Electronic Supplementary Information

Magnesium-Mediated sp^3 C-H Activation in Cascade Cyclization of 1-Arylethynyl-2-Alkyl-*o*-Carboranes: Efficient Synthesis of Carborane-Fused Cyclopentanes

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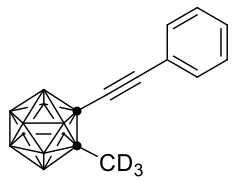
Experimental Section

General information. All reactions were carried out under an atmosphere of dry argon with the rigid exclusion of air and moisture using standard Schlenk techniques or in a glovebox unless otherwise specified. ^{1}H NMR spectra were recorded on a Bruker DPX 400 spectrometer at 400 MHz or a Bruker DPX 500 spectrometer at 500 MHz. ^{2}H NMR spectra were recorded on a Bruker DPX 400 spectrometer at 61 MHz or a Bruker DPX 500 spectrometer at 77 MHz. ^{13}C{^{1}H} NMR spectra were recorded on a Bruker DPX 400 spectrometer at 100 MHz or a Bruker DPX 500 spectrometer at 125 MHz. ^{11}B{^{1}H} NMR spectra were recorded on a Bruker DPX 400 spectrometer at 128 MHz or a Bruker DPX 500 spectrometer at 160 MHz. ^{19}F NMR spectra were recorded on a Bruker DPX 500 spectrometer at 470 MHz. All signals were reported in ppm with reference to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, to external $BF_3{\cdot}OEt_2$ (0.00 ppm) for boron chemical shifts and to external $CFCl_3$ (0.00) for fluorine chemical shifts. The data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quadruplet, p = pentet, m = multiplet or unresolved, dd = doublet of doublets), coupling constant, integration and assignment. Mass spectra were obtained on a Thermo Q Exactive Focus Orbitrap Mass Spectrometer. All organic solvents were freshly distilled from Na-K alloy or CaH_2 immediately prior to use. 1-Arylethynyl-2-alkyl-*o*-carboranes **1**[1] and 3,4,5,6,7,11-D_6-*o*-carborane[2] were synthesized according to the reported literatures. All other chemicals were purchased from either Aldrich or Acros Chemical Co. and used as received unless otherwise specified.

Synthesis of 1a-*d*$_3$. To a THF solution (5 mL) of 1-phenylethynyl-*o*-carborane (244 mg, 1.0 mmol) was slowly added ^{n}BuLi (1.6 M in hexane, 0.69 mL, 1.1 mmol) at 0 ^{o}C, and the mixture was stirred at room temperature for 2 h. After addition of CD_3I (172 mg, 1.2 mmol) at 0^{o}C, the reaction mixture was further stirred at room temperature for 12 h. Reaction was then quenched with water (5 mL) and extracted with diethyl ether (20 mL x 3). The ether solutions were combined and concentrated to dryness in

vacuo. The residue was subjected to flash column chromatography on silica gel (230 - 400 mesh) using *n*-hexane as eluent to give **1a-*d*$_3$**.

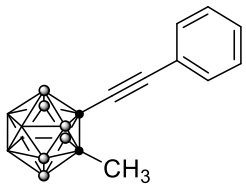


1a-*d*$_3$

1a-*d*$_3$: White solid. Yield: 80%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (m, 2H), 7.42 (m, 1H), 7.37 (m, 2H) (aromatic C*H*). ^{2}H NMR (77 MHz, $CHCl_3$): δ 2.30 (s, 3D) (C*D*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 132.3, 130.0, 128.5, 119.9 (aromatic *C*), 82.5, 81.7 (alkynyl *C*), 66.5 (cage *C*), another cage C and CD_3 carbon were not observed. ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.1 (1B), -6.5 (1B), -8.4 (2B), -10.1 (6B). HRMS (EI): *m/z* calcd for $C_{11}H_{15}{}^{10}B_2{}^{11}B_8D_3[M]^-$: 261.2605. Found: 261.2603.

Synthesis of 1a-*d*$_6$. To a THF solution (5 mL) of 3,4,5,6,7,11-D_6-*o*-carborane (150 mg, 1.0 mmol) was slowly added ^{n}BuLi (1.6 M in hexane, 0.69 mL, 1.1 mmol) at 0 ^{o}C, and the mixture was stirred at room temperature for 2 h. After addition of CuCl (140 mg, 1.4 mmol), the reaction mixture was stirred at 40 ^{o}C for 1 h, to which was added phenylethynyl bromide (252 mg, 1.4 mol). The reaction was further stirred at room temperature for 12 h. After quenching with water (10 mL), the resultant solution was extracted with diethyl ether (20 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (230 - 400 mesh) using *n*-hexane as eluent to give 1-phenylethynyl-3,4,5,6,7,11-D_6-*o*-carborane (245 mg, 98%).

To a THF solution (5 mL) of 1-phenylethynyl-3,4,5,6,7,11-D_6-*o*-carborane (250 mg, 1.0 mmol) was slowly added ^{n}BuLi (1.6 M in hexane, 0.69 mL, 1.1 mmol) at 0 ^{o}C, and the mixture was stirred at room temperature for 2 h. After addition of MeI (171 mg, 1.2 mmol) at 0^{o}C, the reaction mixture was further stirred at room temperature for 12 h. Reaction was then quenched with water (5 mL) and extracted with diethyl ether (20 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (230 - 400 mesh) using *n*-hexane as eluent to give 1-phenylethynyl-2-methyl-3,4,5,6,7,11-D_6-*o*-carborane **1a-*d*$_6$**.

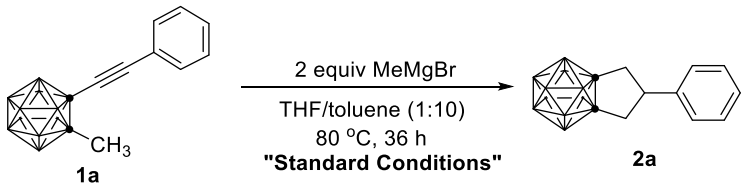


1a-*d*$_6$

1a-*d*$_6$: White solid. Yield: 76%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 (m, 2H), 7.43 (m, 1H), 7.36 (m, 2H) (aromatic C*H*), 2.21 (s, 3H) (C*H*$_3$). ^{2}H{^{11}B} NMR (77 MHz, $CHCl_3$): δ 2.68 (s, 2D), 2.55 (s, 2D), 2.49 (s, 2D) (B*D*). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 132.3, 130.0, 128.5, 119.9 (aromatic *C*), 82.6, 81.6 (alkynyl *C*), 76.6, 66.5 (cage *C*), 23.8 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.4 (1B), -5.9 (1B), -7.8 (2B), -9.6 (6B). HRMS (EI): *m/z* calcd for $C_{11}H_{12}{}^{10}B_2{}^{11}B_8D_6[M]^-$: 264.2794. Found: 264.2789.

Optimization of reaction conditions

Table S1. Optimization of Reaction Conditions[a]



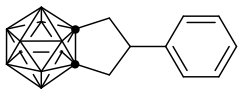
Entry	Deviation from standard conditions	Yield [%][b]
1	None	80
2	MeMgCl in place of MeMgBr	13[c]
3	PhMgCl in place of MeMgBr	30[d]
4	^{n}BuLi in place of MeMgBr	0[c]
5	24 h	60
6	No THF	0[e]
7	No toluene	0[c]
8	1 equiv of MeMgBr	32[c,e]

[a]Reactions were conducted on 0.1 mmol scale of **1a** in 0.8 mL solvent in a closed flask. [b]Isolated yield. [c]A mixture of multi-B-alkylated *o*-carboranes detected by GC-MS. [d]Deboronation detected by ^{11}B NMR. [e]Starting materials recovered.

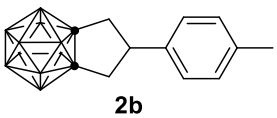
Synthesis of Carborane-Fused Cyclopentanes 2

General synthetic procedure A. Methyl magnesium bromide (3.0 M in Et_2O, 0.067 mL, 0.2 mmol) was added to 1-arylethynyl-2-alkyl-*o*-carborane **1** (0.1 mmol),

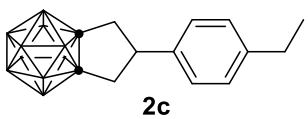
followed by the addition of THF (0.067 mL) and toluene (0.667 mL), and then the Schlenk flask was closed. The mixture was stirred at 80°C for 36 h. Reaction was quenched with water (1 mL) and extracted with diethyl ether (10 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give product **2**.


2a

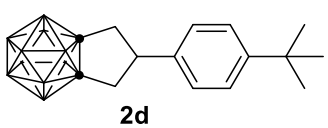
2a: Colorless crystals. 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 (m, 2H), 7.27 (m, 1H), 7.18 (m, 2H) (aromatic C*H*), 4.05 (p, *J* = 9.7 Hz, 1H), 2.90 (dd, *J* = 13.6, 9.6 Hz, 2H), 2.63 (dd, *J* = 13.6, 9.9 Hz, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 140.4, 129.1, 127.6, 127.1 (aromatic *C*), 99.9, 82.3 (cage *C*), 53.1, 43.0 (alkyl *C*). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -7.0 (4B), -10.1 (1B), -11.0 (2B), -12.4 (1B), -13.3 (2B). HRMS: *m/z* calcd for $C_{11}H_{20}{}^{10}B_2{}^{11}B_8$ $[M]^-$: 260.2574. Found 260.2576.


2b

2b: Colorless crystals. 77% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.15 (d, *J* = 7.9 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H) (aromatic C*H*), 4.02 (p, *J* = 9.7 Hz, 1H), 2.87 (dd, *J* = 13.6, 9.7 Hz, 2H), 2.61 (dd, *J* = 13.6, 9.9 Hz, 2H), 2.34 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 137.4, 137.3, 129.7, 126.9 (aromatic *C*), 82.34 (cage *C*), 52.8, 43.1, 21.0 (alkyl *C*). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -6.5 (4B), -9.7 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{12}H_{22}{}^{10}B_2{}^{11}B_8$ $[M]^-$: 274.2730. Found 274.2732.

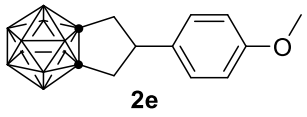

2c

2c: Colorless crystals. 78% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.17 (t, *J* = 6.5 Hz, 2H), 7.09 (m, 2H) (aromatic C*H*), 4.03 (m, 1H), 2.87 (m, 2H), 2.62 (m, 4H), 1.23 (m, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 143.8, 137.6, 128.5, 127.1 (aromatic *C*), 82.4 (cage *C*), 52.8, 43.1, 28.4, 15.5 (alkyl *C*). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -6.5 (4B), -9.7 (1B), -10.5 (2B), -12.0 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{13}H_{24}{}^{10}B_2{}^{11}B_8$ $[M]^-$: 288.2887. Found 288.2890.


2d

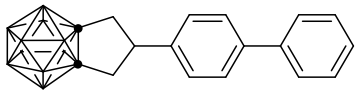
2d: Colorless crystals. 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35 (d, *J* = 8.3 Hz, 2H), 7.11 (d, *J* = 8.2 Hz, 2H) (aromatic C*H*), 4.03 (p, *J* = 9.7 Hz, 1H), 2.87 (dd, *J* = 13.6,

9.6 Hz, 2H), 2.62 (dd, *J* = 13.6, 9.9 Hz, 2H), 1.30 (s, 9H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 150.7, 137.3, 126.8, 125.9 (aromatic *C*), 82.4 (cage *C*), 52.7, 43.0, 34.5, 31.2 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -6.6 (2B), -7.0 (2B), -9.7 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{15}H_{28}{}^{10}B_2{}^{11}B_8$ $[M]^-$: 316.3200. Found 316.3201.

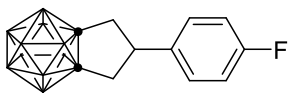


2e

2e: Colorless crystals. 72% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.09 (m, 2H), 6.85 (m, 2H) (aromatic C*H*), 4.01 (p, *J* = 9.7 Hz, 1H), 3.79 (s, 3H), 2.86 (dd, *J* = 13.6, 9.6 Hz, 2H), 2.57 (dd, *J* = 13.6, 9.9 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 158.9, 132.3, 128.2, 114.4 (aromatic *C*), 82.3 (cage *C*), 55.3, 52.5, 43.2 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -6.5 (4B), -9.8 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{12}H_{22}{}^{10}B_2{}^{11}B_8O$ $[M]^-$: 290.2683. Found 290.2679.

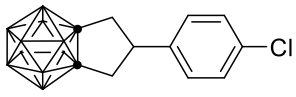

2f

2f: Colorless crystals. 76% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.57 (m, 4H), 7.46 (m, 2H), 7.38 (m, 1H), 7.26 (m, 2H) (aromatic C*H*), 4.11 (m, 1H), 2.94 (dd, *J* = 12.9, 10.2 Hz, 2H), 2.69 (m, 2H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 140.6, 140.3, 139.3, 128.9, 127.7, 127.6, 127.0 (aromatic *C*), 82.3 (cage *C*), 52.8, 43.2 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -6.5 (4B), -9.7 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{17}H_{24}{}^{10}B_2{}^{11}B_8$ $[M]^-$: 336.2887. Found 336.2886.



2g

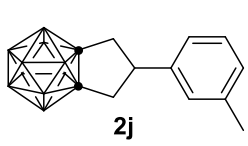
2g: Colorless crystals. 35% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.15 (m, 2H), 7.02 (m, 2H) (aromatic C*H*), 4.04 (p, *J* = 9.7 Hz, 1H), 2.89 (dd, *J* = 13.6, 9.6 Hz, 2H), 2.58 (dd, *J* = 13.6, 9.9 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 162.0 (d, $^{1}J_{C\text{-}F}$ = 246.8 Hz), 136.1 (d, $^{4}J_{C\text{-}F}$ = 3.3 Hz), 128.7 (d, $^{3}J_{C\text{-}F}$ = 8.1 Hz), 115.9 (d, $^{2}J_{C\text{-}F}$ = 21.5 Hz) (aromatic *C*), 82.1 (cage *C*), 52.3, 43.1 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -6.5 (4B), -9.7 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). ^{19}F NMR (470 MHz, $CDCl_3$): δ -114.5 (s, 1F). HRMS: *m/z* calcd for $C_{11}H_{19}{}^{10}B_2{}^{11}B_8F$ $[M]^-$: 278.2479. Found 278.2482.



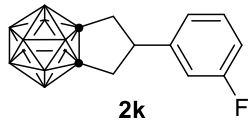
2h

2h: Colorless crystals. 74% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.30 (d, *J* = 8.3 Hz, 2H), 7.11 (d, *J* = 8.3 Hz, 2H) (aromatic C*H*), 4.03 (p, *J* = 9.7 Hz, 1H), 2.90 (dd, *J* = 13.6,

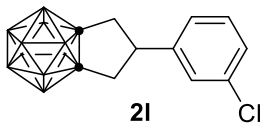
9.7 Hz, 2H), 2.58 (dd, J = 13.6, 9.9 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 138.8, 133.5, 129.2, 128.5 (aromatic *C*), 82.0 (cage *C*), 52.3, 42.9 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -6.4 (4B), -9.7 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{11}H_{19}{}^{10}B_2{}^{11}B_8Cl$ $[M]^-$: 294.2185. Found 294.2182.



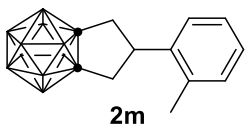
2j: Colorless crystals. 75% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.23 (dd, J = 11.1, 4.8 Hz, 1H), 7.09 (m, 1H), 6.98 (m, 2H) (aromatic C*H*), 4.02 (p, J = 9.7 Hz, 1H), 2.88 (dd, J = 13.6, 9.6 Hz, 2H), 2.63 (dd, J = 13.6, 9.9 Hz, 2H), 2.34 (s, 3H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 140.3, 138.8, 128.9, 128.3, 127.8, 124.1 (aromatic *C*), 82.3 (cage *C*), 53.0, 43.0, 21.4 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -6.5 (4B), -9.7 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{12}H_{22}{}^{10}B_2{}^{11}B_8$ $[M]^-$: 274.2730. Found 274.2733.



2k: Colorless crystals. 72% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.30 (m, 1H), 6.97 (m, 2H), 6.88 (d, J = 9.6 Hz, 1H) (aromatic C*H*), 4.04 (p, J = 9.6 Hz, 1H), 2.91 (dd, J = 13.2, 10.0 Hz, 2H), 2.61 (dd, J = 13.1, 10.3 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 163.0 (d, $^{1}J_{C\text{-}F}$ = 247.4 Hz), 142.8 (d, $^{3}J_{C\text{-}F}$ = 7.0 Hz), 130.7 (d, $^{3}J_{C\text{-}F}$ = 8.4 Hz), 122.7 (d, $^{4}J_{C\text{-}F}$ = 2.8 Hz), 114.6 (d, $^{2}J_{C\text{-}F}$ = 21.0 Hz), 114.1 (d, $^{2}J_{C\text{-}F}$ = 21.8 Hz) (aromatic *C*), 81.9 (cage *C*), 52.5, 42.8 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -6.4 (4B), -9.6 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). ^{19}F NMR (470 MHz, $CDCl_3$): δ -111.7 (s, 1F). HRMS: *m/z* calcd for $C_{11}H_{19}{}^{10}B_2{}^{11}B_8F$ $[M]^-$: 278.2479. Found 278.2482.

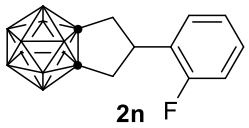


2l: Colorless crystals. 74% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.27 (m, 2H), 7.17 (s, 1H), 7.07 (d, J = 6.9 Hz, 1H) (aromatic C*H*), 4.02 (p, J = 9.7 Hz, 1H), 2.91 (dd, J = 13.6, 9.7 Hz, 2H), 2.61 (dd, J = 13.6, 9.9 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 142.3, 134.9, 130.4, 127.9, 127.4, 125.3 (aromatic *C*), 81.9 (cage *C*), 52.5, 42.8 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -6.4 (4B), -9.6 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{11}H_{19}{}^{10}B_2{}^{11}B_8Cl$ $[M]^-$: 294.2185. Found 294.2184.

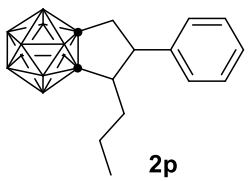


2m: Colorless crystals. 45% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.24 (m, 2H), 7.15 (m, 2H) (aromatic C*H*), 4.33 (p, J = 9.7 Hz, 1H), 2.84 (dd, J = 13.5, 9.6 Hz, 2H), 2.59 (dd, J = 13.5, 9.9 Hz,

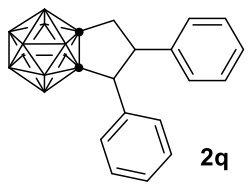
2H), 2.32 (s, 3H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 138.4, 135.4, 130.7, 127.3, 127.0, 126.1 (aromatic *C*), 82.3 (cage *C*), 48.2, 42.3, 19.7 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -6.5 (4B), -9.7 (1B), -10.6 (2B), -11.9 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{12}H_{22}{}^{10}B_2{}^{11}B_8$ $[M]^-$: 274.2730. Found 274.2735.



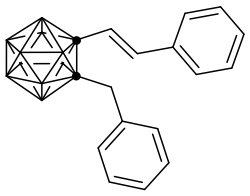
2n: Colorless crystals. 43% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.26 (m, 1H), 7.21 (m, 1H), 7.13 (m, 1H), 7.04 (m, 1H) (aromatic C*H*), 4.28 (p, *J* = 9.8 Hz, 1H), 2.86 (dd, *J* = 13.4, 9.6 Hz, 2H), 2.69 (dd, *J* = 13.4, 10.0 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 160.5 (d, $^{1}J_{C\text{-}F}$ = 246.6 Hz), 129.4 (d, $^{3}J_{C\text{-}F}$ = 8.5 Hz), 128.5 (d, $^{3}J_{C\text{-}F}$ = 4.1 Hz), 126.8 (d, $^{2}J_{C\text{-}F}$ = 13.6 Hz), 124.7 (d, $^{4}J_{C\text{-}F}$ = 3.6 Hz), 116.0 (d, $^{2}J_{C\text{-}F}$ = 22.4 Hz) (aromatic *C*), 82.0 (cage *C*), 46.1, 41.1 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -6.5 (4B), -9.7 (1B), -10.5 (2B), -12.0 (1B), -12.9 (2B). ^{19}F NMR (470 MHz, $CDCl_3$): δ -116.4 (s, 1F). HRMS: *m/z* calcd for $C_{11}H_{19}{}^{10}B_2{}^{11}B_8F$ $[M]^-$: 278.2479. Found 278.2483.



2p: Colorless crystals. 77% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34 (t, *J* = 7.2 Hz, 2H), 7.28 (d, *J* = 7.4 Hz, 1H), 7.19 (d, *J* = 7.2 Hz, 2H) (aromatic C*H*), 3.36 (m, 1H), 2.80 (m, 2H), 2.54 (m, 1H), 1.51 (m, 1H), 1.40 (m, 2H), 1.11 (m, 1H), 0.76 (t, *J* = 6.3 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 140.1, 129.0, 127.7, 127.7 (aromatic *C*), 86.3, 82.1 (cage *C*), 60.5, 53.5, 43.2, 35.5, 20.7, 13.8 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -5.9 (2B), -6.7 (2B), -10.3 (2B), -11.8 (1B), -13.4 (3B). HRMS: *m/z* calcd for $C_{14}H_{26}{}^{10}B_2{}^{11}B_8$ $[M]^-$: 302.3043. Found 302.3045.

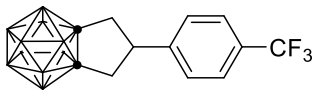


2q: Colorless oil. 27% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30 (m, 5H), 7.20 (m, 3H), 7.12 (d, *J* = 6.8 Hz, 2H) (aromatic C*H*), 4.24 (m, 1H), 4.14 (d, *J* = 10.8 Hz, 1H), 3.01 (dd, *J* = 13.7, 9.0 Hz, 1H), 2.81 (dd, *J* = 13.7, 9.9 Hz, 1H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 139.0, 135.1, 128.9, 128.8, 128.6, 128.0, 127.7, 127.3 (aromatic *C*), 85.9, 80.2 (cage *C*), 59.4, 57.8, 42.3 (alkyl *C*). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -5.9 (1B), -7.1 (3B), -10.3 (4B), -13.4 (2B). HRMS: *m/z* calcd for $C_{17}H_{24}{}^{10}B_2{}^{11}B_8$ $[M]^-$: 336.2887. Found 336.2889.



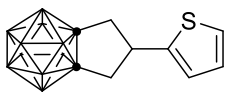
1-Bn-2-C_6H_5CH=C-*o*-$C_2B_{10}H_{12}$ was also isolated as colorless oil in 60% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (m, 2H), 7.42 (m, 3H), 7.31 (m, 3H), 7.12 (m, 2H) (aromatic C*H*), 7.07 (d, *J* = 15.7 Hz, 1H), 6.39 (d, *J* = 15.7 Hz, 1H) (alkenyl C*H*), 3.44 (s, 2H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 141.8, 135.4, 134.2, 130.2, 129.9, 129.0, 128.5, 127.9, 127.2, 120.8 (aromatic *C*), 80.8, 79.8 (cage *C*), 41.3 (*C*H_2). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -3.9 (2B), -10.2 (8B). HRMS: *m/z* calcd for $C_{17}H_{24}{}^{10}B_2{}^{11}B_8$ [M]$^-$: 336.2887. Found 336.2888.

General synthetic procedure B. A suspension of $MgH_2(THF)_{0.23}$[3] (8.5 mg, 0.2 mmol) and 1-arylethynyl-2-methyl-*o*-carborane **1** (0.1 mmol) in a mixed solvent of THF (0.067 mL) and toluene (0.666 mL) in a closed Schlenk was stirred at 80°C for 36 h. Reaction was then quenched with water (1 mL) and extracted with diethyl ether (10 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give product **2**.



2i

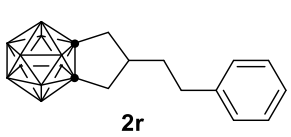
2i: Colorless crystals. 60% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.60 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H) (aromatic C*H*), 4.11 (p, *J* = 9.7 Hz, 1H), 2.94 (dd, *J* = 13.6, 9.7 Hz, 2H), 2.63 (dd, *J* = 13.6, 9.9 Hz, 2H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 144.3, 130.1 (q, $^2J_{C\text{-}F}$ = 32.7 Hz), 127.6, 126.1 (q, $^3J_{C\text{-}F}$ = 3.7 Hz), 124.0 (q, $^1J_{C\text{-}F}$ = 272.1 Hz) (aromatic *C*), 81.8 (cage *C*), 52.5, 42.8 (alkyl *C*). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -6.4 (4B), -9.6 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). ^{19}F NMR (470 MHz, $CDCl_3$): δ -62.7 (s, 3F). HRMS: *m/z* calcd for $C_{12}H_{19}{}^{10}B_2{}^{11}B_8F_3$ [M]$^-$: 328.2448. Found 328.2449.



2o

2o: Colorless crystals. 75% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32 (dd, *J* = 5.0, 2.9 Hz, 1H), 6.99 (m, 1H), 6.91 (dd, *J* = 5.0, 1.3 Hz, 1H) (aromatic C*H*), 4.17 (p, *J* = 9.6 Hz, 1H), 2.90 (dd, *J* = 13.5, 9.6 Hz, 2H), 2.61 (dd, *J* = 13.5, 9.7 Hz, 2H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 141.4, 127.2, 125.9, 120.9 (aromatic *C*), 82.1 (cage *C*), 47.9, 42.4 (alkyl *C*). ^{11}B{^{1}H} NMR

(160 MHz, $CDCl_3$): δ -6.5 (4B), -9.7 (1B), -10.6 (2B), -11.9 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_9H_{18}{}^{10}B_2{}^{11}B_8S$ $[M]^-$: 266.2138. Found 266.2141.



2r: Colorless crystals. 82% yield. ^1H NMR (500 MHz, $CDCl_3$): δ 7.29 (t, J = 7.5 Hz, 2H), 7.21 (t, J = 7.3 Hz, 1H), 7.12 (d, J = 7.2 Hz, 2H) (aromatic C*H*), 2.88 (m, 1H), 2.68 (m, 2H), 2.54 (m, 2H), 2.20 (m, 2H), 1.76 (m, 2H). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ 140.7, 128.6, 128.1, 126.3 (aromatic *C*), 83.0 (cage *C*), 47.4, 41.2, 37.9, 34.2 (alkyl *C*). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -6.8 (4B), -9.5 (1B), -10.7 (2B), -11.5 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{13}H_{24}{}^{10}B_2{}^{11}B_8$ $[M-H]^-$: 287.2808. Found 287.2812.

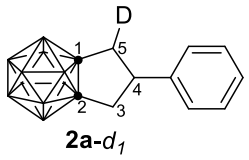
Deuterium labelling experiments

Reaction of 1a with MeMgBr in a mixed solvent of THF-*d*$_8$/toluene-*d*$_8$ (0.8 mL, 1/10 in V/V). A suspension of MeMgBr (3.0 M in Et_2O, 0.067 mL, 0.2 mmol) and 1-phenylethynyl-2-methyl-*o*-carborane (**1a**; 25.8 mg, 0.1 mmol) in a mixed solvent of THF-*d*$_8$ (0.067 mL) and toluene-*d*$_8$ (0.667 mL) in a closed Schlenk flask was stirred at 80°C for 36 h. Reaction was then quenched with water (1 mL) and extracted with diethyl ether (10 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give product **2a** (20.8 mg, 80%).

Reaction of 1a with C_2D_5MgBr. A suspension of C_2D_5MgBr[4] (1.0 M in THF, 0.2 mL, 0.2 mmol) and 1-phenylethynyl-2-methyl-*o*-carborane (**1a**; 25.8 mg, 0.1 mmol) in toluene (0.6 mL) in a closed Schlenk flask was stirred at 80°C for 36 h. Reaction was then quenched with water (1 mL) and extracted with diethyl ether (10 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give product **2a** (13.0 mg, 50%).

Quenching with D_2O. A suspension of MeMgBr (3.0 M in Et_2O, 0.067 mL, 0.2 mmol) and 1-phenylethynyl-2-methyl-*o*-carborane (**1a**; 25.8 mg, 0.1 mmol) in a mixed solvent of THF (0.067 mL) and toluene (0.667 mL) in a closed Schlenk flask was stirred at 80°C for 36 h. Reaction was then quenched with D_2O (1 mL) and extracted with

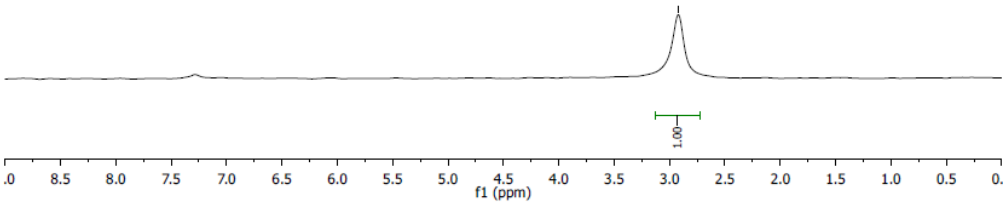
diethyl ether (10 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give product **2a**-d_1 (20.4 mg, 78%).



2a-d_1

2a-d_1: Colorless crystals. 78% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34 (m, 2H), 7.28 (m, 1H), 7.18 (dd, J = 5.2, 3.3 Hz, 2H) (aromatic C*H*), 4.04 (m, 1H), 2.90 (dd, J = 13.6, 9.6 Hz, 1H), 2.63 (dd, J = 13.5, 9.9 Hz, 2H). ^{2}H NMR (77 MHz, $CHCl_3$): 2.92 (s, 1D). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 140.4, 129.1, 127.6, 127.1 (aromatic *C*), 82.3, 82.2 (cage *C*), 53.0, 43.0, 42.7 (t, $J_{C\text{-}D}$ = 21.1 Hz) (alkyl *C*). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -6.5 (4B), -9.7 (1B), -10.6 (2B), -12.0 (1B), -12.9 (2B). HRMS: *m/z* calcd for $C_{11}H_{19}D^{10}B_2{}^{11}B_8$ $[M]^-$: 261.2636. Found 261.2638.

a)



b)

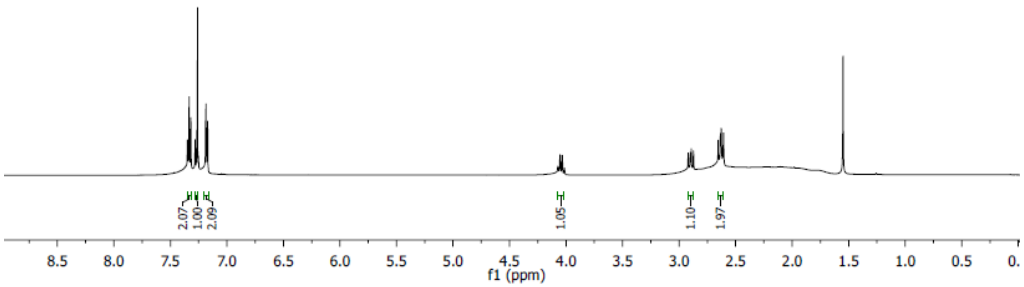
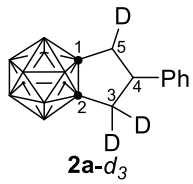


Figure S1. a) ^{2}H NMR spectrum of **2a**-d_1 in $CHCl_3$; b) ^{1}H NMR spectrum of **2a**-d_1 in $CDCl_3$.

Reaction of 1a-d_3 with MeMgBr. A suspension of MeMgBr (3.0 M in Et_2O, 0.067 mL, 0.2 mmol) and 1-(PhC≡C)-2-CD_3-*o*-carborane (**1a**-d_3; 26.1 mg, 0.1 mmol) in a mixed solvent of THF (0.067 mL) and toluene (0.667 mL) in a closed Schlenk flask was stirred at 80°C for 36 h. Reaction was then quenched with water (1 mL) and

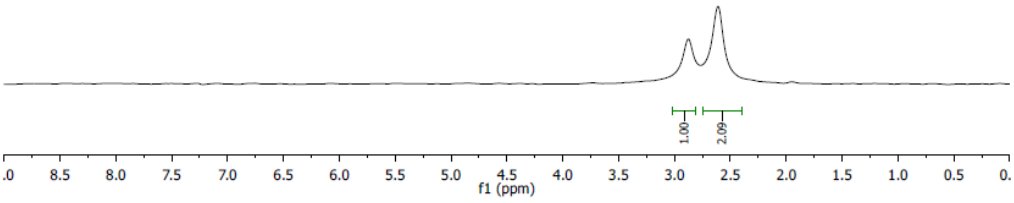
extracted with diethyl ether (10 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give product **2a**-d_3 (20.0 mg, 76%).



2a-d_3

2a-d_3: Colorless crystals. 76% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 (t, J = 7.3 Hz, 2H), 7.28 (d, J = 7.2 Hz, 1H), 7.18 (d, J = 7.3 Hz, 2H) (aromatic C*H*), 4.03 (d, J = 9.5 Hz, 1H), 2.88 (d, J = 9.5 Hz, 1H). ^{2}H NMR (77 MHz, $CHCl_3$): 2.88 (s, 1D), 2.61 (s, 2D). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 140.3, 129.1, 127.6, 127.1 (aromatic *C*), 82.2 (cage *C*), 52.8, 42.7 (t, $J_{C\text{-}D}$ = 21.0 Hz) (alkyl *C*). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -6.9 (4B), -10.1 (1B), -11.0 (2B), -12.5 (1B), -13.3 (2B). HRMS: *m/z* calcd for $C_{11}H_{17}D_3{}^{10}B_2{}^{11}B_8$ $[M]^-$: 263.2762. Found 263.2758.

a)



b)

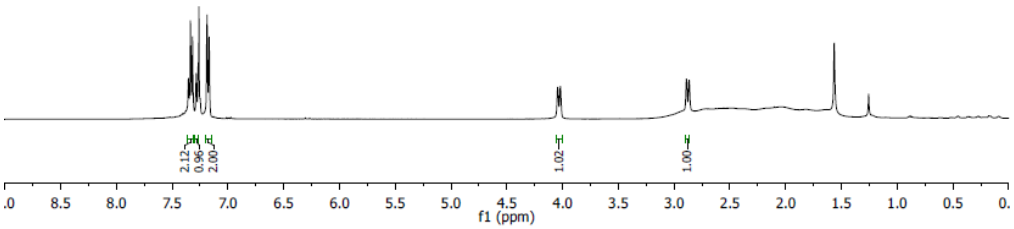
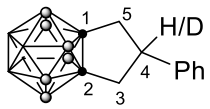


Figure S2. a) ^{2}H NMR spectrum of **2a**-d_3 in $CHCl_3$; b) ^{1}H NMR spectrum of **2a**-d_3 in $CDCl_3$.

Reaction of 1a-d_6 with MeMgBr. A suspension of MeMgBr (3.0 M in Et_2O, 0.067 mL, 0.2 mmol) and 1-phenylethynyl-2-methyl-3,4,5,6,7,11-D_6-*o*-carborane (**1a**-d_6; 26.4mg, 0.1 mmol) in a mixed solvent of THF (0.067 mL) and toluene (0.667 mL) in a closed Schlenk flask was stirred at 80°C for 24 h. Reaction was then quenched with water (1 mL) and extracted with diethyl ether (10 mL x 3). The ether solutions were

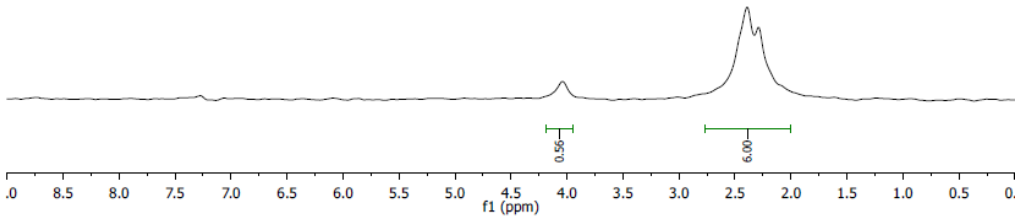
combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give the starting material **1a**-d_6 (10.0 mg, 38%), product **2a**-d_7 (6.7 mg, 25%) and a mixture of **3** and **2a**-d_7 (1.6 mg, 6%). In addition, an inseparable mixture of multi-B-methylated *o*-carboranes **1a**-Me_n (24%) were detected by GC-MS.



2a-d_7

2a-d_7: Colorless crystals. 25% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34 (t, J = 7.4 Hz, 2H), 7.28 (d, J = 7.4 Hz, 1H), 7.18 (d, J = 7.4 Hz, 2H) (aromatic C*H*), 4.04 (p, J = 9.5 Hz, 0.44H), 2.90 (dd, J = 13.6, 9.4 Hz, 2H), 2.63 (dd, J = 13.5, 9.1 Hz, 2H). ^{2}H{^{11}B} NMR (77 MHz, $CDCl_3$): 4.04 (s, 0.56D) (C*D*), 2.39 (s, 4D), 2.29 (s, 2D) (B*D*). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 141.8, 140.4, 140.3, 129.1, 127.6, 127.1 (aromatic *C*), 82.1 (cage *C*), 53.0, 52.7 (t, $J_{C\text{-}D}$ = 20.3 Hz), 42.9 (alkyl *C*). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -6.6 (4B), -9.8 (1B), -10.7 (2B), -12.0 (1B), -13.0 (2B). HRMS: *m/z* calcd for $C_{11}H_{13}D_7{}^{10}B_2{}^{11}B_8$ $[M\text{-}H]^-$: 266.2940. Found 266.2950.

a)



b)

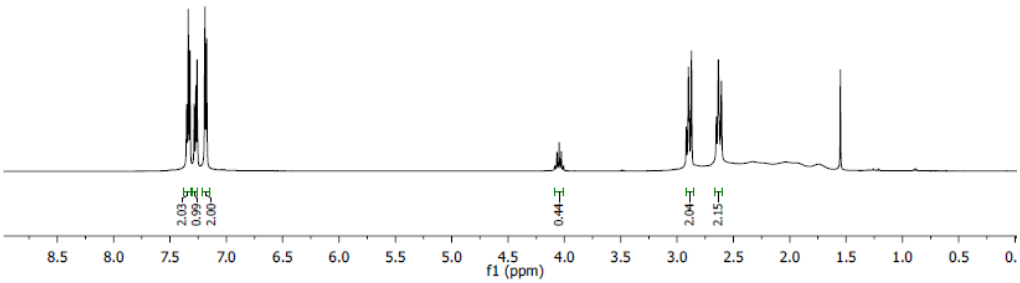
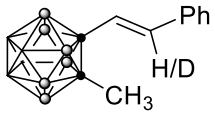


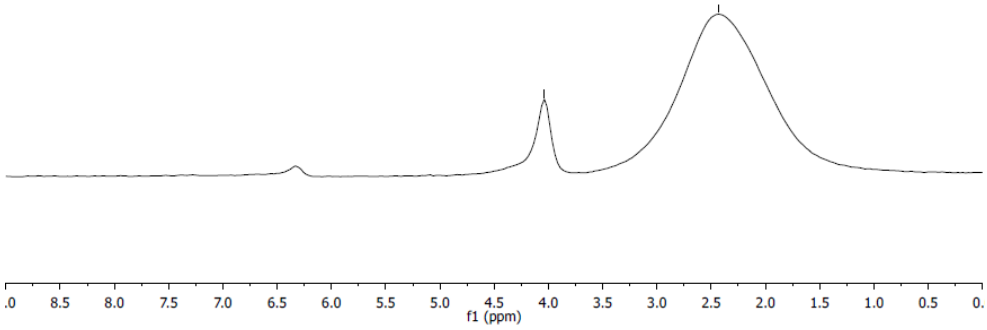
Figure S3. a) ^{2}H{^{11}B} NMR spectrum of **2a**-d_7 in $CHCl_3$; b) ^{1}H NMR spectrum of **2a**-d_7 in $CDCl_3$.



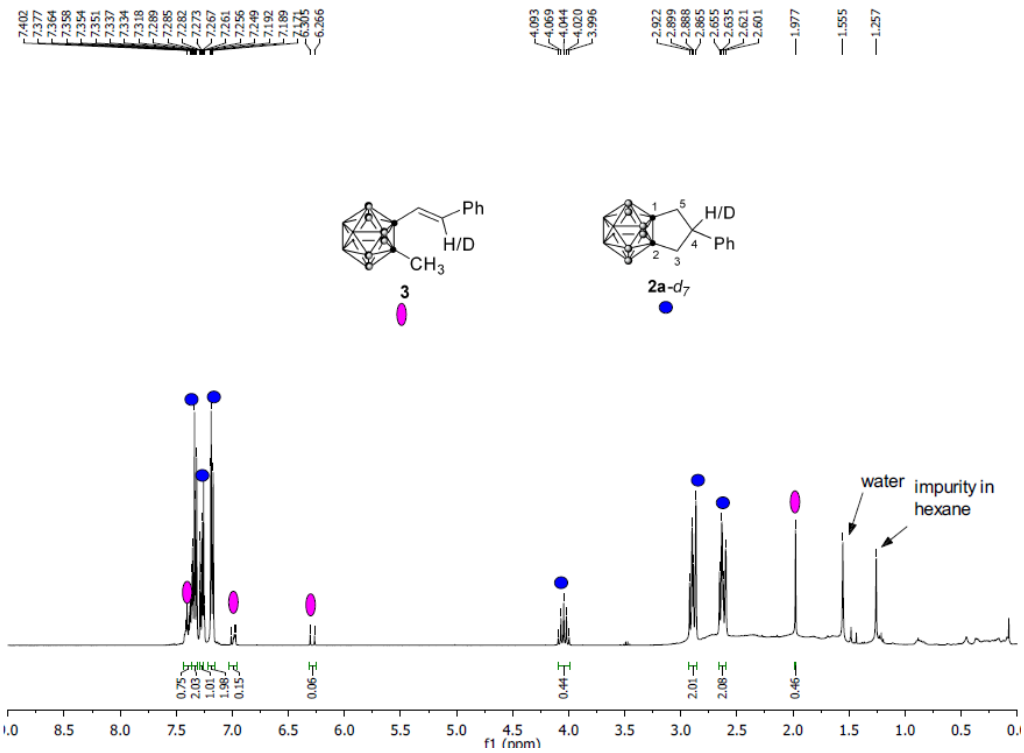
3

3 was obtained as a mixture of **3** with 60% D incorporation and **2a**-d_7 in a molar ration of 0.15:1 by ^{1}H NMR. Compared ^{1}H NMR spectra of the mixture, **2a**-d_7 and 1-phenylethenyl-2-methyl-*o*-carborane, the resonances at 7.40 (m, 0.75H) (aromatic C*H*), 6.98 (m, 0.15H), 6.27 (d, J = 15.6 Hz, 0.06H) (alkenyl C*H*), 1.98 (s, 0.46H) (CH_3) ppm were assigned to **3** (Figure S4b). A resonance at 6.30 ppm in ^{2}H NMR spectrum of the mixture supported the incorporation of D at the alkenyl C (Figure S4a).

a)



b)



c)

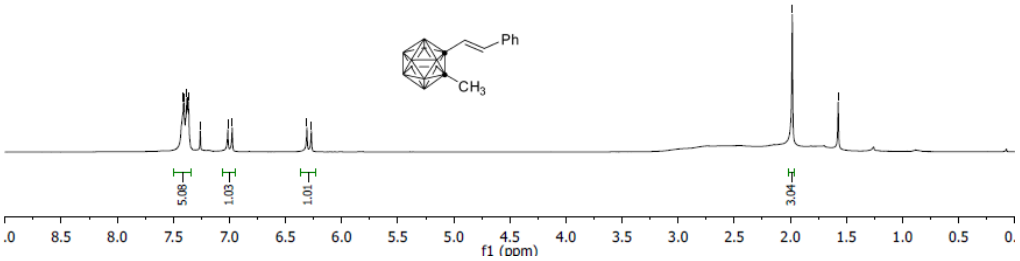
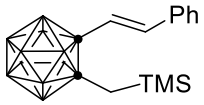


Figure S4. a) ^{2}H NMR spectrum of the mixture of **3** and **2a**-d_7 in $CHCl_3$; b) ^{1}H NMR spectrum of the mixture of **3** and **2a**-d_7 in $CDCl_3$; c) ^{1}H NMR spectrum of 1-phenylethenyl-2-methyl-*o*-carborane in $CDCl_3$.

Control experiments

Reaction of 1a with MeMgBr in the presence of 1,1-diphenylethylene. A suspension of MeMgBr (3.0 M in Et_2O, 0.067 mL, 0.2 mmol), 1-phenylethynyl-2-methyl-*o*-carborane (**1a**; 25.8 mg, 0.1 mmol) and 1,1-diphenylethylene (36.0 mg, 0.2 mmol) in a mixed solvent of THF (0.067 mL) and toluene (0.667 mL) in a closed Schlenk flask was stirred at 80^{o}C for 36 h. Reaction was then quenched with water (1 mL) and extracted with diethyl ether (10 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give product **2a** (20.8 mg, 80%).

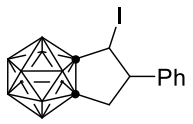
Quenching with TMSCl. A suspension of MeMgBr (3.0 M in Et_2O, 0.067 mL, 0.2 mmol) and 1-phenylethynyl-2-methyl-*o*-carborane (**1a**; 25.8 mg, 0.1 mmol) in a mixed solvent of THF (0.067 mL) and toluene (0.667 mL) in a closed Schlenk flask was stirred at 80^{o}C for 18 h. Reaction mixture was then treated with TMSCl (21.7 mg, 0.2 mmol). After further stirring at room temperature for 12 h, the reaction was quenched with water and extracted with diethyl ether (10 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give product **2a** (9.9 mg, 38%) and **4** (11.6 mg, 35%).



4

4: Colorless crystals. 35% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45 (m, 2H), 7.39 (m, 3H) (aromatic C*H*), 6.98 (d, *J* = 15.7 Hz, 1H), 6.31 (d, *J* = 15.7 Hz, 1H) (alkenyl C*H*), 1.59 (s, 2H), 0.14 (s, 9H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 141.4, 134.4, 129.7, 128.9, 127.2, 121.2 (aromatic and alkenyl *C*), 81.4, 81.1 (cage *C*), 26.3 (*C*H_2). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -4.0 (1B), -5.1 (1B), -9.0 (2B), -10.6 (6B). HRMS: *m/z* calcd for $C_{14}H_{28}{}^{10}B_2{}^{11}B_8Si$ [M-H]$^-$: 331.2892. Found 331.2885.

Quenching with I_2. A suspension of MeMgBr (3.0 M in Et_2O, 0.067 mL, 0.2 mmol) and 1-phenylethynyl-2-methyl-*o*-carborane (**1a**; 25.8 mg, 0.1 mmol) in a mixed solvent of THF (0.067 mL) and toluene (0.667 mL) in a closed Schlenk flask was stirred at 80^{o}C for 36 h. Reaction mixture was then treated with I_2 (50.8 mg, 0.2 mmol). After further stirring at room temperature for 12 h, the reaction was quenched with water and extracted with diethyl ether (10 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give product **5** (25.1 mg, 65%).



5

5: Colorless crystals. 65% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.37 (m, 3H), 7.24 (m, 2H) (aromatic C*H*), 4.71 (d, *J* = 9.6 Hz, 1H), 4.03 (q, *J* = 9.8 Hz, 1H), 2.78 (d, *J* = 9.8 Hz, 2H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 136.8, 129.3, 129.1, 128.5, 127.6, 127.1 (aromatic *C*), 84.0, 82.2 (cage *C*), 65.9, 42.9, 29.7 (alkyl *C*). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -5.6 (1B), -6.5 (3B), -7.9 (1B), -9.4 (1B), -10.4(1B), -13.1 (3B). HRMS: *m/z* calcd for $C_{11}H_{19}{}^{10}B_2{}^{11}B_8I$ [M-H]$^-$: 385.1462. Found 385.1461.

Reaction of 1i with MeMgBr. A suspension of MeMgBr (3.0 M in Et_2O, 0.067 mL, 0.2 mmol) and 1-[(4-trifluoromethyl)phenylethynyl]-2-methyl-*o*-carborane (**1i**; 32.6 mg, 0.1 mmol) in a mixed solvent of THF (0.067 mL) and toluene (0.667 mL) in a closed Schlenk flask was stirred at 80^{o}C for 36 h. Reaction was then quenched with D_2O (1 mL) and extracted with diethyl ether (10 mL x 3). The ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give **2i**-d_1

(2.3 mg, 7%) and **1i** (26.1 mg, 80%) without any D incorporation, suggesting that the cage-CH_3 proton was not deprotonated by MeMgBr.

X-ray structure determination. The data of **2a**, **2p** and **2r** were collected on a Bruker APEX DUO diffractometer. An empirical absorption correction was applied using the SADABS program.[5] 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 on F^2 using the SHELXTL program package.[6] All hydrogen atoms were geometrically fixed using the riding model. Crystal data and details of data collection and structure refinements were given in Table S2.

CCDC 1998059-1998061 (**2a**, **2p** and **2r**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S2. Crystal Data and Summary of Data Collection and Refinement

	2a	**2p**	**2r**
formula	$C_{11}H_{20}B_{10}$	$C_{14}H_{26}B_{10}$	$C_{13}H_{24}B_{10}$
crystal size (mm)	0.50×0.40×0.30	0.50×0.40×0.30	0.50×0.40×0.30
fw	260.37	302.45	288.42
crystal system	Monoclinic	Monoclinic	Orthorhombic
space group	$P2_1/c$	$P2_1/n$	$Pca2_1$
a, Å	7.7202(4)	9.7246(5)	18.2149(7)
b, Å	21.9059(12)	9.0634(4)	8.1437(4)
c, Å	9.0867(6)	21.3352(10)	12.0108(4)
α, deg	90	90	90
β, deg	98.1207(17)	96.9612(15)	90
γ, deg	90	90	90
V, Å^3	1521.31(15)	1866.58(15)	1781.64(13)
Z	4	4	4
D_{calcd}, Mg/m^3	1.137	1.076	1.075
radiation (λ) Å	0.71073	0.71073	0.71073
2θ range, deg	2.448 to 25.238	2.423 to 25.250	2.236 to 25.249
μ, mm^{-1}	0.054	0.052	0.052
F(000)	544	640	608
no. of obsd reflns	2749	3366	3208
no. of params refnd	190	217	208
goodness of fit	1.054	1.107	1.064
R1	0.0701	0.0624	0.0409
wR2	0.1889	0.1804	0.1066

Reference

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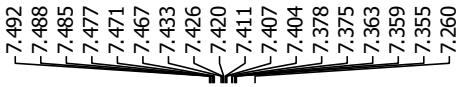

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Receiver Gain	36
Relaxation Delay	1.0000
Pulse Width	12.8000
Acquisition Time	4.0894
Spectrometer Frequency	400.23
Spectral Width	8012.8
Lowest Frequency	-1544.9
Nucleus	1H
Acquired Size	32768
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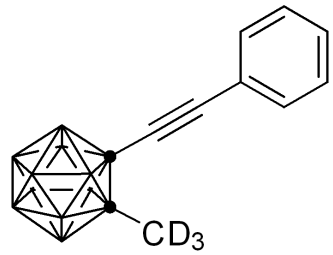
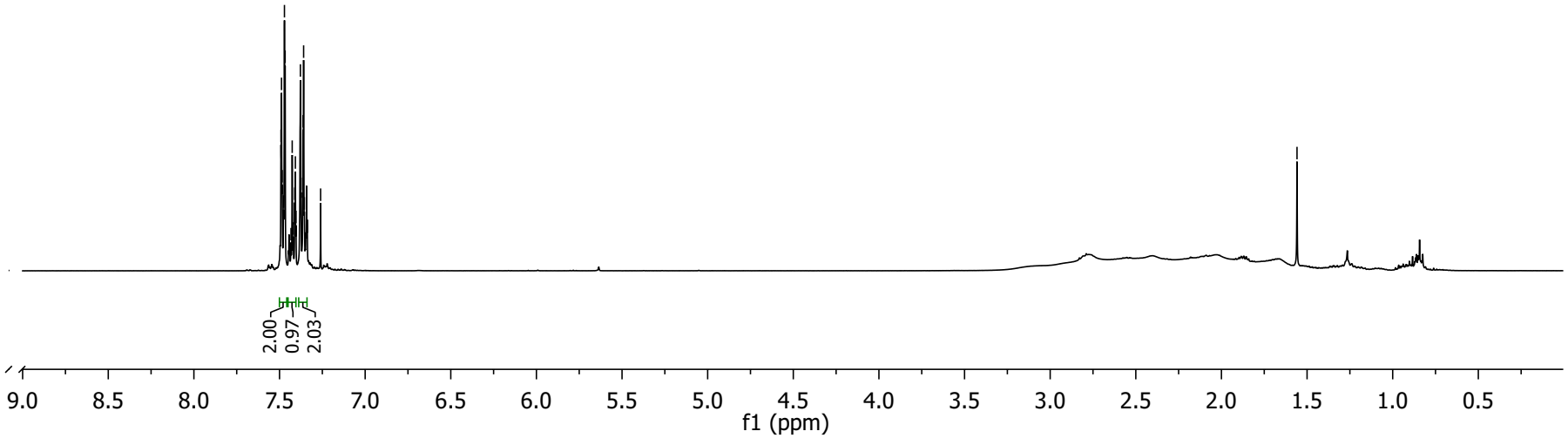
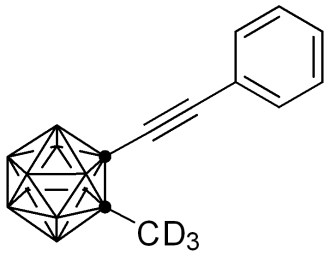


1a-d_3





1a-d_3

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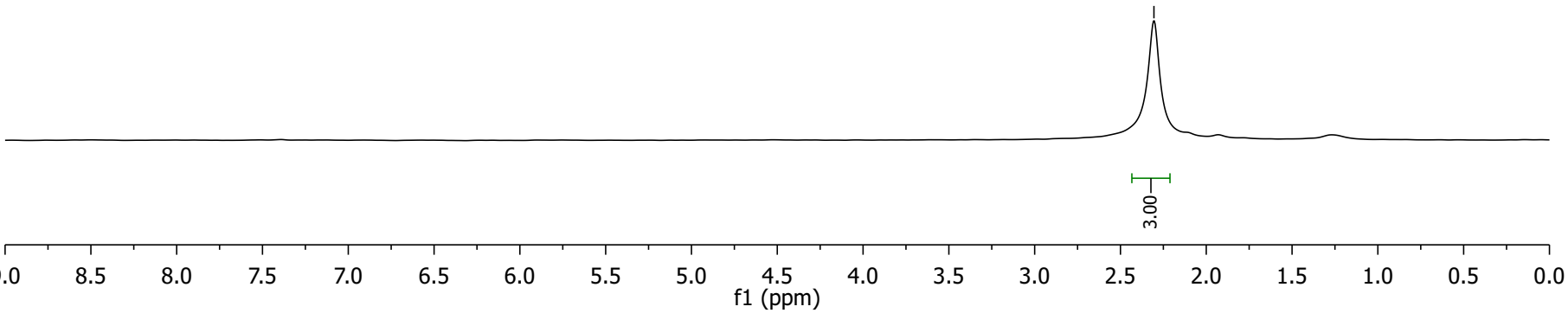

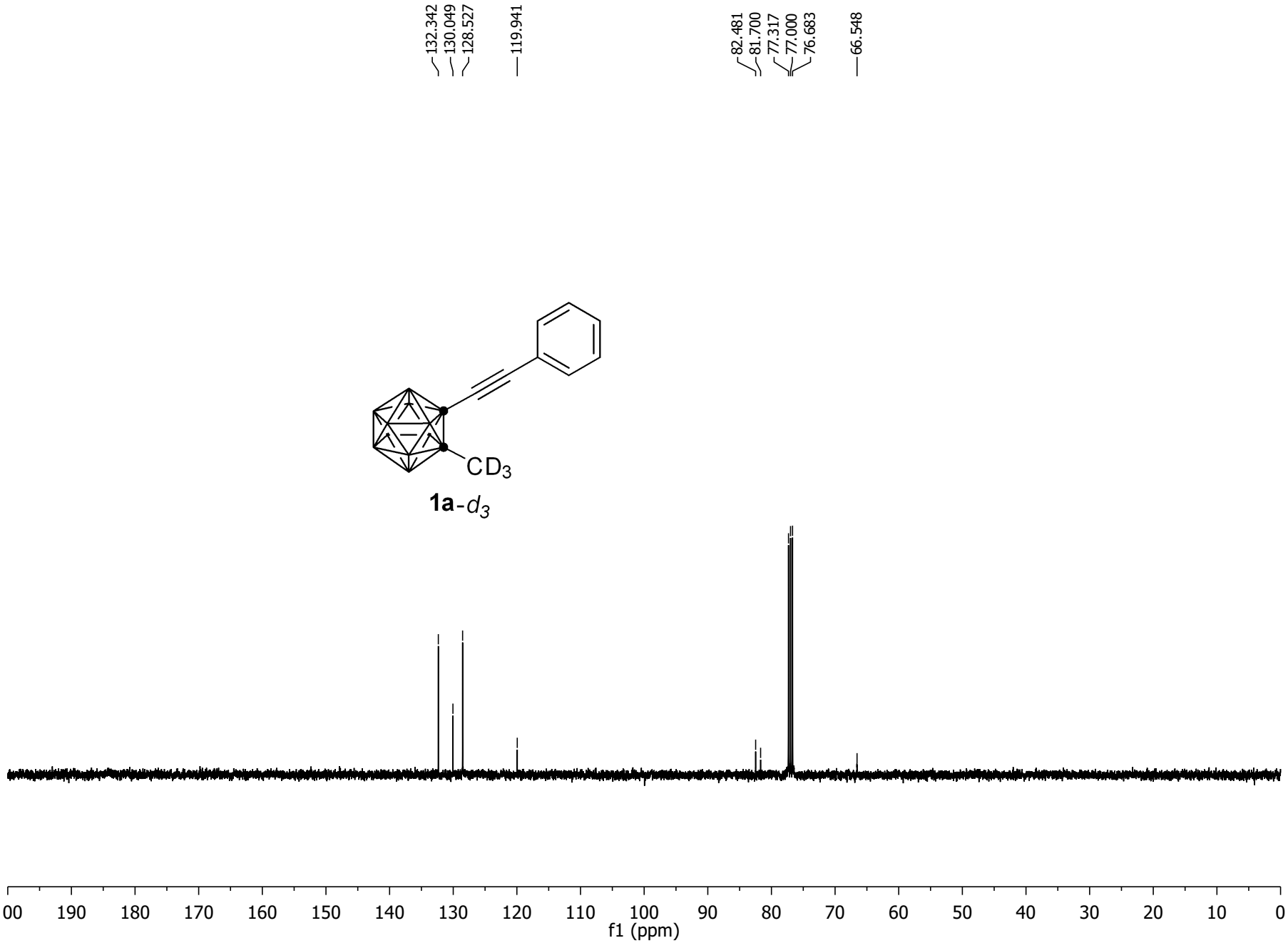

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Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	24
Receiver Gain	203
Relaxation Delay	2.0000
Pulse Width	9.5000
Acquisition Time	1.1010
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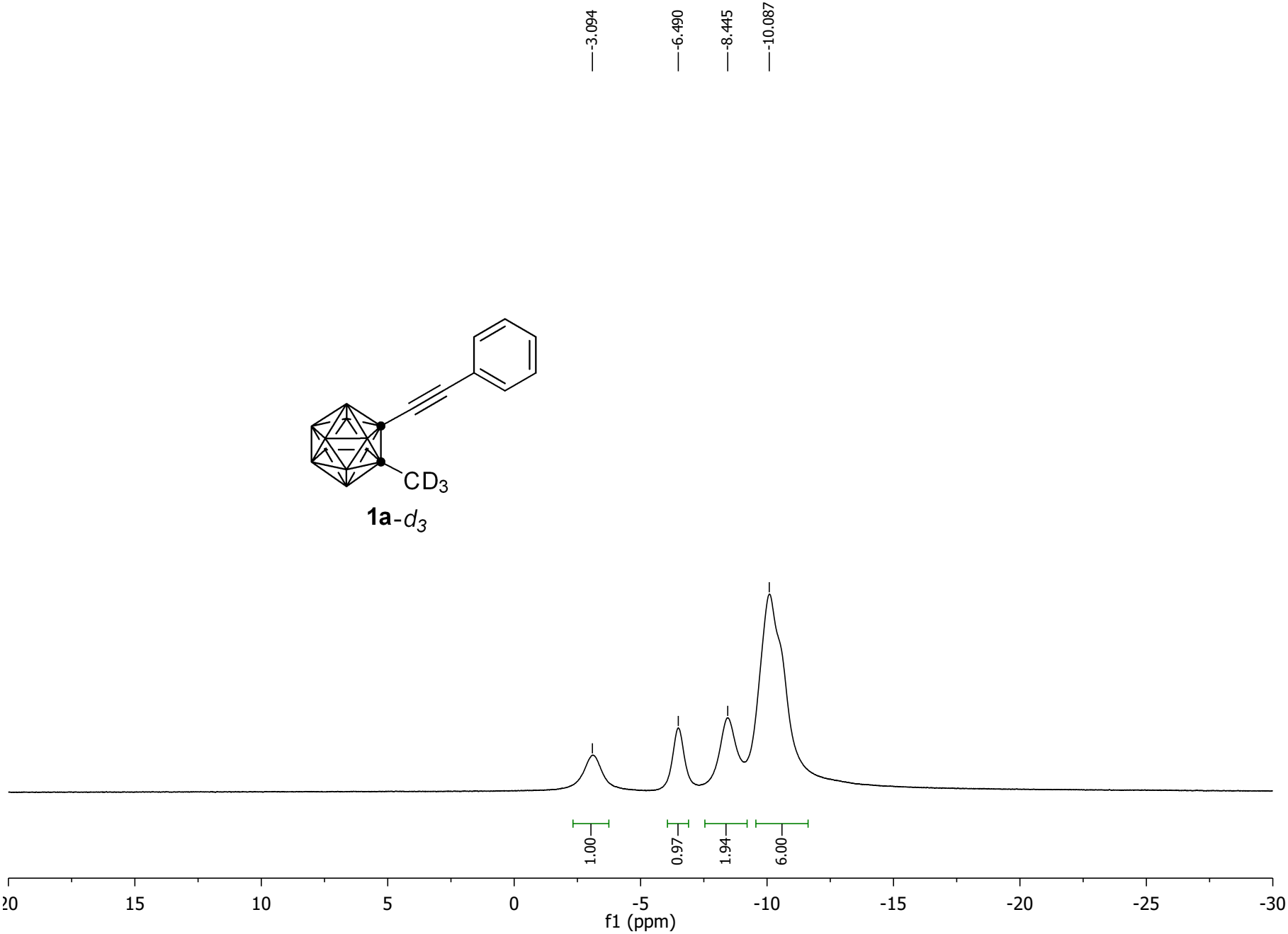
Spectral Width	29761.9
Lowest Frequency	-4822.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



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Receiver Gain	181
Relaxation Delay	2.0000
Pulse Width	7.5000
Acquisition Time	1.3631
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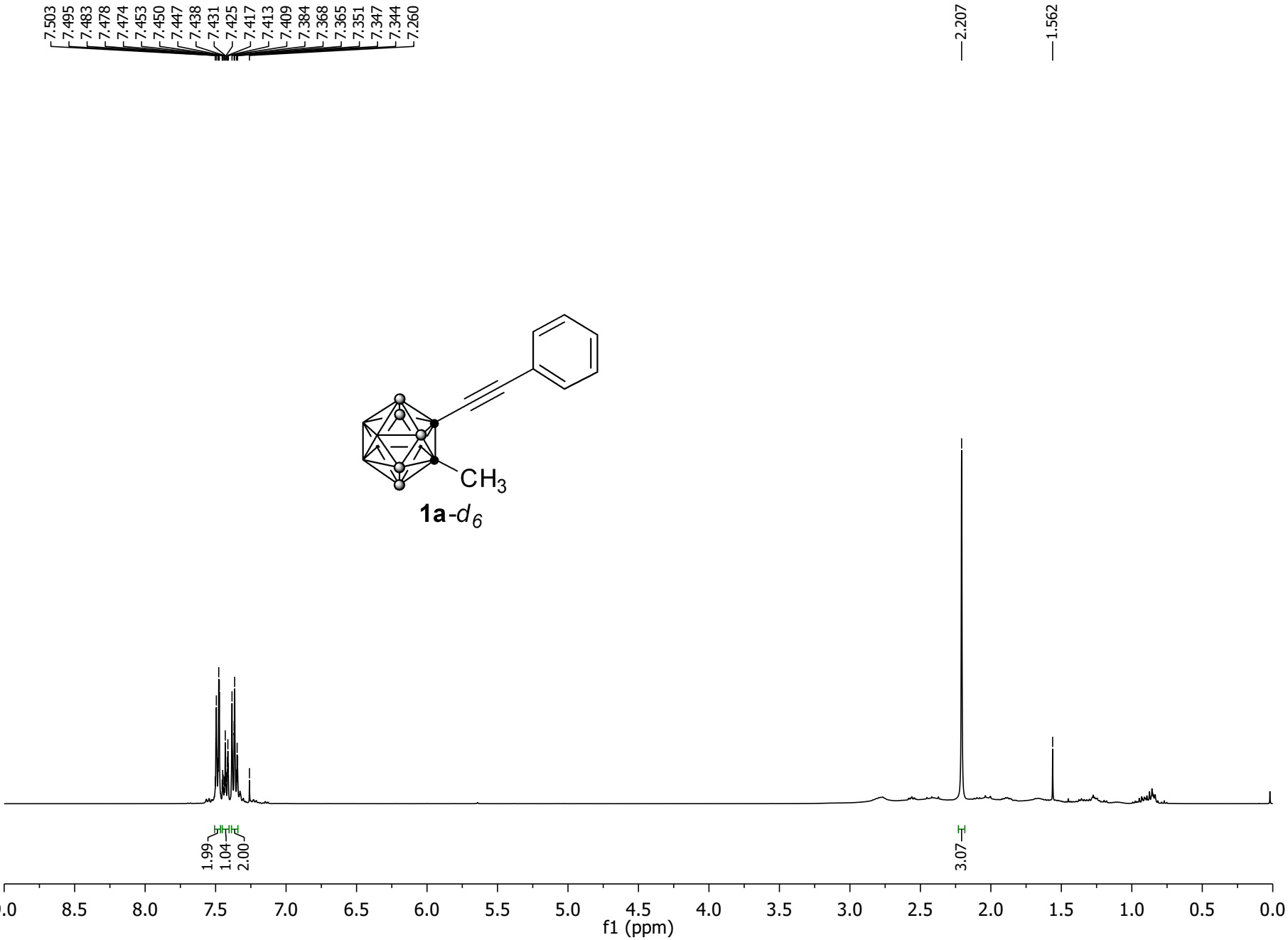
Nucleus	11B
Acquired Size	32768
Spectral Size	65536



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Receiver Gain	64
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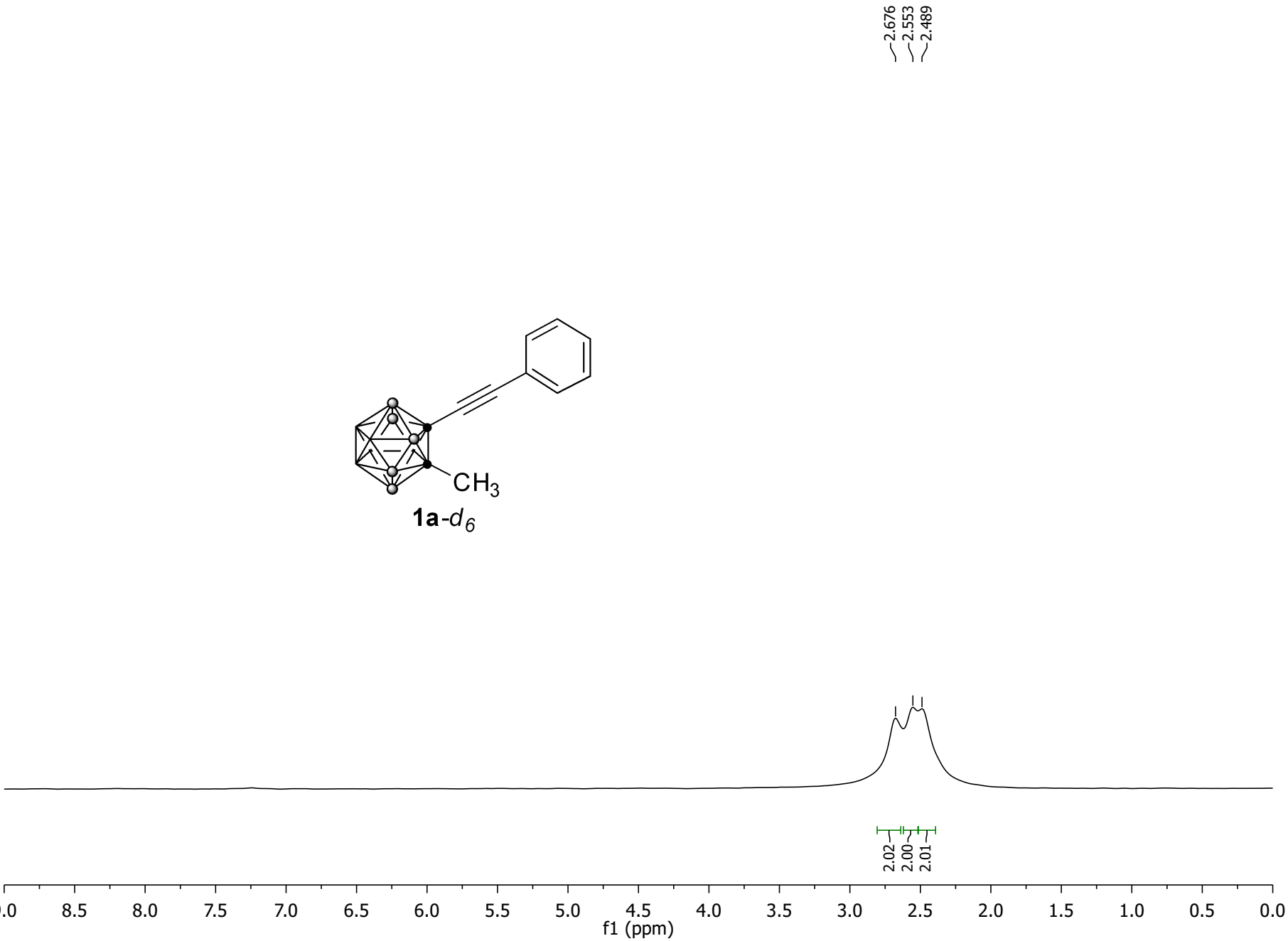

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Temperature	295.4
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Experiment	1D
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Receiver Gain	207
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Acquisition Time	0.9996
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Lowest Frequency	-212.1
Nucleus	2H
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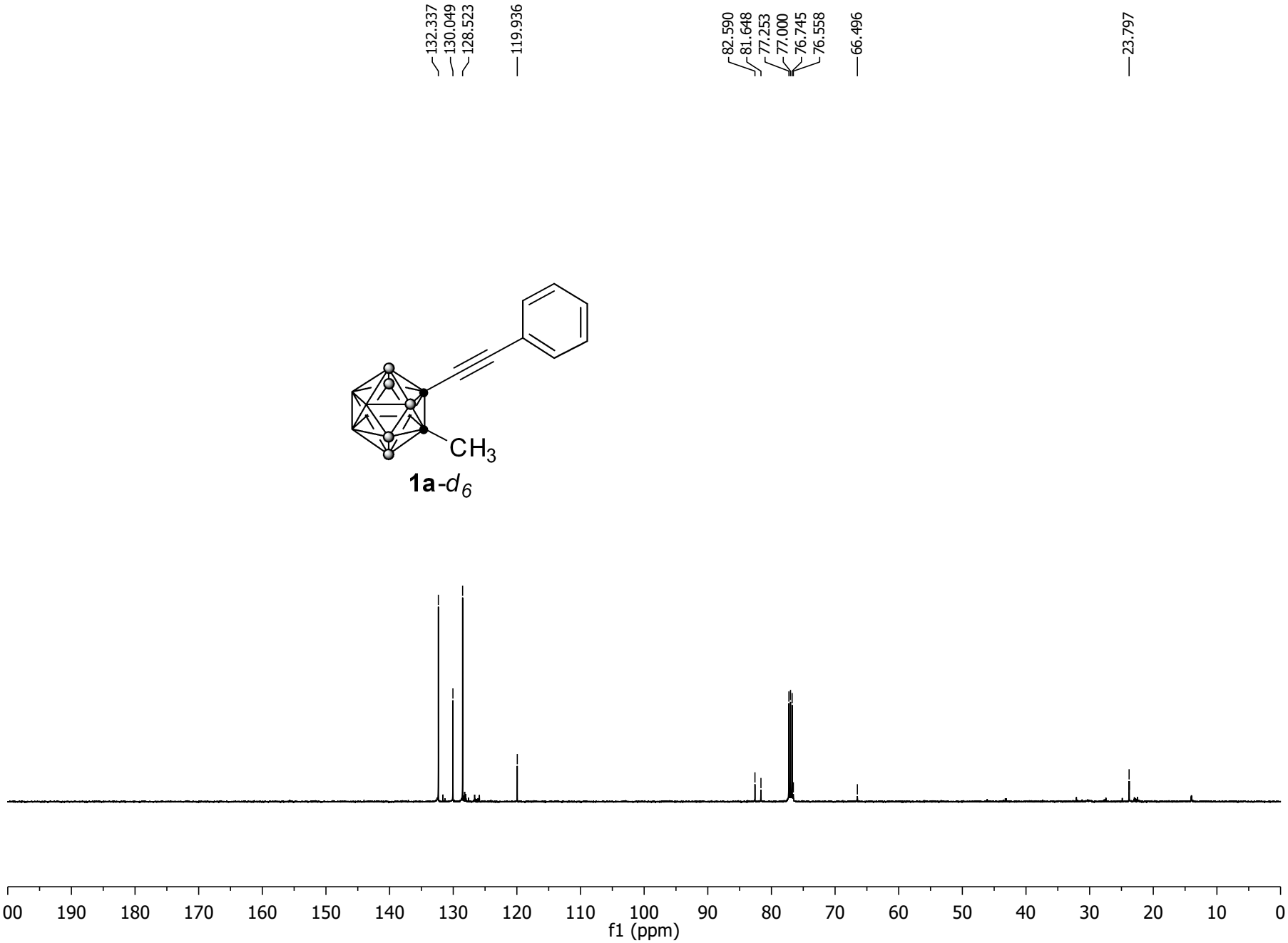

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Solvent	CDCl3
Temperature	298.0
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Experiment	1D
Number of Scans	32
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
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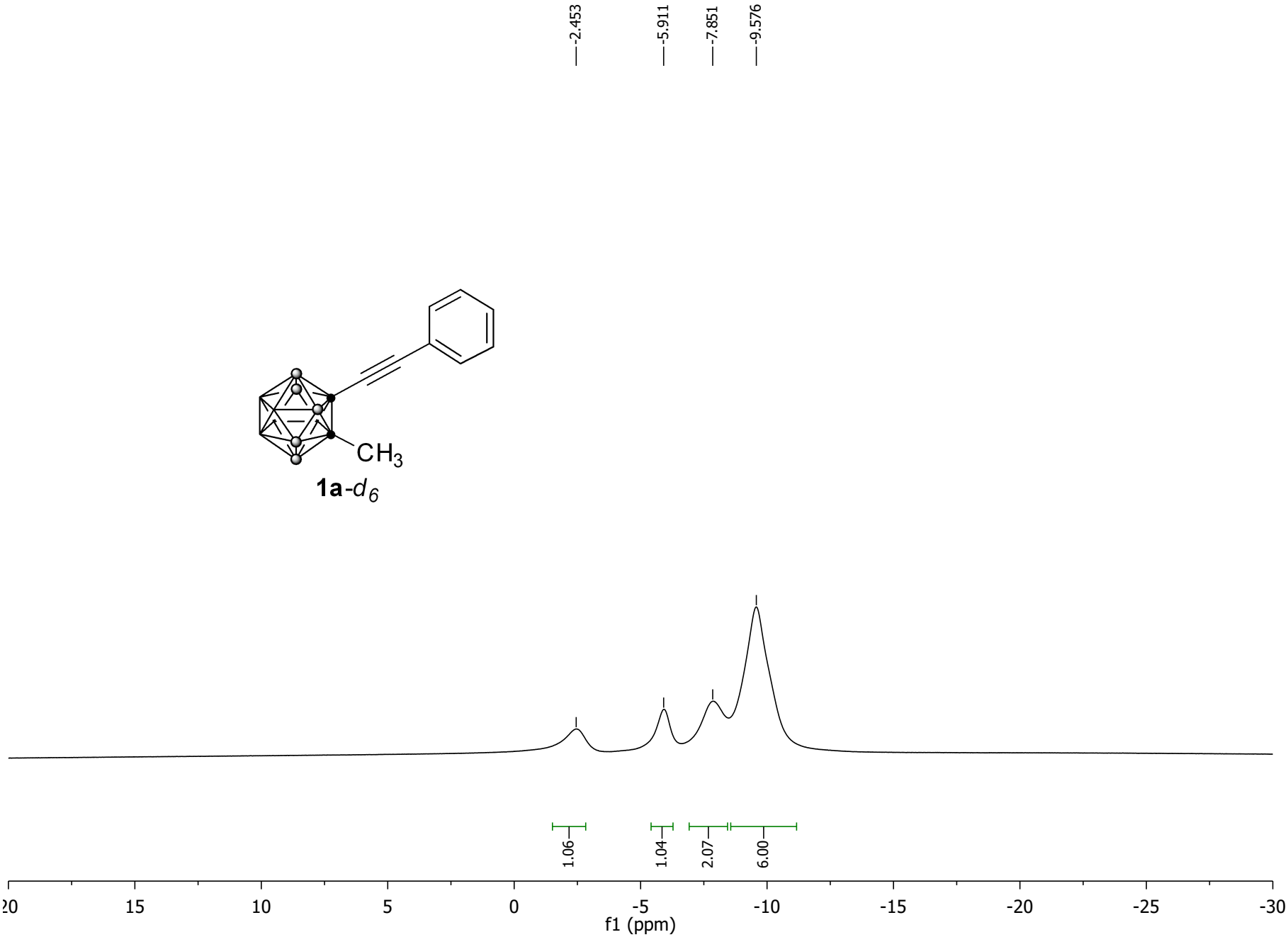
Lowest Frequency	-2313.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



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Solvent	CDCl3
Temperature	294.6
Pulse Sequence	zgig
Experiment	1D
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Relaxation Delay	1.0000
Pulse Width	28.5000
Acquisition Time	1.2845
Spectrometer Frequency	128.38
Spectral Width	25510.2
Lowest Frequency	-12755.3
Nucleus	11B
Acquired Size	32768
Spectral Size	65536

Parameter	Value
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Solvent	CDCl3
Temperature	295.3
Pulse Sequence	zg30
Experiment	1D
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Pulse Width	12.8000
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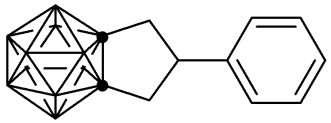
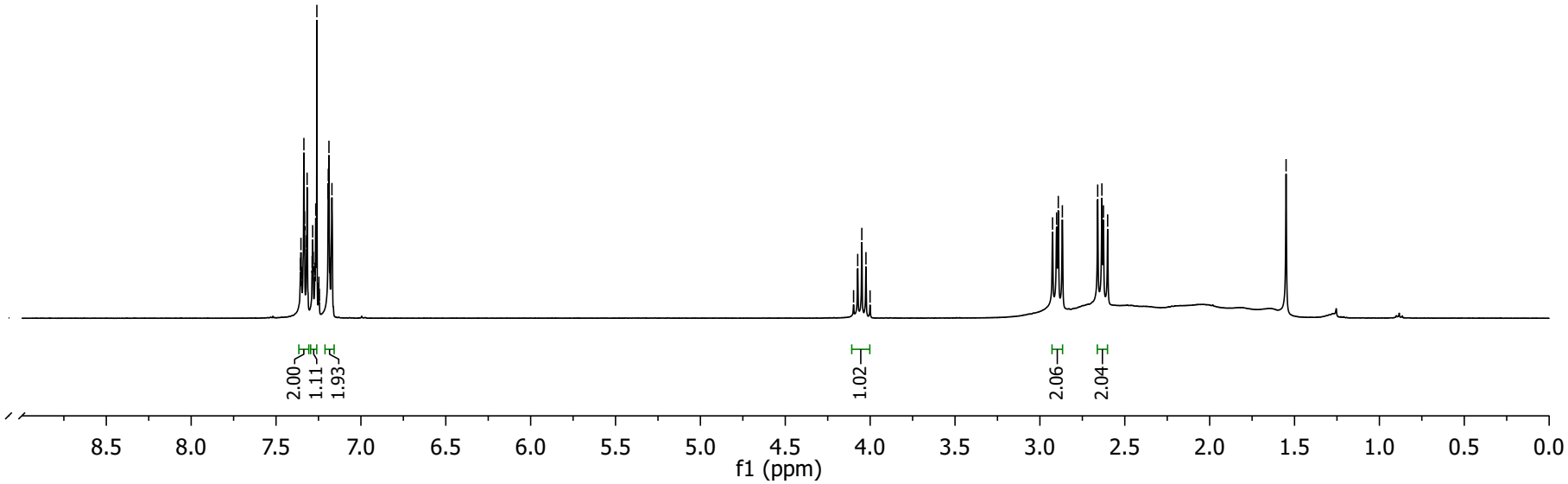
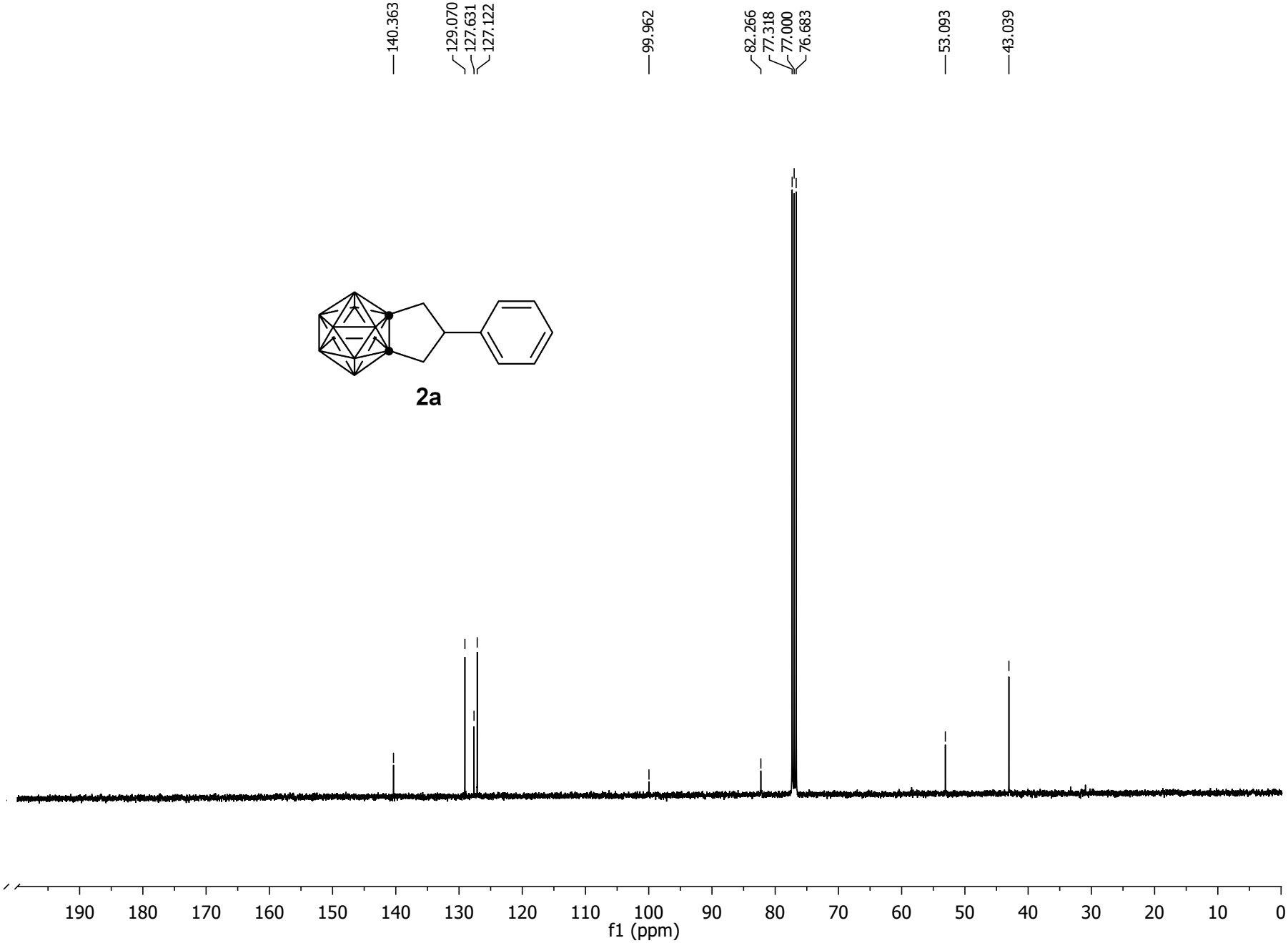


2a





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Receiver Gain	144
Relaxation Delay	2.0000
Pulse Width	9.5000
Acquisition Time	1.1010
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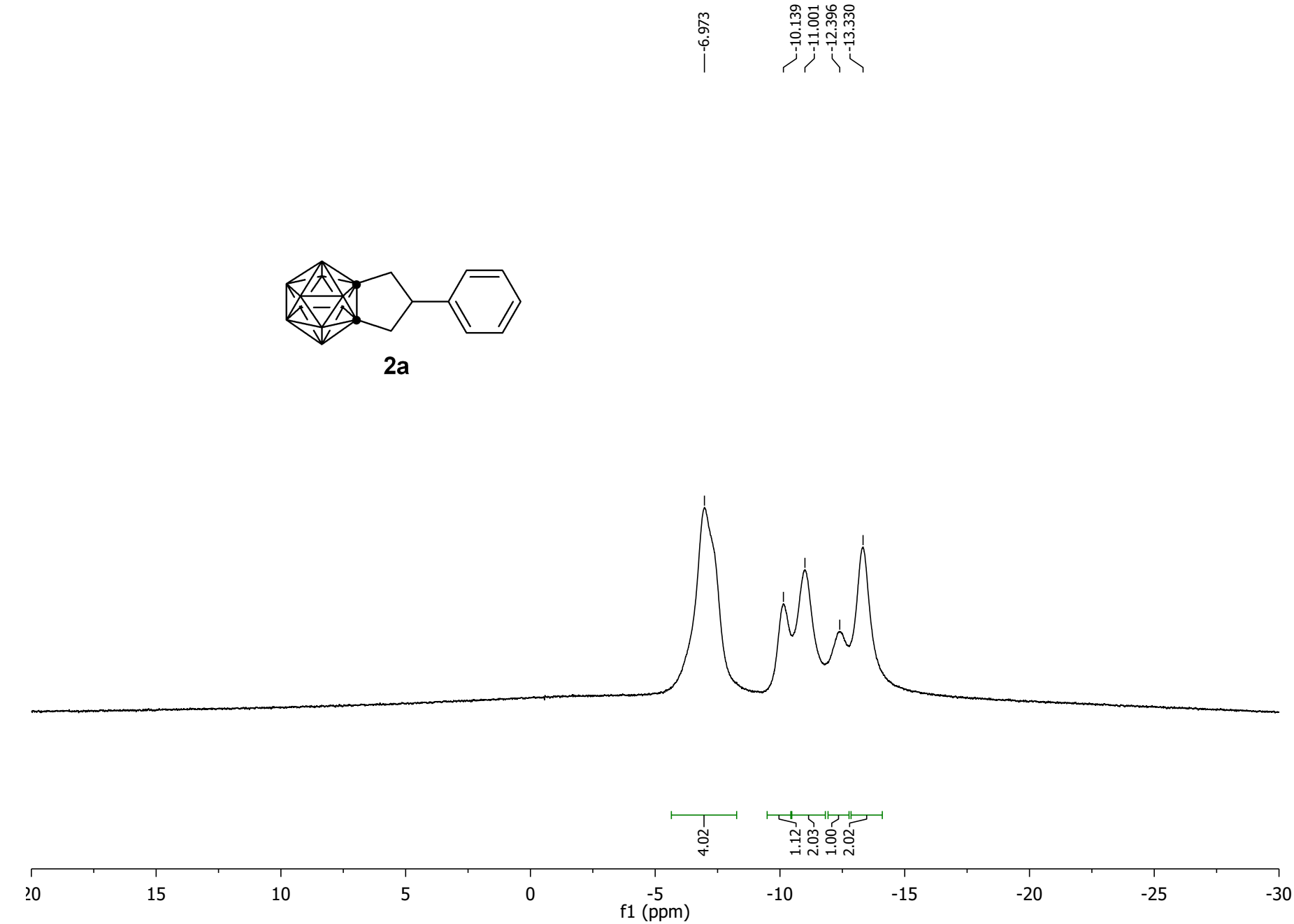
Spectral Width	29761.9
Lowest Frequency	-4821.0
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie-6171-1-p-cdcl3-B
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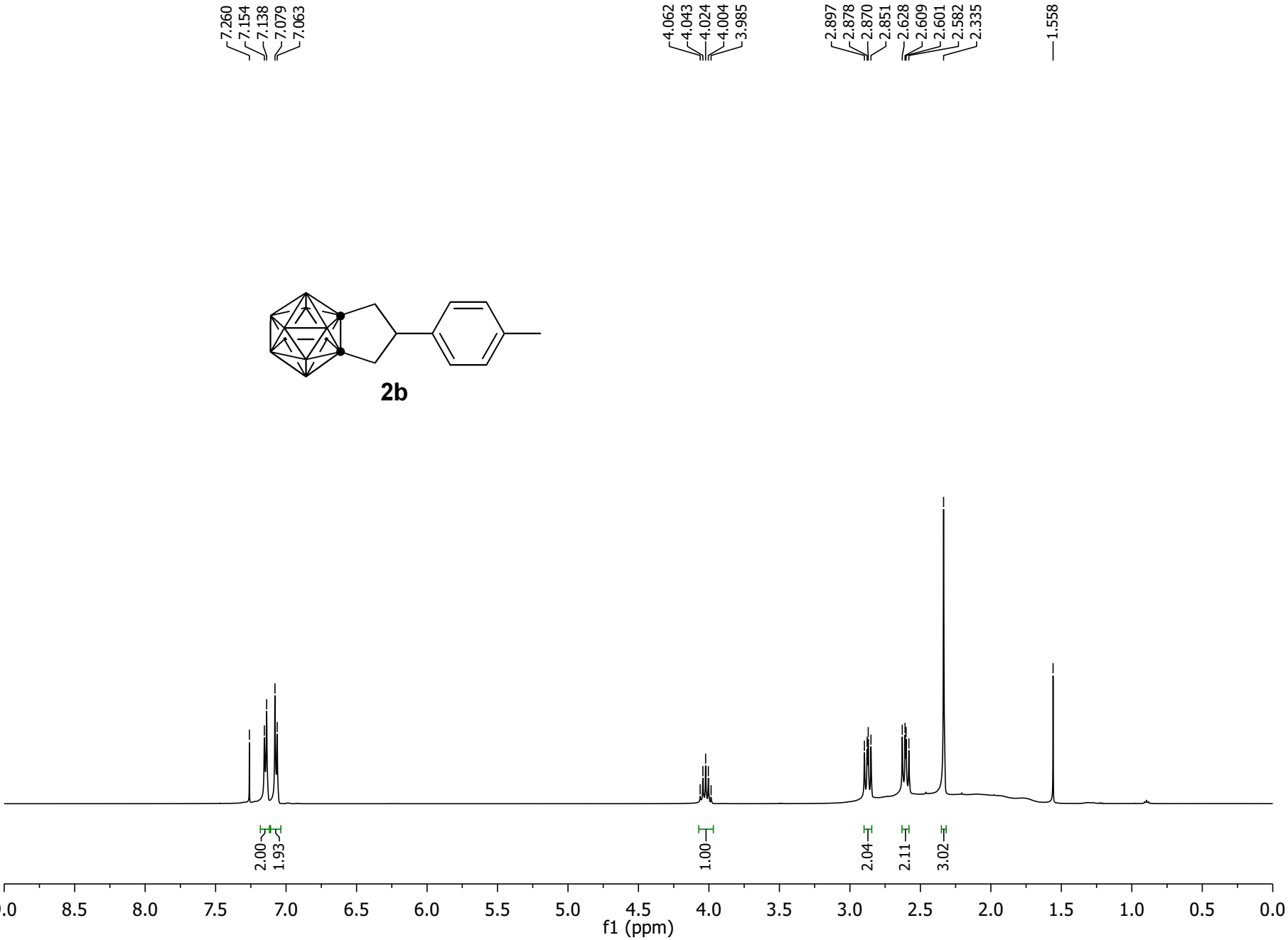
Solvent	CDCl3
Temperature	295.6
Pulse Sequence	zgdc
Experiment	1D
Number of Scans	32
Receiver Gain	362
Relaxation Delay	2.0000
Pulse Width	7.5000
Acquisition Time	1.3631
Spectrometer Frequency	128.41
Spectral Width	24038.5
Lowest Frequency	-12091.7
Nucleus	11B
Acquired Size	32768
Spectral Size	65536



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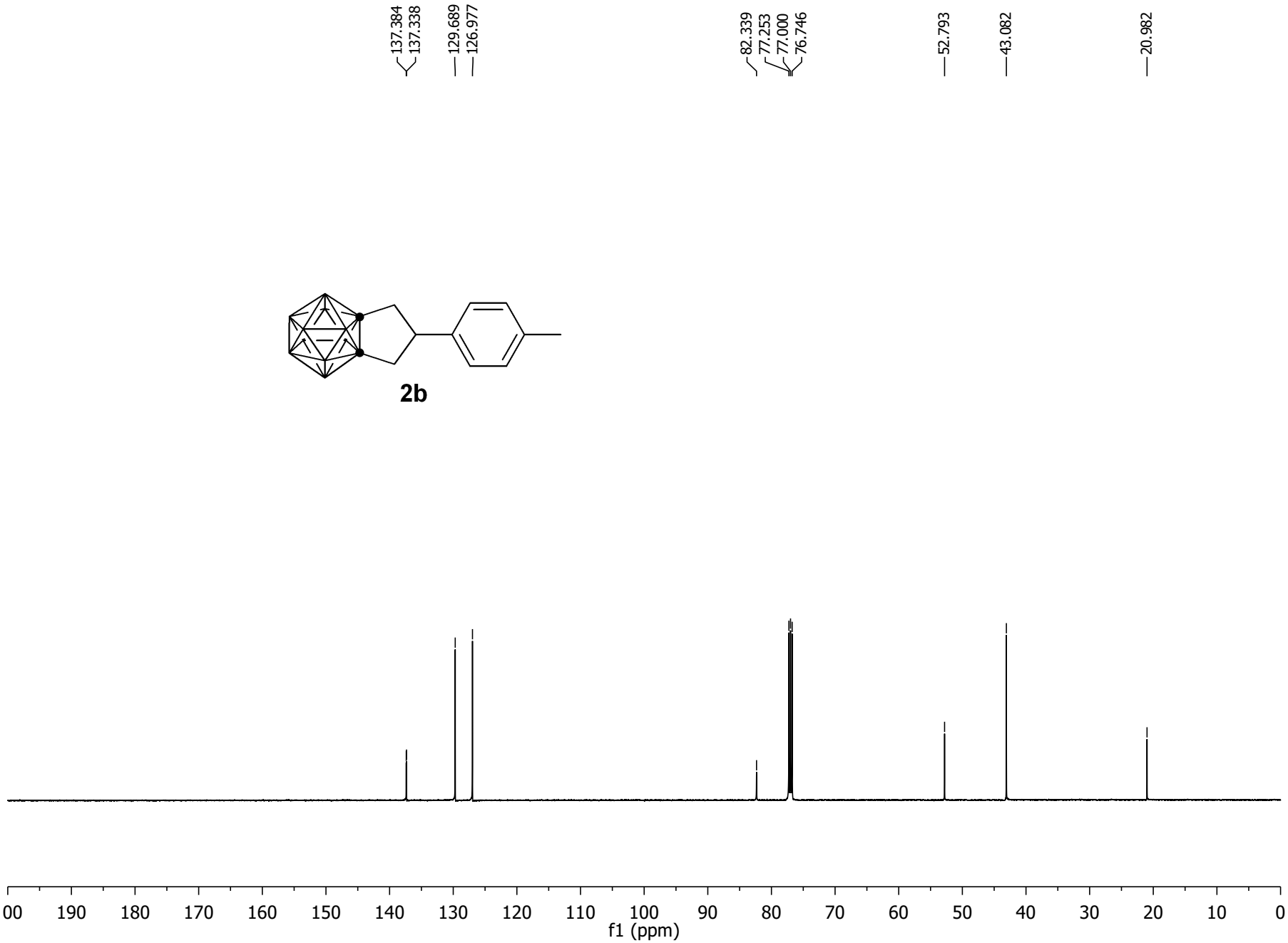

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Experiment	1D
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Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
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Nucleus	13C
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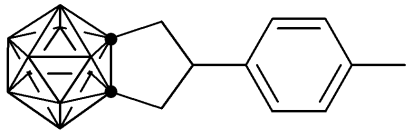
Spectral Size	65536



2b

Parameter	Value
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Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
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Relaxation Delay	1.0000
Pulse Width	15.0000
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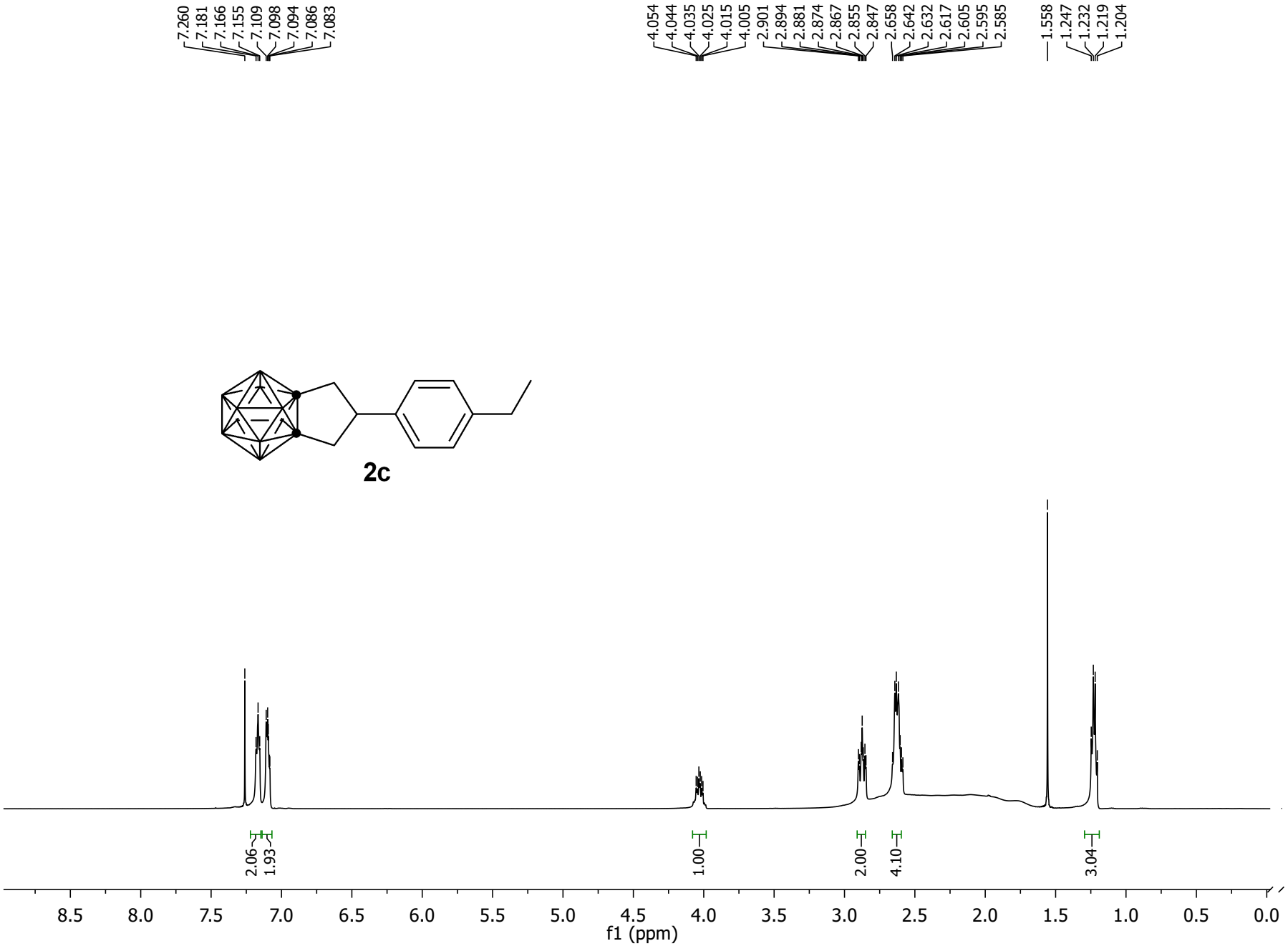
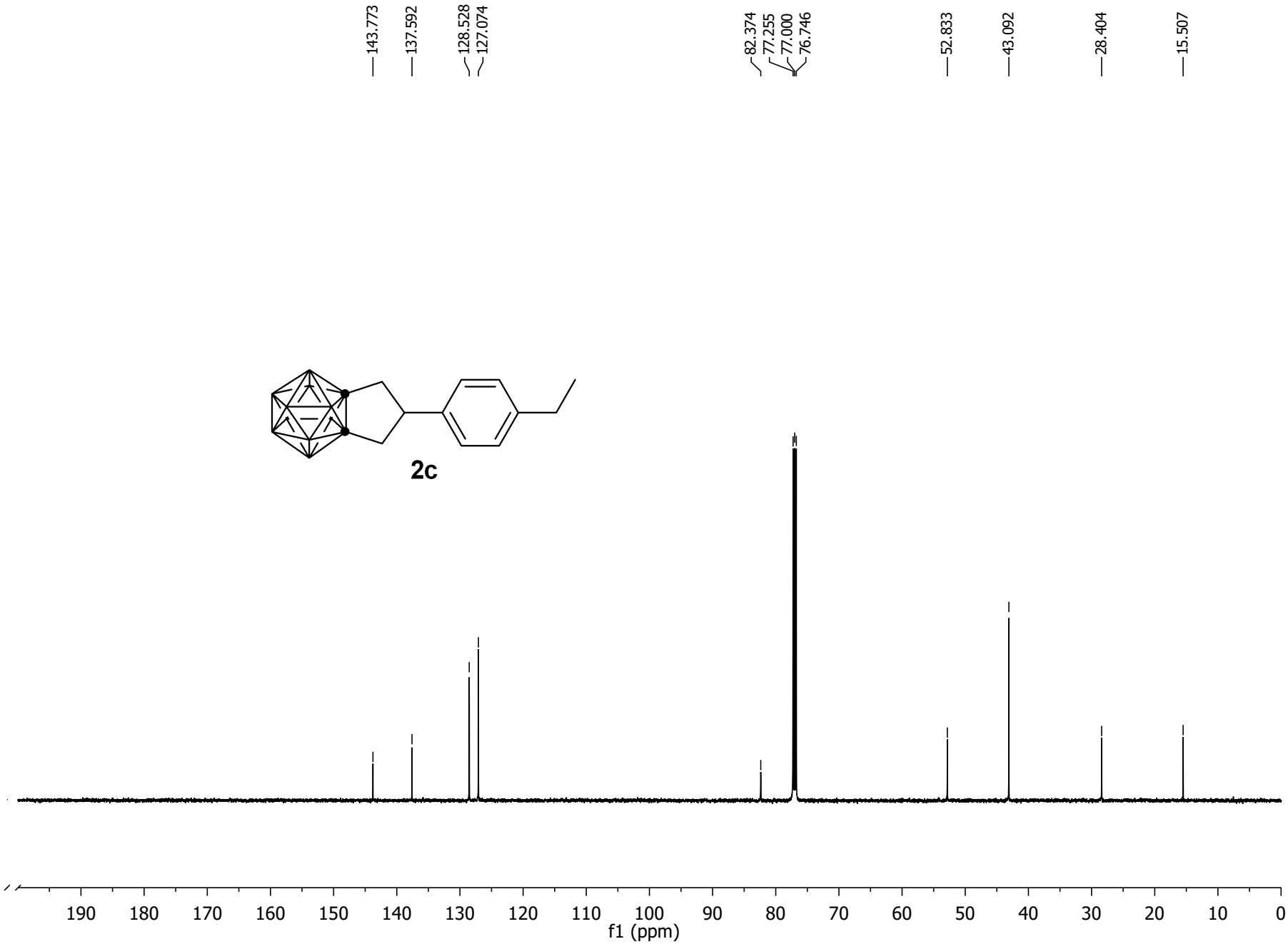
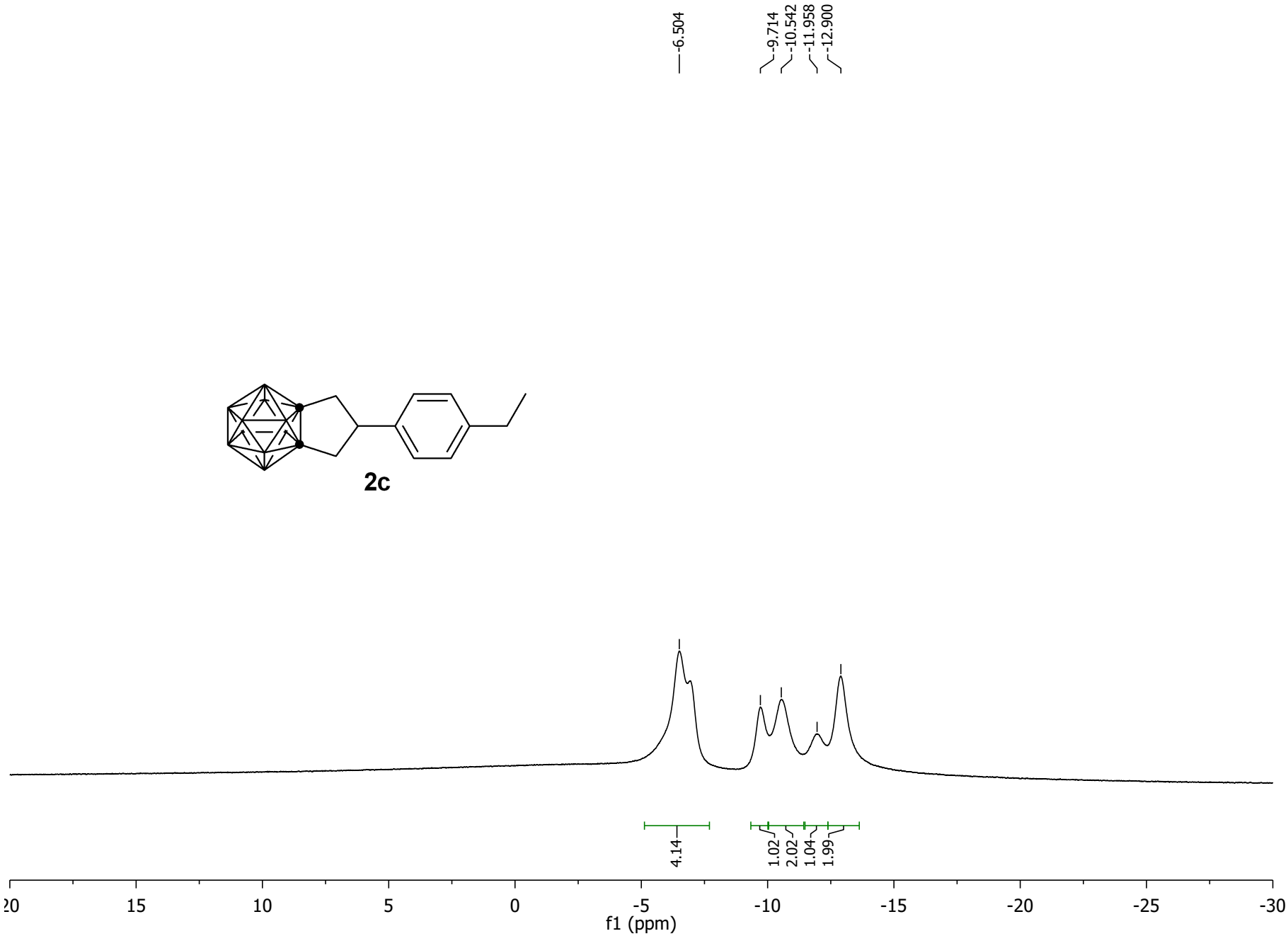
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



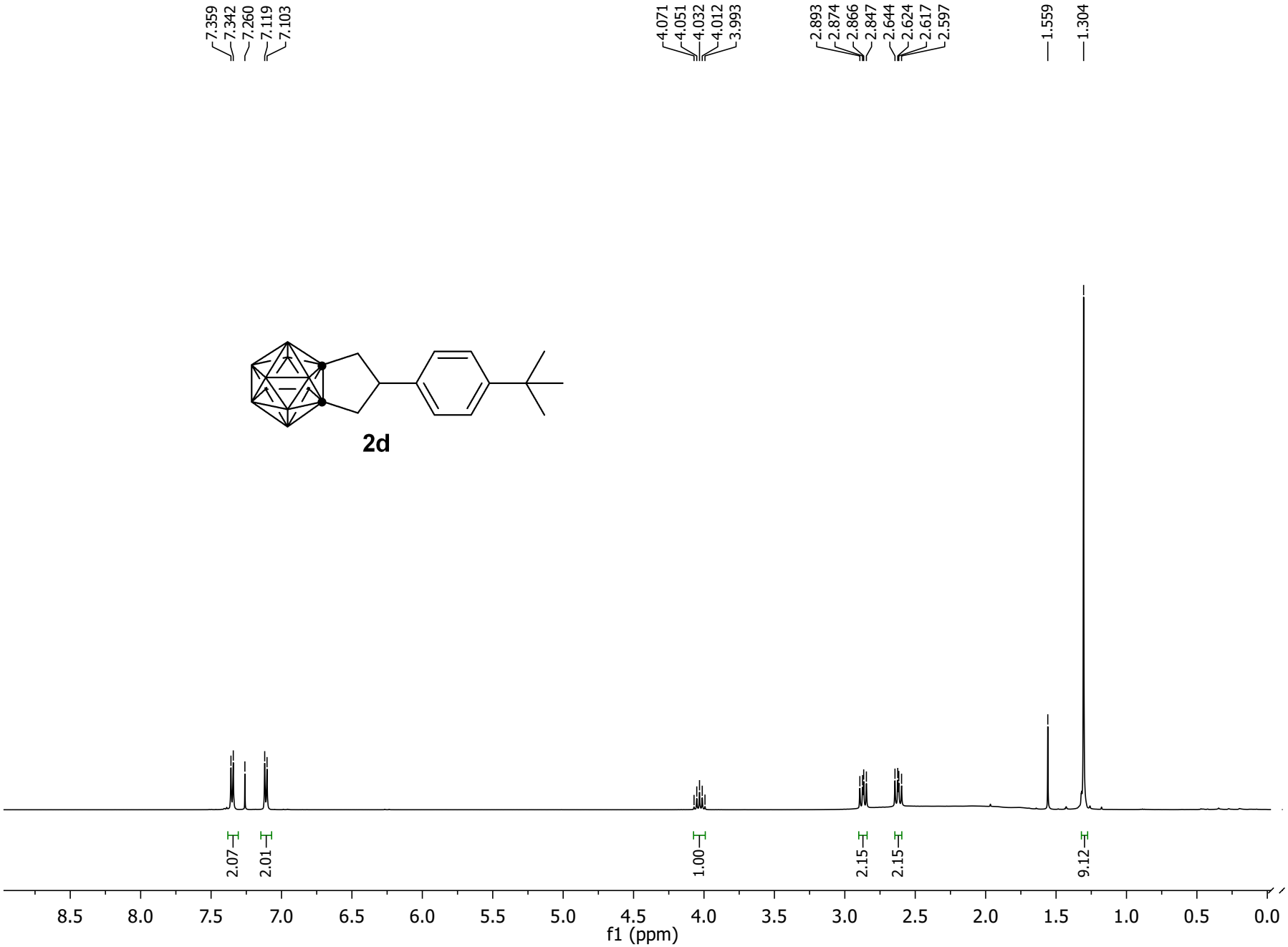
Parameter	Value
Title	zhjie181220-4-Et-wu-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	31
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



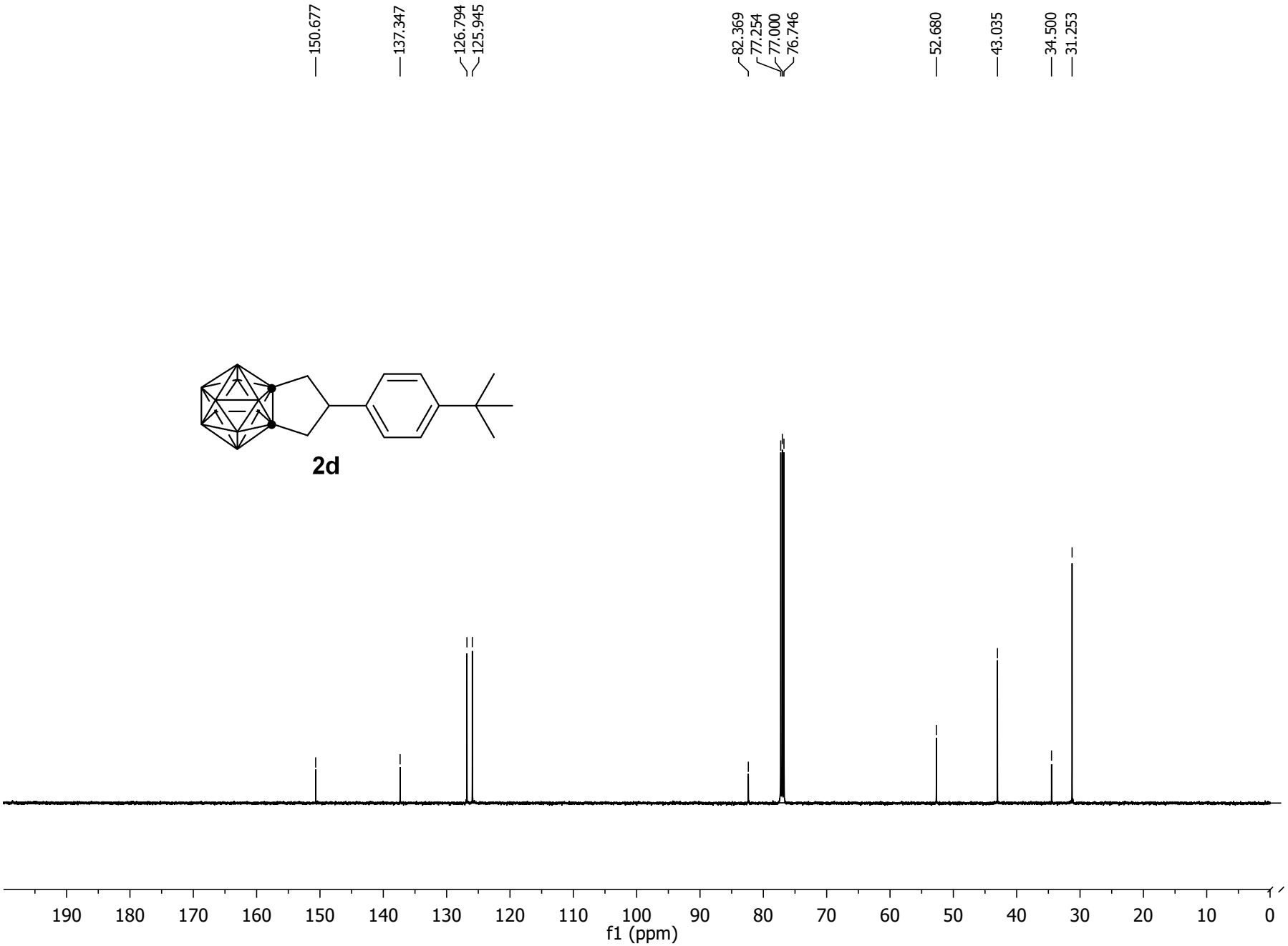
Parameter	Value
Title	zhjie181220-4-Et-wu-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	128
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2309.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



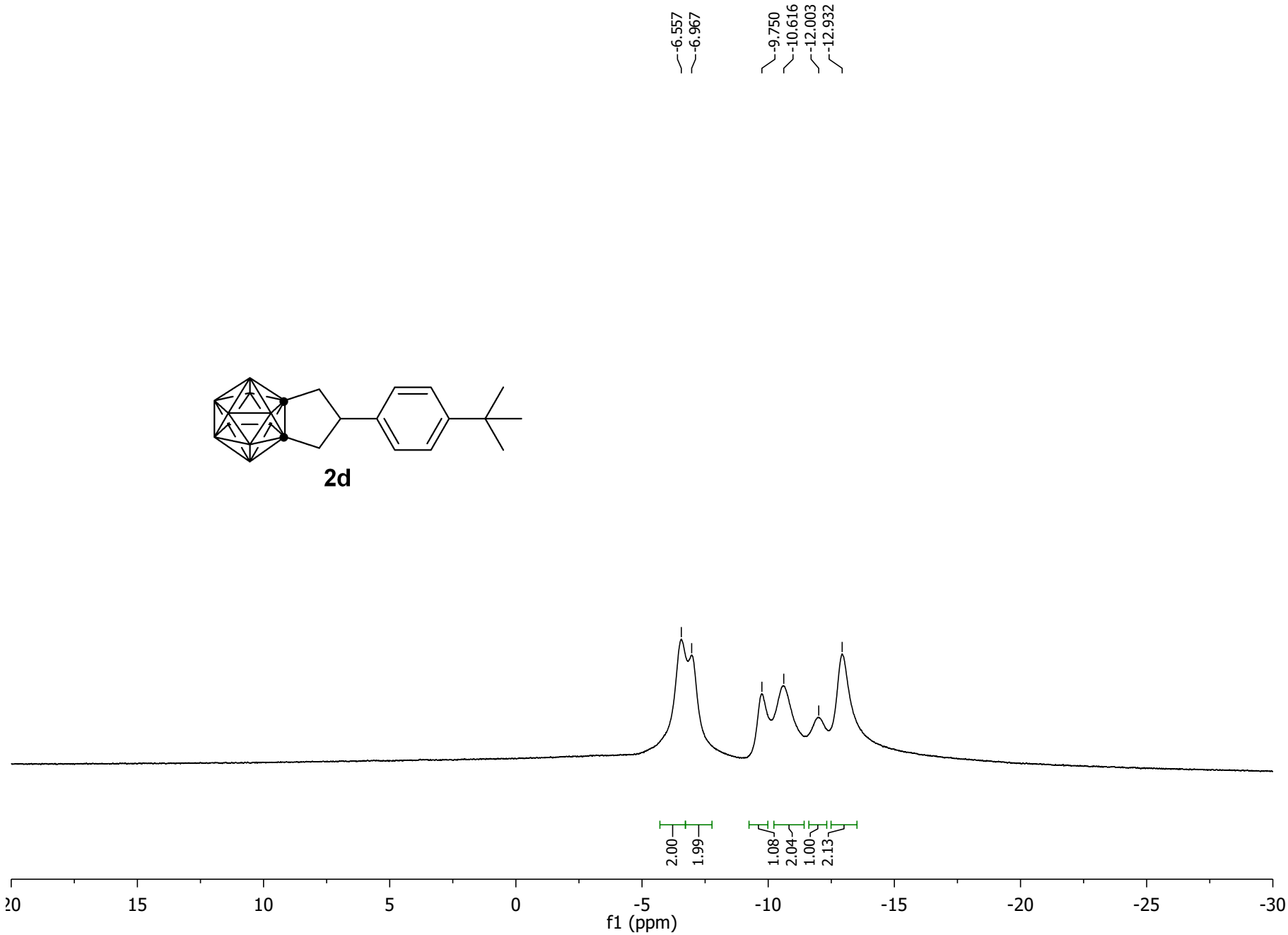
Parameter	Value
Title	zhjie181220-4-Et-wu-cdcl3-B
Spectrometer	spect
Solvent	None
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



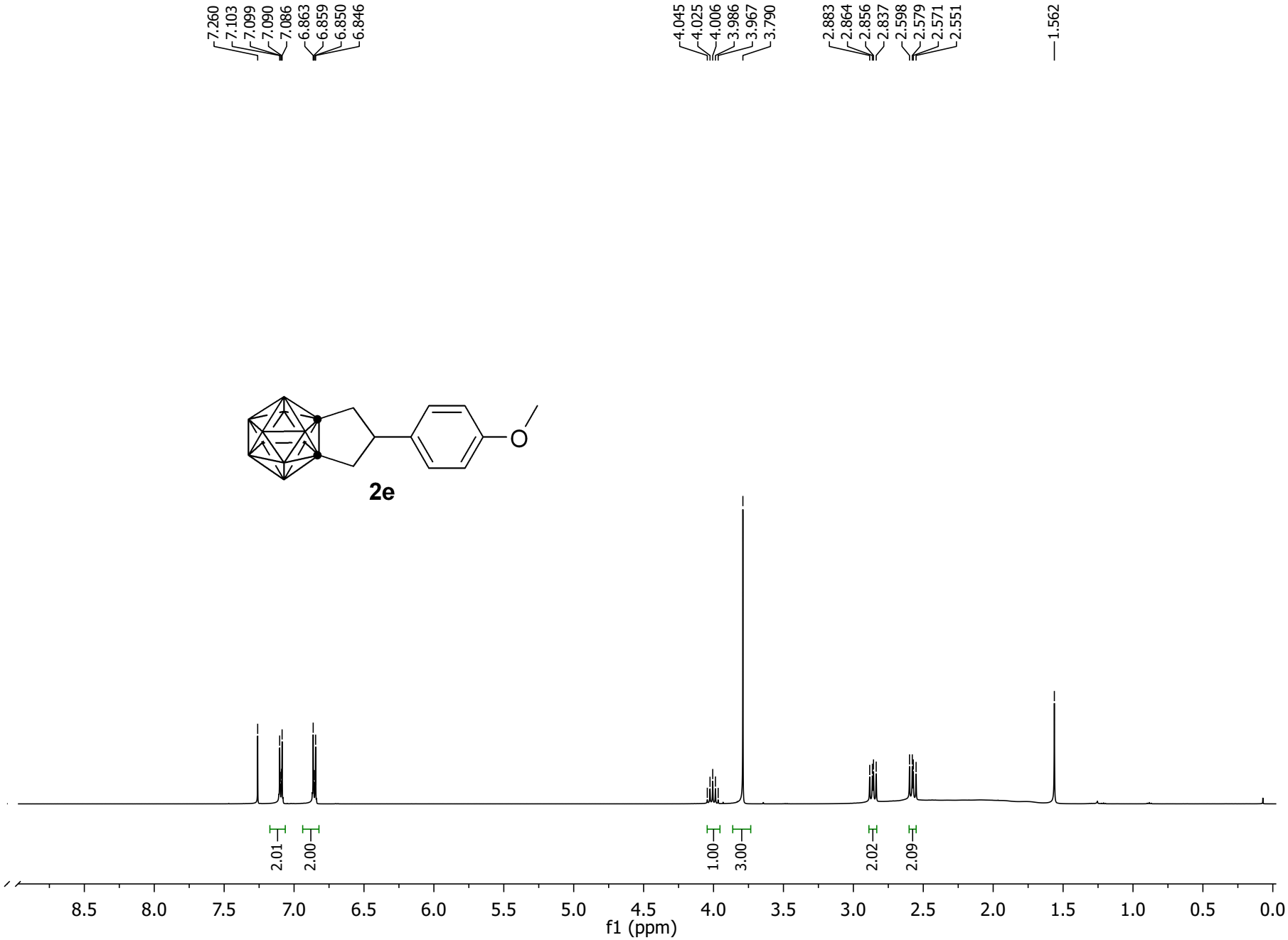
Parameter	Value
Title	zhjie181220-4-tBu-wu-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	31
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



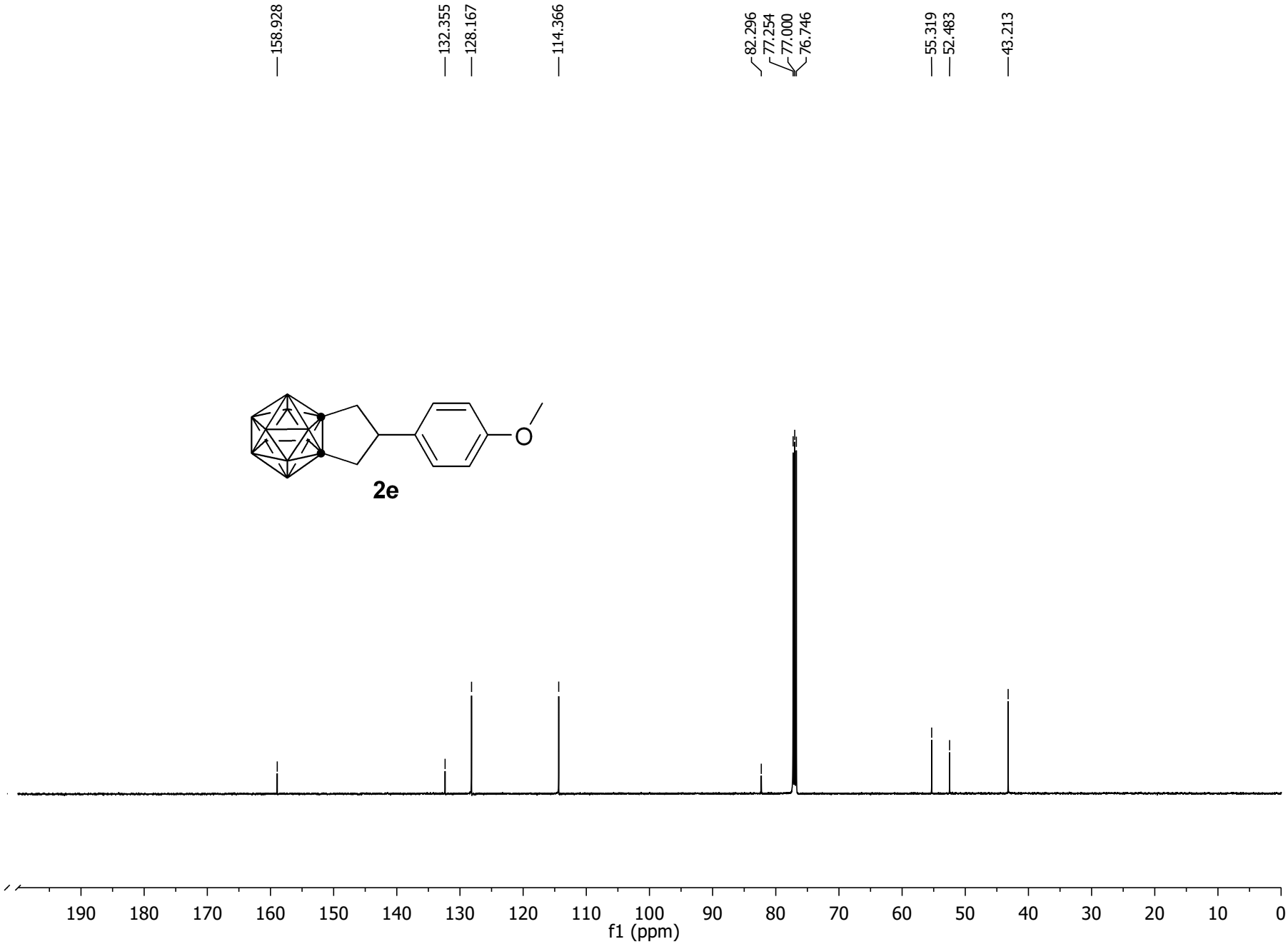
Parameter	Value
Title	zhjie181220-4-tBu-wu-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	88
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2309.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



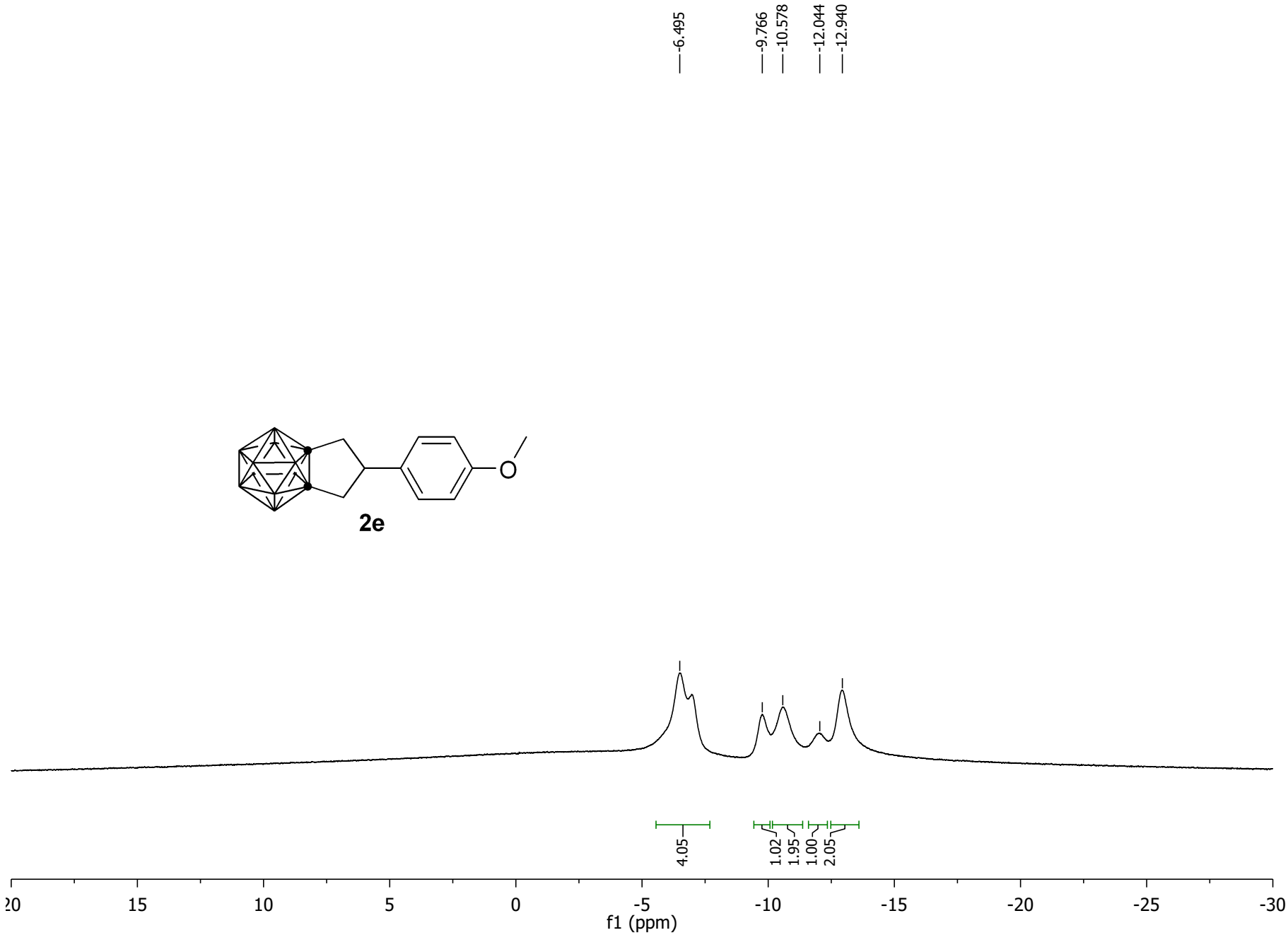
Parameter	Value
Title	zhjie181220-4-tBu-wu-cdcl3-B
Spectrometer	spect
Solvent	None
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



Parameter	Value
Title	zhjie190314-4-MeO-wu-p-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	51
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

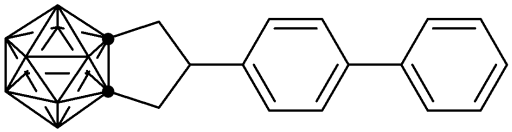


Parameter	Value
Title	zhjie190314-4-MeO-wu-p-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	256
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.77
Spectral Width	29761.9
Lowest Frequency	-2308.4
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie190314-4-MeO-wu-p-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

Parameter	Value
Title	zhjie181116-wu-4-Ph-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	31
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1921.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



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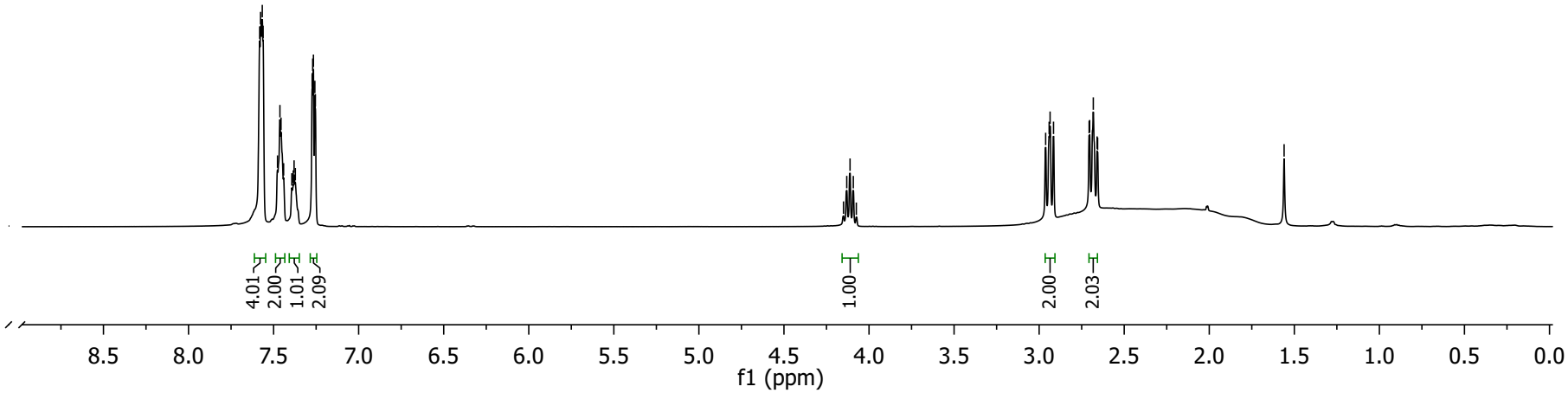
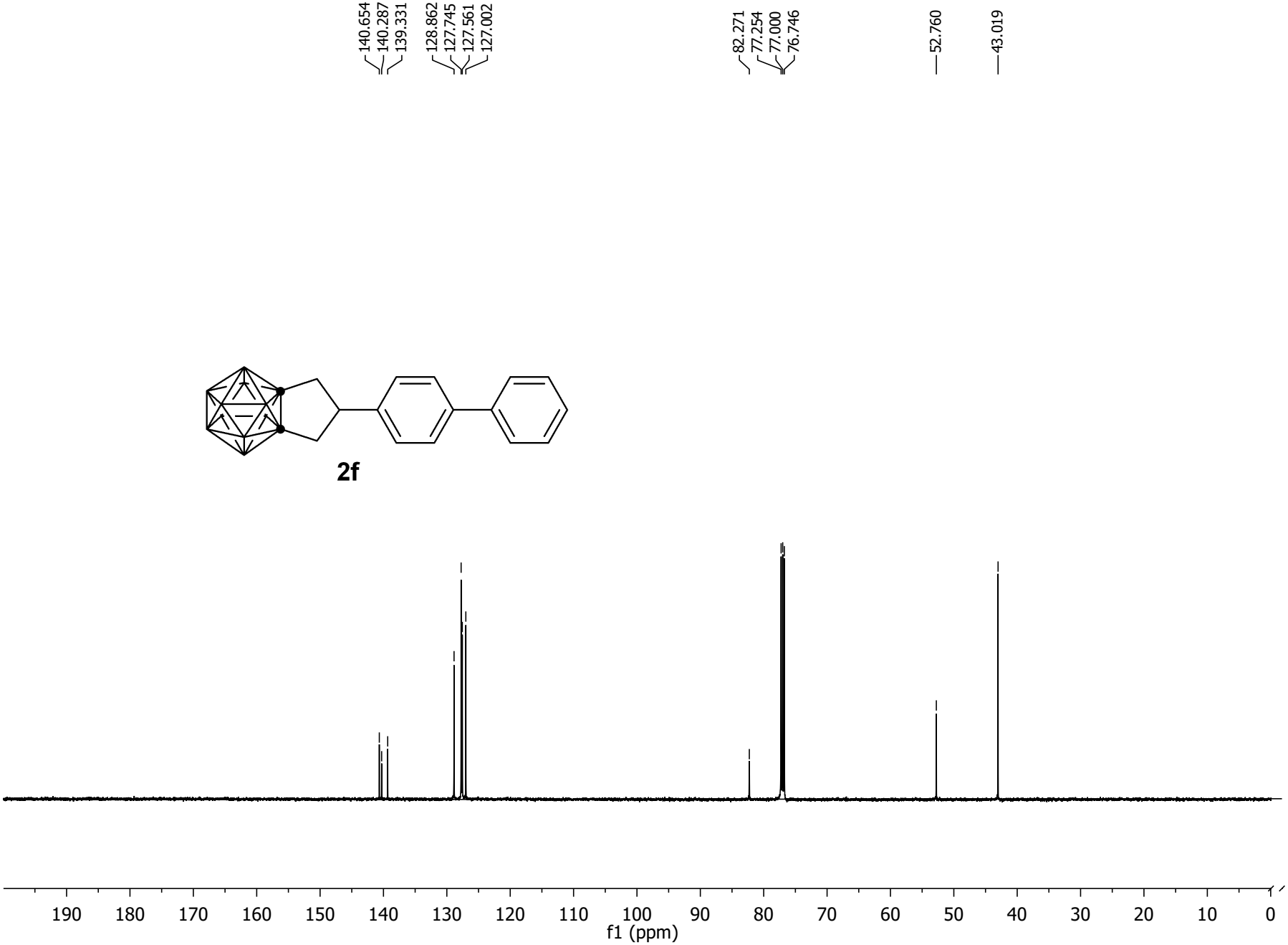
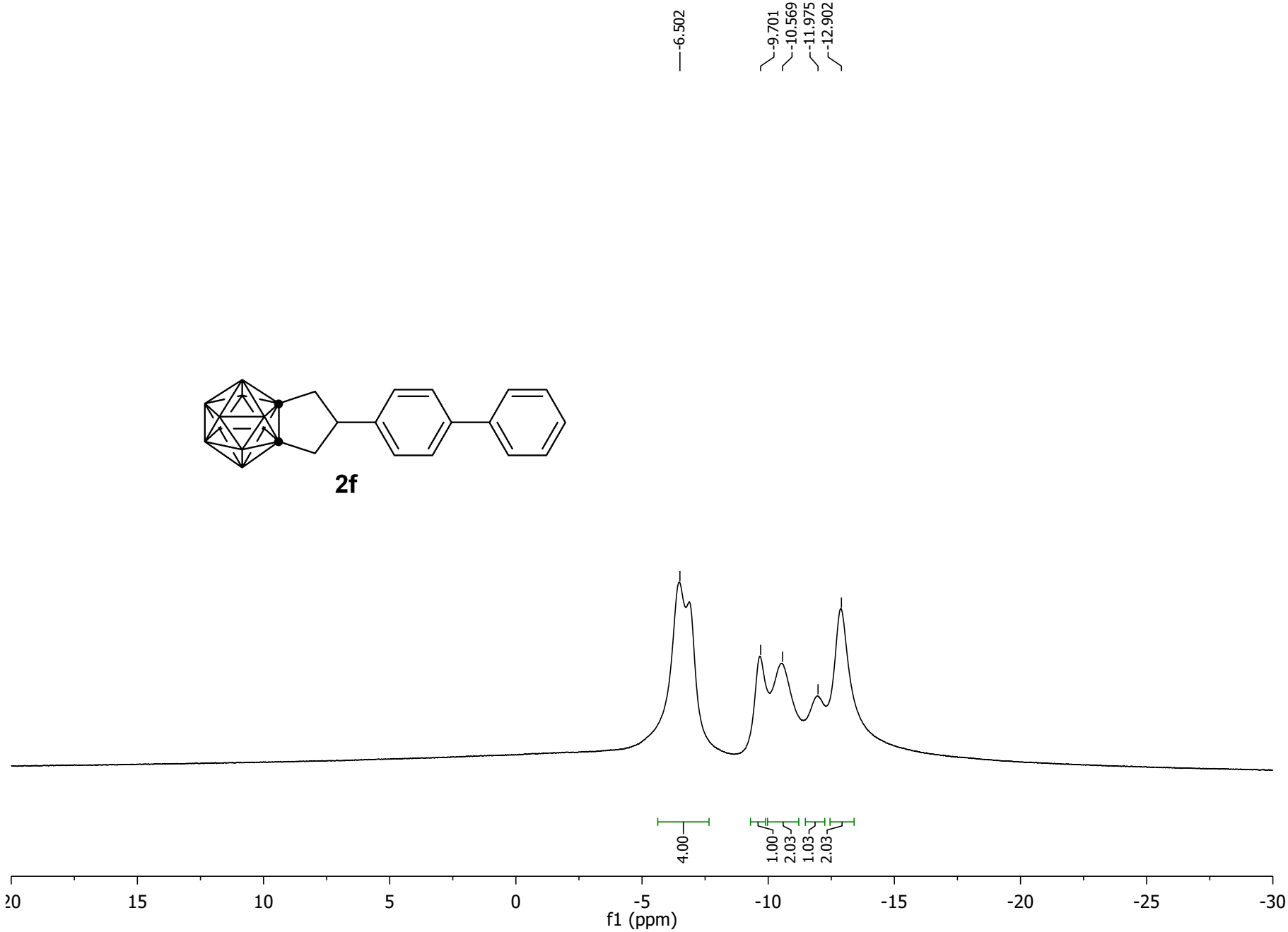


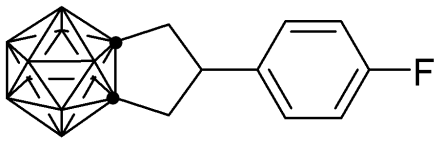


Parameter	Value
Title	zhjie181116-wu-4-Ph-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	100
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2310.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie181116-wu-4-Ph-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	32
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

Parameter	Value
Title	zhjie190613-4-F-wu-p-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	31
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



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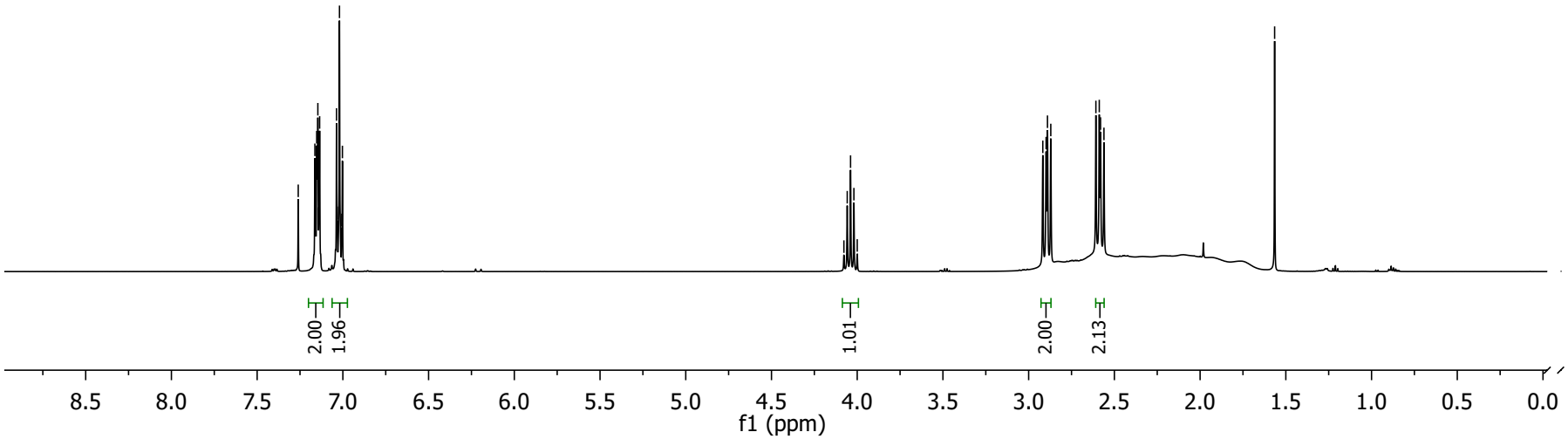
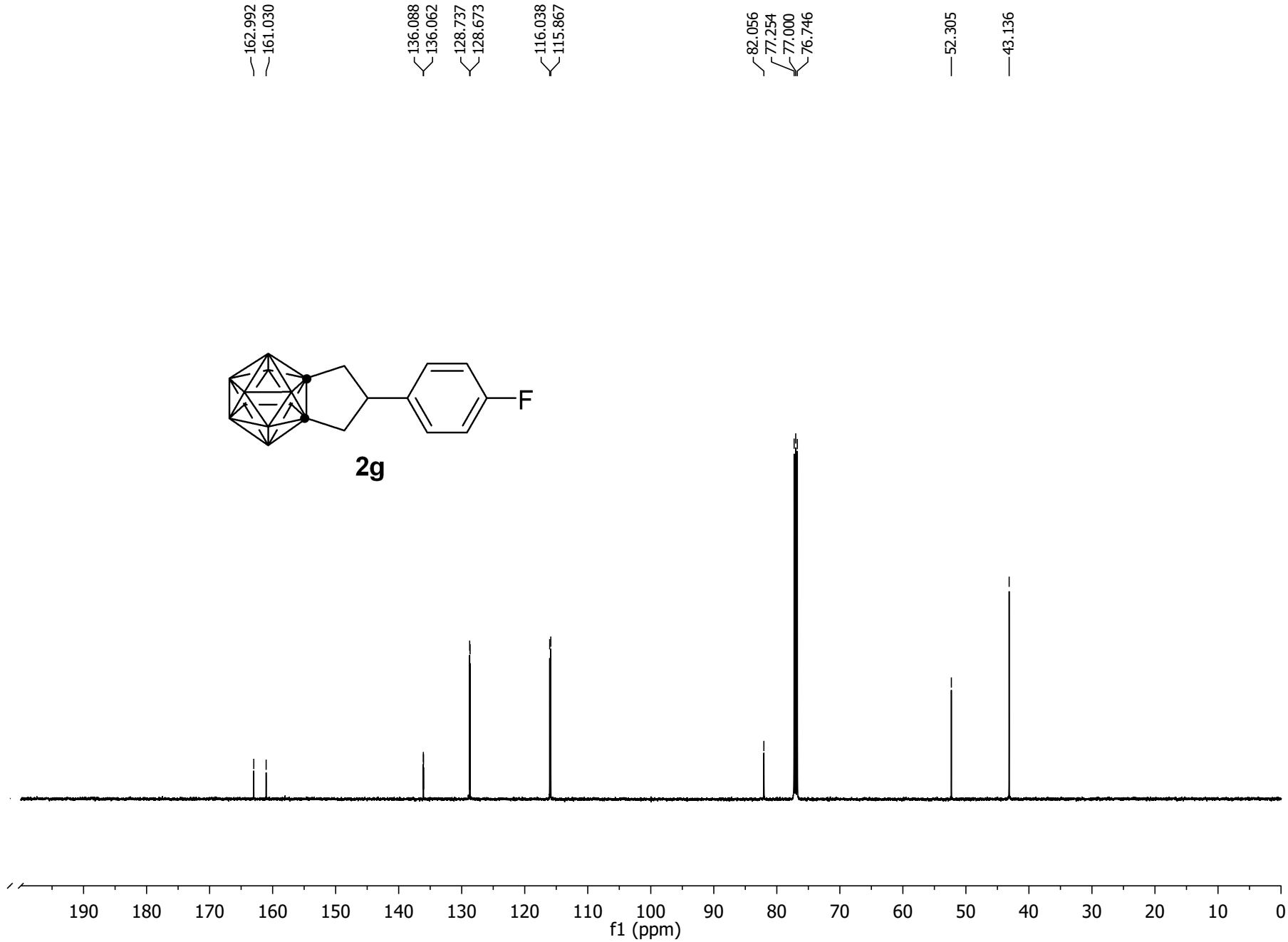
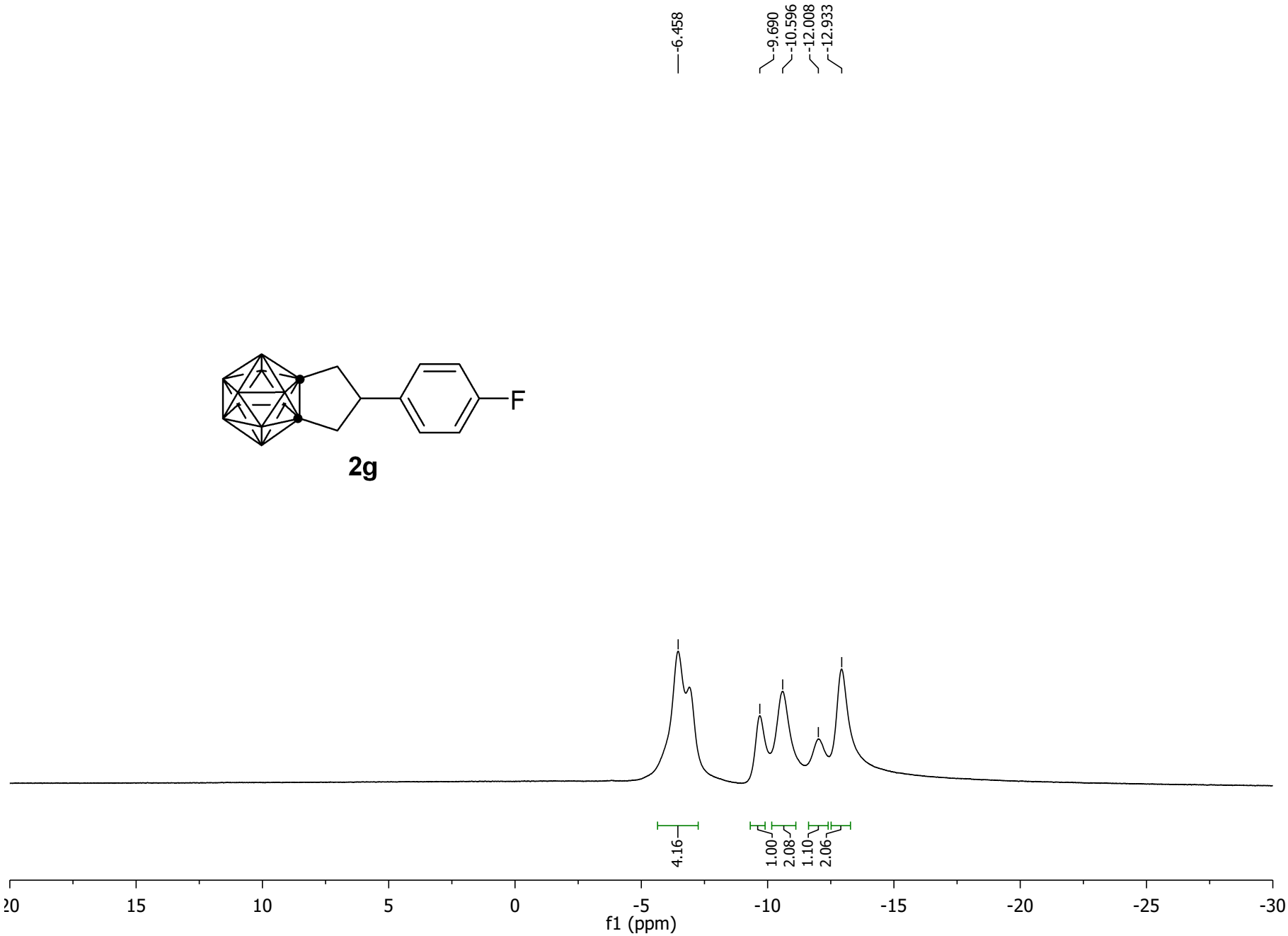
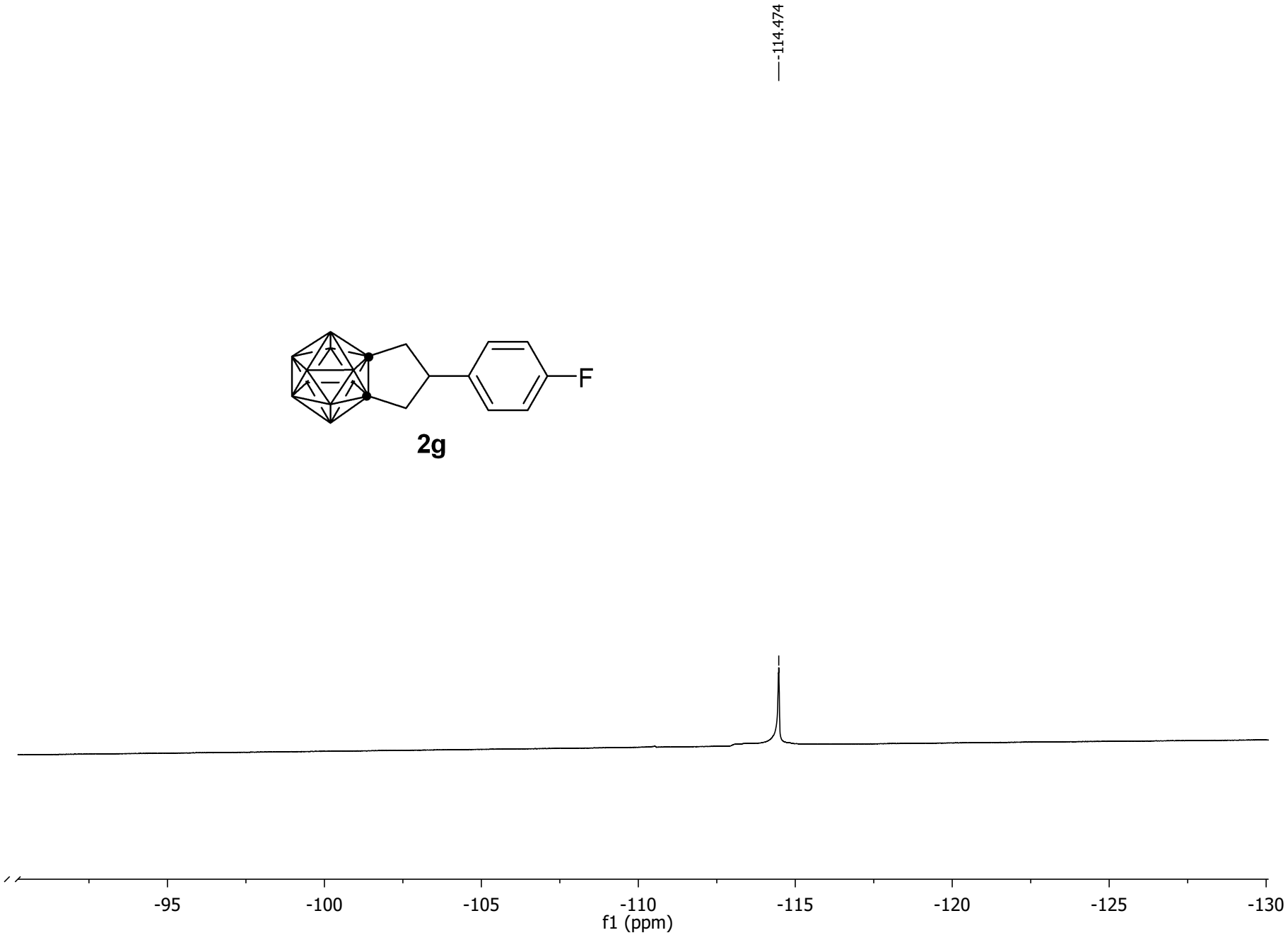




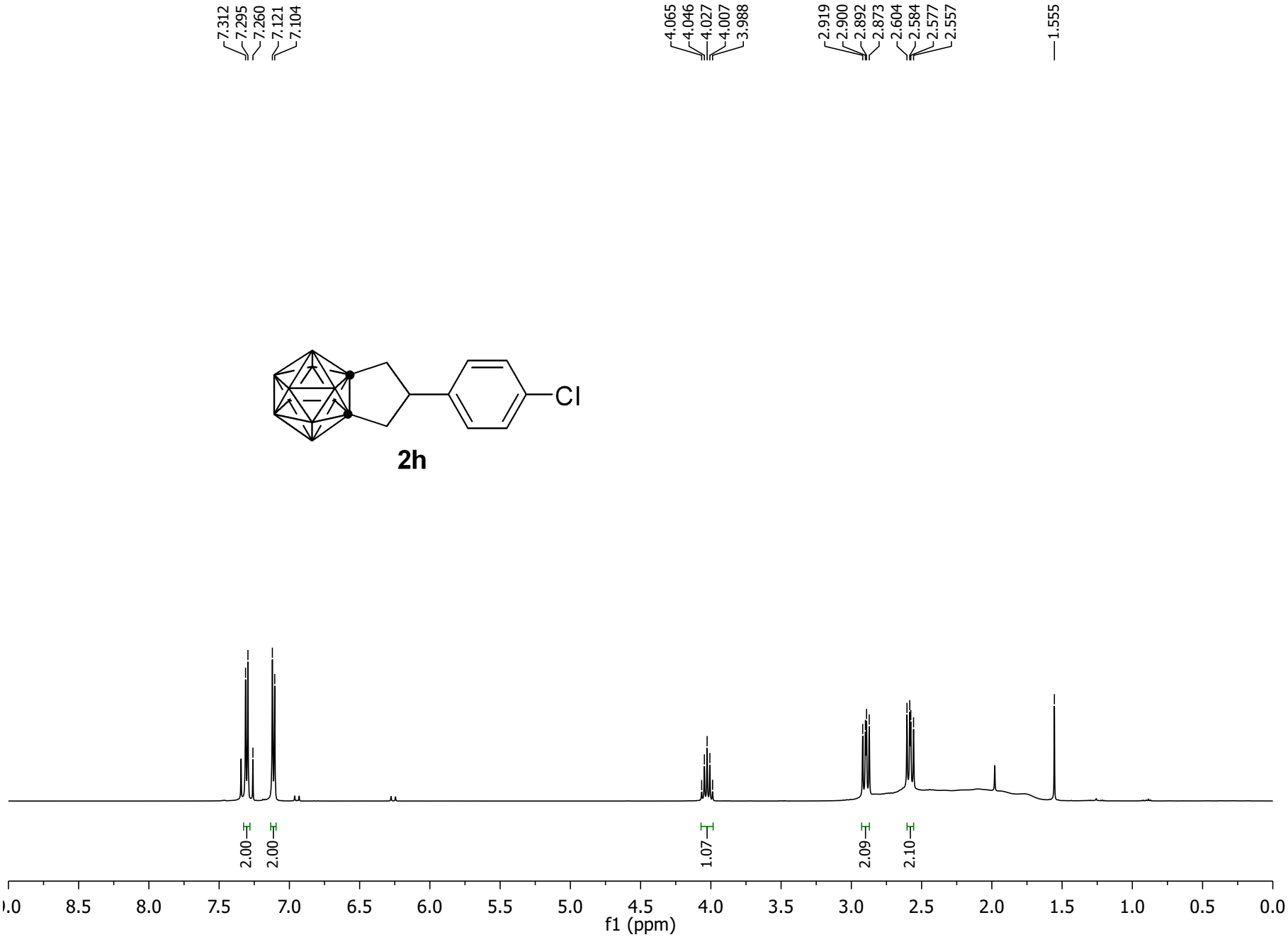
Parameter	Value
Title	zhjie190613-4-F-wu-p-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	64
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2310.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



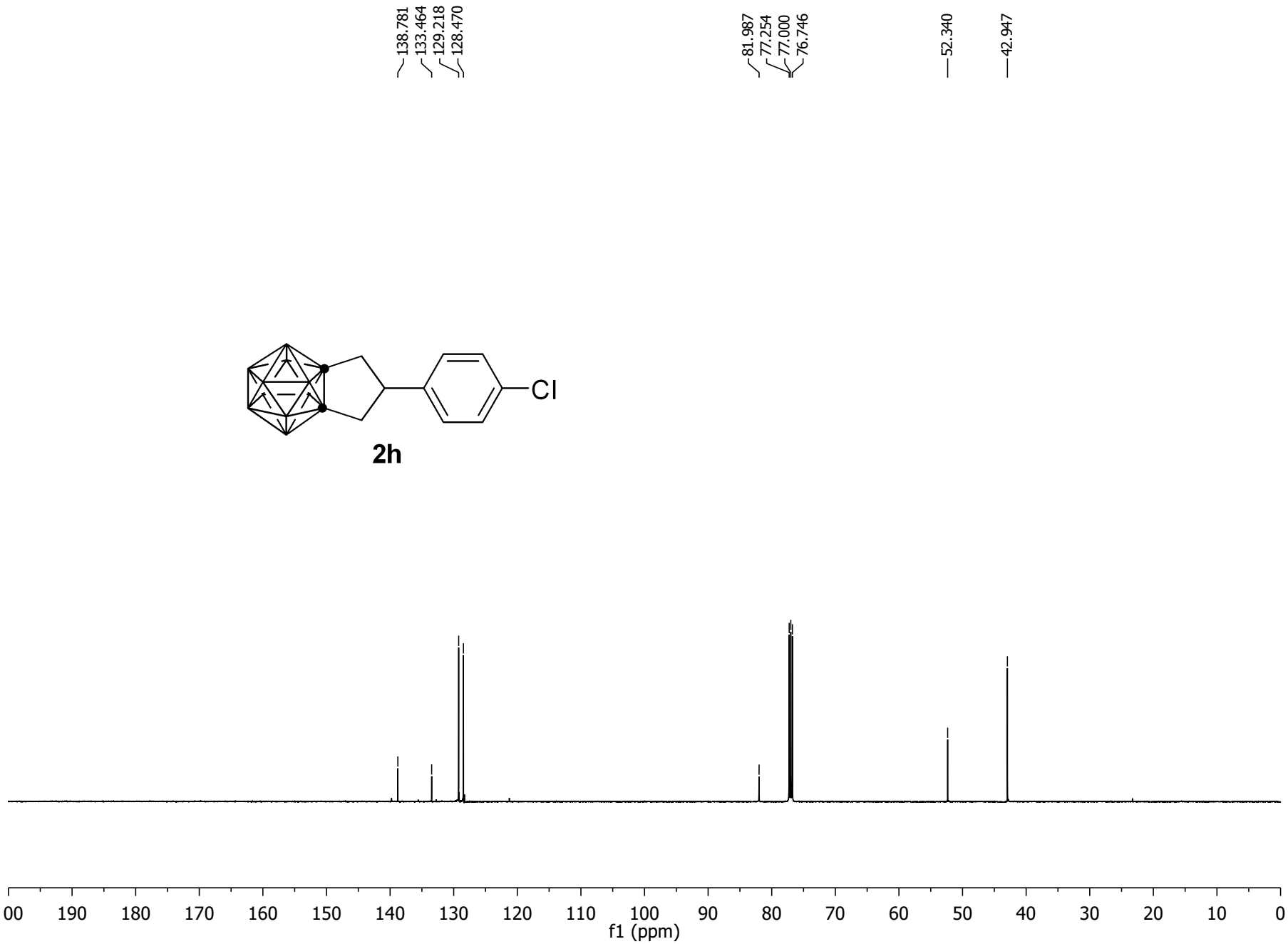
Parameter	Value
Title	zhjie190613-4-F-wu-p-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



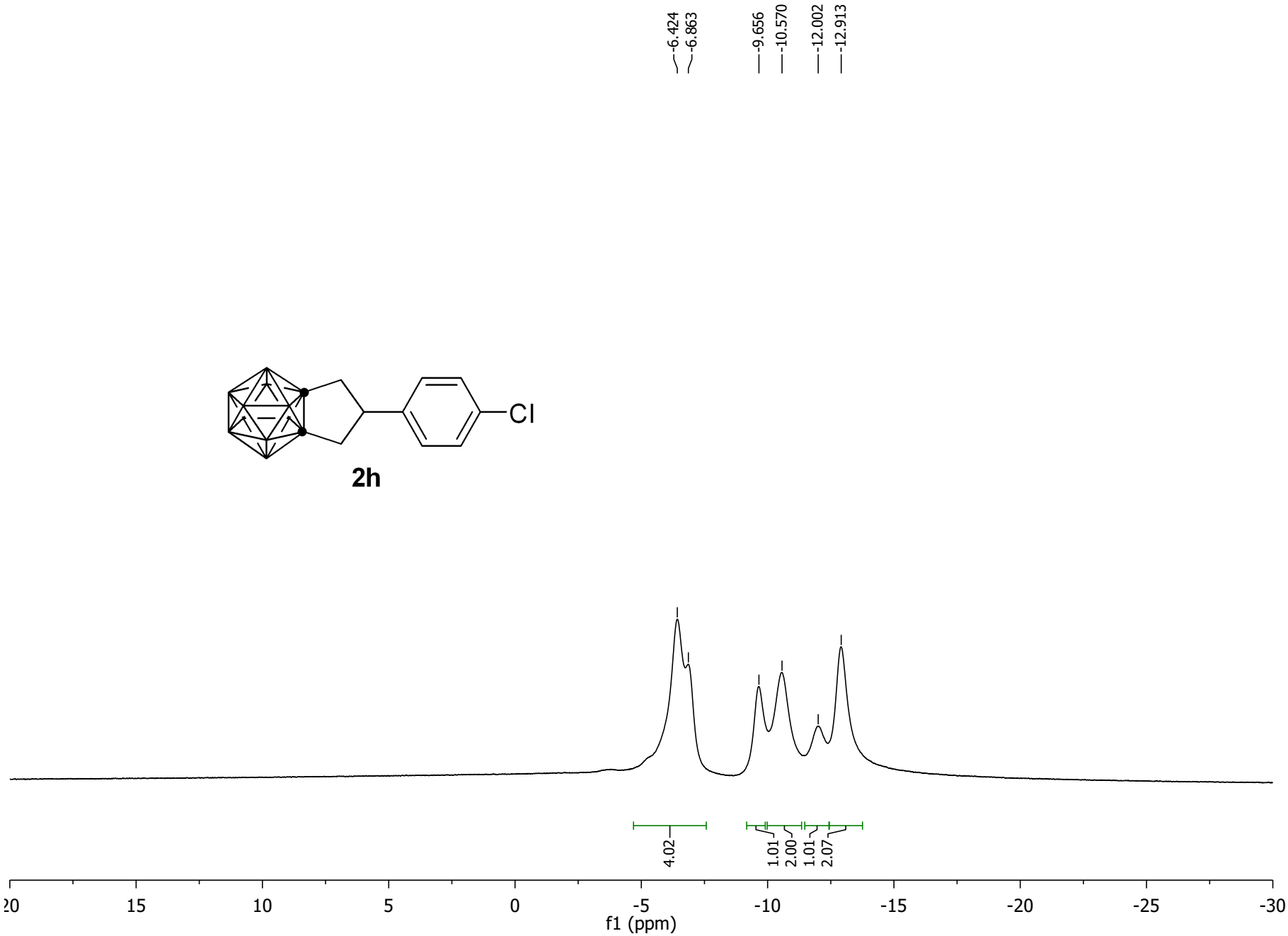
Parameter	Value
Title	zhjie190618-4-F-wu-cdcl3-F(c)
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgflqn
Experiment	1D
Number of Scans	16
Receiver Gain	7
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.5767
Spectrometer Frequency	470.59
Spectral Width	113636.4
Lowest Frequency	-103877.4
Nucleus	19F
Acquired Size	65536
Spectral Size	131072



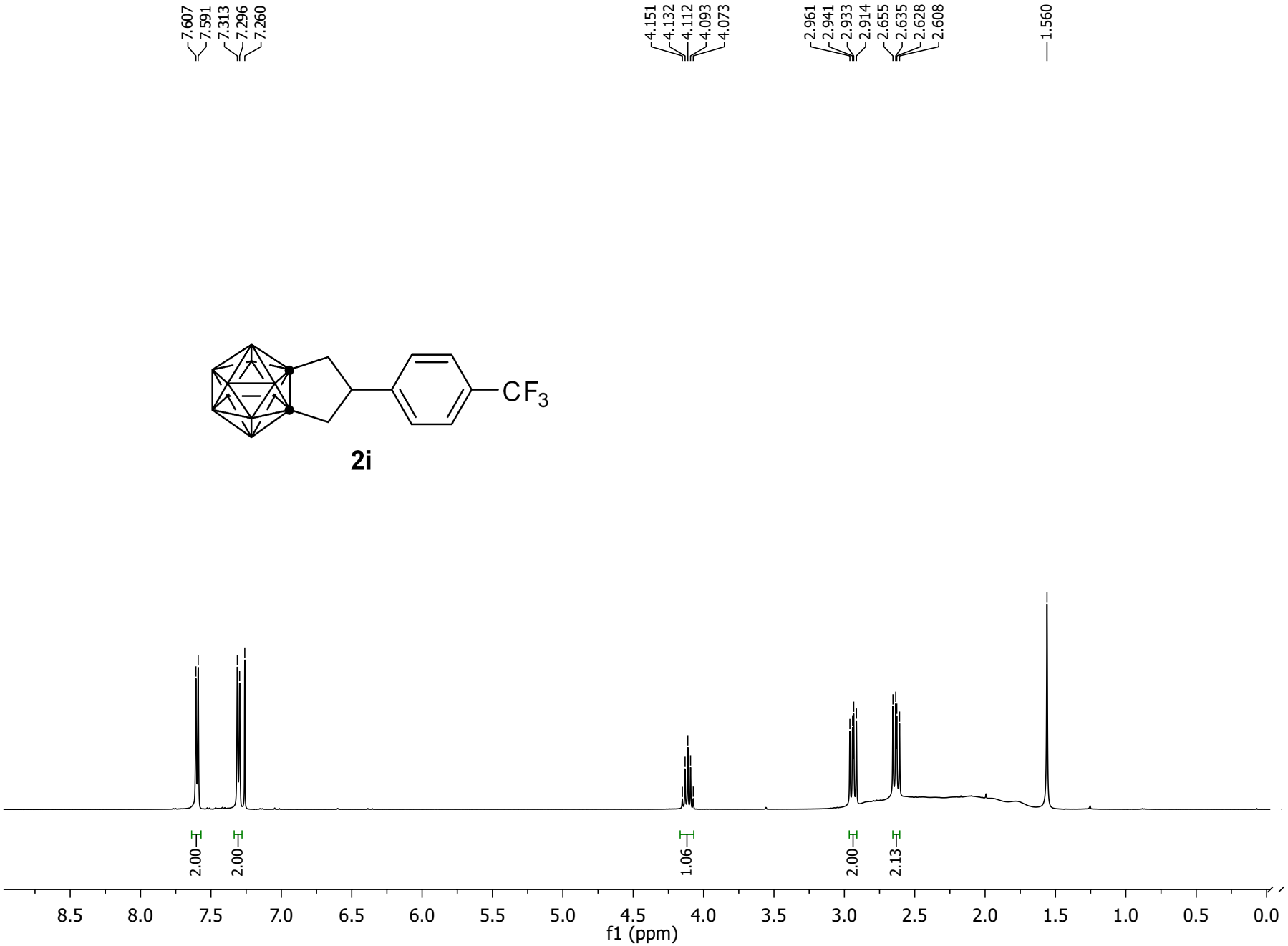
Parameter	Value
Title	zhjie190102-4-Cl-wu-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	31
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



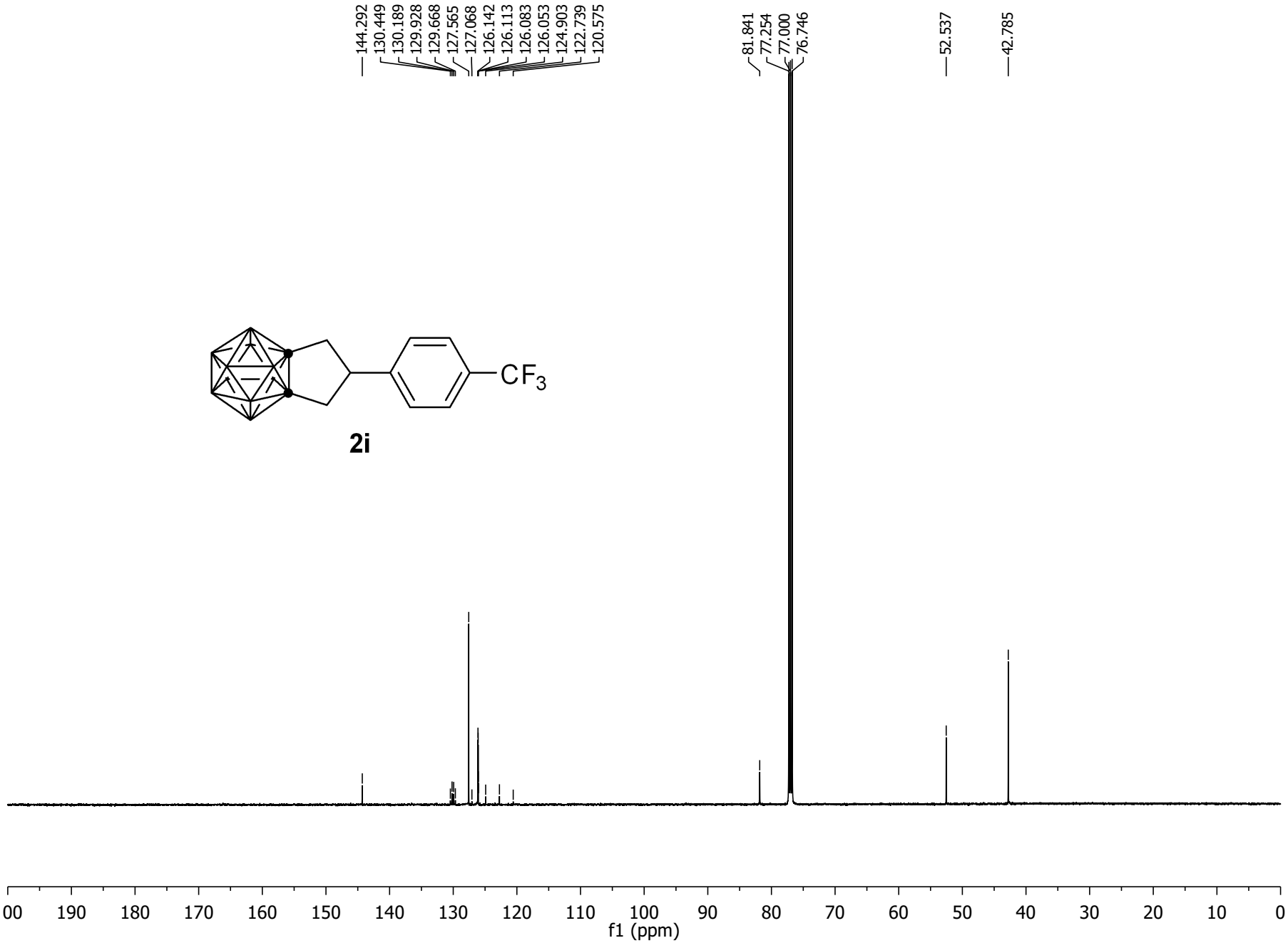
Parameter	Value
Title	zhjie190102-4-Cl-wu-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	128
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.77
Spectral Width	29761.9
Lowest Frequency	-2309.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



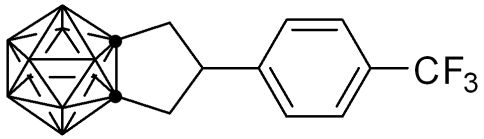
Parameter	Value
Title	zhjie190102-4-Cl-wu-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



Parameter	Value
Title	zhjie190710-4-CF3-wu-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	32
Receiver Gain	64
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie190708-4-CF3-wu-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	800
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2308.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



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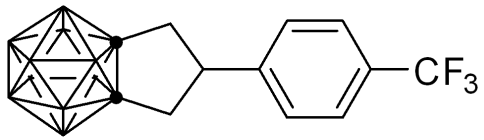
Parameter	Value
Title	zhjie190618-4-CF3-wu-p-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



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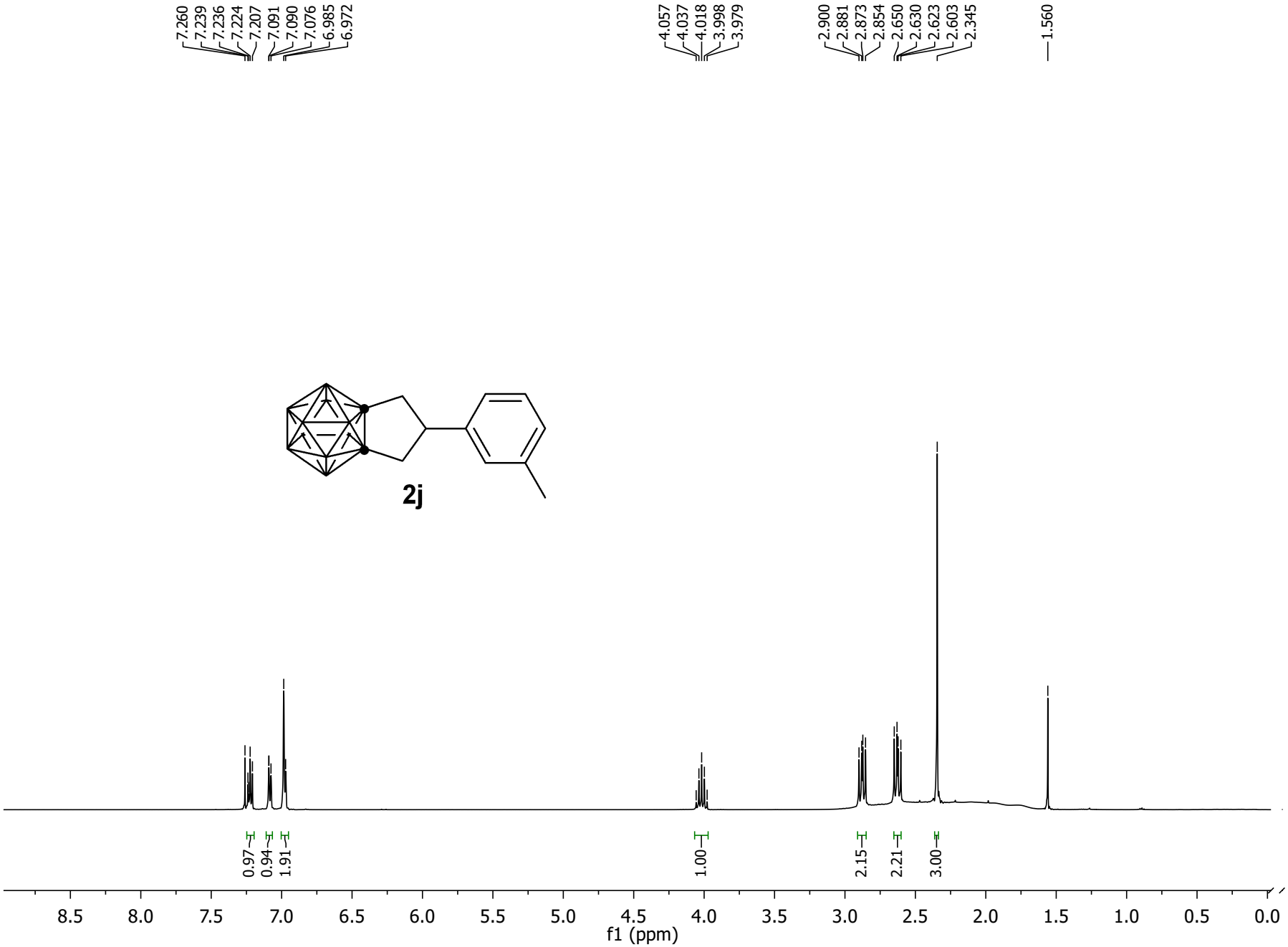
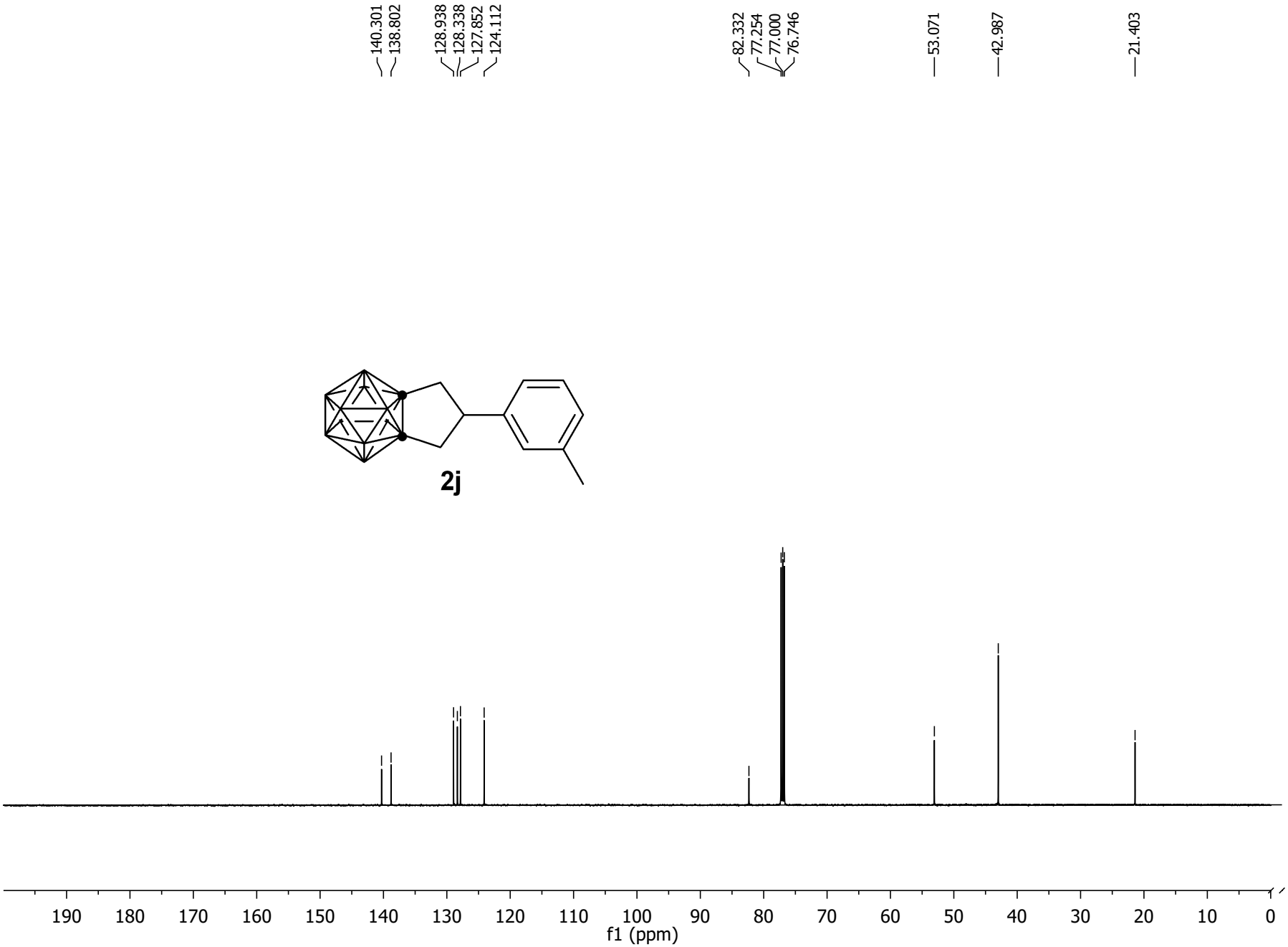
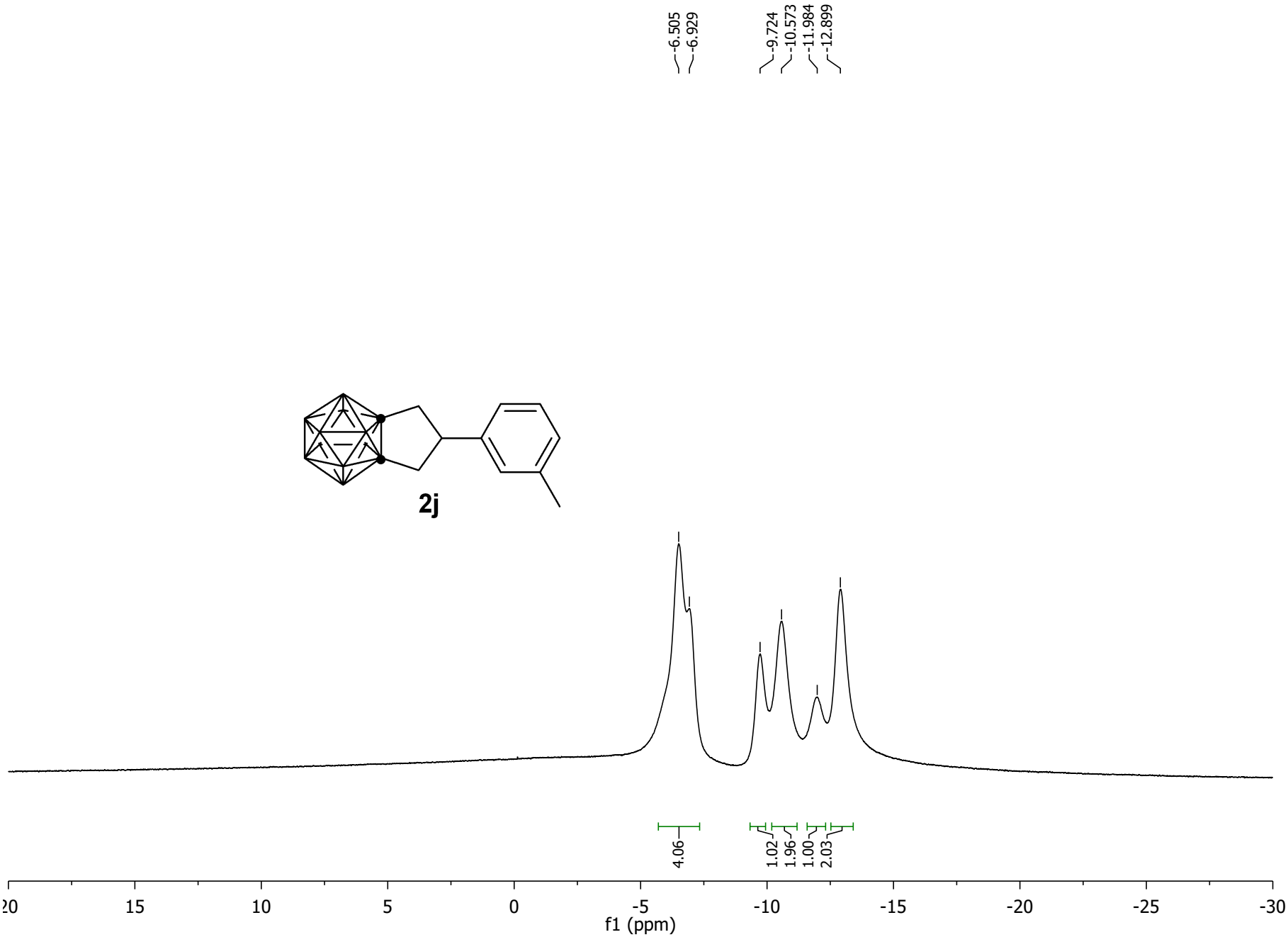
Parameter	Value
Title	zhjie190710-4-CF3-wu-cdcl3-F
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgflqn
Experiment	1D
Number of Scans	32
Receiver Gain	7
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.5767
Spectrometer Frequency	470.59
Spectral Width	113636.4
Lowest Frequency	-103877.4
Nucleus	19F
Acquired Size	65536
Spectral Size	131072



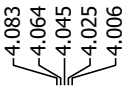
Parameter	Value
Title	zhjie190313-3-Me-wu-p-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	31
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

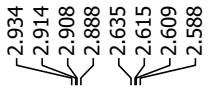


Parameter	Value
Title	zhjie190313-3-Me-wu-p-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	128
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2310.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

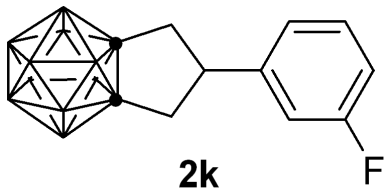


Parameter	Value
Title	zhjie190313-3-Me-wu-p-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768





Parameter	Value
Title	zhjie190315-3-f-wu-p-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	31
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1925.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



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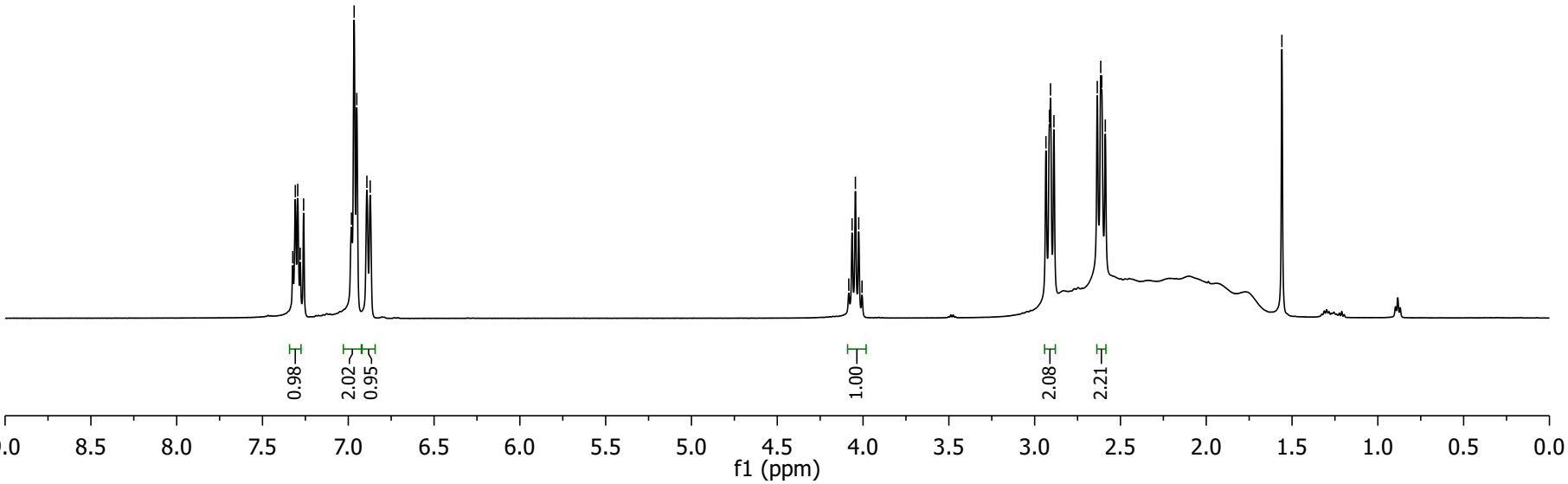
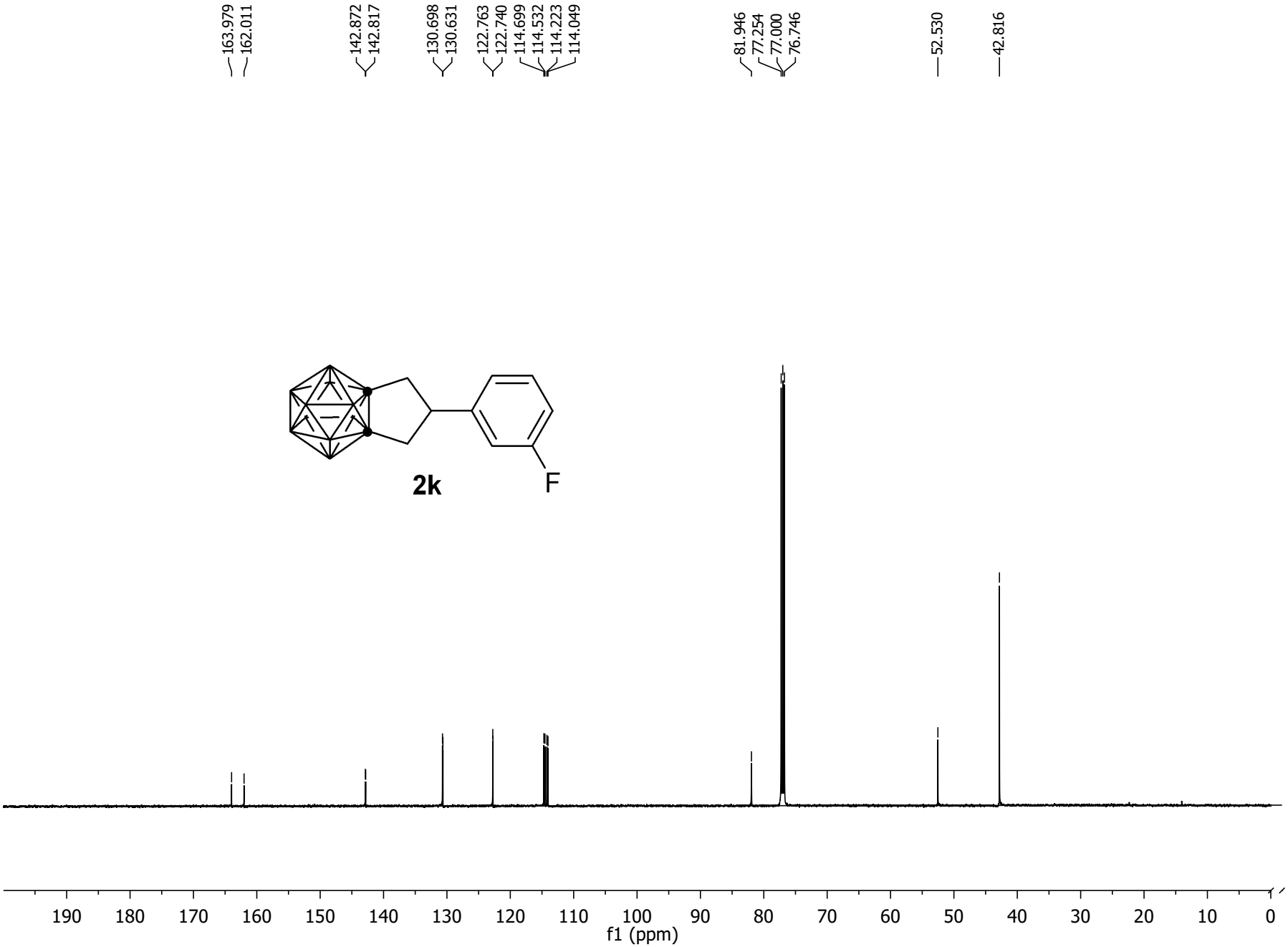
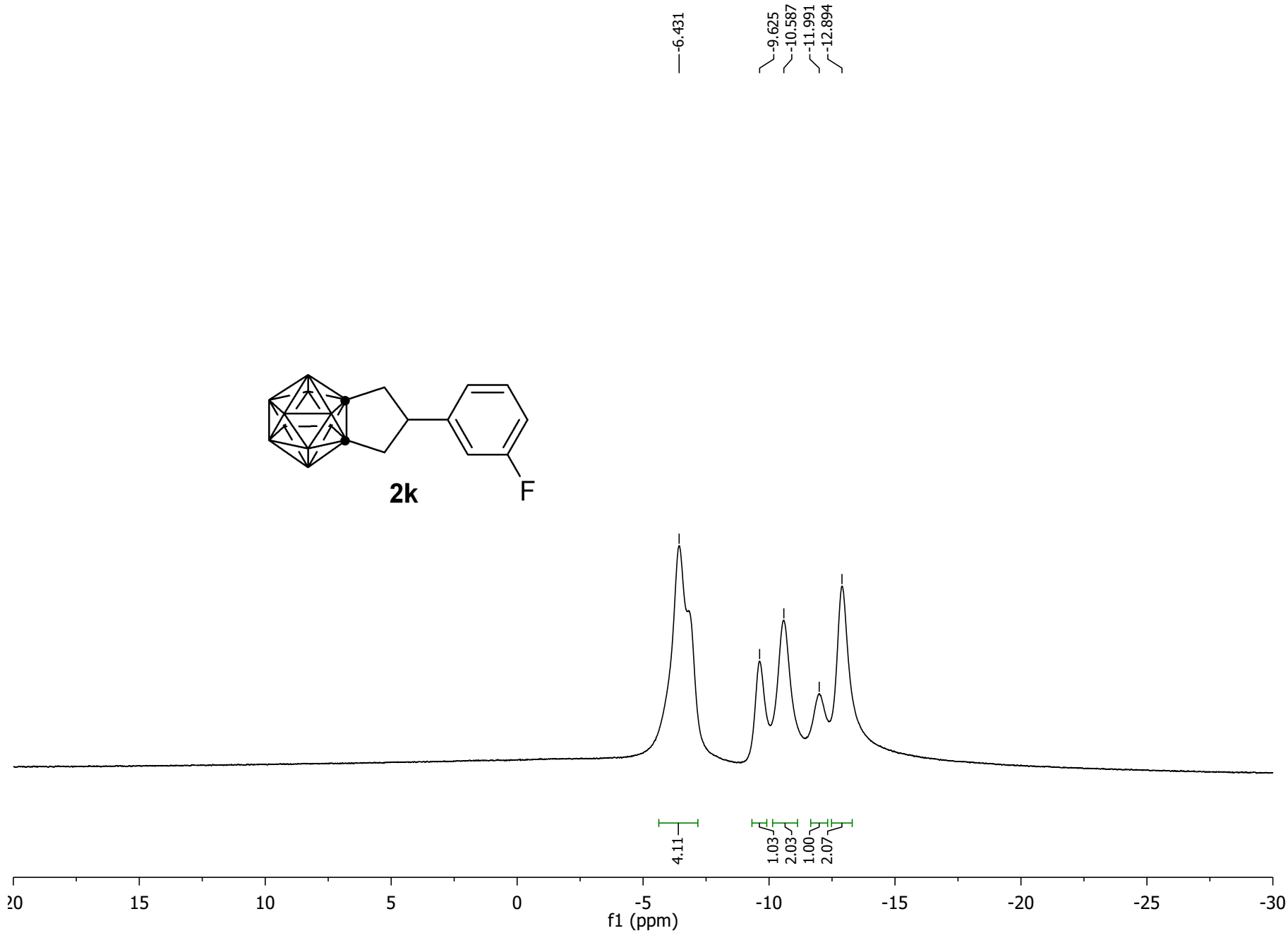
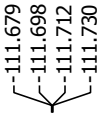




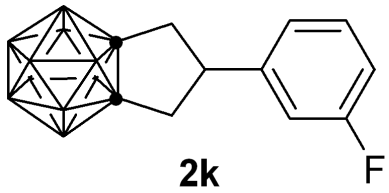
Parameter	Value
Title	zhjie190315-3-f-wu-p-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	256
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.77
Spectral Width	29761.9
Lowest Frequency	-2308.9
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie190315-3-f-wu-p-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



Parameter	Value
Title	zhjie190315-3-f-wu-p-cdcl3-F
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgflqn
Experiment	1D
Number of Scans	16
Receiver Gain	7
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.5767
Spectrometer Frequency	470.55
Spectral Width	113636.4
Lowest Frequency	-103877.4
Nucleus	19F
Acquired Size	65536
Spectral Size	131072



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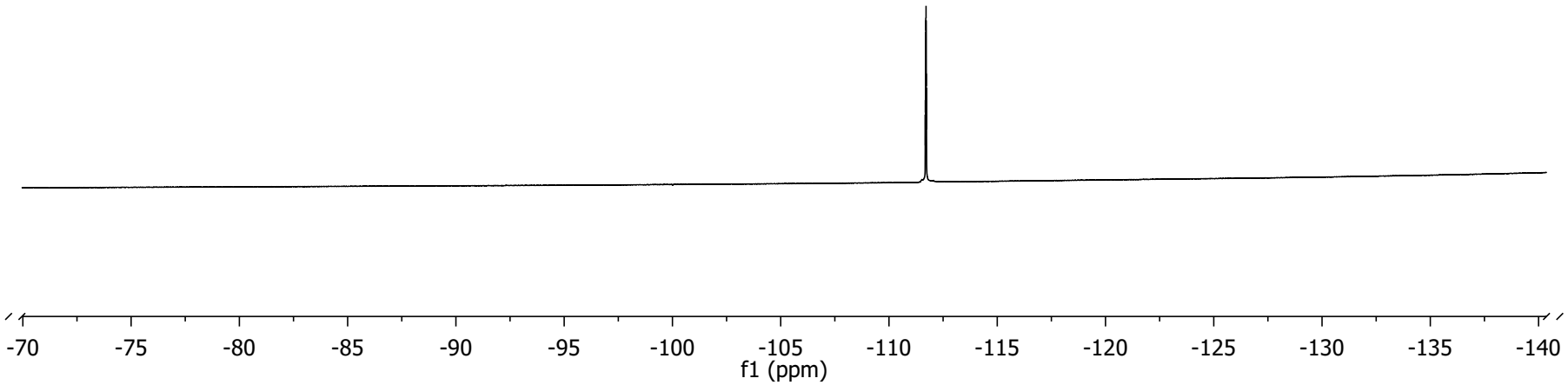
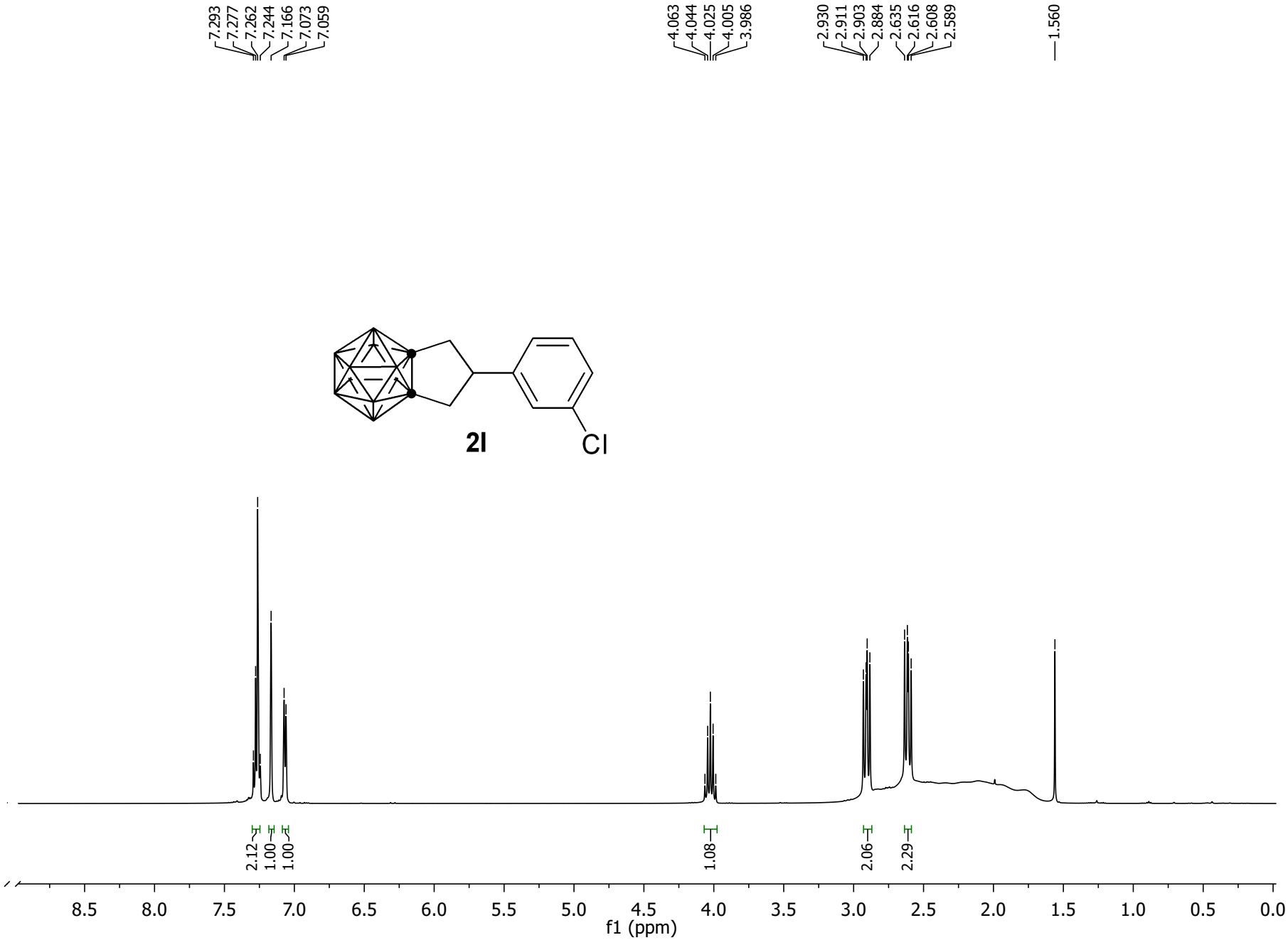
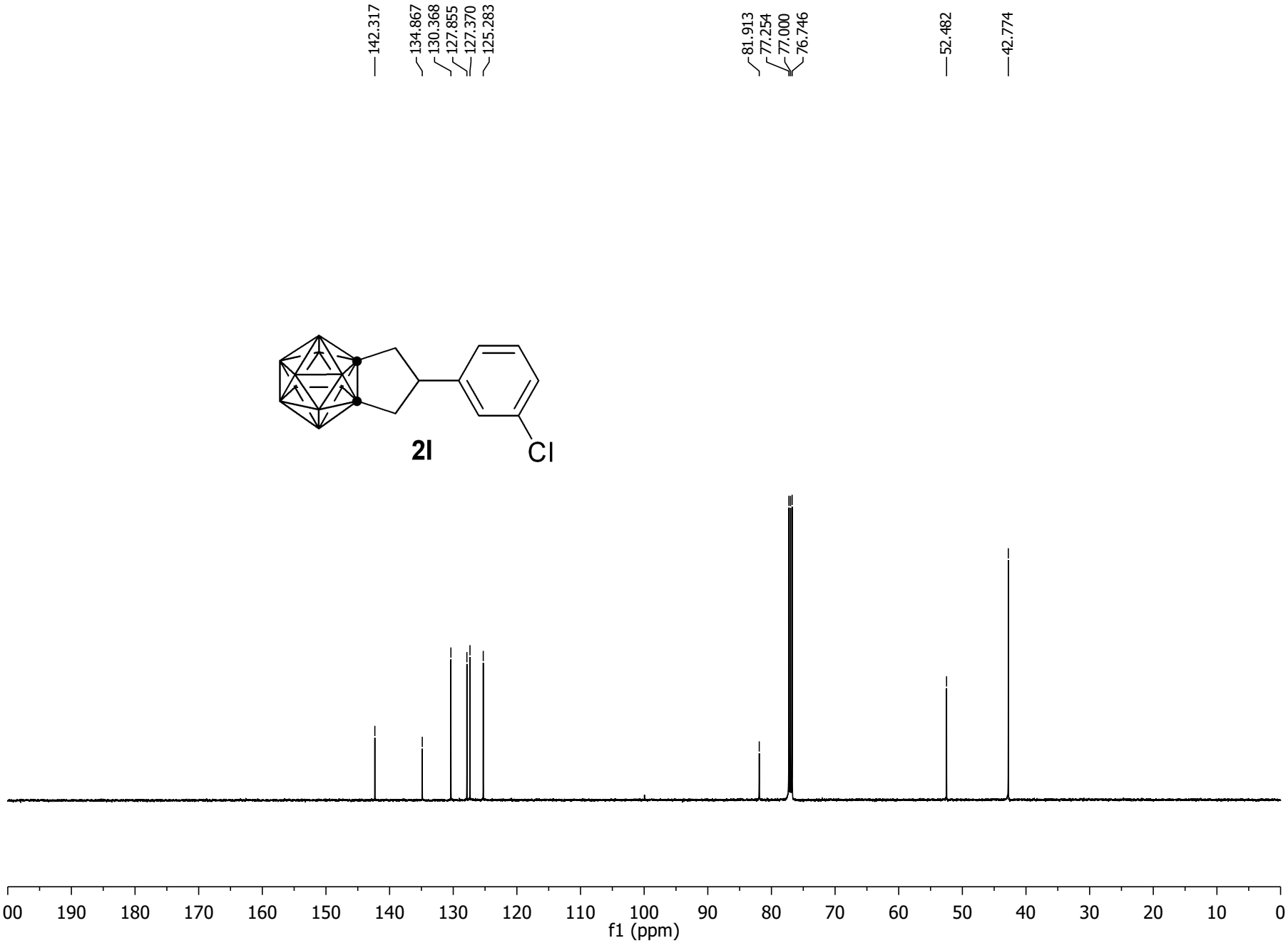
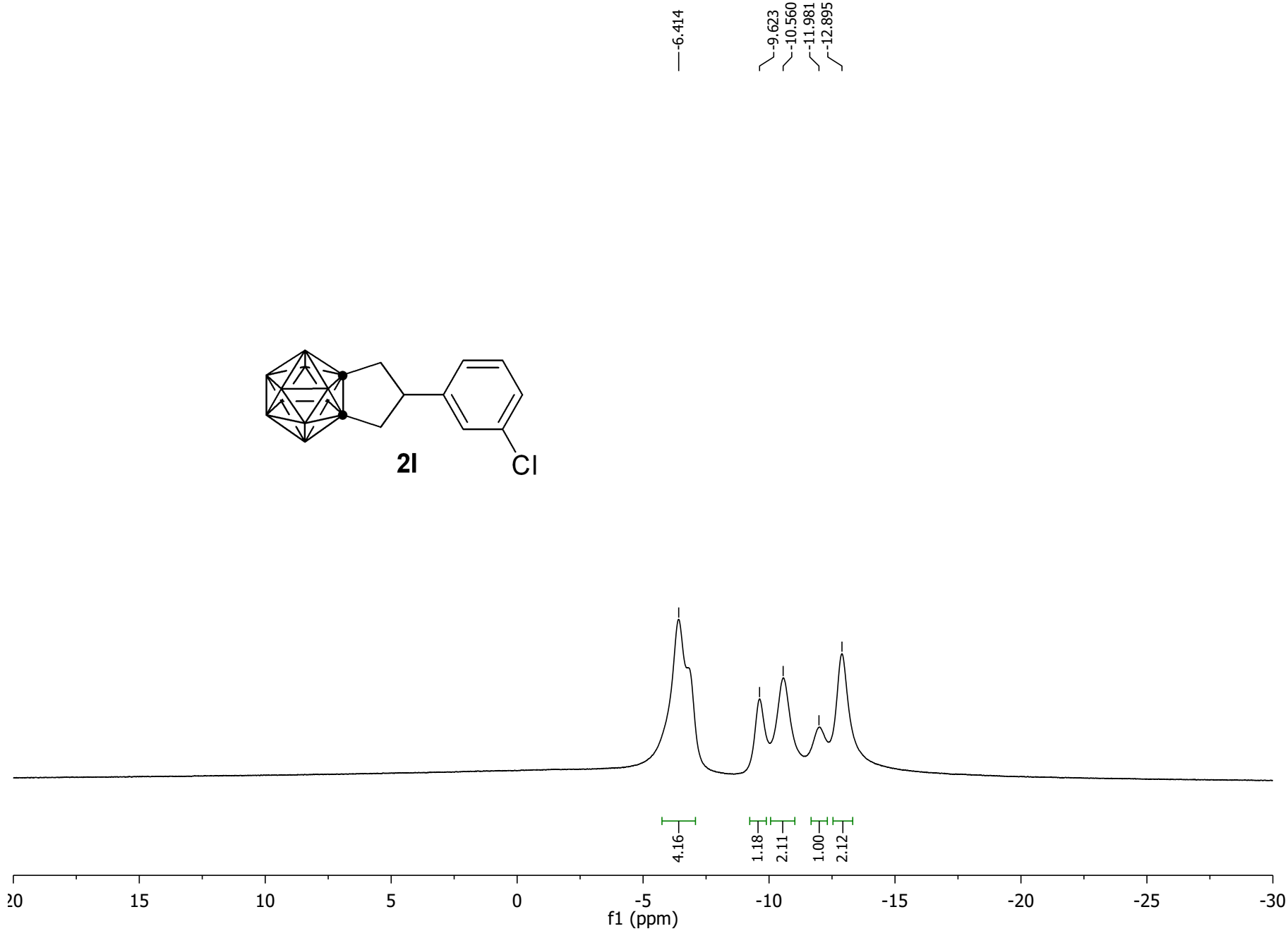




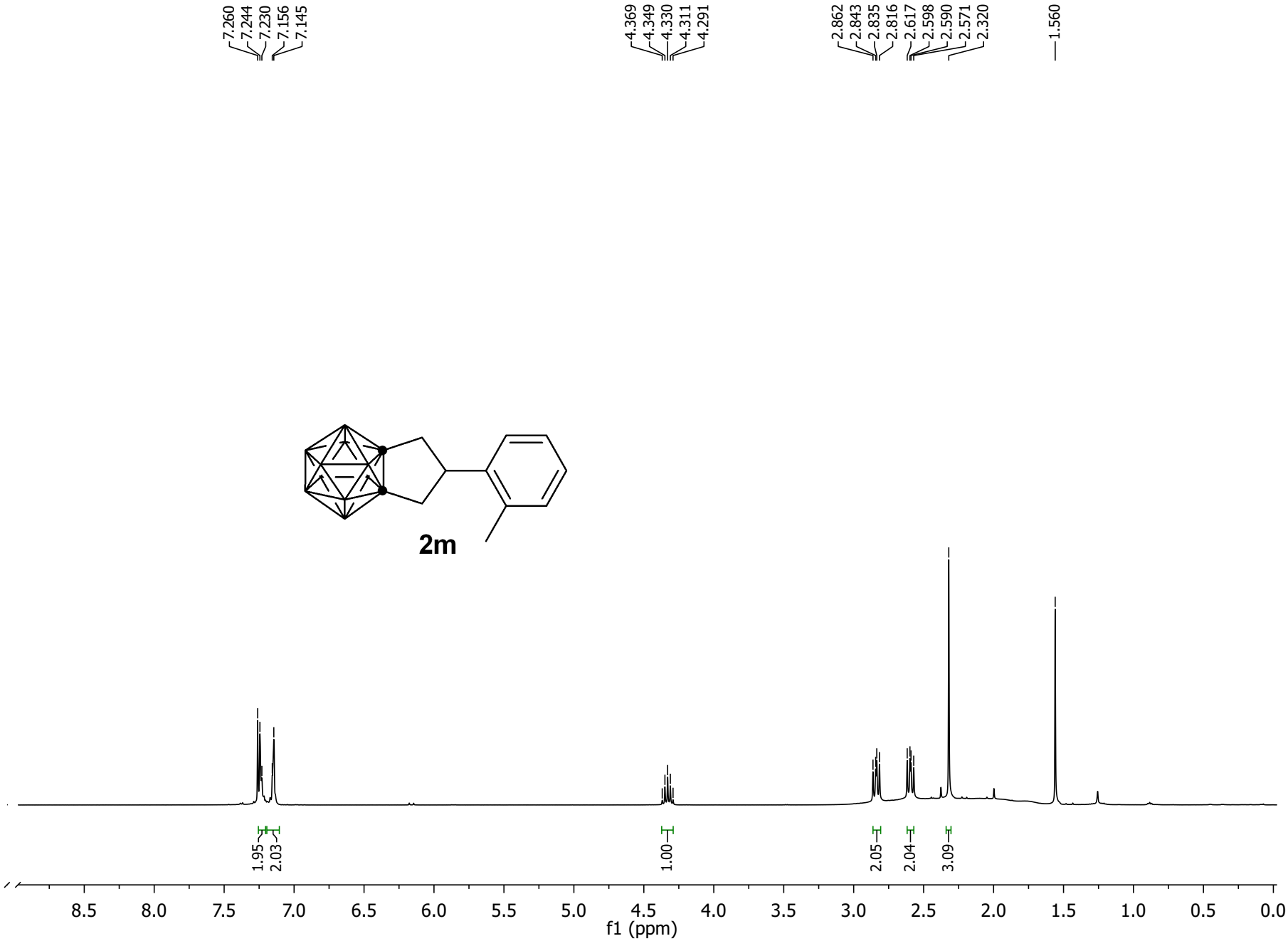
Parameter	Value
Title	zhjie190313-3-Cl-wu-p-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	31
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1923.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



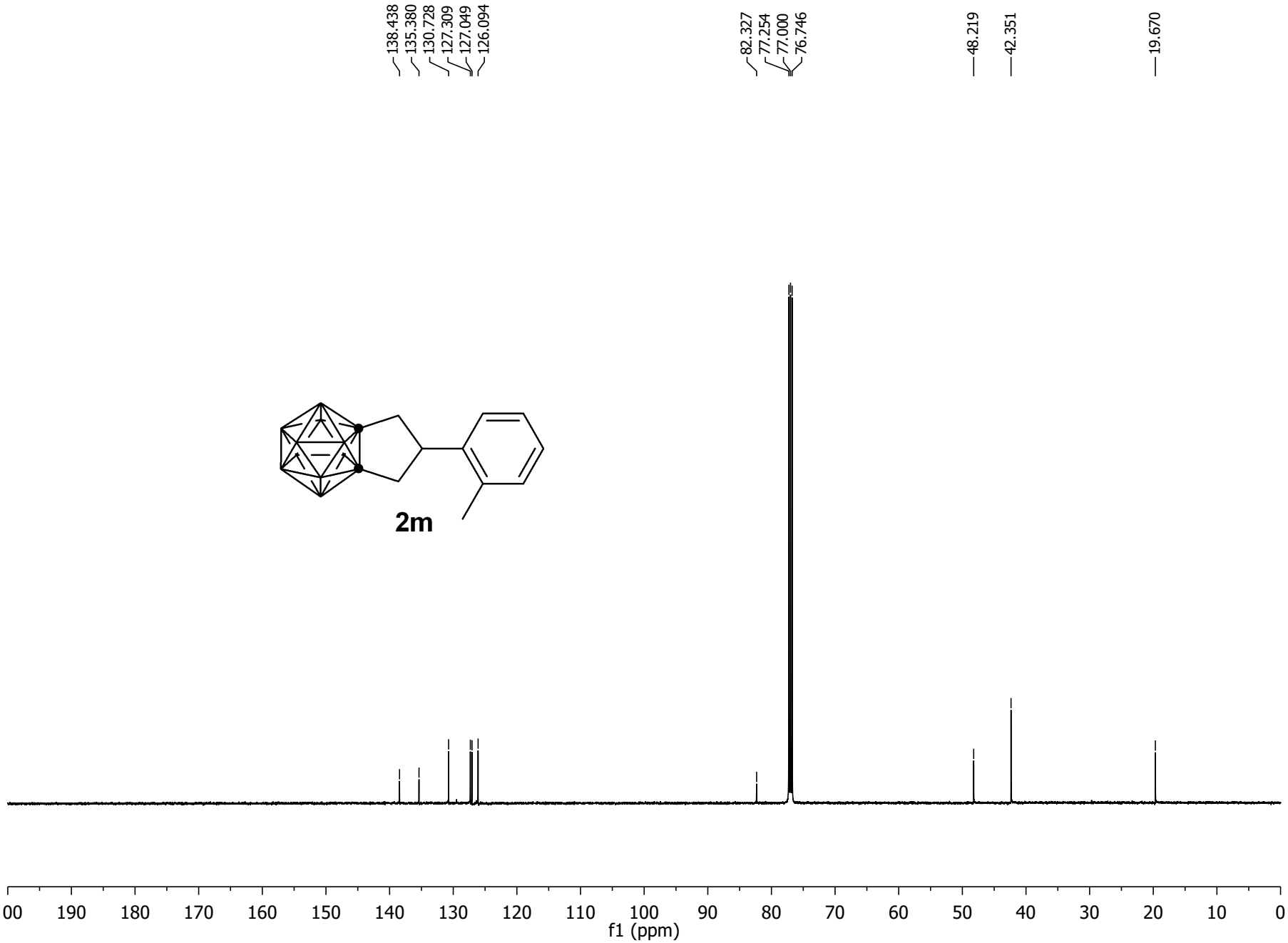
Parameter	Value
Title	zhjie190313-3-Cl-wu-p-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	128
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2311.0
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



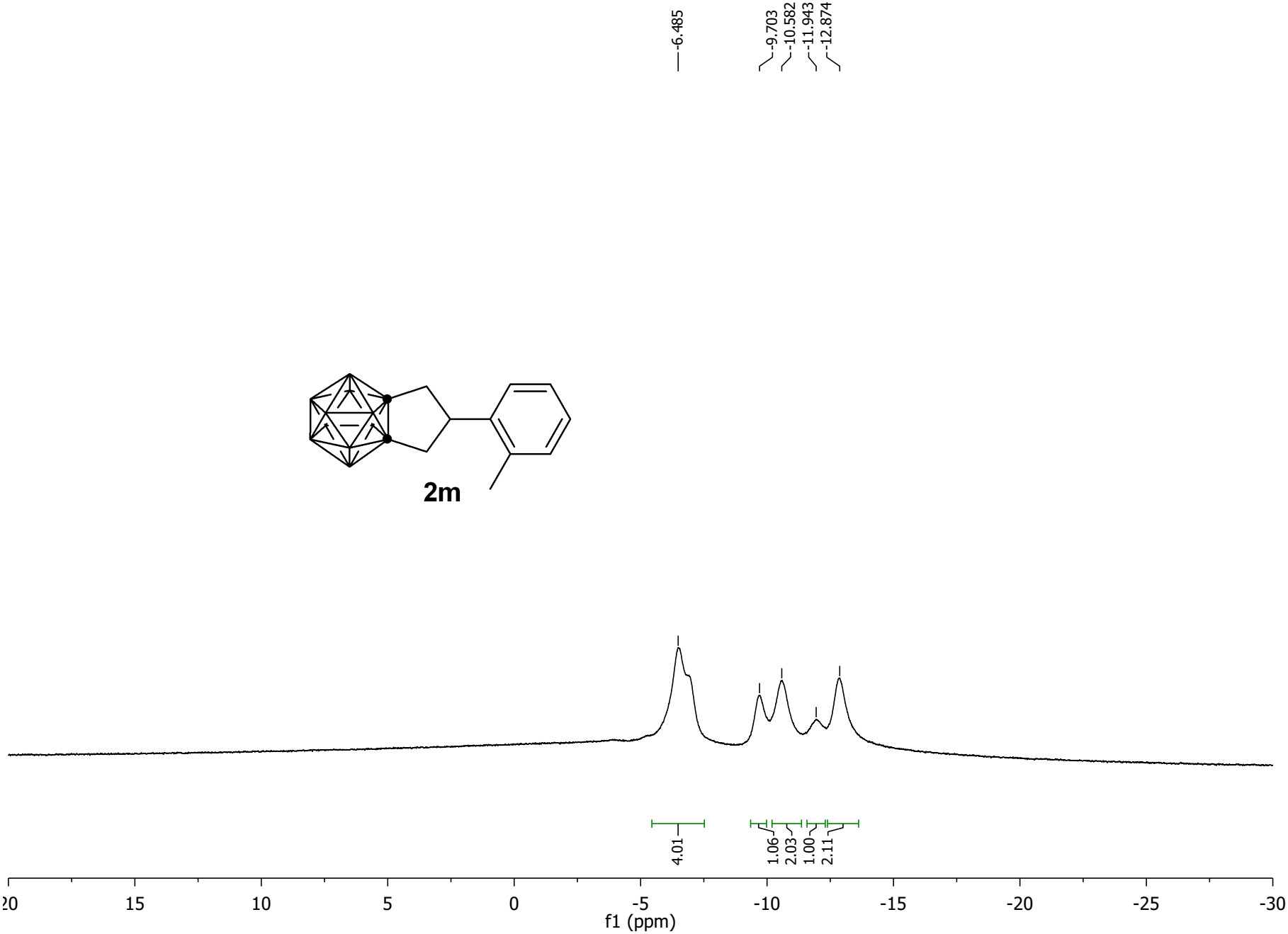
Parameter	Value
Title	zhjie190313-3-Cl-wu-p-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



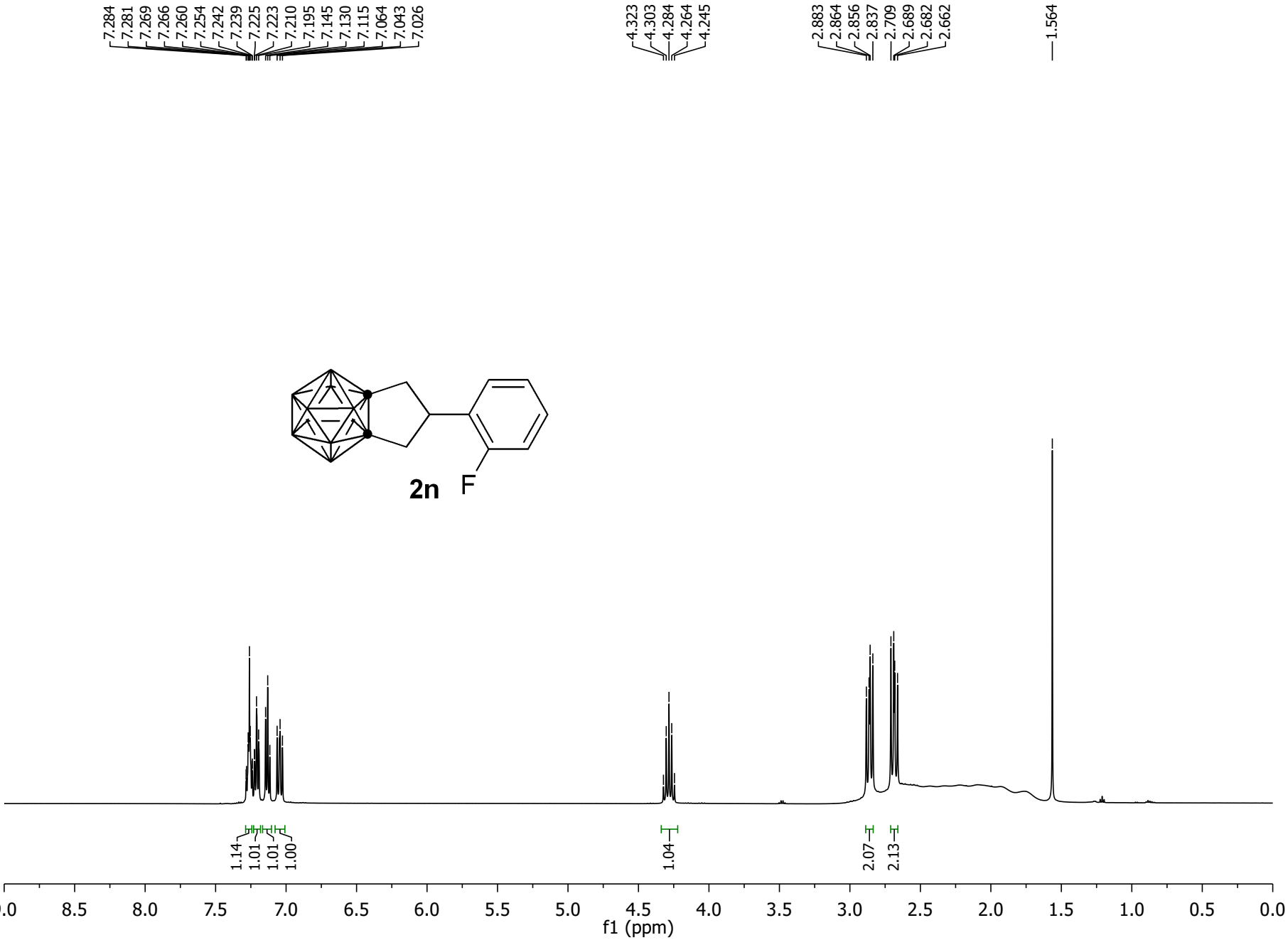
Parameter	Value
Title	zhjie190314-2-Me-wu-p-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	57
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



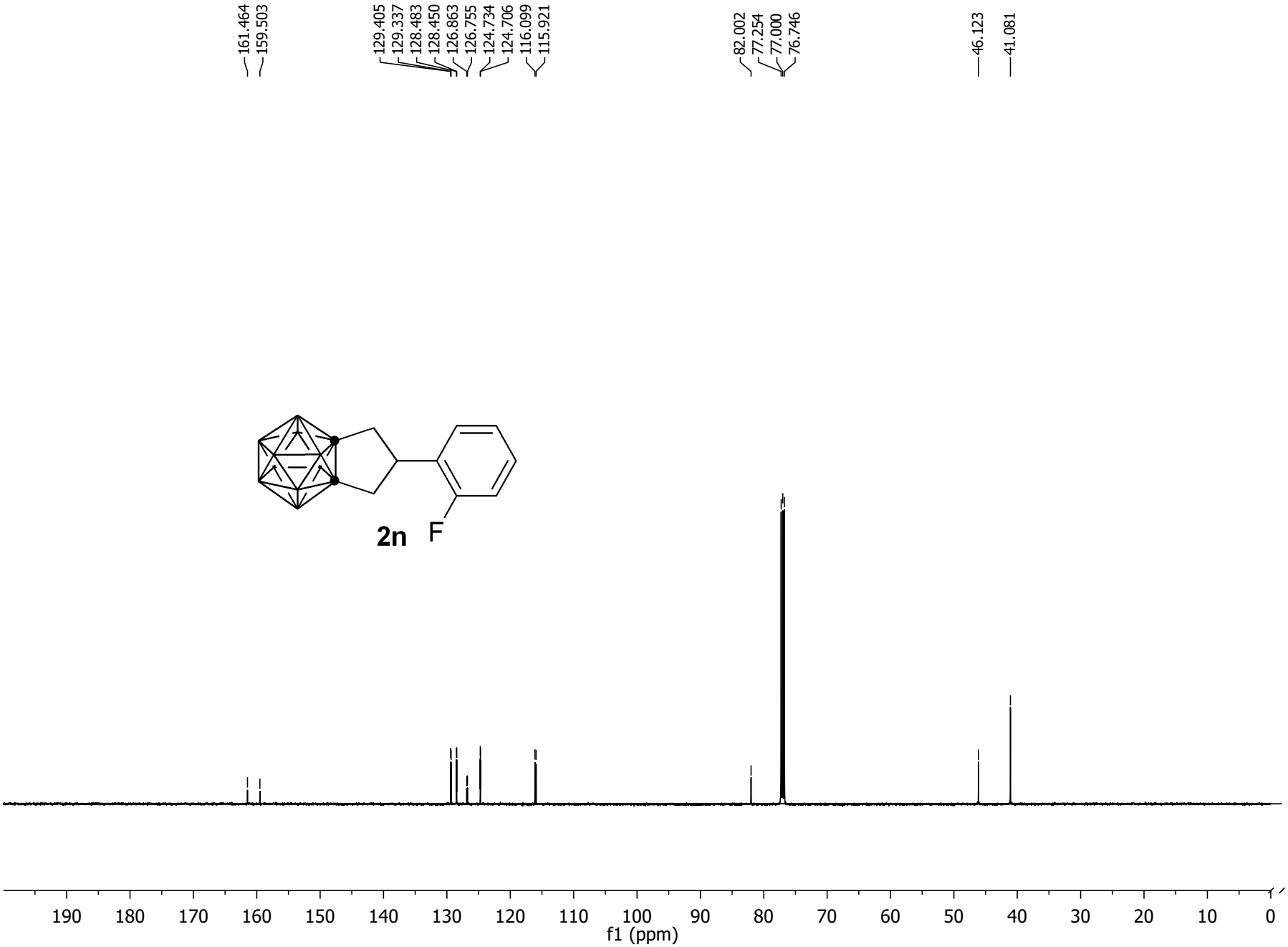
Parameter	Value
Title	zhjie190314-2-Me-wu-p-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	300
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.77
Spectral Width	29761.9
Lowest Frequency	-2308.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



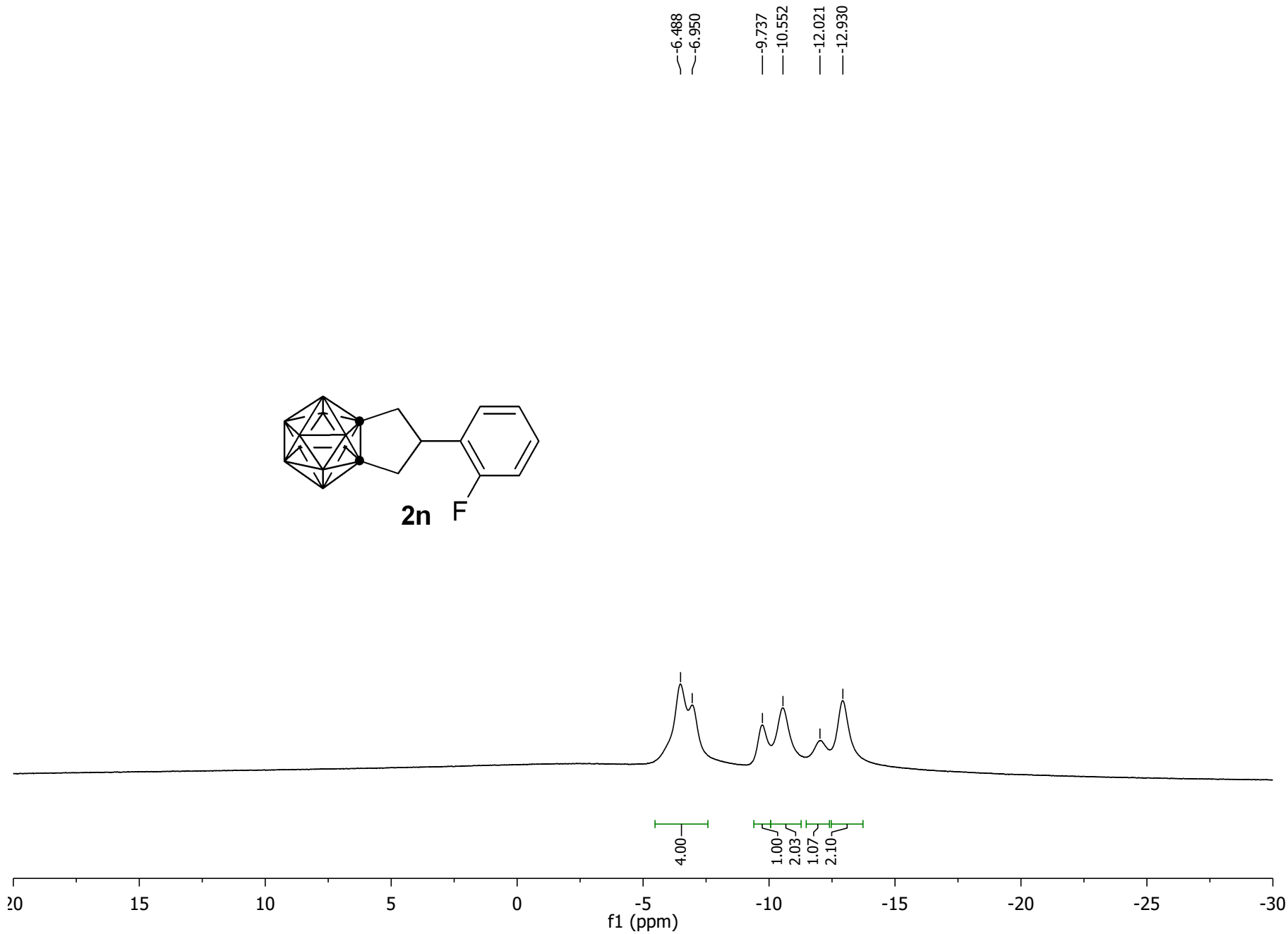
Parameter	Value
Title	zhjie190314-2-Me-wu-p-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



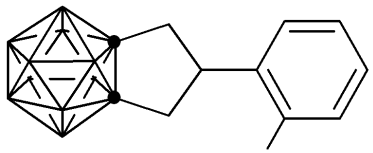
Parameter	Value
Title	zhjie190613-2-F-wu-P-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	31
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie190613-2-F-wu-P-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	128
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2309.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie190613-2-F-wu-P-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



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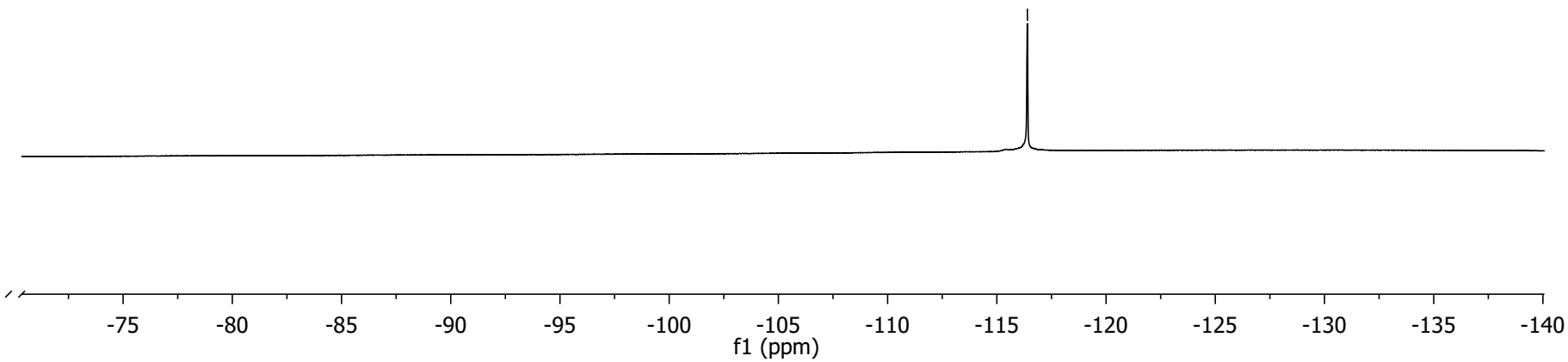
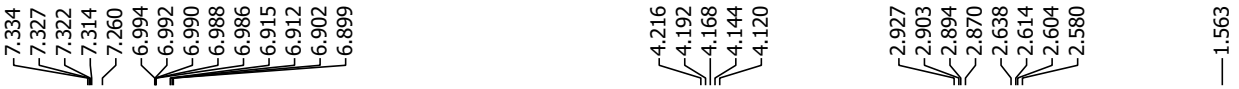
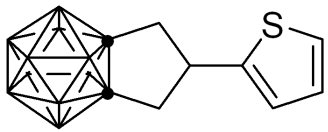
-116.399

Parameter	Value
Title	zhjie190618-2-F-wu-cdcl3-F
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgflqn
Experiment	1D
Number of Scans	32
Receiver Gain	7
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.5767
Spectrometer Frequency	470.59
Spectral Width	113636.4
Lowest Frequency	-103877.4
Nucleus	19F
Acquired Size	65536
Spectral Size	131072





Parameter	Value
Title	zhjie191101-wup-thiophene-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	295.4
Pulse Sequence	zg30
Experiment	1D
Number of Scans	24
Receiver Gain	181
Relaxation Delay	1.0000
Pulse Width	14.5000
Acquisition Time	4.0894
Spectrometer Frequency	400.23
Spectral Width	8012.8
Lowest Frequency	-1545.0
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



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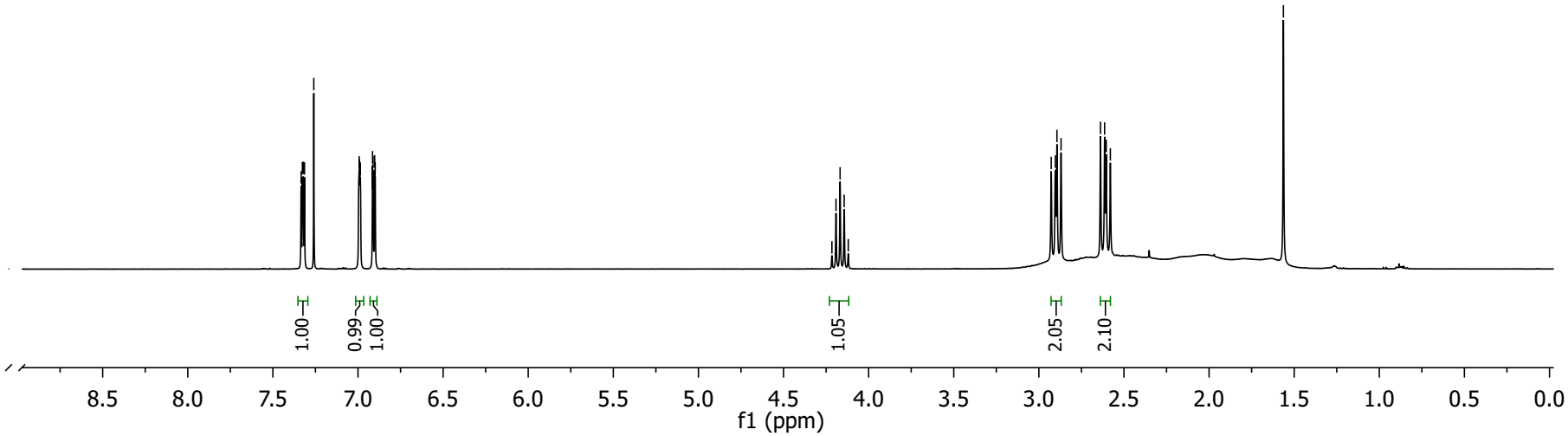
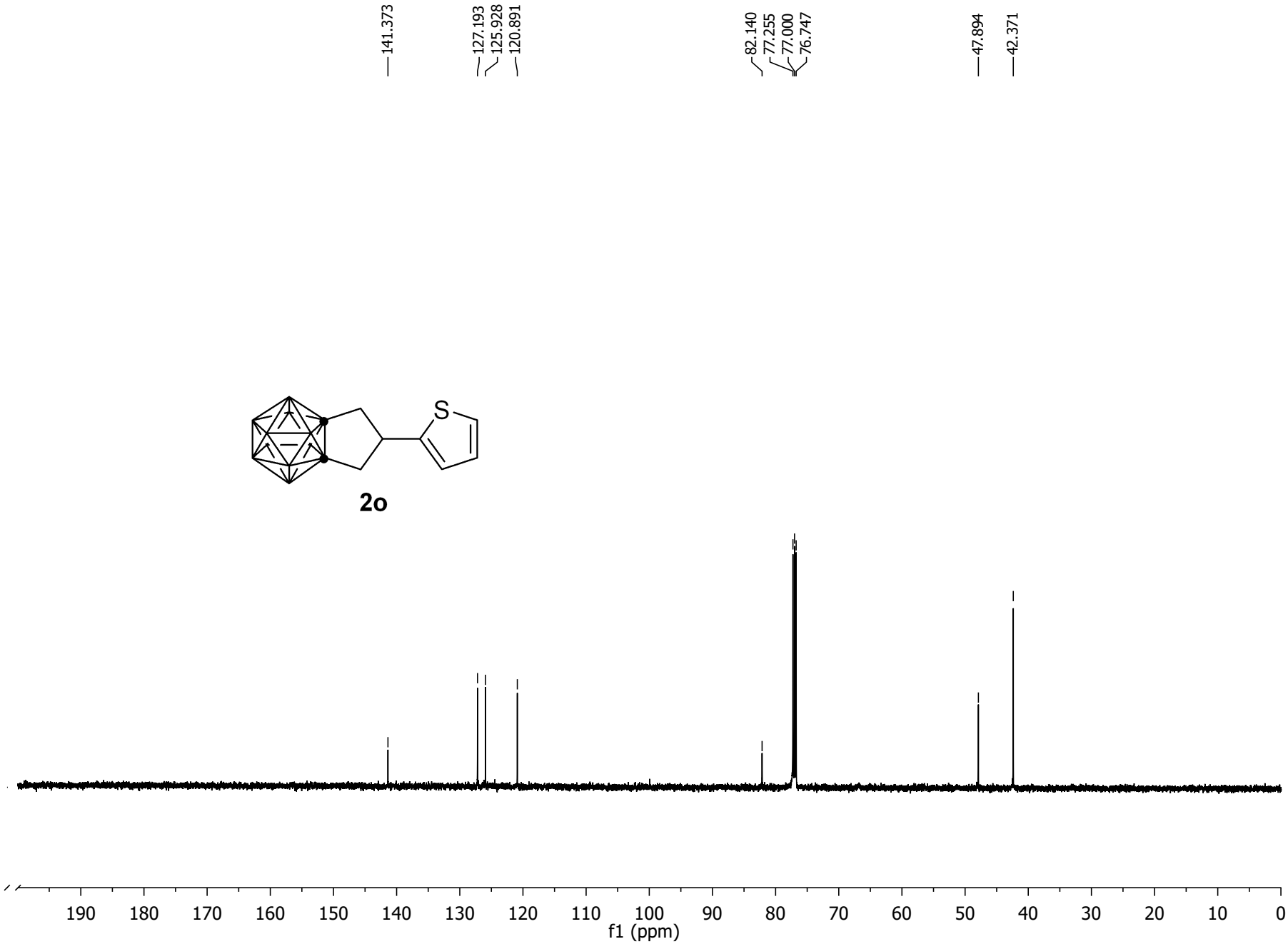
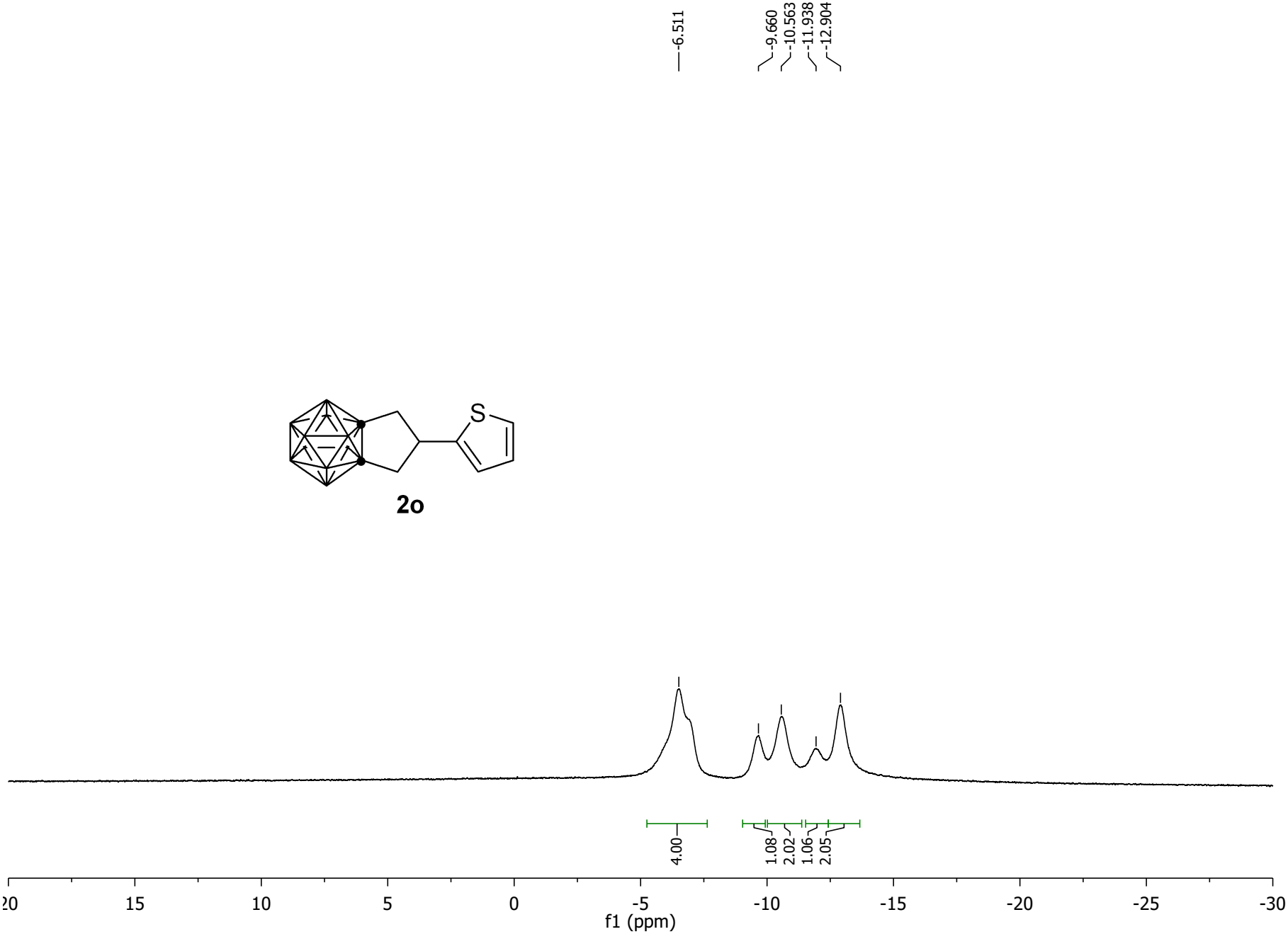


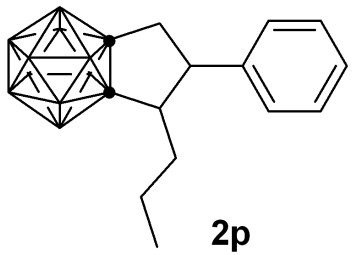


Parameter	Value
Title	zhjie190921-wu-thiophene-p-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	295.2
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	110
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	9.7500
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2312.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie191101-wup-thiophene-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	295.3
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	16.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

Parameter	Value
Title	zhjie190313-ynePh-Bu-wu-p-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	51
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



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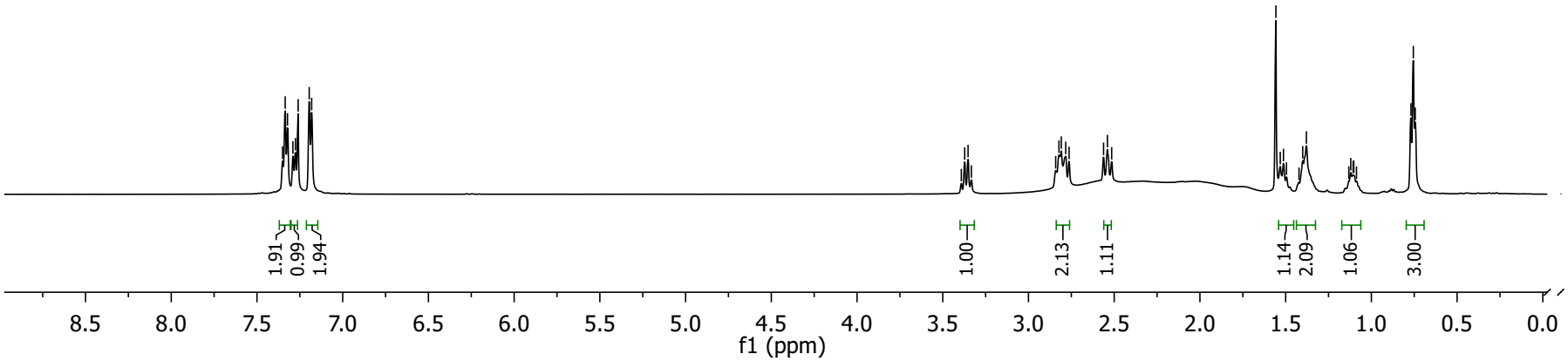
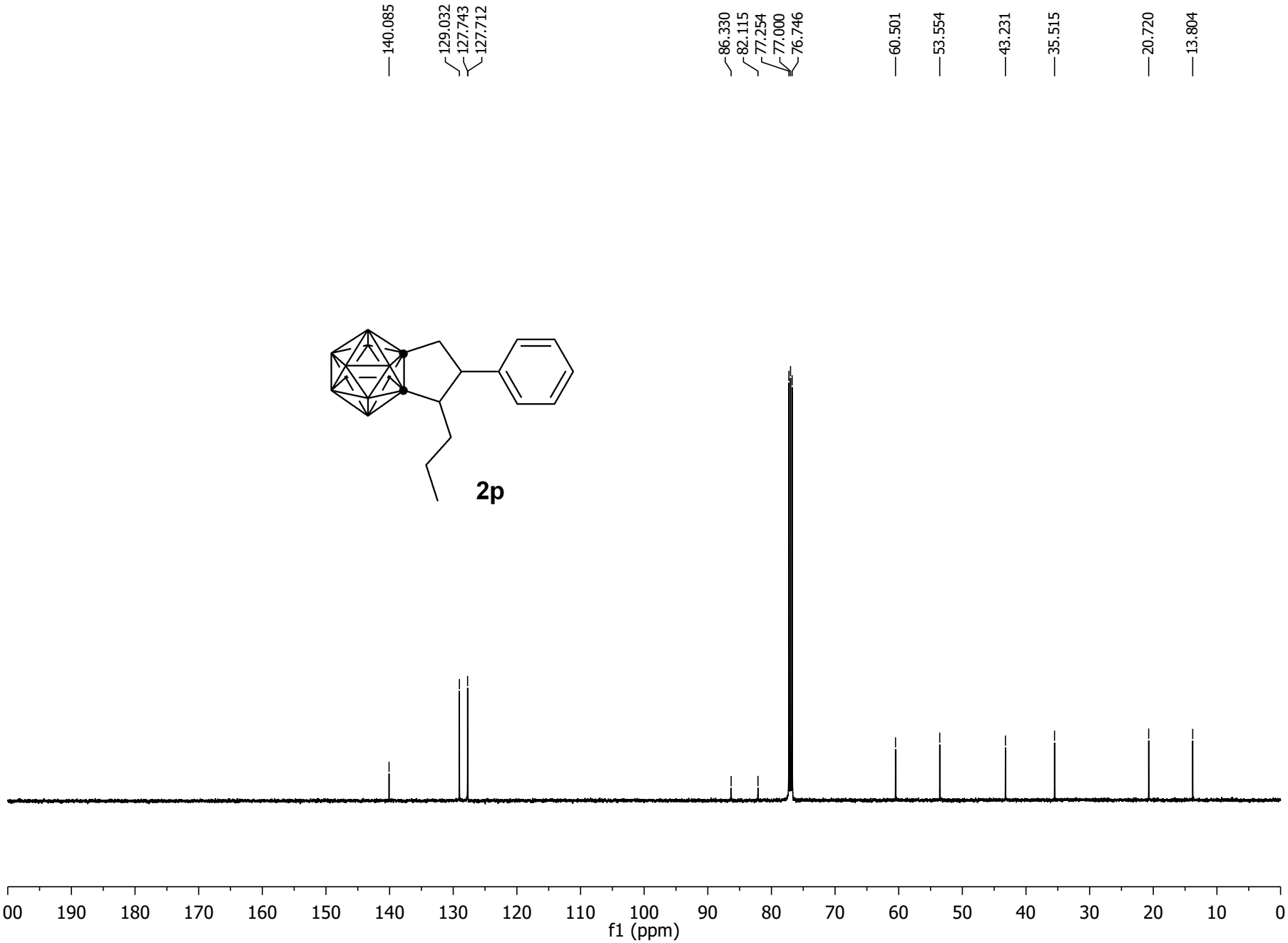
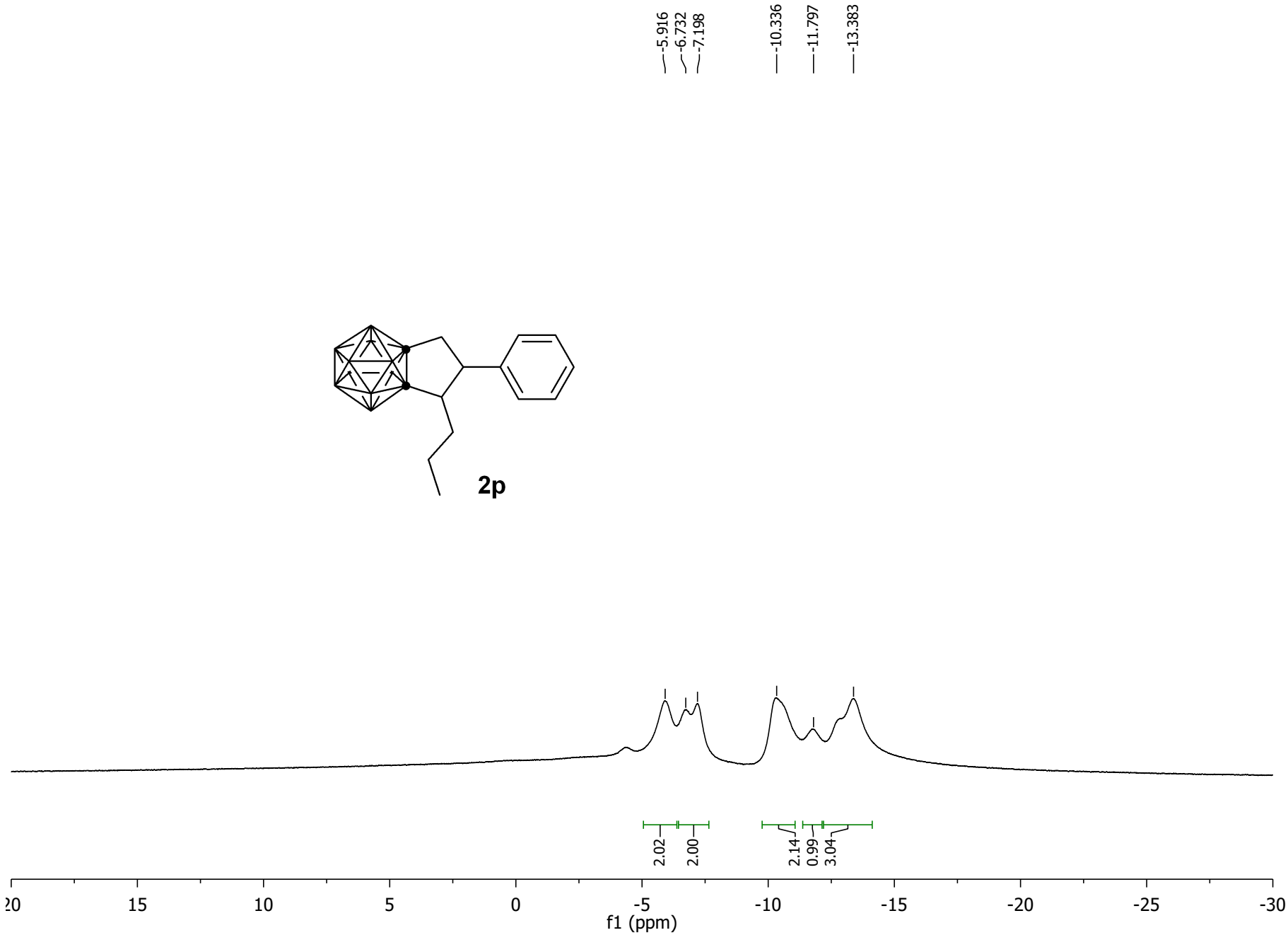
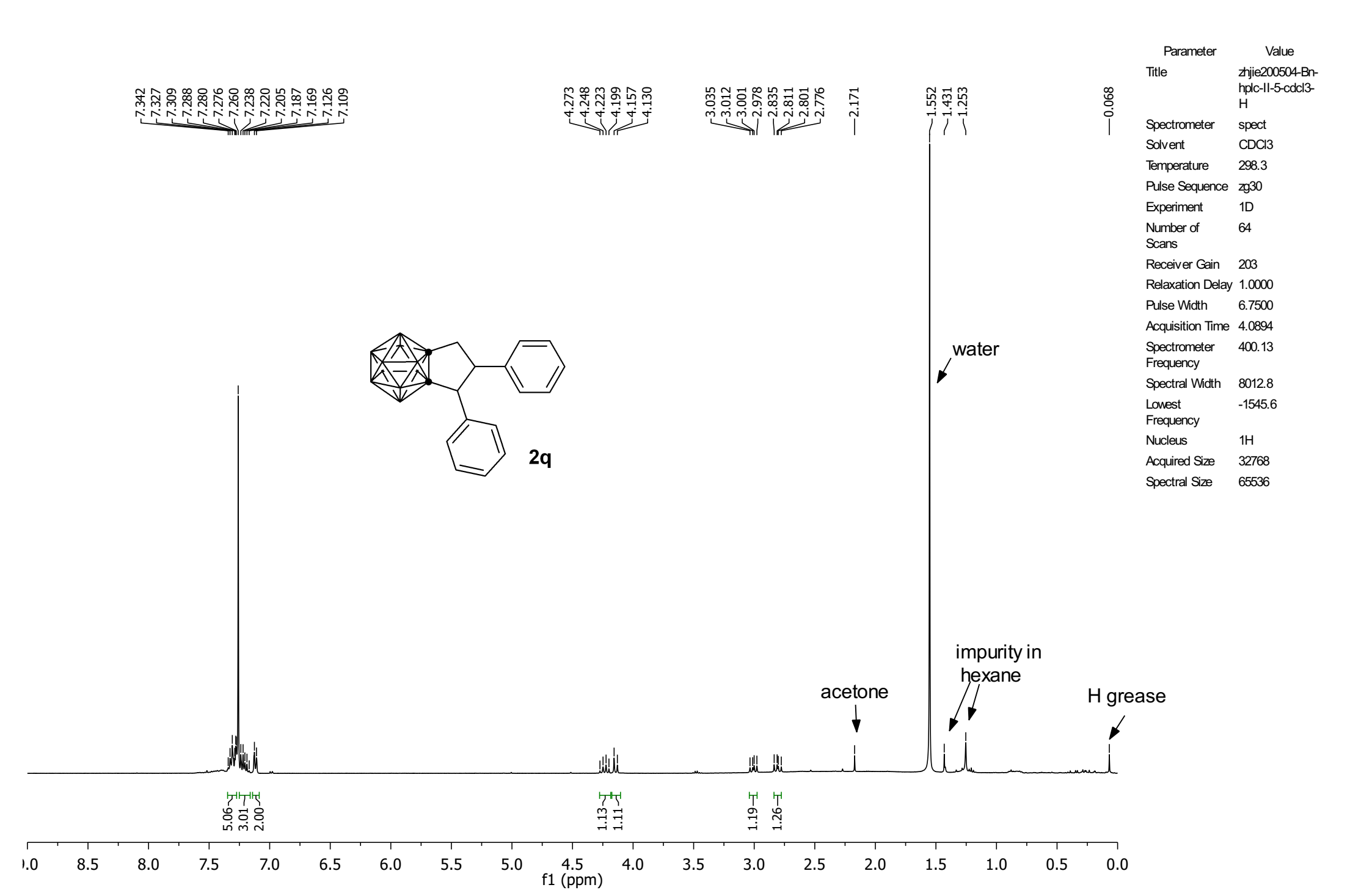




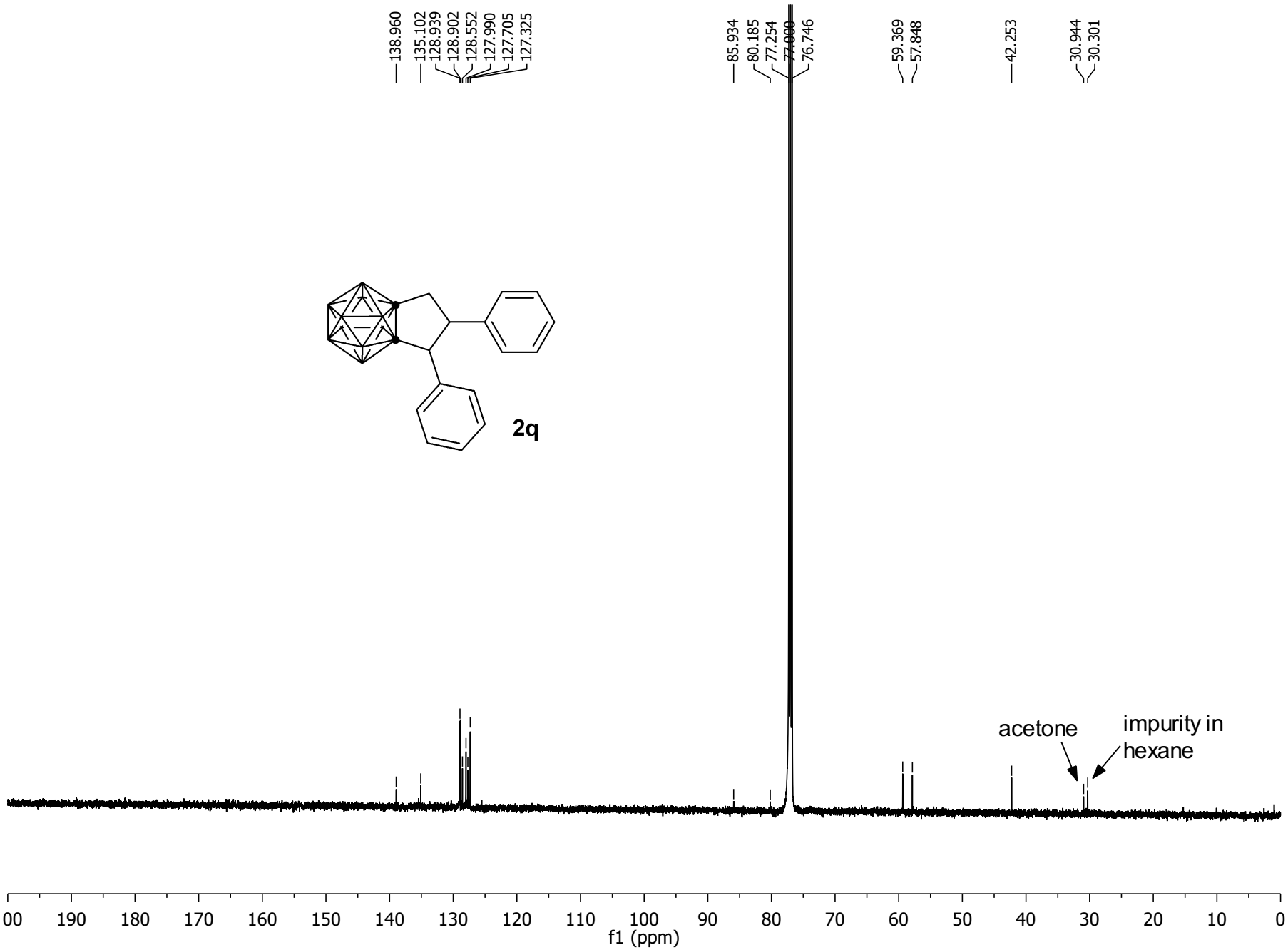
Parameter	Value
Title	zhjie190313-ynePh-Bu-wu-p-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	128
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2309.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



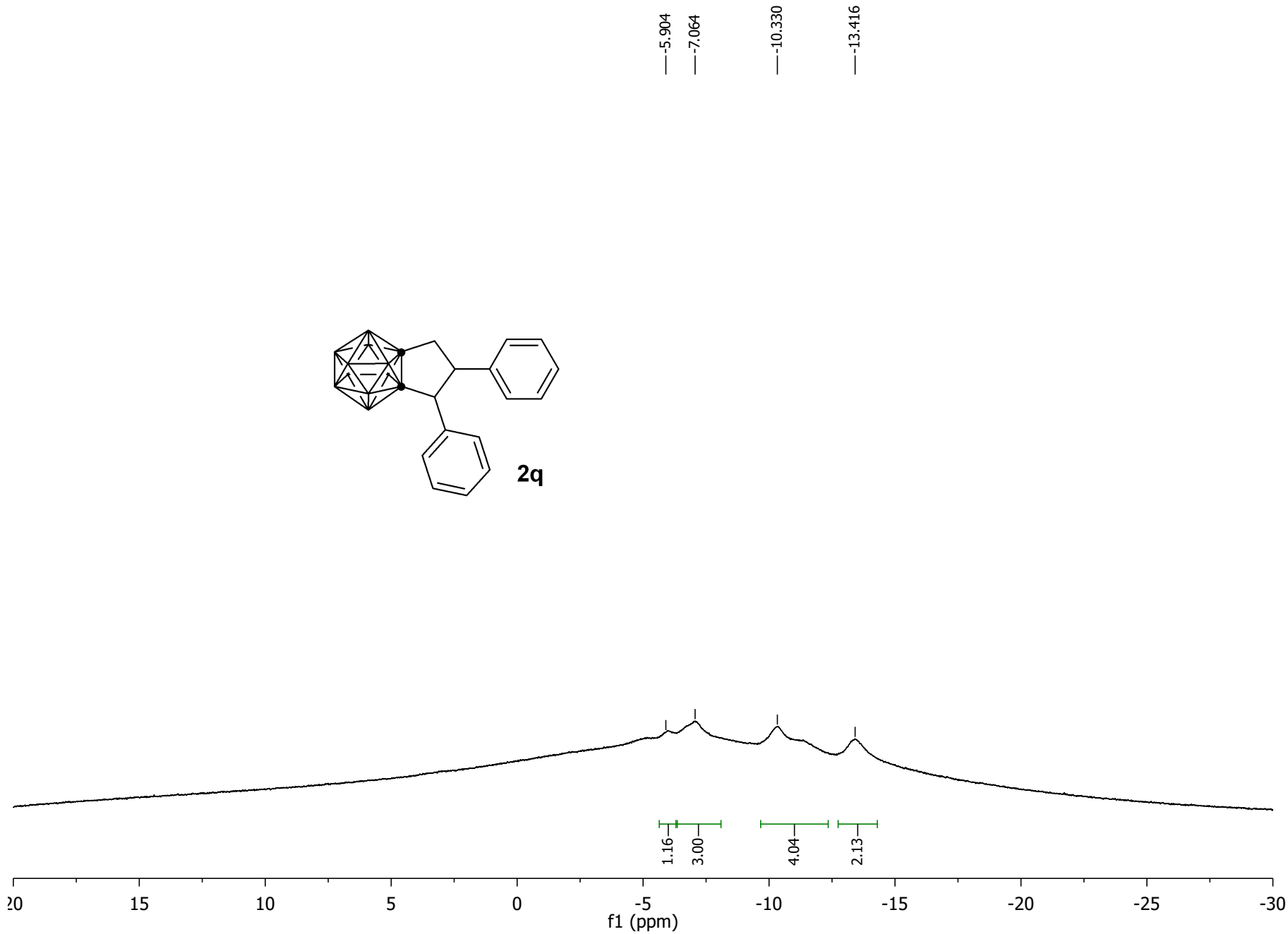
Parameter	Value
Title	zhjie190102-4-Br-wu-cdcl3-B
Spectrometer	spect
Solvent	None
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



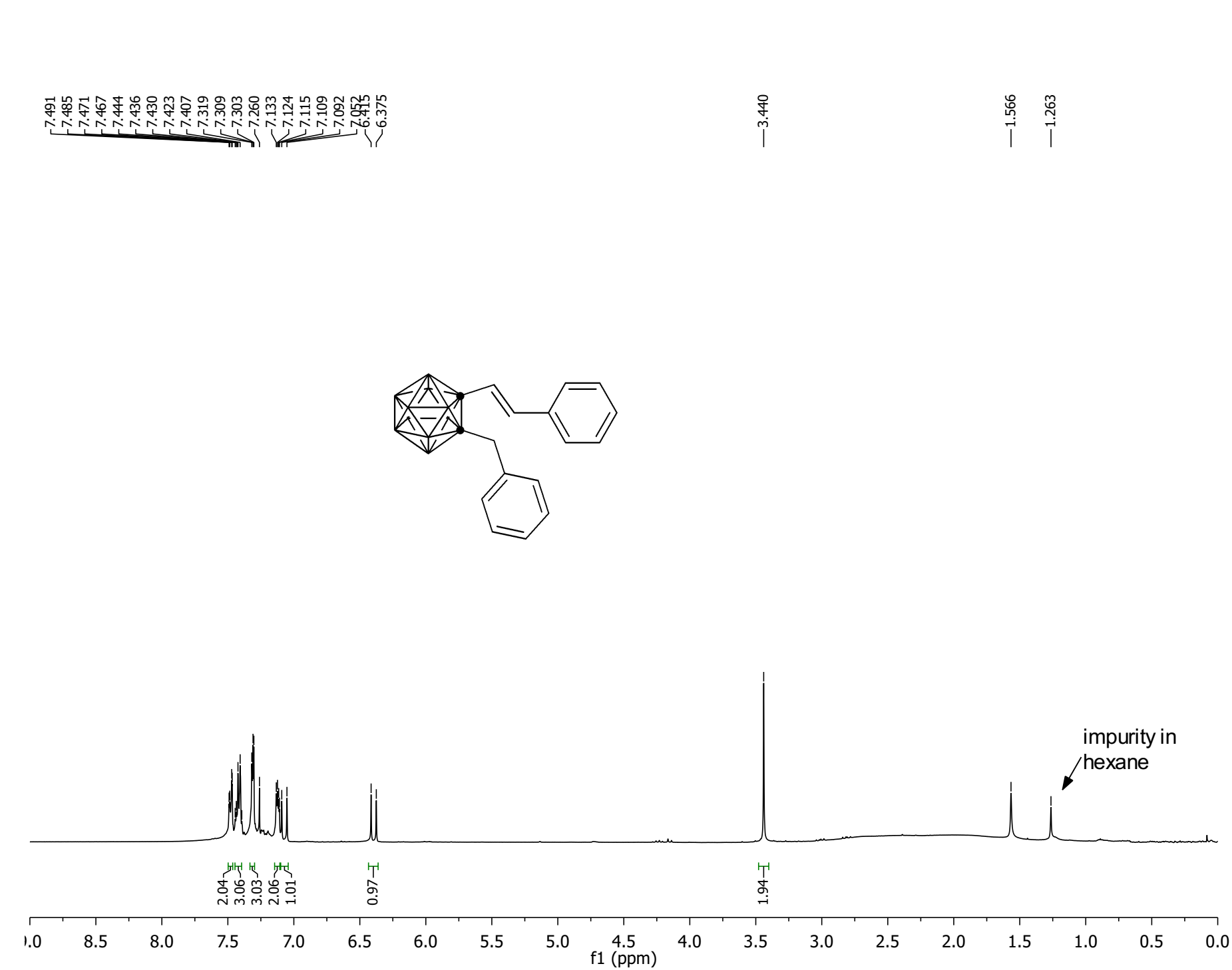
Parameter	Value
Title	zhjie200504-Bn-hplc-II-5-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.3
Pulse Sequence	zg30
Experiment	1D
Number of Scans	64
Receiver Gain	203
Relaxation Delay	1.0000
Pulse Width	6.7500
Acquisition Time	4.0894
Spectrometer Frequency	400.13
Spectral Width	8012.8
Lowest Frequency	-1545.6
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



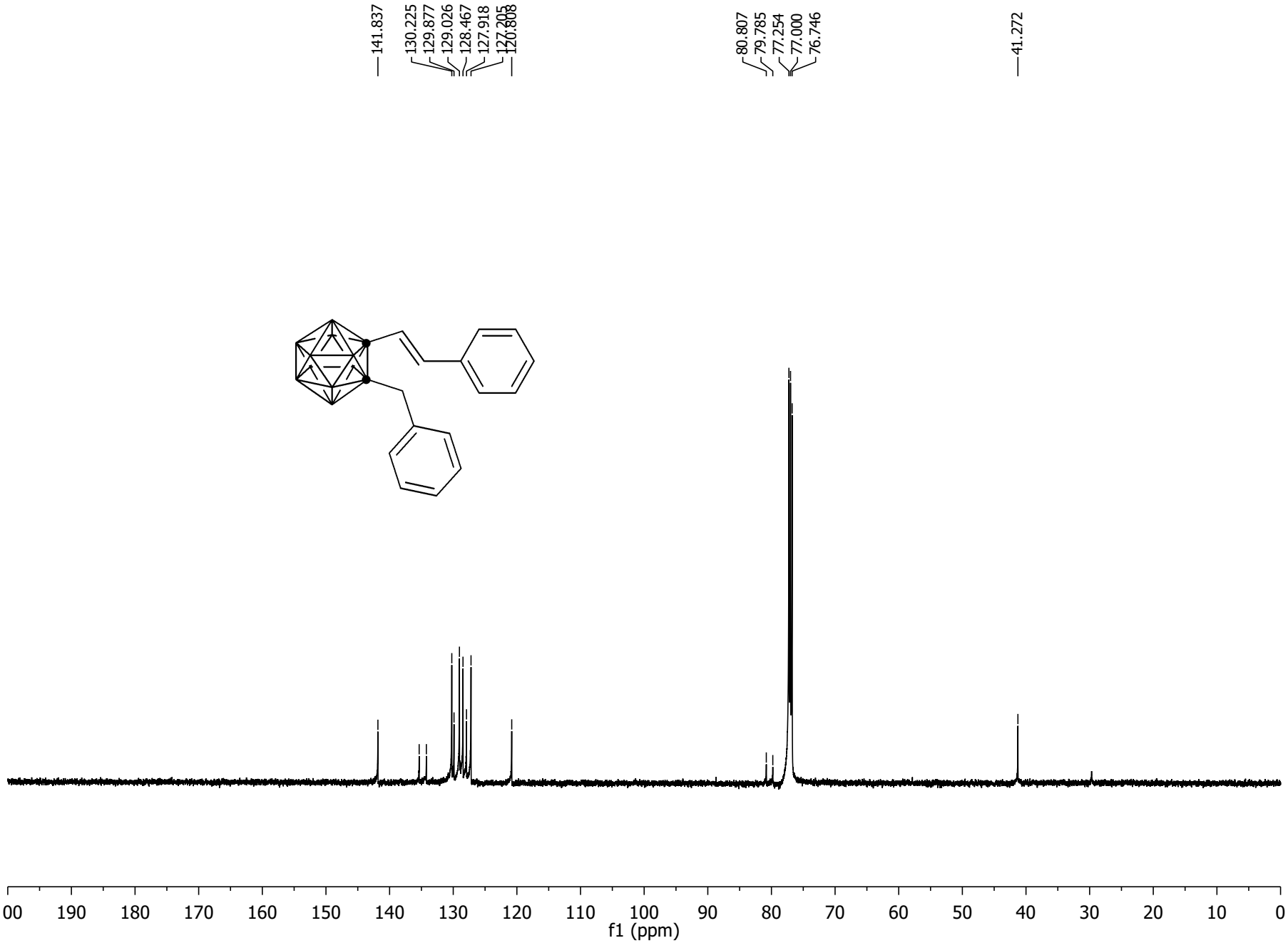
Parameter	Value
Title	zhjie200505-bnhplc-5-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	295.1
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	8000
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	9.7500
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2308.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



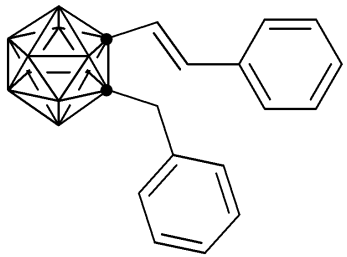
Parameter	Value
Title	zhjie200505-bnhplc-5-cdcl3-B
Spectrometer	spect
Solvent	None
Temperature	295.2
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	500
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	16.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



Parameter	Value
Title	zhjie190115-Bn-p1-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	294.9
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	90
Relaxation Delay	1.0000
Pulse Width	12.8000
Acquisition Time	4.0894
Spectrometer Frequency	400.23
Spectral Width	8012.8
Lowest Frequency	-1544.8
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

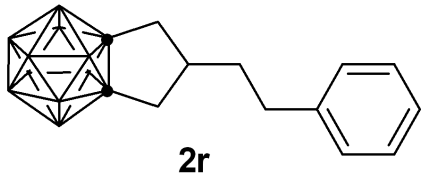


Parameter	Value
Title	zhjie190102-c1Bn-wu-p1-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	256
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.77
Spectral Width	29761.9
Lowest Frequency	-2310.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie190102-c1Bn-wu-p1-cdcl3-B
Spectrometer	spect
Solvent	None
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

Parameter	Value
Title	zhjie-7175-CH2CH2Ph-p2-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	31
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



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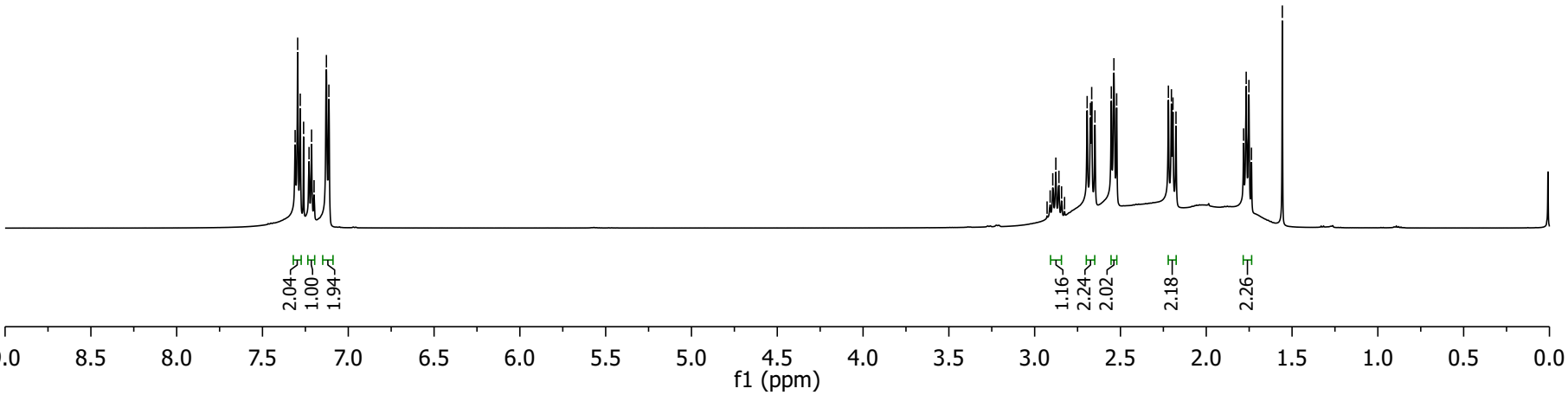
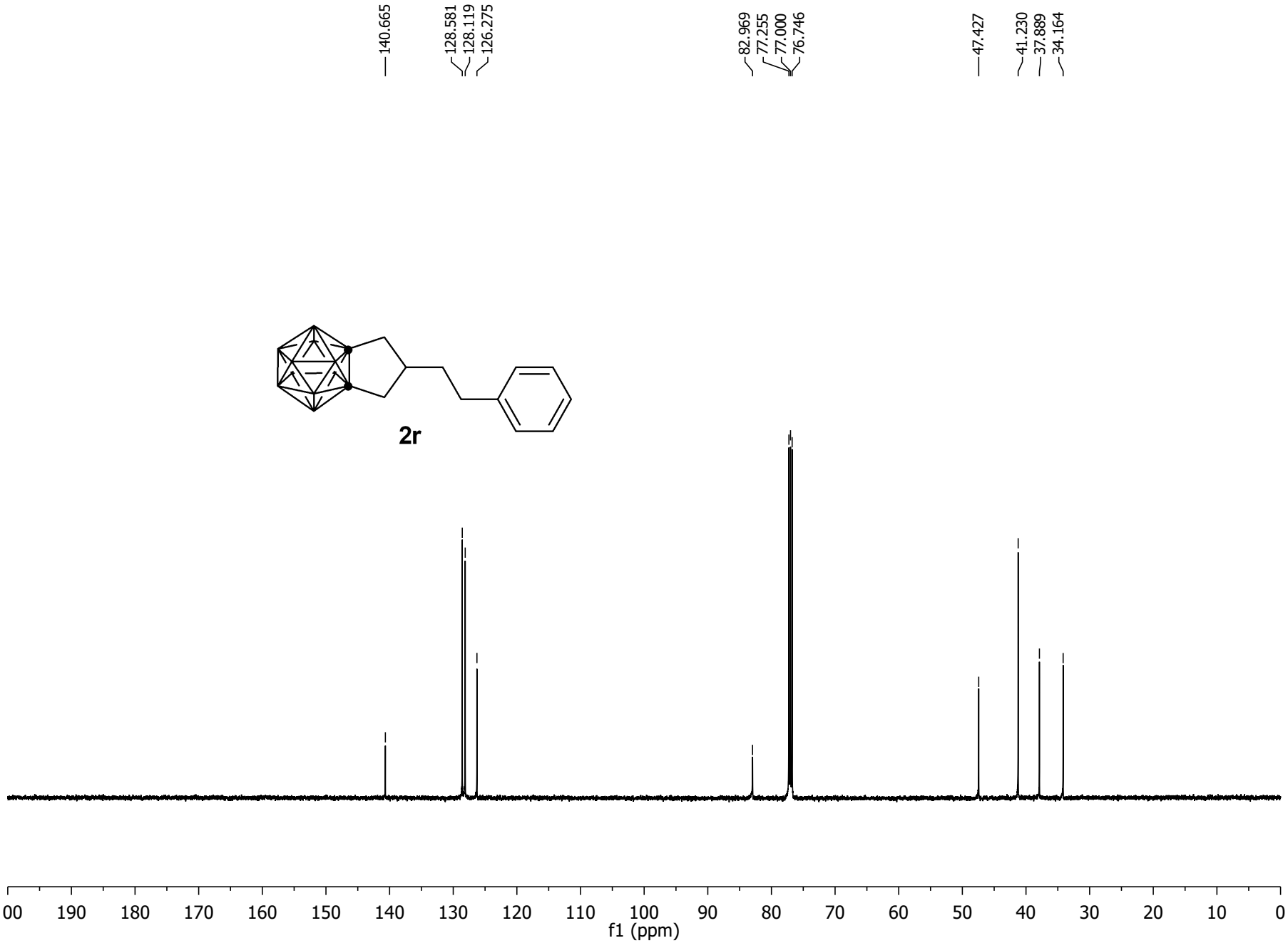
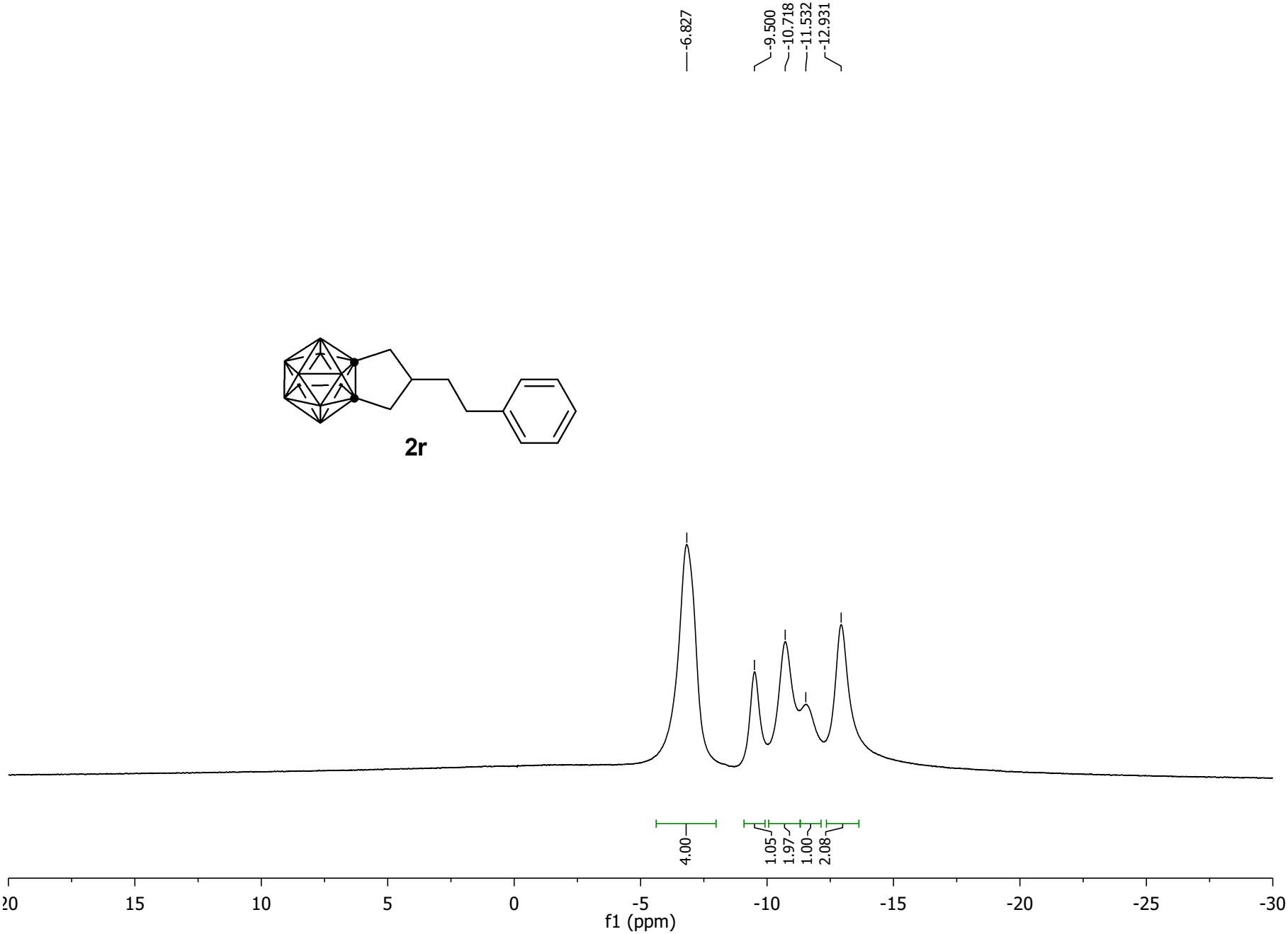


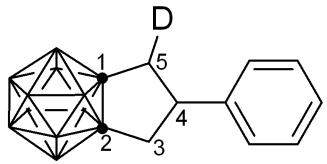


Parameter	Value
Title	zhjie-7175-CH2CH2Ph-p2-cdcl3-C-
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	64
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2310.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

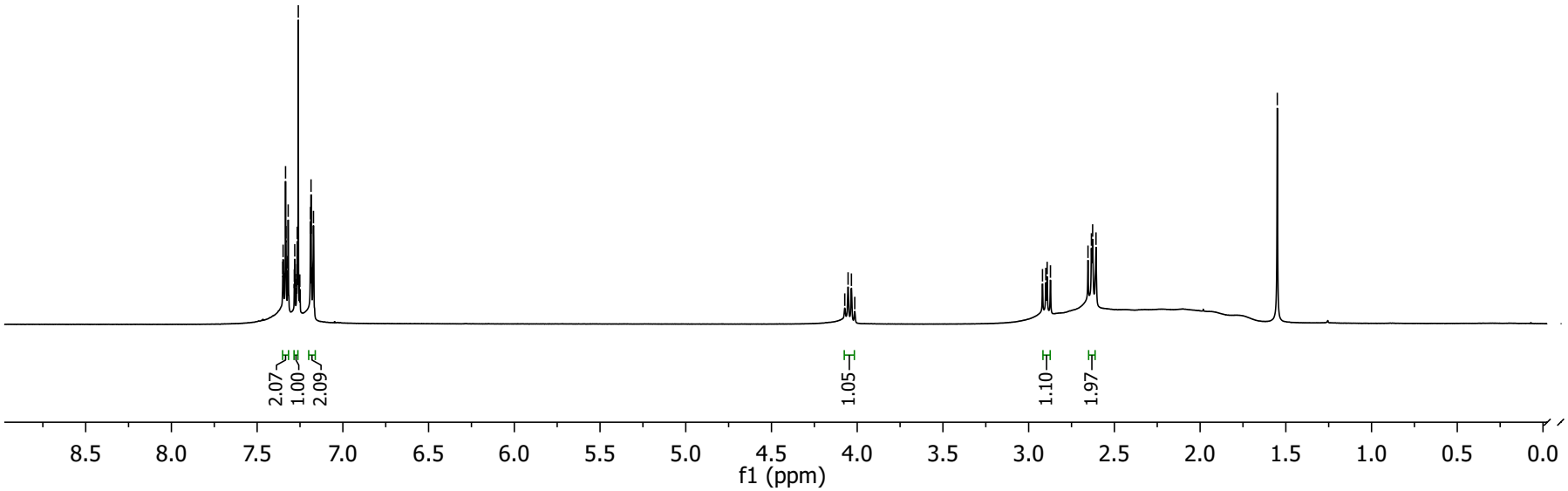


Parameter	Value
Title	zhjie-7175-CH2CH2Ph-p2-cdcl3-B-
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

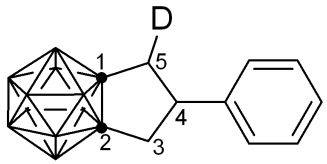
Parameter	Value
Title	zhjie181116-wu-D-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	93
Relaxation Delay	1.0000
Pulse Width	11.2500
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



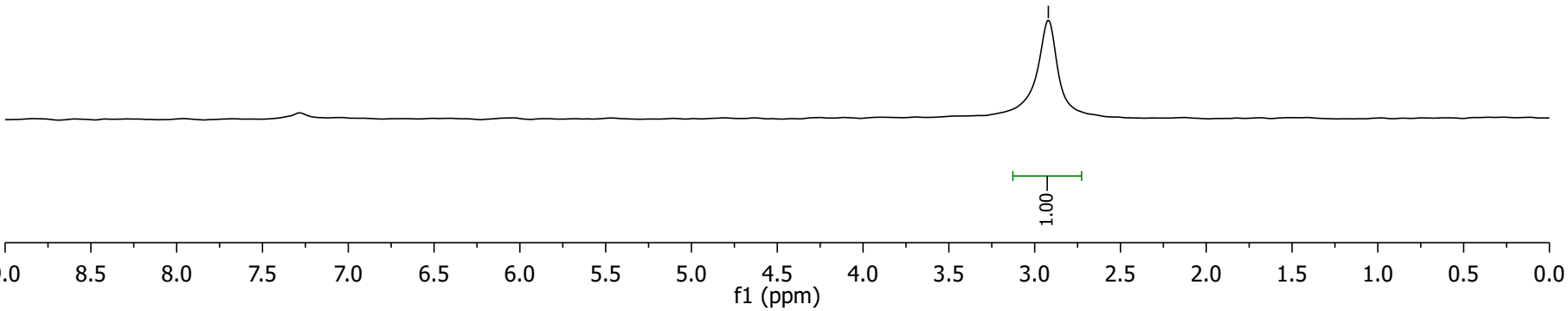
2a-d_1

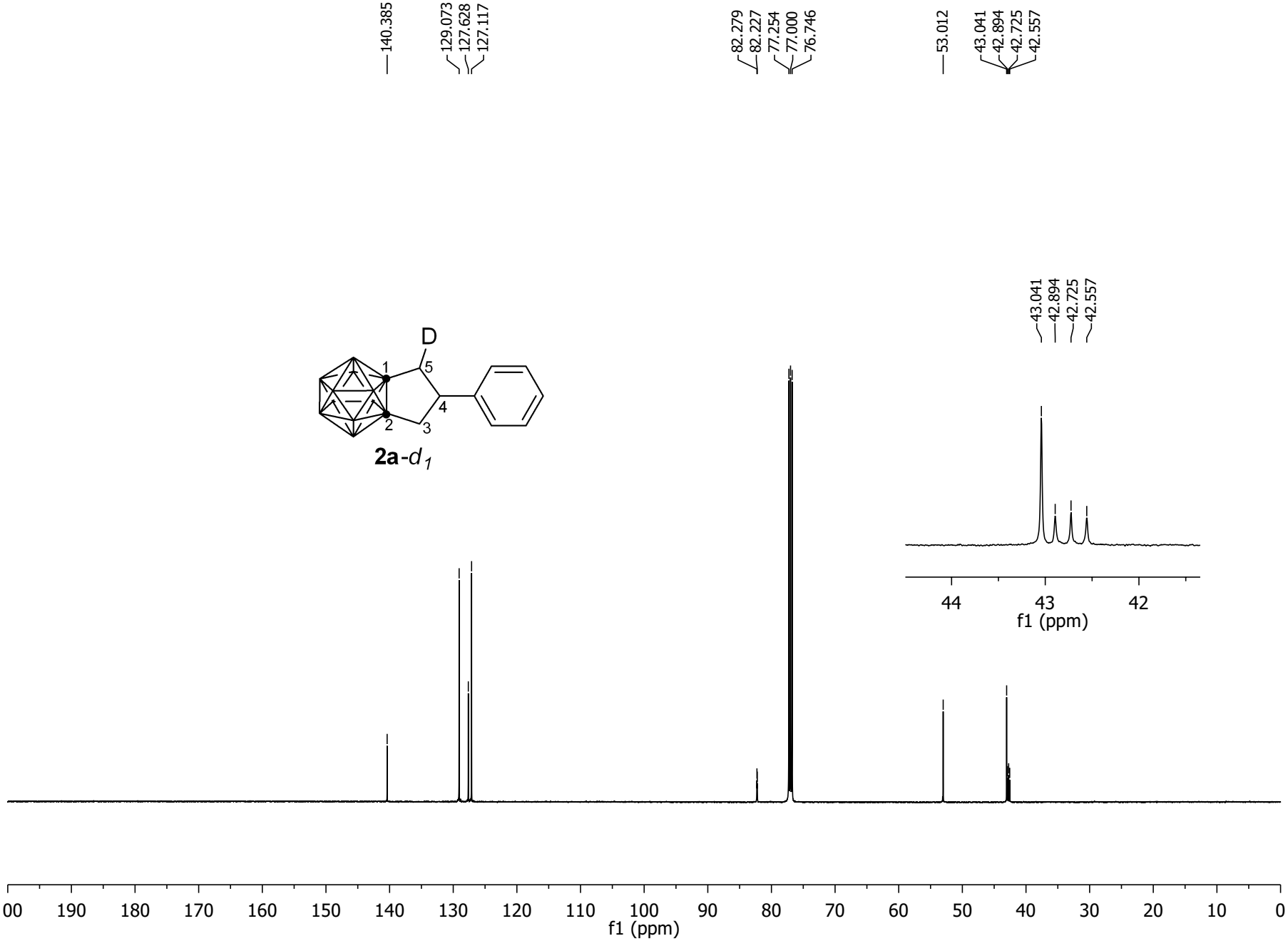


Parameter	Value
Title	CF-20200327-Research Service Xie 51
Spectrometer	spect
Solvent	CDCl3
Temperature	295.1
Pulse Sequence	zg2h
Experiment	1D
Number of Scans	32
Receiver Gain	64
Relaxation Delay	0.0500
Pulse Width	300.0000
Acquisition Time	0.9996
Spectrometer Frequency	76.77
Spectral Width	1535.6
Lowest Frequency	-212.0
Nucleus	2H
Acquired Size	1535
Spectral Size	4096

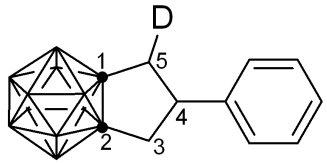


2a-d_1



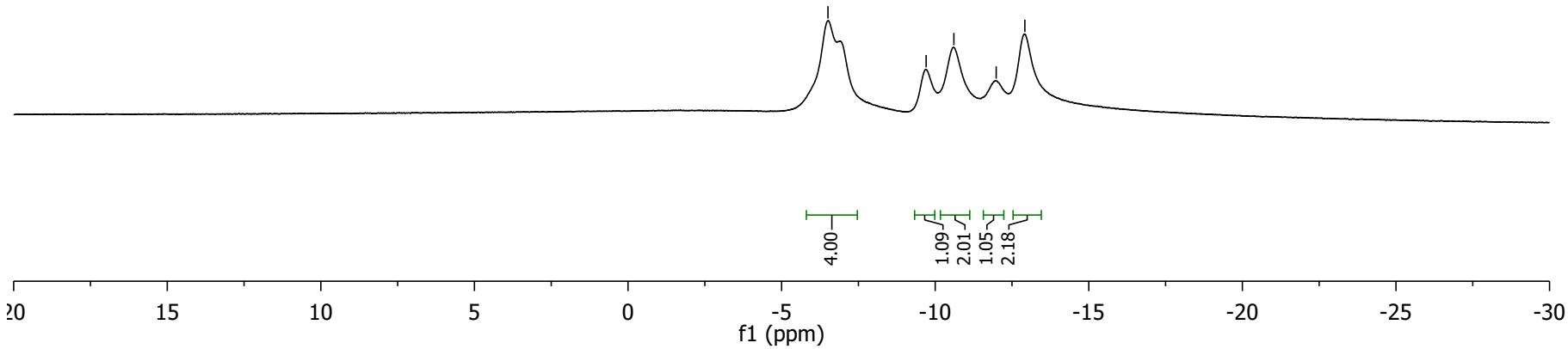


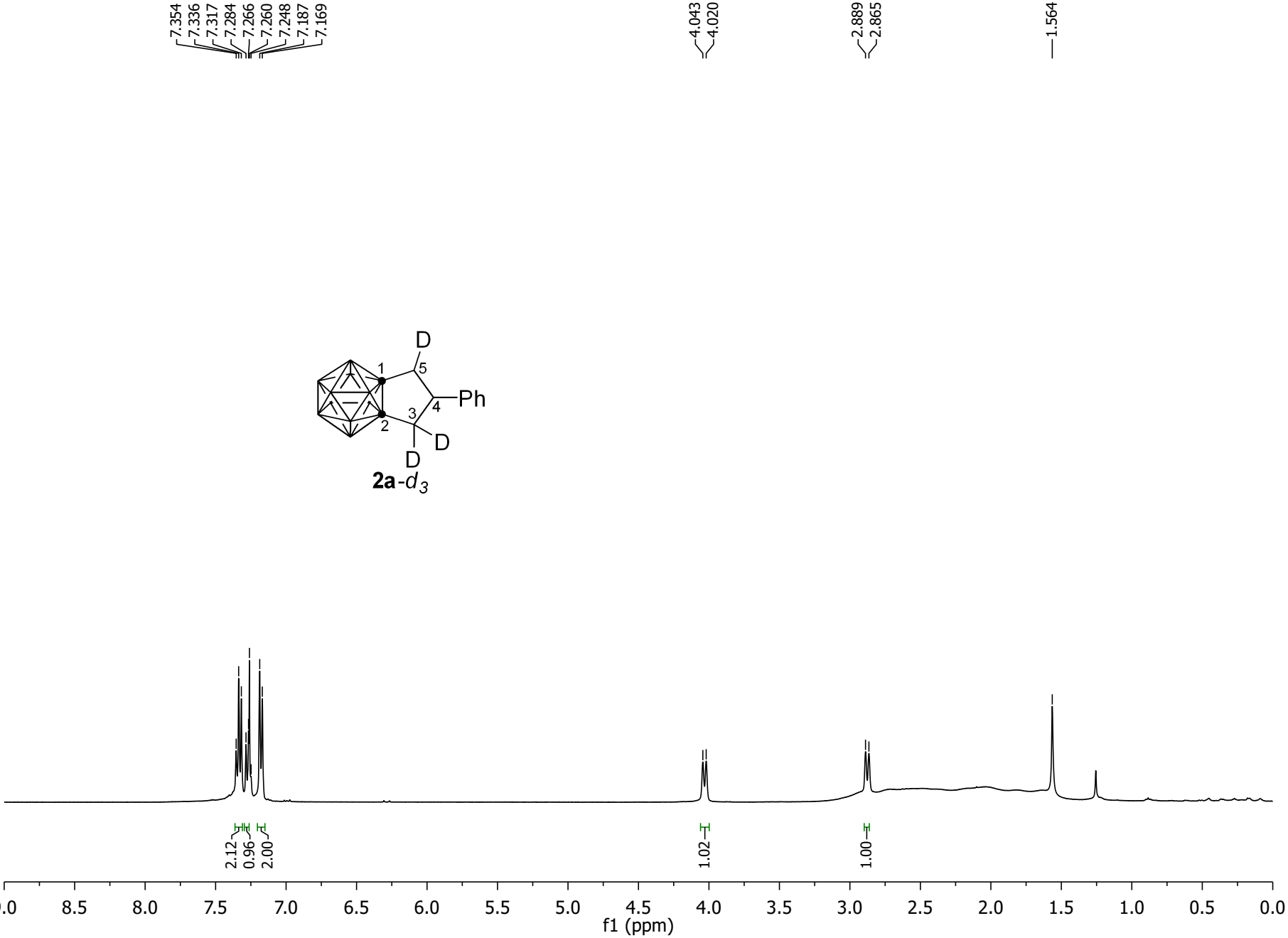
Parameter	Value
Title	zhjie181116-wu-D-cdcl3-C-2
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	1024
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2309.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



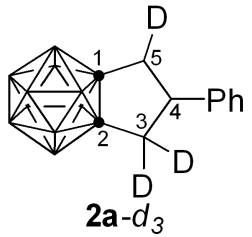
2a-d_1

Parameter	Value
Title	zhjie181116-wu-D-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	32
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



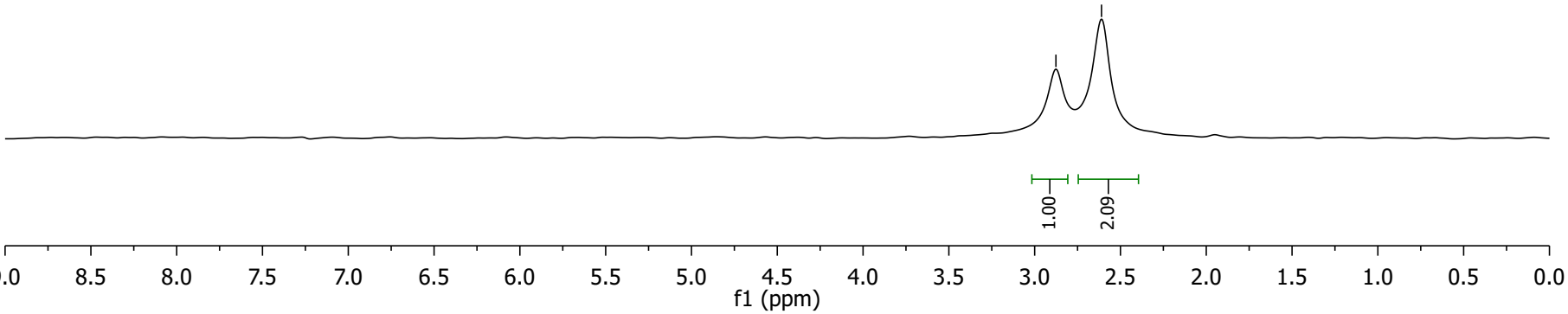


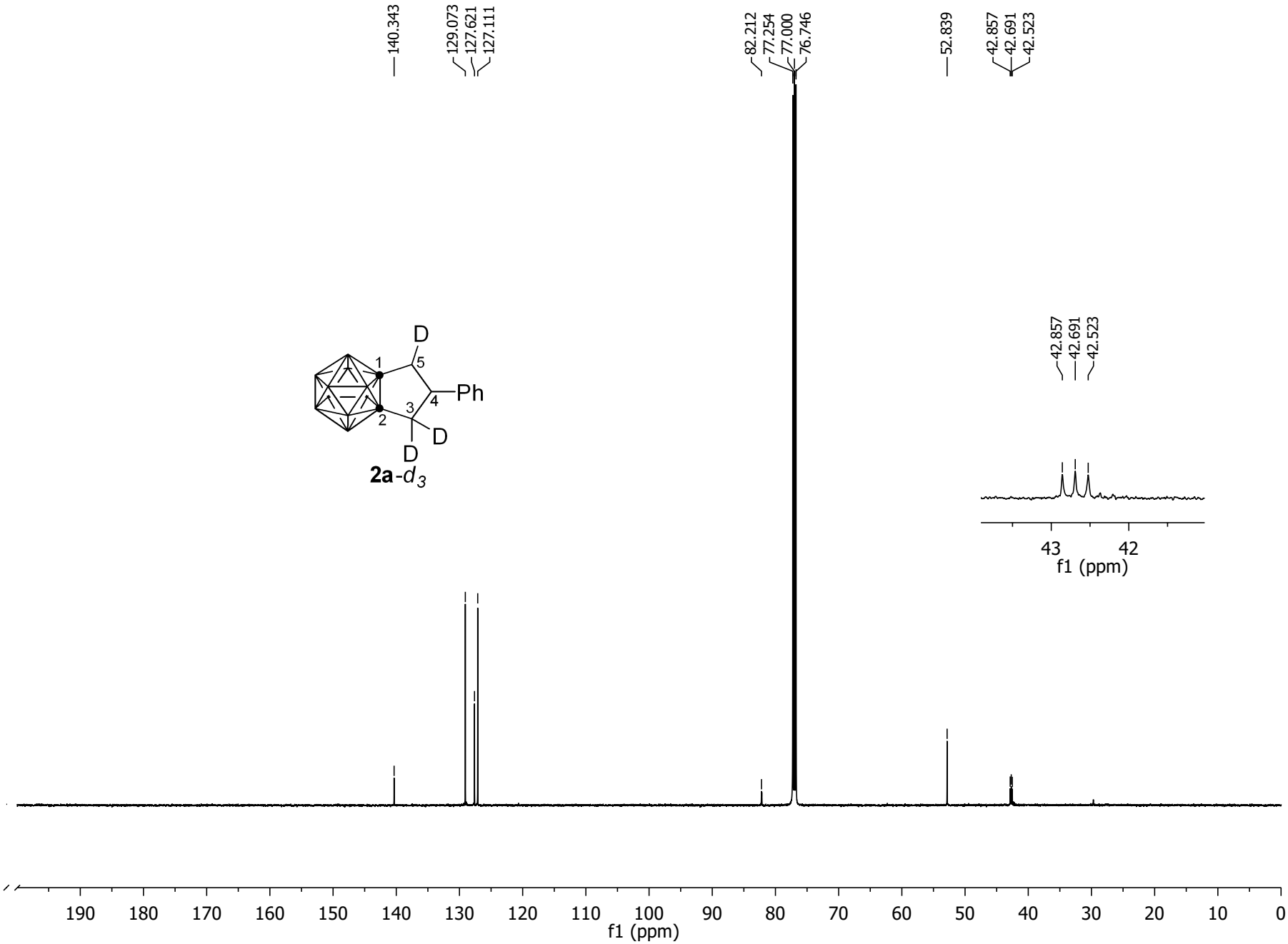
Parameter	Value
Title	zhjie-7041-2-cd3wu-l6-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	294.9
Pulse Sequence	zg30
Experiment	1D
Number of Scans	33
Receiver Gain	144
Relaxation Delay	1.0000
Pulse Width	12.8000
Acquisition Time	4.0894
Spectrometer Frequency	400.23
Spectral Width	8012.8
Lowest Frequency	-1545.5
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



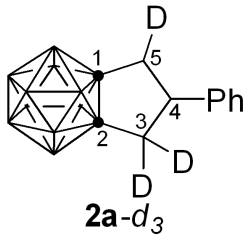
2a-d_3

Parameter	Value
Title	CF-20200327-Research Service Xie 52
Spectrometer	spect
Solvent	CDCl3
Temperature	295.2
Pulse Sequence	zg2h
Experiment	1D
Number of Scans	32
Receiver Gain	64
Relaxation Delay	0.0500
Pulse Width	300.0000
Acquisition Time	0.9996
Spectrometer Frequency	76.77
Spectral Width	1535.6
Lowest Frequency	-212.0
Nucleus	2H
Acquired Size	1535
Spectral Size	4096



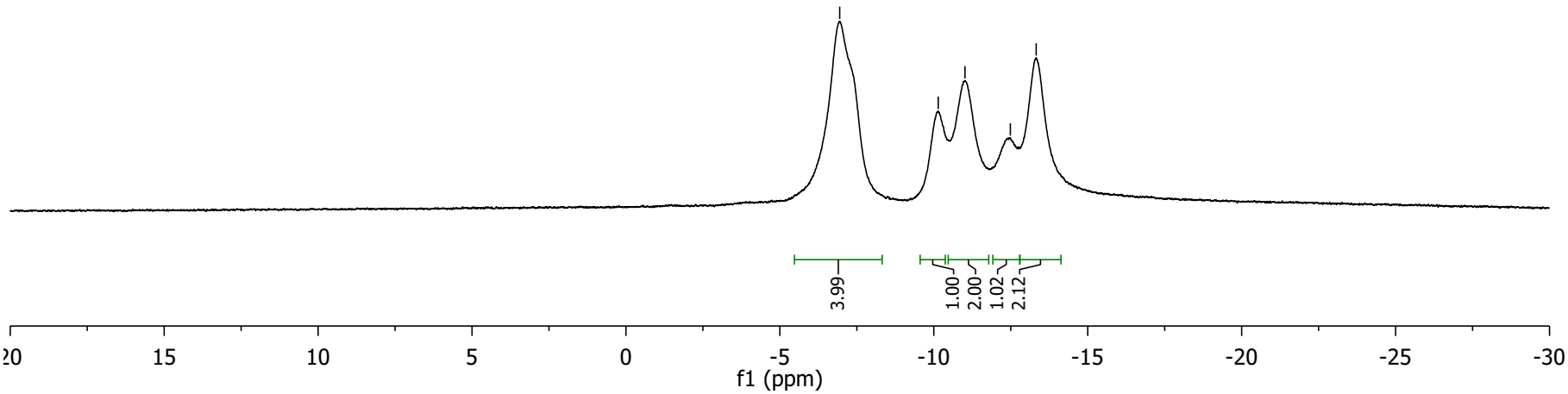


Parameter	Value
Title	zhjie-7041-2-I6-cd3wu-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	799
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2309.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

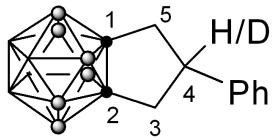


2a-d_3

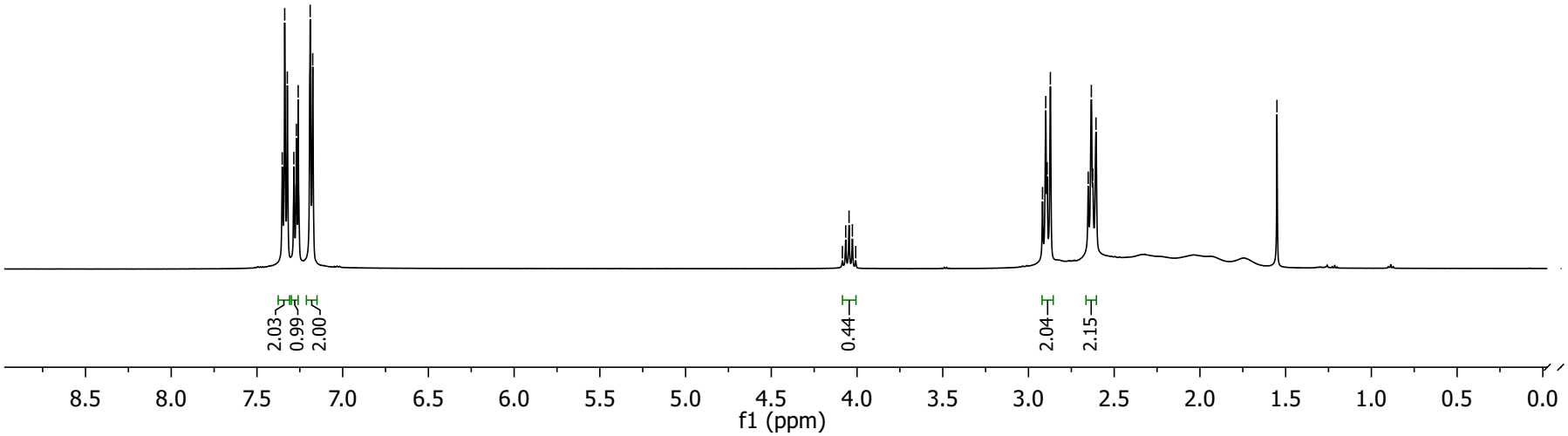
Parameter	Value
Title	zhjie-7041-2-cd3wu-l6-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	295.3
Pulse Sequence	zgdc
Experiment	1D
Number of Scans	24
Receiver Gain	287
Relaxation Delay	2.0000
Pulse Width	7.5000
Acquisition Time	1.3631
Spectrometer Frequency	128.41
Spectral Width	24038.5
Lowest Frequency	-12091.7
Nucleus	11B
Acquired Size	32768
Spectral Size	65536

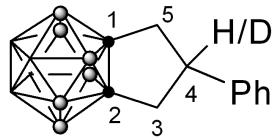


Parameter	Value
Title	zhije-8153-wud7-cry-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	295.2
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	103
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1924.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



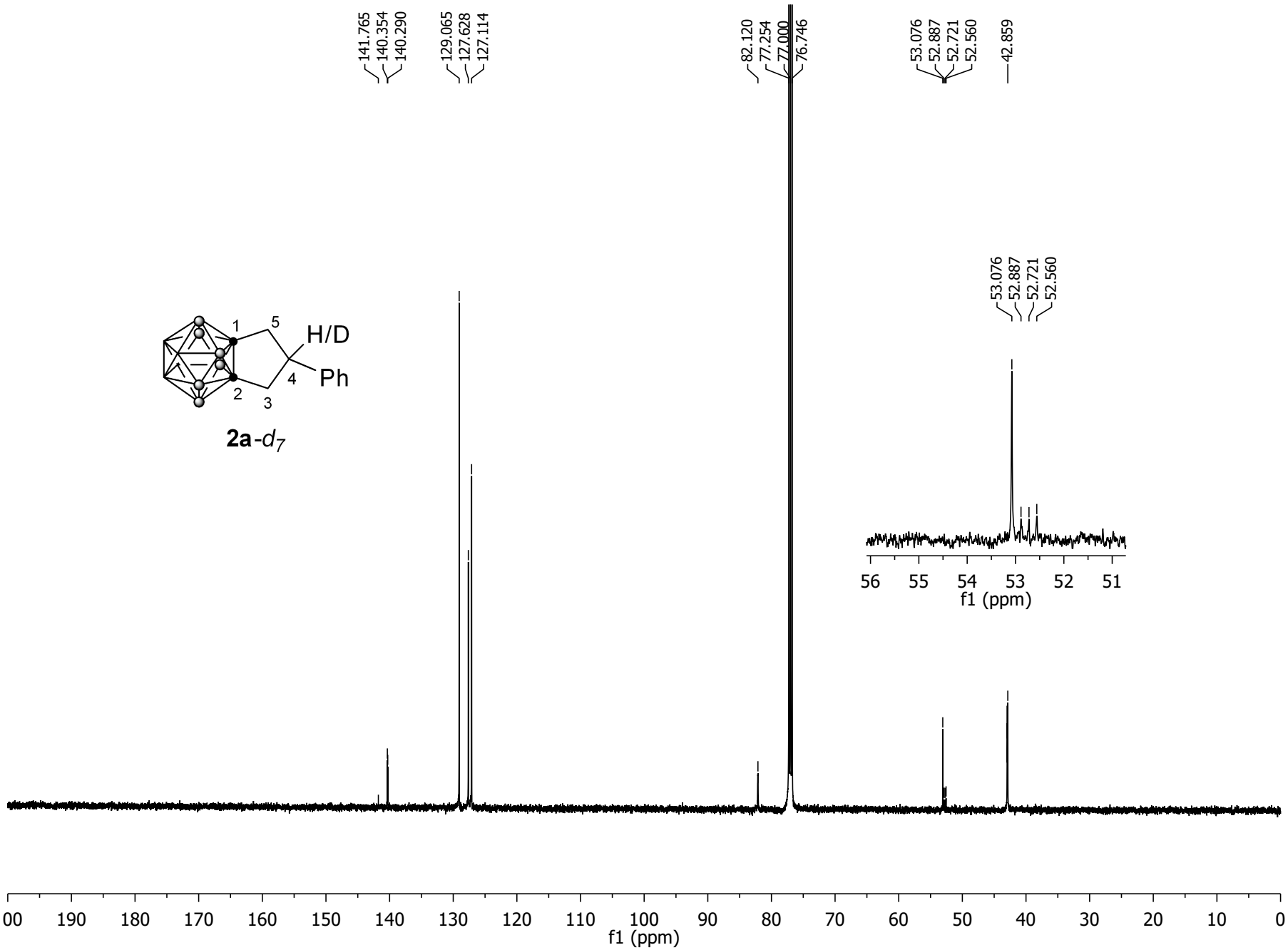
2a-d_7



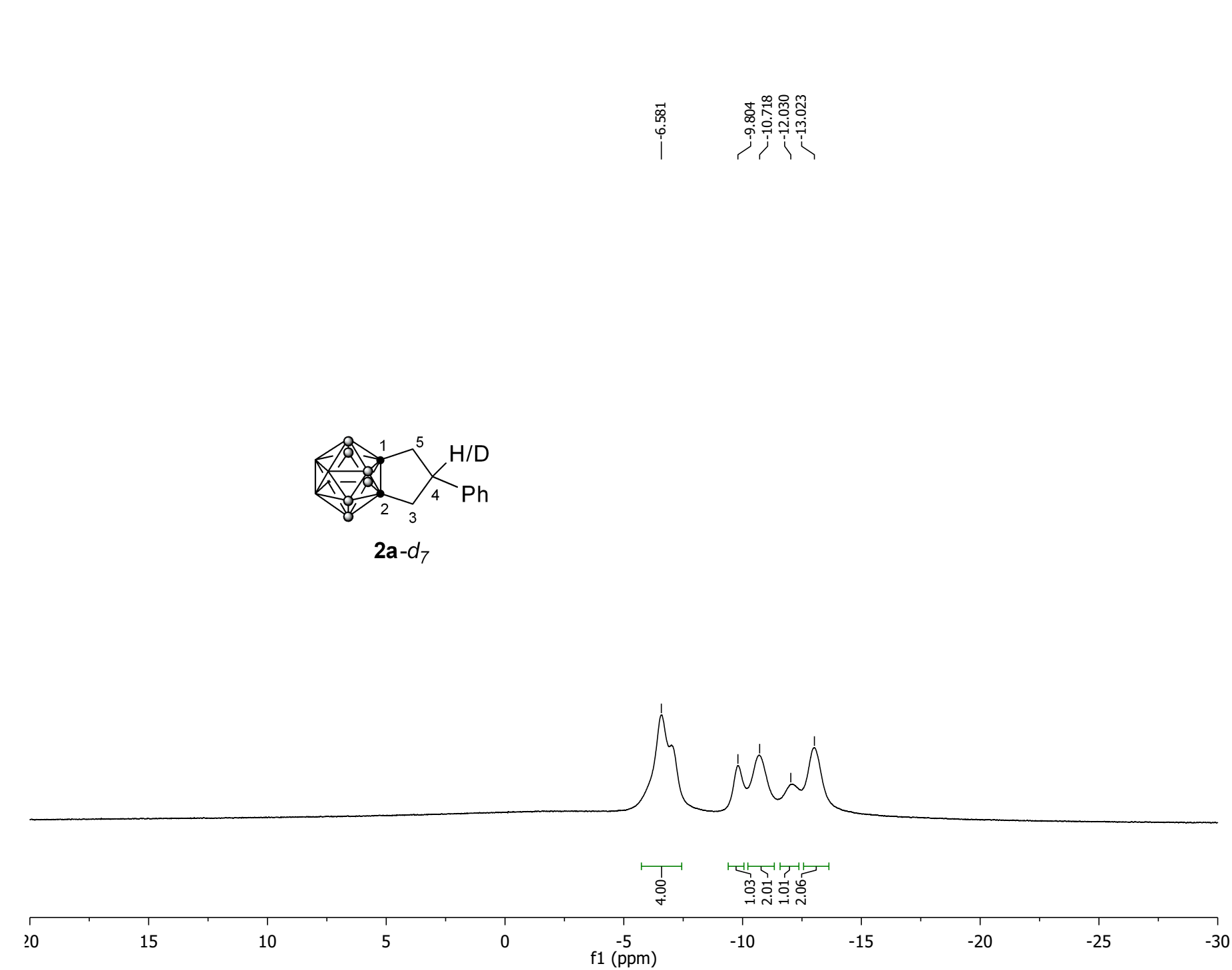


2a-d_7

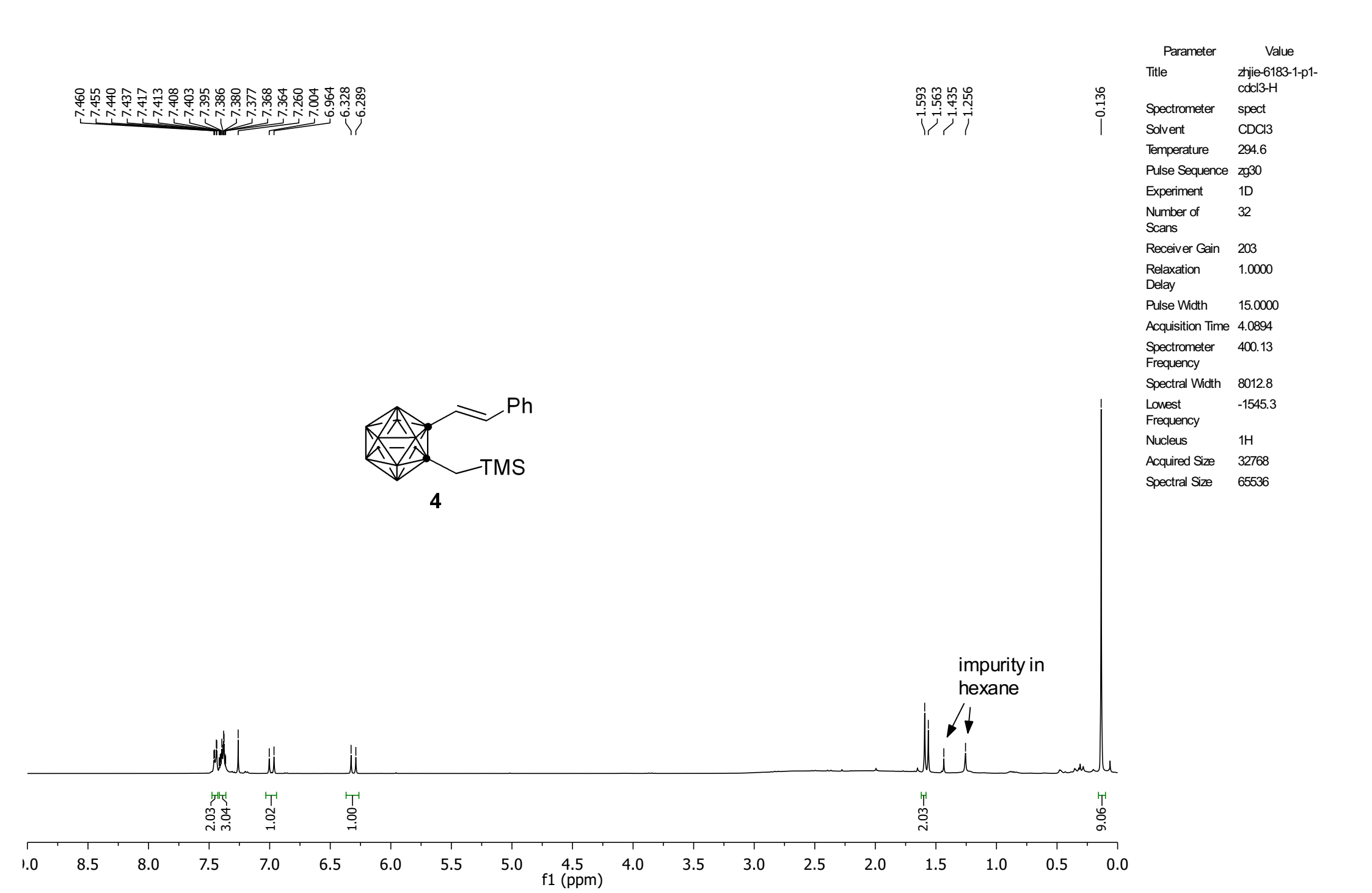
Parameter	Value
Title	CF-20200327-Research Service Xie 55
Spectrometer	spect
Solvent	CDCl3
Temperature	295.4
Pulse Sequence	zgig2h
Experiment	1D
Number of Scans	32
Receiver Gain	207
Relaxation Delay	0.0500
Pulse Width	300.0000
Acquisition Time	0.9996
Spectrometer Frequency	76.77
Spectral Width	1535.6
Lowest Frequency	-226.5
Nucleus	2H
Acquired Size	1535
Spectral Size	4096



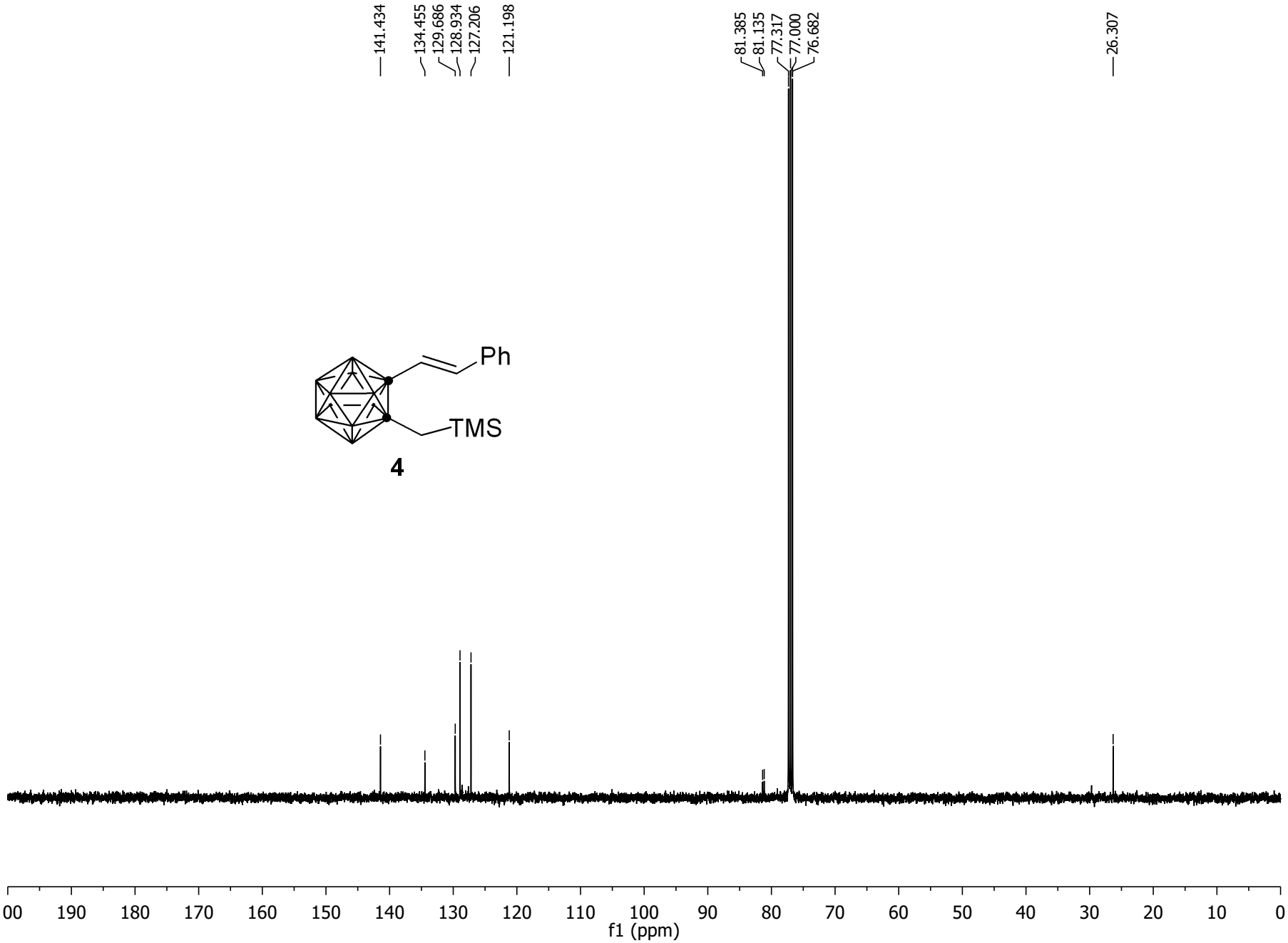
Parameter	Value
Title	zhije-8153-wud7-cry-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	295.2
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	1024
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	9.7500
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2311.0
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



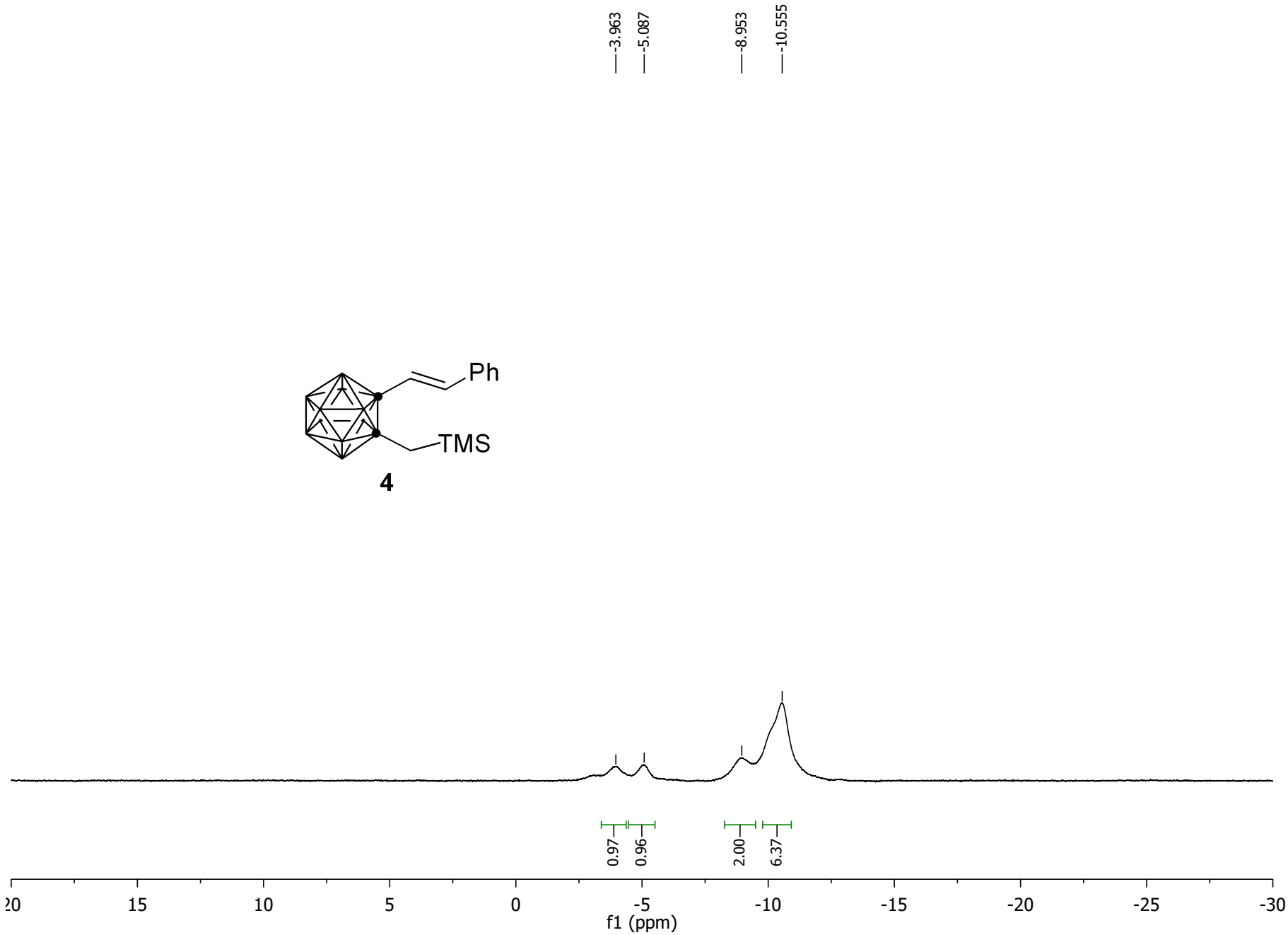
Parameter	Value
Title	zhije-8153-wud7-cry-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	295.1
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	32
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	16.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



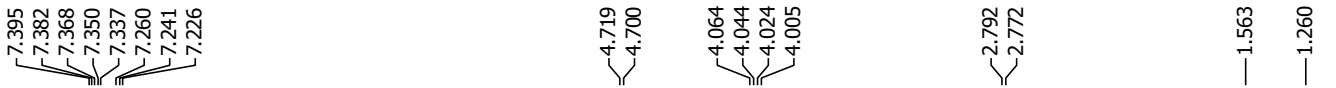
Parameter	Value
Title	zhjie-6183-1-p1-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	294.6
Pulse Sequence	zg30
Experiment	1D
Number of Scans	32
Receiver Gain	203
Relaxation Delay	1.0000
Pulse Width	15.0000
Acquisition Time	4.0894
Spectrometer Frequency	400.13
Spectral Width	8012.8
Lowest Frequency	-1545.3
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



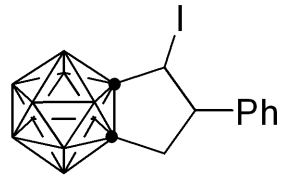
Parameter	Value
Title	zhjie-6183-1-p1-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	294.6
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	288
Receiver Gain	203
Relaxation Delay	2.0000
Pulse Width	9.5000
Acquisition Time	1.3631
Spectrometer Frequency	100.61
Spectral Width	24038.5
Lowest Frequency	-1961.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie-6183-1-wu-tms-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	295.1
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	128
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	16.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



Parameter	Value
Title	zhjie-6183-2-wu-l-cdcl3-H
Spectrometer	spect
Solvent	CDCl3
Temperature	295.2
Pulse Sequence	zg30
Experiment	1D
Number of Scans	12
Receiver Gain	93
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	3.2768
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1911.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



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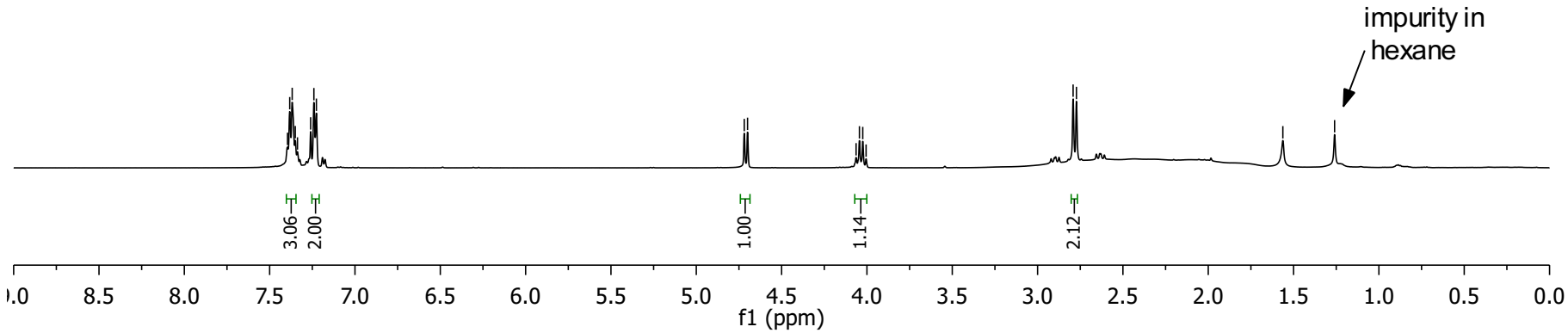
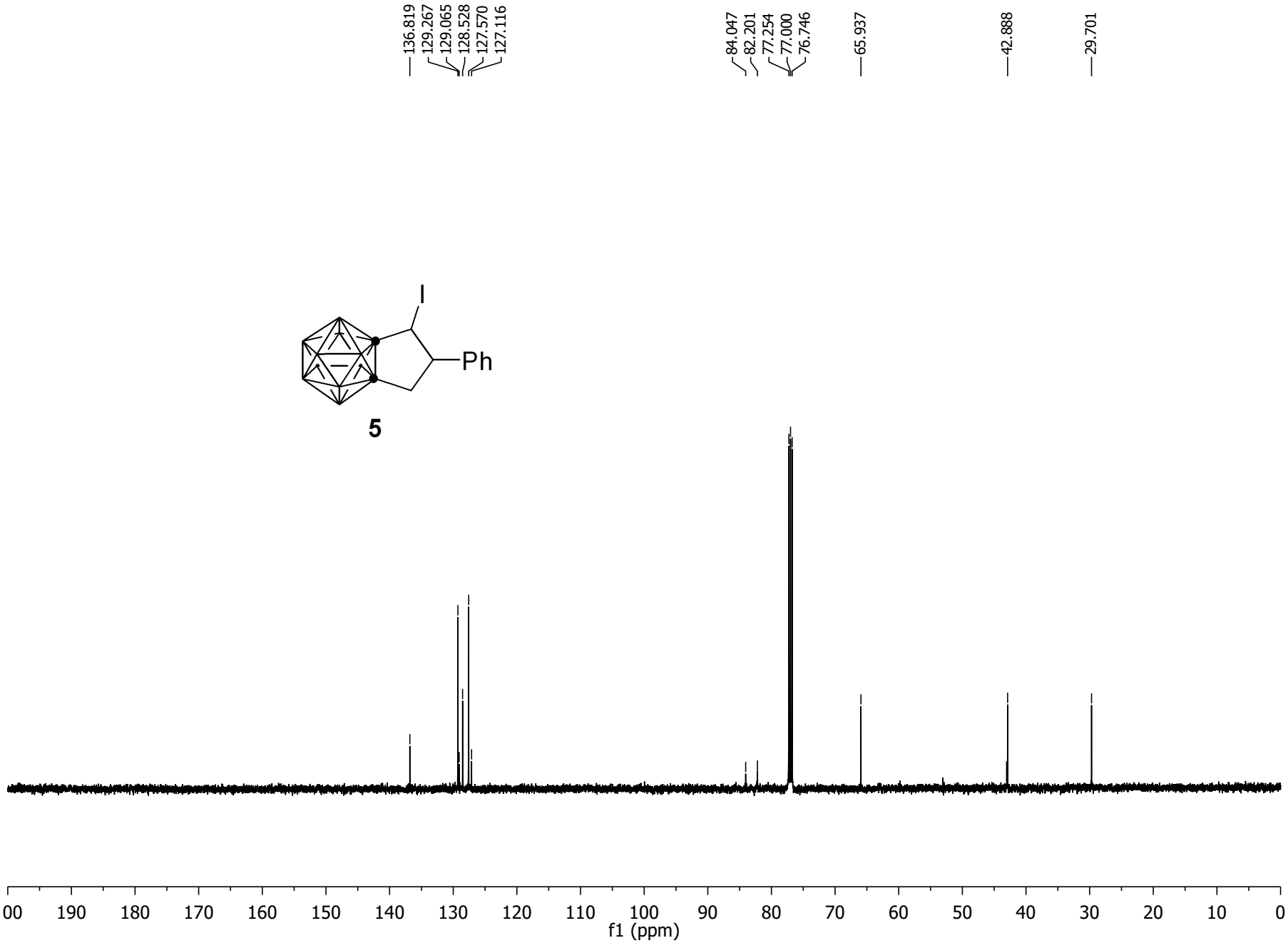
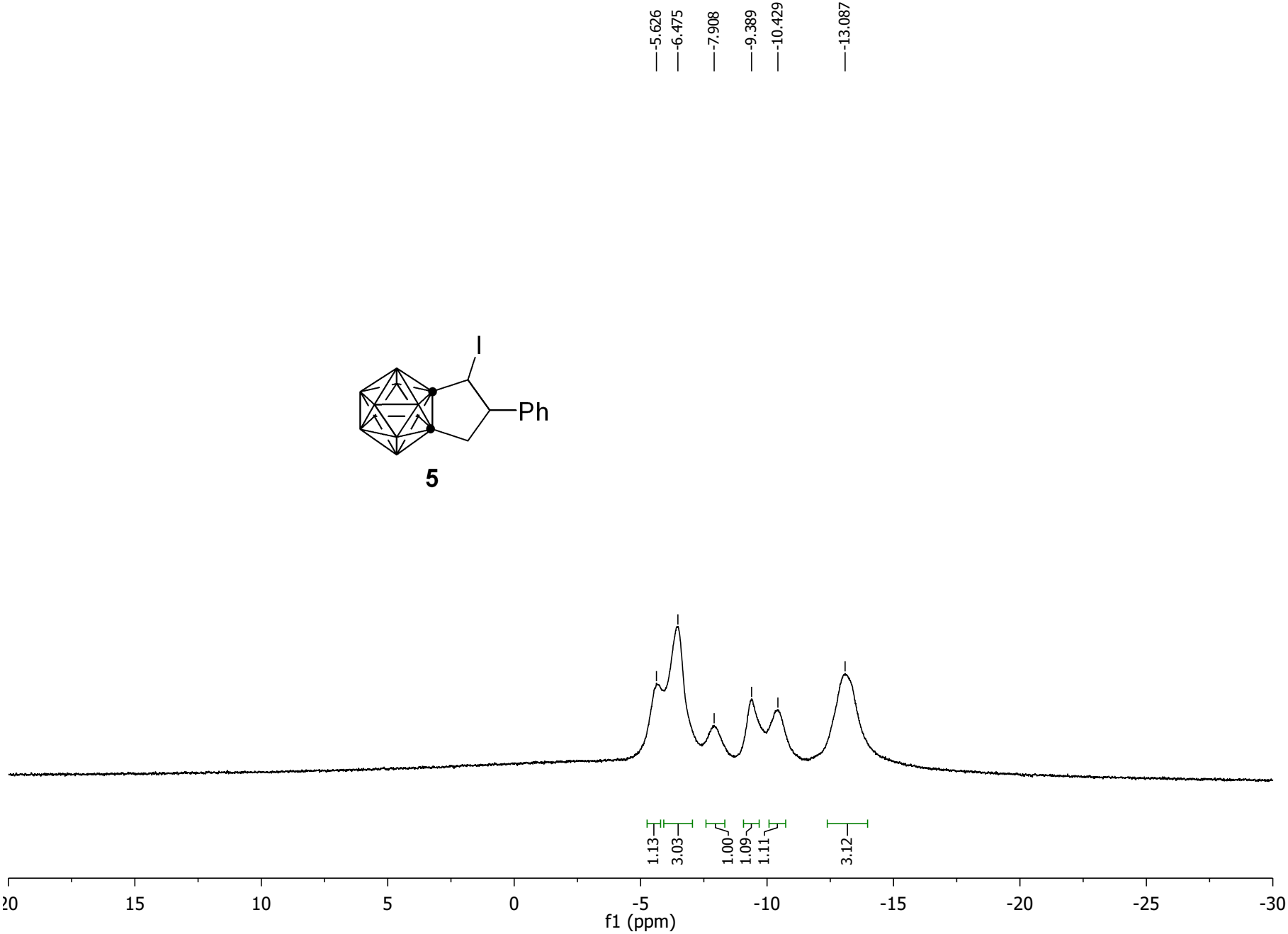




Parameter	Value
Title	zhjie-6183-2-wu-l-cdcl3-C
Spectrometer	spect
Solvent	CDCl3
Temperature	295.1
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	128
Receiver Gain	207
Relaxation Delay	2.0000
Pulse Width	9.7500
Acquisition Time	1.1010
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2311.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Title	zhjie-6183-2-wu-I-cdcl3-B
Spectrometer	spect
Solvent	CDCl3
Temperature	295.3
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	207
Relaxation Delay	1.0000
Pulse Width	16.0000
Acquisition Time	0.6816
Spectrometer Frequency	160.46
Spectral Width	24038.5
Lowest Frequency	-12040.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768