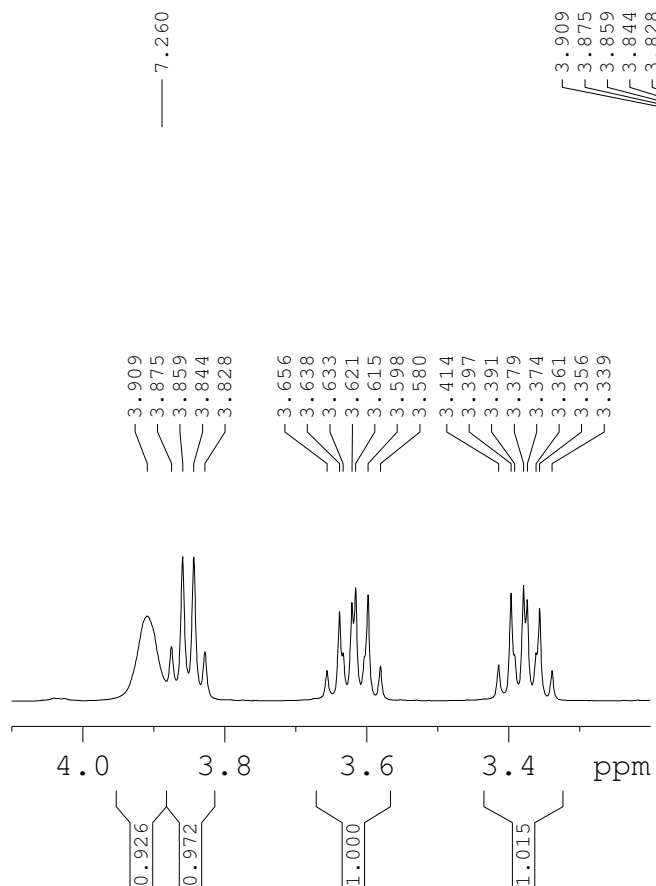
NAME wrx0319-2-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100510
Time 12.04
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgdc
TD 4000
SOLVENT CDC13
NS 116
DS 4
SWH 25510.203 Hz
FIDRES 6.377551 Hz
AQ 0.0784500 sec
RG 203
DW 19.600 usec
DE 6.50 usec
TE 294.3 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 14.50 usec
PL1 -4.00 dB
SFO1 128.3776076 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.80 dB
PL2W 13.17734718 W
PL12W 0.10960442 W
SFO2 400.1316005 MHz
SI 2048
SF 128.3776263 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

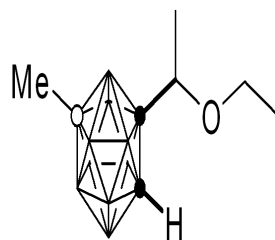


wrx0323-1-H-CDC13

*m*-6ea

NAME wrx0323-1-H-CDC13
 EXPNO 1
 PROCNO 1
 Date_ 20100515
 Time 16.29
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2768500 sec
 RG 28.5
 DW 50.000 usec
 DE 6.50 usec
 TE 294.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 -2.00 dB
 PL1W 13.17734718 W
 SFO1 400.1318000 MHz
 SI 65536
 SF 400.1300056 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



m-6ea

77.318
77.000
76.683
75.393
— 65.990
— 51.493

— 19.793
— 15.150

wrx0323-1-C-CDC13

```

NAME      wrx0323-1-C-CDC13
EXPNO     1
PROCNO    1
Date_     20100515
Time      16.33
INSTRUM   spect
PROBHD    5 mm PABBI 1H/
PULPROG   zgdc
TD         131072
SOLVENT   CDC13
NS         176
DS         0
SWH        29761.904 Hz
FIDRES     0.227065 Hz
AQ         2.2020595 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE         295.0 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

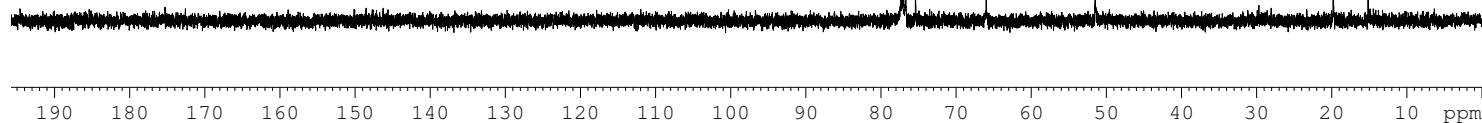
===== CHANNEL f1 =====
NUC1       13C
P1         3.50 usec
PL1        -0.60 dB
PL1W       41.24164963 W
SFO1       100.6227690 MHz

```

```

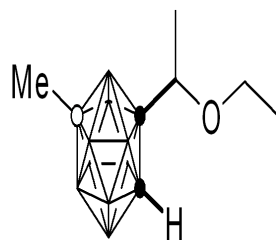
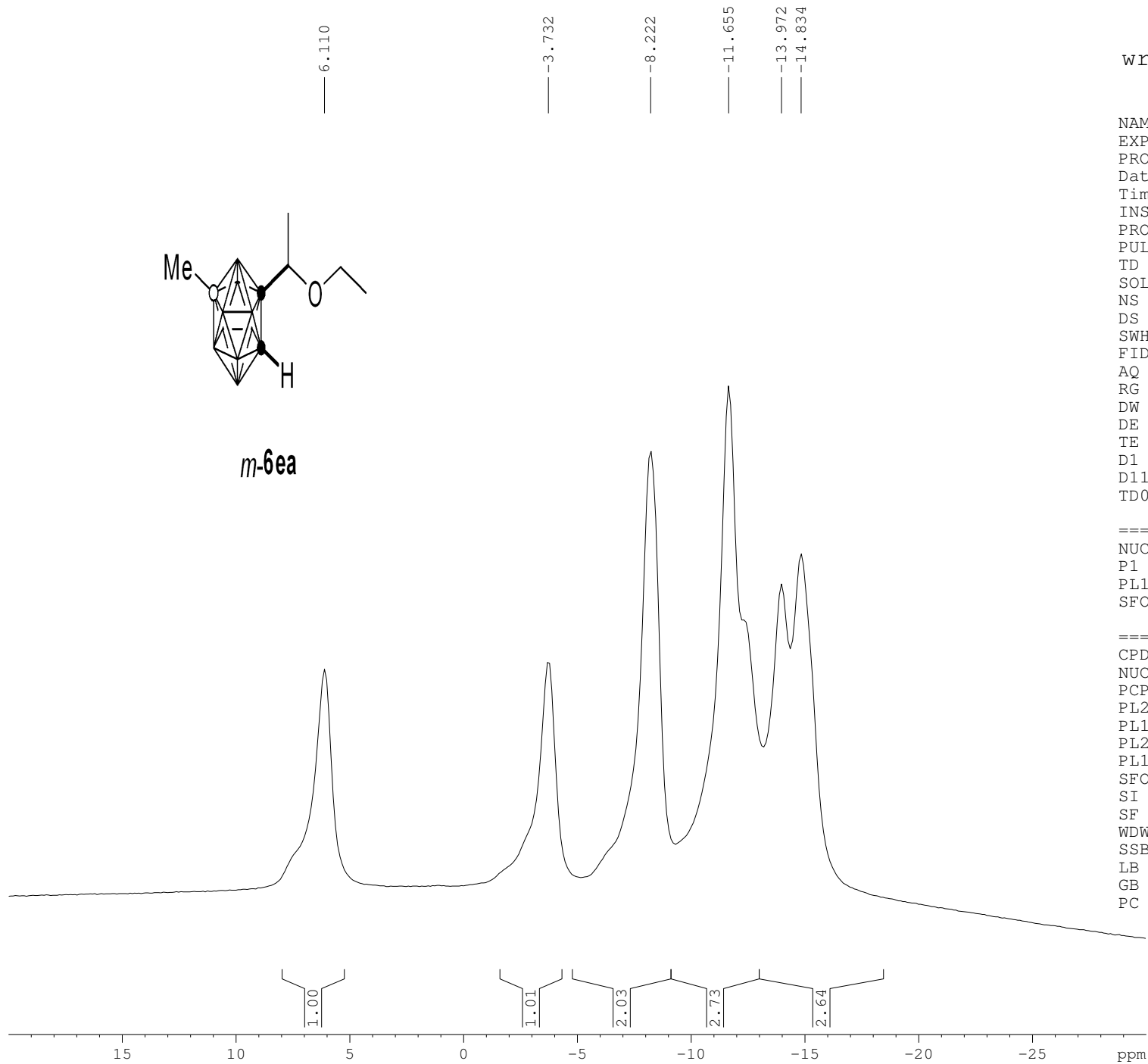
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2      90.00 usec
PL2         0.00 dB
PL12        16.10 dB
PL2W        8.31434441 W
PL12W       0.20409293 W
SFO2       400.1320007 MHz
SI          131072
SF         100.6127711 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40

```



S108

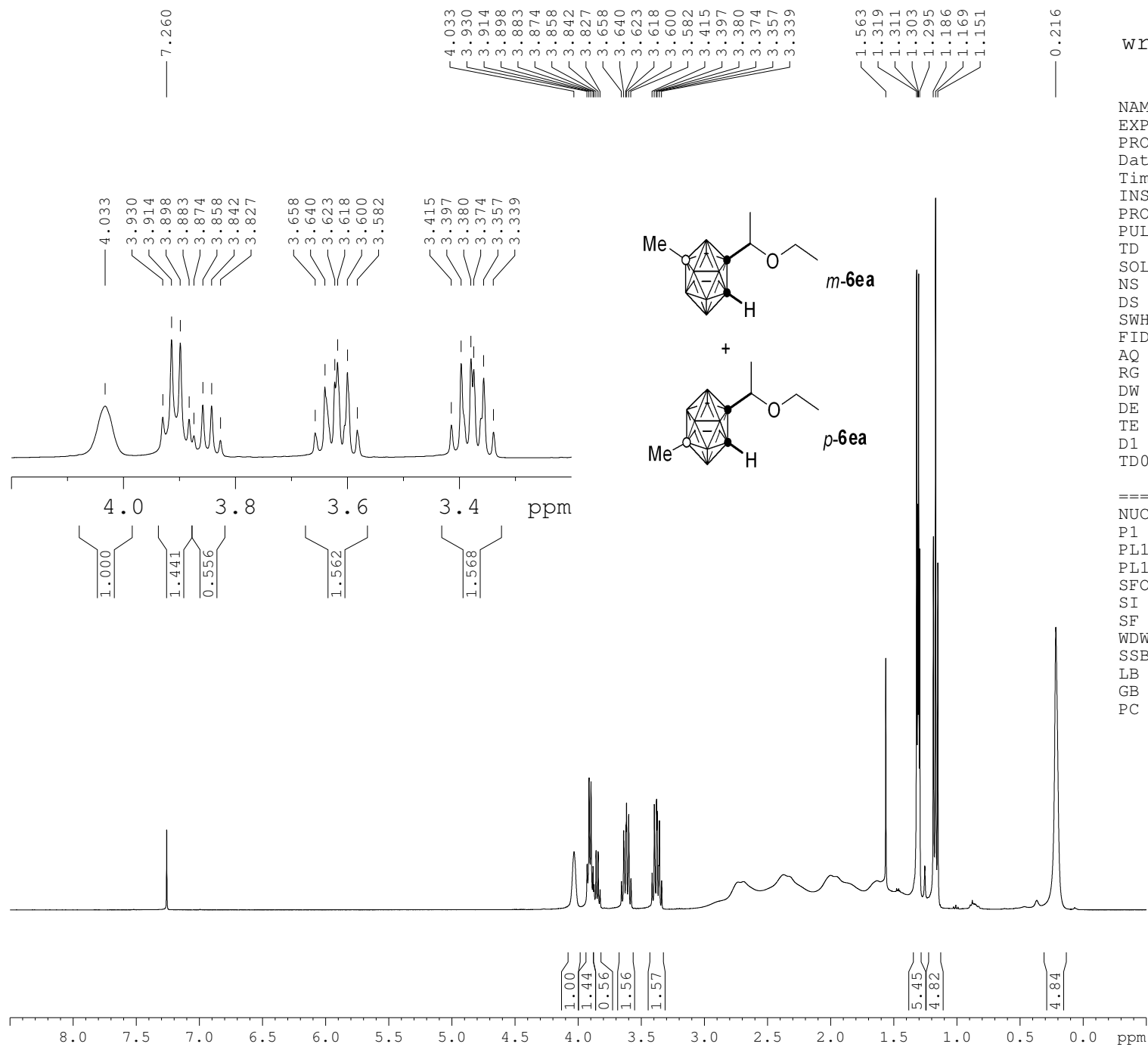
wrx0323-1-B-CDC13

*m*-6ea

NAME wrx0323-1-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100517
Time 11.59
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgdc
TD 4000
SOLVENT CDC13
NS 104
DS 4
SWH 25510.203 Hz
FIDRES 6.377551 Hz
AQ 0.0784500 sec
RG 203
DW 19.600 usec
DE 6.50 usec
TE 294.6 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 14.50 usec
PL1 -4.00 dB
SFO1 128.3776076 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.80 dB
PL2W 13.17734718 W
PL12W 0.10960442 W
SFO2 400.1316005 MHz
SI 2048
SF 128.3776263 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



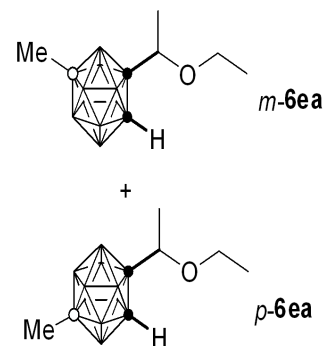
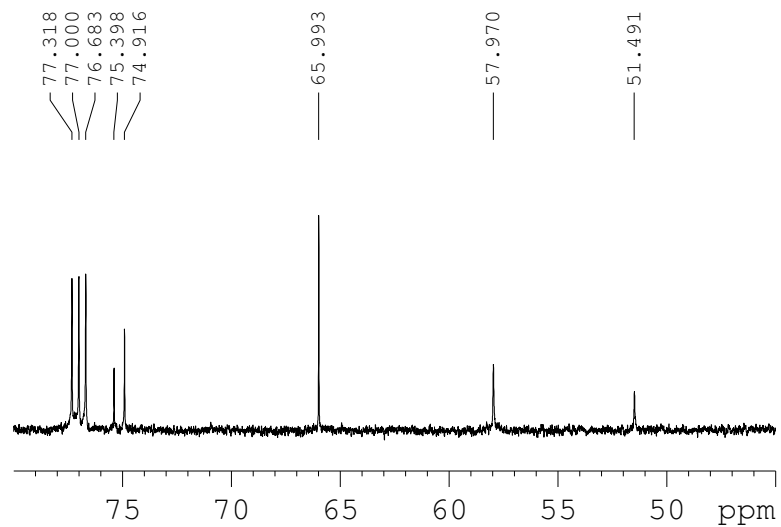
wrx0320-1-H-CDC13

NAME wrx0320-1-H-CDC13
 EXPNO 1
 PROCNO 1
 Date_ 20100525
 Time 17.59
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg
 TD 65536
 SOLVENT CDC13
 NS 13
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 28.5
 DW 62.400 usec
 DE 6.50 usec
 TE 294.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 -2.00 dB
 PL1W 13.17734718 W
 SFO1 400.1316005 MHz
 SI 65536
 SF 400.1300053 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

77.318
77.000
76.683
75.398
74.916
65.993
57.970
51.491
20.009
19.796
15.154

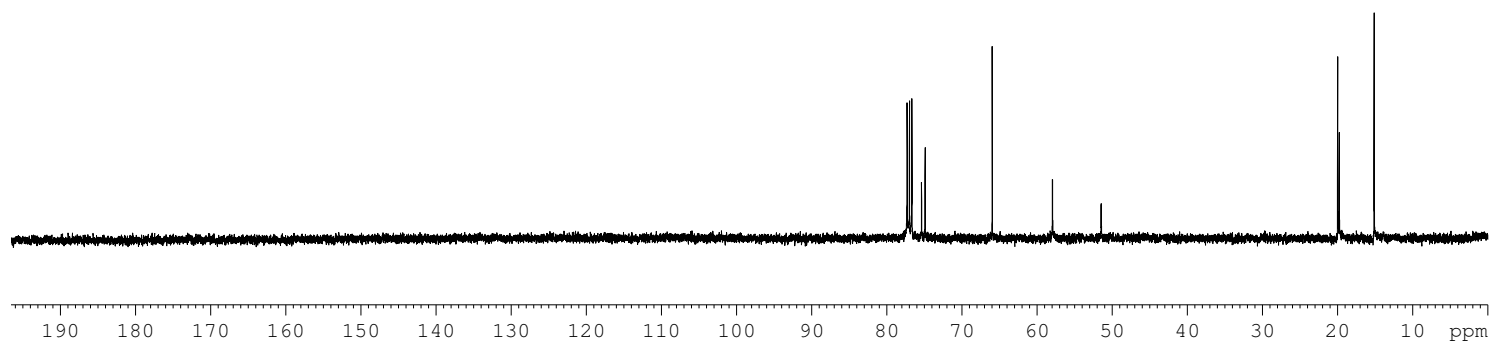
wrx0320-1-C-CDC13



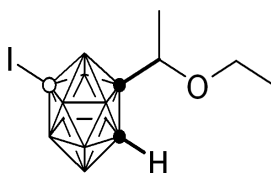
NAME wrx0320-1-C-CDC13
EXPNO 1
PROCNO 1
Date_ 20100525
Time 18.16
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgdc
TD 131072
SOLVENT CDC13
NS 803
DS 0
SWH 29761.904 Hz
FIDRES 0.227065 Hz
AQ 2.2020595 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 294.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 14.50 usec
PL1 -4.00 dB
PL1W 90.22689819 W
SFO1 100.6227690 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.80 dB
PL2W 13.17734718 W
PL12W 0.10960442 W
SFO2 400.1320007 MHz
SI 131072
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



— 7.260

*m*-6fa

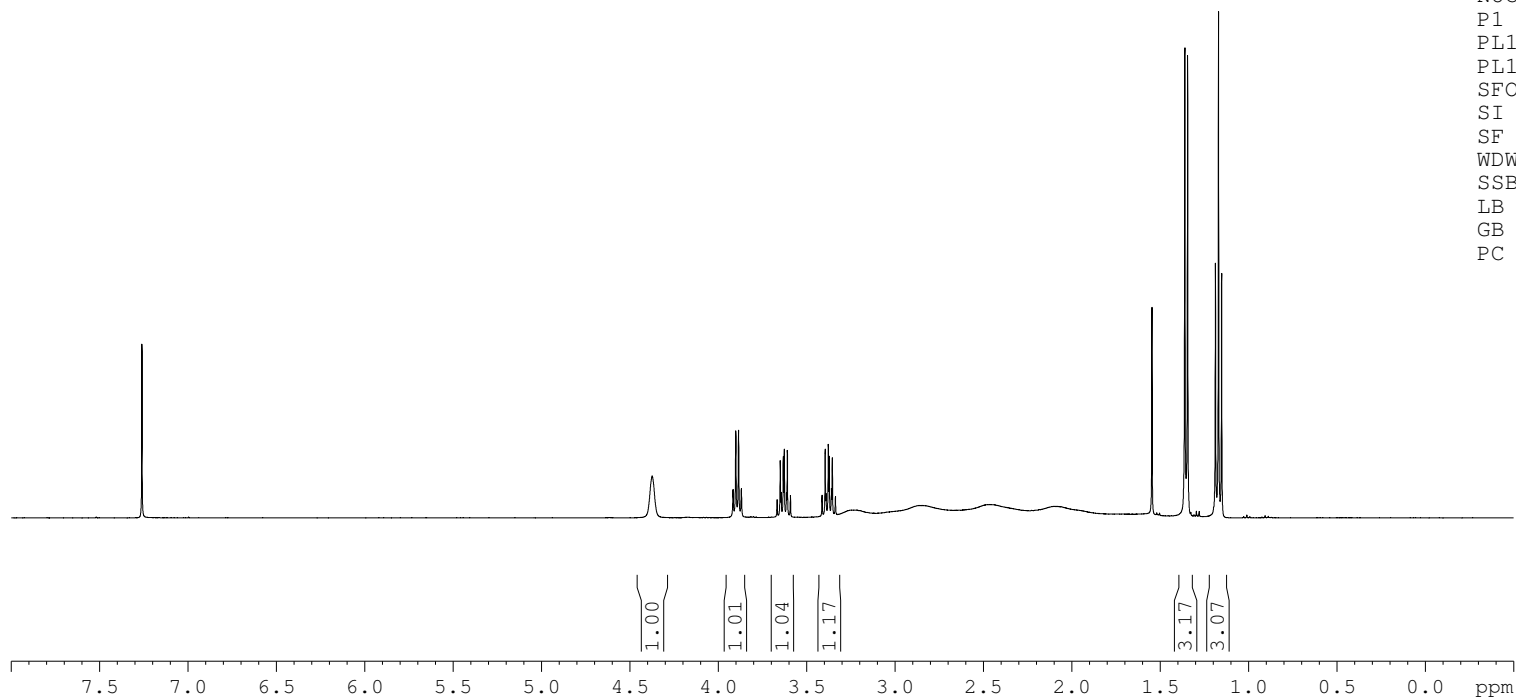
4.374
3.917
3.902
3.886
3.870
3.650
3.645
3.633
3.627
3.615
3.610
3.592
3.413
3.396
3.390
3.378
3.373
3.361
3.355

1.547
1.361
1.345
1.188
1.170
1.153

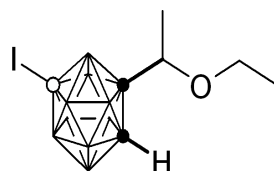
wrx0270-1r-H-CDC13

NAME wrx0270-1r-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100310
Time 12.49
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S112

*m*-6fa

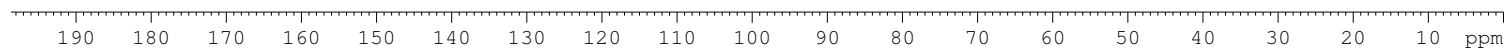
78.981
77.318
77.000
76.683
75.076
66.063
54.930
19.818
15.113

wrx0270-1b-C-CDCl3

NAME wrx0270-1b-C-CDCl3
EXPNO 1
PROCNO 1
Date_ 20100310
Time 1.08
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgdc
TD 131072
SOLVENT CDCl3
NS 444
DS 0
SWH 29761.904 Hz
FIDRES 0.227065 Hz
AQ 2.2020595 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 3.50 usec
PL1 -0.60 dB
PL1W 41.24164963 W
SFO1 100.6227690 MHz

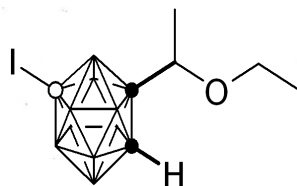
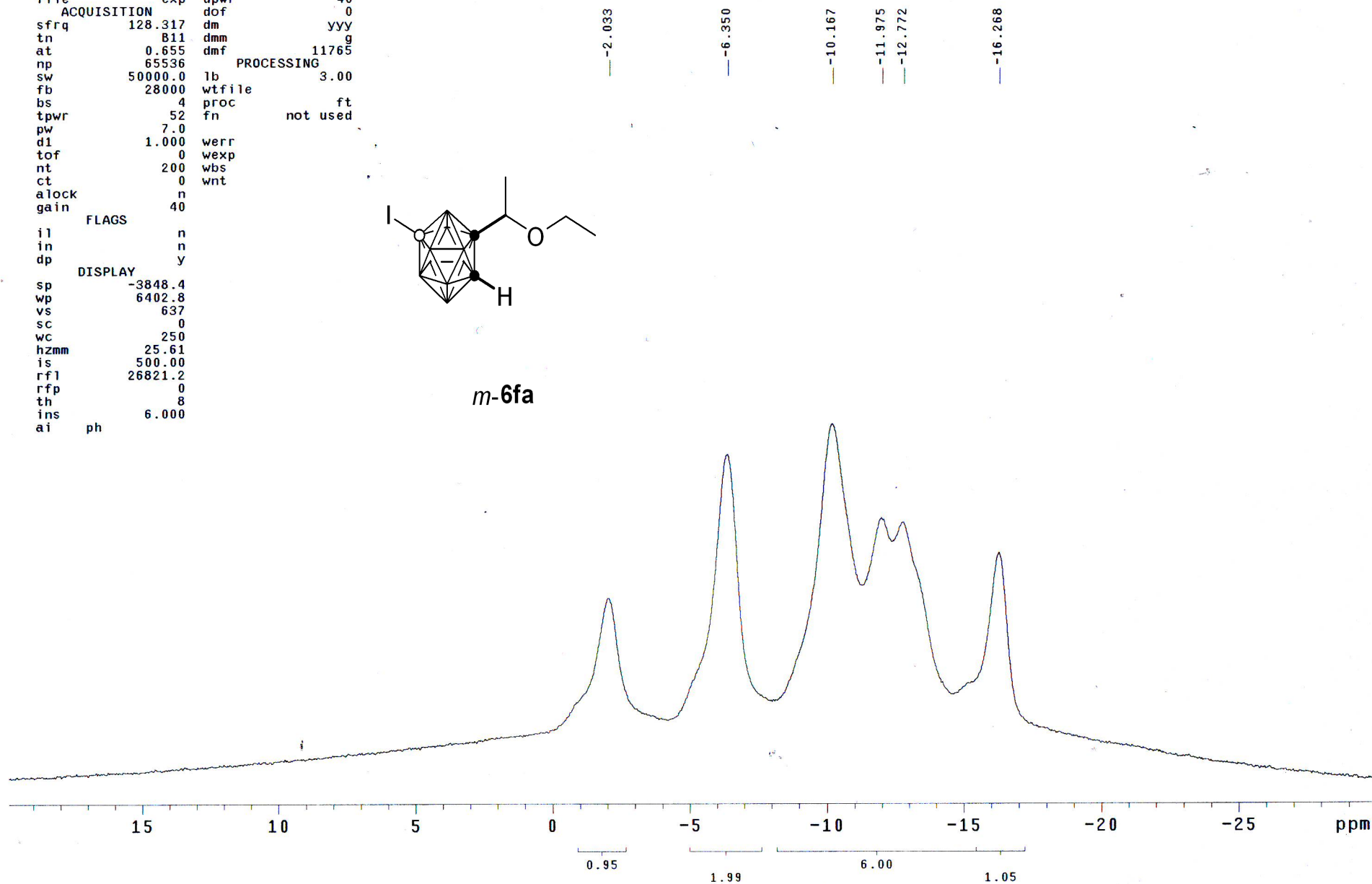
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL2W 8.31434441 W
PL12W 0.20409293 W
SFO2 400.1320007 MHz
SI 131072
SF 100.6127707 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



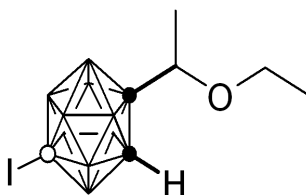
wrx0270-1b-B-CDC13

exp1 s2pu1

SAMPLE		DEC. & VT	
date	Mar 10 2010	dfrq	399.951
solvent	CDC13	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	128.317	dm	YYY
tn	B11	dmm	g
at	0.655	dmf	11765
np	65536	PROCESSING	
sw	50000.0	lb	3.00
fb	28000	wtfile	
bs	4	proc	ft
tpwr	52	fn	not used
pw	7.0		
d1	1.000	werr	
tof	0	wexp	
nt	200	wbs	
ct	0	wnt	
alock	n		
gain	40		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-3848.4		
wp	6402.8		
vs	637		
sc	0		
wc	250		
hzmm	25.61		
is	500.00		
rfl	26821.2		
rfl	0		
th	8		
ins	6.000		
ai	ph		

*m*-6fa

— 7.260

*p*-6fa

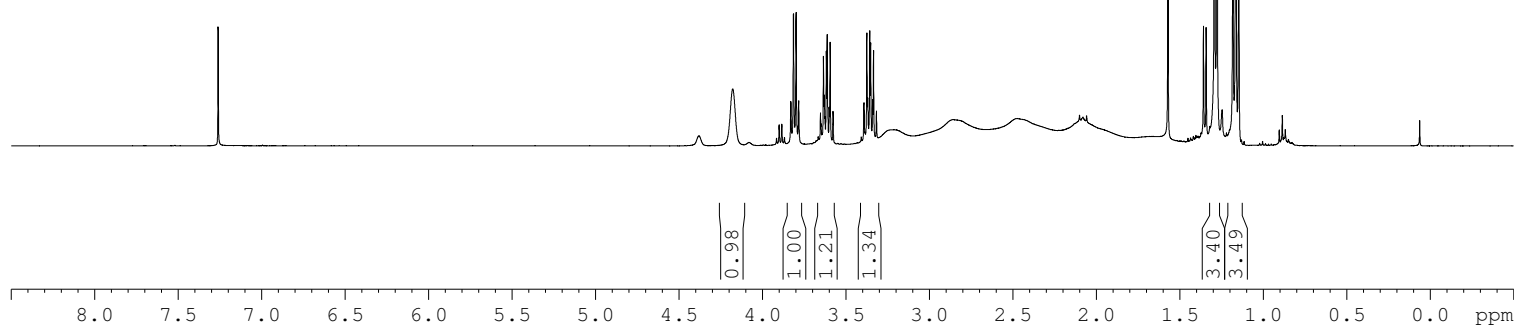
4.179
3.831
3.815
3.799
3.784
3.653
3.636
3.631
3.618
3.613
3.601
3.595
3.578
3.393
3.376
3.370
3.358
3.353
3.341
3.335
3.318

1.571
1.293
1.278
1.182
1.165
1.147

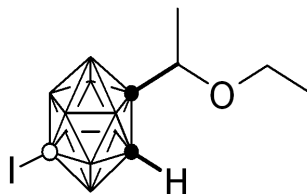
wrx0270-2-H-CDC13

NAME wrx0270-2-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100313
Time 16.36
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PL1 0.00 dB
PL1W 8.31434441 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S115

*p-6fa*

77.317
76.999
76.682
75.360
— 66.024
— 59.456

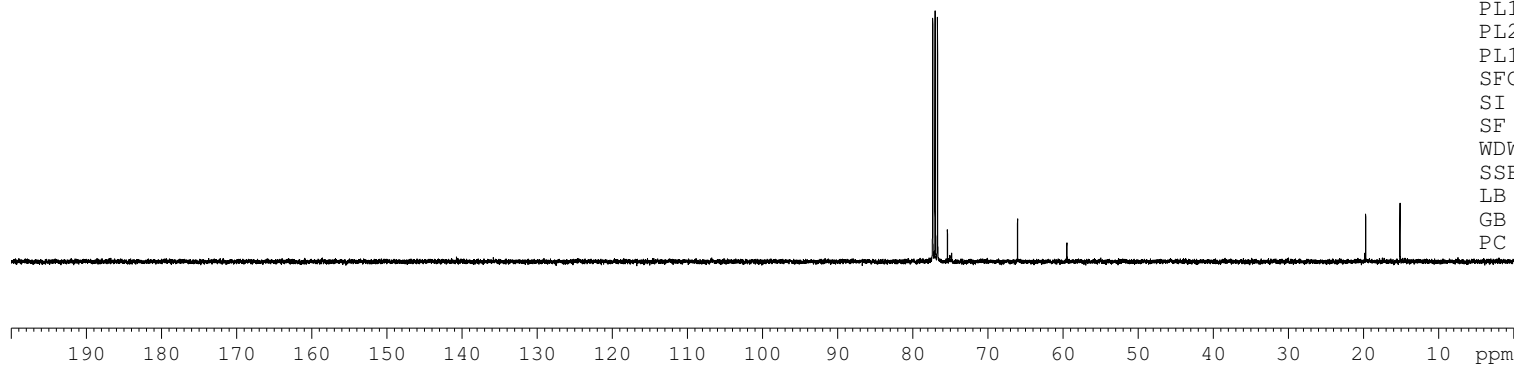
— 19.682
— 15.114

wrx0270-2-C-CDC13

NAME wrx0270-2-C-CDC13
EXPNO 1
PROCNO 1
Date_ 20100313
Time 16.39
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgdc
TD 131072
SOLVENT CDC13
NS 200
DS 0
SWH 29761.904 Hz
FIDRES 0.227065 Hz
AQ 2.2020595 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

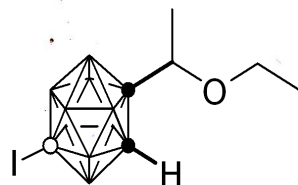
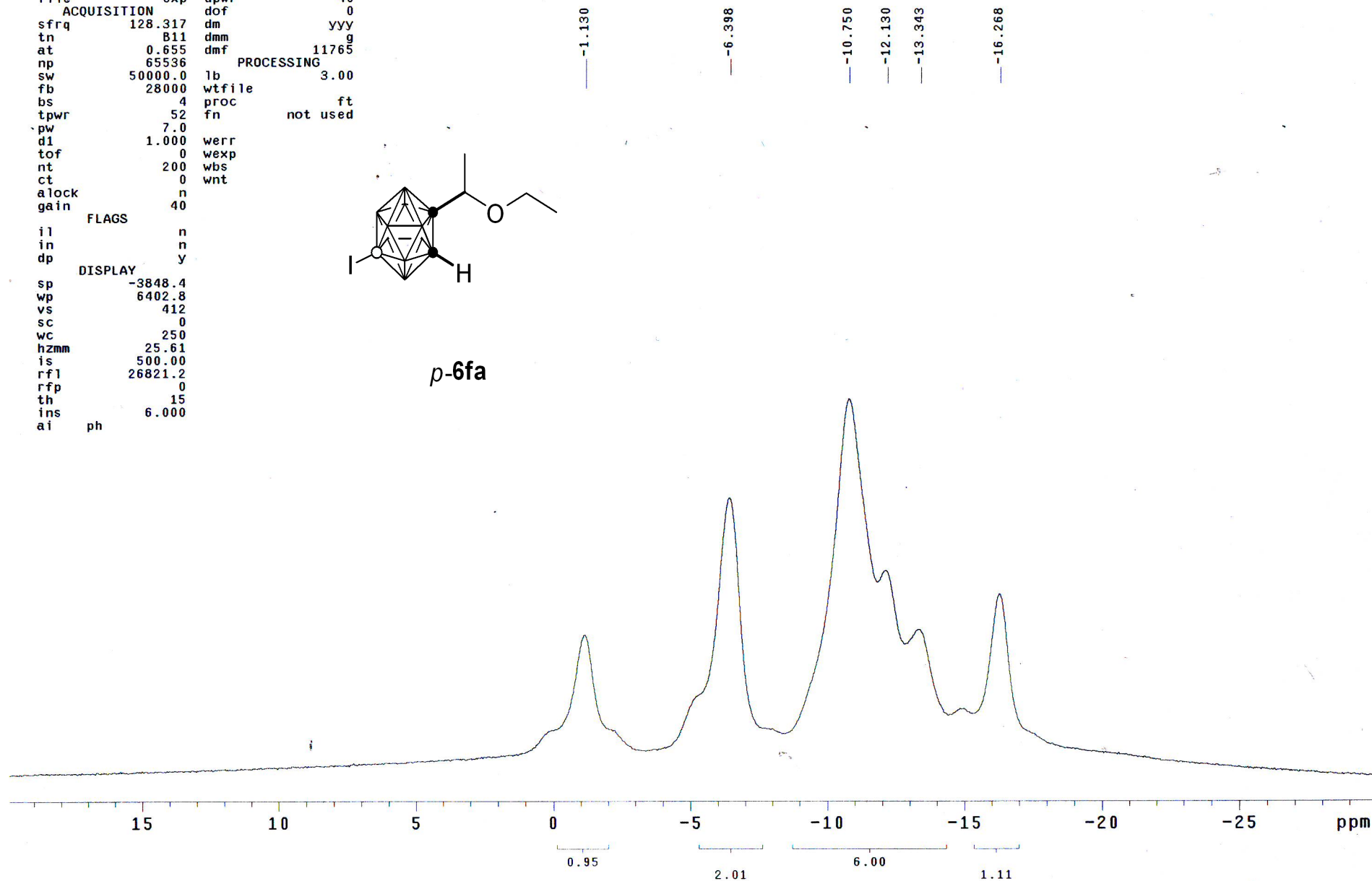
===== CHANNEL f1 =====
NUC1 13C
P1 3.50 usec
PL1 -0.60 dB
PL1W 41.24164963 W
SFO1 100.6227690 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL2W 8.31434441 W
PL12W 0.20409293 W
SFO2 400.1320007 MHz
SI 131072
SF 100.6127735 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

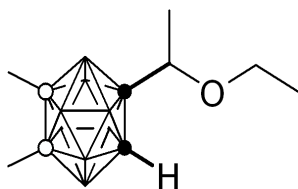


exp1 s2pu1

SAMPLE DEC. & VT
date Mar 13 2010 dfrq 399.951
solvent CDC13 dn H1
file exp dpwr 40
ACQUISITION dof 0
sfrq 128.317 dm yyy
tn 811 dmm g
at 0.655 dmf 11765
np 65536 PROCESSING
sw 50000.0 lb 3.00
fb 28000 wtfile
bs 4 proc ft
tpwr 52 fn not used
pw 7.0
d1 1.000 werr
tof 0 wexp
nt 200 wbs
ct 0 wnt
alock n
gain 40
FLAGS
il n
in n
dp y
DISPLAY
sp -3848.4
wp 6402.8
vs 412
sc 0
wc 250
hzmm 25.61
is 500.00
rfl 26821.2
rfp 0
th 15
ins 6.000
ai ph

*p-6fa*

— 7.260



6ga

3.911
3.895
3.879
3.864
3.652
3.634
3.629
3.616
3.611
3.599
3.594
3.576
3.414
3.397
3.392
3.380
3.374
3.362
3.357
3.339

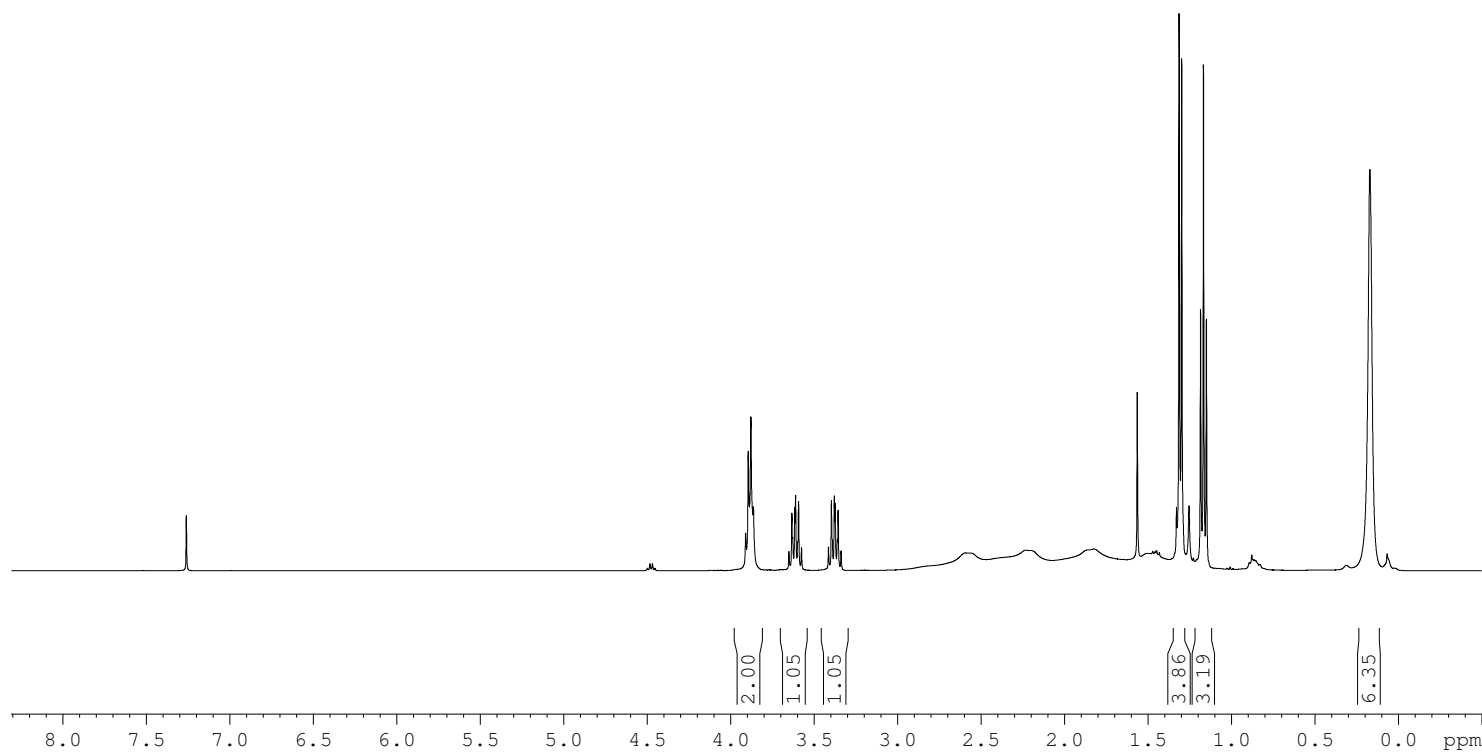
1.565
1.314
1.298
1.185
1.168
1.151

— 0.171

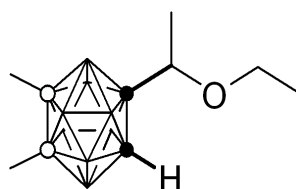
wrx0330-1-H-CDC13

NAME wrx0330-1-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100531
Time 19.17
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 40.3
DW 62.400 usec
DE 6.50 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1

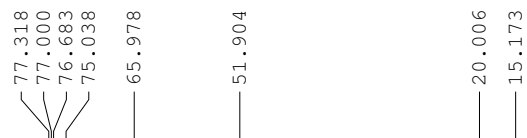
===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S118



6ga



wrx0330-1-C-CDC13

```

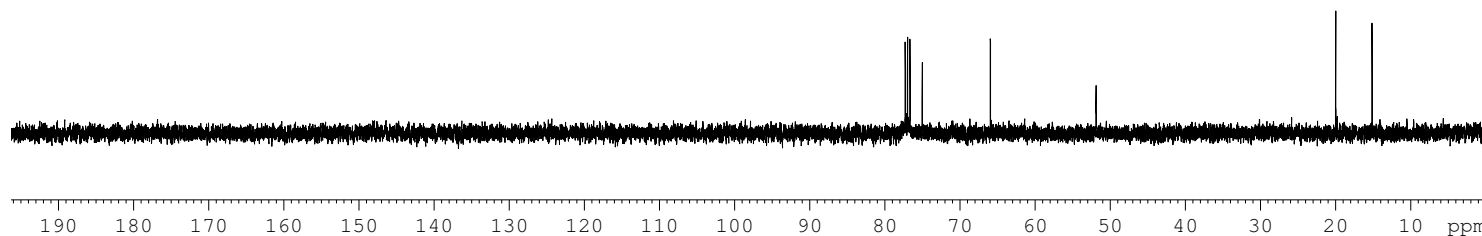
NAME      wrx0330-1-C-CDC13
EXPNO      1
PROCNO     1
Date_      20100531
Time       19.21
INSTRUM    spect
PROBHD     5 mm PABBI 1H/
PULPROG    zgdc
TD         131072
SOLVENT    CDC13
NS         42
DS         0
SWH        29761.904 Hz
FIDRES     0.227065 Hz
AQ         2.2020595 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE         294.7 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1       13C
P1         14.50 usec
PL1        -4.00 dB
PL1W       90.22689819 W
SFO1       100.6227690 MHz
  
```

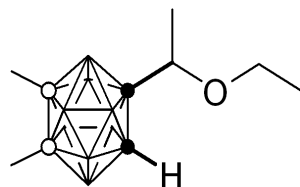
```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -2.00 dB
PL12       18.80 dB
PL2W       13.17734718 W
PL12W      0.10960442 W
SFO2       400.1320007 MHz
SI         131072
SF         100.6127707 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



S119

wrx0330-1-B-CDC13



6ga

— 6.058
— 5.287

— -7.245

— -12.089

— -13.314

— -14.180

— -16.023

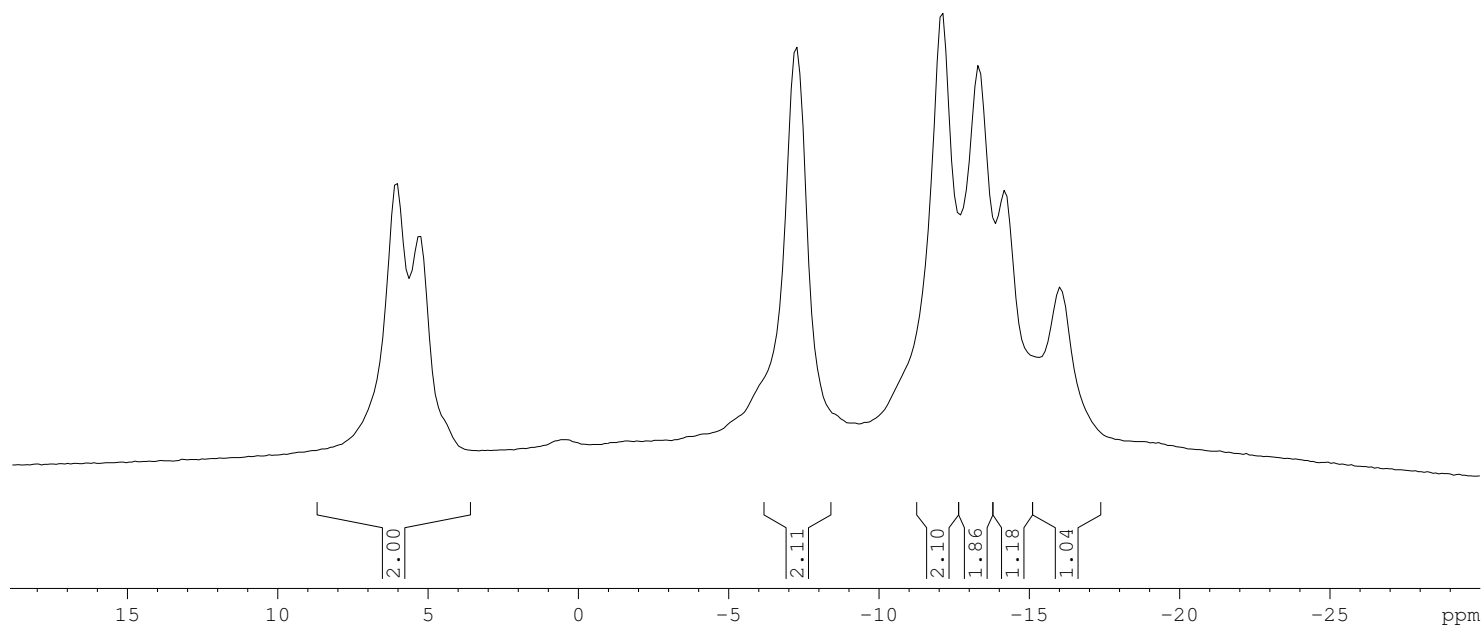
Current Data Parameters
NAME wrx0330-1-B-CDC13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100531
Time 13.32
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgdc
TD 4000
SOLVENT CDC13
NS 133
DS 4
SWH 25510.203 Hz
FIDRES 6.377551 Hz
AQ 0.0784500 sec
RG 203
DW 19.600 usec
DE 6.50 usec
TE 294.6 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1

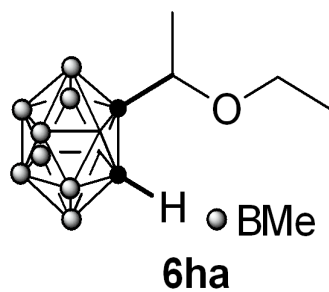
===== CHANNEL f1 =====
NUC1 11B
P1 14.50 usec
PL1 -4.00 dB
SFO1 128.3776076 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.80 dB
PL2W -1.#IND0000 W
PL12W -1.#IND0000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 2048
SF 128.3776263 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



— 7.260



3.821
3.805
3.789
3.773
3.635
3.618
3.613
3.600
3.595
3.583
3.578
3.560
3.454
3.436
3.418
3.414
3.401
3.396
3.379

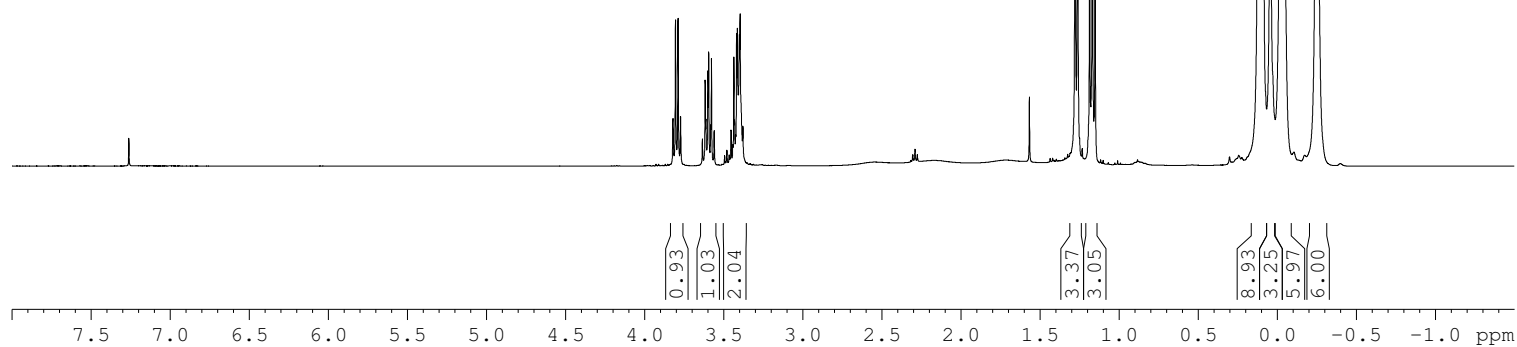
1.567
1.279
1.263
1.187
1.169
1.152

0.119
0.108
0.091
0.044
-0.019
-0.045
-0.248

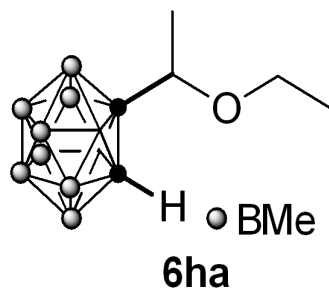
wrx0257-1-H-CDC13

NAME wrx0257-1-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100226
Time 21.57
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 22.6
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PL1 0.00 dB
PL1W 8.31434441 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S121



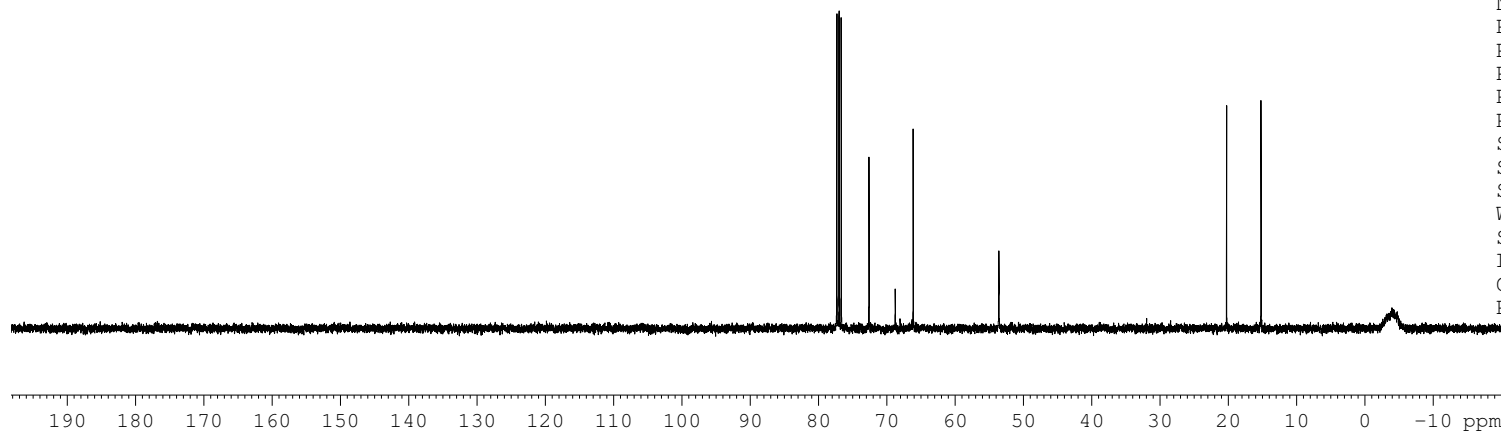
77.318
77.001
76.683
72.615
68.777
66.150
53.593
20.238
15.200
-4.055
-4.742

wrx0257-1-C-CDC13

NAME wrx0257-1-C-CDC13
EXPNO 1
PROCNO 1
Date_ 20100226
Time 21.59
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgdc
TD 131072
SOLVENT CDC13
NS 72
DS 0
SWH 29761.904 Hz
FIDRES 0.227065 Hz
AQ 2.2020595 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

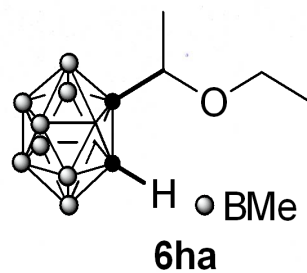
===== CHANNEL f1 =====
NUC1 13C
P1 3.50 usec
PL1 -0.60 dB
PL1W 41.24164963 W
SFO1 100.6227690 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL2W 8.31434441 W
PL12W 0.20409293 W
SFO2 400.1320007 MHz
SI 131072
SF 100.6127697 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



exp1 s2pu1

SAMPLE DEC. & VT
date Feb 26 2010 dfrq 399.951
solvent CDC13 dn H1
file exp dpwr 40
ACQUISITION dof 0
sfrq 128.317 dm yyy
tn 811 dmm g
at 0.655 dmf 11765
np 65536 PROCESSING
sw 50000.0 lb 3.00
fb 28000 wtfile
bs 4 proc ft
tpwr 52 fn not used
pw 7.0
d1 1.000 werr
tof 0 wexp
nt 200 wbs
ct 0 wnt
alock n
gain 40
FLAGS
il n
in n
dp y
DISPLAY
sp -3863.6
wp 7725.8
vs 173
sc 0
wc 250
hzmm 30.90
is 500.00
rfl 26821.2
rfp 0
th 8
ins 2.000
ai ph

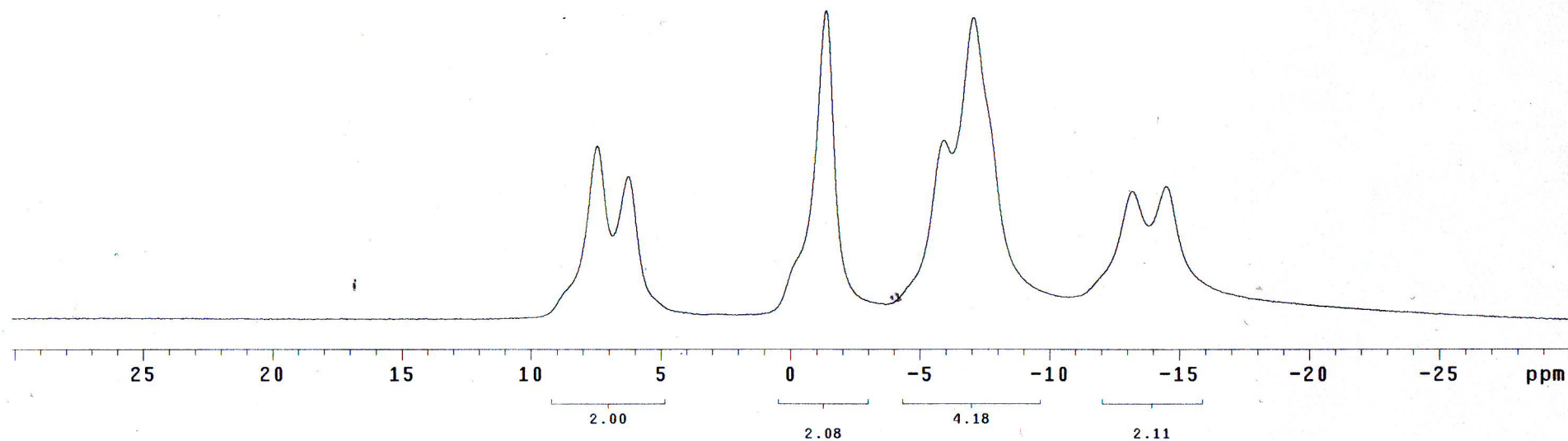


7.468
6.291

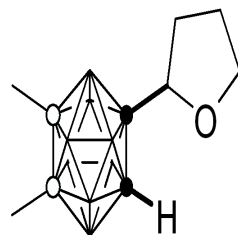
-1.332

-5.922
-7.064

-13.176
-14.484



7.260



6gj

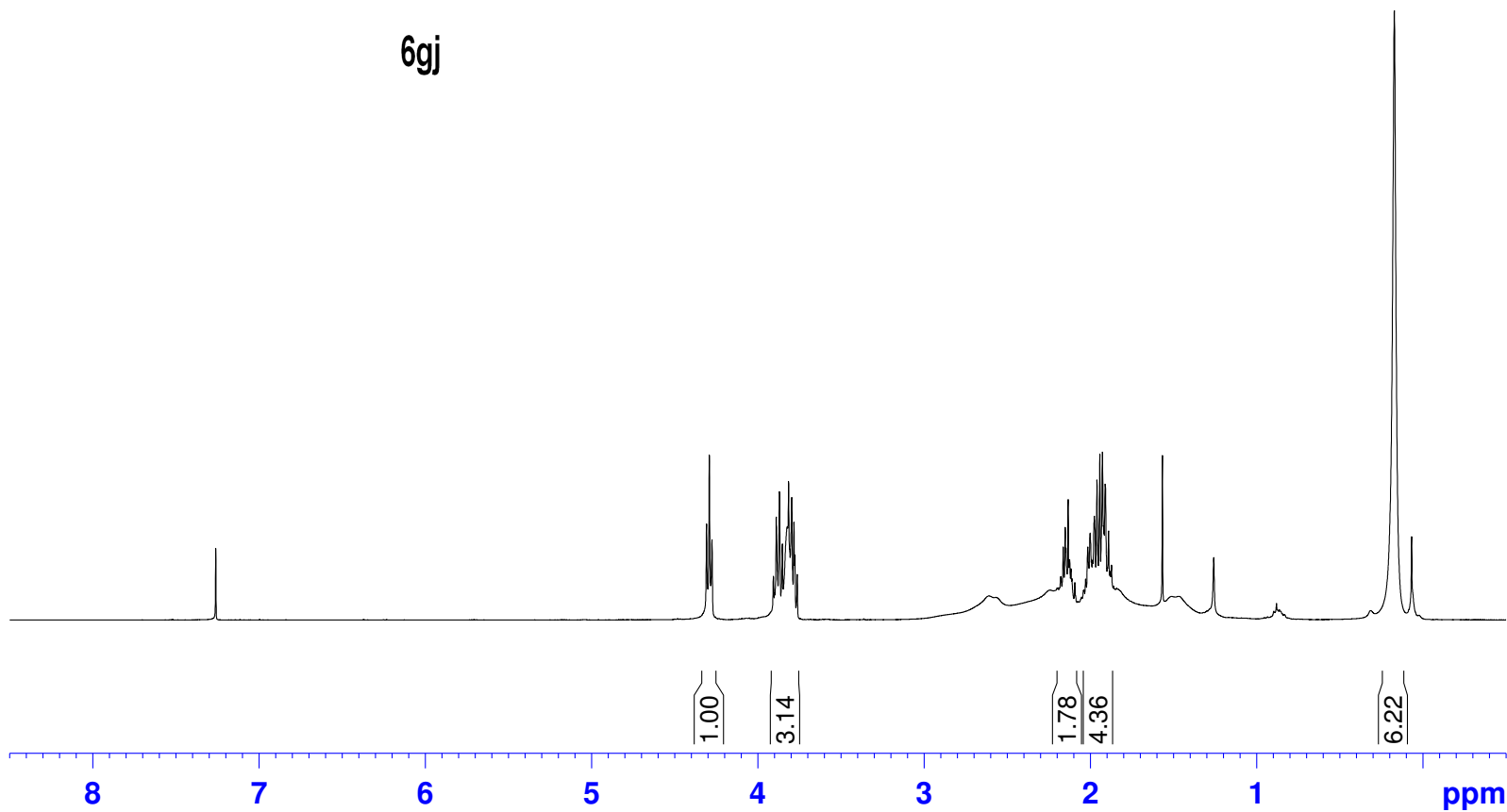
4.308
4.292
4.275
3.906
3.898
3.889
3.869
3.852
3.823
3.815
3.796
3.783
3.776
3.763
2.163
2.151
2.146
2.133
2.124
2.015
2.001
1.960
1.943
1.927
1.911
1.891

0.173

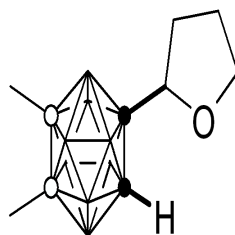
wrx0348-1-H-CDC13

NAME wrx0348-1-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100720
Time 16.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 36
DW 60.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -1.00 dB
PL1W 13.56617069 W
SFO1 400.1924713 MHz
SI 32768
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S124



6gj

78.89
77.32
77.00
76.68
70.76
69.54

52.54

32.93

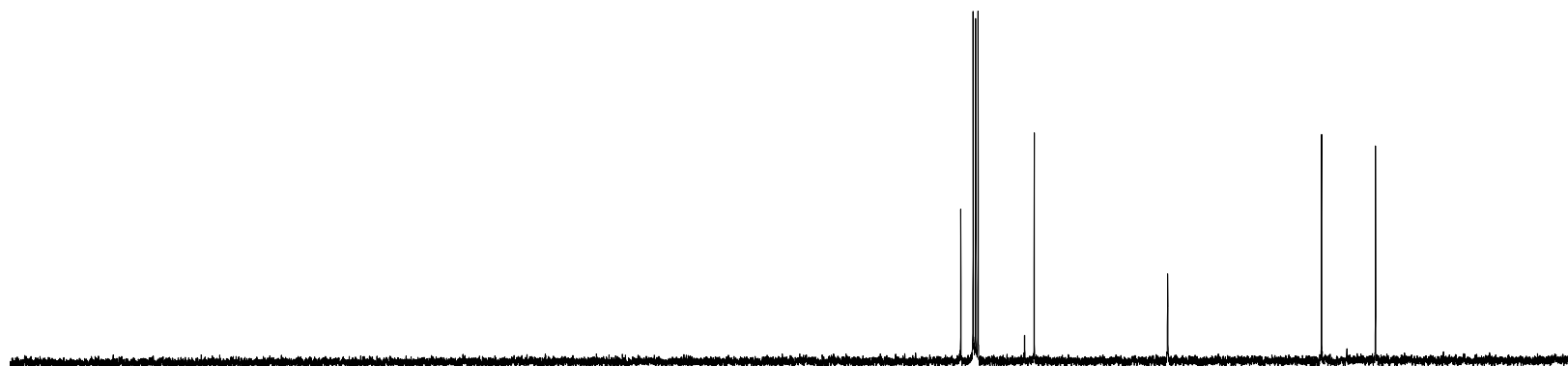
26.06

wrx0348-1-C-CDC13

NAME wrx0348-1-C-CDC13
EXPNO 1
PROCNO 1
Date_ 20100720
Time 16.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 84
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6379183 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL13 18.62 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
PL13W 0.14806664 W
SFO2 400.1916008 MHz
SI 32768
SF 100.6278591 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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

wrx0348-1-B-CDC13

```

NAME      wrx0348-1-B-CDC13
EXPNO     1
PROCNO    1
Date_     20100720
Time      16.21
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgdc
TD         65536
SOLVENT    CDC13
NS         28
DS         0
SWH        25510.203 Hz
FIDRES     0.389255 Hz
AQ         1.2845556 sec
RG         181
DW         19.600 usec
DE         6.50 usec
TE         298.6 K
D1         5.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

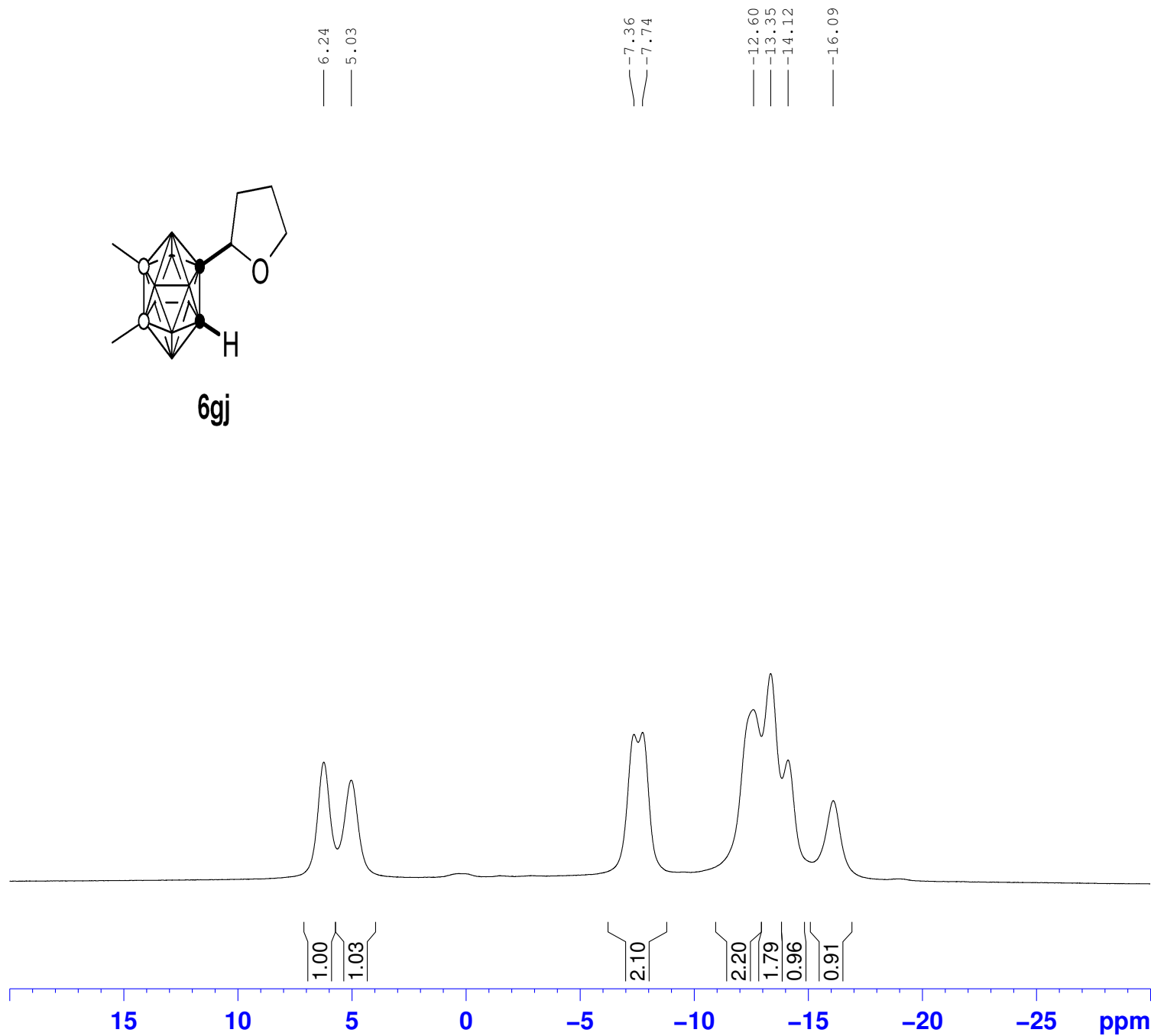
===== CHANNEL f1 =====
NUC1       11B
P1         7.60 usec
PL1        -3.00 dB
PL1W       55.13059616 W
SFO1       128.3968556 MHz

```

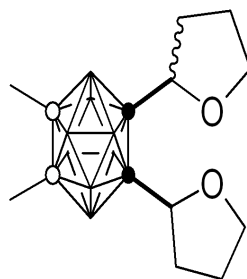
```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -1.00 dB
PL12       15.16 dB
PL2W       13.56617069 W
PL12W      0.32844096 W
SFO2       400.1916008 MHz
SI         32768
SF         128.3969002 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40

```



— 7.260

**8gj**

4.533
4.516
4.499
3.889
3.873
3.868
3.857
3.853
3.846
3.836
3.827

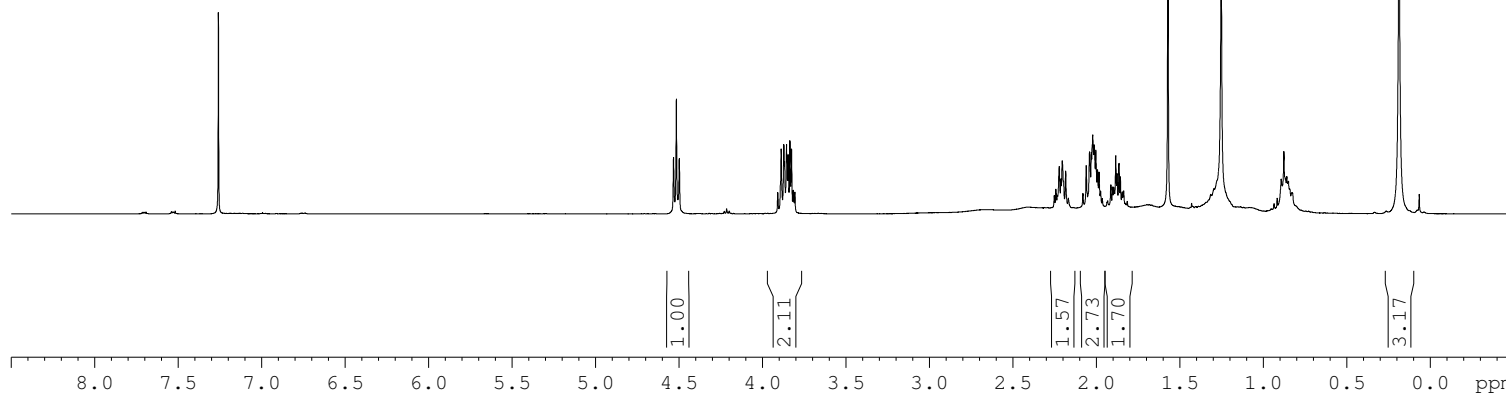
2.223
2.205
2.184
2.061
2.026
2.022
2.014
2.004
1.984
1.913
1.904
1.897
1.884
1.865
1.837
1.571

— 0.187

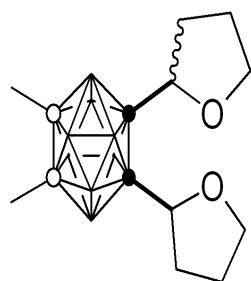
wrx0348-1.5-H-CDC13

NAME wrx0348-1.5-H-CDC13
EXPNO 1
PROCNO 1
Date_ 20100724
Time 15.23
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1

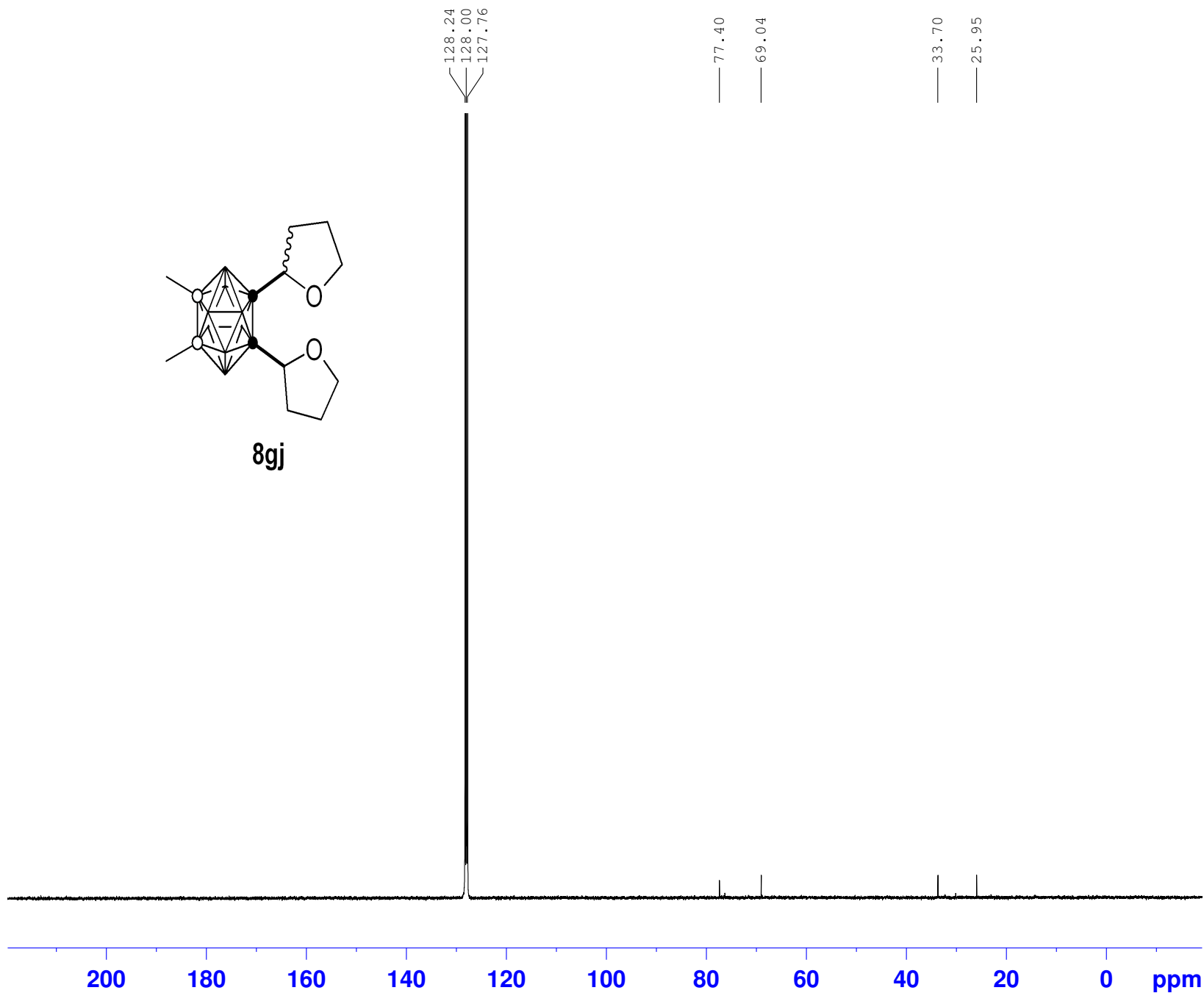
===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



wrx0348-1.5-C-C6D6



8gj



```
NAME wrx0348-1.5-C-C6D6
EXPNO 1
PROCNO 1
Date_ 20100724
Time 17.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 272
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
```

```
===== CHANNEL f1 =====
NUC1 13C
P1 9.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6379183 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL13 18.62 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
PL13W 0.14806664 W
SFO2 400.1916008 MHz
SI 32768
SF 100.6278253 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

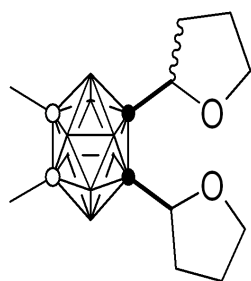
S128

wrx0348-1.5-B-CDC13

NAME wrx0348-1.5-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100724
Time 16.02
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgdc
TD 4000
SOLVENT DMSO
NS 296
DS 4
SWH 25510.203 Hz
FIDRES 6.377551 Hz
AQ 0.0784500 sec
RG 128
DW 19.600 usec
DE 6.50 usec
TE 294.4 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 11B
P1 10.00 usec
PL1 -4.00 dB
PL1W 63.09573364 W
SFO1 128.3776076 MHz

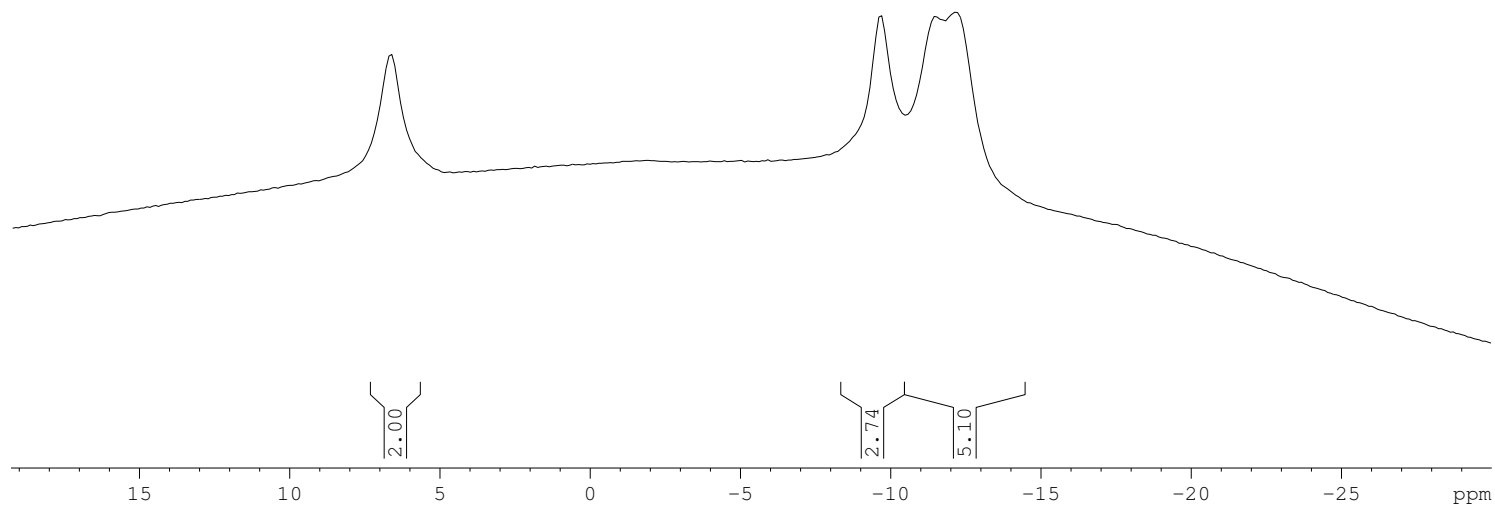
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.80 dB
PL2W 13.17734718 W
PL12W 0.10960442 W
SFO2 400.1316005 MHz
SI 2048
SF 128.3775515 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

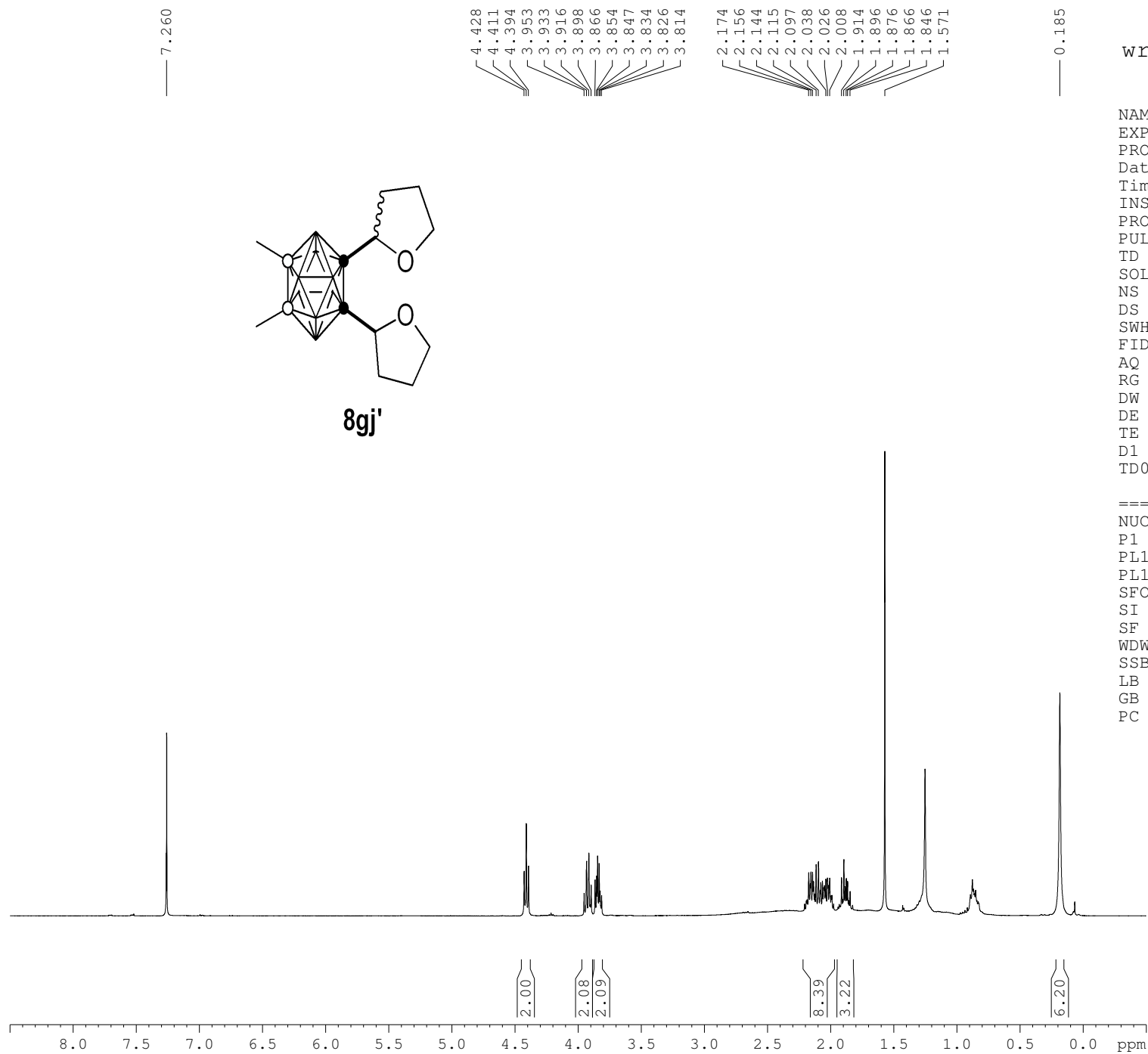
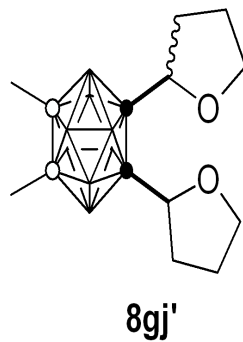


8gj

— 6.633

— -9.661
— -11.487
— -12.160

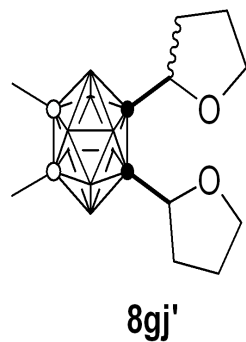




wrx0348-2-H-CDC13

NAME wrx0348-2-H-CDC13
 EXPNO 1
 PROCNO 1
 Date_ 20100722
 Time 18.59
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 161
 DW 62.400 usec
 DE 6.50 usec
 TE 294.6 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 -2.00 dB
 PL1W 13.17734718 W
 SFO1 400.1316005 MHz
 SI 65536
 SF 400.1300052 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



128.238
127.995
127.752

77.607

68.942

33.542

25.952

wrx0348-2-C-C6D6

```

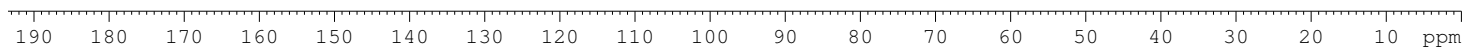
NAME      wrx0348-2-C-C6D6
EXPNO     1
PROCNO    1
Date_     20100723
Time      20.06
INSTRUM   spect
PROBHD    5 mm PABBI 1H/
PULPROG   zgdc
TD         131072
SOLVENT   C6D6
NS         374
DS         0
SWH        29761.904 Hz
FIDRES     0.227065 Hz
AQ         2.2020595 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE         294.5 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1       13C
P1         14.50 usec
PL1        -4.00 dB
PL1W       90.22689819 W
SFO1       100.6227690 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2      80.00 usec
PL2        -2.00 dB
PL12       18.80 dB
PL2W       13.17734718 W
PL12W      0.10960442 W
SFO2       400.1320007 MHz
SI         131072
SF         100.6127511 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

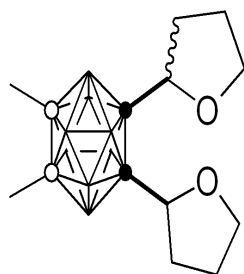


wrx0348-2-B-CDC13

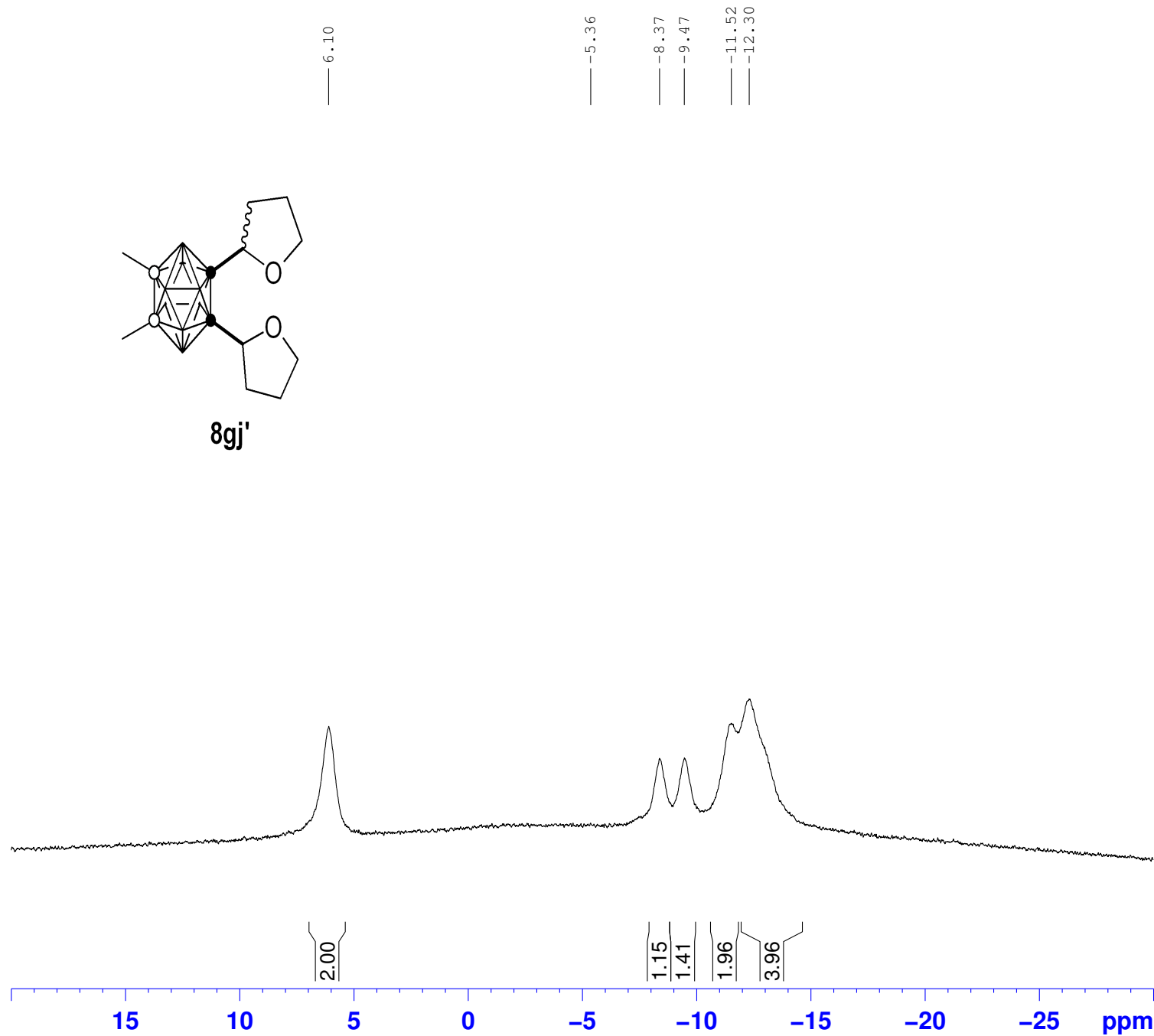
NAME wrx0348-2-B-CDC13
EXPNO 1
PROCNO 1
Date_ 20100723
Time 10.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 65536
SOLVENT CDC13
NS 12
DS 0
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 512
DW 19.600 usec
DE 6.50 usec
TE 298.1 K
D1 5.00000000 sec
D11 0.03000000 sec
TD0 1

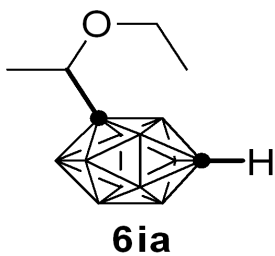
===== CHANNEL f1 =====
NUC1 11B
P1 7.60 usec
PL1 -3.00 dB
PL1W 55.13059616 W
SFO1 128.3968556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
SFO2 400.1916008 MHz
SI 32768
SF 128.3969002 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



8gj'





3.577
3.559
3.541
3.537
3.525
3.519
3.509
3.502
3.491
3.474
3.456
3.451
3.439
3.434
3.416

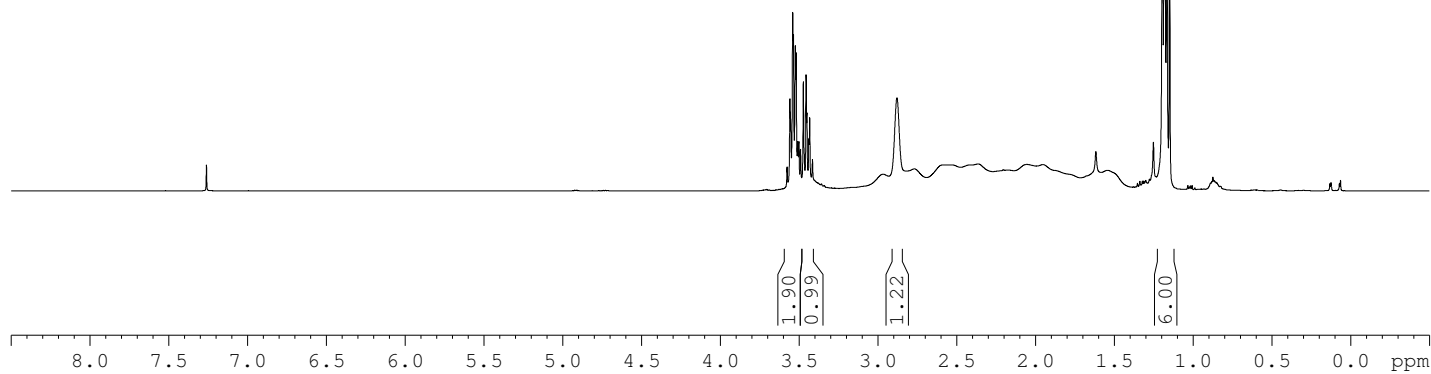
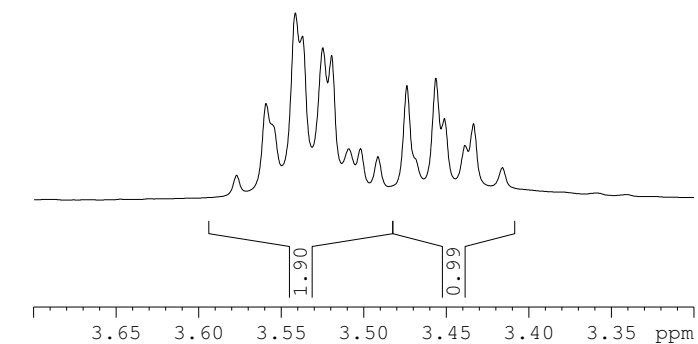
3.577
3.559
3.541
3.537
3.525
3.519
3.509
3.502
3.491
3.474
3.456
3.451
3.439
3.434
3.416
2.880

1.195
1.183
1.180
1.167
1.149

wrx0408-1-H-CDCl3

NAME wrx0408-1-H-CDCl3
EXPNO 1
PROCNO 1
Date_ 20100930
Time 22.33
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 8
DW 62.400 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1316005 MHz
SI 65536
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S133

81.47
77.32
77.00
76.68
76.11

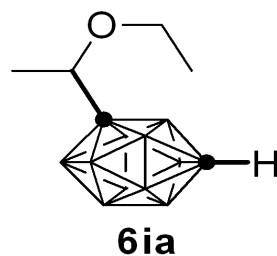
66.30

54.18

21.09

15.09

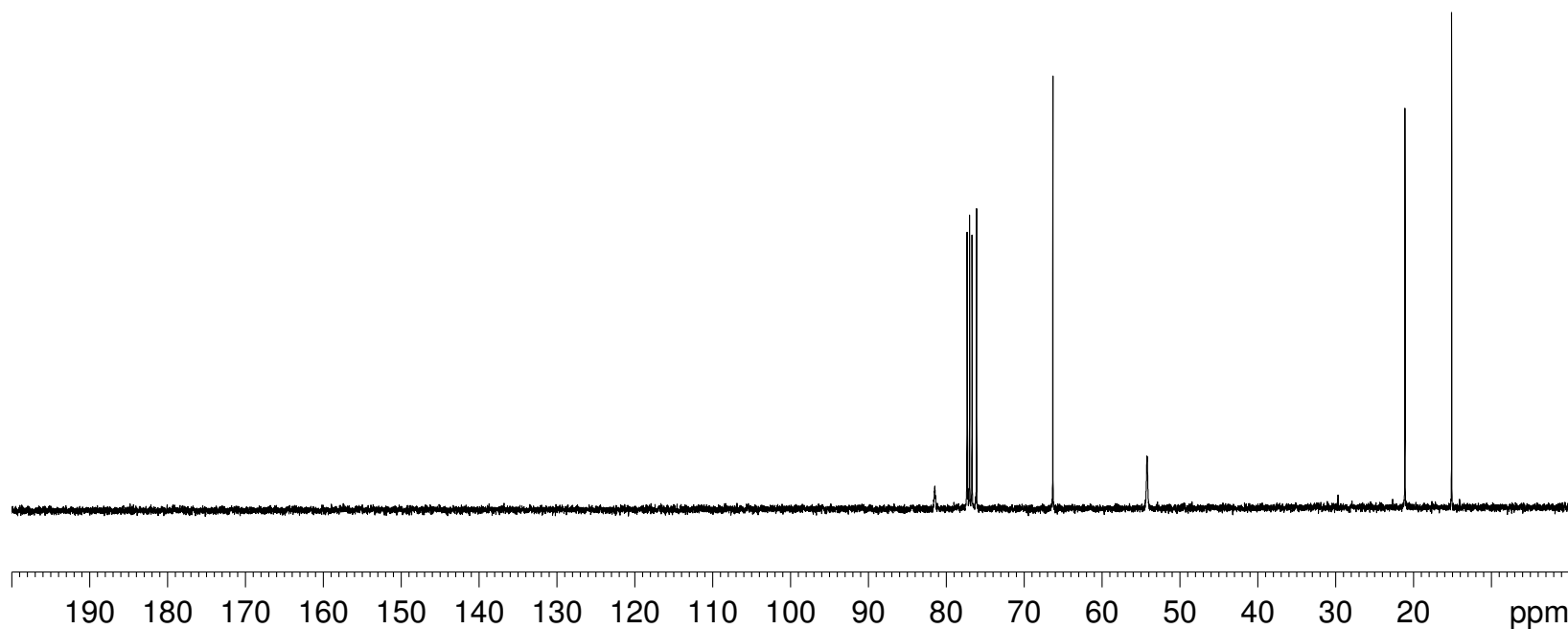
wrx0408-1-C-CDCl3

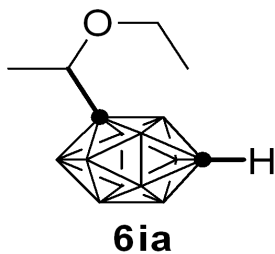


NAME wrx0408-1-C-CDCl3
EXPNO 1
PROCNO 1
Date_ 20100831
Time 9.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 120
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6379183 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL13 18.62 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
PL13W 0.14806664 W
SFO2 400.1916008 MHz
SI 32768
SF 100.6278603 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





— -4.066
 — -7.896
 — -10.466
 — -11.466
 — -12.940
 — -15.045
 — -15.418

wrx0408-1-B-CDC13

```

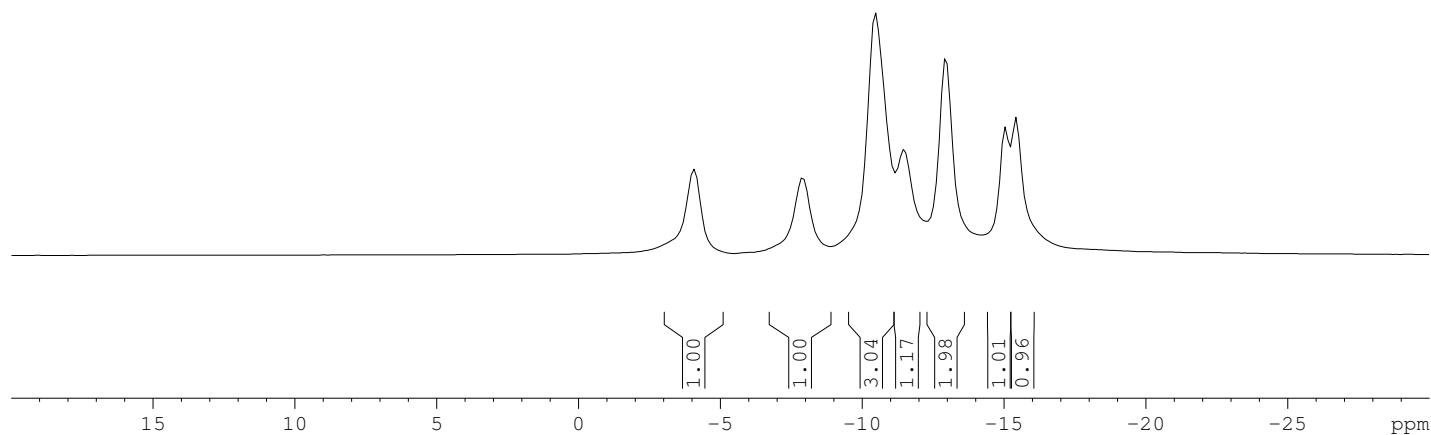
NAME      wrx0408-1-B-CDC13
EXPNO      1
PROCNO     1
Date_      20100930
Time       23.37
INSTRUM    spect
PROBHD     5 mm PABBI 1H/
PULPROG    zgdc
TD         4000
SOLVENT    CDC13
NS         120
DS         4
SWH        25510.203 Hz
FIDRES     6.377551 Hz
AQ         0.0784500 sec
RG         114
DW         19.600 usec
DE         6.50 usec
TE         294.7 K
D1         0.10000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1       11B
P1         10.00 usec
PL1        -4.00 dB
PL1W       63.09573364 W
SFO1       128.3776076 MHz
  
```

```

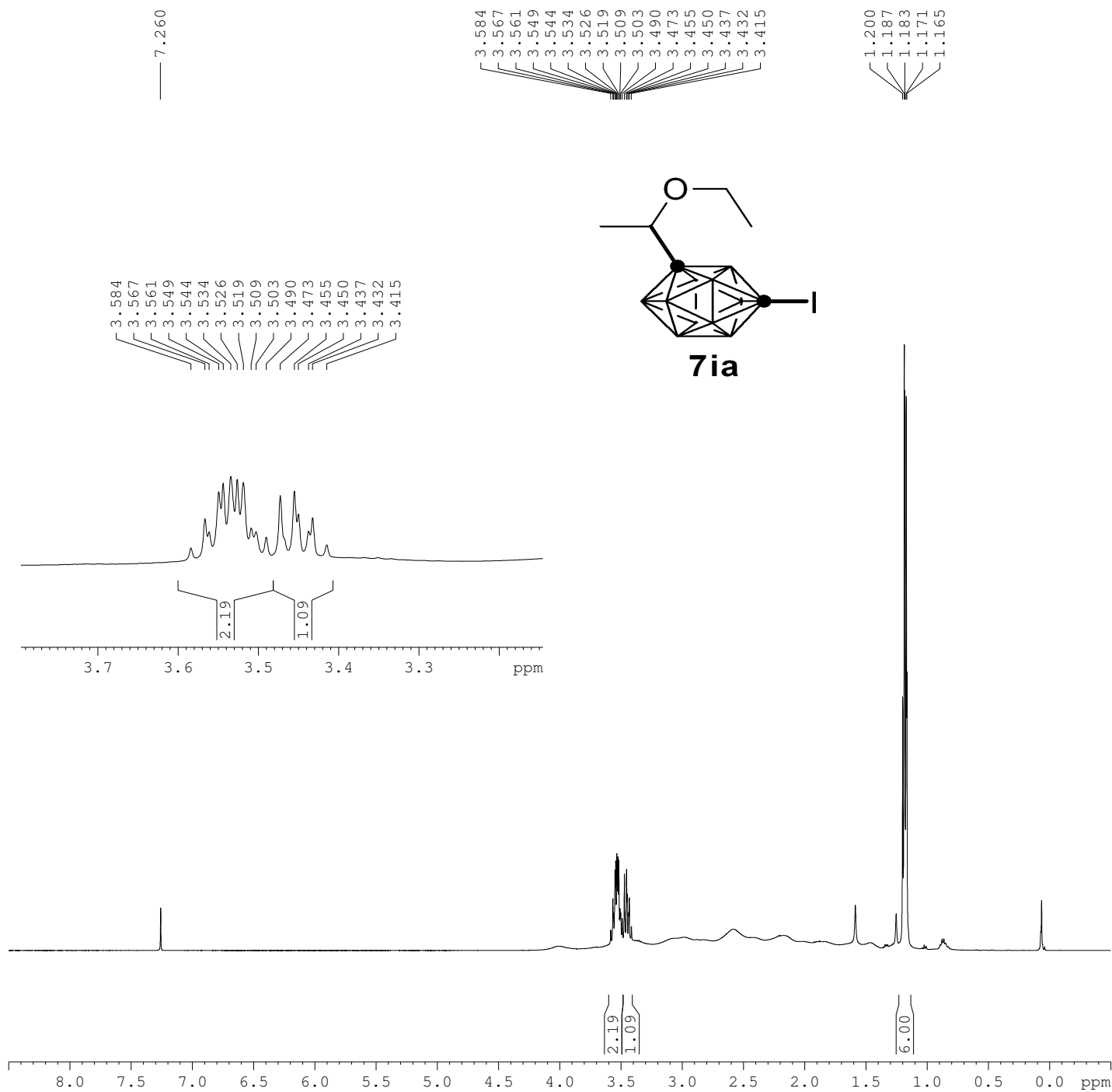
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -2.00 dB
PL12       18.80 dB
PL2W       13.17734718 W
PL12W      0.10960442 W
SFO2       400.1316005 MHz
SI         2048
SF         128.3775017 MHz
WDW        EM
SSB        0
LB         2.00 Hz
GB         0
PC         1.40
  
```



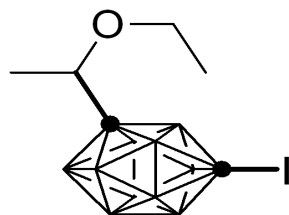
wrx0411-1-H-CDCl3

NAME wrx0411-1-H-CDCl3
 EXPNO 1
 PROCNO 1
 Date_ 20101005
 Time 17.59
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2768500 sec
 RG 32
 DW 50.000 usec
 DE 6.50 usec
 TE 294.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 -2.00 dB
 PL1W 13.17734718 W
 SFO1 400.1318000 MHz
 SI 65536
 SF 400.1300052 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



S136

**7ia**

84.16
77.32
77.00
76.68
76.03
66.38

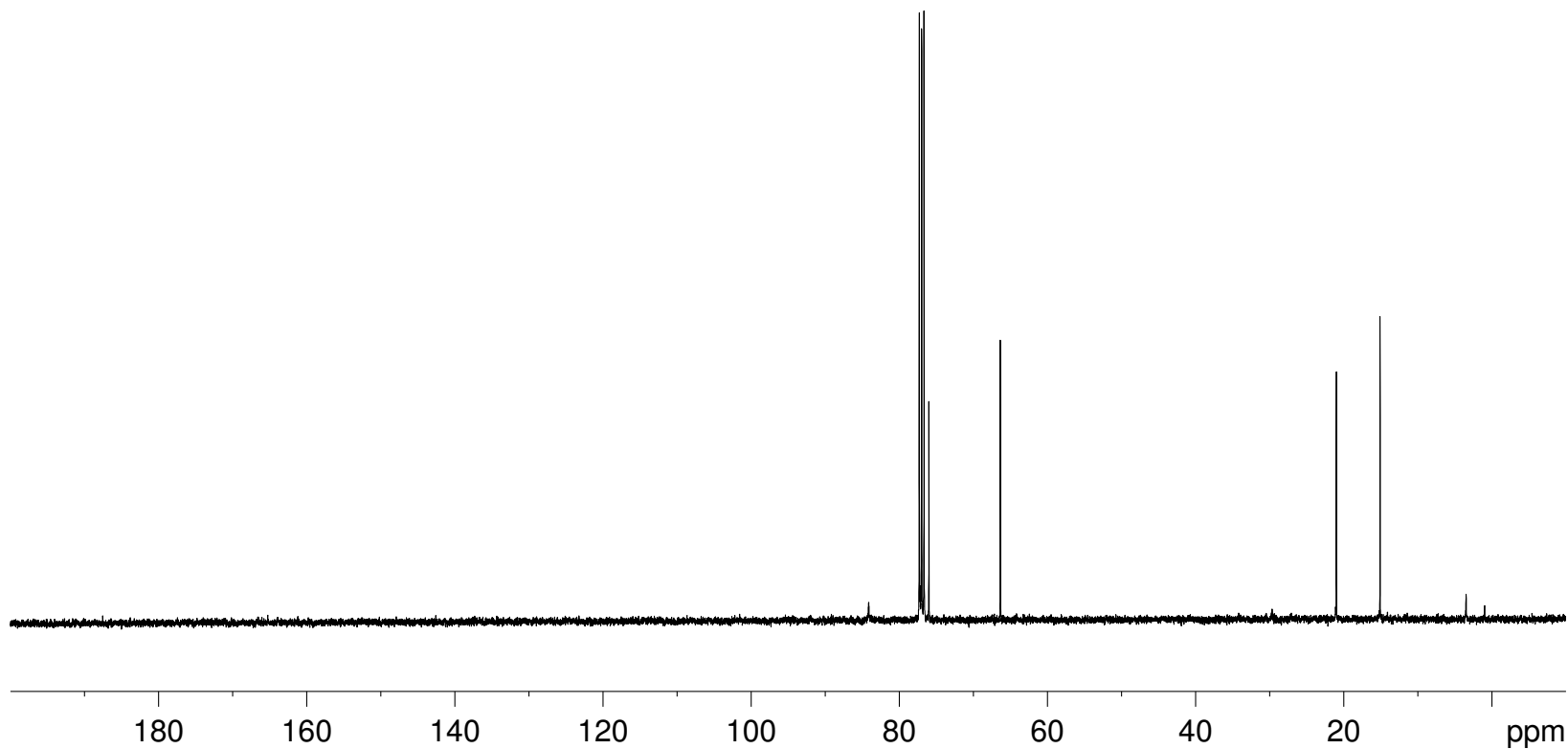
21.01
15.12
3.50

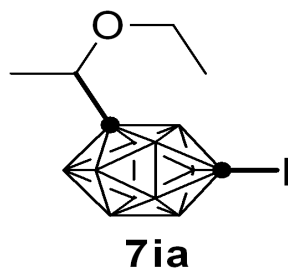
wrx0411-1-C-CDCl3

NAME wrx0411-1-C-CDCl3
EXPNO 1
PROCNO 1
Date_ 20101004
Time 14.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 360
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.90 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6379183 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.16 dB
PL13 18.62 dB
PL2W 13.56617069 W
PL12W 0.32844096 W
PL13W 0.14806664 W
SFO2 400.1916008 MHz
SI 32768
SF 100.6278592 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





— 4.33
— 7.43
— 9.16
— 10.81
— 11.64
— 12.28

wrx0411-1-B-CDC13

```

NAME      wrx0411-1-B-CDC13
EXPNO     1
PROCNO    1
Date_     20101004
Time      15.11
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgdc
TD        65536
SOLVENT   DMSO
NS        12
DS        0
SWH       25510.203 Hz
FIDRES    0.389255 Hz
AQ        1.2845556 sec
RG        228
DW        19.600 usec
DE        6.50 usec
TE        298.1 K
D1        5.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

```

===== CHANNEL f1 =====
NUC1      11B
P1        7.60 usec
PL1       -3.00 dB
PL1W      55.13059616 W
SFO1      128.3968556 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -1.00 dB
PL12      15.16 dB
PL2W      13.56617069 W
PL12W     0.32844096 W
SFO2      400.1916008 MHz
SI        32768
SF        128.3969002 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40
  
```

