Supporting Information

Palladium catalyzed regioselective mono-alkenylation of *o*-carboranes via Heck type coupling reaction of cage B-H bond

Ji Wu, Ke Cao*, Tao-Tao Xu, Xiao-Juan Zhang, Linhai Jiang, Junxiao Yang and Yawen Huang

State Key Laboratory Cultivation Base for Nonmetal Composite and Functional Materials & School of Materials Science and Engineering, Southwest University of Science and Technology, Mianyang, 621010, P. R. China

E-mail: caoke@swust.edu.cn

Context

General information

1b[1], 1c[2], 1d[2], 1e[3] were synthesized according to literature methods. THF was dried and freshly distilled over sodium before used. Styrenes were synthesized via Wittig reaction. Other materials were purchased from J&K Scientific and used as received unless otherwise specified. All reactions under standard conditions were monitored by thin-layer chromatography (TLC) on gel F254 plates. The silica gel (200-300 meshes) is used for column chromatography, and the distillation range of petroleum ether is 60-90^{o}C. ^{1}H NMR, ^{13}C{^{1}H} NMR, ^{11}B NMR and ^{11}B{^{1}H} NMR spectra were recorded on the Bruker 600MHz instruments. All ^{1}H NMR and ^{13}C NMR spectral data are reported in *ppm* relative to tetramethylsilane (TMS) as internal standard, and ^{11}B NMR spectral data are referenced to external BF_3•Et_2O. HRMS data were measured with ESI techniques.

Experiment

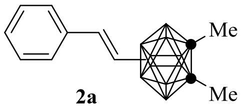
General procedure for palladium catalyzed arylation of *o*-carboranes:

To a 10 mL dried flask were sequentially added *o*-carborane (0.25 mmol), THF (1 mL), $Pd(OAc)_2$ (5.6 mg, 0.025 mmol), AgOAc (83.5 mg, 0.5 mmol), styrene (0.75 mmol) under argon atmosphere. After the reaction mixture was stirred at 80^{o}C for 48h, the reaction mixture was cooled to room temperature and filtered through a short silica gel column using CH_2Cl_2 as eluent. After evaporation of the solvent, the residue was purified by column chromatography on 200-300 mesh silica gel with petroleum ether as eluent.

Reference:

1. Heying, T. L., Jr., Ager, J. W., Clark, S. L., Alexander, R. P., Papetti, S., Reid, J. A., Trotz, S. I. *Inorg. Chem.*, **2**, 1097-1105 (1963).
2. Paxson, T. E., Kaloustian, M. K., Tom, G. M., Wiersema, R. J., Hawthorne, M. F. *J. Am. Chem. Soc.*, **94**, 4882-4888 (1972).
3. Armstrong, A. F., Valliant, J. F. *Inorg. Chem.*, **46**, 2148-2158 (2007).

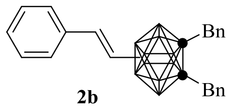
Spectroscopic data for products:



2a

An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.

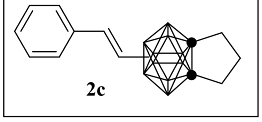
^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.42-7.40 (d, *J* = 12Hz, 2H), 7.38-7.36 (d, *J* = 12Hz, 2H), 7.31-7.26 (m, 4H), 7.21-7.16 (m, 2H), 6.75-6.72 (d, *J* = 18Hz, 1H), 6.60-6.57 (d, *J* = 18Hz, 1H), 6.44-6.41 (d, *J* = 18Hz, 1H), 6.35-6.32(d, *J* = 18Hz, 1H), 2.05 (brs, 12H); ^{13}C{^{1}H} NMR (150MHz, $CDCl_3$, *ppm*): δ 140.0, 138.9, 128.4, 128.3, 127.2, 126.9, 126.2, 126.1, 79.1, 67.4, 23.4, 23.2. 22.5; ^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, *ppm*): δ 3.3 (1B, -*B(9)*-CH), -1.6 (1B, -*B(8)*-CH), -4.9 (3B), -9.1 (2B), -10.3 (7B), -11.5 (2B); HRMS: calculated for $C_{12}B_{10}H_{23}$ (M^{+}+H) 275.2795; found: 275.2797.



2b

An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.1.

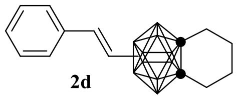
^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.38-7.35 (m, 14H), 7.30-7.21 (m, 16H), 6.64-6.61 (d, *J* = 18Hz, 1H), 6.48-6.45 (d, *J* = 18Hz, 1H), 6.37-6.34 (d, *J* = 18Hz, 1H), 6.25-6.22 (d, *J* = 18Hz, 1H), 3.66 (s, 3H), 3.65 (s, 2H), 3.64 (s, 2H), 3.63 (s, 1H); ^{13}C{^{1}H} NMR (150MHz, $CDCl_3$, *ppm*): δ 139.9, 138.8, 138.7, 135.1, 135.0, 134.9, 131.1, 130.4, 128.8, 128.7, 128.6, 128.3, 128.2, 128.1, 127.1, 126.9, 126.1, 124.4, 77.9, 73.7, 41.4, 41.3, 40.7; ^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, *ppm*): δ 4.5 (1B, -*B(9)*-CH), -0.8 (1B, -*B(8)*-CH), -3.6 (3B), -10.7 (11B); HRMS: calculated for $C_{24}B_{10}H_{31}$ (M^{+}+H) 427.3418; found: 427.3423.



2c

An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.

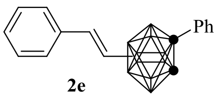
^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.42-7.41 (m, 2H), 7.38-7.36 (m, 2H), 7.30-7.27 (m, 6H), 7.21-7.17 (m, 2H), 6.76-6.73 (d, *J* = 18Hz, 1H), 6.60-6.57 (d, *J* = 18Hz, 1H), 6.47-6.44 (d, *J* = 18Hz, 1H), 6.35-6.32 (d, *J* = 18Hz, 1H), 2.54-2.50 (m, 8H), 2.46-2.41 (m, 4H); ^{13}C{^{1}H} NMR (150MHz, $CDCl_3$, *ppm*): δ 139.9, 138.8, 128.4, 128.3, 127.2, 126.9, 126.2, 126.1, 82.8, 82.4, 78.6, 34.7, 34.6, 33.9, 32.3, 31.9; ^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, *ppm*): δ 2.1 (1B, -*B(9)*-CH), 1.2 (1B, -*B(8)*-CH), -6.1 (3B), -7.5 (2B), -9.0 (2B), -9.4 (2B), -11.7 (3B), -12.2 (4B); HRMS: calculated for $C_{13}B_{10}H_{23}$ (M^++H) 287.2796; found: 287.2797.



2d

An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.

^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.42-7.40 (m, 2H), 7.37-7.36 (m, 2H), 7.30-7.25 (m, 4H), 7.20-7.15 (m, 2H), 6.76-6.73 (d, *J* = 18Hz, 1H), 6.59-6.56 (d, *J* = 18Hz, 1H), 6.47-6.44 (d, *J* = 18Hz, 1H), 6.34-6.31 (d, *J* = 18Hz, 1H), 2.46-2.45 (m, 8H), 1.60-1.59 (m, 8H); ^{13}C{^{1}H} NMR (150MHz, $CDCl_3$, *ppm*): δ 139.9, 138.8, 128.4, 128.3, 127.2, 126.9, 126.2, 126.1, 71.7, 67.2, 32.8, 32.7, 32.1, 19.8, 19.7, 19.6; ^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, *ppm*): δ 3.0 (1B, -*B(9)*-CH), -0.1 (1B, -*B(8)*-CH), -5.1 (2B), -8.7 (2B), -9.6 (2B), -10.1 (4B), -12.1 (3B), -14.5 (2B); HRMS: calculated for $C_{14}B_{10}H_{25}$ (M^++H) 301.2952; found: 301.2954.

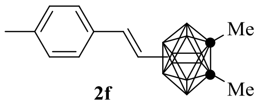


2e

An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.

^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.52-7.51 (m, 4H), 7.43-7.39 (m, 6H), 7.36 -7.31 (m, 7H), 7.29-7.25 (m, 3H), 6.94-6.91 (d, *J* = 18Hz, 1H), 6.66-6.63 (d, *J* = 18Hz, 1H), 6.42-6.39 (d, *J* = 18Hz, 1H), 6.41-6.38 (d, *J* = 18Hz, 1H), 4.05 (s, 1H), 3.87 (s, 1H);

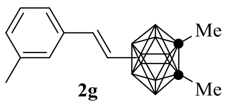
$^{13}C\{^1H\}$ NMR (150MHz, $CDCl_3$, *ppm*): δ 143.3, 139.0, 130.4, 129.9, 128.9, 128.8, 128.6, 128.5, 128.3, 128.0, 127.6, 127.5, 127.1, 126.4, 126.2, 79.3, 60.9, 54.4; $^{11}B\{^1H\}$ NMR (192 MHz, $CDCl_3$, *ppm*): δ 6.6 (1B, *-B(9)*-CH), -2.2 (1B, *-B(8)*-CH), -3.7 (2B), -8.5 (2B), -10.8 (3B), -13.5 (2B); HRMS: calculated for $C_{16}B_{10}H_{23}$ (M^++H) 323.2797; found: 323.2797.



2f

An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.1.

^1H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.31-7.30 (m, 2H), 7.27-7.26 (m, 2H), 7.11-7.10 (m, 2H), 7.08-7.07 (m, 2H), 6.72-6.69 (d, *J* = 18Hz, 1H), 6.57-6.54 (d, *J* = 18Hz, 1H), 6.37-6.34 (d, *J* = 18Hz, 1H), 6.28-6.25 (d, *J* = 18Hz, 1H), 2.33 (s, 3H), 2.31 (s, 3H), 2.05 (brs, 12H); $^{13}C\{^1H\}$ NMR (150MHz, $CDCl_3$, *ppm*): δ 139.9, 138.8, 136.9, 136.7, 129.1, 128.9, 126.1, 126.0, 71.9, 67.3, 23.4, 23.2, 22.5, 21.2, 21.1; $^{11}B\{^1H\}$ NMR (192 MHz, $CDCl_3$, *ppm*): δ 3.8 (1B, *-B(9)*-CH), -1.1 (1B, *-B(8)*-CH), -4.5 (3B), -8.8 (3B), -9.9 (8B), -11.2 (2B); HRMS: calculated for $C_{13}B_{10}H_{25}$ (M^++H) 289.2951; found: 289.2954.

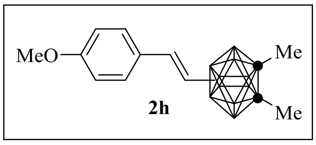


2g

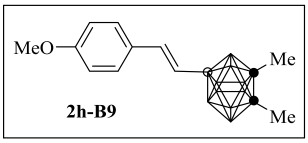
An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.4.

^1H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.24 (s, 1H), 7.23-7.20 (m, 2H), 7.18-7.14 (m, 3H), 7.02-6.98 (m, 2H), 6.71-6.68 (d, *J* = 18Hz, 1H), 6.56-6.53 (d, *J* = 18Hz, 1H), 6.42-6.39 (d, *J* = 18Hz, 1H), 6.33-6.30 (d, *J* = 18Hz, 1H), 2.33 (s, 3H), 2.31 (s, 3H), 2.05 (brs, 12H); $^{13}C\{^1H\}$ NMR (150MHz, $CDCl_3$, *ppm*): δ 140.1, 138.9, 137.8, 137.7, 128.3, 128.2, 127.9, 127.8, 126.8, 123.4, 71.9, 67.3, 23.4, 23.2, 22.5, 21.4, 21.3; $^{11}B\{^1H\}$ NMR (192 MHz, $CDCl_3$, *ppm*): δ 3.7 (1B, *-B(9)*-CH), -1.2 (1B, *-B(8)*-CH), -4.5 (2B), -8.7 (2B), -9.9 (5B), -11.2 (2B); HRMS: calculated for $C_{13}B_{10}H_{25}$ (M^++H)

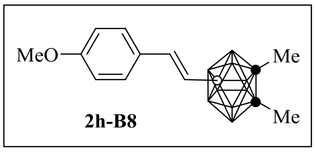
289.2950; found: 289.2954.



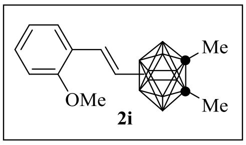
A separable B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.1.



^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.31-7.30 (d, *J* = 6Hz, 2H), 6.81-6.80 (d, *J* = 6Hz, 2H), 6.53-6.50 (d, *J* = 18Hz, 1H), 6.18-6.15 (d, *J* = 18Hz, 1H), 3.79 (s, 3H), 2.05 (brs, 6H); ^{13}C{^{1}H} NMR (150MHz, $CDCl_3$, *ppm*): δ 158.8, 138.3, 127.3, 113.7, 71.9, 67.1, 55.3, 23.4, 22.5; ^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, *ppm*): δ 3.5 (1B, -*B(9)*-CH), -5.1 (2B), -9.2 (2B), -10.3 (5B); HRMS: calculated for $C_{13}B_{10}H_{25}O_1$ (M^++H) 305.2905; found: 305.2903.

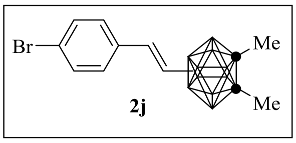


^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.34-7.33 (d, *J* = 6Hz, 2H), 6.84-6.83 (d, *J* = 6Hz, 2H), 6.68-6.65 (d, *J* = 18Hz, 1H), 6.27-6.24 (d, *J* = 18Hz, 1H), 3.80 (s, 3H), 2.05 (s, 6H); ^{13}C{^{1}H} NMR (150MHz, $CDCl_3$, *ppm*): δ 158.8, 139.3, 127.3, 113.8, 71.7, 55.3, 23.2; ^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, *ppm*): δ -1.3 (1B, -*B(9)*-CH), -4.9 (2B), -8.9 (1B), -9.7 (1B), -10.4 (1B), -11.6 (3B).



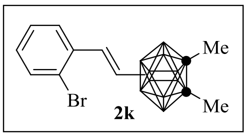
An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.6.

^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.51-7.50 (d, *J* = 6Hz, 1H), 7.47-7.46 (d, *J* = 6Hz, 1H), 7.18-7.15 (m, 2H), 7.13-7.10 (d, *J* = 18Hz, 1H), 6.98-6.95 (d, *J* = 18Hz, 1H), 6.91-6.88 (m, 2H), 6.86-6.81 (m, 2H), 6.42-6.39 (d, *J* = 18Hz, 1H), 6.33-6.30 (d, *J* = 18Hz, 1H), 3.84 (s, 3H), 3.82 (s, 3H), 2.05 (brs, 12H); ^{13}C{^{1}H} NMR (150MHz, CDCl$_3$, *ppm*): δ 156.5, 134.2, 133.1, 128.2, 127.9, 126.1, 126.0, 120.5, 120.4, 110.9, 110.8, 71.9, 67.1, 55.5, 23.4, 23.2, 22.5; $^{11}B\{^1H\}$ NMR (192 MHz, CDCl$_3$, *ppm*): δ 3.6 (1B, -*B(9)*-CH), -1.3 (1B, -*B(8)*-CH), -4.8 (2B), -9.1 (2B), -9.7 (3B), -10.4 (4B), -11.5 (3B); HRMS: calculated for $C_{13}B_{10}H_{25}O_1$ (M^++H) 305.2899; found: 305.2903.



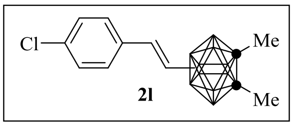
An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.

^1H NMR (600MHz, CDCl$_3$, *ppm*): δ 7.41-7.40 (d, *J* = 6Hz, 2H), 7.38-7.37 (d, *J* = 6Hz, 2H), 7.27-7.21 (m, 4H), 6.66-6.63 (d, *J* = 18Hz, 1H), 6.51-6.48 (d, *J* = 18Hz, 1H), 6.42-6.39 (d, *J* = 18Hz, 1H), 6.33-6.30 (d, *J* = 18Hz, 1H), 2.05 (brs, 12H); $^{13}C\{^1H\}$ NMR (150MHz, CDCl$_3$, *ppm*): δ 138.8, 137.7, 137.6, 131.4, 131.3, 130.8, 127.7, 120.8, 120.6, 72.1, 67.7, 23.4, 23.2, 22.5; $^{11}B\{^1H\}$ NMR (192 MHz, CDCl$_3$, *ppm*): δ 3.0 (1B, -*B(9)*-CH), -1.8 (1B, -*B(8)*-CH), -4.9 (2B), -9.1 (2B), -10.3 (4B), -11.4 (4B); HRMS: calculated for $C_{12}B_{10}H_{22}Br$ (M^++H) 353.1899; found: 353.1903.



An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.1.

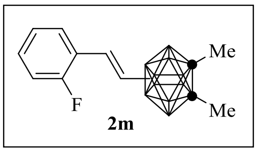
^1H NMR (600MHz, CDCl$_3$, *ppm*): δ 7.56-7.55 (m, 1H), 7.52-7.50 (m, 2H), 7.49-7.48 (m, 1H), 7.25-7.19 (m, 2H), 7.07-7.02 (m, 3H), 6.95-6.92 (d, *J* = 18Hz, 1H), 6.37-6.34 (d, *J* = 18Hz, 1H), 6.29-6.26 (d, *J* = 18Hz, 1H), 2.06 (s, 8H), 2.05 (s, 4H); $^{13}C\{^1H\}$ NMR (150MHz, CDCl$_3$, *ppm*): δ 138.6, 137.5, 132.8, 132.7, 128.4, 128.2, 127.3, 127.2, 126.8, 126.7, 123.6, 123.5, 72.1, 68.4, 23.4, 23.2, 22.5; $^{11}B\{^1H\}$ NMR (192 MHz, CDCl$_3$, *ppm*): δ 2.9 (1B, -*B(9)*-CH), -1.9 (1B, -*B(8)*-CH), -4.9 (2B), -9.1 (3B), -10.3 (3B), -11.4 (5B); HRMS: calculated for $C_{12}B_{10}H_{22}Br$ (M^++H) 353.1902; found: 353.1903.



2l

An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.

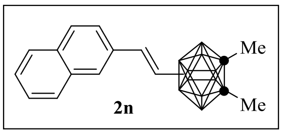
^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.33-7.32 (d, *J* = 6Hz, 2H), 7.29-2.38 (d, *J* = 6Hz, 2H), 7.25-7.22 (m, 4H), 6.68-6.65 (d, *J* = 18Hz, 1H), 6.53-6.50 (d, *J* = 18Hz, 1H), 6.41-6.38 (d, *J* = 18Hz, 1H), 6.31-6.28 (d, *J* = 18Hz, 1H), 2.05 (brs, 12H); ^{13}C{^{1}H} NMR (150MHz, $CDCl_3$, *ppm*): δ 138.7, 137.6, 132.7, 132.5, 128.5, 128.4, 127.4, 127.3, 72.1, 67.6, 23.4, 23.2, 22.5; ^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, *ppm*): δ 3.4 (1B, -*B(9)*-CH), -1.4 (1B, -*B(8)*-CH), -4.5 (3B), -8.7 (2B), -9.9 (6B), -11.1 (2B); HRMS: calculated for $C_{12}B_{10}H_{22}Cl$ (M^{+}+H) 309.2407; found: 309.2408.



2m

An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.

^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.53-7.51 (dd, *J* = 6Hz, 1H), 7.49-7.47 (dd, *J* = 6Hz, 1H), 7.16-7.12 (m, 2H), 7.08-6.97 (m, 4H), 6.95-6.92 (d, *J* = 18Hz, 1H), 6.80-6.77 (d, *J* = 18Hz, 1H), 6.49-6.46 (d, *J* = 18Hz, 1H), 6.40-6.37 (d, *J* = 18Hz, 1H), 2.06 (s, 8H), 2.05 (s, 4H); ^{13}C{^{1}H} NMR (150MHz, $CDCl_3$, *ppm*): δ 160.9, 159.2, 130.6, 128.3, 128.1, 126.6, 123.9, 123.8, 115.6, 115.5, 115.4, 72.1, 67.6, 23.4, 23.2, 22.5; ^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, *ppm*): δ 3.5 (1B, -*B(9)*-CH), -1.4 (1B, -*B(8)*-CH), -4.5 (2B), -8.7 (2B), -9.9 (2B), -11.1 (5B); HRMS: calculated for $C_{12}B_{10}H_{22}F$ (M^{+}+H) 293.2699; found: 293.2703.

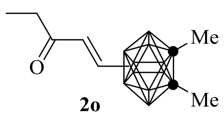


2n

An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.

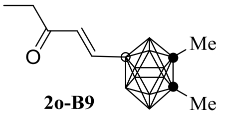
^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.81-7.61 (m, 9H), 7.46-7.39 (m, 5H), 6.91-6.88

(d, J = 18Hz, 1H), 6.77-6.74 (d, J = 18Hz, 1H), 6.57-6.54 (d, J = 18Hz, 1H), 6.48-6.45 (d, J = 18Hz, 1H), 2.07 (s, 9H), 2.06 (s, 3H); $^{13}C\{^1H\}$ NMR (150MHz, $CDCl_3$, *ppm*): δ 144.5, 140.1, 138.9, 133.7, 132.9, 132.8, 128.0, 127.9, 127.8, 127.6, 127.5, 126.0, 125.9, 125.5, 125.4, 123.6, 123.5, 72.0, 67.4, 23.4, 23.2, 22.5; HRMS: calculated for $C_{16}B_{10}H_{25}$ (M^++H) 325.2953; found: 325.2954.



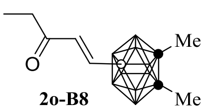
2o

A separable B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.6.



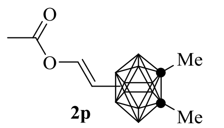
2o-B9

^1H NMR (600MHz, $CDCl_3$, *ppm*): δ 6.88-6.85 (d, J = 18Hz, 1H), 6.25-6.22 (d, J = 18Hz, 1H), 2.58-2.54 (q, J = 6Hz, 2H), 2.04 (brs, 6H), 1.07-1.05 (t, J = 6Hz, 3H); $^{13}C\{^1H\}$ NMR (150MHz, $CDCl_3$, *ppm*): δ 204.7, 138.5, 72.5, 32.3, 23.3, 22.6, 8.2; $^{11}B\{^1H\}$ NMR (192 MHz, $CDCl_3$, *ppm*): δ 1.7 (1B, -*B(9)*-CH), -5.2 (2B), -8.9 (2B), -10.3 (5B); HRMS: calculated for $C_9B_{10}H_{23}O$ (M^++H) 255.2746; found: 255.2747.



2o-B8

^1H NMR (600MHz, $CDCl_3$, *ppm*): δ 6.98-6.95 (d, J = 18Hz, 1H), 6.40-6.37 (d, J = 18Hz, 1H), 2.61-2.58 (q, J = 6Hz, 2H), 2.04 (s, 6H), 1.10-1.08 (t, J = 6Hz, 3H); $^{13}C\{^1H\}$ NMR (150MHz, $CDCl_3$, *ppm*): δ 201.4, 139.4, 72.6, 32.5, 23.2, 8.1; $^{11}B\{^1H\}$ NMR (192 MHz, $CDCl_3$, *ppm*): δ -3.1 (1B, -*B(8)*-CH), -4.9 (2B), -8.9 (1B), -9.8 (1B), -10.1 (3B), -11.1 (2B); HRMS: calculated for $C_9B_{10}H_{23}O$ (M^++H) 255.2744; found: 255.2747.



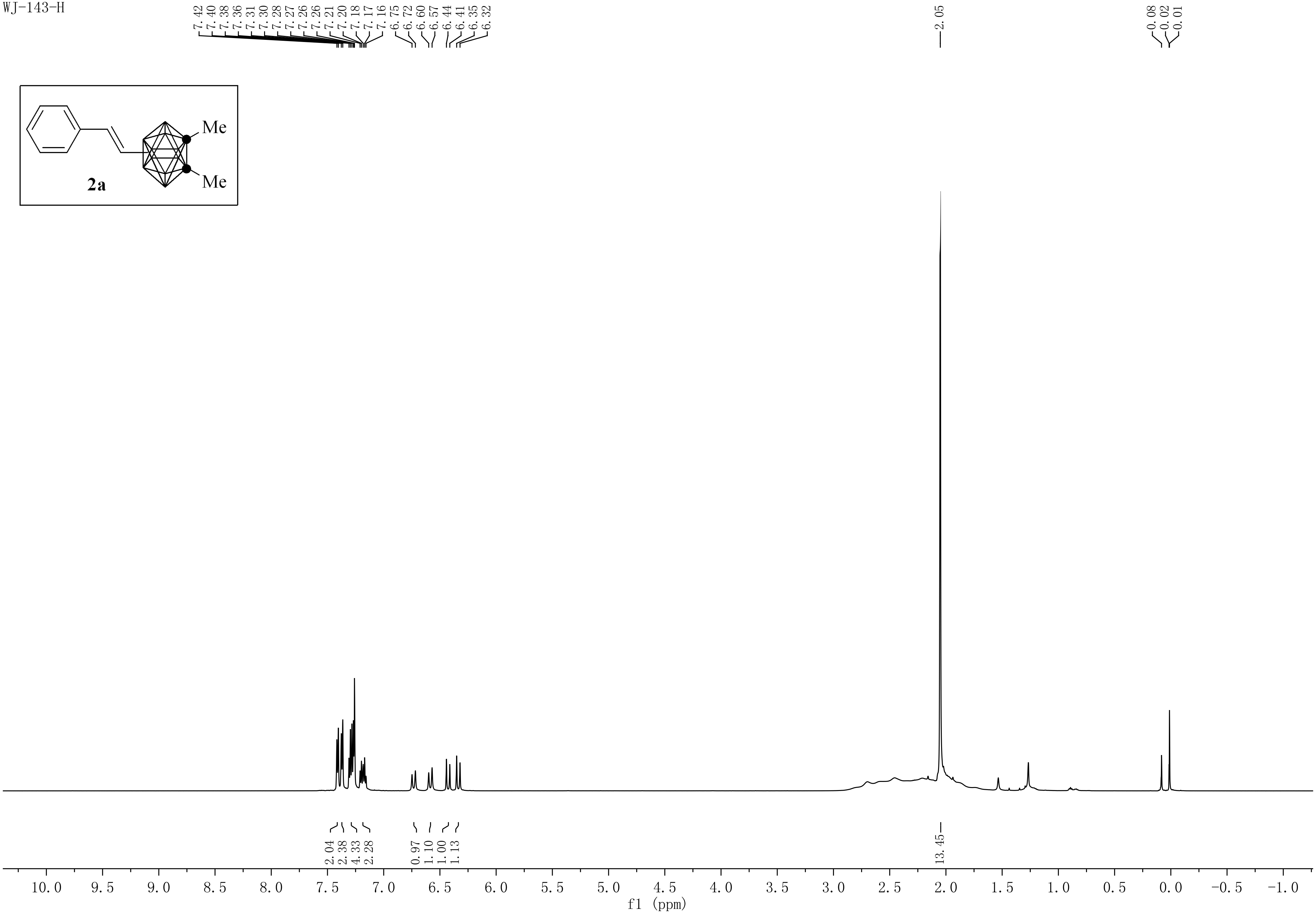
2p

An inseparable mixture of B8 and B9 isomers was obtained. The ratio of B8/B9 is about 1:1.4.

^{1}H NMR (600MHz, $CDCl_3$, *ppm*): δ 7.20-7.17 (d, J = 18Hz, 1H), 7.06-7.03 (d, J = 18Hz, 1H), 5.33-5.30 (d, J = 18Hz, 1H), 5.23-5.20 (d, J = 18Hz, 1H), 2.10 (s, 3H), 2.07 (s, 3H), 2.03 (brs, 12H); $^{13}C\{^{1}H\}$ NMR (150MHz, $CDCl_3$, *ppm*): δ 168.1, 141.2, 140.4, 72.1, 67.8, 23.3, 23.1, 22.5, 20.8; $^{11}B\{^{1}H\}$ NMR (192 MHz, $CDCl_3$, *ppm*): δ 1.6 (1B, -*B(9)*-CH), -3.3 (1B, -*B(8)*-CH), -4.9 (2B), -9.0 (2B), -10.3 (5B), -11.4 (3B); HRMS: calculated for $C_8B_{10}H_{21}O_2$ (M^++H) 257.2541; found: 257.2539.

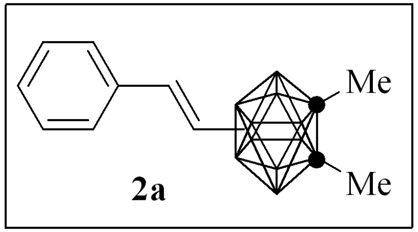
Copies of ^{1}H NMR, $^{13}C\{^{1}H\}$ NMR, ^{11}B NMR and ^{11}B{H} NMR:

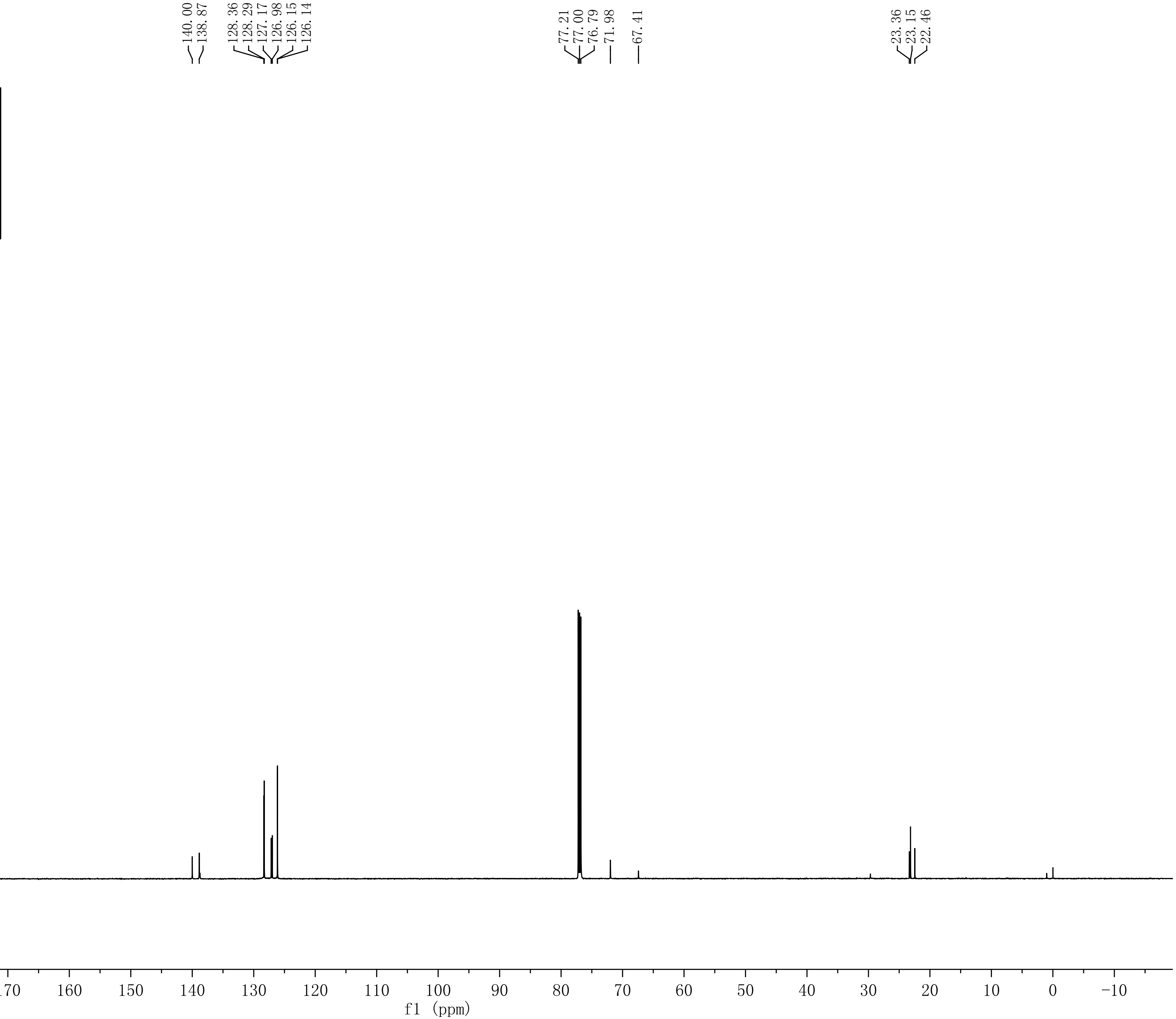
WJ-143-H



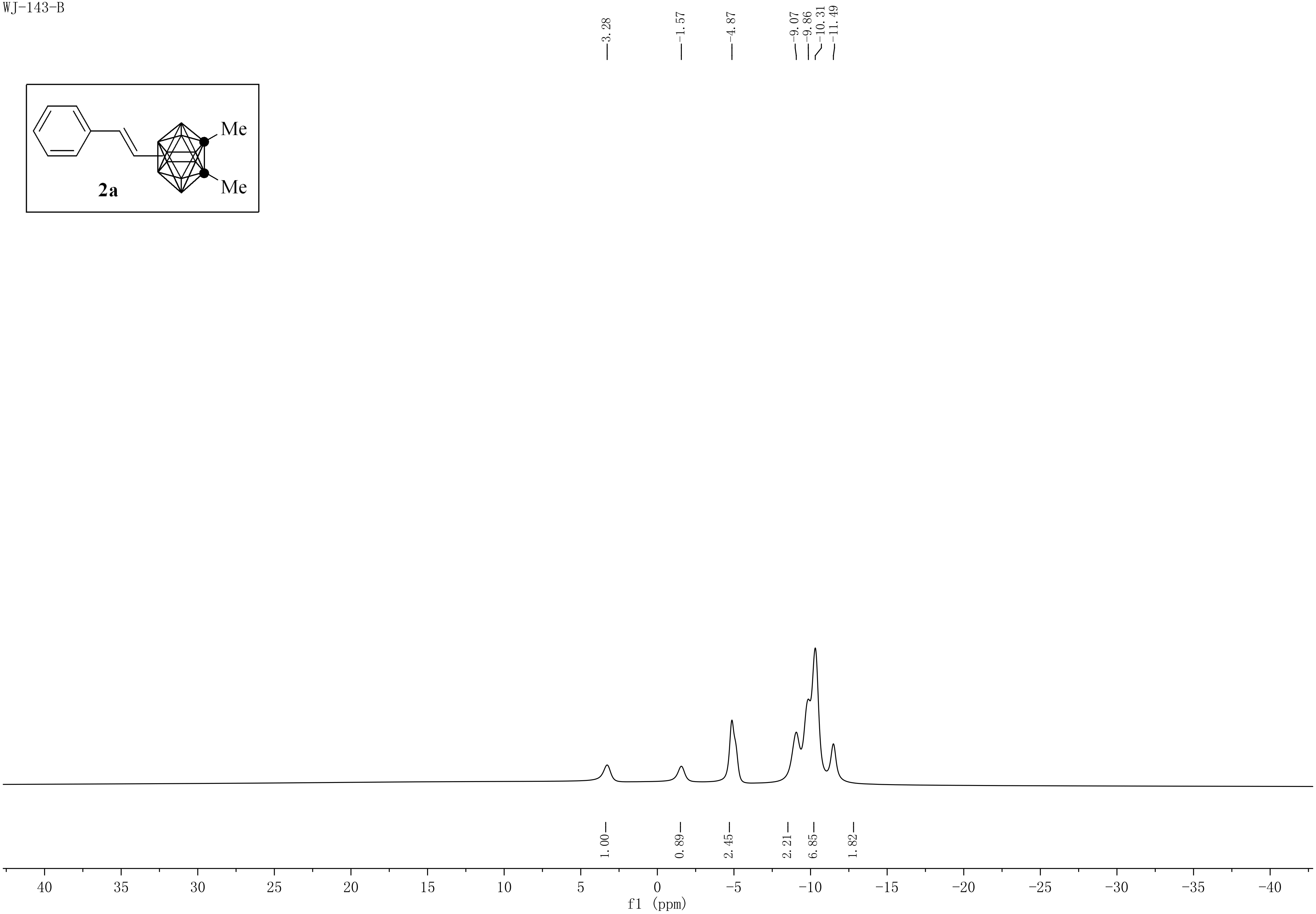
7.42 7.40 7.38 7.36 7.31 7.30 7.28 7.27 7.26 7.26 7.21 7.20 7.18 7.17 7.16 6.75 6.72 6.60 6.57 6.44 6.41 6.35 6.32
2.05
0.08 0.02 0.01
Me
Me
2a
2.04 2.38 4.33 2.28
0.97 1.10 1.00 1.13
13.45
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

WJ-143-C

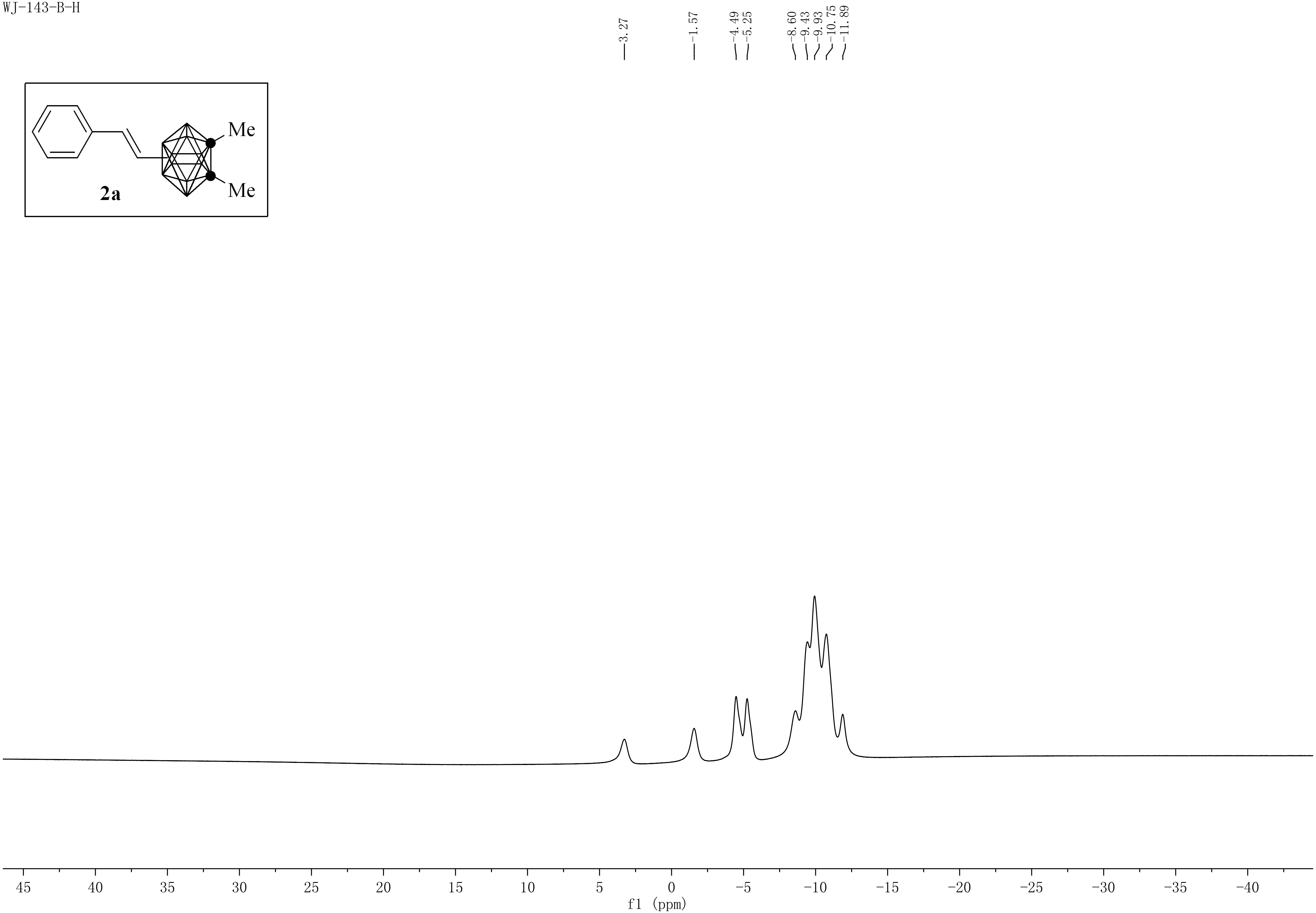

Me
Me
2a


140.00
138.87
128.36
128.29
127.17
126.98
126.15
126.14
77.21
77.00
76.79
71.98
67.41
23.36
23.15
22.46
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

WJ-143-B

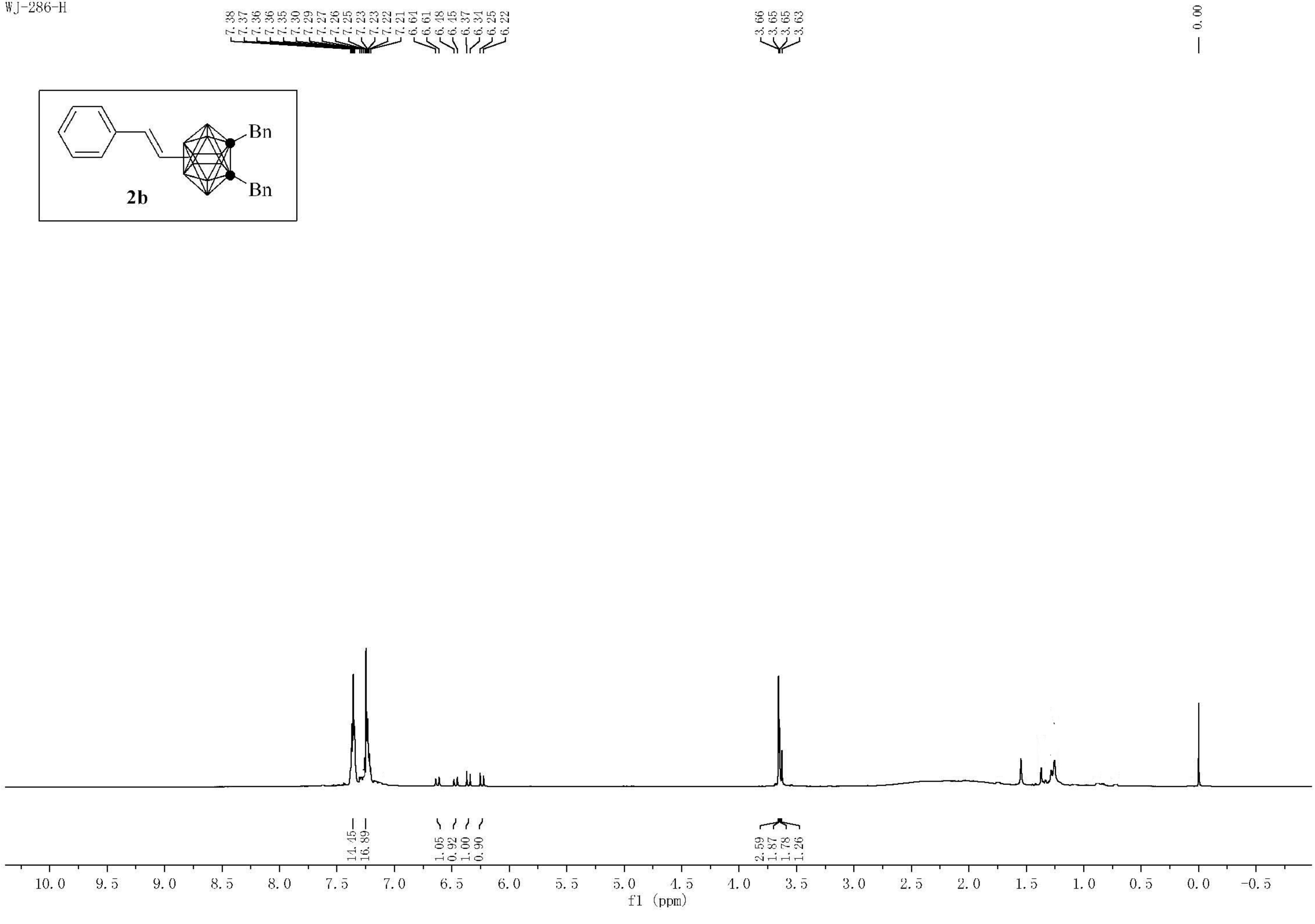

3.28
-1.57
-4.87
-9.07
-9.86
-10.31
-11.49
Me
Me
2a
1.00
0.89
2.45
2.21
6.85
1.82
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
f1 (ppm)

WJ-143-B-H



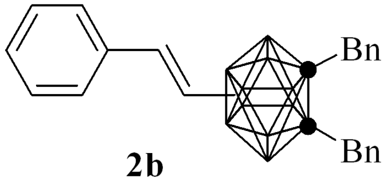
3.27
-1.57
-4.49
-5.25
-8.60
-9.43
-9.93
-10.75
-11.89
Me
Me
2a
45 40 35 30 25 20 15 10 5 0 −5 −10 −15 −20 −25 −30 −35 −40
f1 (ppm)

WJ-286-H

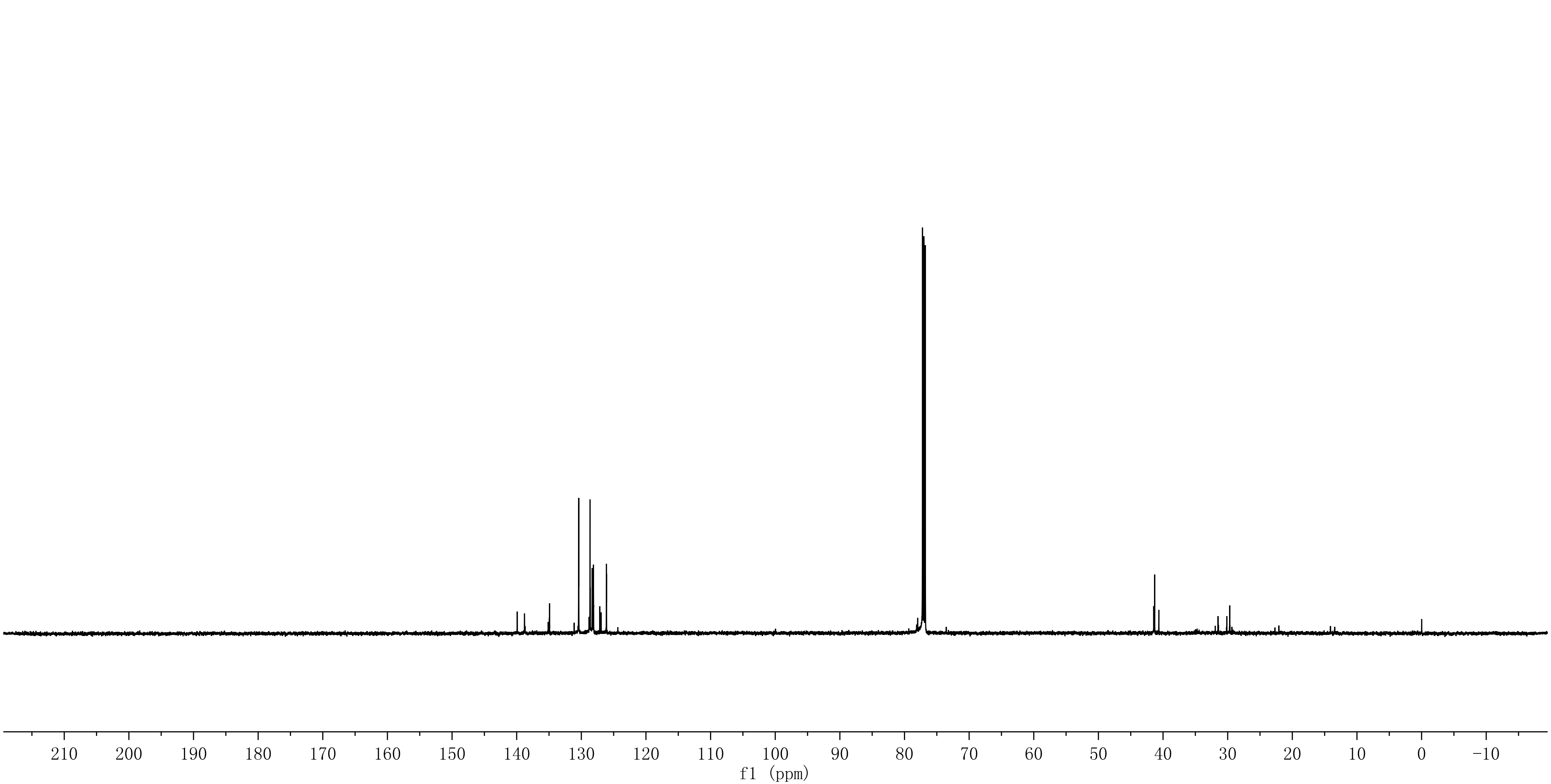


7.38 7.37 7.36 7.36 7.35 7.30 7.29 7.27 7.26 7.25 7.23 7.23 7.22 7.21 6.64 6.61 6.48 6.45 6.37 6.34 6.25 6.22
3.66 3.65 3.65 3.63
0.00
Bn
Bn
2b
14.45
16.89
1.05
0.92
1.00
0.90
2.59
1.87
1.78
1.26
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

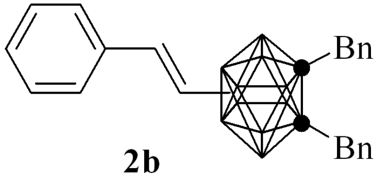
WJ-286-C



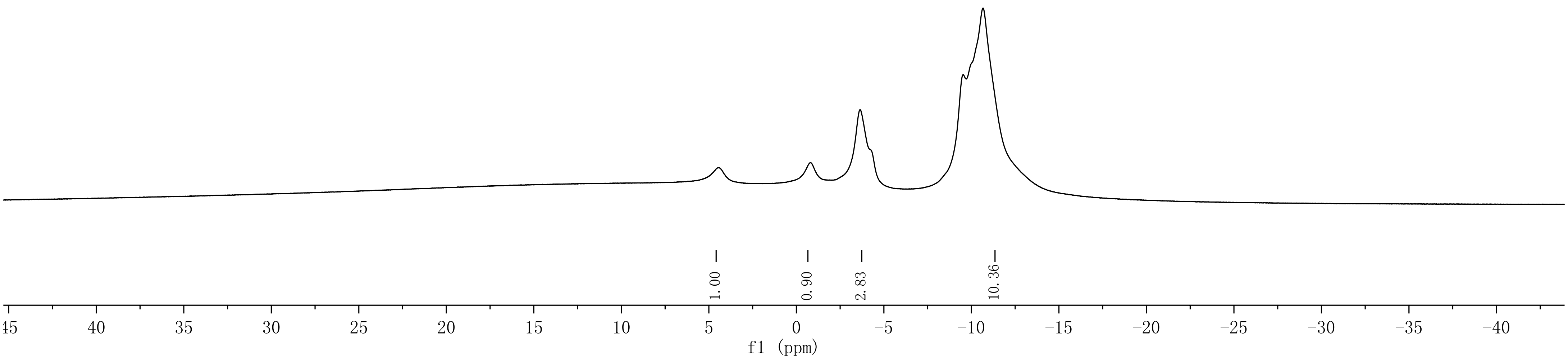
2b


139.93
138.79
138.71
135.12
134.97
134.95
134.92
131.11
130.42
130.40
128.80
128.65
128.64
128.62
128.33
128.24
128.12
128.11
128.10
127.14
126.94
126.12
126.10
124.36
77.97
77.21
77.00
76.79
73.65
41.44
41.36
41.30
40.65
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

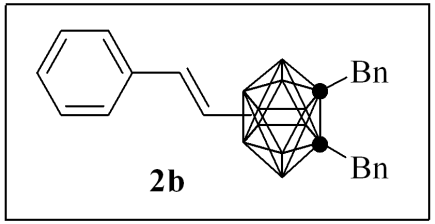
WJ-286-B


Bn
Bn

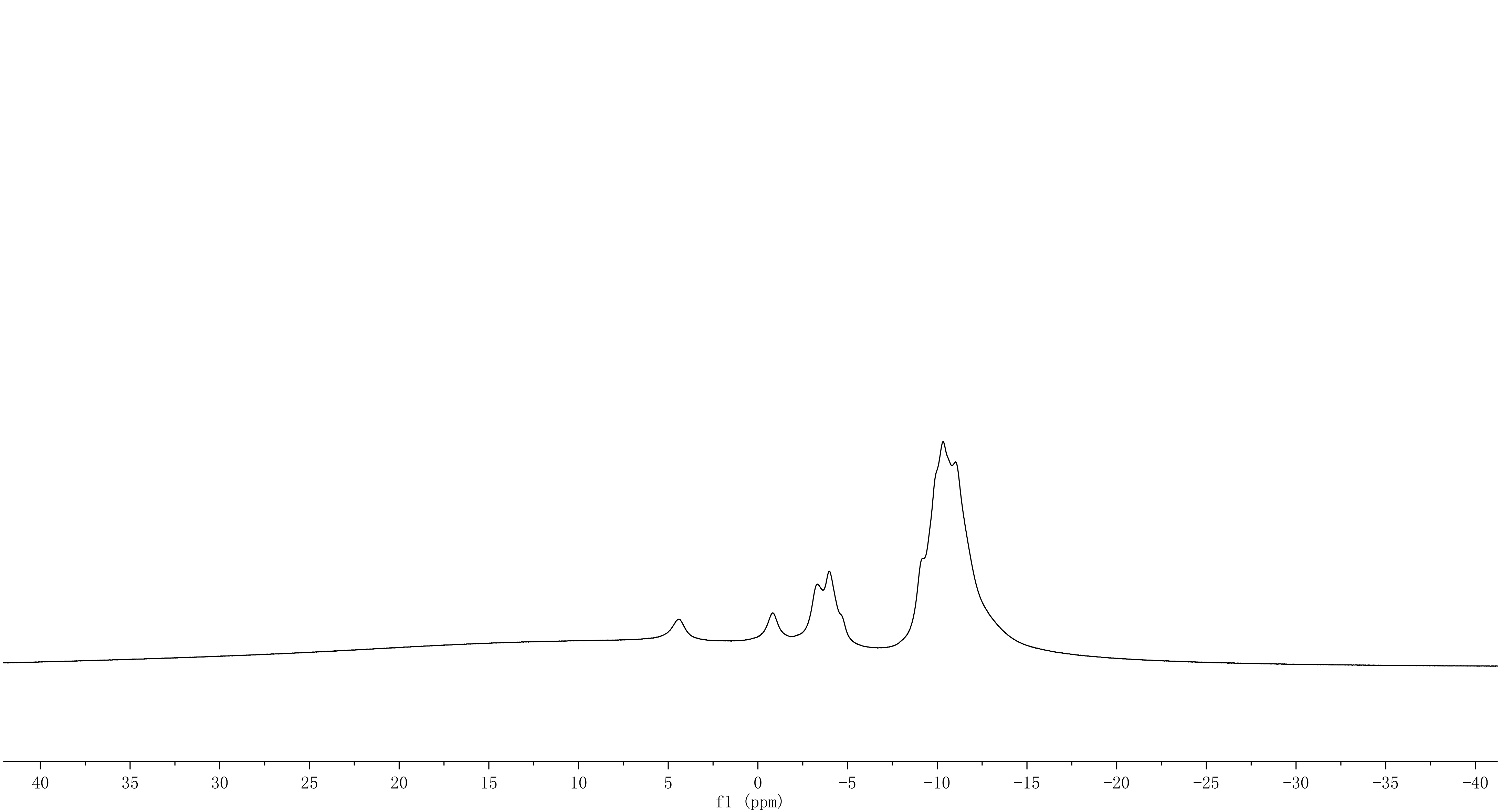
2b


4.46
0.80
-3.63
-9.53
-10.66
1.00
0.90
2.83
10.36
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
f1 (ppm)

WJ-286-B-H

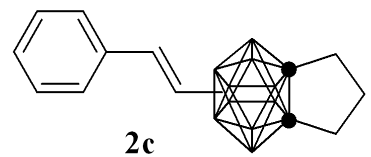


Bn
Bn
2b

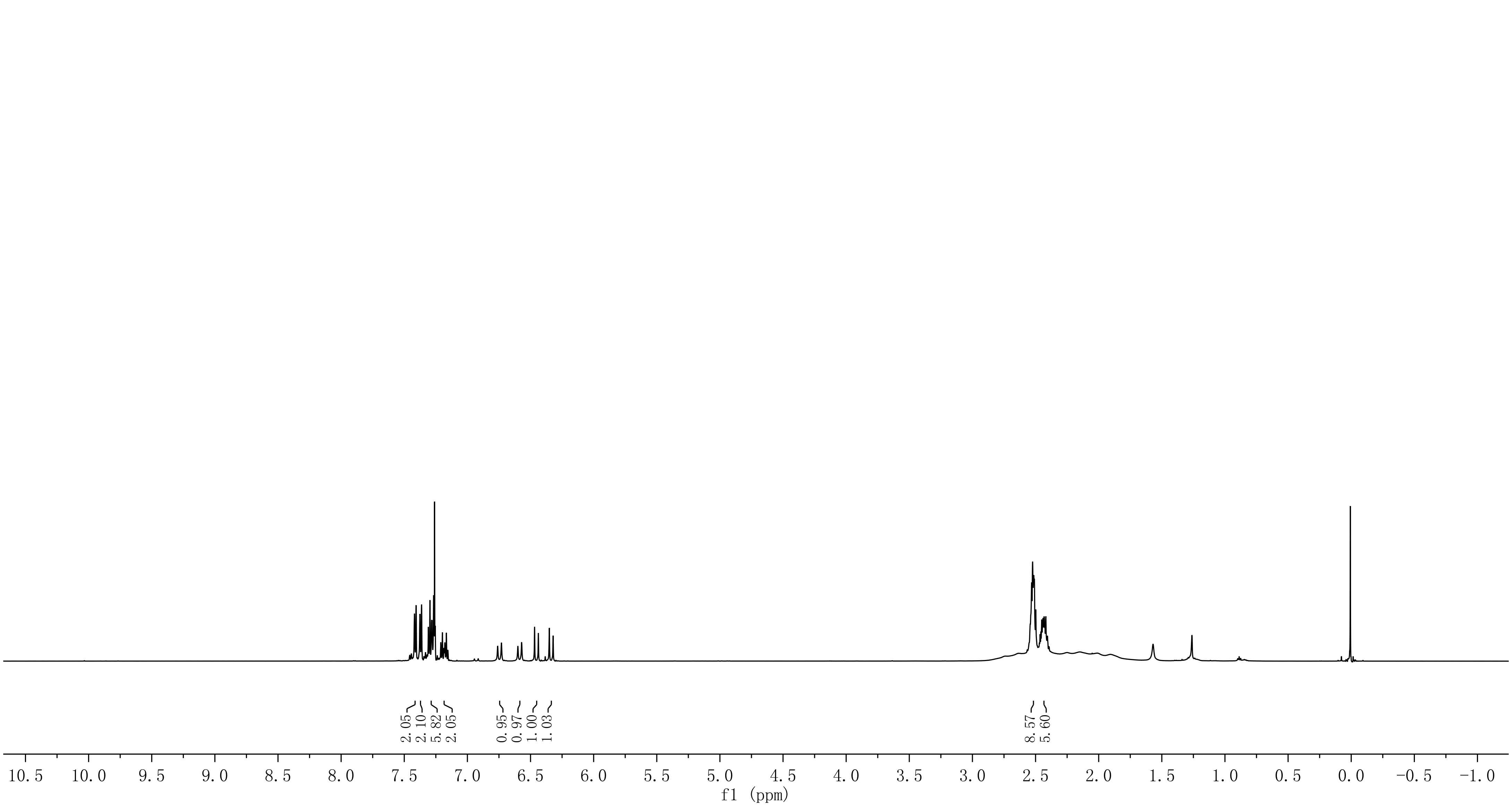


4.42
0.82
-3.32
-3.97
-10.33
-11.02
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
f1 (ppm)

WJ-258-H

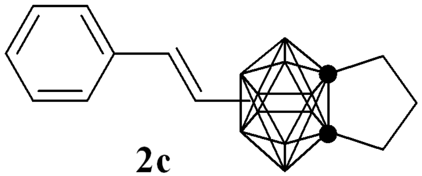


2c

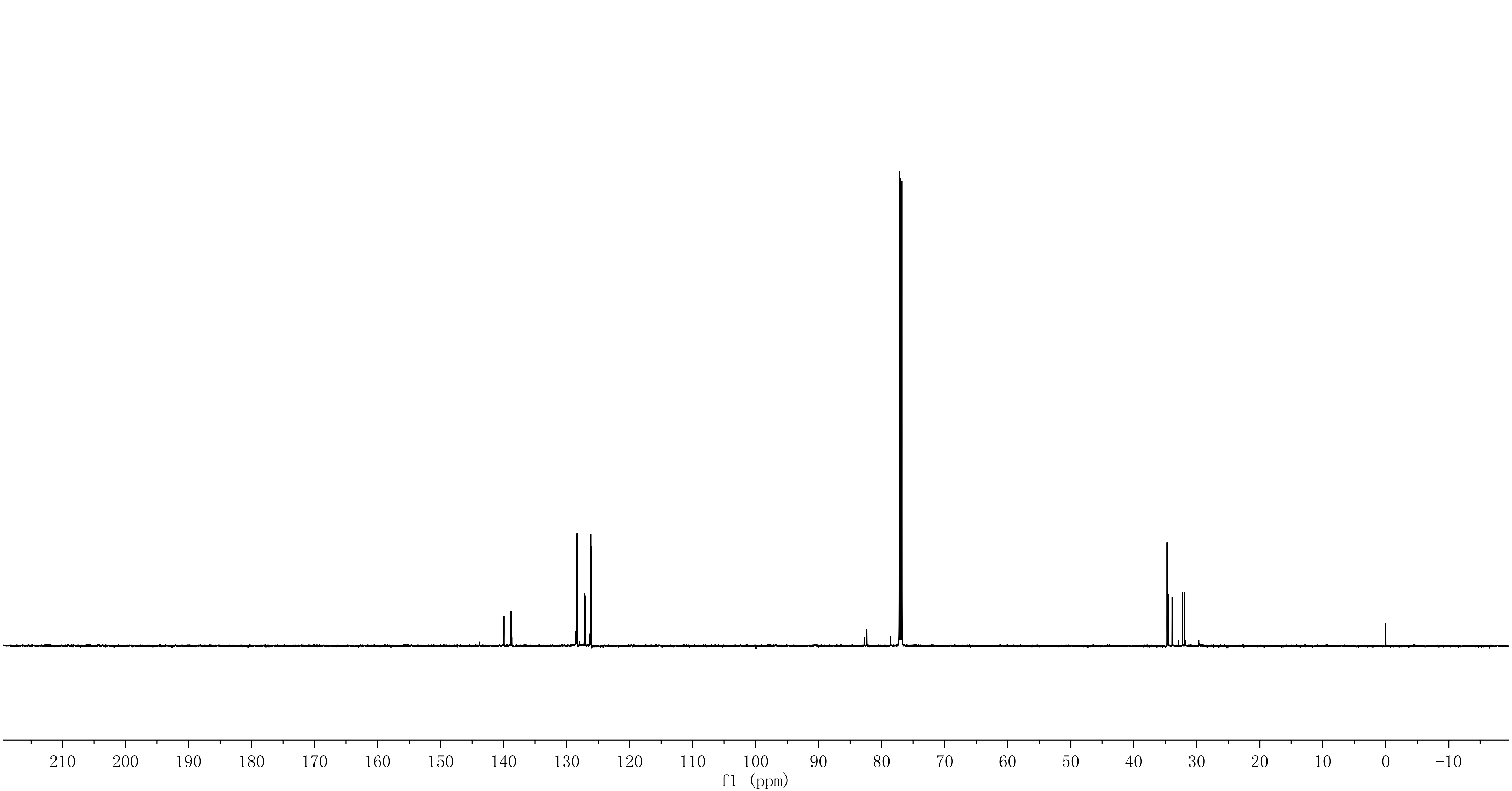


7.42
7.41
7.38
7.36
7.31
7.30
7.28
7.28
7.27
7.26
7.25
7.21
7.20
7.18
7.17
6.76
6.73
6.60
6.57
6.47
6.44
6.35
6.32
2.54
2.53
2.52
2.51
2.51
2.50
2.46
2.46
2.45
2.44
2.43
2.43
2.43
2.42
2.41
0.01
2.05
2.10
5.82
2.05
0.95
0.97
1.00
1.03
8.57
5.60
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

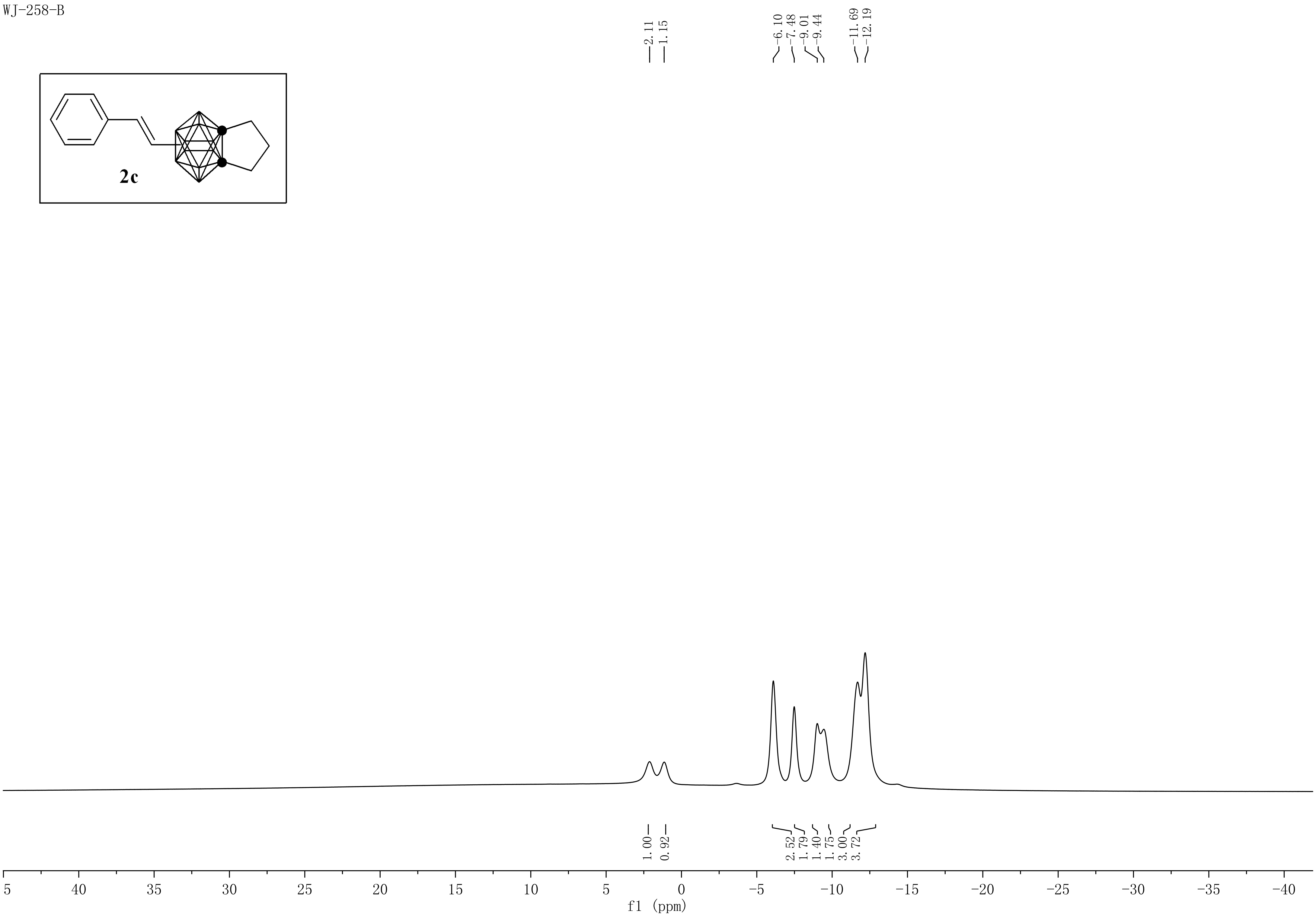
WJ-258-C



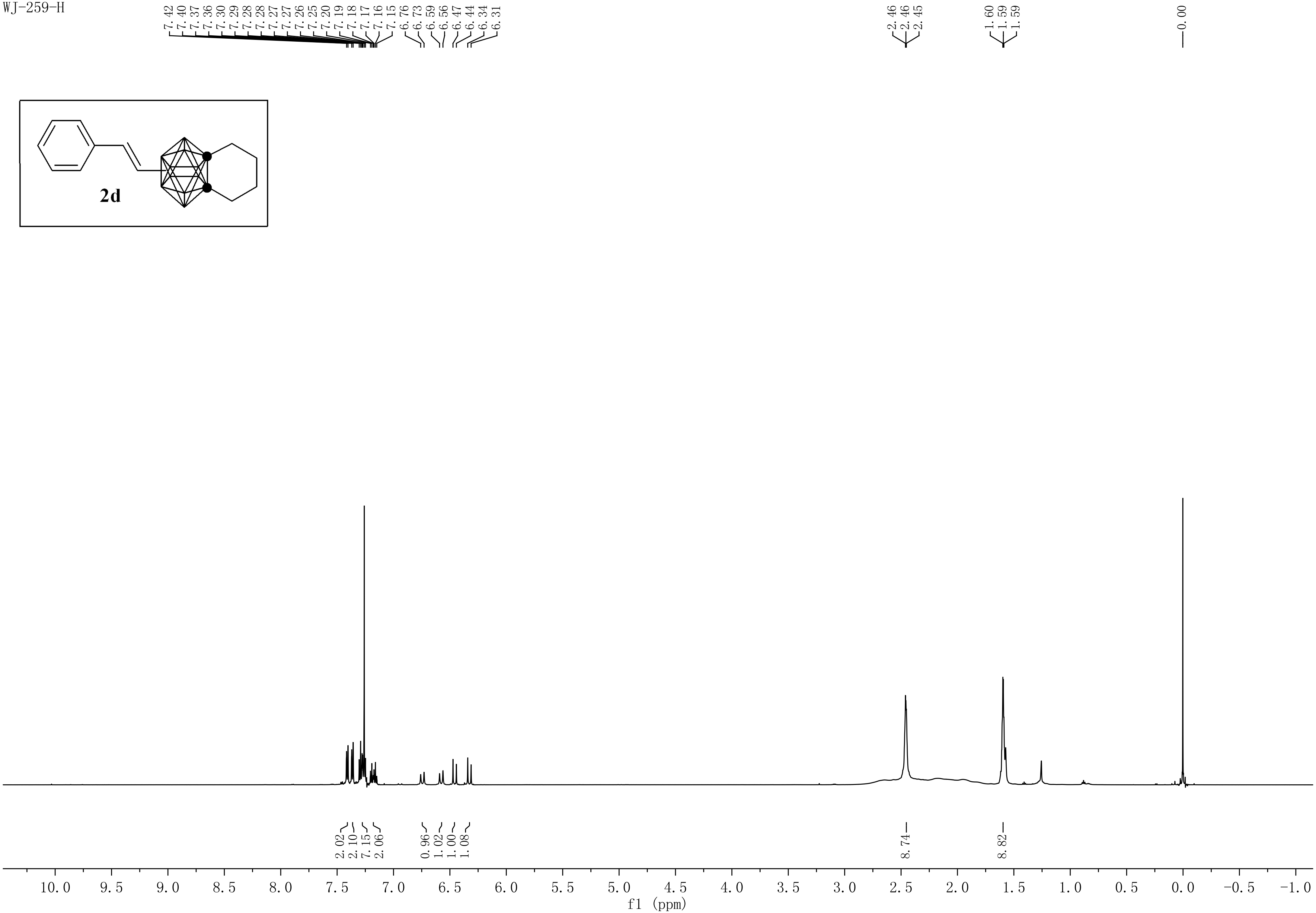
2c



139.96
138.84
128.36
128.28
127.18
126.96
126.16
126.12
82.77
82.37
78.59
77.21
77.00
76.79
34.72
34.55
33.87
32.29
31.94
-0.02
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

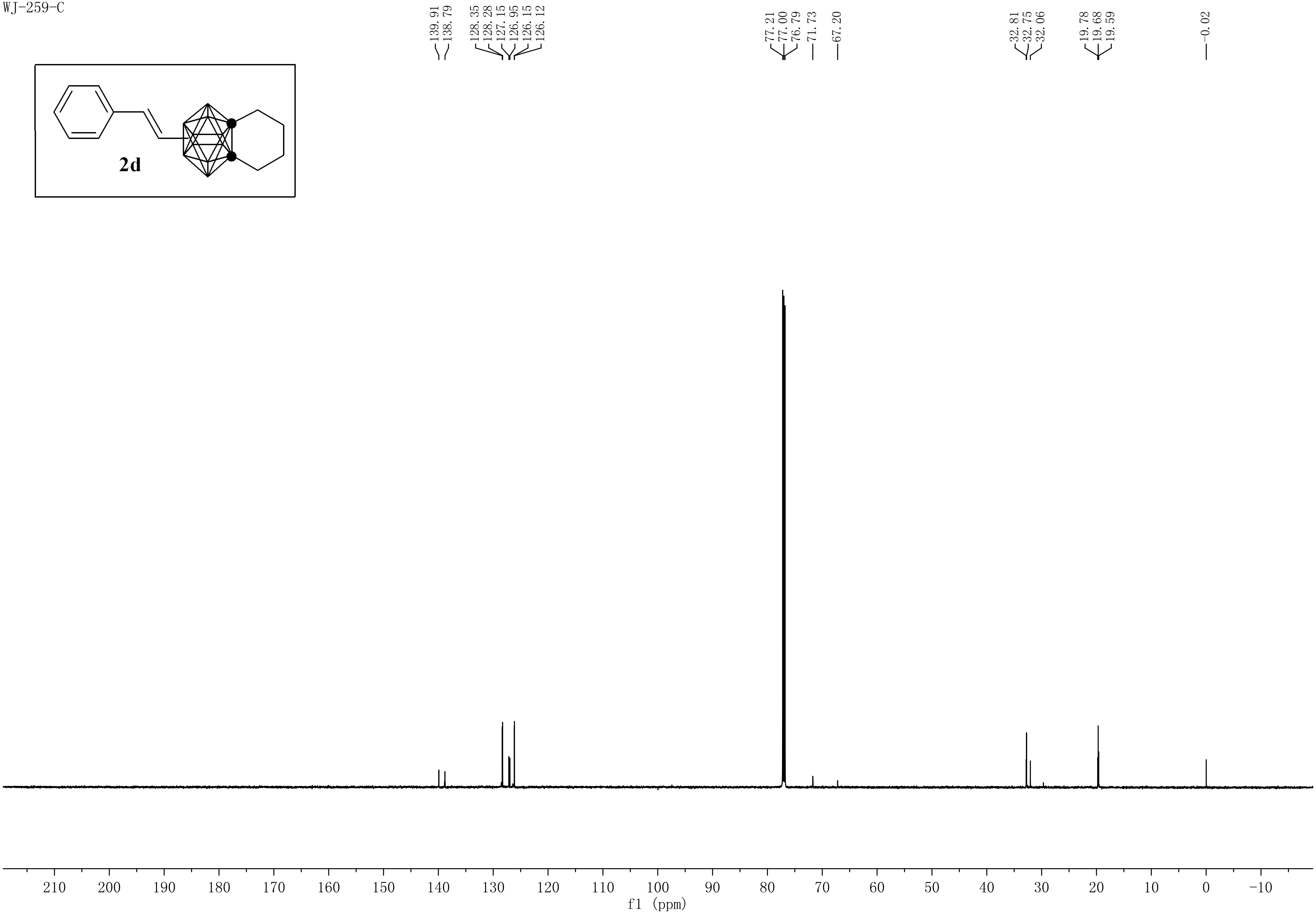

WJ-258-B
2c
2.11
1.15
-6.10
-7.48
-9.01
-9.44
-11.69
-12.19
1.00
0.92
2.52
1.79
1.40
1.75
3.00
3.72
5
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
f1 (ppm)

WJ-259-H

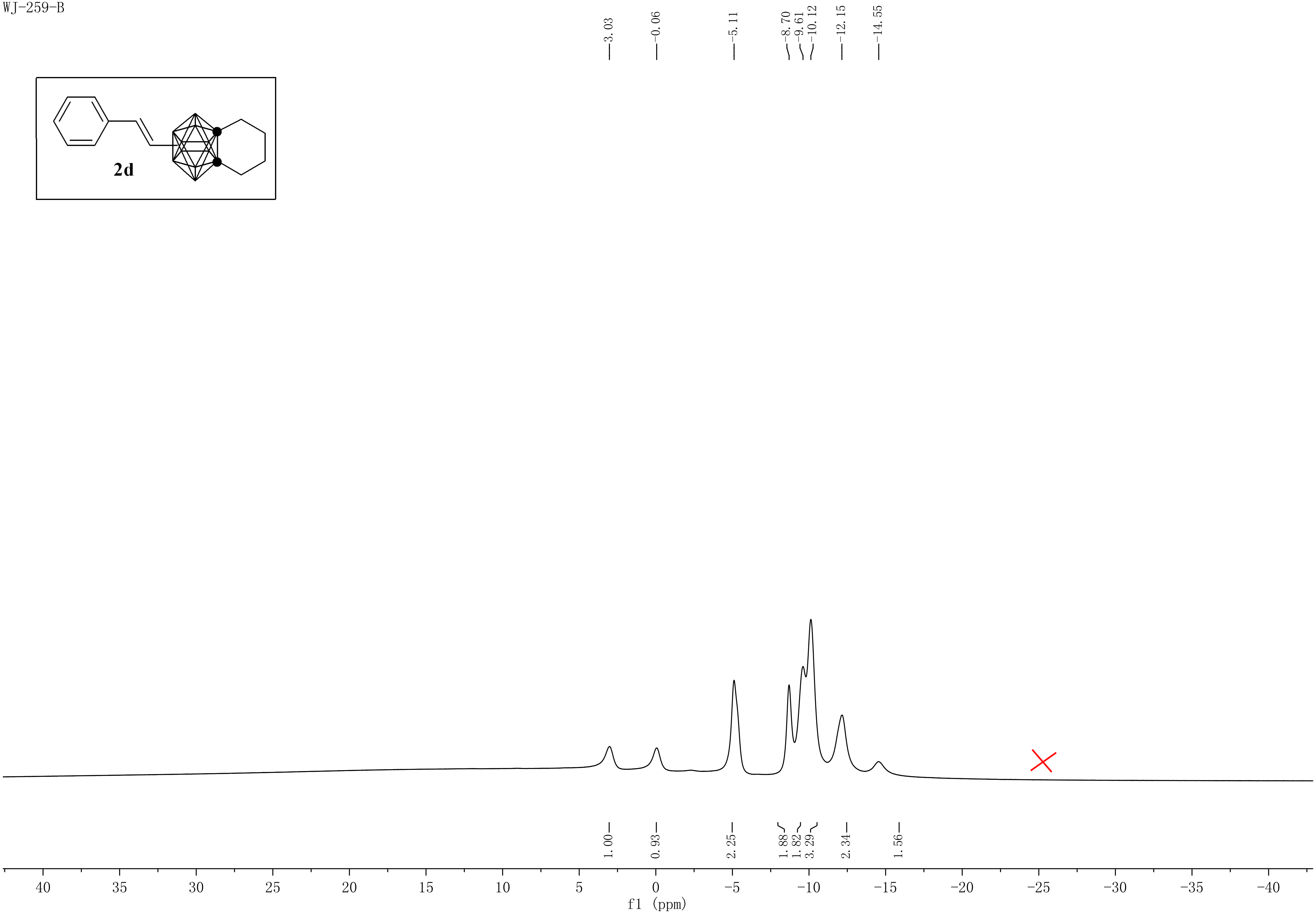

7.42
7.40
7.37
7.36
7.30
7.29
7.28
7.28
7.27
7.27
7.26
7.25
7.20
7.19
7.18
7.17
7.16
7.15
6.76
6.73
6.59
6.56
6.47
6.44
6.34
6.31
2.46
2.46
2.45
1.60
1.59
1.59
0.00
2d
2.02
2.10
7.15
2.06
0.96
1.02
1.00
1.08
8.74
8.82
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

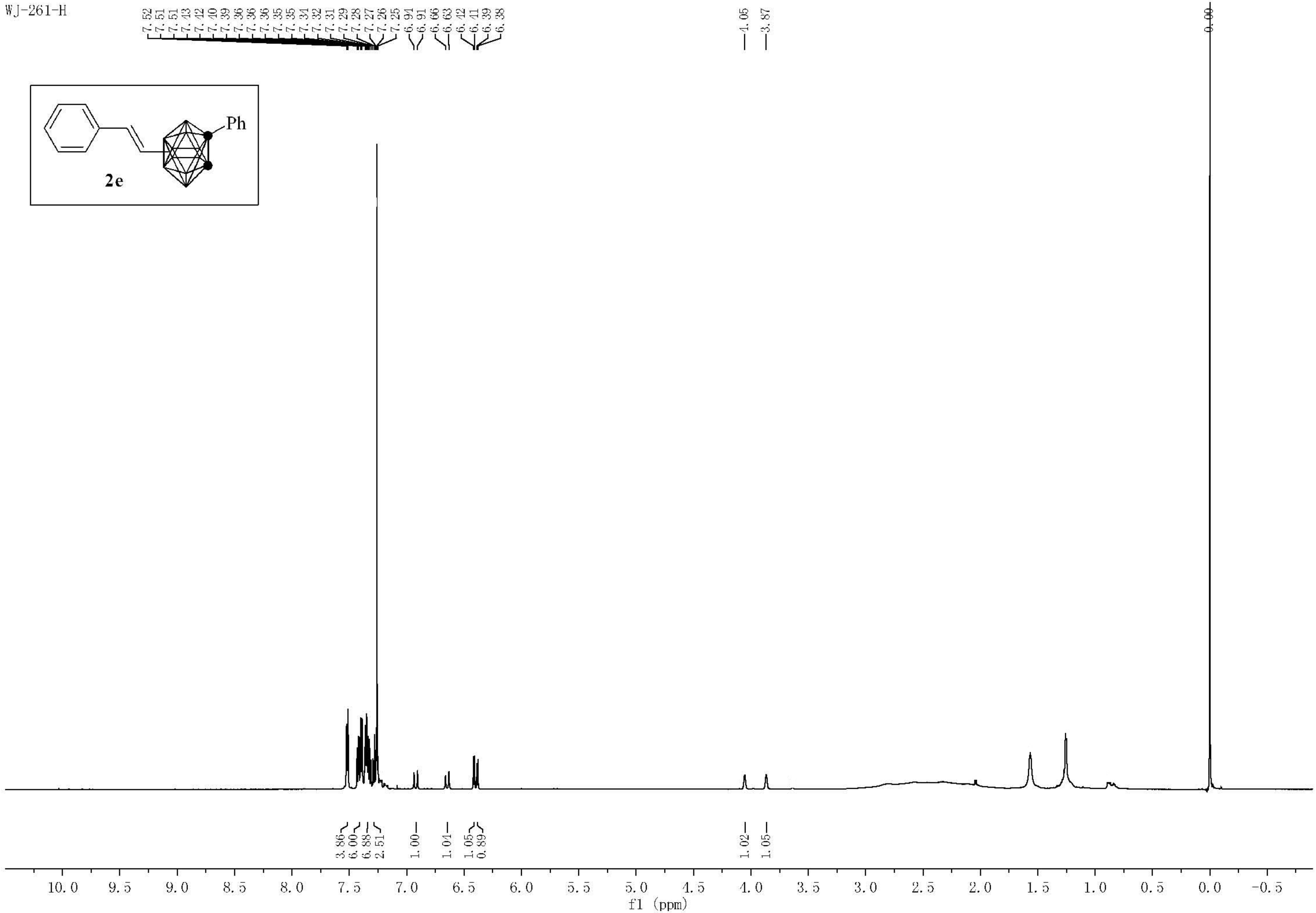
WJ-259-C

2d

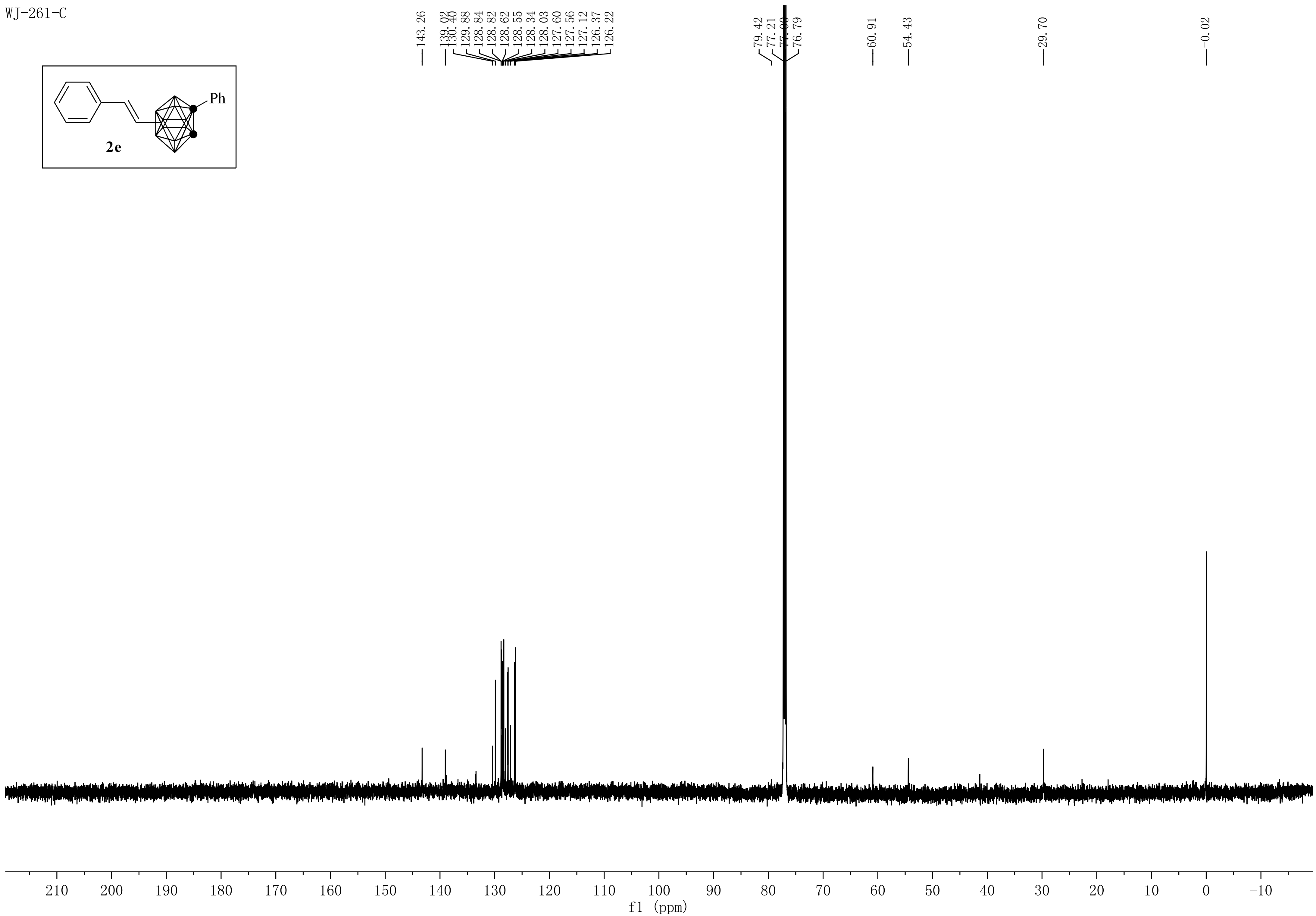

139.91
138.79
128.35
128.28
127.15
126.95
126.15
126.12
77.21
77.00
76.79
71.73
67.20
32.81
32.75
32.06
19.78
19.68
19.59
-0.02
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

WJ-259-B

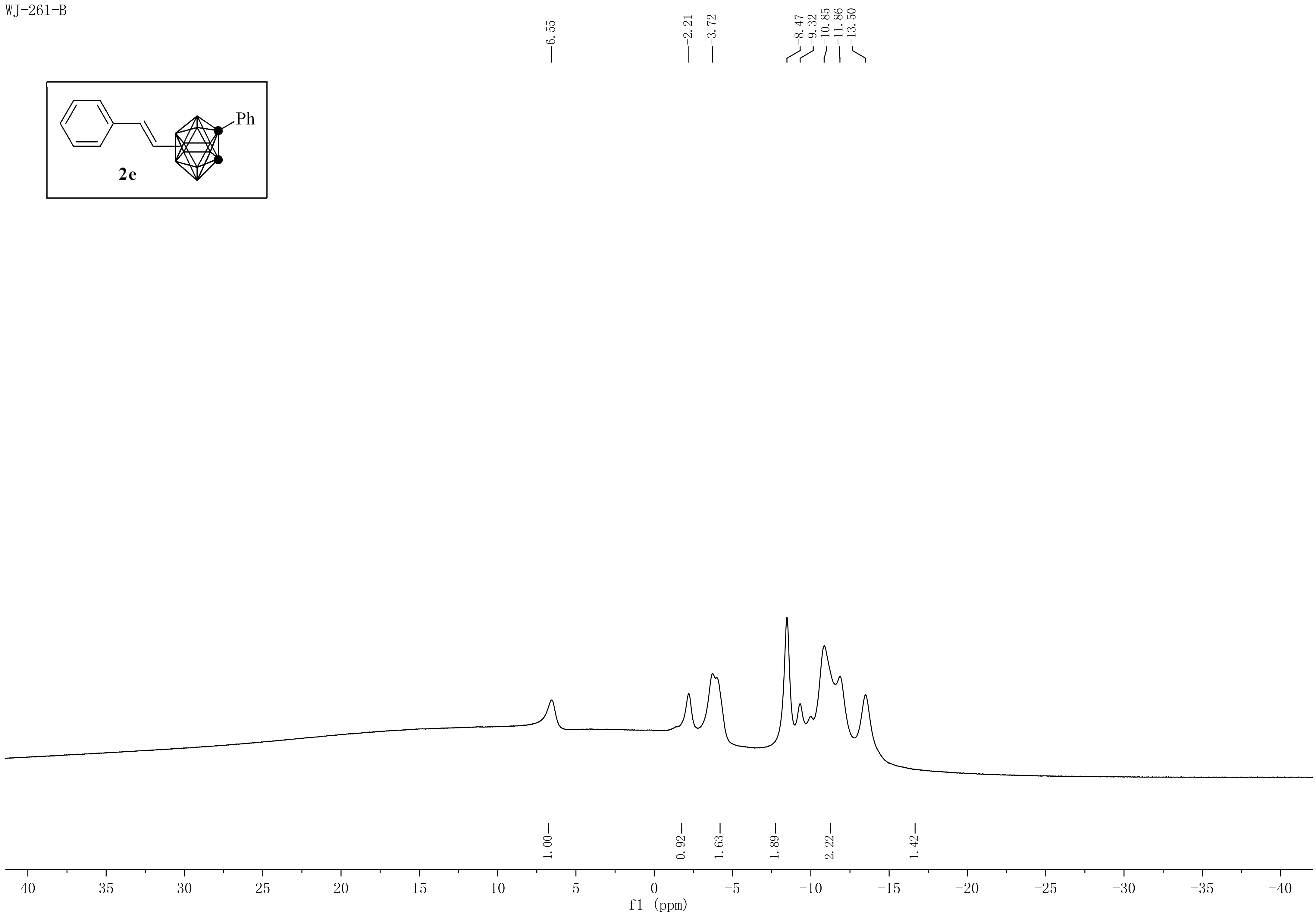

3.03
0.06
-5.11
-8.70
-9.61
-10.12
-12.15
-14.55
2d
1.00
0.93
2.25
1.88
1.82
3.29
2.34
1.56
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
f1 (ppm)



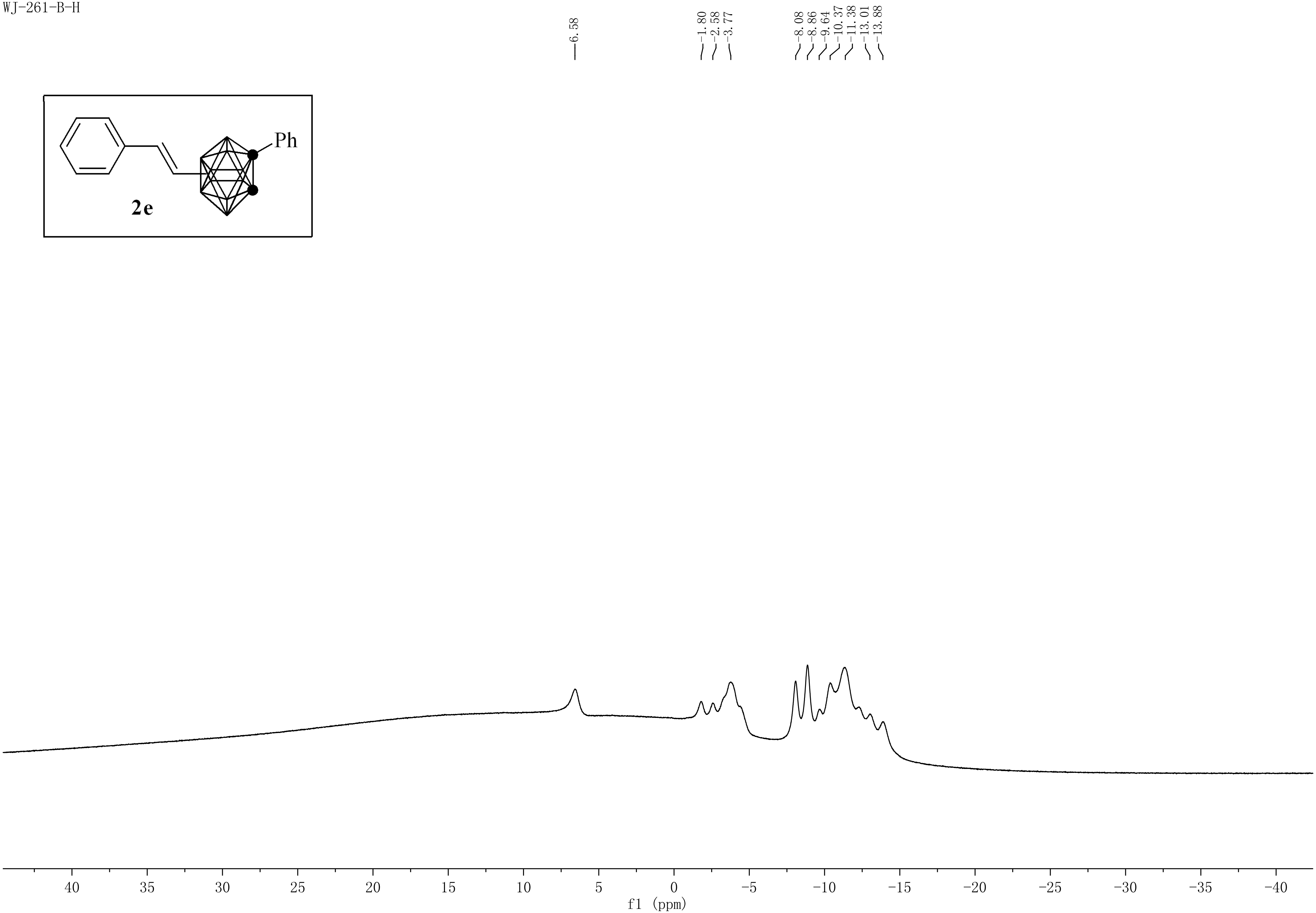
WJ-261-H
7.52
7.51
7.51
7.43
7.42
7.40
7.39
7.36
7.36
7.36
7.35
7.35
7.31
7.32
7.31
7.29
7.28
7.27
7.26
7.25
6.94
6.91
6.66
6.63
6.42
6.41
6.39
6.38
4.05
3.87
0.00
Ph
2e
3.86
6.00
6.88
2.51
1.00
1.04
1.05
0.89
1.02
1.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



WJ-261-C
143.26
139.02
130.40
129.88
128.84
128.82
128.62
128.55
128.34
128.03
127.60
127.56
127.12
126.37
126.22
79.42
77.21
77.00
76.79
60.91
54.43
29.70
-0.02
Ph
2e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

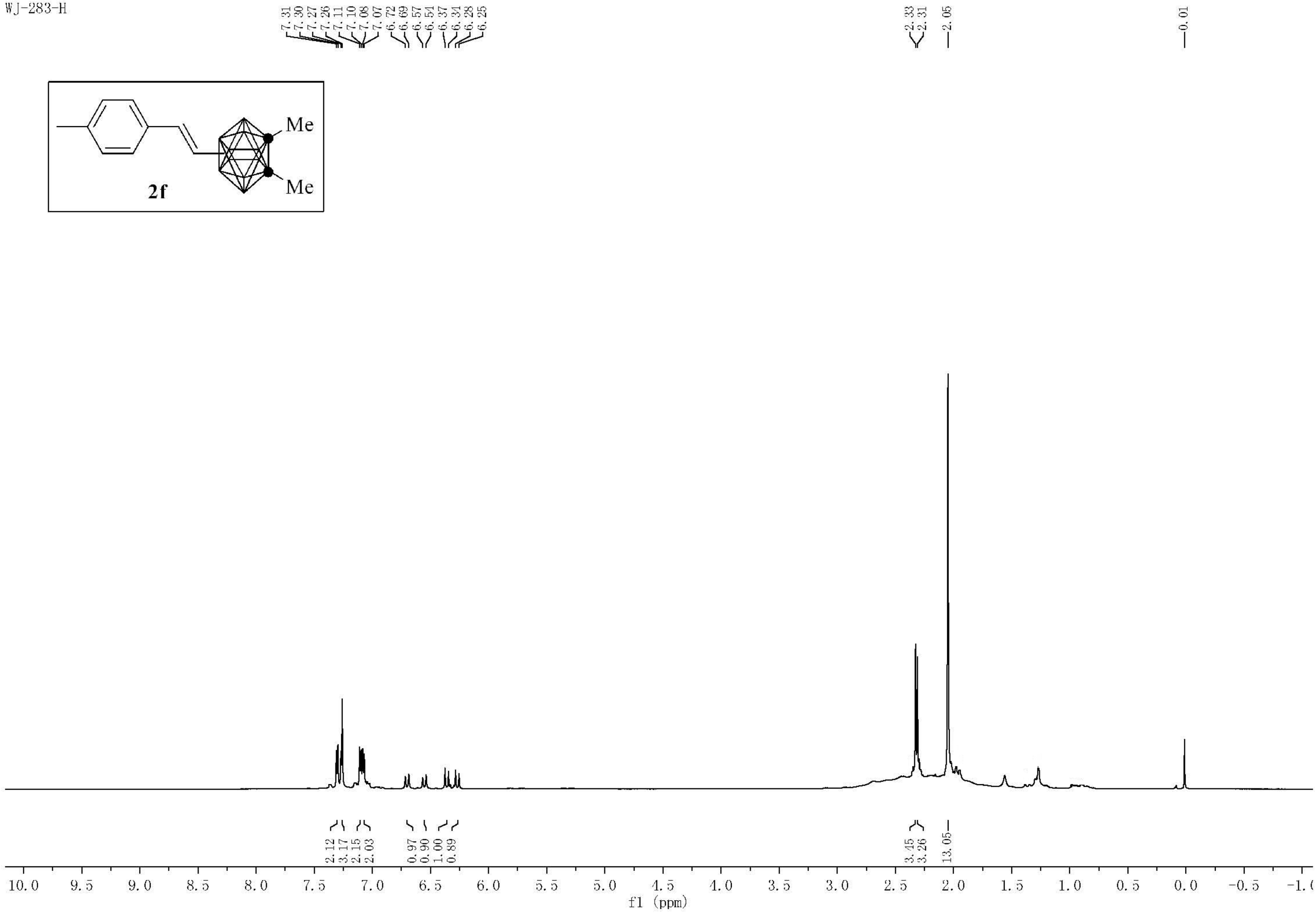

WJ-261-B
6.55
-2.21
-3.72
-8.47
-9.32
-10.85
-11.86
-13.50
Ph
2e
1.00
0.92
1.63
1.89
2.22
1.42
40 35 30 25 20 15 10 5 0 −5 −10 −15 −20 −25 −30 −35 −40
f1 (ppm)

WJ-261-B-H



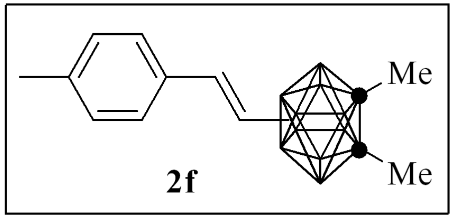
6.58
-1.80
-2.58
-3.77
-8.08
-8.86
-9.64
-10.37
-11.38
-13.01
-13.88
Ph
2e
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
f1 (ppm)

WJ-283-H



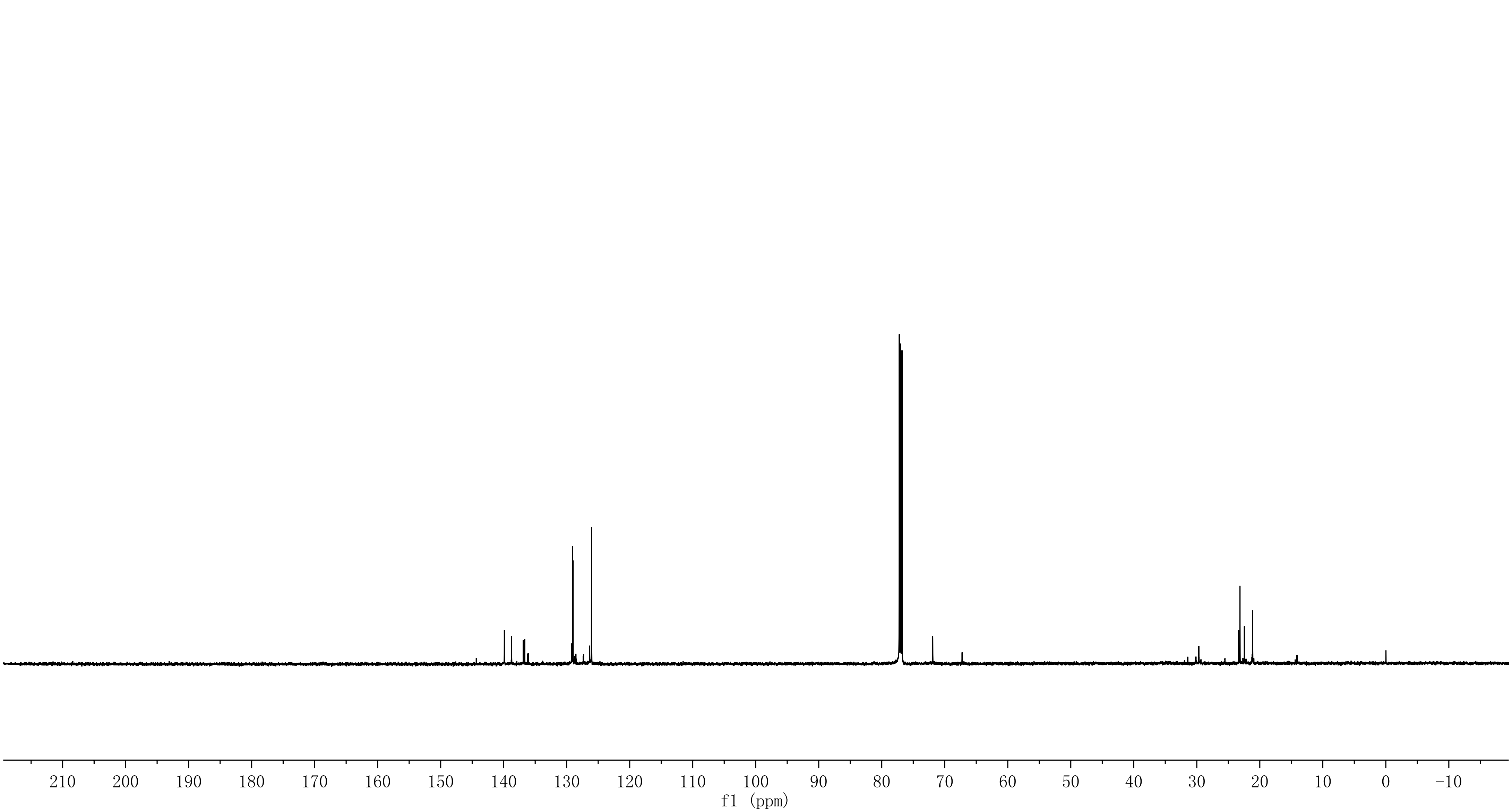
7.31
7.30
7.27
7.26
7.11
7.10
7.08
7.07
6.72
6.69
6.57
6.54
6.37
6.31
6.28
6.25
2.33
2.31
2.05
0.01
Me
Me
2f
2.12
3.17
2.15
2.03
0.97
0.90
1.00
0.89
3.45
3.26
13.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

WJ-283-C



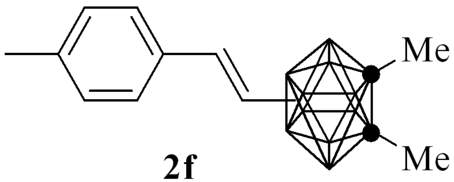
Me
Me

2f

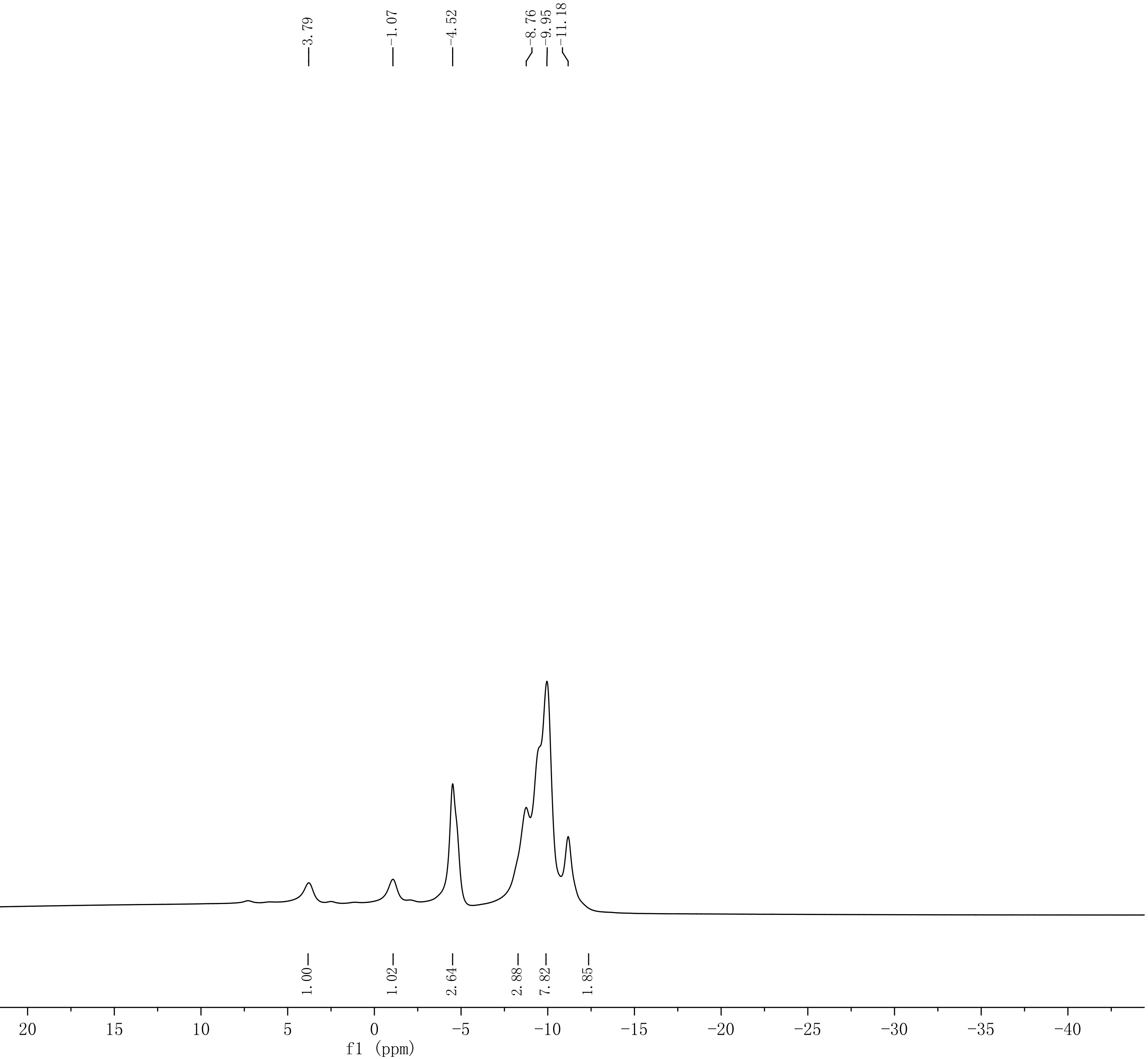


139.88
138.75
136.88
136.66
129.05
128.98
126.06
126.04
77.21
77.00
76.79
71.92
67.25
23.36
23.15
22.45
21.16
21.13
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

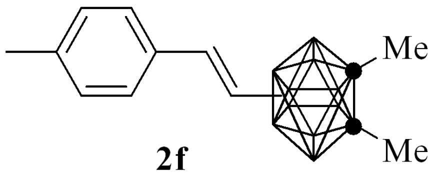
WJ-283-B


Me
Me

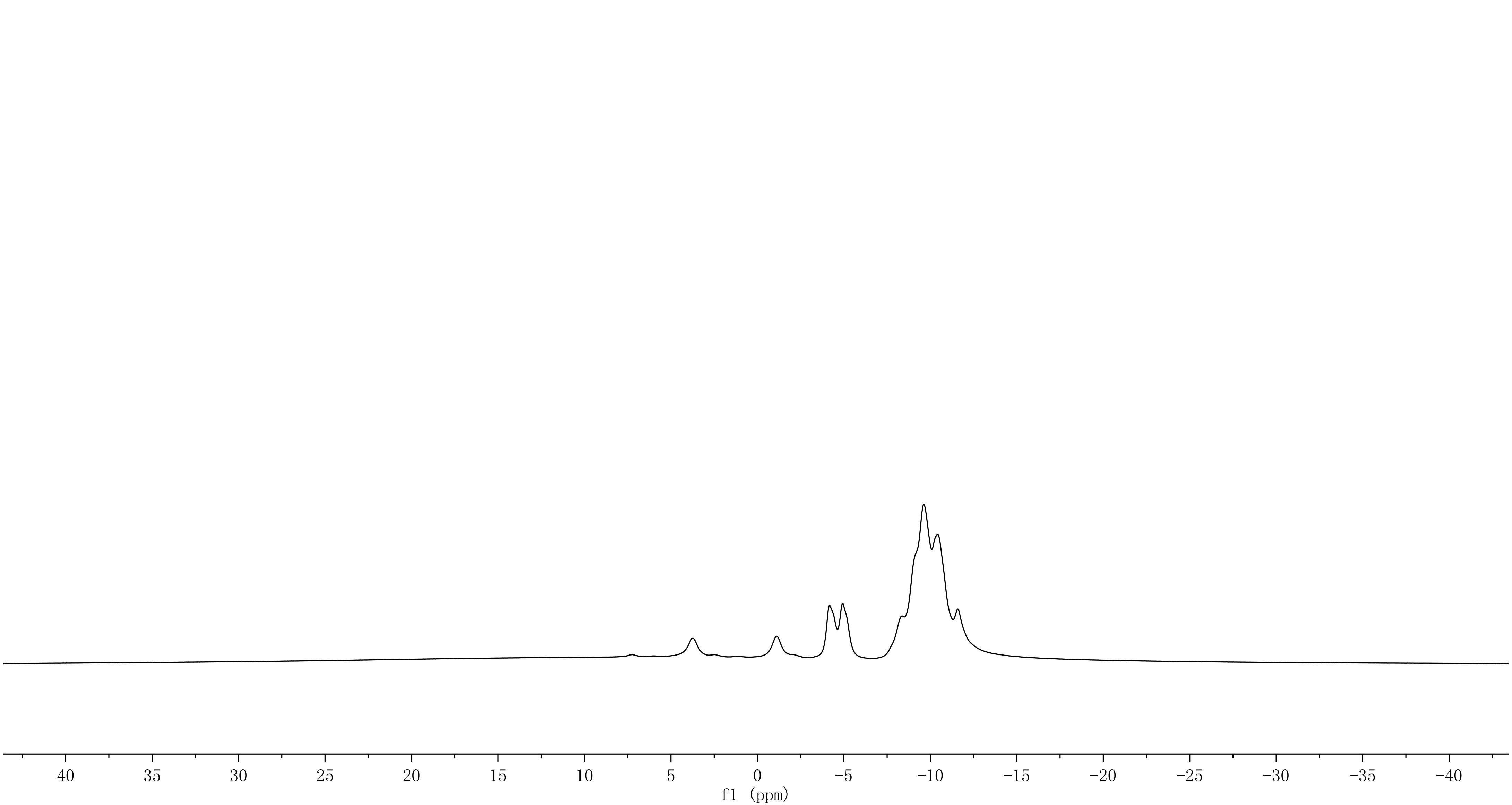
2f

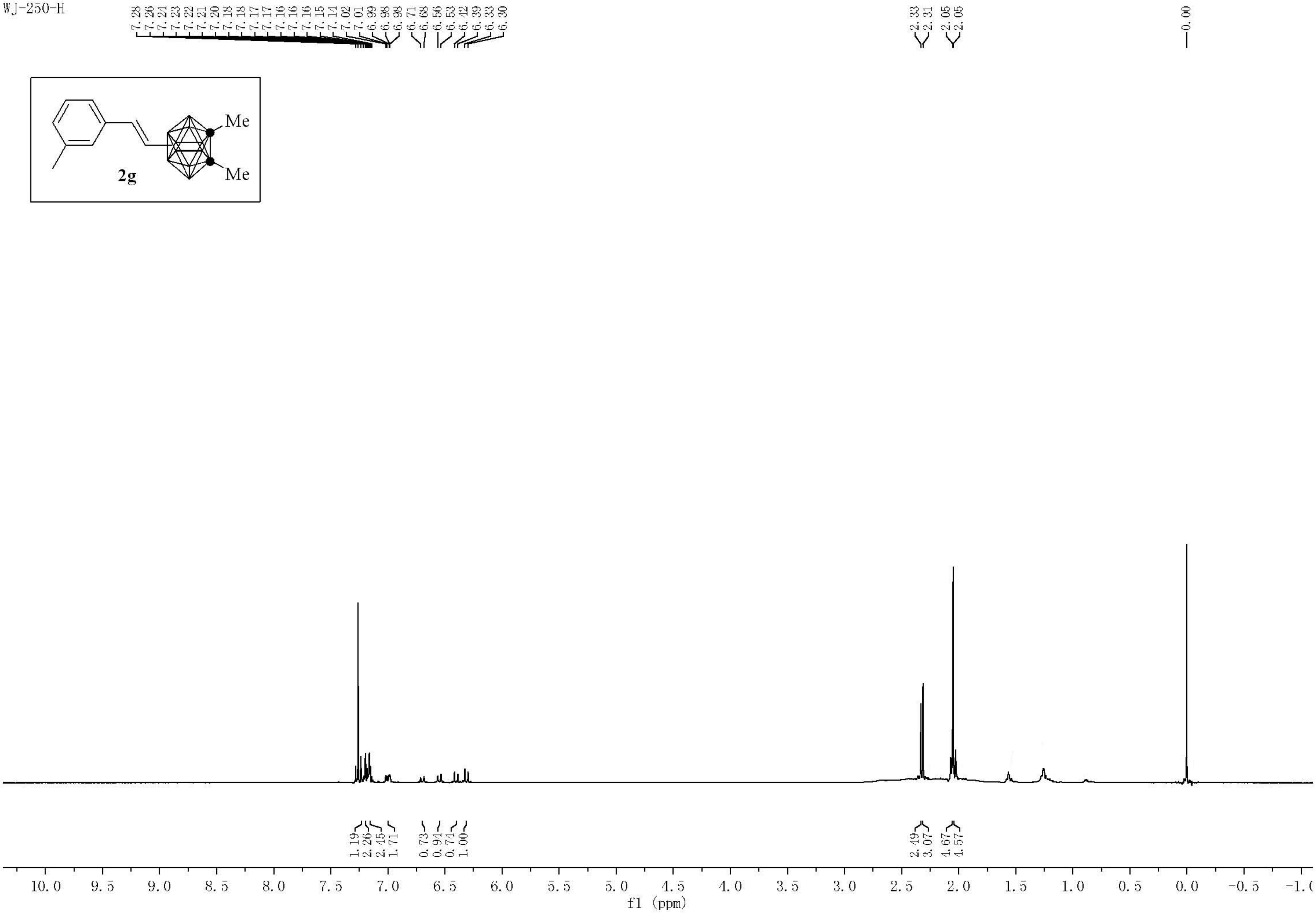

3.79
-1.07
-4.52
-8.76
-9.95
-11.18
1.00
1.02
2.64
2.88
7.82
1.85
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
f1 (ppm)

WJ-283-B-H

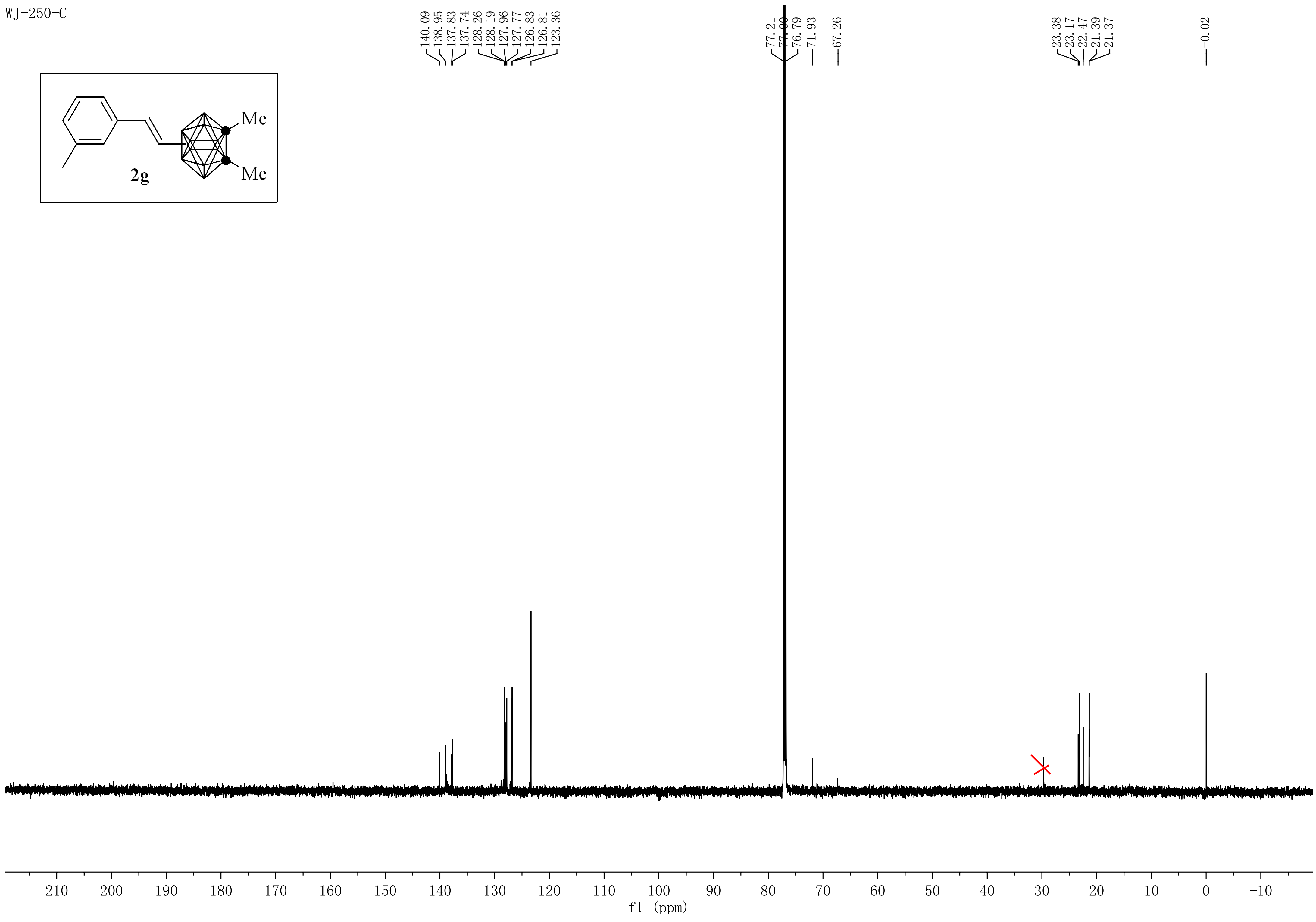

Me
Me

2f

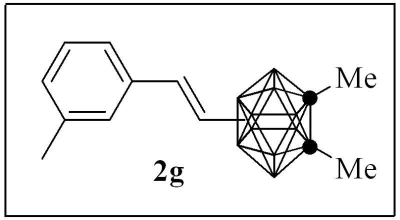

3.74
-1.11
-4.17
-4.93
-8.35
-9.63
-10.43
-11.59
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
f1 (ppm)

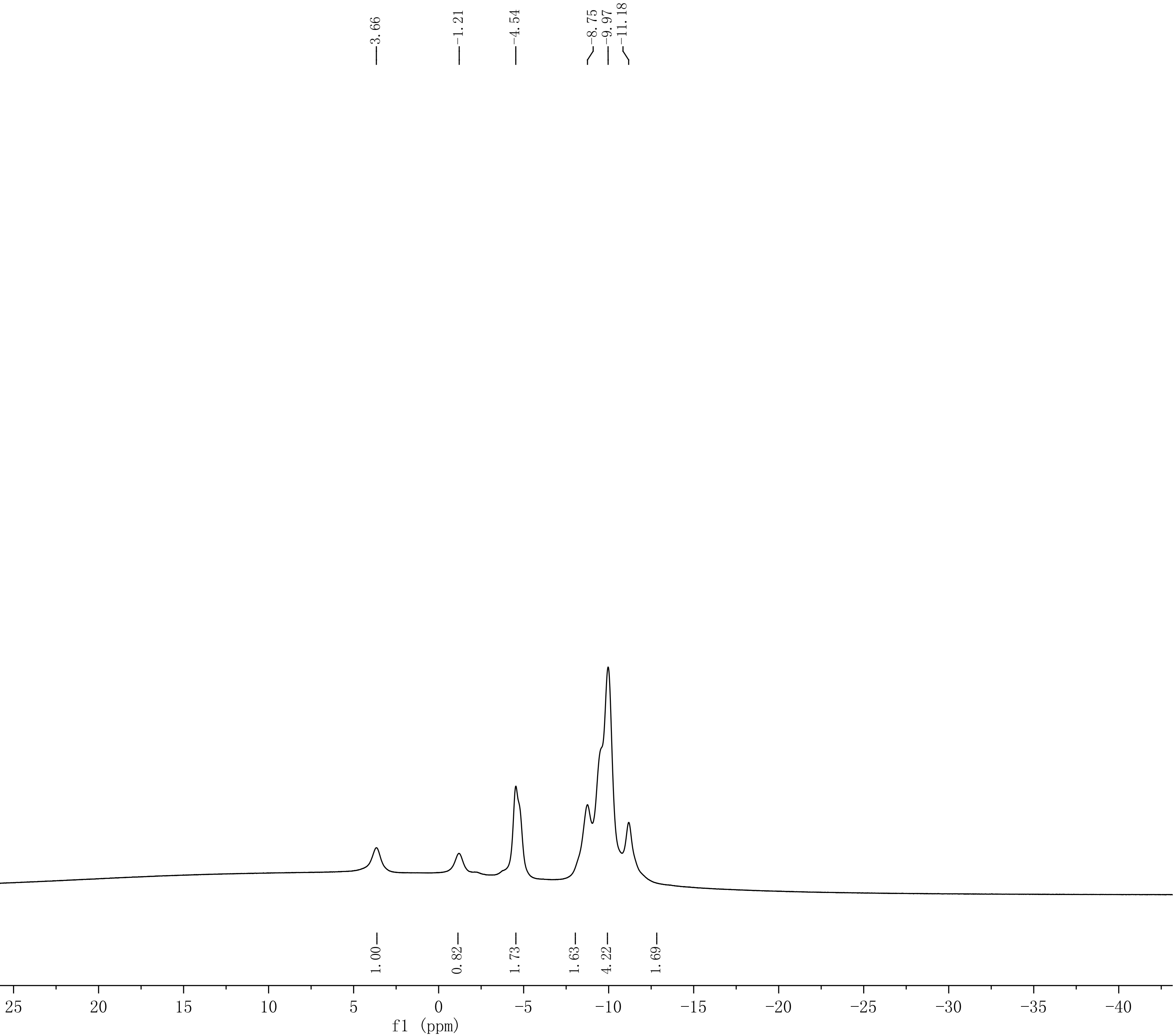


WJ-250-H
7.28 7.26 7.24 7.23 7.22 7.21 7.20 7.18 7.18 7.17 7.17 7.16 7.16 7.16 7.15 7.14 7.02 7.01 6.99 6.98 6.98 6.71 6.68 6.56 6.53 6.42 6.39 6.33 6.30
2.33 2.31 2.05 2.05
0.00
Me
Me
2g
1.19 2.26 2.45 1.71 0.73 0.91 0.74 1.00
2.49 3.07 4.67 4.57
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

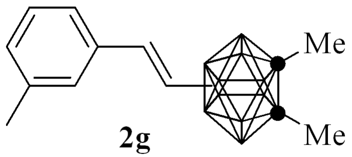

WJ-250-C
140.09
138.95
137.83
137.74
128.26
128.19
127.96
127.77
126.83
126.81
123.36
77.21
77.00
76.79
71.93
67.26
23.38
23.17
22.47
21.39
21.37
-0.02
Me
Me
2g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

WJ-250-B

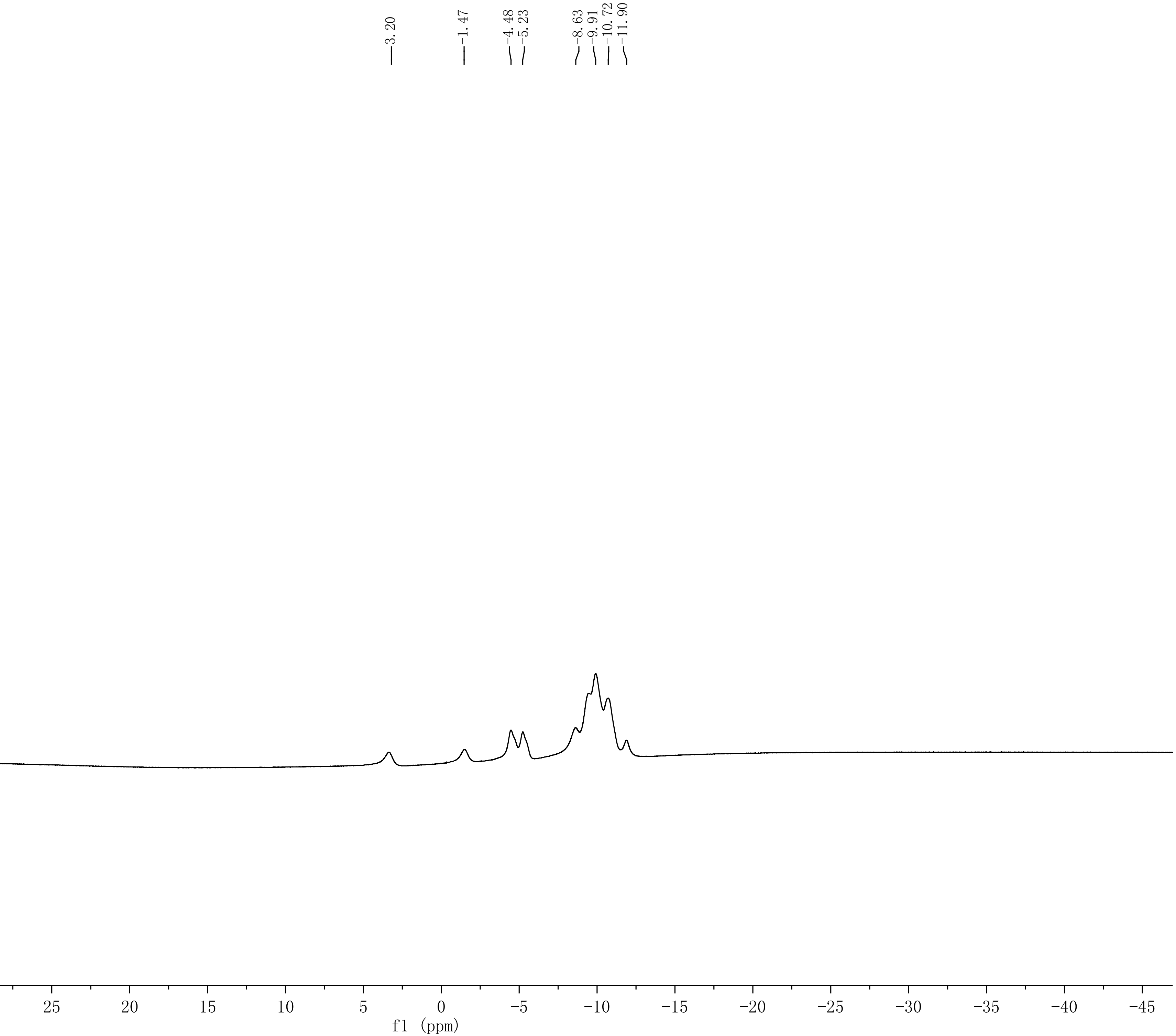

Me
Me
2g


3.66
-1.21
-4.54
-8.75
-9.97
-11.18
1.00
0.82
1.73
1.63
4.22
1.69
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
f1 (ppm)

WJ-250-B-H

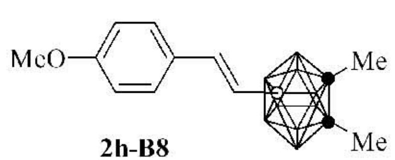


2g

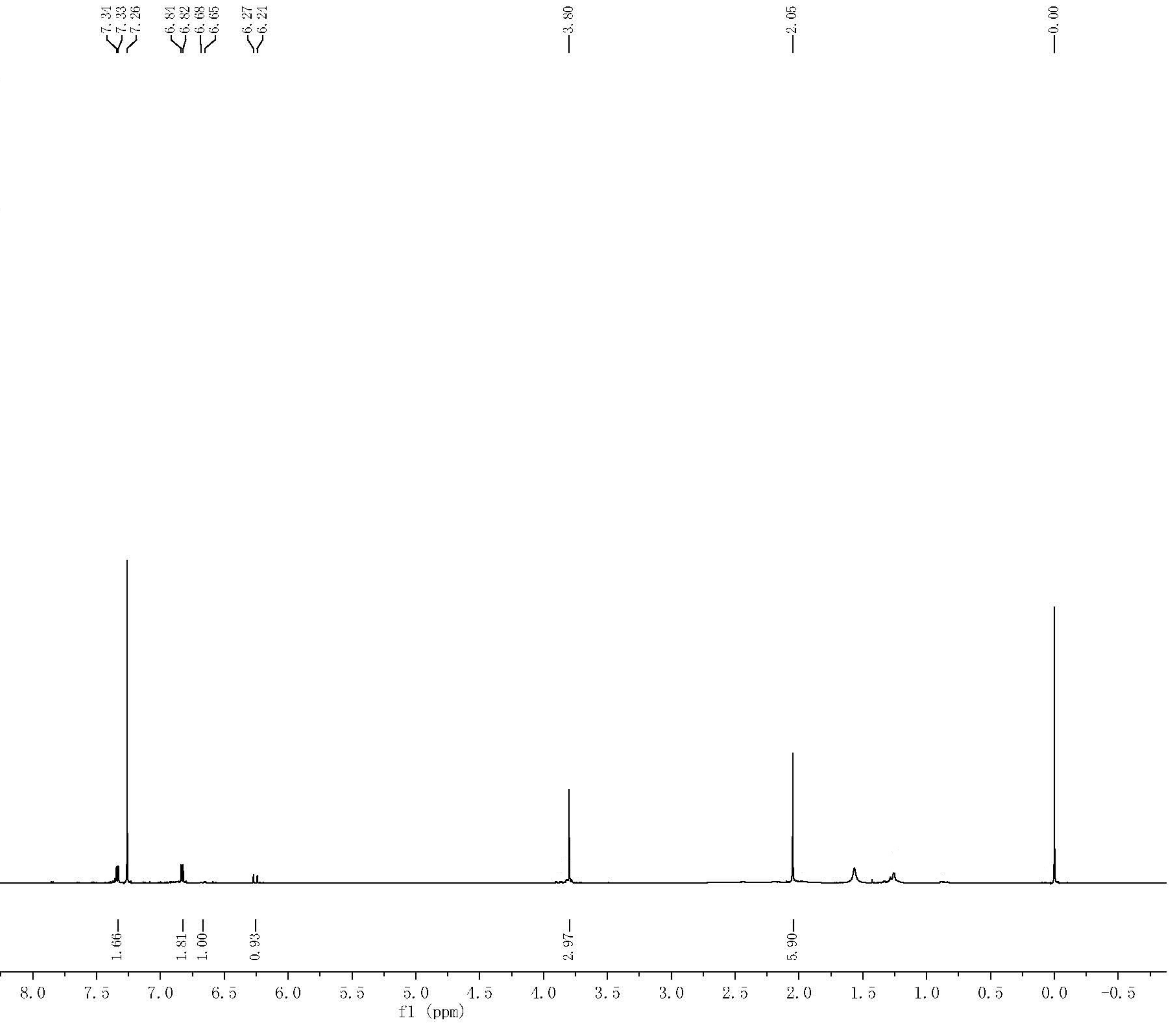


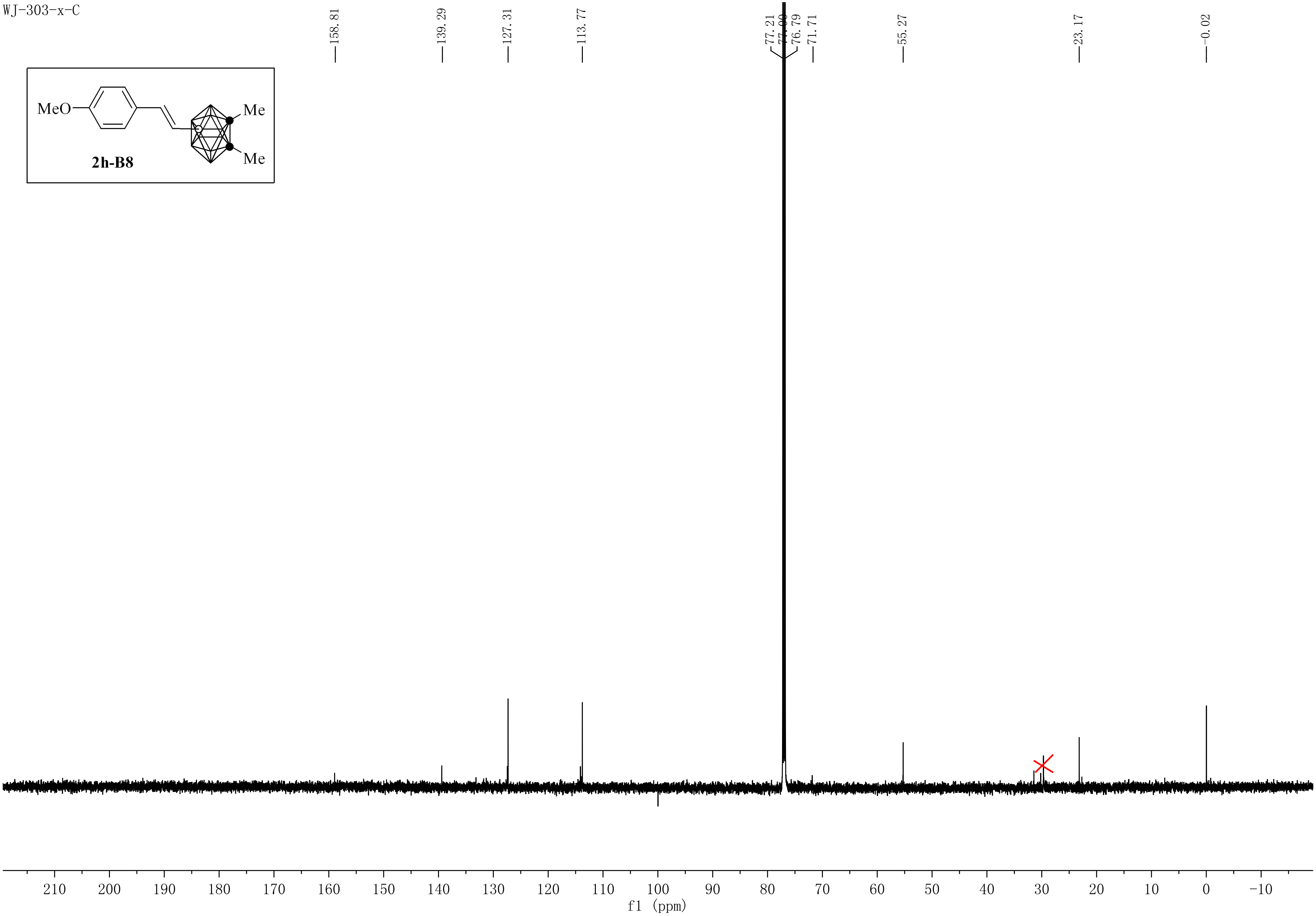
3.20
-1.47
-4.48
-5.23
-8.63
-9.91
-10.72
-11.90
45
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
−45
f1 (ppm)

WJ-303-x-H

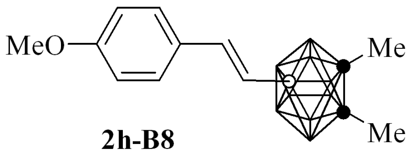


2h-B8

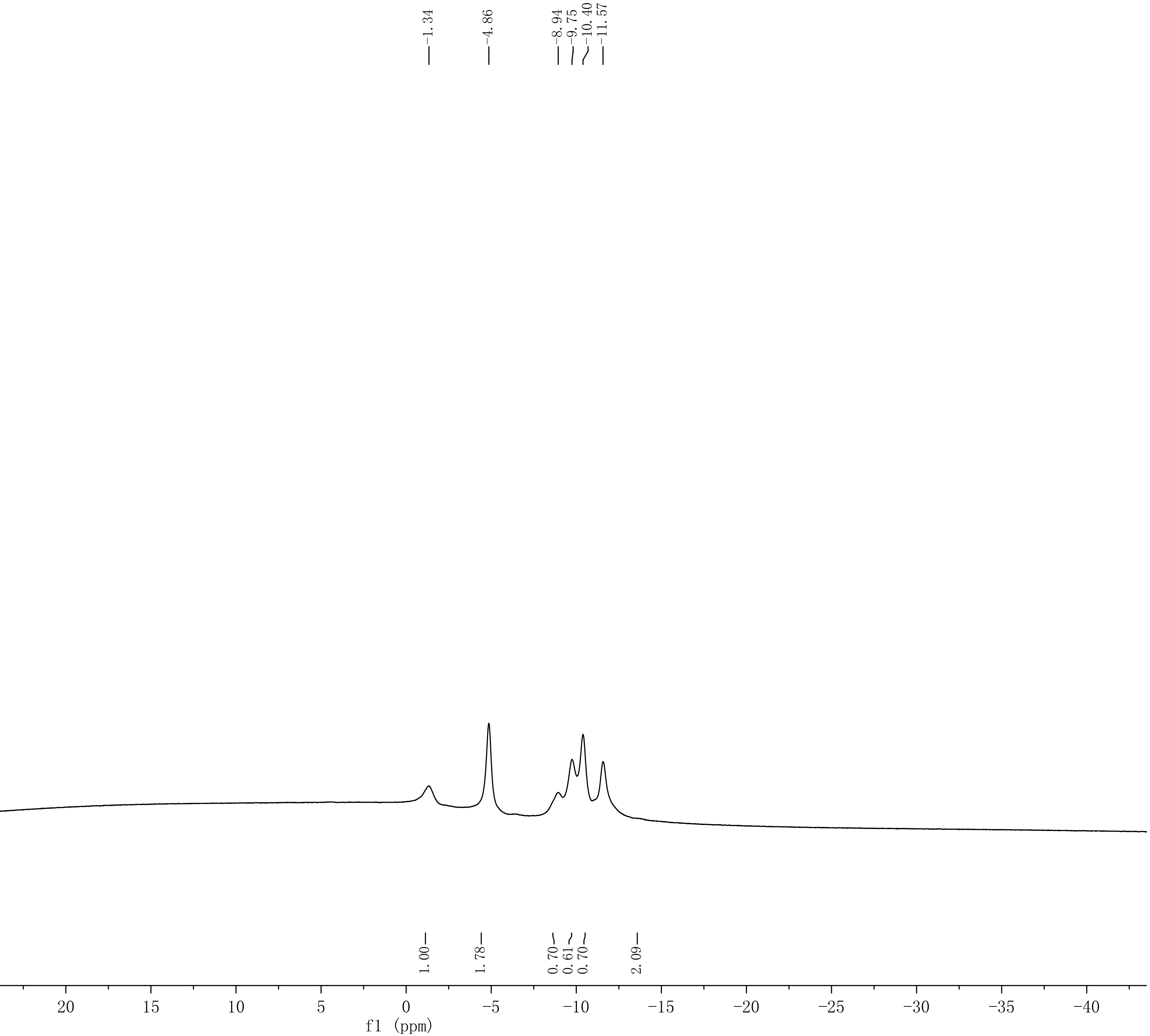



WJ-303-x-C
158.81
139.29
127.31
113.77
77.21
77.00
76.79
71.71
55.27
23.17
-0.02
MeO
Me
Me
2h-B8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

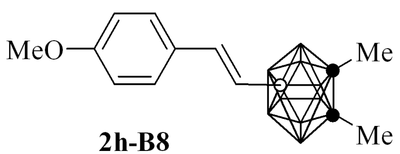
WJ-303-x-B



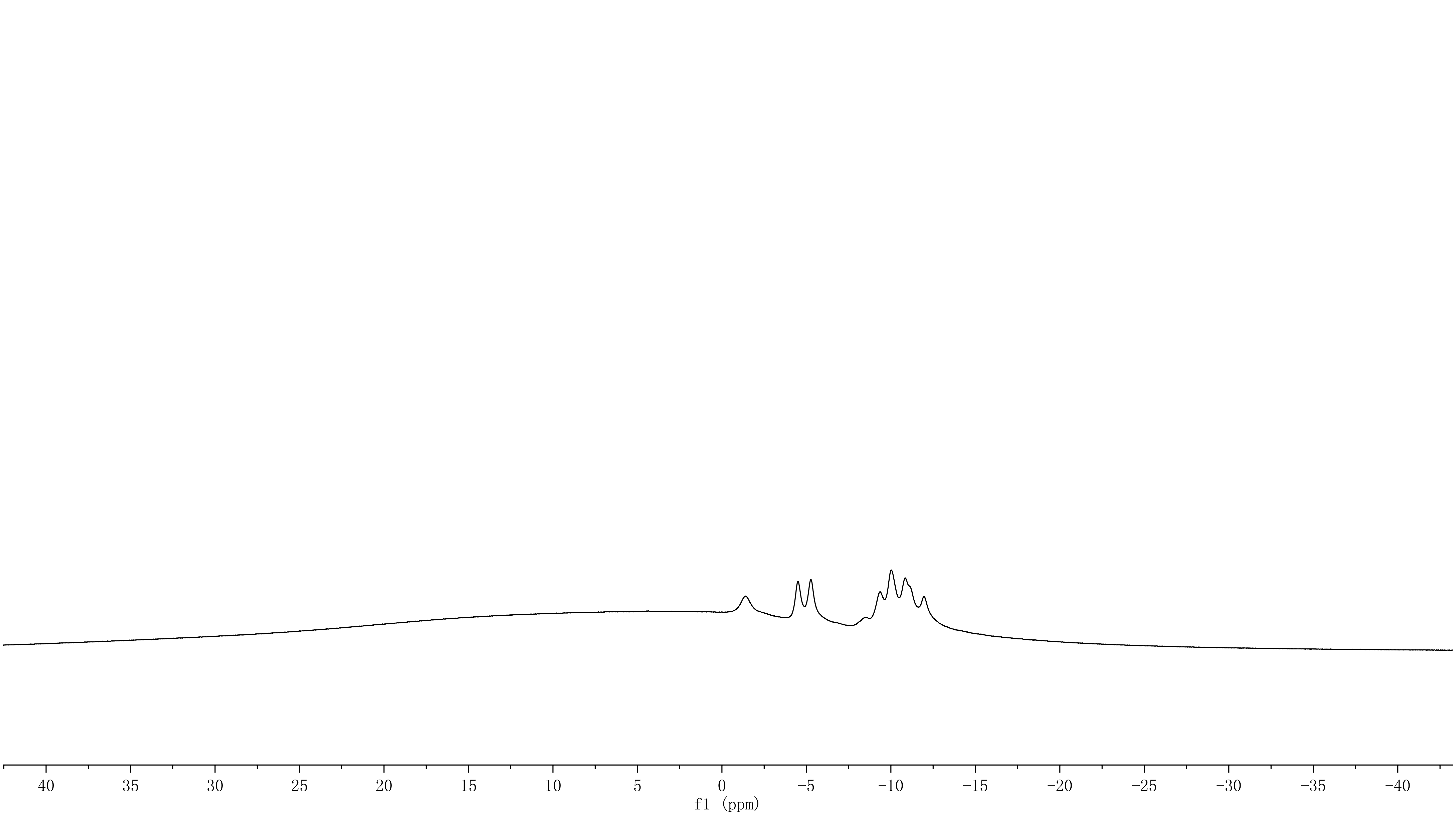
2h-B8



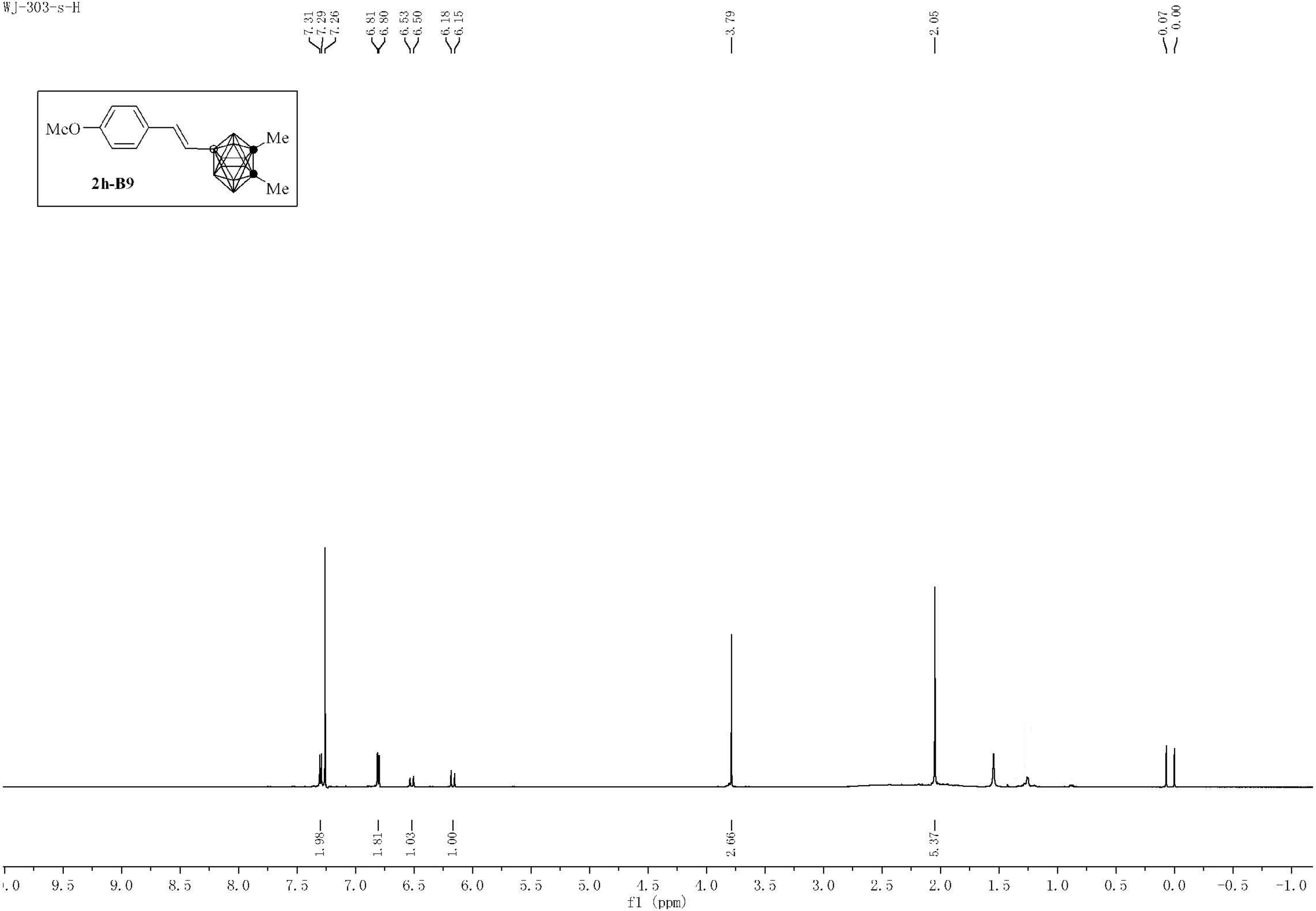
WJ-303-x-B-H

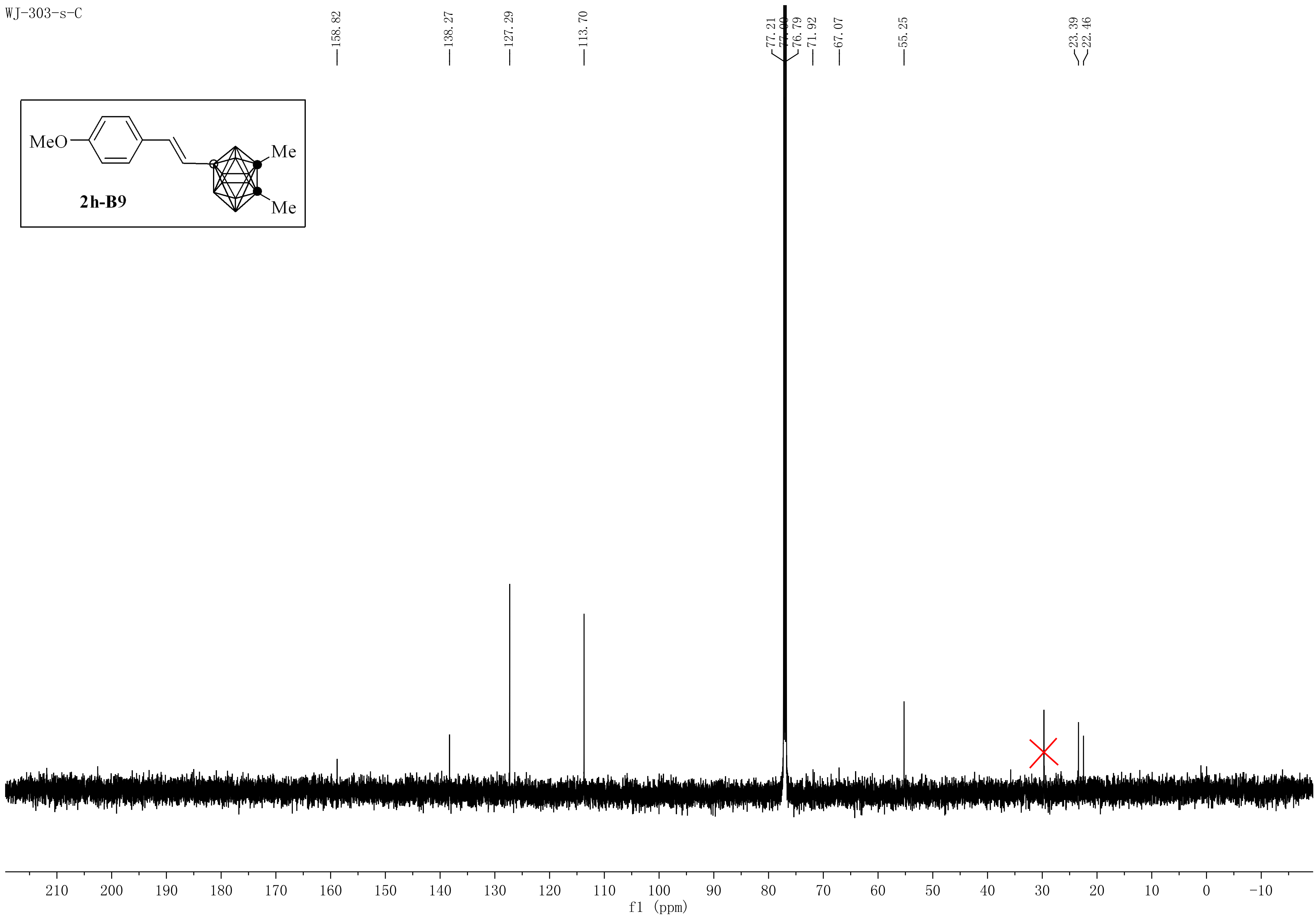


2h-B8

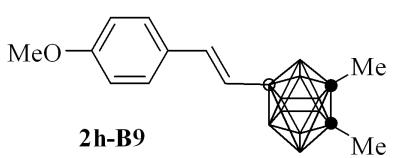


WJ-303-s-H

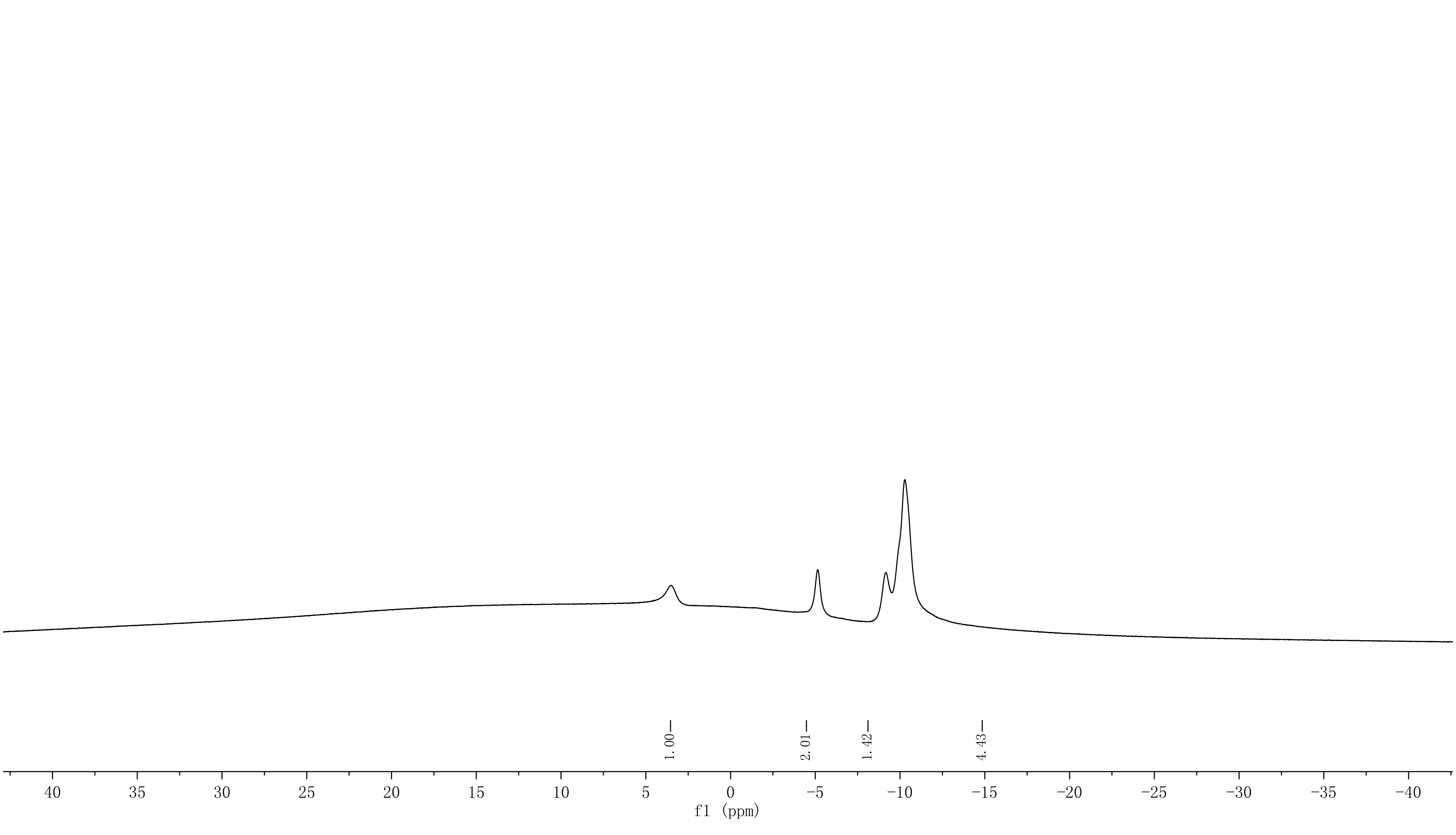

7.31
7.29
7.26
6.81
6.80
6.53
6.50
6.18
6.15
3.79
2.05
0.07
0.00
MeO
Me
Me
2h-B9
1.98
1.81
1.03
1.00
2.66
5.37
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


WJ-303-s-C
158.82
138.27
127.29
113.70
77.21
77.00
76.79
71.92
67.07
55.25
23.39
22.46
MeO
Me
Me
2h-B9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

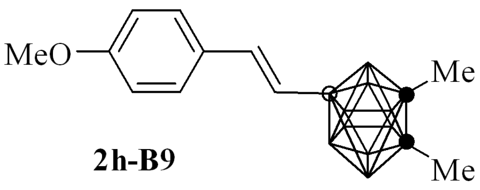
WJ-303-s-B



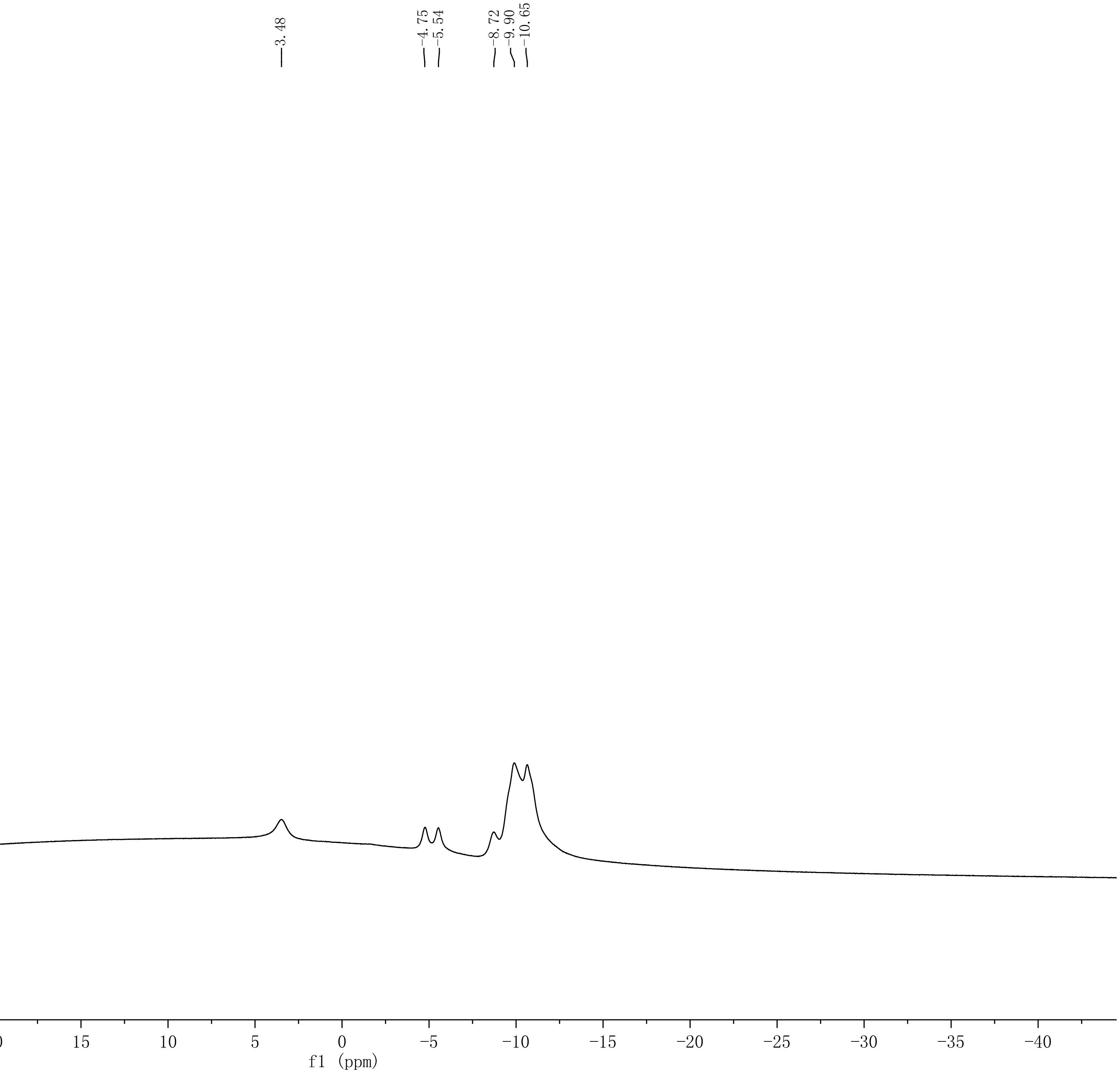
2h-B9

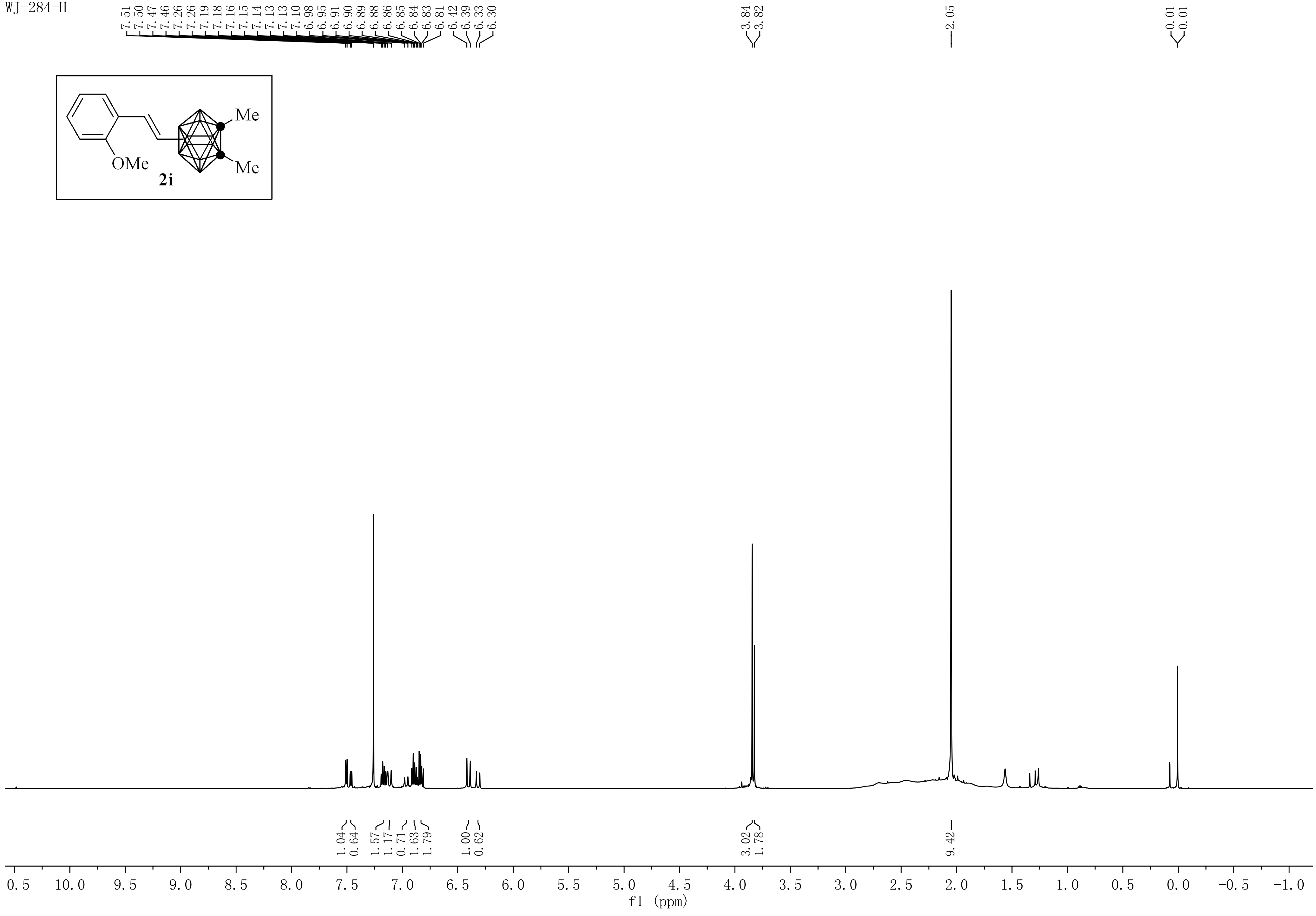


WJ-303-s-B-H

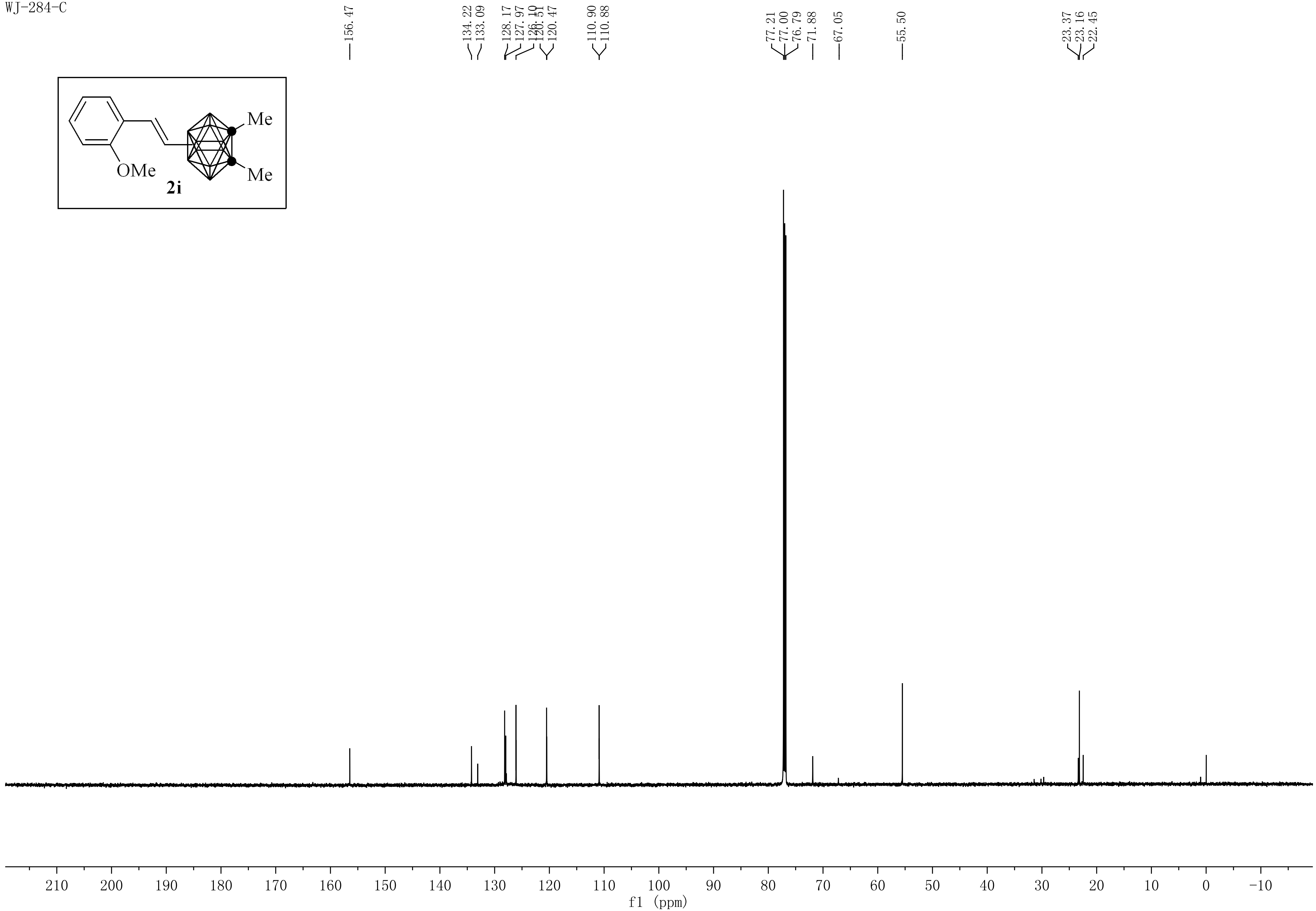


2h-B9

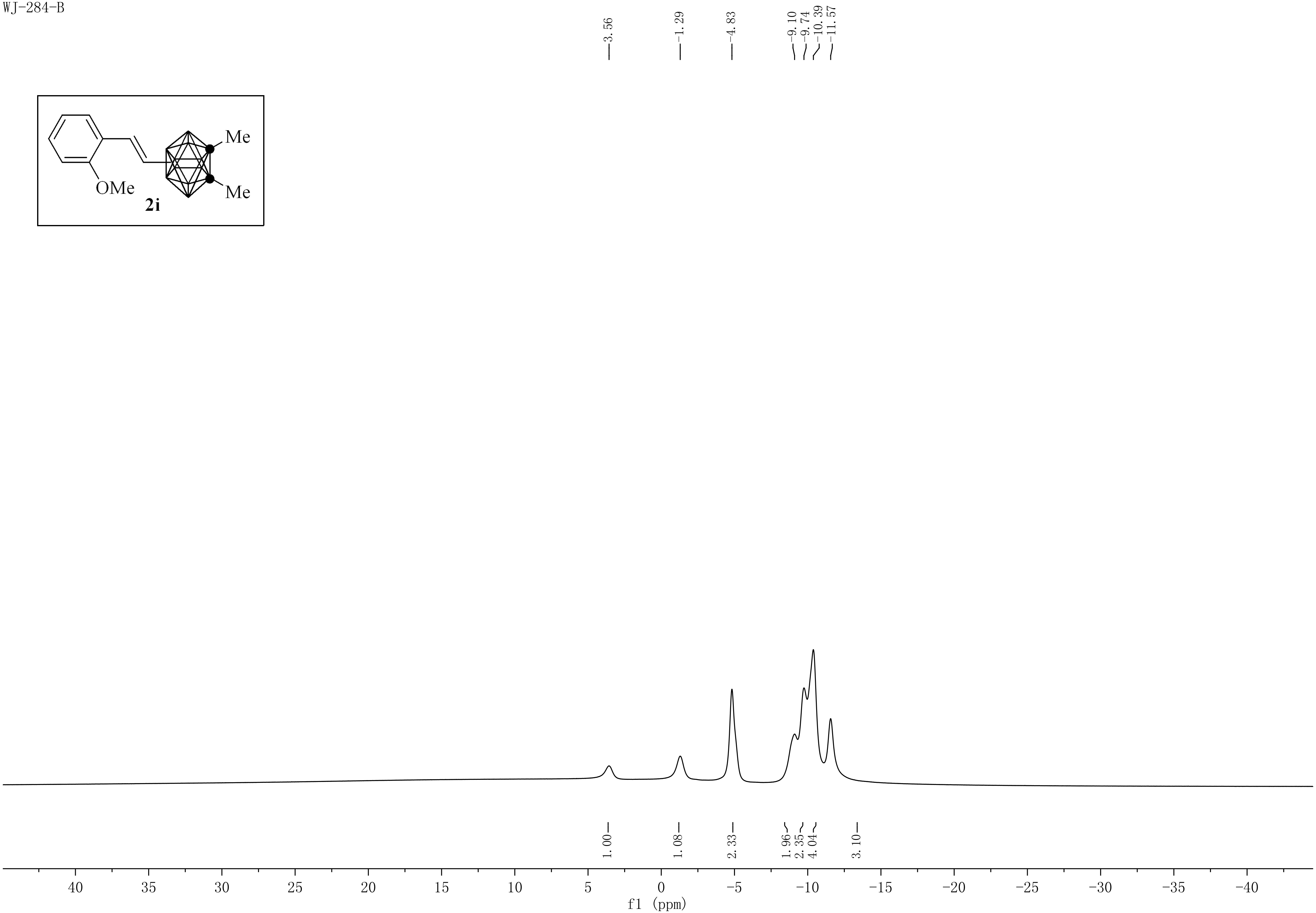




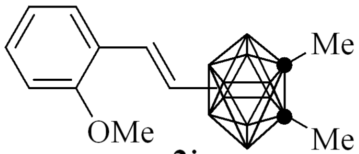
WJ-284-H
7.51
7.50
7.47
7.46
7.26
7.26
7.19
7.18
7.16
7.15
7.14
7.13
7.13
7.10
6.98
6.95
6.91
6.90
6.89
6.88
6.86
6.85
6.84
6.83
6.81
6.42
6.39
6.33
6.30
3.84
3.82
2.05
0.01
0.01
Me
Me
OMe
2i
1.04
0.64
1.57
1.17
0.71
1.63
1.79
1.00
0.62
3.02
1.78
9.42
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


WJ-284-C
156.47
134.22
133.09
128.17
127.97
126.10
120.51
120.47
110.90
110.88
77.21
77.00
76.79
71.88
67.05
55.50
23.37
23.16
22.45
Me
OMe
Me
2i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

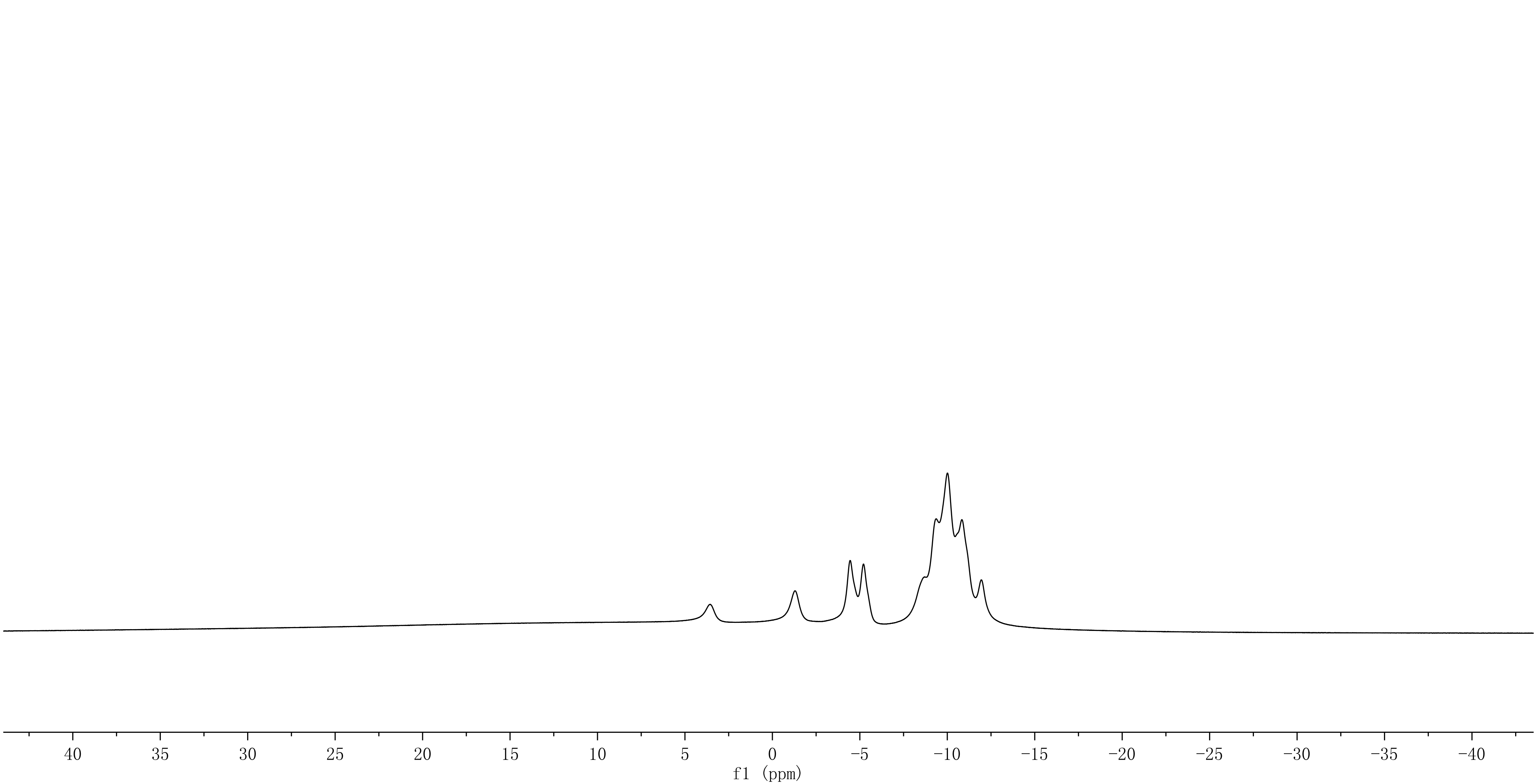
WJ-284-B


3.56
-1.29
-4.83
-9.10
-9.74
-10.39
-11.57
Me
Me
OMe
2i
1.00
1.08
2.33
1.96
2.35
4.04
3.10
40 35 30 25 20 15 10 5 0 −5 −10 −15 −20 −25 −30 −35 −40
f1 (ppm)

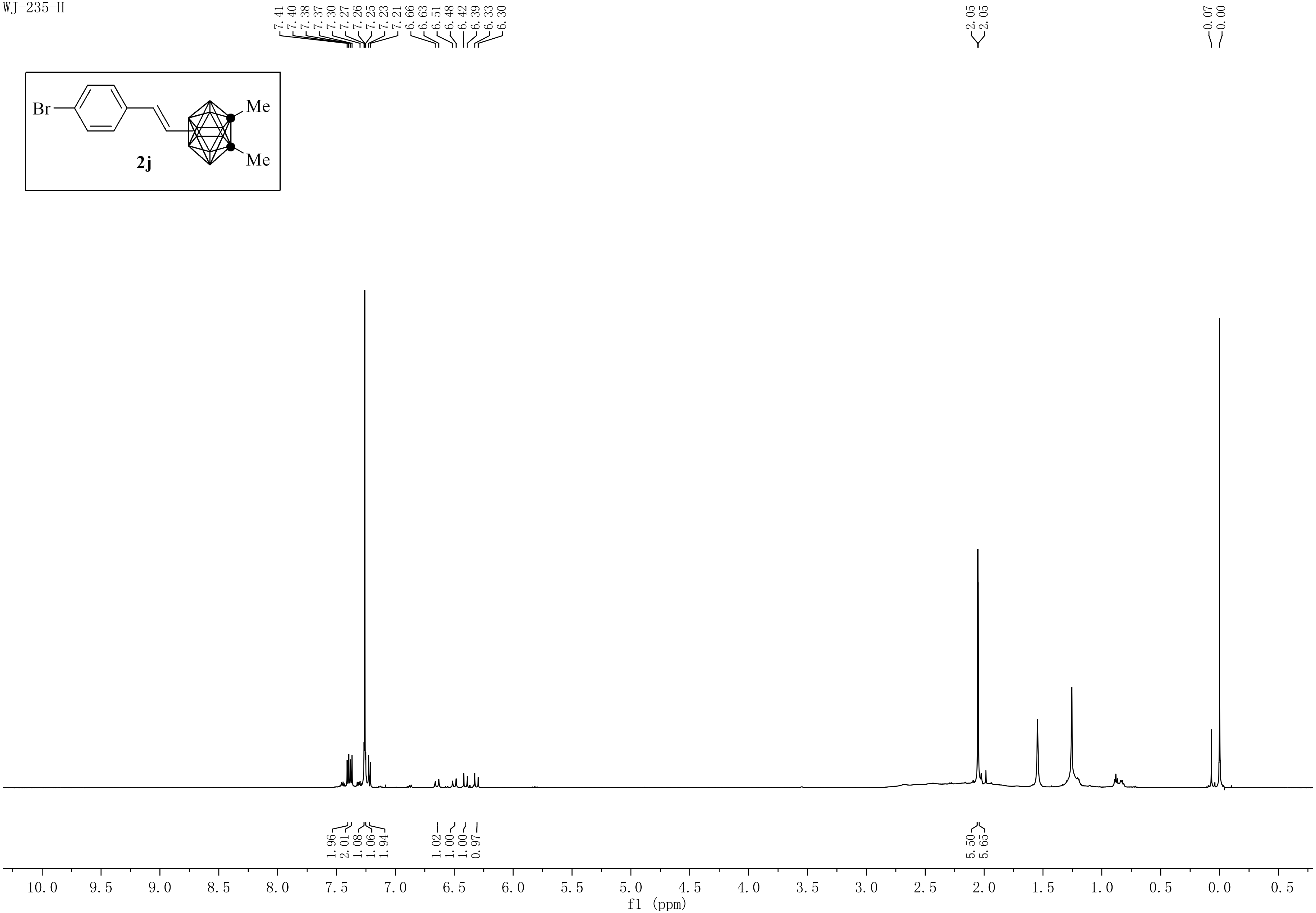
WJ-284-B-H



2i

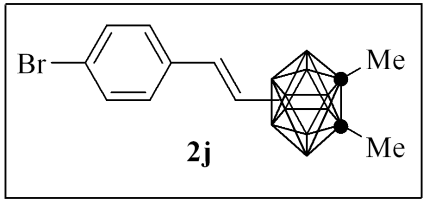

3.58
-1.28
-4.45
-5.21
-9.37
-10.01
-10.84
-11.94
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
f1 (ppm)

WJ-235-H

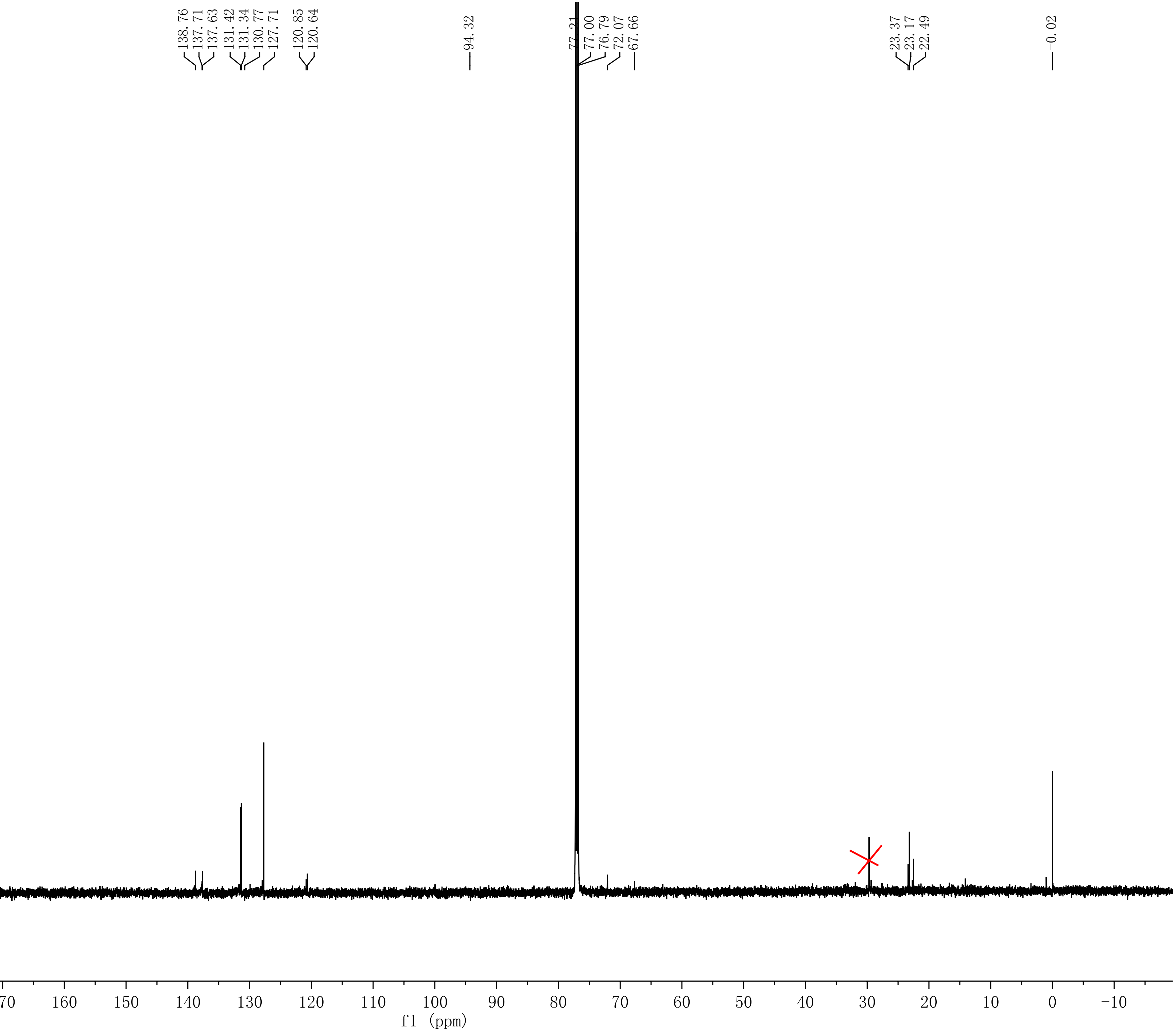


7.41
7.40
7.38
7.37
7.30
7.27
7.26
7.25
7.23
7.21
6.66
6.63
6.51
6.48
6.42
6.39
6.33
6.30
2.05
2.05
0.07
0.00
Br
Me
Me
2j
1.96
2.01
1.08
1.06
1.94
1.02
1.00
1.00
0.97
5.50
5.65
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

WJ-235-C

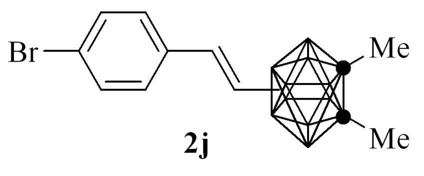


Br
Me
Me
2j



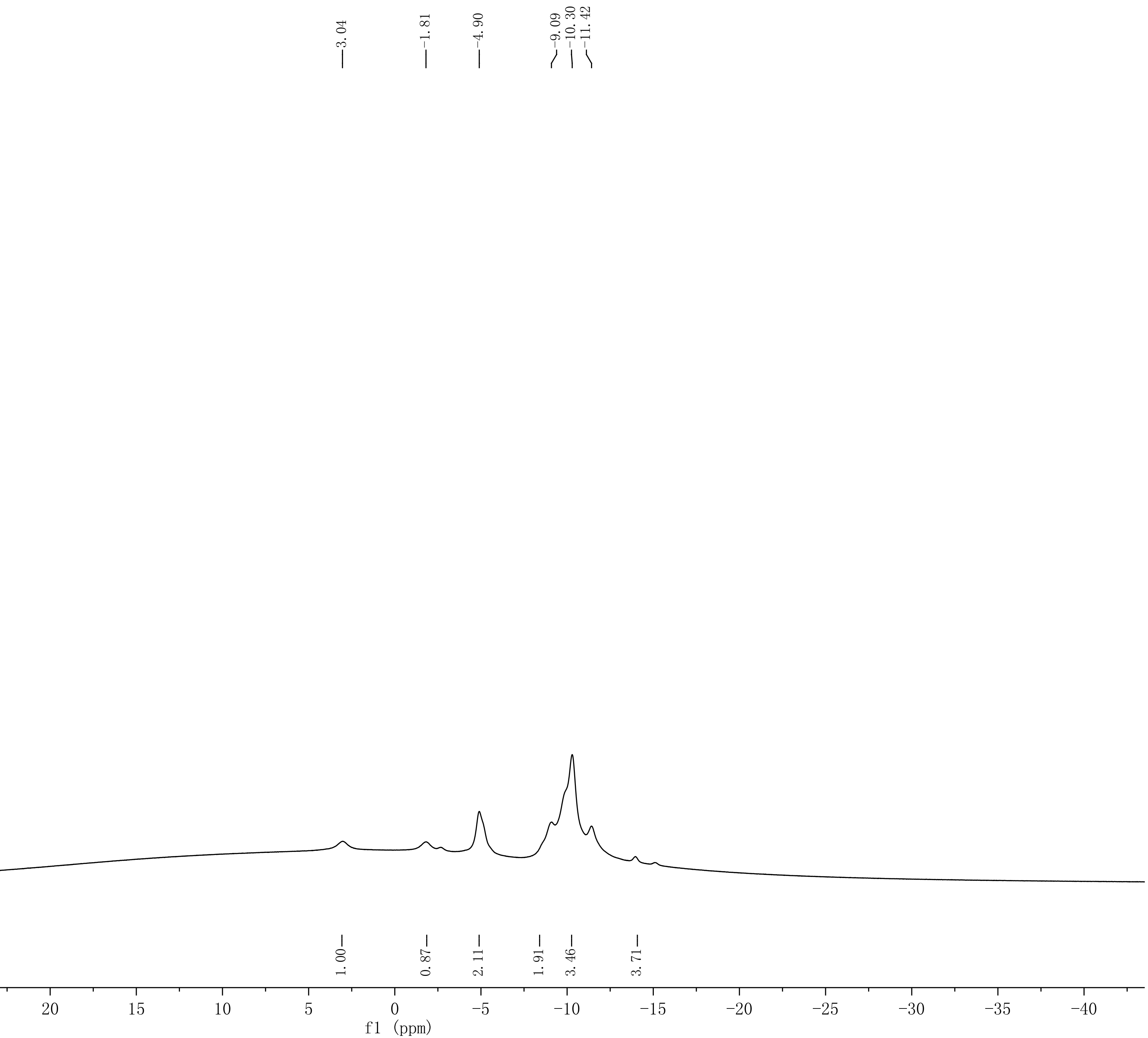
138.76
137.71
137.63
131.42
131.34
130.77
127.71
120.85
120.64
94.32
77.21
77.00
76.79
72.07
67.66
23.37
23.17
22.49
-0.02
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

WJ-235-B



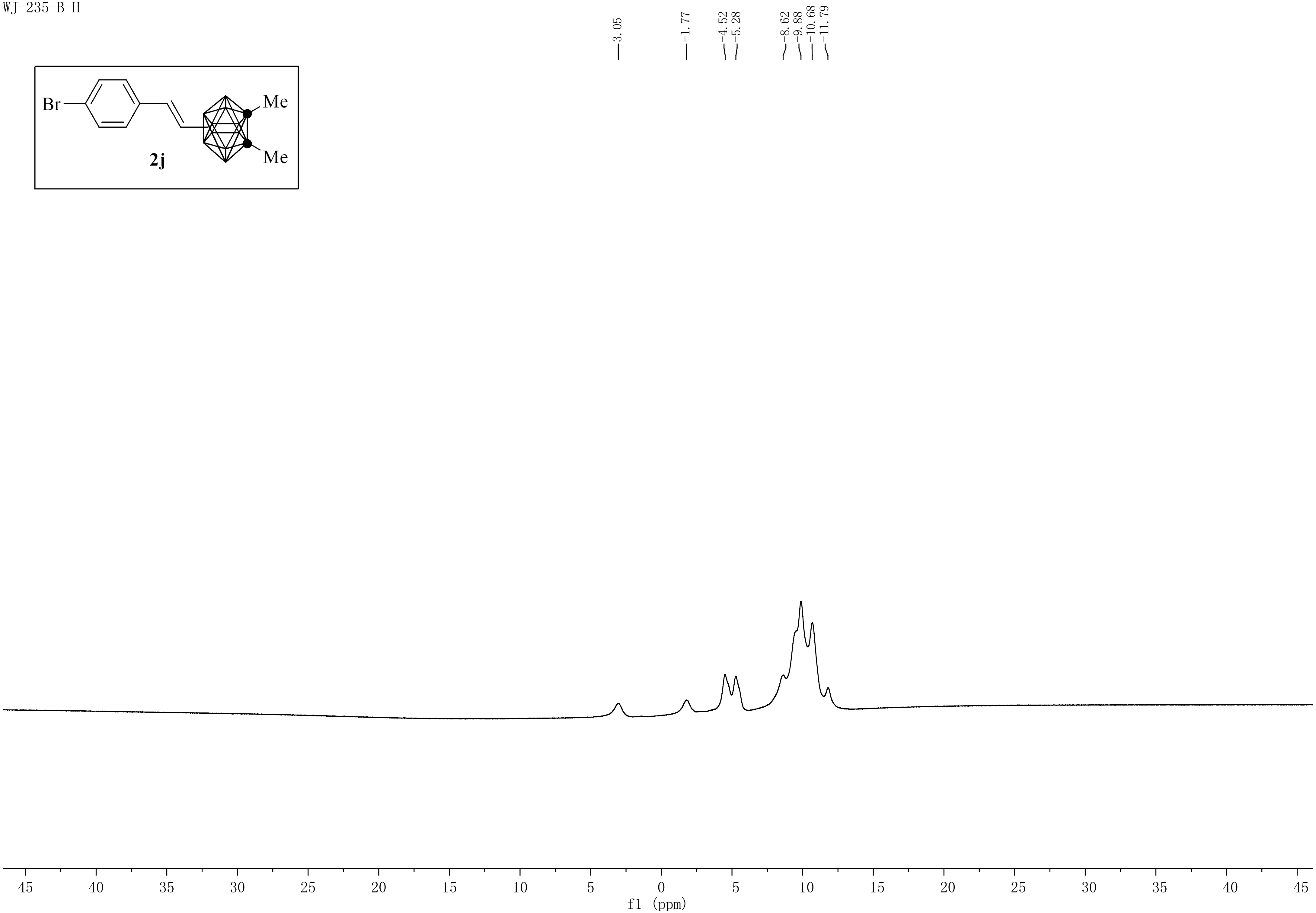
Br
Me
Me

2j

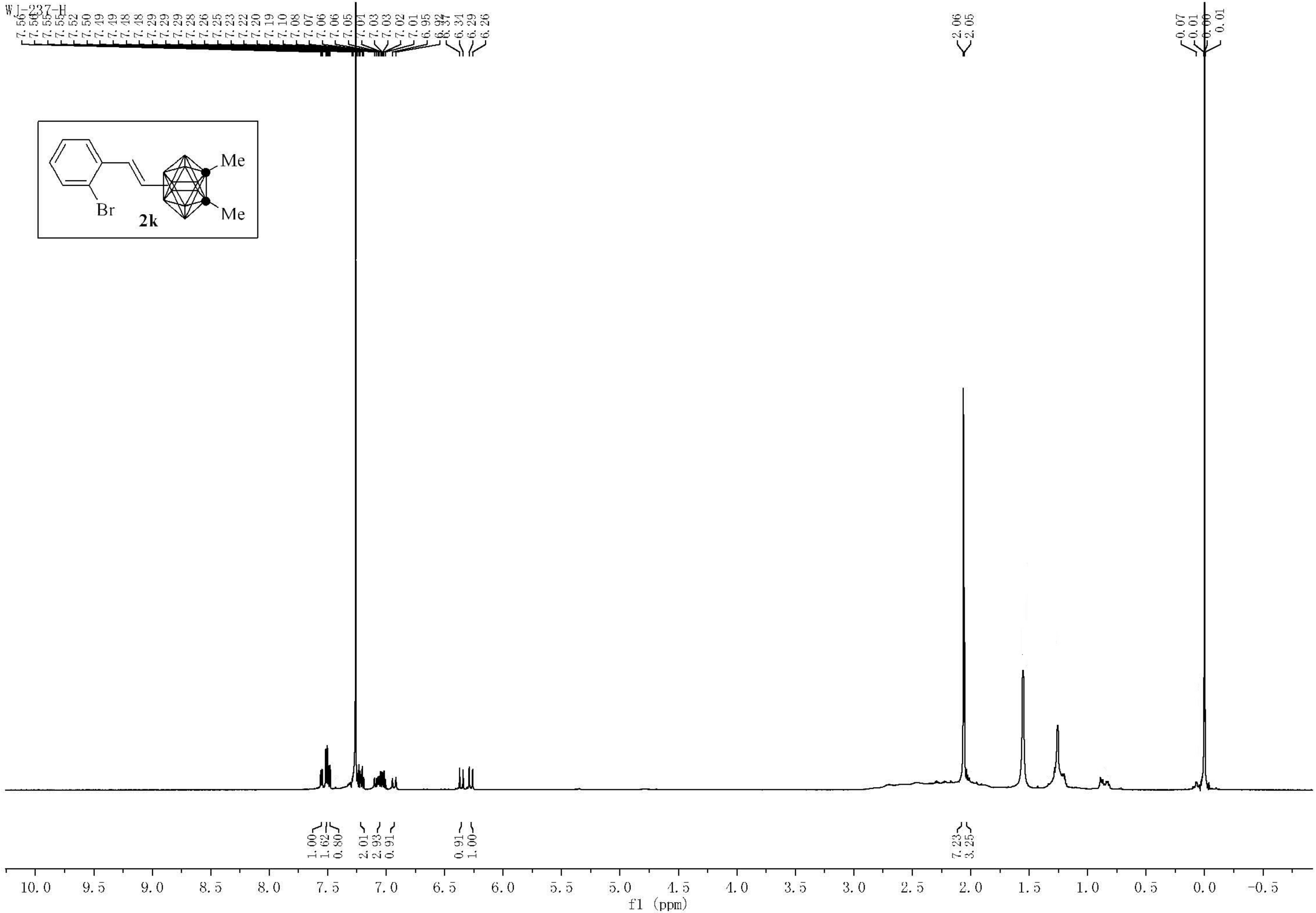


3.04
-1.81
-4.90
-9.09
-10.30
-11.42
1.00
0.87
2.11
1.91
3.46
3.71
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
f1 (ppm)

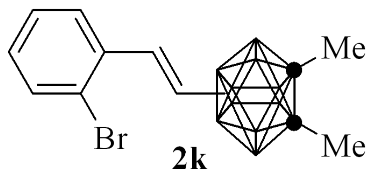
WJ-235-B-H



Br
Me
Me
2j
3.05
-1.77
-4.52
-5.28
-8.62
-9.88
-10.68
-11.79
45 40 35 30 25 20 15 10 5 0 −5 −10 −15 −20 −25 −30 −35 −40 −45
f1 (ppm)

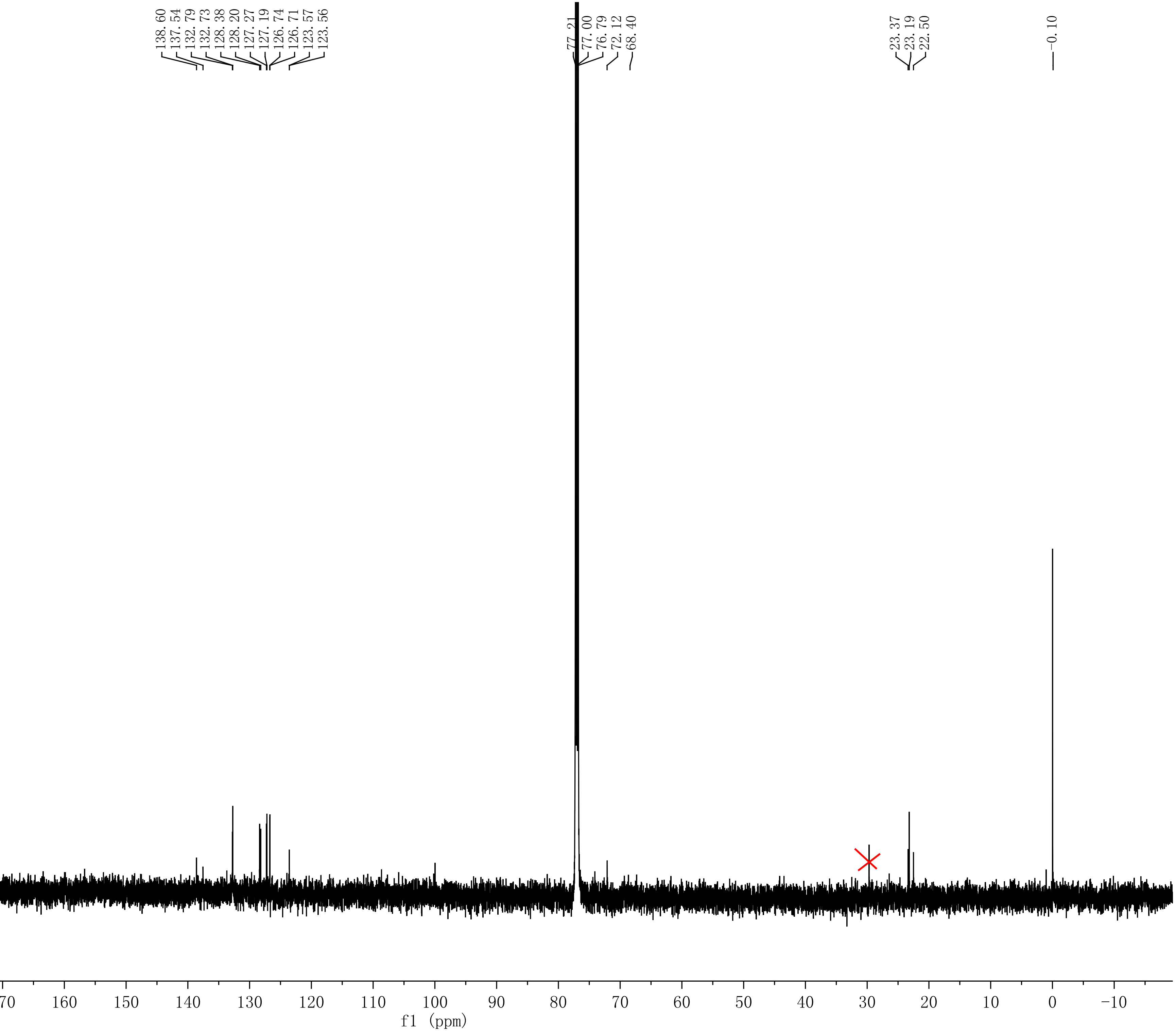

WJ-237-H
7.56
7.56
7.55
7.55
7.52
7.50
7.49
7.49
7.48
7.48
7.29
7.29
7.29
7.28
7.26
7.25
7.23
7.22
7.20
7.19
7.10
7.08
7.07
7.06
7.06
7.05
7.04
7.03
7.03
7.02
7.01
6.95
6.92
6.37
6.34
6.29
6.26
2.06
2.05
0.07
0.01
0.00
0.01
Me
Me
Br
2k
1.00
1.62
0.80
2.01
2.93
0.91
0.91
1.00
7.23
3.25
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

WJ-237-C



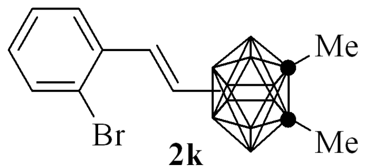
Me
Br
Me

2k

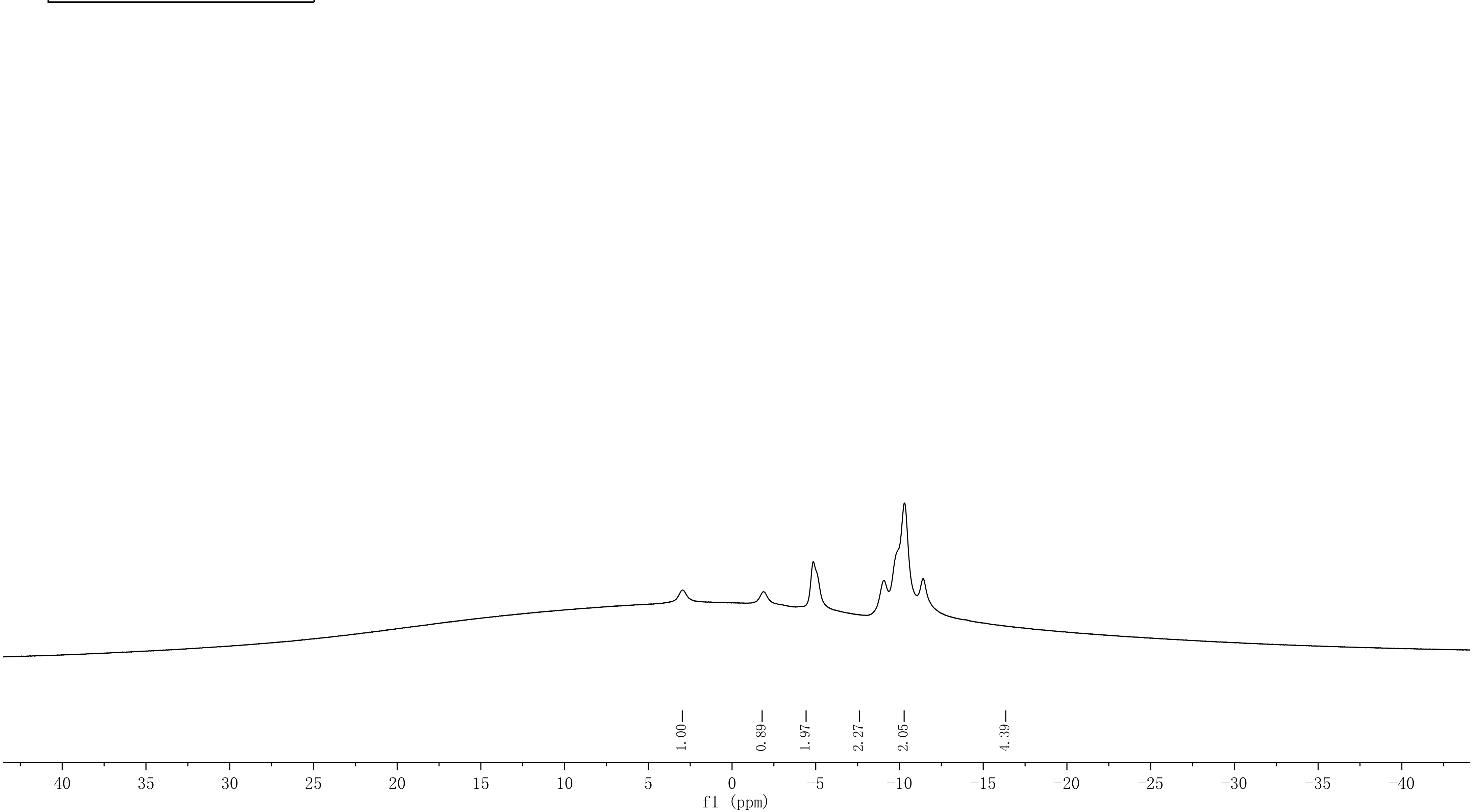


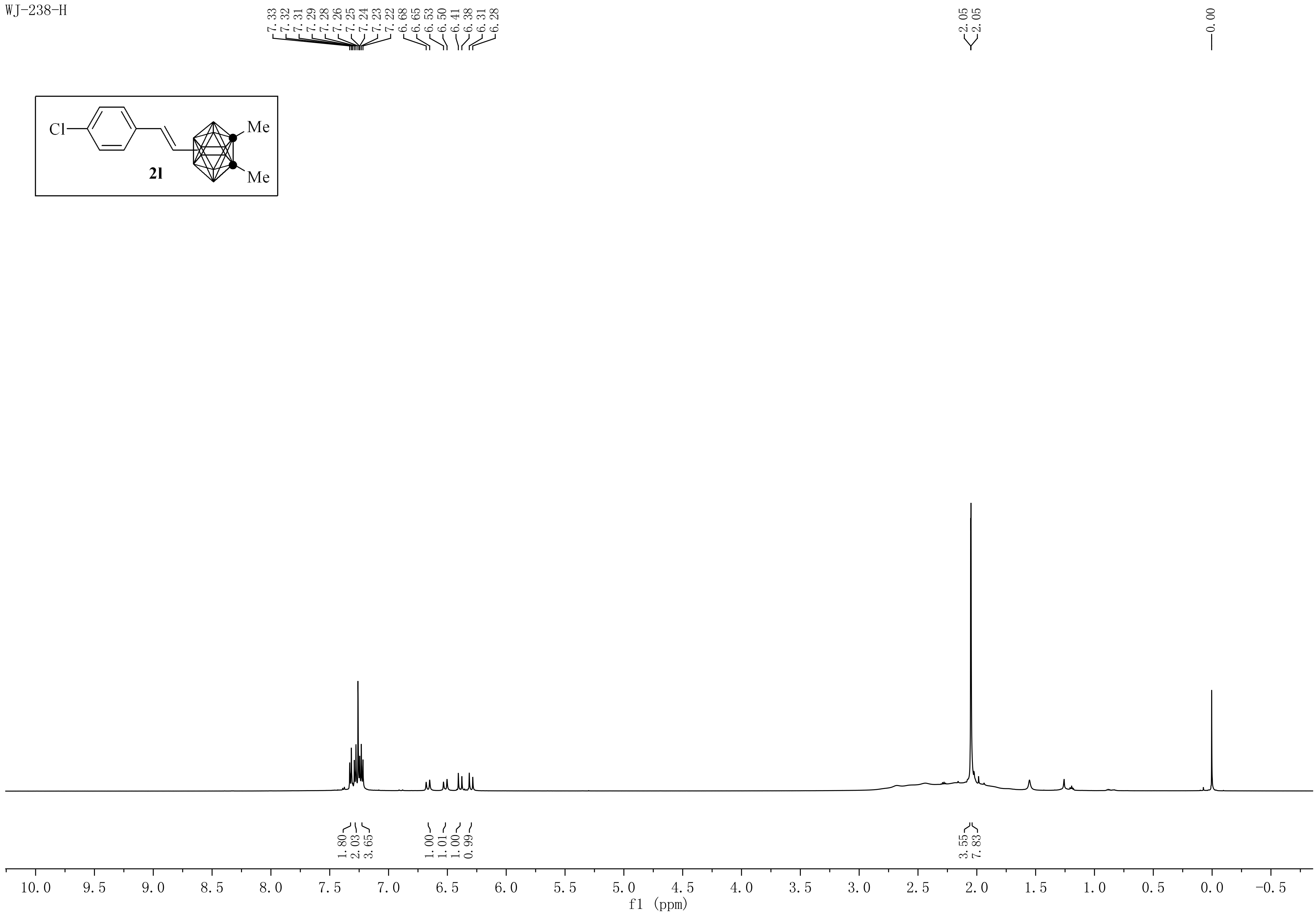
138.60
137.54
132.79
132.73
128.38
128.20
127.27
127.19
126.74
126.71
123.57
123.56
77.21
77.00
76.79
72.12
68.40
23.37
23.19
22.50
-0.10
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

WJ-237-B

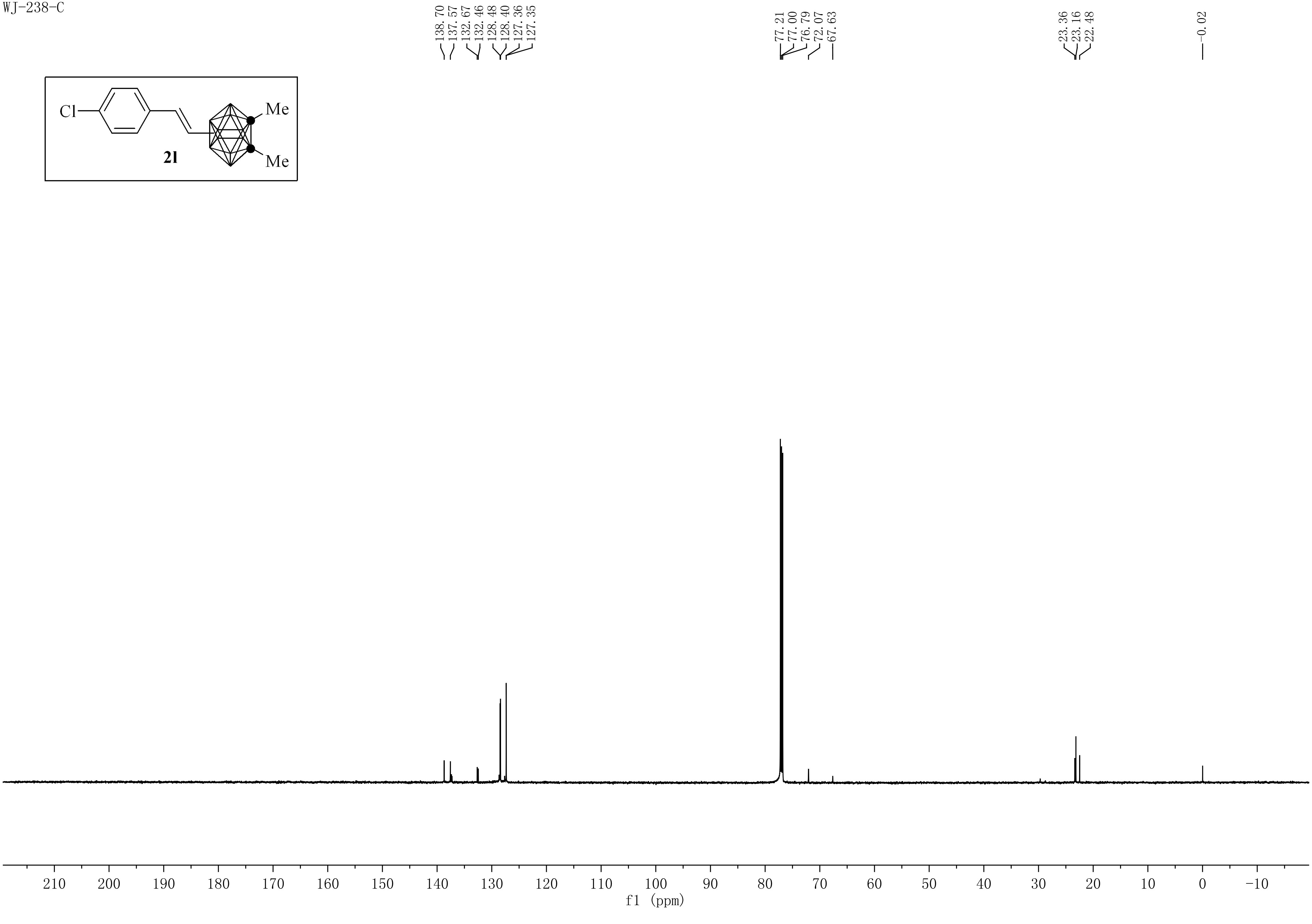

Me
Br
Me

2k

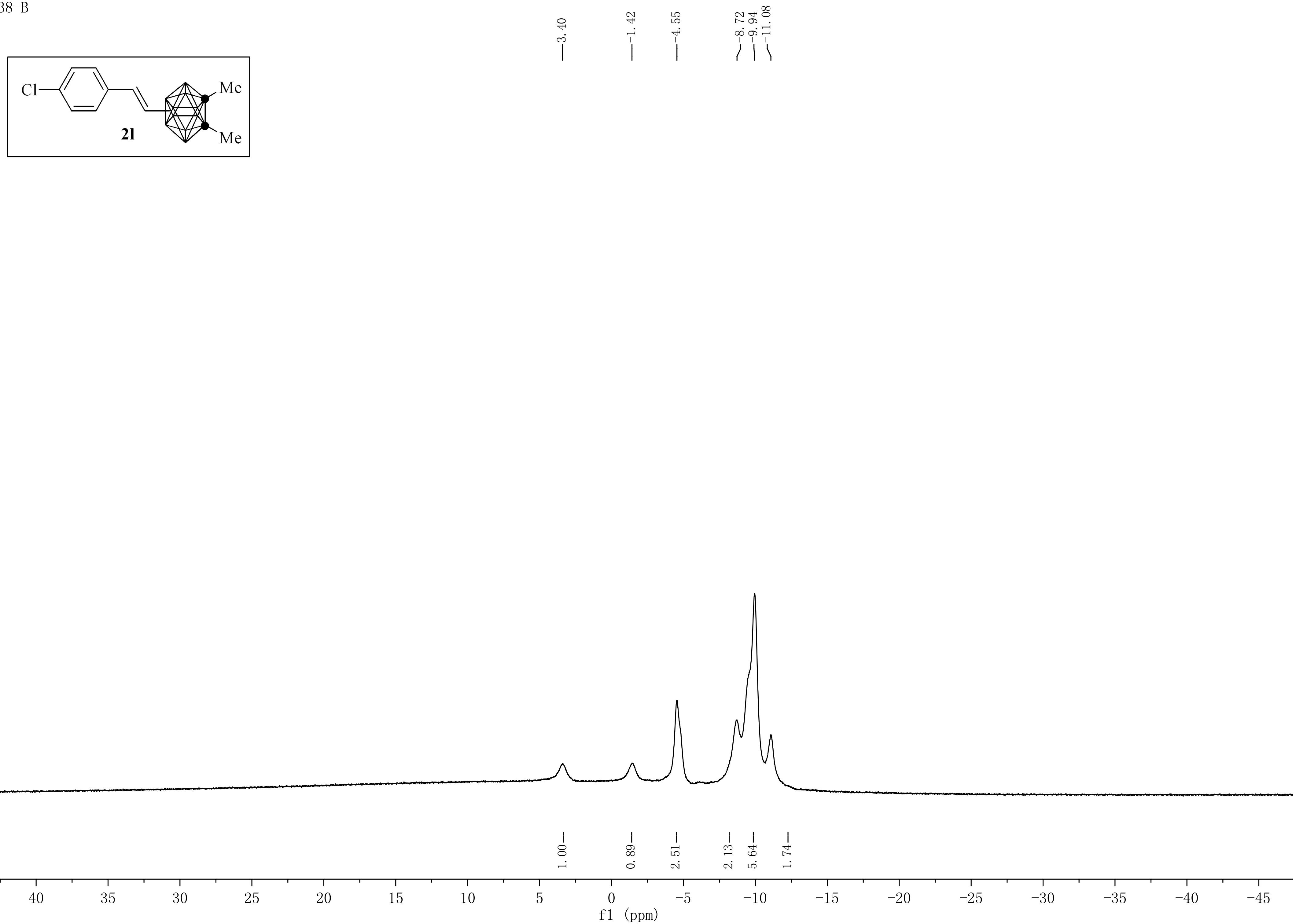

2.94
-1.88
-4.85
-9.07
-10.30
-11.41
1.00
0.89
1.97
2.27
2.05
4.39
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
f1 (ppm)


WJ-238-H
7.33
7.32
7.31
7.29
7.28
7.26
7.25
7.24
7.23
7.22
6.68
6.65
6.53
6.50
6.41
6.38
6.31
6.28
2.05
2.05
0.00
Cl
Me
Me
2l
1.80
2.03
3.65
1.00
1.01
1.00
0.99
3.55
7.83
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

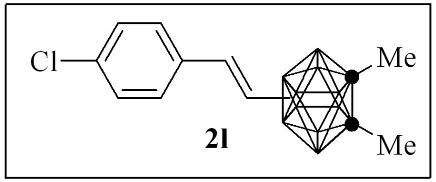
WJ-238-C


138.70
137.57
132.67
132.46
128.48
128.40
127.36
127.35
77.21
77.00
76.79
72.07
67.63
23.36
23.16
22.48
-0.02
Cl
Me
Me
2l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

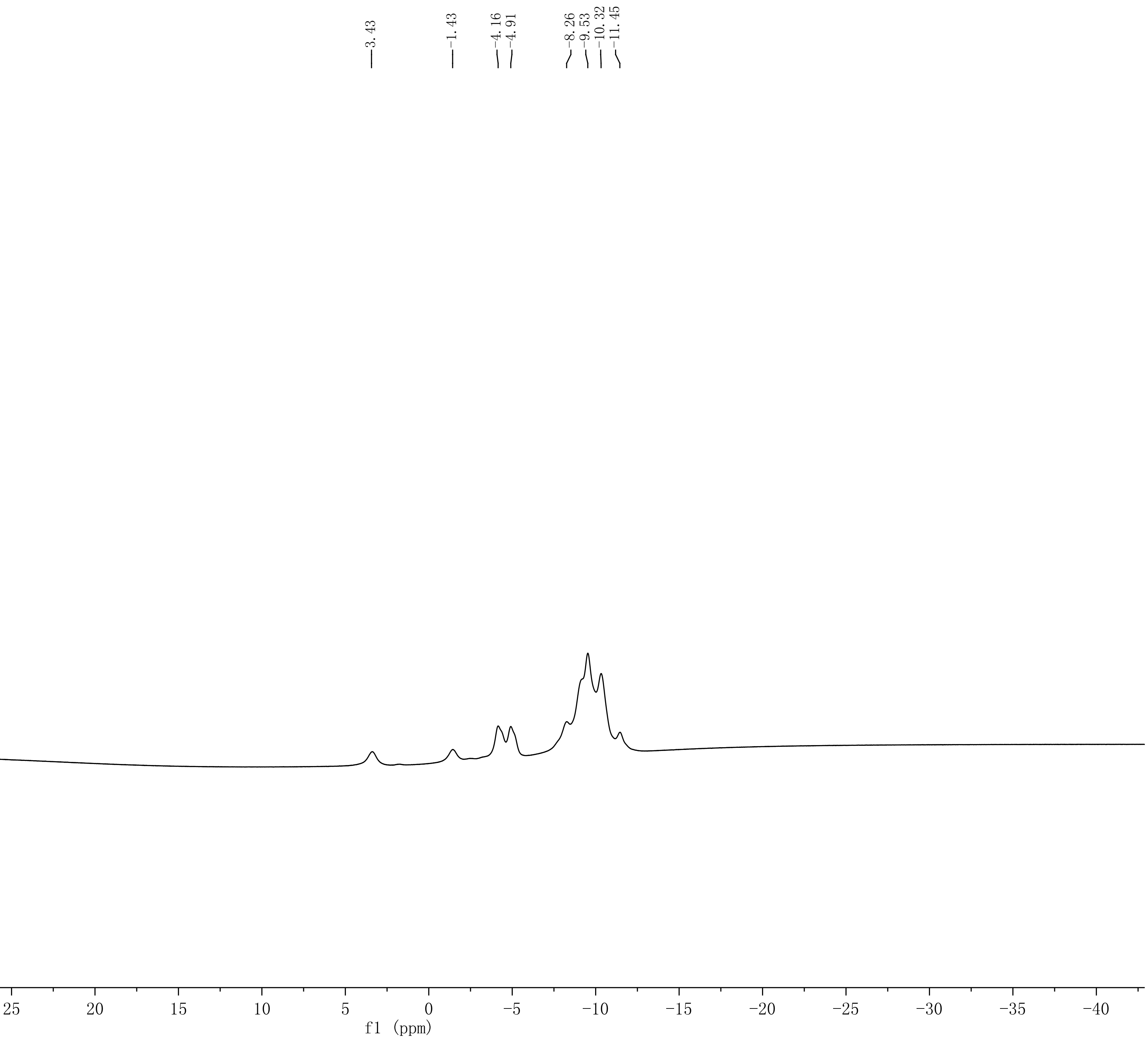
WJ-238-B

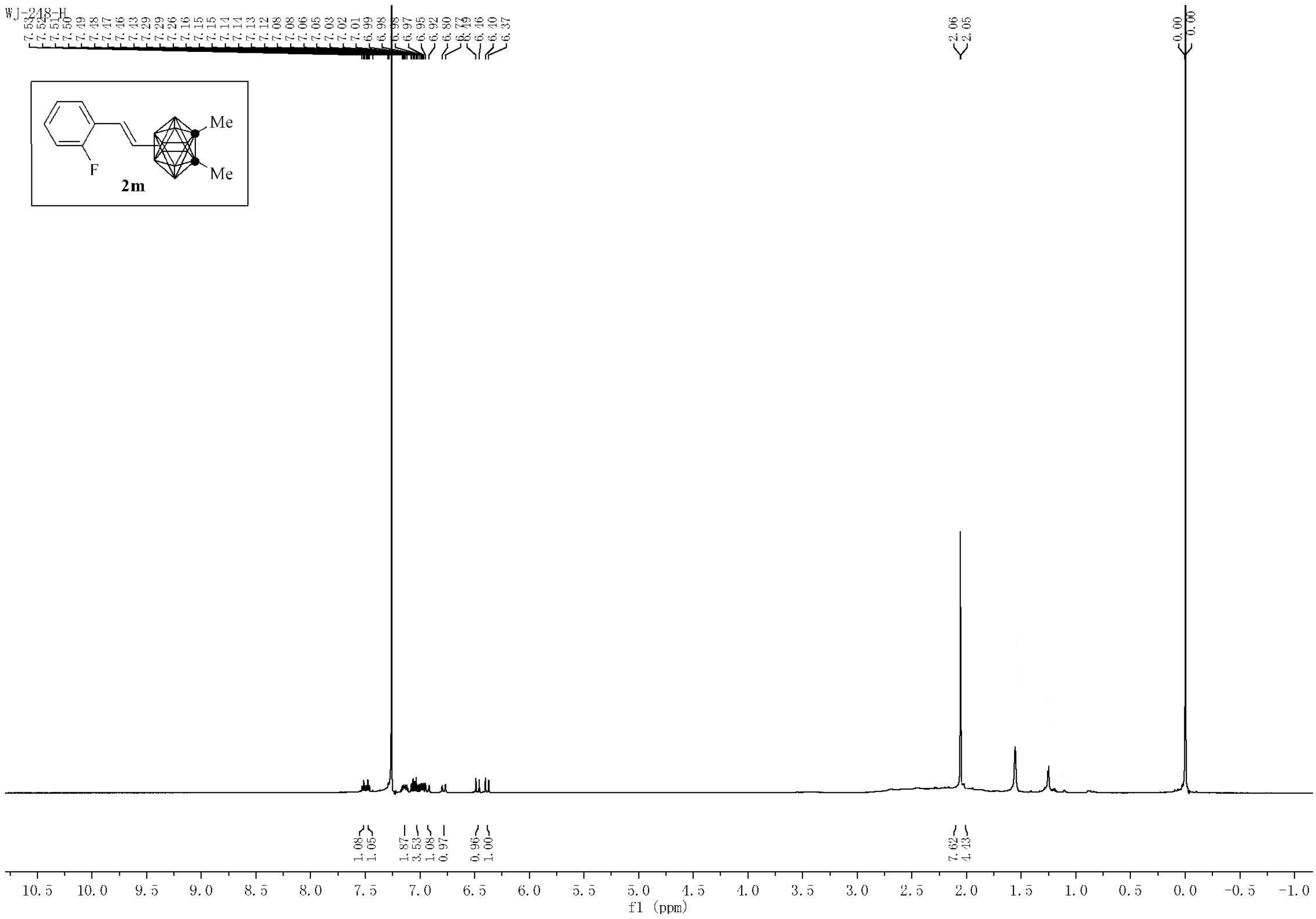

Cl
Me
Me
2l
3.40
-1.42
-4.55
-8.72
-9.94
-11.08
1.00
0.89
2.51
2.13
5.64
1.74
40 35 30 25 20 15 10 5 0 −5 −10 −15 −20 −25 −30 −35 −40 −45
f1 (ppm)

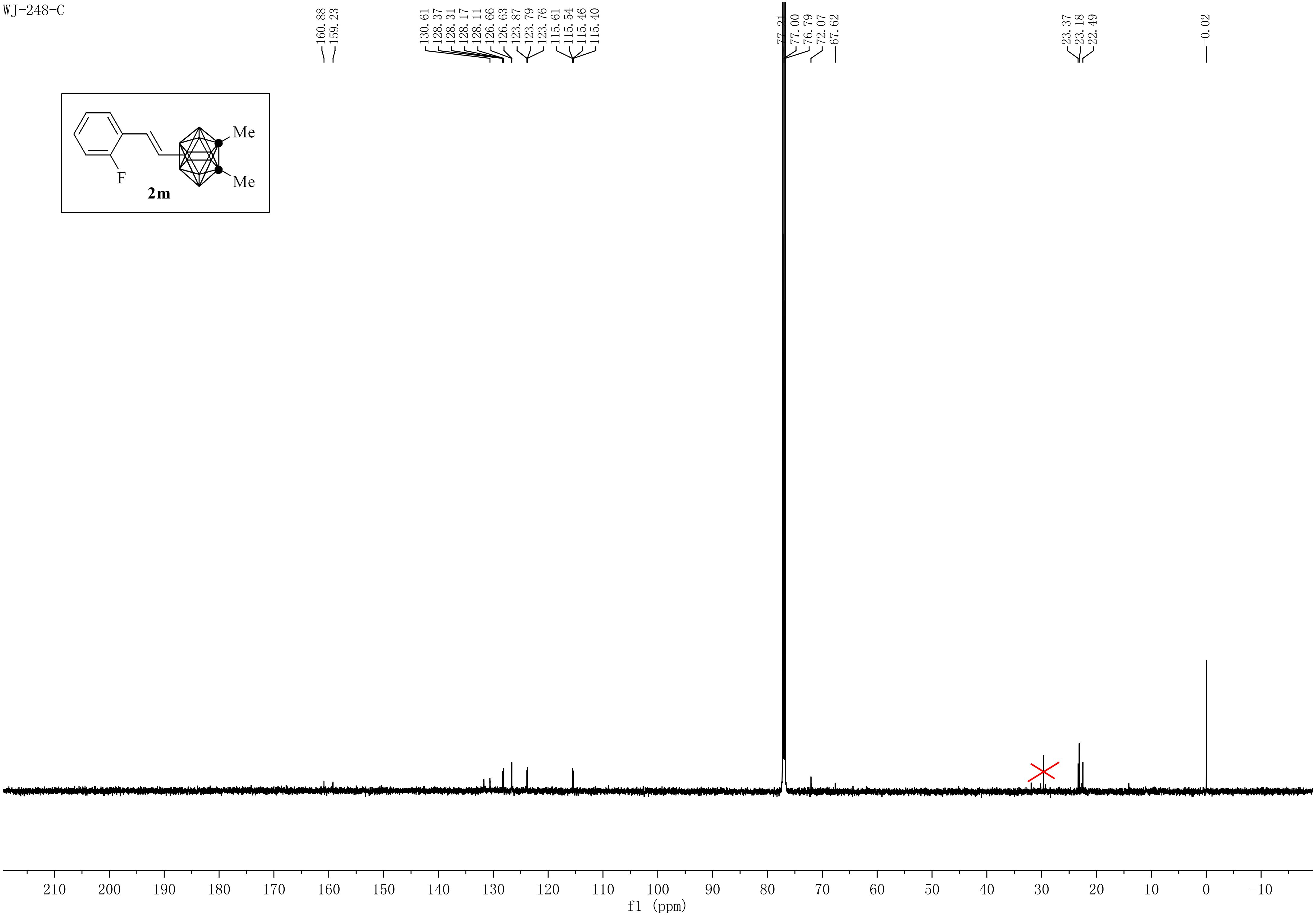
WJ-238-B-H


Cl
Me
Me

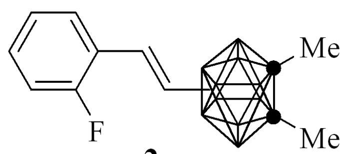
2l


3.43
-1.43
-4.16
-4.91
-8.26
-9.53
-10.32
-11.45
45
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
f1 (ppm)


WJ-248-H
7.53 7.52 7.51 7.50 7.49 7.48 7.47 7.46 7.43 7.29 7.26 7.16 7.15 7.15 7.14 7.14 7.13 7.12 7.08 7.08 7.06 7.05 7.03 7.02 7.01 6.99 6.98 6.98 6.97 6.95 6.92 6.80 6.77 6.49 6.46 6.40 6.37
2.06 2.05
0.00 0.00
Me
Me
F
2m
1.08 1.05 1.87 3.53 1.08 0.97 0.96 1.00
7.62 4.13
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

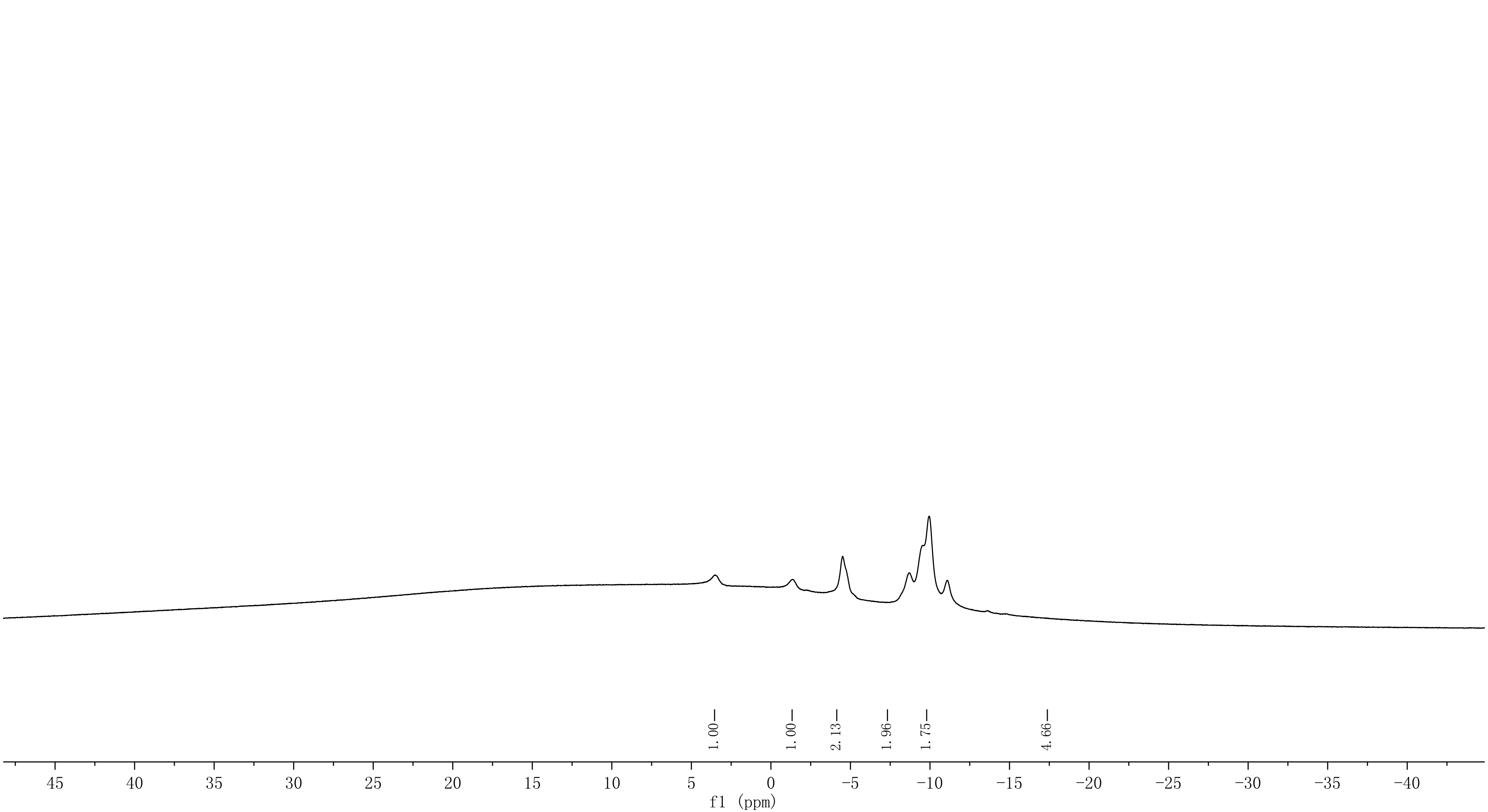

WJ-248-C
160.88
159.23
130.61
128.37
128.31
128.17
128.11
126.66
126.63
123.87
123.79
123.76
115.61
115.54
115.46
115.40
77.21
77.00
76.79
72.07
67.62
23.37
23.18
22.49
-0.02
Me
Me
F
2m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

WJ-248-B



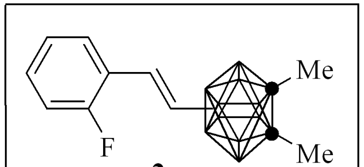
Me
Me
F

2m

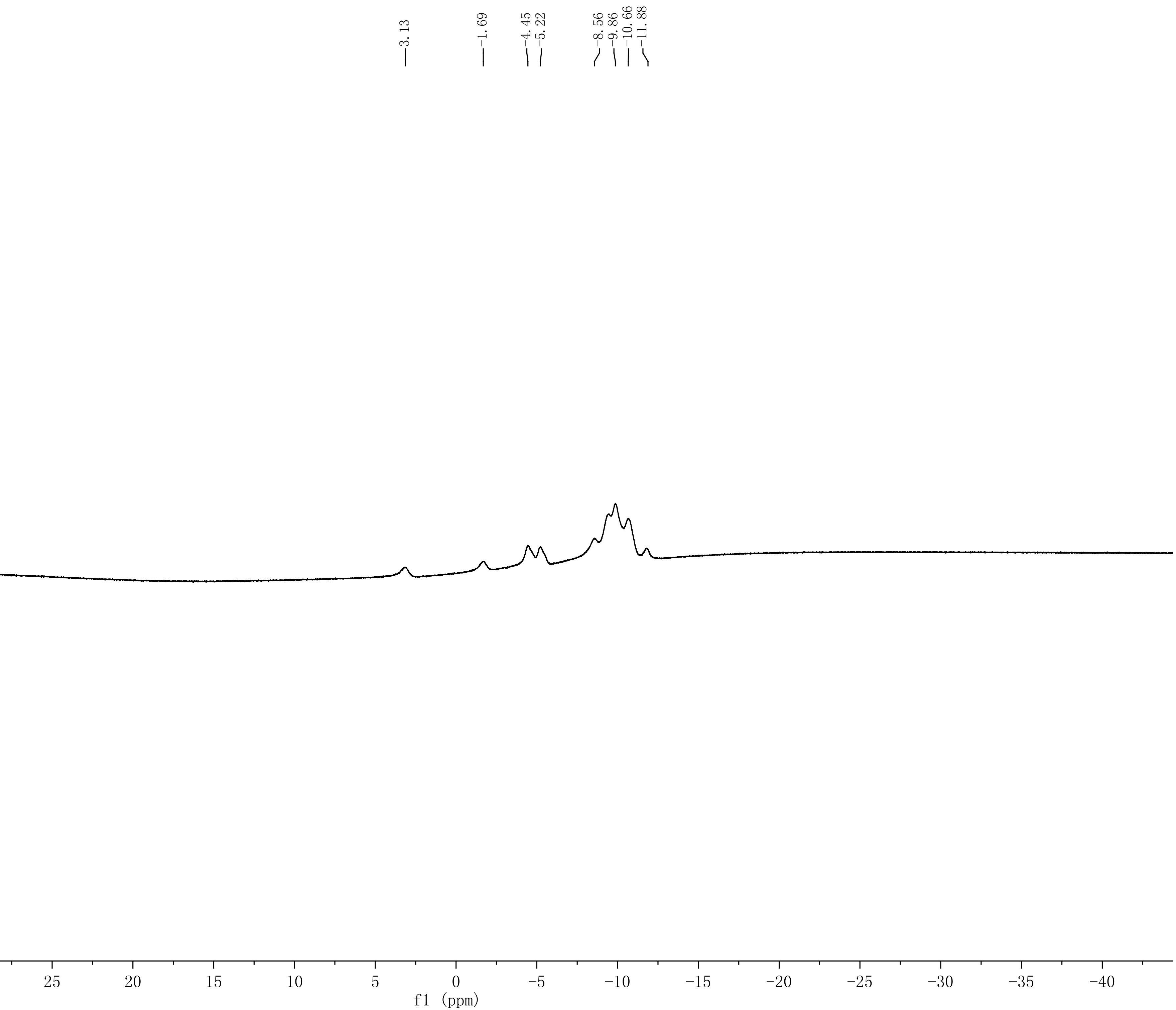


3.52
-1.37
-4.51
-8.72
-9.95
-11.08
1.00
1.00
2.13
1.96
1.75
4.66
45
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
f1 (ppm)

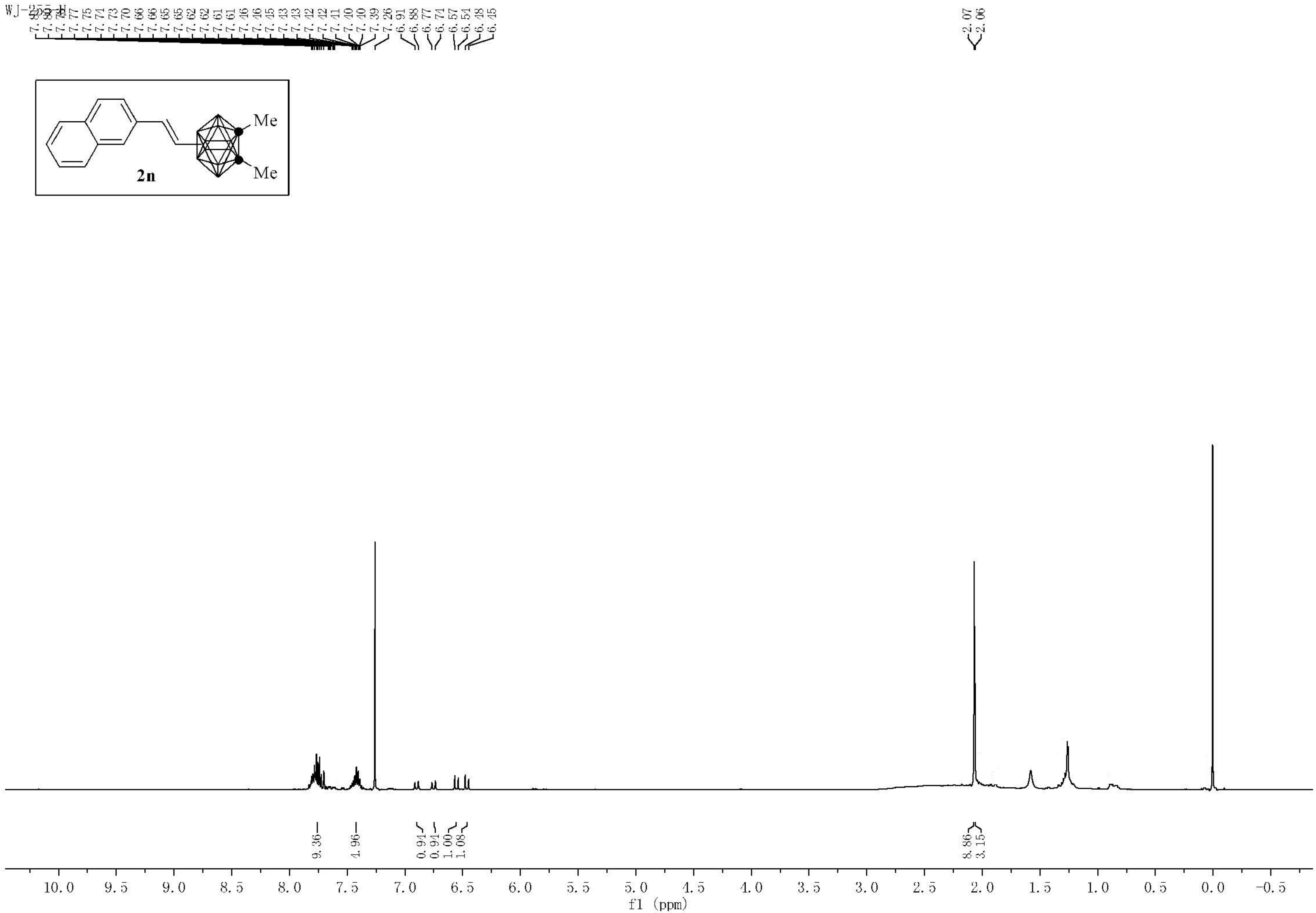
WJ-248-B-H



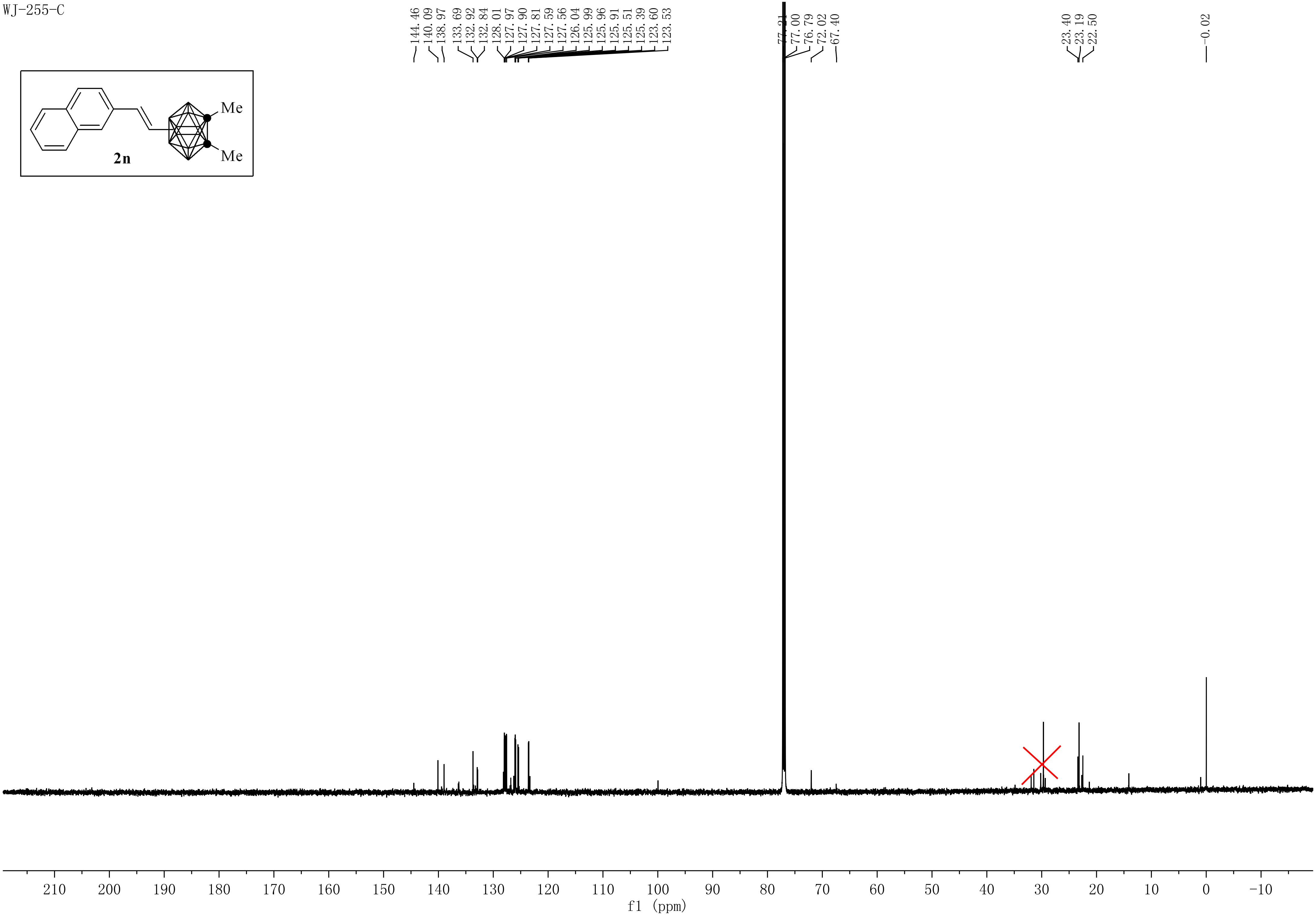
2m

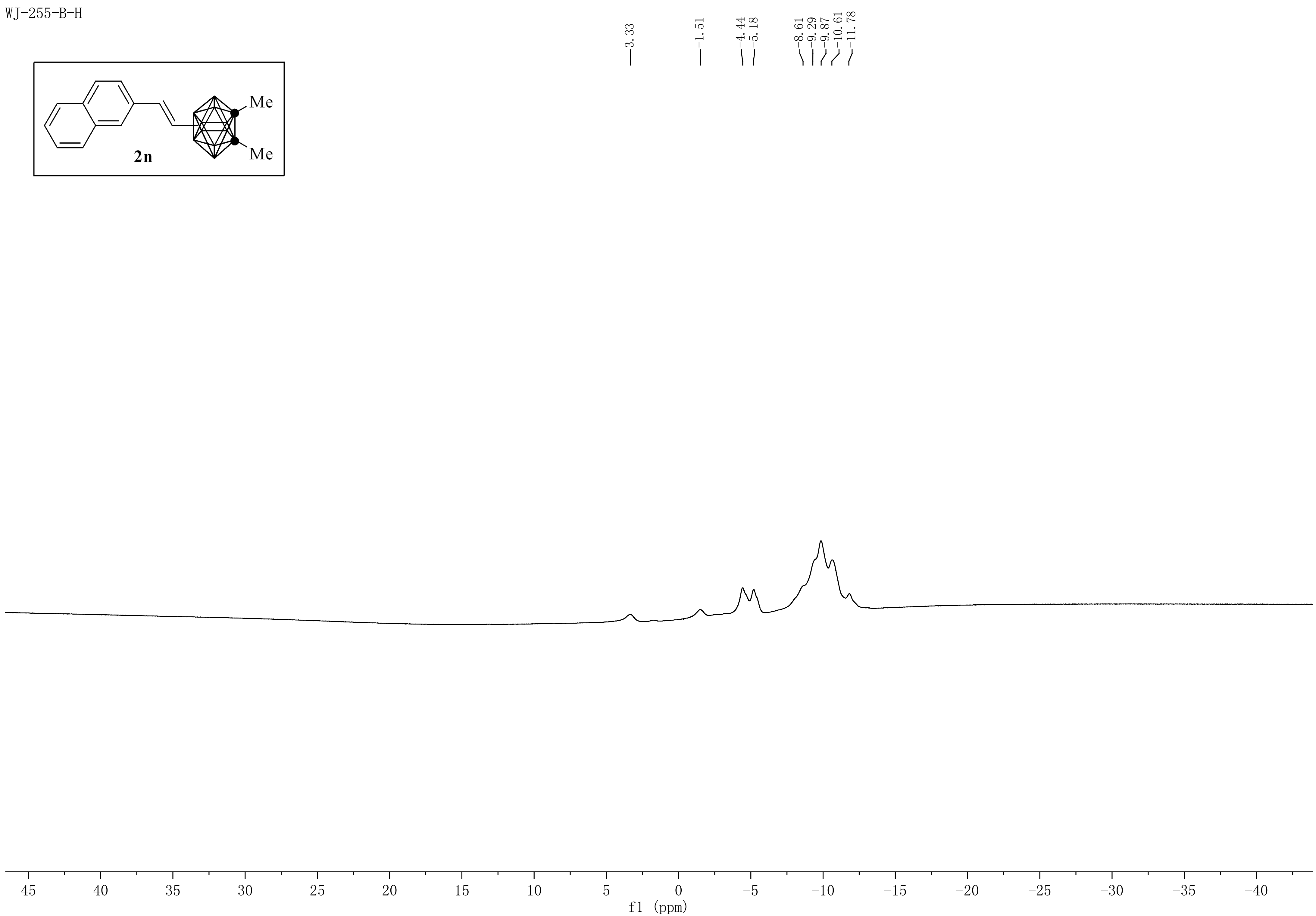


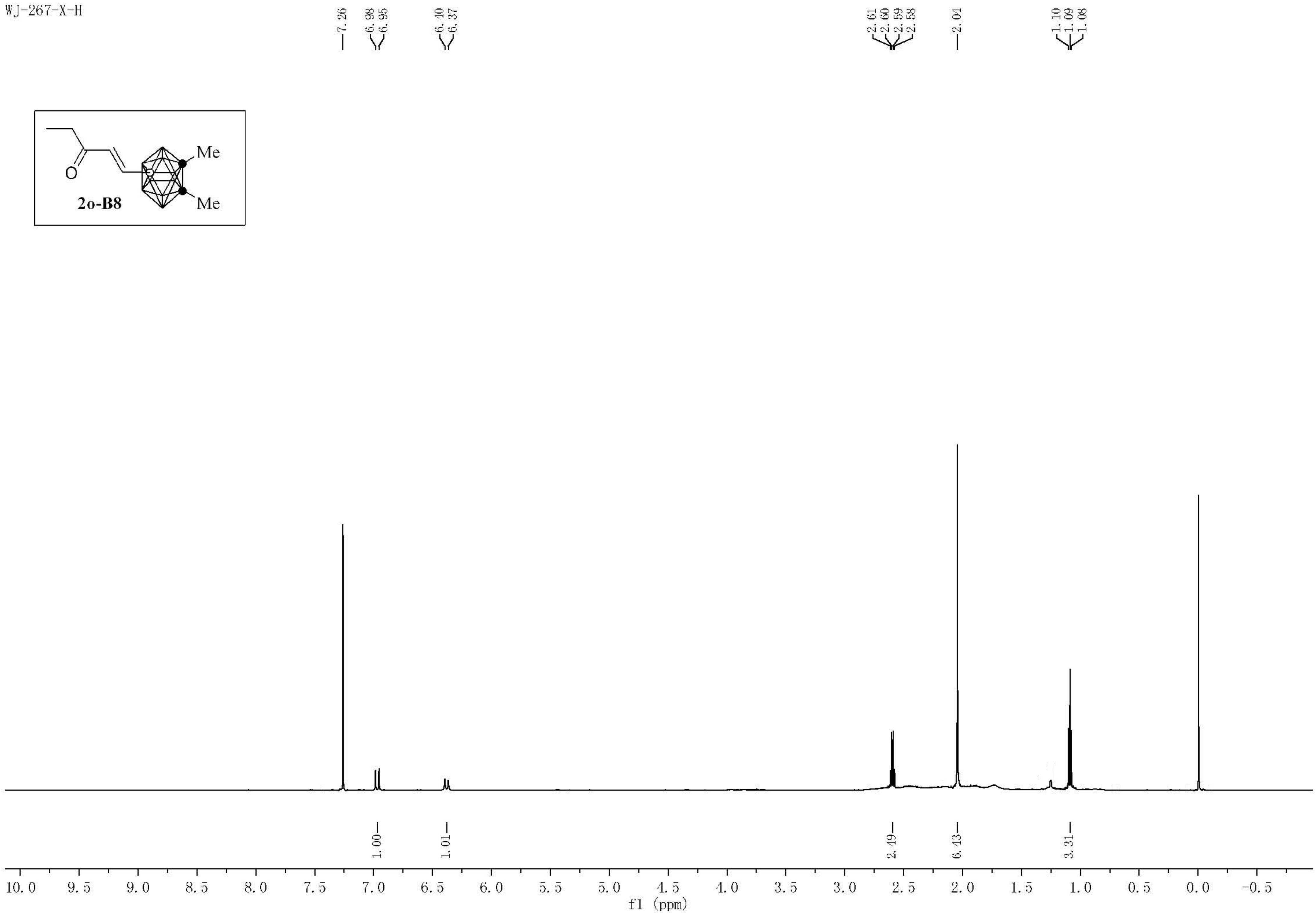
3.13
-1.69
-4.45
-5.22
-8.56
-9.86
-10.66
-11.88
45 40 35 30 25 20 15 10 5 0 −5 −10 −15 −20 −25 −30 −35 −40
f1 (ppm)

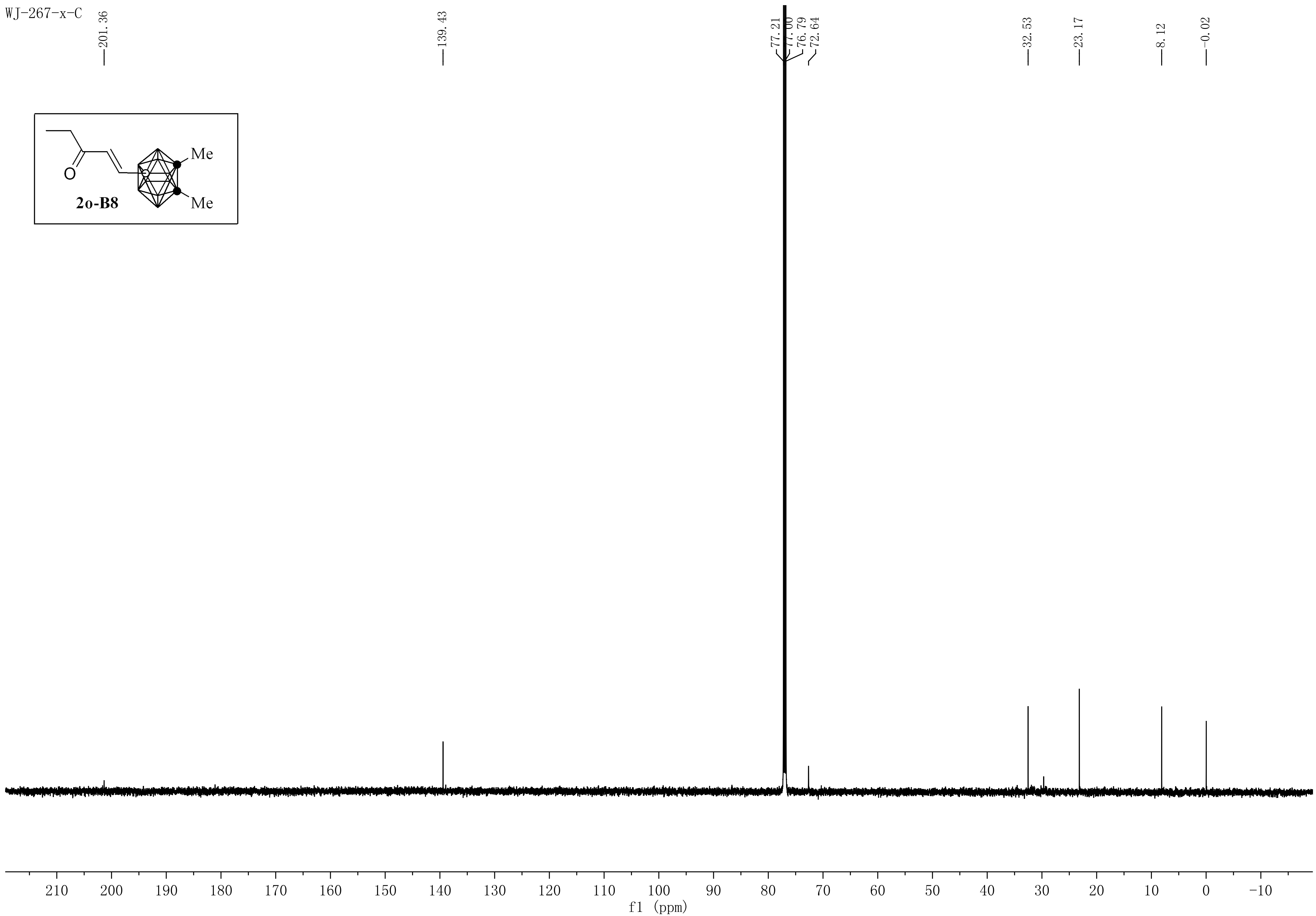

WJ-255-H
2n
Me
Me
7.26
2.07
2.06
9.36
4.96
0.91
0.94
1.00
1.08
8.86
3.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

WJ-255-C

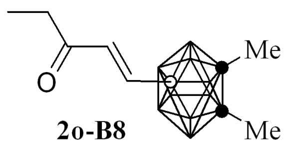

Me
Me
2n
144.46
140.09
138.97
133.69
132.92
132.84
128.01
127.97
127.90
127.81
127.59
127.56
126.04
125.99
125.96
125.91
125.51
125.39
123.60
123.53
77.21
77.00
76.79
72.02
67.40
23.40
23.19
22.50
-0.02
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


WJ-255-B-H
3.33
-1.51
-4.44
-5.18
-8.61
-9.29
-9.87
-10.61
-11.78
Me
Me
2n
45
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
f1 (ppm)

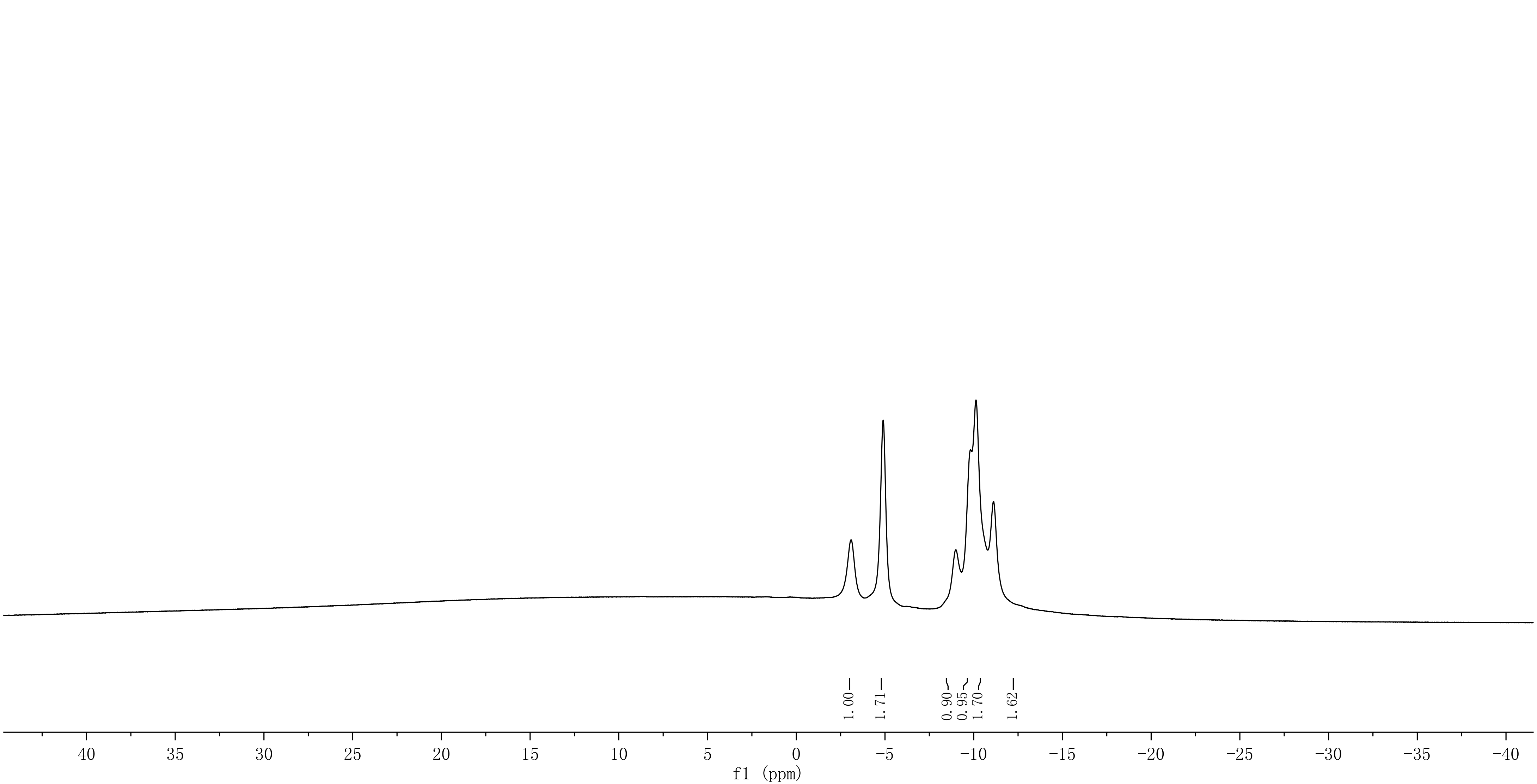

WJ-267-X-H
7.26
6.98
6.95
6.40
6.37
2.61
2.60
2.59
2.58
2.04
1.10
1.09
1.08
Me
Me
O
2o-B8
1.00
1.01
2.49
6.43
3.31
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


WJ-267-x-C
201.36
139.43
77.21
77.00
76.79
72.64
32.53
23.17
8.12
-0.02
Me
O
2o-B8
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

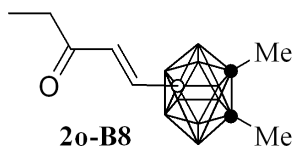
WJ-267-X-B



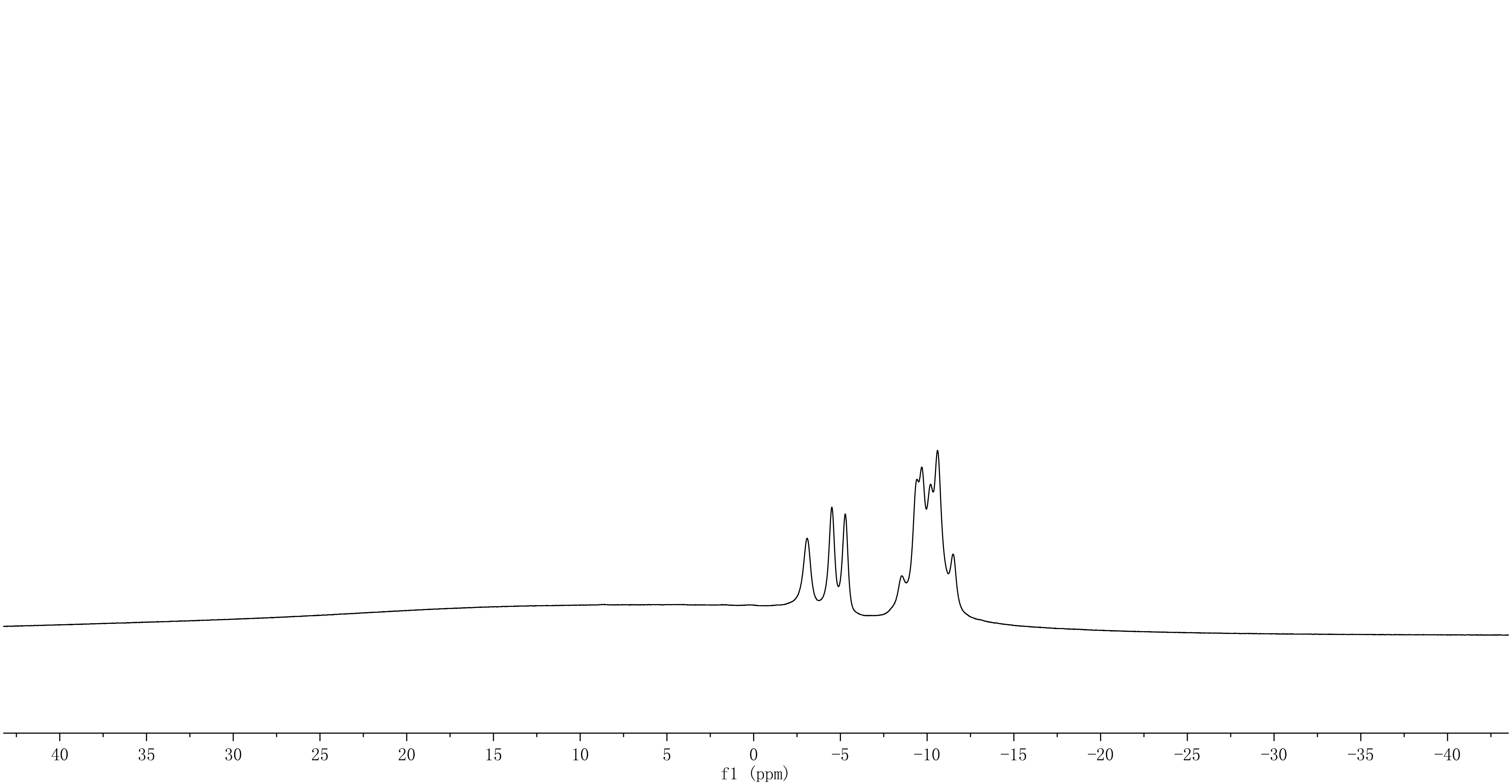
2o-B8



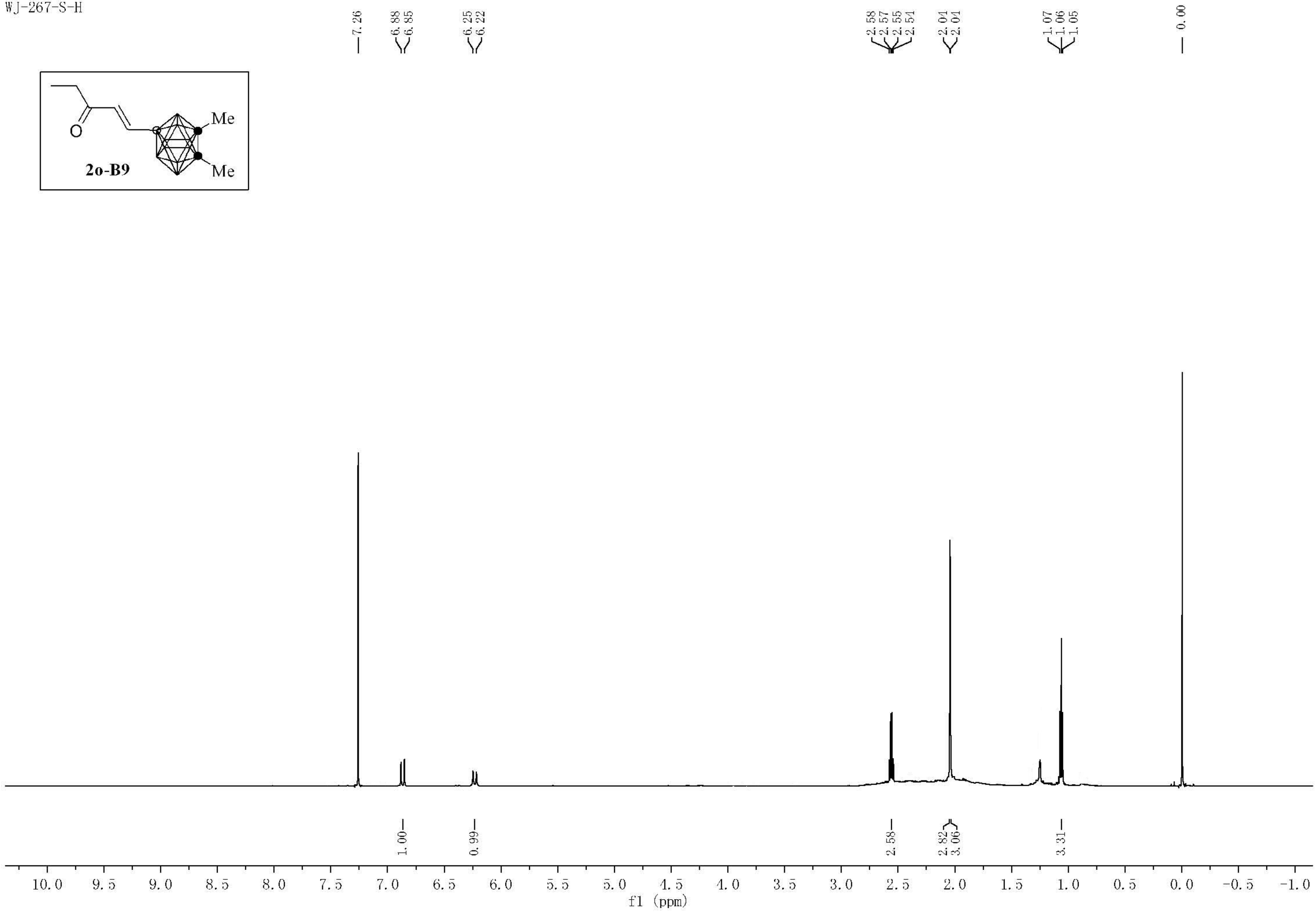
WJ-267-X-B-H

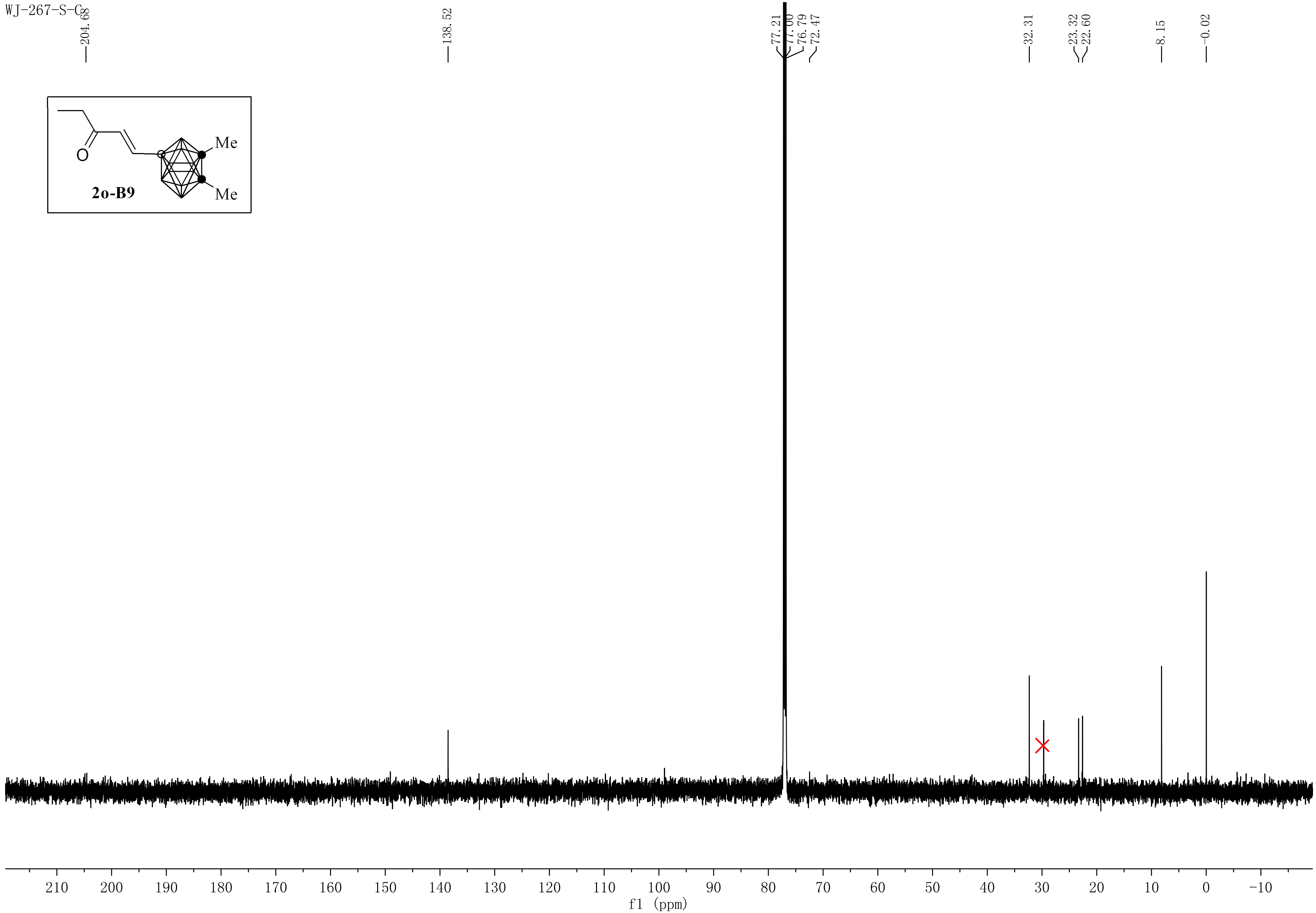


2o-B8

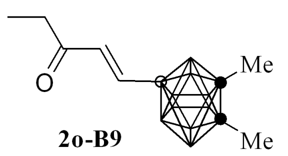


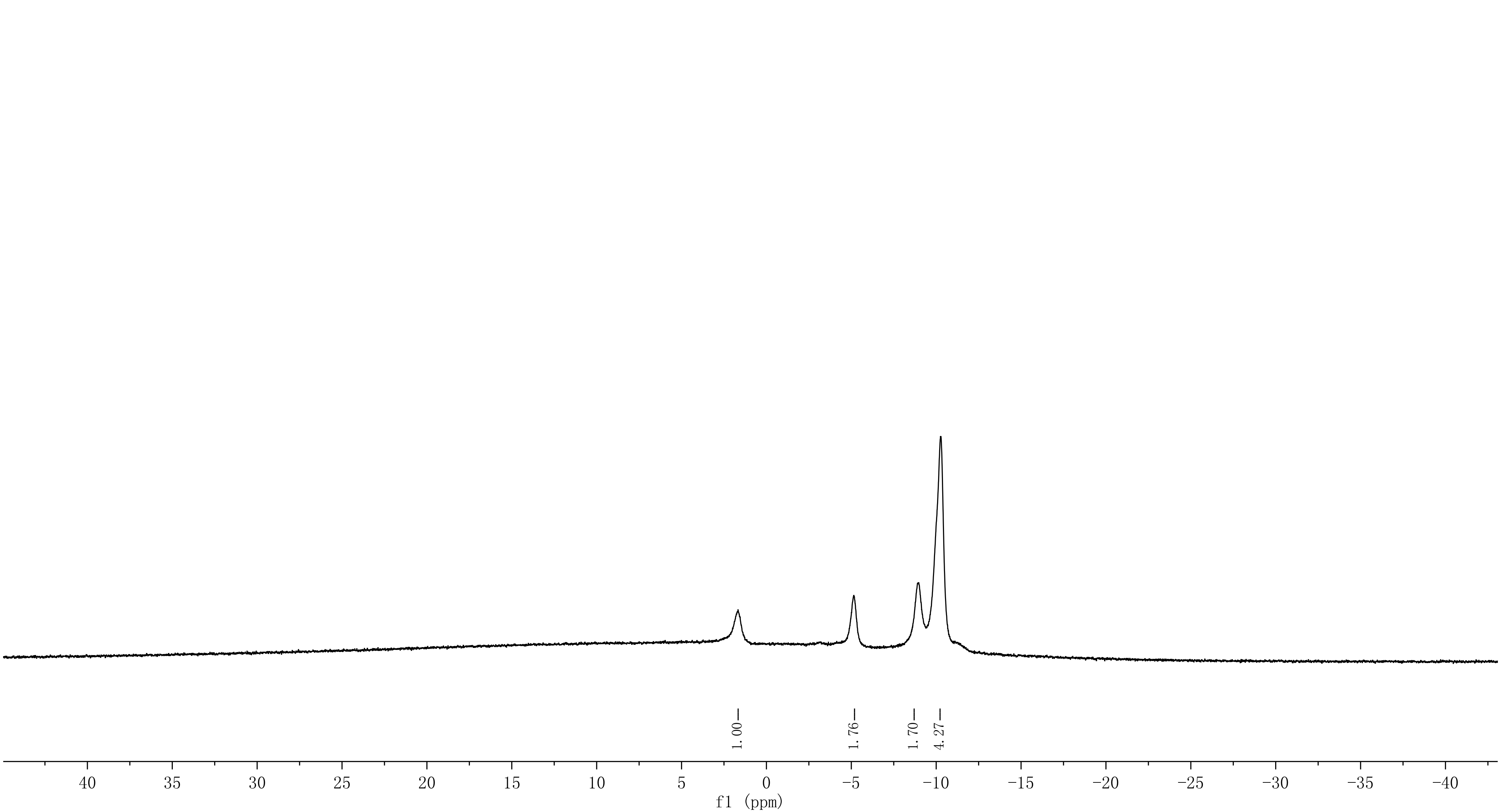
WJ-267-S-H


7.26
6.88
6.85
6.25
6.22
2.58
2.57
2.55
2.54
2.04
2.04
1.07
1.06
1.05
0.00
Me
Me
2o-B9
1.00
0.99
2.58
2.82
3.06
3.31
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

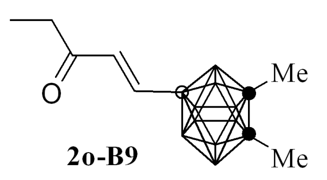

WJ-267-S-C
204.68
138.52
77.21
77.00
76.79
72.47
32.31
23.32
22.60
8.15
-0.02
Me
O
Me
2o-B9
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

WJ-267-S-B

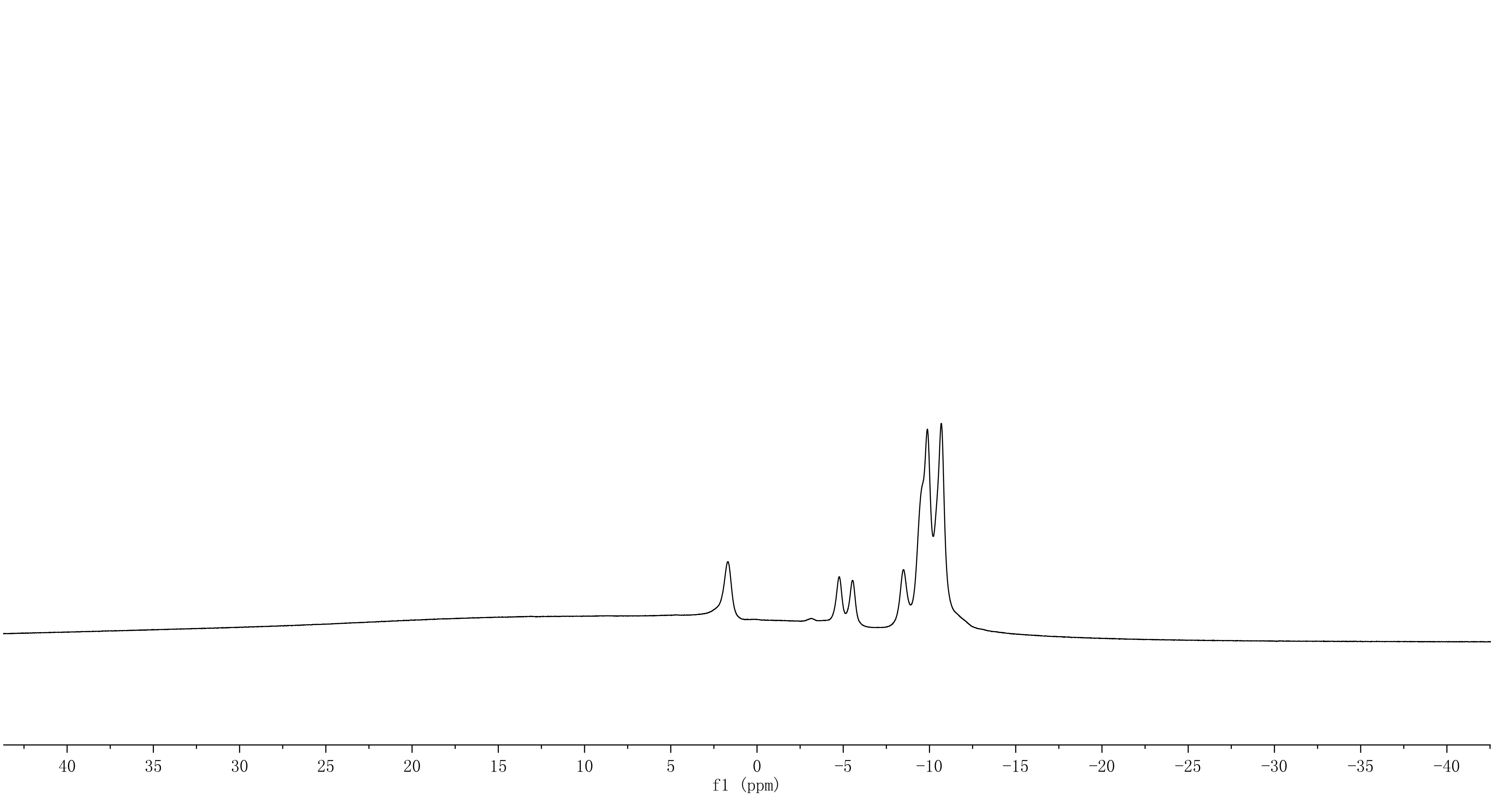

2o-B9



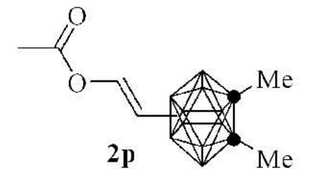
WJ-267-S-B-H



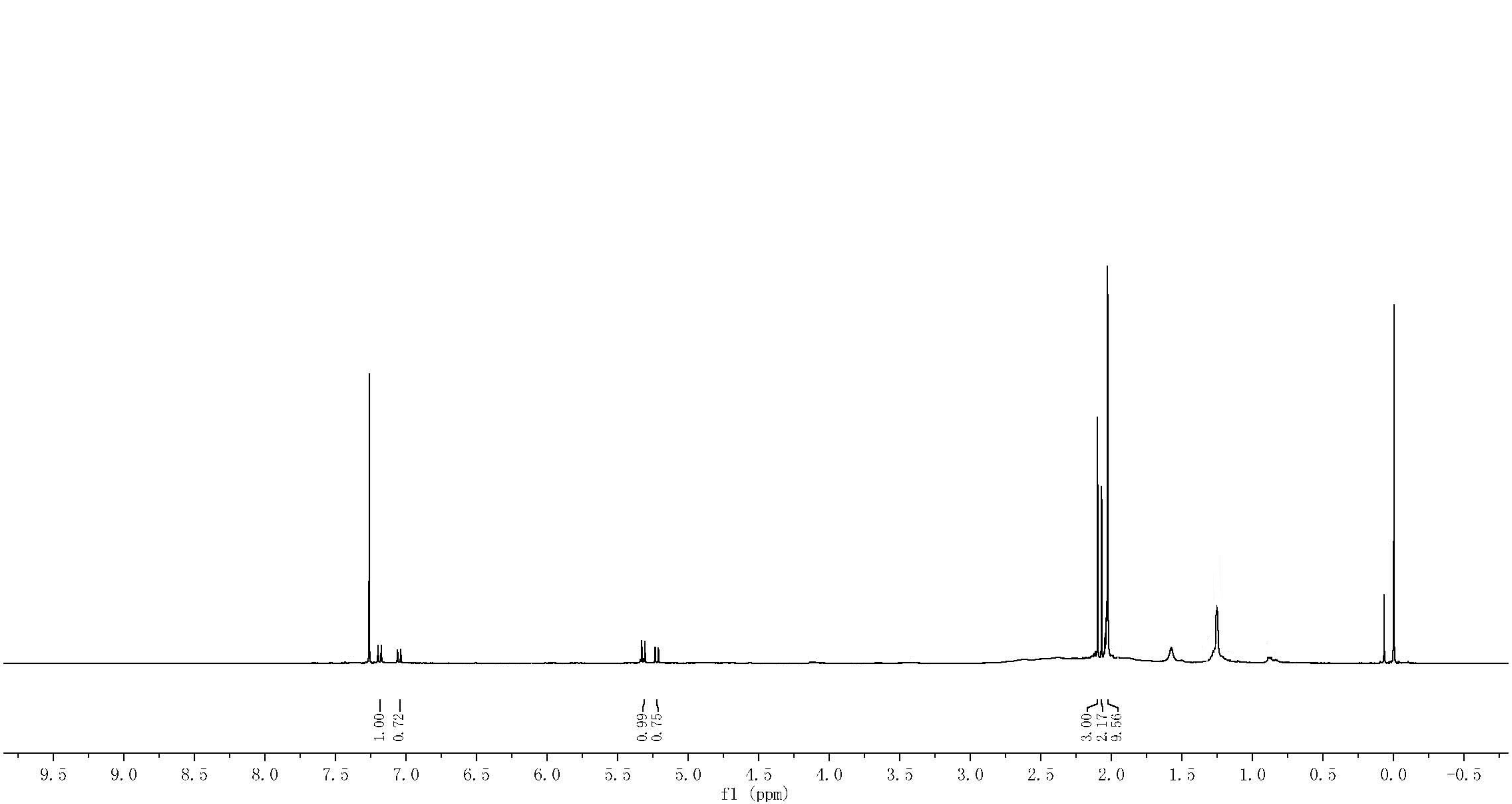
2o-B9

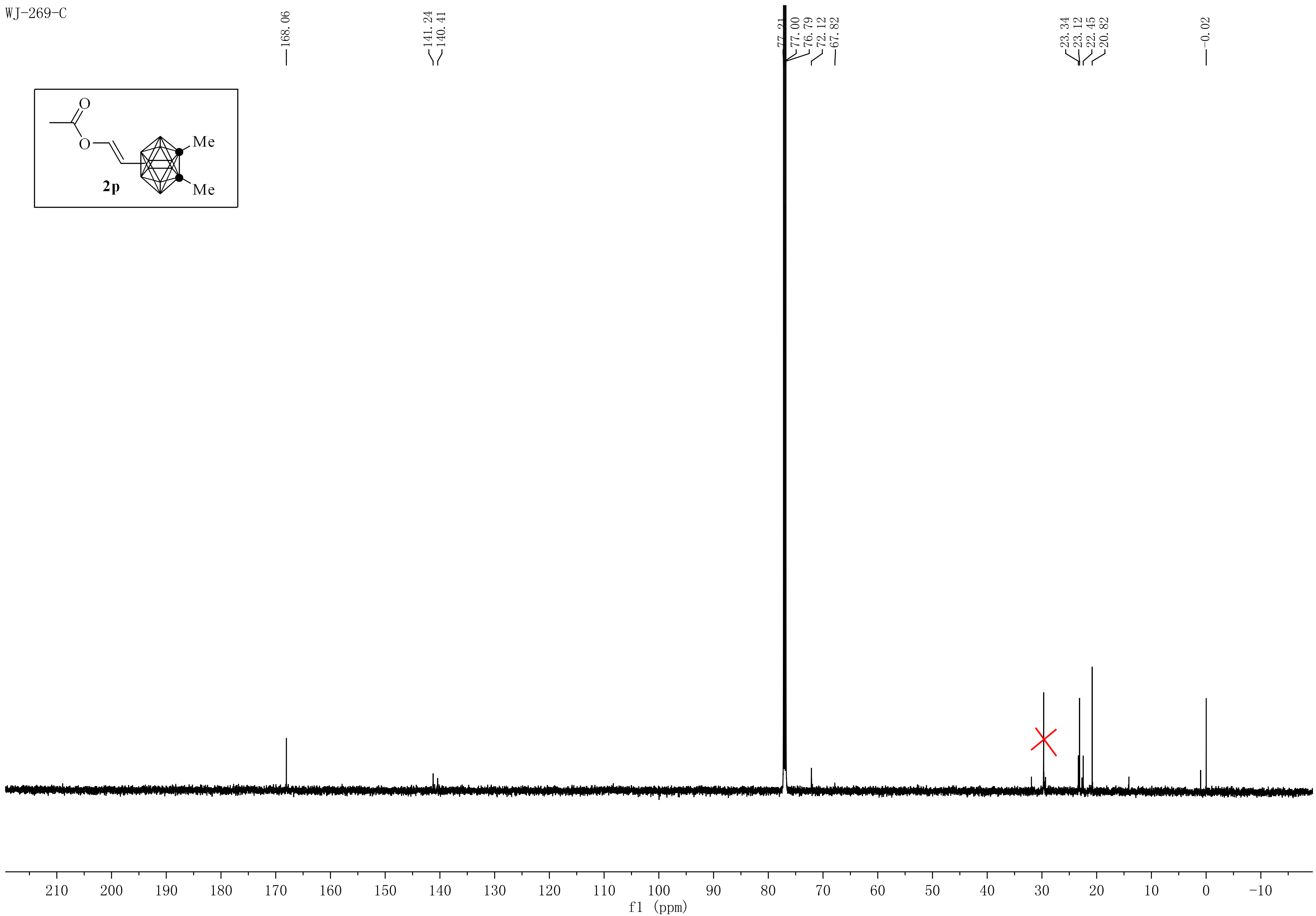


WJ-269-H


O
O
Me
Me

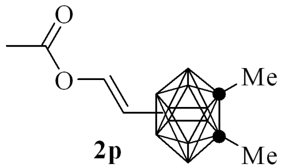
2p


7.26
7.20
7.17
7.06
7.01
5.33
5.31
5.23
5.21
2.10
2.07
2.03
0.00
1.00
0.72
0.99
0.75
3.00
2.17
9.56
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

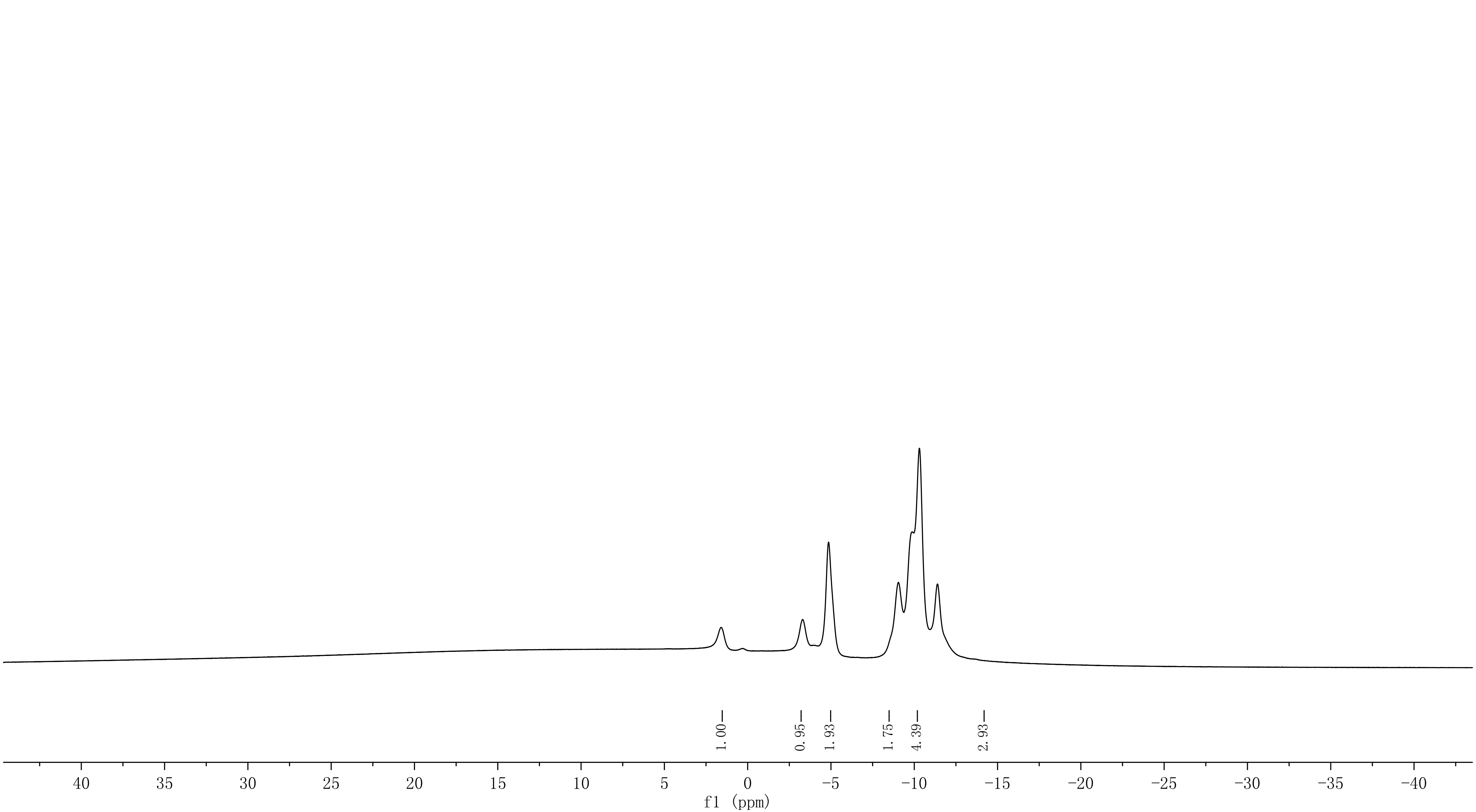


WJ-269-C
168.06
141.24
140.41
77.21
77.00
76.79
72.12
67.82
23.34
23.12
22.45
20.82
-0.02
O
O
Me
Me
2p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

WJ-269-B

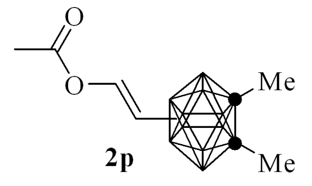


2p

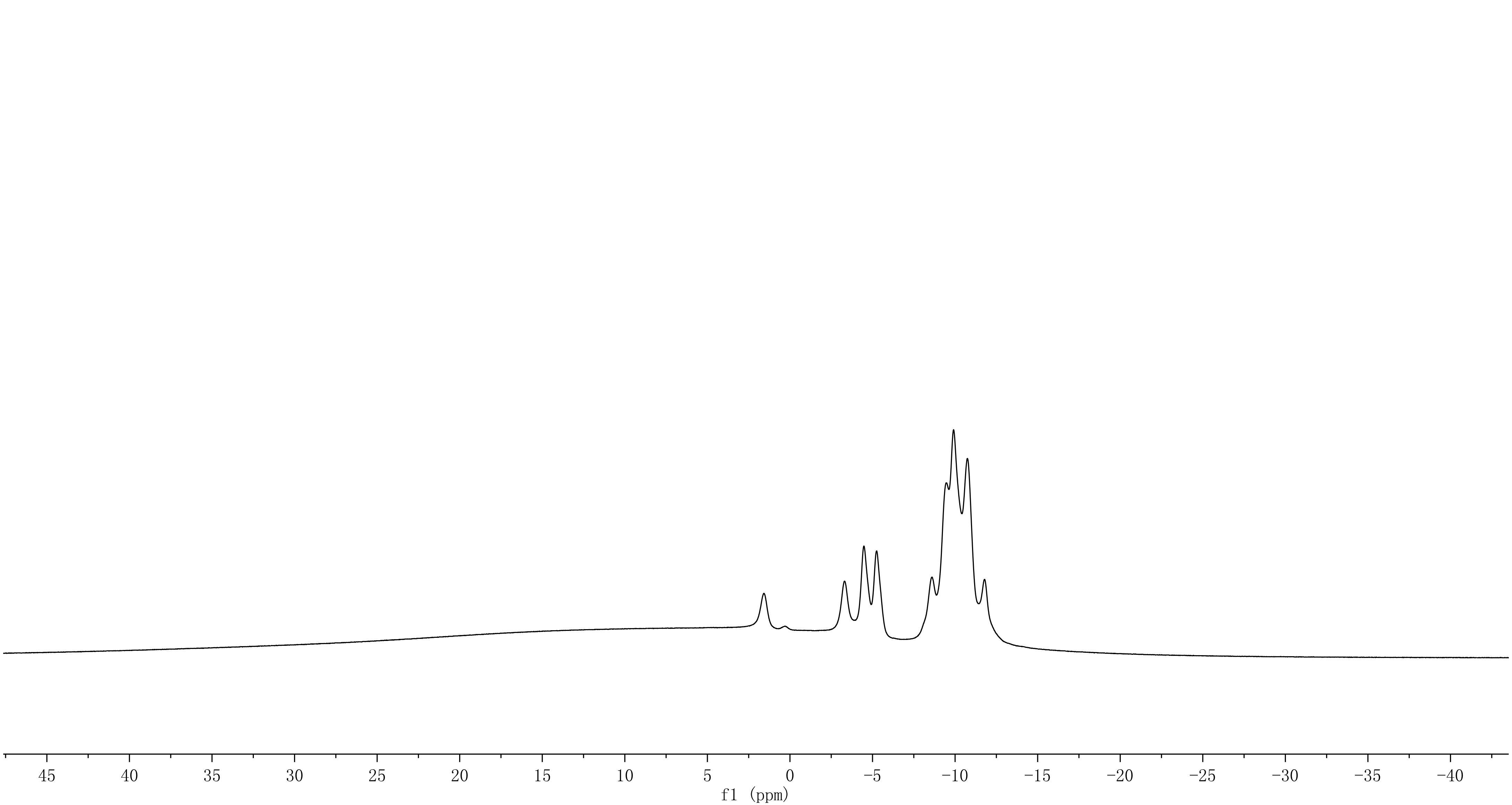


1.60
-3.30
-4.86
-9.04
-9.86
-10.31
-11.40
1.00
0.95
1.93
1.75
4.39
2.93
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
f1 (ppm)

WJ-269-B-H



2p



1.59
3.31
4.48
5.25
8.60
9.46
9.91
10.74
11.79
45
40
35
30
25
20
15
10
5
0
−5
−10
−15
−20
−25
−30
−35
−40
f1 (ppm)