Supporting Information

Iridium Catalyzed Selective Amination of B(4)-H for Synthesis of *o*-Carborane Fused Indolines

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Context

1. General information

2. Experimental

3. Spectroscopic date for products

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

General information

1a-1j, 4a-4e were synthesized according to literature method[1-2]. Other materials were purchased from Acros, J&K and Aladdin, 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) was used for column chromatography, and the distillation range of petroleum ether was 60-90 °C. ^{1}H NMR, $^{13}C\{^{1}H\}$, $^{11}B\{^{1}H\}$ NMR and ^{11}B NMR spectra were recorded on the Bruker 400、500 or 600 MHz instruments. All ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectral data were reported in *ppm* relative to tetramethylsilane (TMS) as an internal standard, and $^{11}B\{^{1}H\}$ and ^{11}B NMR spectra data are referenced to external BF_3•Et_2O. HRMS data were measured with ESI techniques. Additionally, for $^{13}C\{^{1}H\}$ NMR, the peak at about 30 *ppm* is an unidentified impurity originated from commercialized *o*-carborane, even if the *o*-carborane is purified by sublimation, this impurity is still irremovable.

Experimental

General procedure for the synthesis of 1a-1j, 4a-4e (Take 1a as an example) [1-2]**.**

To a 50 mL dried flask, 3-benzamide-*o*-carborane (263 mg, 1 mmol), MeCN (5 mL), MeOH (5mL), [Bis(trifluoroacetoxy)iodo]benzene (PIFA, 430 mg, 1 mmol) were sequentially added under argon atmosphere. The reaction mixture was stirred at room temperature for 12 h. Then the mixture was filtered through a short silica gel column using ethyl acetate as eluent. After evaporation of the solvent, the residue was purified by column chromatography on a 200-300 mesh silica gel with petroleum ether/EtOAc=10:1 (v/v) as an eluent, the desired product **1a** was obtained with 83 % yield (243.2 mg).

Typical procedure for the synthesis of 3a-3j, 5a-5e (Take 3a as an example).

To a 10 mL dried flask, **1a** (29.4 mg, 0.1 mmol), HFIP (1 mL), $[Cp^*IrCl_2]_2$ (4 mg, 0.005 mmol), AgOAc (50.1 mg, 0.3 mmol) were sequentially added under argon atmosphere. The reaction mixture was stirred at reflux temperature in the oil bath for 24 h. Then the mixture was led to room temperature and filtered through a

short silica gel column using ethyl acetate as eluent. After evaporation of the solvent, the residue was purified by column chromatography on a 200-300 mesh silica gel with petroleum ether/EtOAc=10:1 (v/v) as an eluent, the desired product **3a** was obtained with 67 % yield (19.6 mg).

Synthesis of 3a on 1 mmol scale.

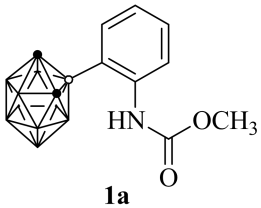
To a 50 mL dried flask, **1a** (294 mg, 1 mmol), HFIP (10 mL), $[Cp^*IrCl_2]_2$ (40 mg, 0.05 mmol), AgOAc (501 mg, 3 mmol) were sequentially added under argon atmosphere. The reaction mixture was stirred at reflux temperature in the oil bath for 24 h. Then the mixture was led to room temperature and filtered through a short silica gel column using ethyl acetate as eluent. After evaporation of the solvent, the residue was purified by column chromatography on a 200-300 mesh silica gel with petroleum ether/EtOAc=10:1 (v/v) as an eluent, the desired product **3a** was obtained with 45 % yield (131.4 mg).

Reference:

[1] K. Cao, J. Wu, C.-Y. Zhang, L. Ding, J. Yang, Iridium Catalyzed Selective Arylation of B(3)-H Bond of *o*-Carborane via B-H/C-H Activation *ChemistrySelect* **2021**, *6*, 10178-10181.

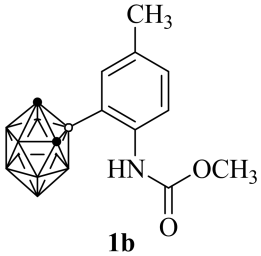
[2] H. Song, W. Chen, Y. Wang, Y. Qin, Preparation of Alkyl Carbamate of 1-Protected Indole-3-methylamine as a Precursor of Indole-3-methylamine. *Synth. Commun*. **2005**, *35*, 2735-2748.

Spectroscopic data for materials and products



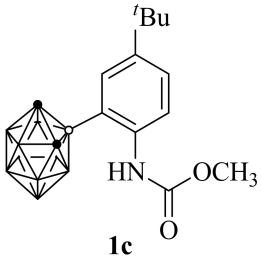
1a

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.87-7.86 (d, 1H, *J* = 5 Hz), 7.55 (s, 1H), 7.43-7.40 (m, 1H), 7.31-7.29 (d, 1H, *J* = 5 Hz), 7.13-7.10 (m, 1H), 3.86 (s, 2H, *Cage C-H*), 3.80 (s, 3H, *OCH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 154.9 (*C=O*), 142.3, 133.4, 131.0, 124.4, 123.2 (*aryl C*) , 57.2, 52.6 (*Cage C*); ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.1 (2B), -6.5 (1B) (*B-C*), -9.1 (1B), -11.1 (1B), -12.6 (2B), -13.0 (2B), -13.8 (1B).



1b

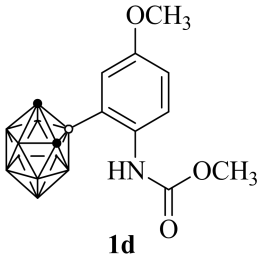
^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.64 (m, 1H), 7.31 (s, 1H), 7.23-7.21 (d, 1H, *J* = 10 Hz), 7.13 (s, 1H), 3.87 (s, 2H, *Cage C-H*), 3.78 (s, 3H, *OCH_3*), 2.32 (s, 3H, *CH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 155.2 (*C=O*), 139.4, 134.3, 131.6, 124.2, 124.1 (*aryl C*), 57.1, 52.6 (*Cage C*), 20.9; ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.2 (2B), -6.4 (1B) (*B-C*), -9.0 (1B), -11.2 (1B), -12.6 (2B), -13.2 (3B).



1c

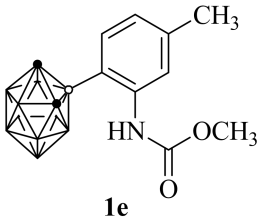
^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.66-7.64 (m, 1H), 7.46-7.44 (m, 1H), 7.38 (s, 1H), 7.26 (s, 1H), 3.88 (s, 2H, *Cage C-H*), 3.78 (s, 3H, *OCH_3*), 1.31 (s, 9H, *CH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 155.3 (*C=O*), 147.6, 139.1, 130.8, 128.2, 124.1 (*aryl C*), 57.0, 52.6 (*Cage C*), 34.5, 31.3; ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$,

ppm): -2.3 (2B), -6.2 (1B) (*B-C*), -8.9 (1B), -11.3 (1B), -12.6 (2B), -13.3 (3B).



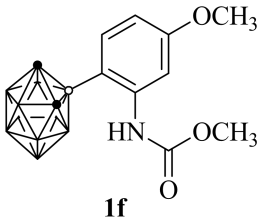
1d

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.49 (s, 1H), 6.99 (s, 1H), 6.94-6.92 (m, 2H), 3.88 (s, 2H, *Cage C-H*), 3.81 (s, 3H, *OCH_3*), 3.76 (s, 3H, *OCH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 157.0 (*C=O*), 155.9, 134.0, 127.1, 120.9, 115.1 (*aryl C*), 56.9 (*Cage C*), 55.5 (*OCH_3*), 52.7 (*Cage C*); ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.3 (2B), -6.6 (1B) (*B-C*), -8.8 (1B), -11.1 (1B), -12.6 (2B), -13.3 (3B).



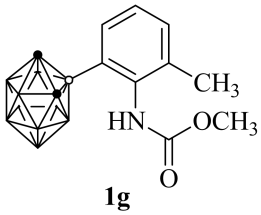
1e

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.67 (s, 1H), 7.49 (s, 1H), 7.19-7.18 (d, 1H, *J* = 5 Hz), 6.94-6.93 (d, 1H, *J* = 5 Hz), 3.84 (s, 2H, *Cage C-H*), 3.79 (s, 3H, *OCH_3*), 2.35 (s, 3H, *CH_3*); ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 154.9 (*C=O*), 142.0, 141.4, 133.4, 125.4, 123.9 (*aryl C*), 57.2, 52.5 (*Cage C*), 21.3; ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.2 (2B), -6.3 (1B) (*B-C*), -9.2 (1B), -11.3 (1B), -12.6 (2B), -13.1 (3B).



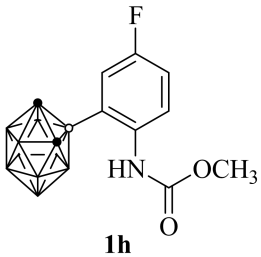
1f

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.71 (s, 1H), 7.61 (s, 1H), 7.15-7.13 (d, 1H, *J* = 10 Hz), 6.65-6.63 (m, 1H), 3.83 (s, 2H, *Cage C-H*), 3.80 (s, 6H, *OCH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 161.7 (*C=O*), 154.6, 144.0, 134.2, 110.9, 106.9 (*aryl C*), 57.2 (*Cage C*), 55.3 (*OCH_3*), 52.5 (*Cage C*); ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.2 (2B), -6.1 (1B) (*B-C*), -9.5 (1B), -11.5 (1B), -12.7 (2B), -13.1 (3B).



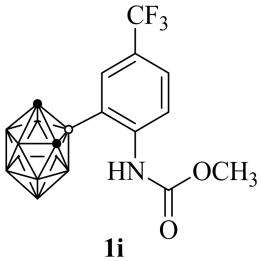
1g

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.49-7.48 (d, 1H, *J* = 5 Hz), 7.33-7.31 (d, 1H, *J* = 5 Hz), 7.25-7.22 (dd, 1H, *J* = 5 Hz, 5 Hz), 6.37 (s, 1H), 3.91 (s, 2H, *Cage C-H*), 3.77 (s, 3H, *OCH_3*), 2.28 (s, 3H, *CH_3*); ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 156.0 (*C=O*), 137.5, 133.7, 132.7, 127.7, 123.6 (*aryl C*), 56.7, 53.0 (*Cage C*), 18.4; ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.5 (2B), -6.2 (1B) (*B-C*), -8.5 (1B), -11.4 (1B), -12.5 (2B), -13.6 (3B).



1h

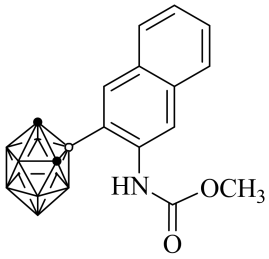
^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.71 (s, 1H), 7.22 (s, 1H), 7.14-7.07 (m, 2H), 3.86 (s, 2H, *Cage C-H*), 3.79 (s, 3H, *OCH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 159.6 (*J* = 245 Hz), 155.3 (*C=O*), 137.7, 126.5 , 120.3 (*J* = 21.3 Hz), 117.7（*J* = 21.3 Hz) (*aryl C*), 57.0, 52.8 (*Cage C*); ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.0 (2B), -7.2 (1B) (*B-C*), -9.0 (1B), -10.8 (1B), -12.7 (2B), -13.0 (2B), -13.8 (1B).



1i

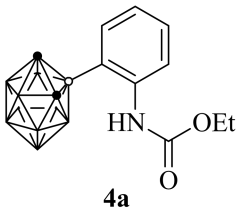
^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.24-8.22 (d, 1H, *J* = 10 Hz), 8.04 (s, 1H), 7.67-7.65 (d, 1H, *J* = 10 Hz), 7.38 (s, 1H), 3.88 (s, 2H, *Cage C-H*), 3.83 (s, 3H, *OCH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 154.1 (*C=O*), 146.0, 129.4 (*J* = 3.8 Hz), 128.0 (*J* = 3.8 Hz), 125.4 (*J* = 32.5 Hz), 123.9 (*J* = 270 Hz), 121.3 (*aryl C*), 57.4, 52.8 (*Cage C*); ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -1.7 (2B), -7.3 (1B)

(*B-C*), -9.4 (1B), -10.5 (1B), -12.7 (5B).



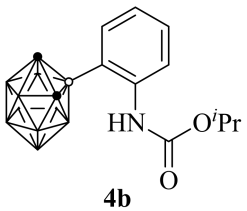
1j

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.31 (s, 1H), 7.81 (s, 1H), 7.79-7.77 (d, 1H, *J* = 10 Hz), 7.73-7.72 (d, 1H, *J* = 10 Hz), 7.68 (s, 1H), 7.51-7.48 (m, 1H), 7.44-7.41 (m, 1H), 3.97 (s, 2H, *Cage C-H*), 3.83 (s, 3H, *OCH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 155.0 (*C=O*), 138.0, 134.7, 134.5, 130.0, 127.7, 127.5, 127.4, 125.8, 120.0 (*aryl C*), 57.6, 52.6 (*Cage C*); ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.0 (2B), -6.4 (1B) (*B-C*), -9.1 (1B), -11.0 (1B), -12.5 (5B).



4a

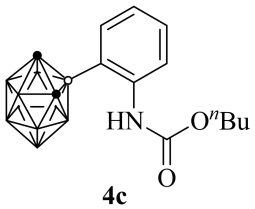
^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.81 (s, 1H), 7.46 (s, 1H), 7.42-7.38 (m, 1H), 7.34-7.32 (d, 1H, *J* = 5 Hz), 7.13-7.10 (dd, 1H, *J* = 5 Hz, 5 Hz), 4.26-4.21 (m, 2H, *OCH_2*), 3.88 (s, 2H, *Cage C-H*), 1.34-1.31 (dd, 3H, *J* = 5 Hz, 5 Hz, *CH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 154.6 (*C=O*), 142.1, 133.7, 130.9, 124.5, 123.7 (*aryl C*), 61.5, 57.2 (*Cage C*), 14.6; ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.2 (2B), -6.4 (1B) (*B-C*), -9.1 (1B), -11.1 (1B), -12.5 (2B), -13.1 (3B).



4b

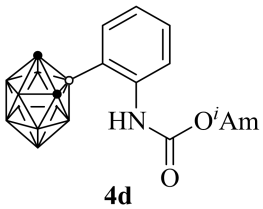
^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.78-7.76 (d, 1H, *J* = 10 Hz), 7.43-7.40 (m, 1H), 7.36-7.35 (d, 1H, *J* = 10 Hz), 7.31 (s, 1H), 7.15-7.12 (m, 1H), 5.04-4.99 (m, 1H, *OCH*), 3.88 (s, 2H, *Cage C-H*), 1.32-1.30 (d, 6H, *J* = 10 Hz, *CH_3*); ^{13}C{^{1}H} NMR

(125 MHz, $CDCl_3$, *ppm*): δ 154.4 (*C=O*), 142.1, 133.9, 130.9, 124.7, 124.2 (*aryl C*), 69.1, 57.1 (*Cage C*), 22.1; $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -2.2 (2B), -6.3 (1B) (*B-C*), -9.0 (1B), -11.1 (1B), -12.6 (2B), -13.2 (3B).



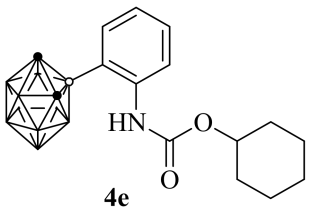
4c

^1H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.79-7.78 (m, 1H), 7.46 (s, 1H), 7.42-7.39 (dd, 1H, *J* = 5 Hz, 5 Hz), 7.34-7.33 (d, 1H, *J* = 5 Hz), 7.14-7.11 (dd, 1H, *J* = 5Hz, 5 Hz), 4.19-4.16 (dd, 2H, *J* = 5 Hz, 5 Hz, *OCH_2*), 3.87 (s, 2H, *Cage C-H*), 1.77-1.64 (m, 2H, *CH_2*), 1.46-1.39 (m, 2H, *CH_2*), 0.98-0.95 (dd, 3H, *J* = 5 Hz, 5 Hz, *CH_3*); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, *ppm*): δ 154.8 (*C=O*), 142.1, 133.7, 130.9, 124.6, 123.8 (*aryl C*), 65.4, 57.2 (*Cage C*), 31.0, 19.0, 13.7; $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -2.1 (2B), -6.4 (1B) (*B-C*), -9.1 (1B), -11.1 (1B), -12.6 (2B), -13.1 (3B).



4d

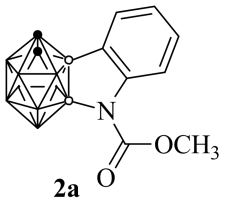
^1H NMR (600 MHz, $CDCl_3$, *ppm*): δ 7.78-7.76 (d, 1H, *J* = 12 Hz), 7.48 (s, 1H), 7.42-7.37 (m, 1H), 7.34-7.33 (d, 1H, *J* = 12 Hz), 7.14-7.10 (m, 1H), 4.22-4.19 (dd, 2H, *J* = 12 Hz, 12 Hz, *OCH_2*), 3.88 (s, 2H, *Cage C-H*), 1.76-1.70 (m, 1H, *CH*), 1.61-1.56 (m, 2H, *CH_2*), 0.96-0.94 (dd, 6H, *J* = 12 Hz, *CH_3*); $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, *ppm*): δ 154.7 (*C=O*), 142.1, 133.6, 130.9, 124.6, 123.8 (*aryl C*), 70.1 (*OCH_2*), 64.2, 57.2 (*Cage C*), 37.6, 25.1, 22.5; $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -2.1 (2B), -6.4 (1B) (*B-C*), -9.1 (1B), -11.1 (1B), -12.6 (2B), -13.1 (3B).



4e

^1H NMR (500 MHz, $CDCl_3$, *ppm*): δ 7.76-7.75 (d, 1H, *J* = 5 Hz), 7.43-7.40 (m, 1H),

7.38-7.37 (d, 1H, *J* = 5 Hz), 7.31 (s, 1H), 7.15-7.12 (m, 1H), 4.78-4.73 (m, 1H, *OCH*), 3.89 (s, 2H, *Cage C-H*), 1.93-1.89 (m, 2H), 1.76-1.74 (m, 2H), 1.52-1.47 (m, 2H), 1.43-1.35 (m, 2H), 1.33-1.27 (m, 2H); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, *ppm*): δ 154.4 (*C=O*), 142.0, 134.0, 130.9, 124.7, 124.3 (*aryl C*), 73.8 (*OCH*), 57.1 (*Cage C*), 31.8, 25.4, 23.7; $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -2.3 (2B), -6.5 (1B) (*B-C*), -9.1 (1B), -11.2 (1B), -12.6 (2B), -13.3 (3B).



2a

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.62-8.61 (d, 1H, *J* = 10 Hz), 7.47-7.44 (dd, 1H, *J* = 10 Hz, 10 Hz), 7.33-7.32 (d, 1H, *J* = 10 Hz), 7.08-7.05 (dd, 1H, *J* = 10 Hz, 10 Hz), 3.99 (s, 2H, *Cage C-H*), 3.81 (s, 3H, *OCH_3*); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, *ppm*): δ 157.6, 155.5, 130.0, 126.1, 121.5, 119.0 (*aryl C*), 52.4, 50.3 (*Cage C*), 44.0 (*OCH_3*); $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -3.4 (2B), -2.9 (2B), -4.5 (1B), -11.5 (2B), -15.8 (2B), -20.0 (1B). HRMS (ESI) m/z calcd for $C_{10}B_{10}H_{16}NO_2^-$ $(M-H)^-$ 291.21534, found 291.21472.

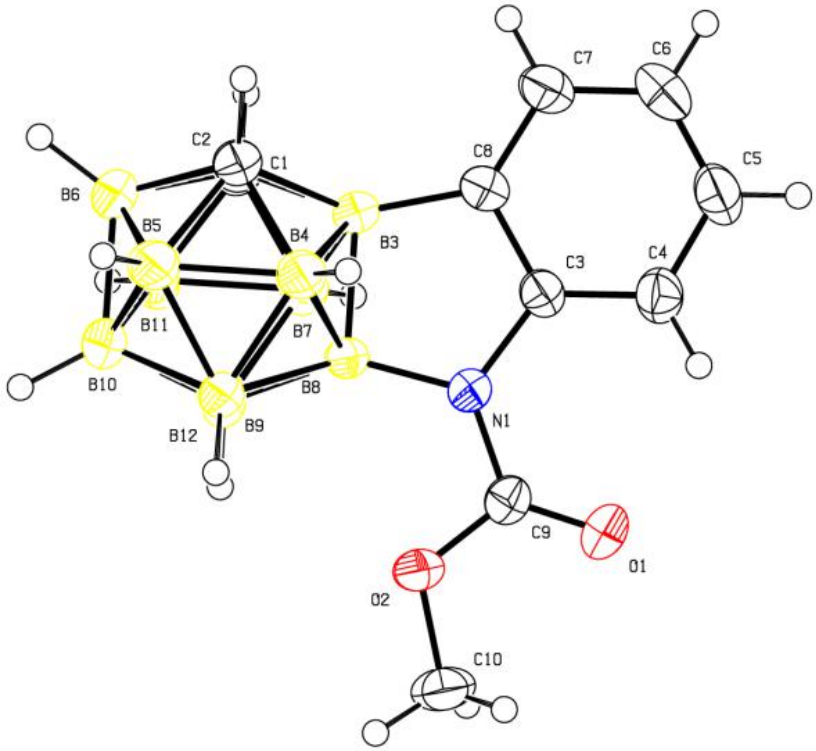
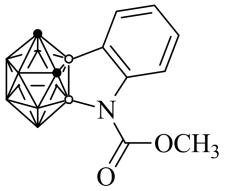


Figure S1. Crystal Structures of 2a.



3a

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.48-8.47 (d, 1H, *J* = 10 Hz), 7.48-7.43 (m, 2H), 7.10-7.07 (m, 1H), 4.04 (s, 1H, *Cage C-H*), 3.84 (s, 3H, *OCH_3*), 3.02 (s, 1H, *Cage C-H*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 156.0, 155.1, 130.5, 128.3, 122.2, 118.7 (*aryl C*), 58.2 (*Cage C*), 52.7 (*OCH_3*), 52.0 (*Cage C*); ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -1.9 (2B), -4.0 (2B), -7.6 (1B), -13.4 (1B), -14.6 (1B), -16.2 (2B), -19.4 (1B). HRMS (ESI) m/z calcd for $C_{10}B_{10}H_{16}NO_2^-$ $(M-H)^-$ 291.21534, found 291.21521.

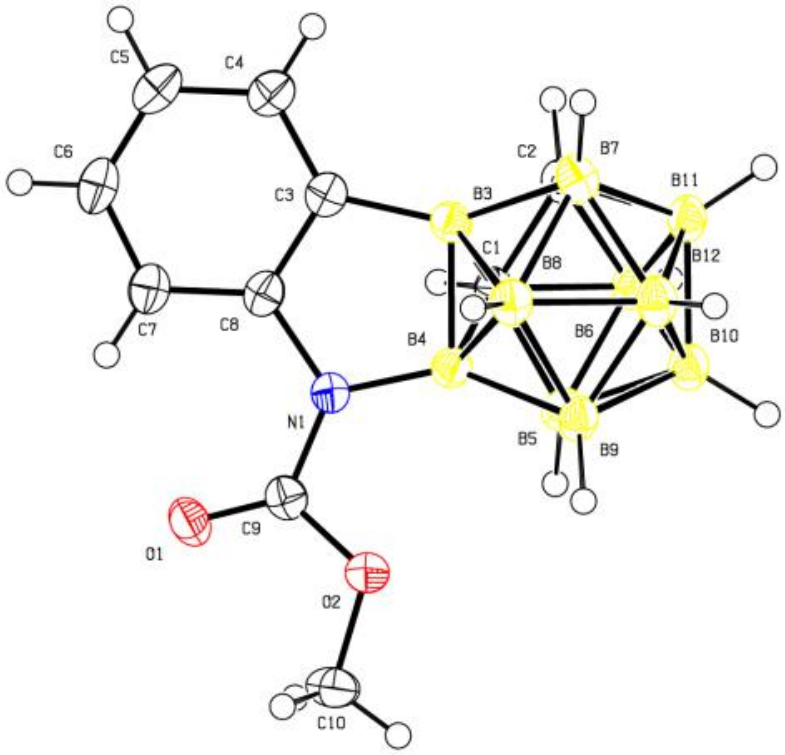
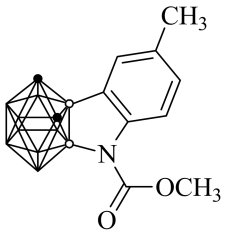


Figure S2. Crystal Structures of 3a.



3b

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.35-8.33 (d, 1H, *J* = 10 Hz), 7.28 (s, 1H), 7.24 (m, 1H), 4.01 (s, 1H, *Cage C-H*), 3.82 (s, 3H, *OCH_3*), 3.01 (s, 1H, *Cage C-H*), 2.34 (s, 3H, *CH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 155.1, 153.8, 131.6, 131.2, 128.8, 118.4 (*aryl C*), 58.3 (*Cage C*), 52.6 (*OCH_3*), 51.9 (*Cage C*), 20.6; ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.0 (1B), -2.7 (1B), -4.2 (2B), -7.6 (1B), -13.4 (1B), -14.7 (1B), -16.3 (2B), -19.5 (1B). HRMS (ESI) m/z calcd for $C_{11}B_{10}H_{18}NO_2^-$ $(M-H)^-$ 305.23099, found 305.23129.

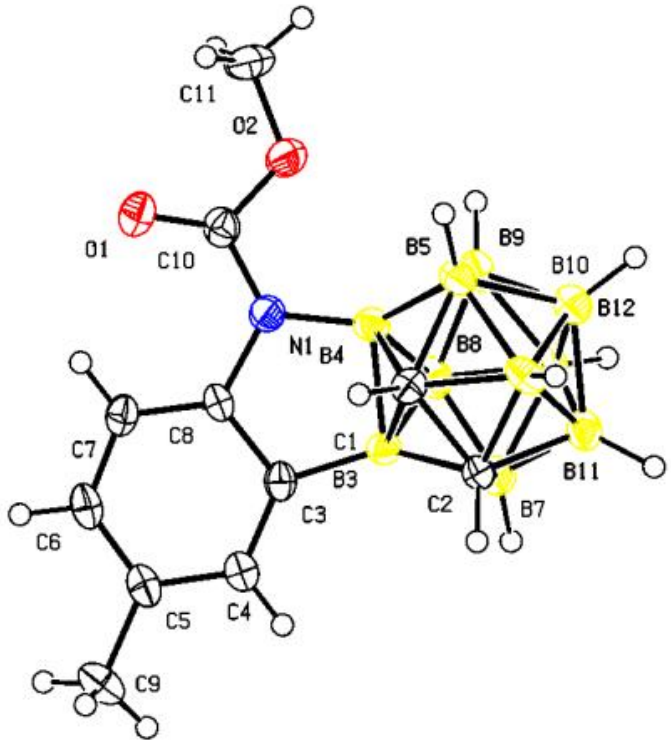
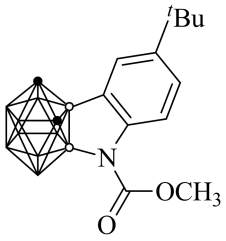


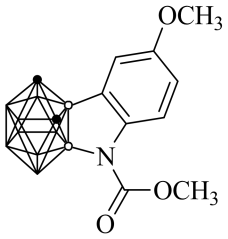
Figure S3. Crystal Structures of 3b.



3c

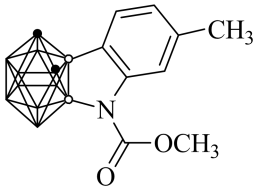
^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.37-8.35 (d, 1H, *J* = 10 Hz), 7.48-7.47 (m, 1H), 7.45 (s,1H), 4.06 (s, 1H, *Cage C-H*), 3.82 (s, 3H, *OCH_3*), 3.04 (s, 1H, *Cage C-H*), 1.33 (s, 9H, *CH_3*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 155.1, 153.7, 144.9,

127.7, 124.8, 118.2 (*aryl C*), 58.4 (*Cage C*), 52.6 (*OCH_3*), 51.9 (*Cage C*), 34.3, 31.5; $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -2.0 (1B), -2.9 (1B), -4.3 (2B), -7.7 (1B), -13.6 (1B), -14.8 (1B), -16.5 (2B), -19.6 (1B). HRMS (ESI) m/z calcd for $C_{14}B_{10}H_{24}NO_2^-$ $(M-H)^-$ 347.27794, found 347.27808.



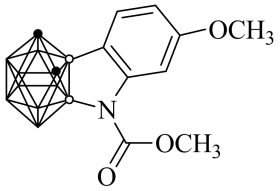
3d

^1H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.40-8.38 (m, 1H), 7.00-6.98 (m, 2H), 4.02 (s, 1H, *Cage C-H*), 3.83-3.81 (m, 6H, *OCH_3*), 3.03 (s, 1H, *Cage C-H*); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, *ppm*): δ 155.2, 154.8, 149.6, 119.6, 115.9, 113.5 (*aryl C*), 58.3 (*Cage C*), 55.7 (*OCH_3*), 52.6 (*OCH_3*), 51.9 (*Cage C*); $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -1.8 (1B), -2.5 (1B), -4.0 (1B), -4.9 (1B), -7.5 (1B), -13.4 (1B), -14.6 (1B), -16.3 (2B), -19.5 (1B). HRMS (ESI) m/z calcd for $C_{11}B_{10}H_{18}NO_3^-$ $(M-H)^-$ 321.22590, found 321.22592.



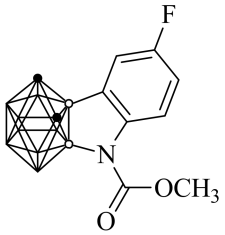
3e

^1H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.34 (s, 1H), 7.35-7.34 (d, 1H, *J* = 5 Hz), 6.91-6.90 (d, 1H, *J* = 5 Hz), 4.01 (s, 1H, *Cage C-H*), 3.83 (s, 3H, *OCH_3*), 3.00 (s, 1H, *Cage C-H*), 2.40 (s, 3H, *CH_3*); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, *ppm*): δ 156.3, 155.2, 141.0, 127.9, 123.1, 119.5 (*aryl C*), 58.5 (*Cage C*), 52.6 (*OCH_3*), 51.9 (*Cage C*), 22.1; $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -1.8 (1B), -2.6 (1B), -4.1 (2B), -7.4 (1B), -13.4 (1B), -14.7 (1B), -16.2 (2B), -19.4 (1B). HRMS (ESI) m/z calcd for $C_{11}B_{10}H_{18}NO_2^-$ $(M-H)^-$ 305.23099, found 305.23080.



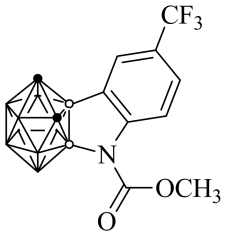
3f

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.18-8.17 (m, 1H), 7.34-7.33 (d, 1H, *J* = 10 Hz), 6.66-6.64 (m, 1H), 4.00 (s, 1H, *Cage C-H*), 3.85 (s, 3H, *OCH₃*), 3.84 (s, 3H, *OCH₃*), 3.03 (s, 1H, *Cage C-H*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 162.0, 157.8, 155.2, 128.7, 109.3, 104.5 (*aryl C*), 58.8 (*Cage C*), 55.4 (*OCH₃*), 52.6 (*OCH₃*), 51.8 (*Cage C*); ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -1.8 (1B), -2.6 (1B), -4.2 (2B), -7.3 (1B), -13.4 (1B), -14.9 (1B), -16.4 (2B), -19.4 (1B). HRMS (ESI) m/z calcd for $C_{11}B_{10}H_{18}NO_3^-$ $(M-H)^-$ 321.22590, found 321.22559.



3h

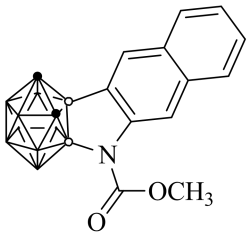
^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.46-8.44 (m, 1H), 7.17-7.12 (m, 2H), 4.04 (s, 1H, *Cage C-H*), 3.84 (s, 3H, *OCH₃*), 3.03 (s, 1H, *Cage C-H*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 158.2 (*J* = 242.5 Hz), 155.1, 152.0, 119.9 (*J* = 7.5 Hz), 117.1 (*J* = 22.5 Hz), 114.8 (*J* = 22.5 Hz) (*aryl C*), 58.0 (*Cage C*), 52.7 (*OCH₃*), 52.0 (*Cage C*); ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -1.8 (2B), -3.9 (1B), -5.4 (1B), -7.6 (1B), -13.2 (1B), -14.2 (1B), -16.1 (2B), -19.3 (1B). HRMS (ESI) m/z calcd for $C_{10}B_{10}H_{15}NO_2F^-$ $(M-H)^-$ 309.20592, found 309.20621.



3i

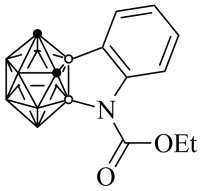
^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.60-8.58 (d, 1H, *J* = 10 Hz), 7.73 (s, 1H), 7.70-7.69 (m, 1H), 4.10 (s, 1H, *Cage C-H*), 3.87 (s, 3H, *OCH₃*), 3.03 (s, 1H, *Cage*

C-H); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, *ppm*): δ 158.5, 154.9, 133.1, 132.1, 127.7 (*J* = 3.8 Hz), 125.4 (*J* = 3.8 Hz), 124.3 (*J* = 32.5 Hz), 118.6 (*aryl C*), 57.9 (*Cage C*), 53.0 (*OCH_3*), 52.3 (*Cage C*); $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -1.9 (2B), -3.7 (1B), -5.4 (1B), -7.6 (1B), -13.2 (1B), -14.0 (1B), -16.0 (2B), -19.1(1B). HRMS (ESI) m/z calcd for $C_{11}B_{10}H_{15}NO_2F_3^-$ $(M-H)^-$ 359.20272, found 359.20285.



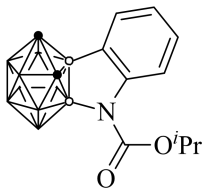
3j

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.89 (s, 1H), 7.97 (s, 1H), 7.87-7.86 (d, 1H, *J* = 10 Hz), 7.80-7.79 (d, 1H, *J* = 10 Hz), 7.52-7.49 (m, 1H), 7.44-7.41 (m, 1H), 4.11 (s, 1H, *Cage C-H*), 3.89 (s, 3H, *OCH_3*), 3.15 (s, 1H, *Cage C-H*); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, *ppm*): δ 155.3, 151.2, 134.7, 128.6, 128.3, 127.7, 127.2, 125.1, 115.7, 100.9 (*aryl C*), 59.0 (*Cage C*), 52.7 (*OCH_3*), 52.3 (*Cage C*); $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -1.4 (1B), -2.3 (1B), -3.8 (1B), -5.0 (1B), -7.2 (1B), -13.8 (2B), -16.0 (2B), -19.3 (1B). HRMS (ESI) m/z calcd for $C_{14}B_{10}H_{18}NO_2^-$ $(M-H)^-$ 341.23099, found 341.23138.



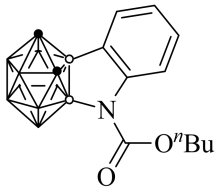
5a

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.49-8.47 (d, 1H, *J* = 10 Hz), 7.48-7.42 (m, 2H), 7.09-7.06 (m, 1H), 4.31-4.25 (m, 2H, *OCH_2*), 4.04 (s, 1H, *Cage C-H*), 3.03 (s, 1H, *Cage C-H*), 1.37-1.34 (m, 3H, *CH_3*); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, *ppm*): δ 156.1, 154.6, 130.5, 128.3, 122.1, 118.7 (*aryl C*), 61.8 (*OCH_2*), 58.3 (*Cage C*), 52.0 (*Cage C*), 14.2; $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -1.8 (2B), -4.1 (2B), -7.5 (1B), -13.2 (1B), -14.5 (1B), -16.2 (2B), -19.4 (1B). HRMS (ESI) m/z calcd for $C_{11}B_{10}H_{18}NO_2^-$ $(M-H)^-$ 305.23099, found 305.23114.



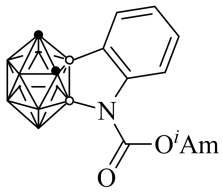
5b

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.50-8.48 (d, 1H, *J* = 10 Hz), 7.47-7.41 (m, 2H), 7.08-7.05 (m, 1H), 5.08-5.03 (m, 1H, *OCH*), 4.03 (s, 1H, *Cage C-H*), 3.01 (s, 1H, *Cage C-H*), 1.35-1.34 (d, 6H, *J* = 5 Hz, *CH₃*); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 156.1, 154.1, 130.5, 128.3, 122.0, 118.6 (*aryl C*), 69.6, 58.2 (*Cage C*), 52.0 (*Cage C*), 22.0, 21.9; ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.1 (2B), -4.3 (1B), -5.0 (1B), -7.8 (1B), -13.4 (1B), -14.7 (1B), -16.4 (2B), -19.6 (1B). HRMS (ESI) m/z calcd for $C_{12}B_{10}H_{20}NO_2^-$ $(M-H)^-$ 319.24664, found 319.24670.



5c

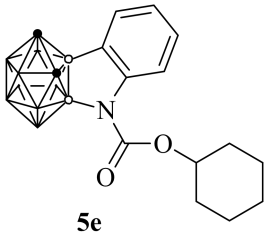
^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.50-8.48 (d, 1H, *J* = 10 Hz), 7.48-7.42 (m, 2H), 7.09-7.06 (m, 1H), 4.26-4.18 (m, 2H, *OCH₂*), 4.04 (s, 1H, *Cage C-H*), 3.02 (s, 1H, *Cage C-H*), 1.74-1.69 (m, 2H, *CH₂*), 1.51-1.43 (m, 2H, *CH₂*), 0.98-0.95 (dd, 3H, *J* = 5 Hz, 5 Hz, *CH₃*) ; ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, *ppm*): δ 156.1, 154.8, 130.5, 128.3, 122.1, 118.7 (*aryl C*), 65.8 (*OCH₂*), 58.3 (*Cage C*), 52.0 (*Cage C*), 30.7, 19.2, 13.7; ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$, *ppm*): -2.1 (2B), -4.3 (2B), -7.8 (1B), -13.5 (1B), -14.7 (1B), -16.4 (2B), -19.6 (1B). HRMS (ESI) m/z calcd for $C_{13}B_{10}H_{22}NO_2^-$ $(M-H)^-$ 333.26229, found 333.26224.



5d

^{1}H NMR (600 MHz, $CDCl_3$, *ppm*): δ 8.50-8.48 (d, 1H, *J* = 12 Hz), 7.48-7.42 (m, 2H), 7.09-7.06 (m, 1H), 4.27-4.24 (m, 2H, *OCH₂*), 4.04 (s, 1H, *Cage C-H*), 3.02 (s, 1H, *Cage C-H*), 1.82-1.77 (m, 1H, *CH*), 1.64-1.60 (m, 2H, *CH₂*), 0.96-0.95 (d, 6H, *J* = 6

Hz, *CH₃*) ; $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$, *ppm*): δ 156.1, 154.8, 130.5, 128.3, 122.1, 118.7 (*aryl C*), 64.6, 58.3 (*Cage C*), 52.0 (*Cage C*), 37.4, 24.9, 22.5, 22.4; $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -2.1 (2B), -4.2 (2B), -7.7 (1B), -13.5 (1B), -14.7 (1B), -16.4 (2B), -19.5 (1B). HRMS (ESI) m/z calcd for $C_{14}H_{25}B_{10}NO_2$ Na^+ $(M+Na)^+$ 370.2781, found 370.2792.



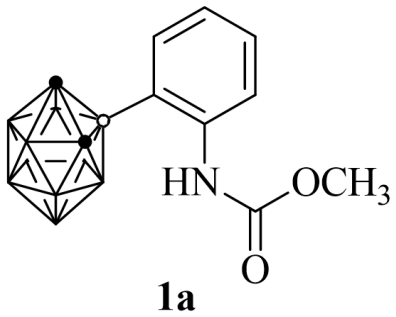
5e

^{1}H NMR (500 MHz, $CDCl_3$, *ppm*): δ 8.51-8.50 (d, 1H, *J* = 10 Hz), 7.47-7.42 (m, 2H), 7.08-7.05 (m, 1H), 4.86-4.81 (m, 1H, *OCH*), 4.03 (s, 1H, *Cage C-H*), 3.02 (s, 1H, *Cage C-H*), 1.94-1.92 (m, 2H, *CH₂*), 1.78-1.77 (m, 2H, *CH₂*), 1.61-1.53 (m, 4H, *CH₂*), 1.43-1.37 (m, 2H, *CH₂*); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, *ppm*): δ 156.2, 130.5, 128.2, 122.0, 118.7, 103.4 (*aryl C*), 74.5, 58.2 (*Cage C*), 52.0 (*Cage C*), 31.6, 25.4, 23.6; $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$, *ppm*): -2.0 (2B), -4.3 (2B), -7.7 (1B), -13.4 (1B), -14.7 (1B), -16.4 (2B), -19.6 (1B). HRMS (ESI) m/z calcd for $C_{15}H_{25}B_{10}NO_2Na^+$ $(M+Na)^+$ 382.2781, found 382.2787.

Table S1. Crystal data and Summary of Data Collection and Refinement for **2a**、**3a** and **3b**.

Compound No.	**2a**	**3a**	**3b**
Formula	$C_{10}H_{17}B_{10}NO_2$	$C_{10}H_{17}B_{10}NO_2$	$C_{11}H_{19}B_{10}NO_2$
Formula weight	291.35	291.35	305.37
Temperature, K	170.0	170.0	170.0
Wavelength, Å	0.71073	0.71073	0.71073
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a, Å	7.0289(5)	10.7495(4)	21.480(2)
b, Å	19.6397(15)	11.4159(5)	12.8355(12)
c, Å	11.4366(9)	12.8872(5)	12.6104(13)
α,deg	90	90	90
β, deg	97.502(3)	107.2450(10)	105.394(3)
γ,deg	90	90	90
V, $Å^3$	1565.3(2)	1510.36(11)	3352.0(6)
Z	4	4	8
D, $g\cdot cm^{-3}$	1.236	1.281	1.210
μ, mm^{-1}	0.071	0.073	0.069
F(000)	600.0	600.0	1264.0
Crystal size,mm^3	0.15 × 0.08 × 0.05	0.15 × 0.08 × 0.05	0.15 × 0.08 × 0.05
Independent reflections	3548	3056	6821
Data/restraints/parameters	3548/0/209	3056/0/209	6821/0/437
R_1	0.0608	0.0552	0.1045
wR_2	0.1711	0.1442	0.2232
Goodness-of-fit on F^2	1.031	1.054	1.055

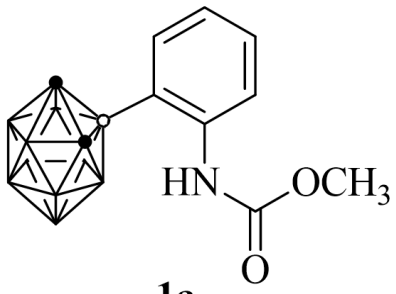
ZCY-1627-H



1a

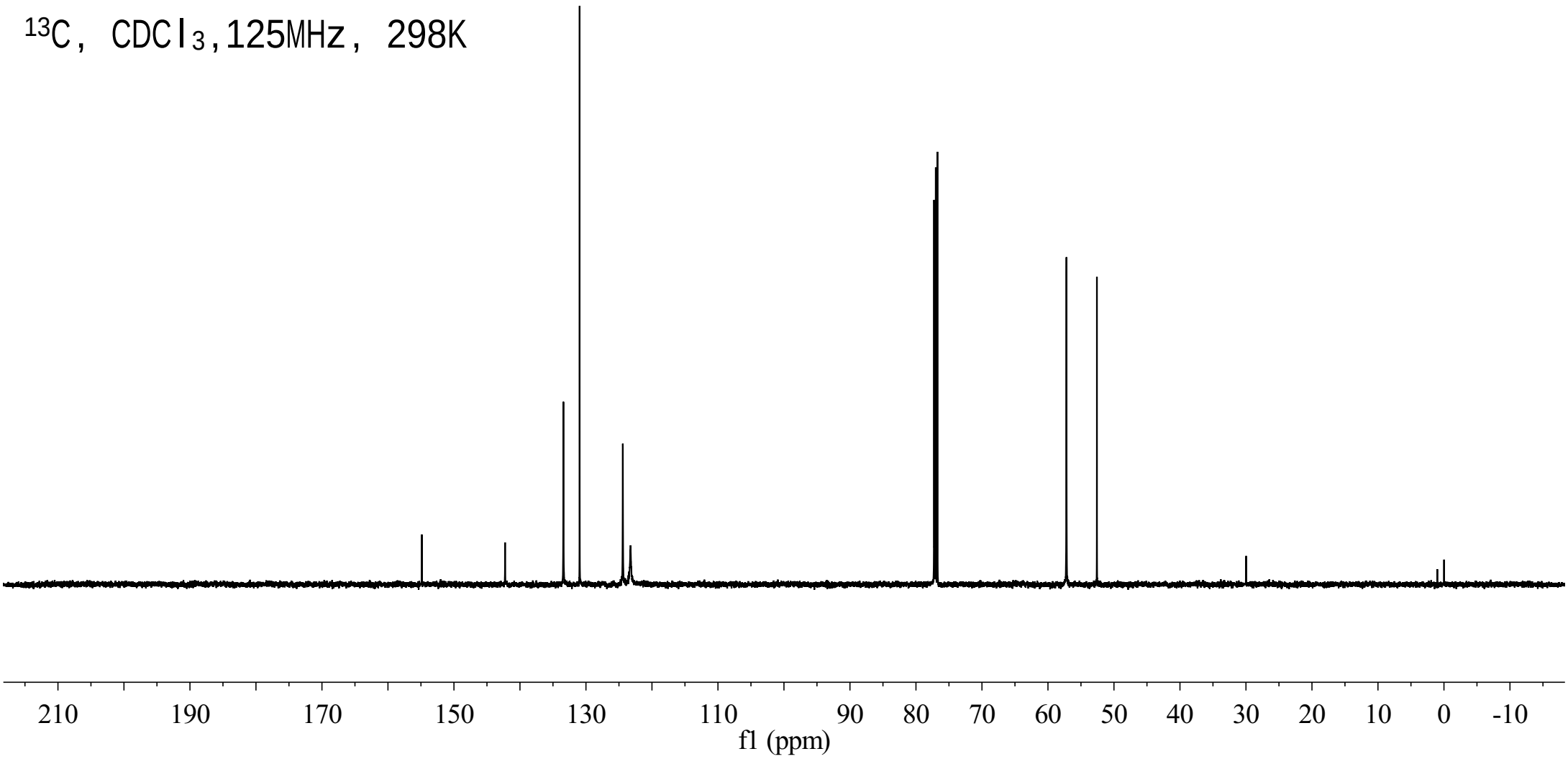
^{1}H, $CDCl_3$, 500MHz, 298K

ZCY-1627-C

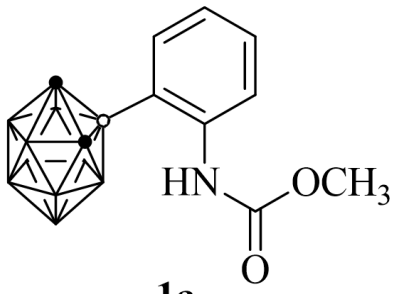


1a

^{13}C, $CDCl_3$, 125MHz, 298K

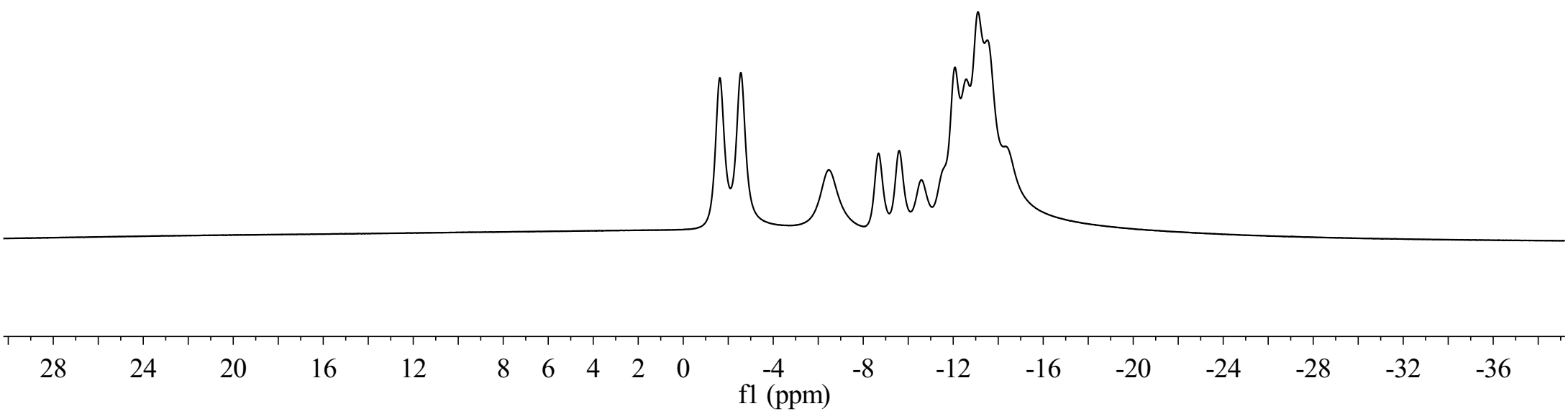


ZCY-1627-B

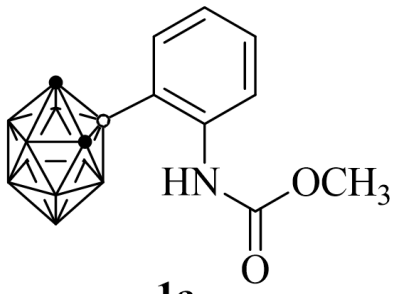


1a

^{11}B, $CDCl_3$, 160MHz, 298K



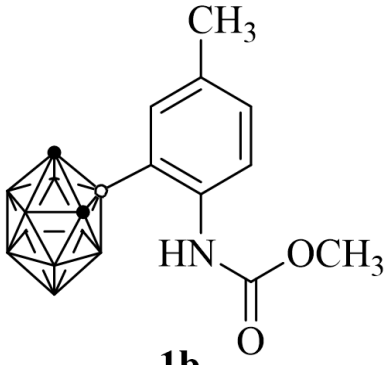
ZCY-1627-B{H}



1a

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

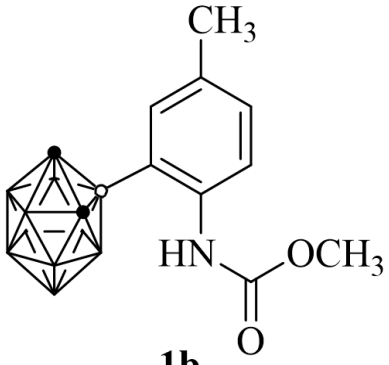
ZCY-1639-H



1b

^{1}H, $CDCl_3$, 500MHz, 298K

ZCY-1639-C



1b

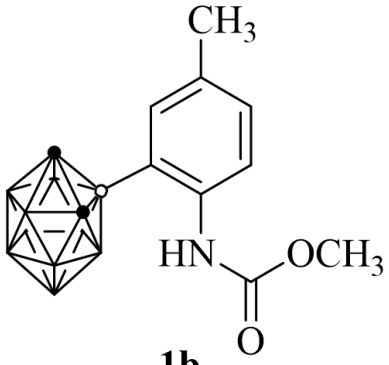
^{13}C, $CDCl_3$, 125MHz, 298K

155.22
139.39
134.27
131.61
124.16
124.12
77.25
77.00
76.75
57.06
52.57
20.87
-0.03

210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

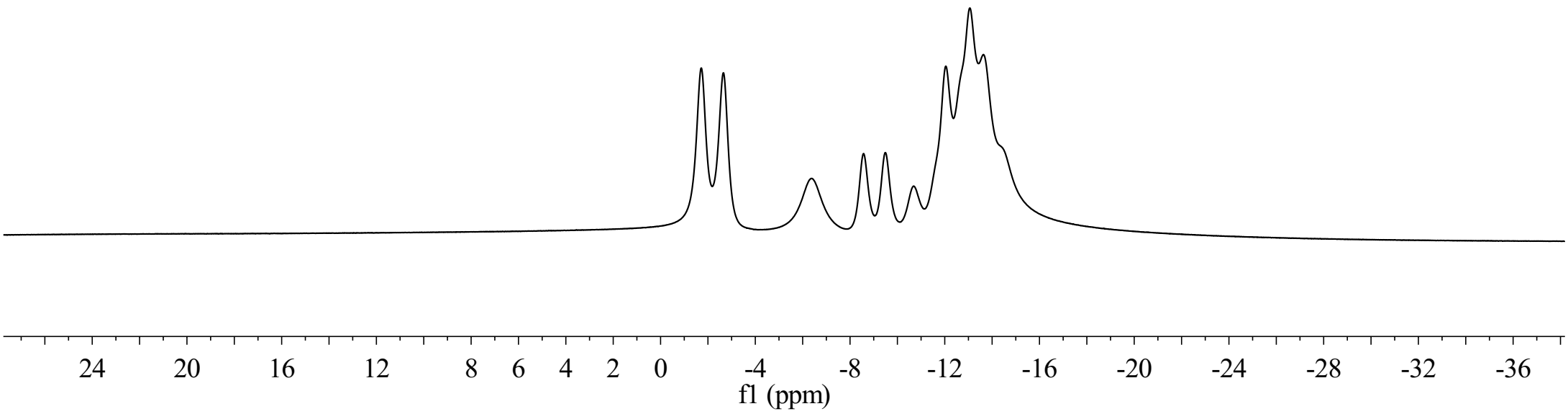
ZCY-1639-B



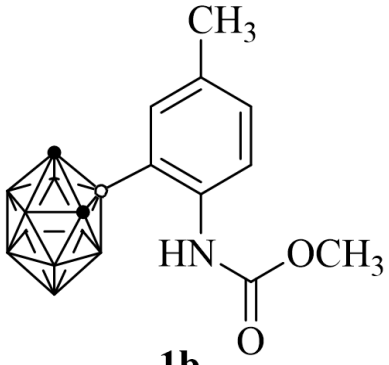
1b

-1.72
-2.65
-6.39
-8.57
-9.49
-10.69
-12.04
-13.06
-13.64

^{11}B, $CDCl_3$, 160MHz, 298K



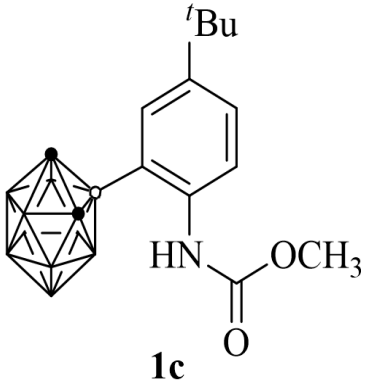
ZCY-1639-B{H}



1b

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

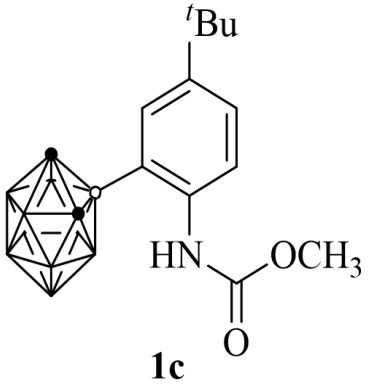
ZCY-1681-H



1c

^{1}H, CDCl$_3$,500MHz, 298K

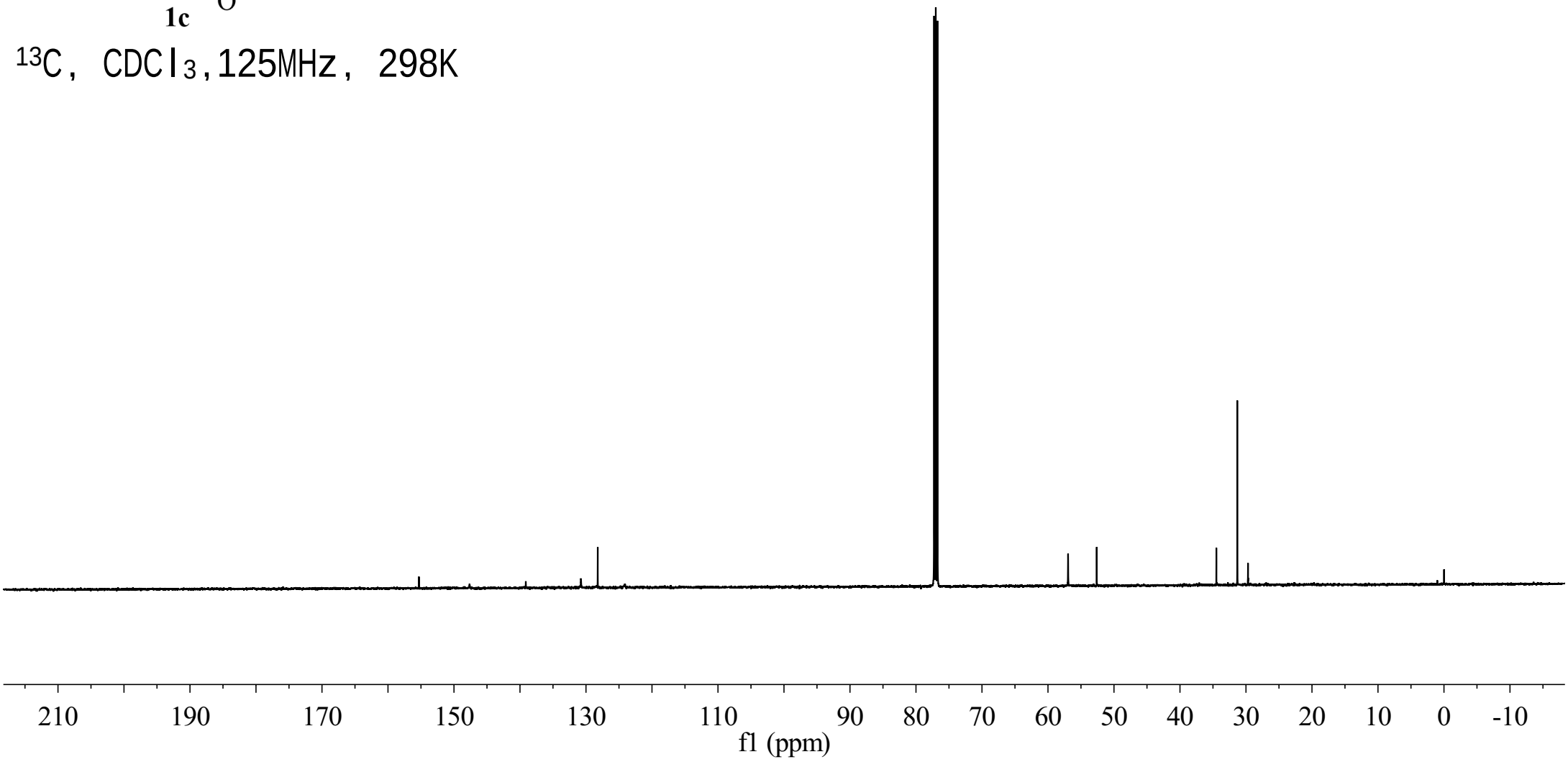
ZCY-1681-C



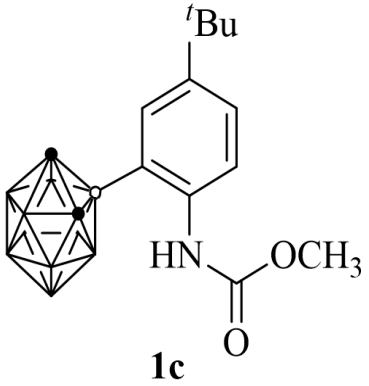
1c

^{13}C, $CDCl_3$, 125MHz, 298K

155.31
147.64
139.12
130.77
128.22
124.10
77.25
77.00
76.75
56.95
52.62
34.49
31.32
-0.02



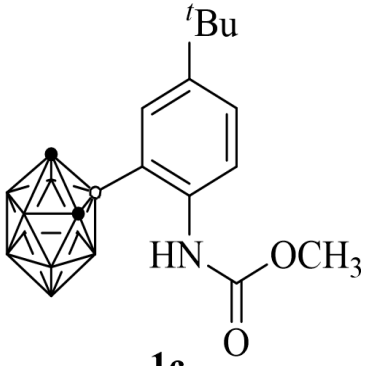
ZCY-1681-B



1c

^{11}B, $CDCl_3$, 160MHz, 298K

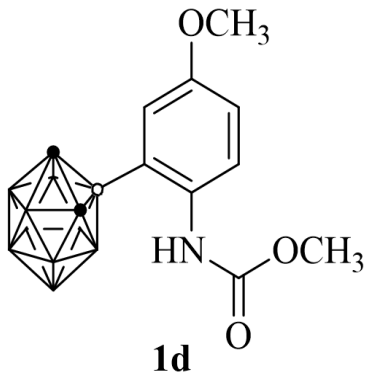
ZCY-1681-B{H}



1c

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

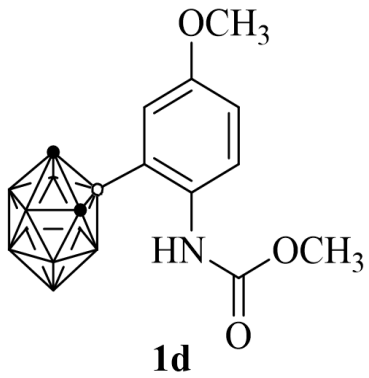
ZCY-1637-H



1d

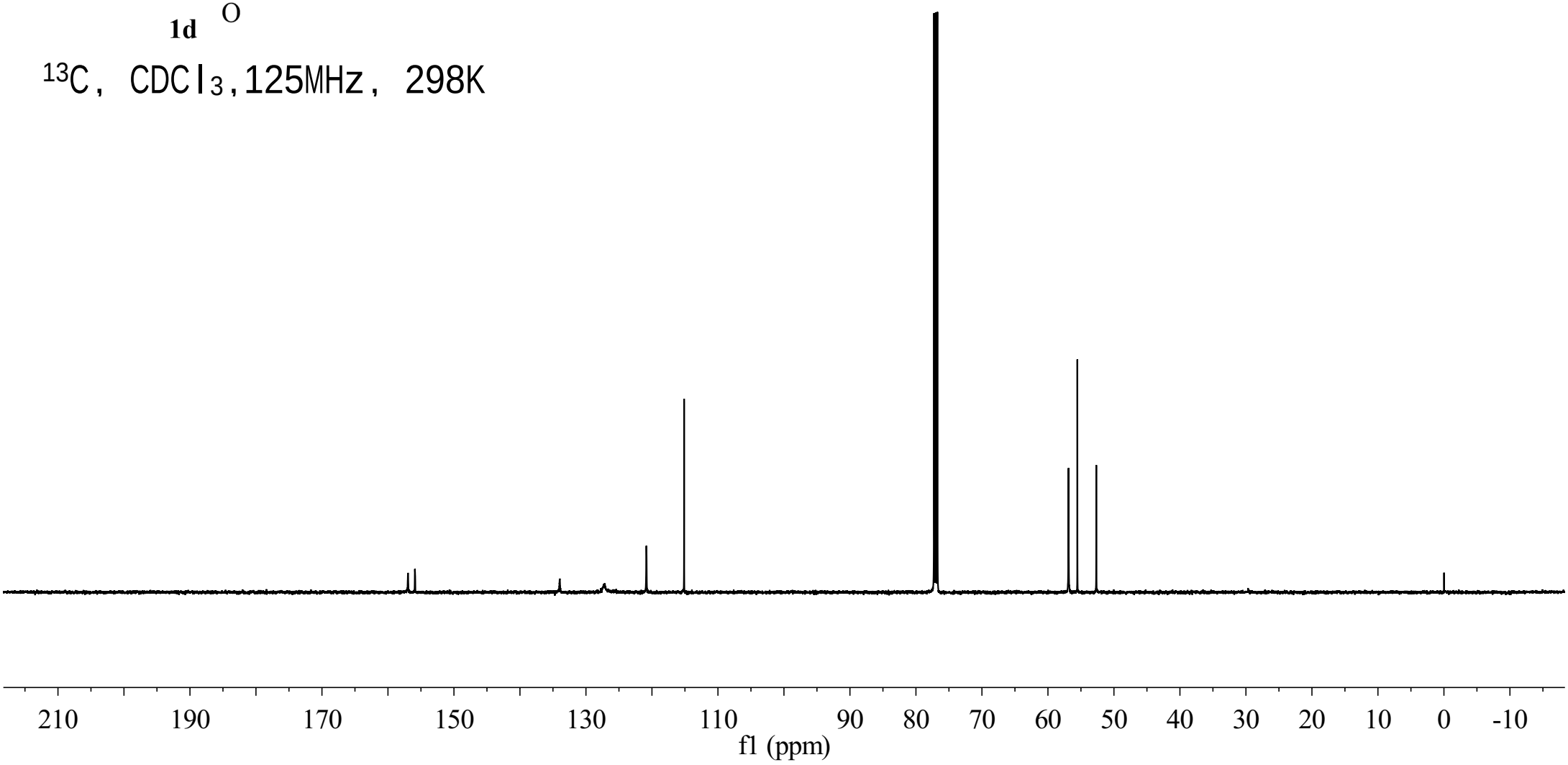
^{1}H, $CDCl_3$, 500MHz, 298K

ZCY-1637-C

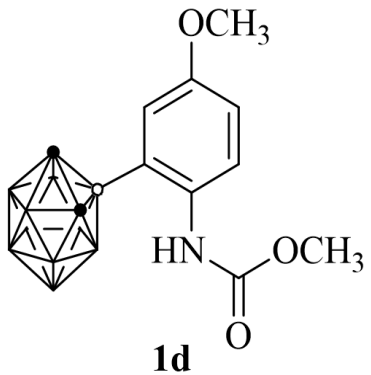


1d

^{13}C, $CDCl_3$, 125MHz, 298K



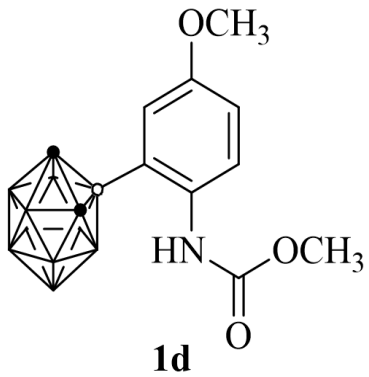
ZCY-1637-B



1d

^{11}B, $CDCl_3$, 160MHz, 298K

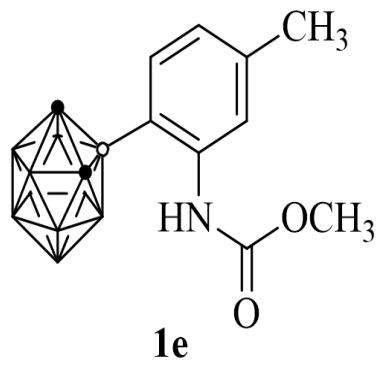
ZCY-1637-B{H}



1d

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

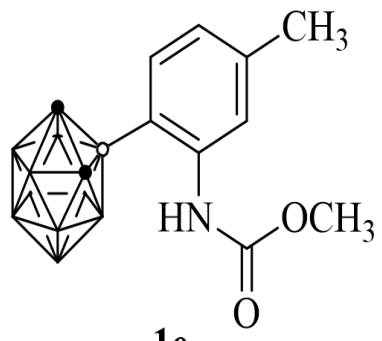
ZCY-1641-H



1e

^{1}H, $CDCl_3$, 500MHz, 298K

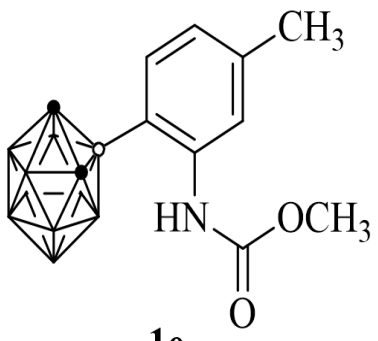
ZCY-1641-C



1e

^{13}C, $CDCl_3$, 125MHz, 298K

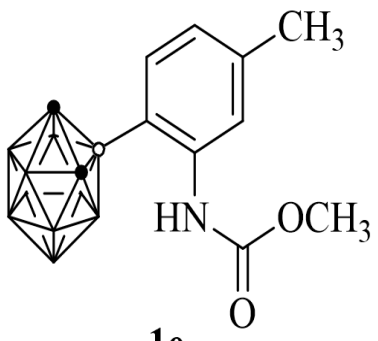
ZCY-1641-B



1e

^{11}B, $CDCl_3$, 160MHz, 298K

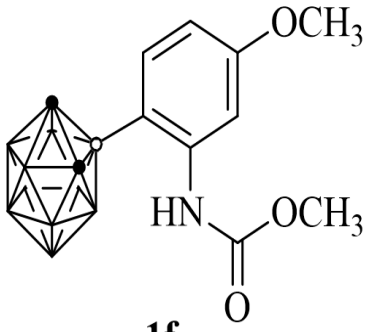
ZCY-1641-B{H}



1e

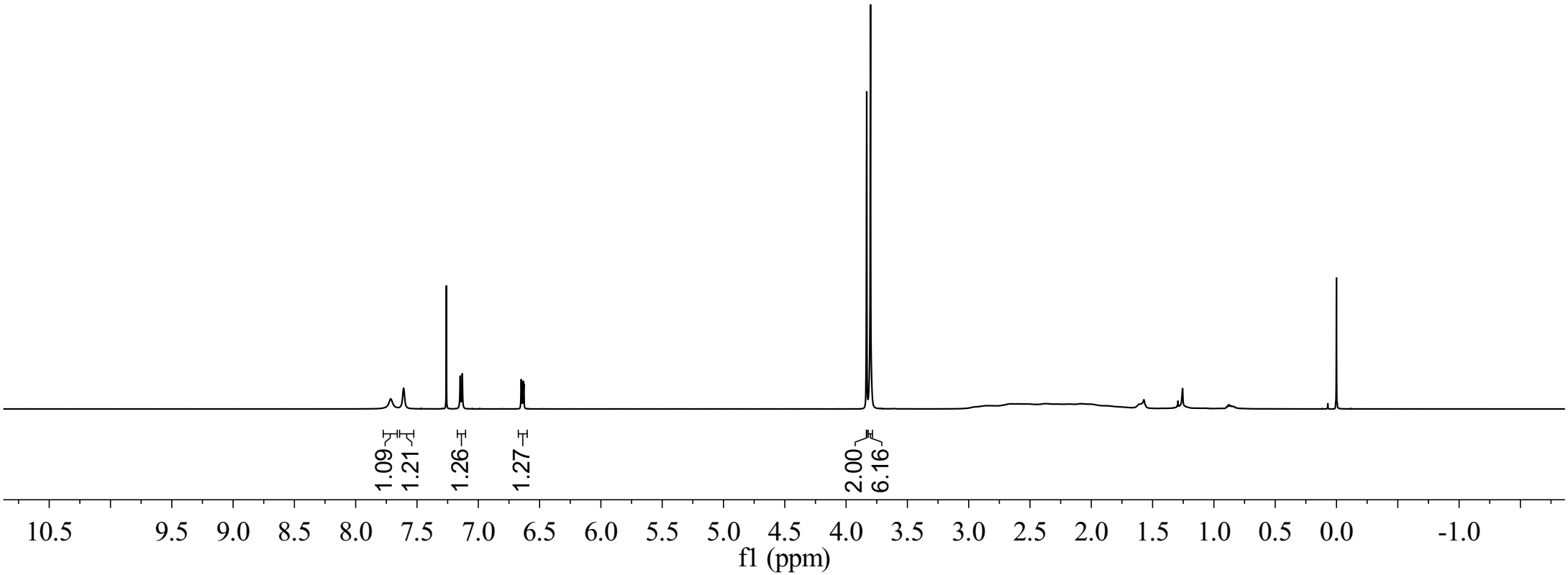
$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

ZCY-1670-H

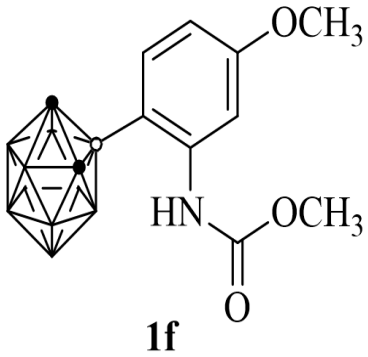


1f

^{1}H, $CDCl_3$, 500MHz, 298K

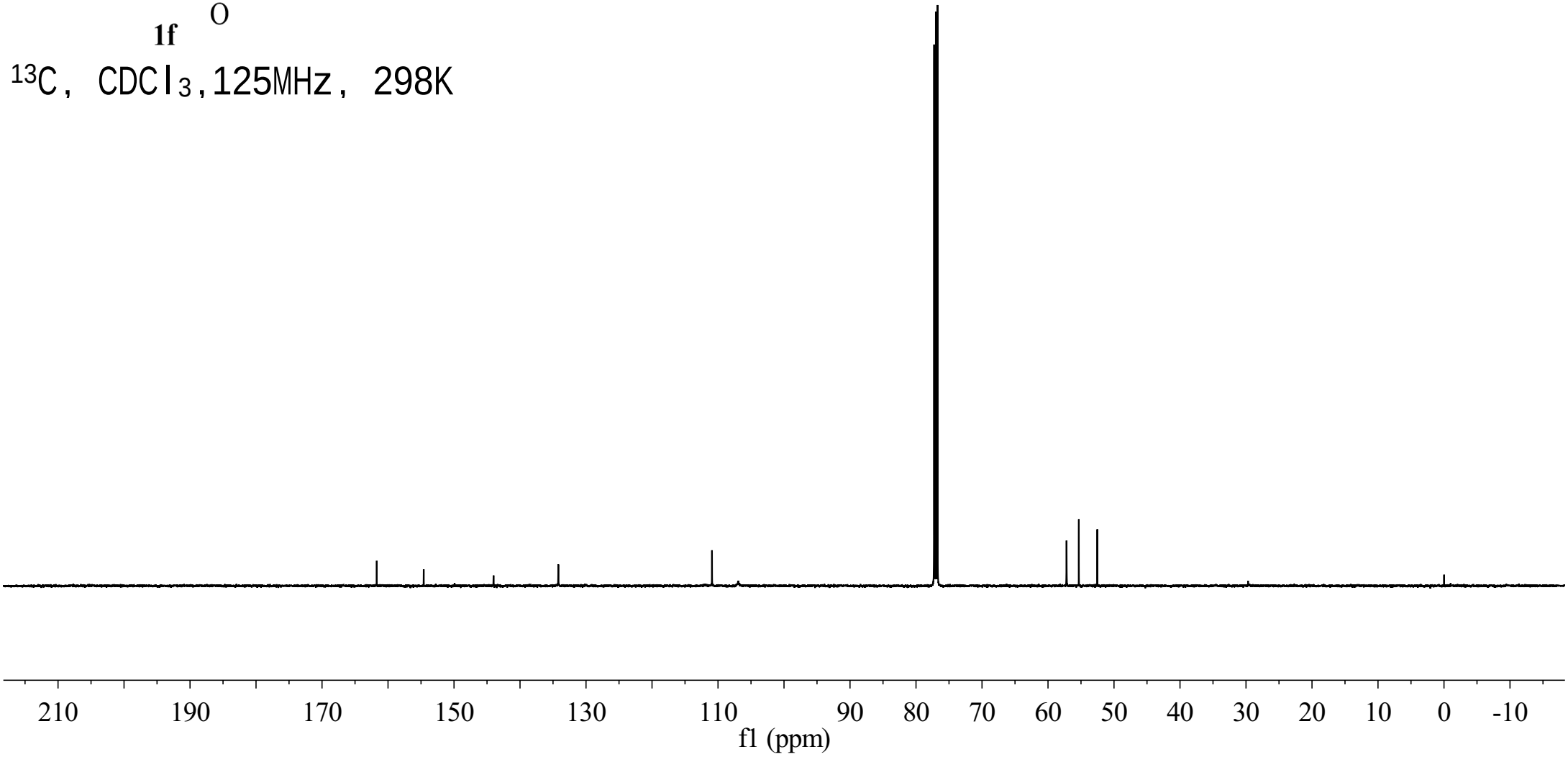


ZCY-1670-C

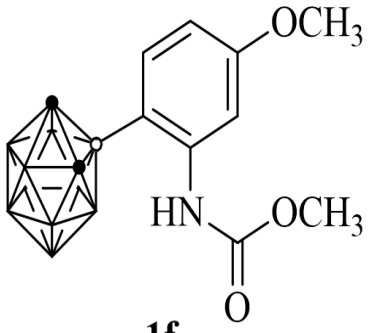


1f

^{13}C, $CDCl_3$, 125MHz, 298K

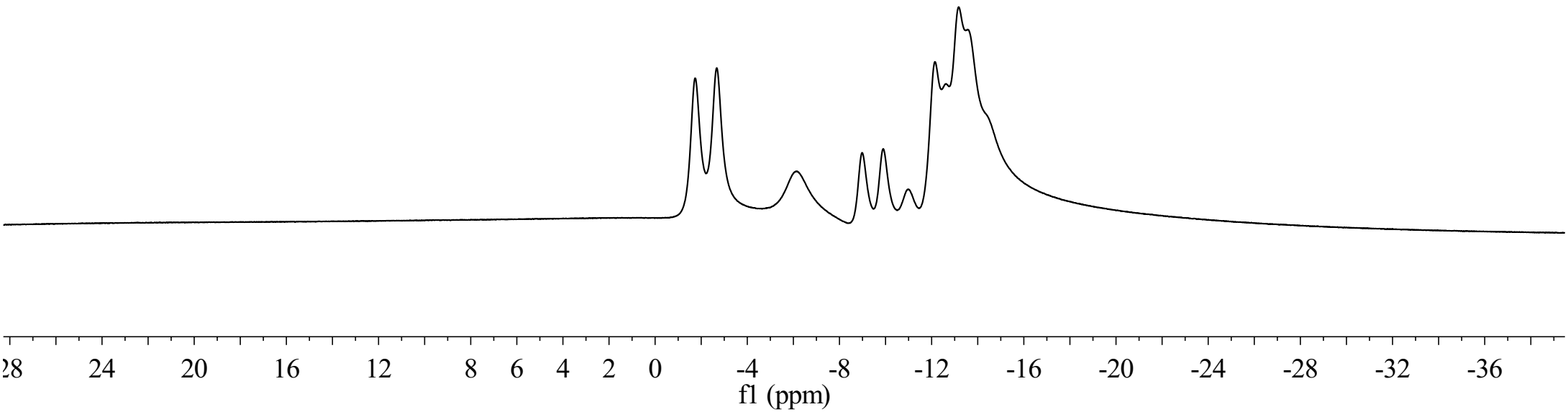


ZCY-1670-B

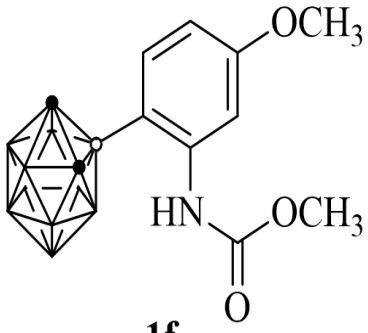


1f

^{11}B, $CDCl_3$, 160MHz, 298K



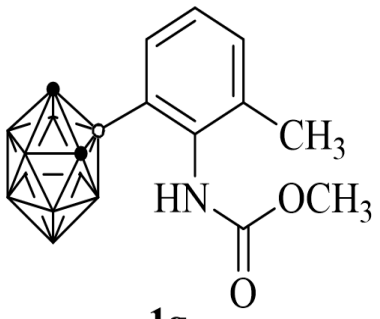
ZCY-1670-B{H}



1f

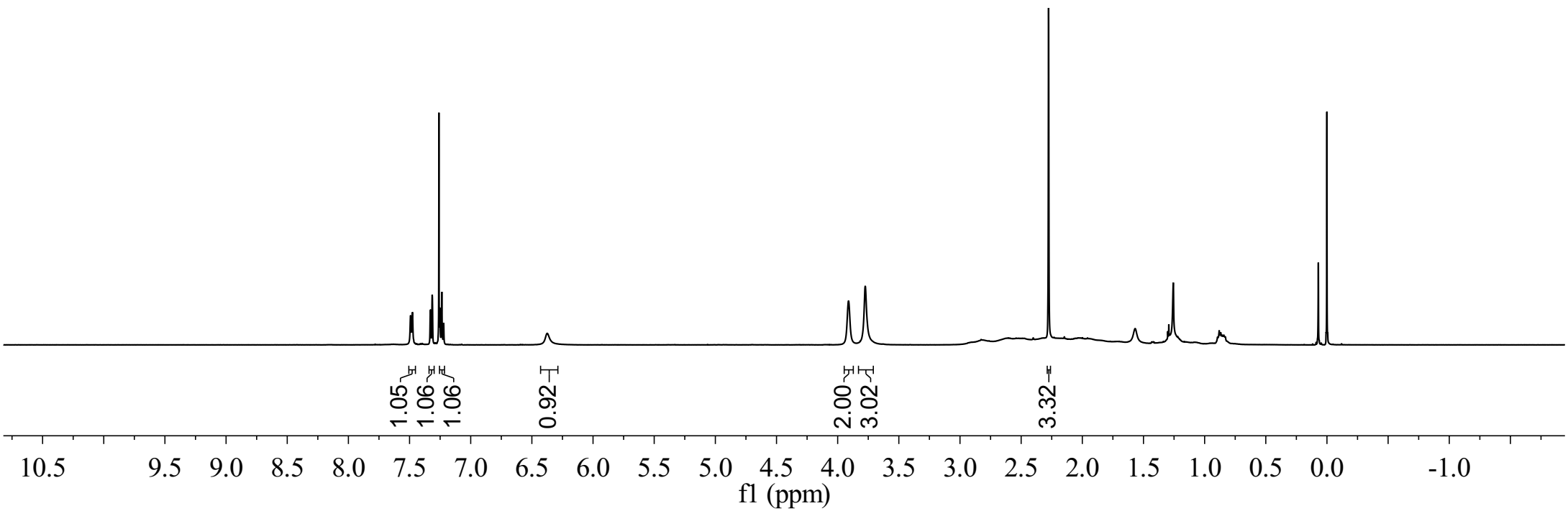
$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

ZCY-1671-H

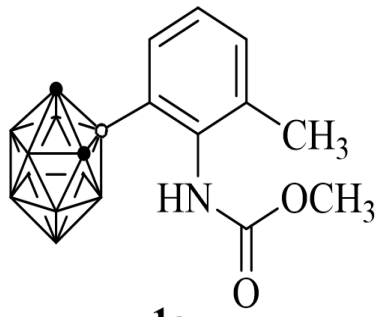


1g

^{1}H, $CDCl_3$, 500MHz, 298K



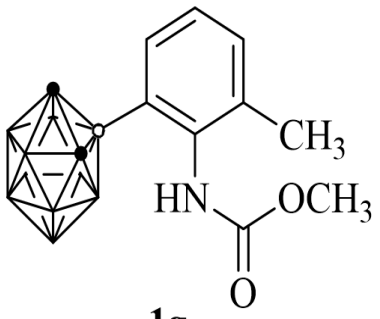
ZCY-1671-C



1g

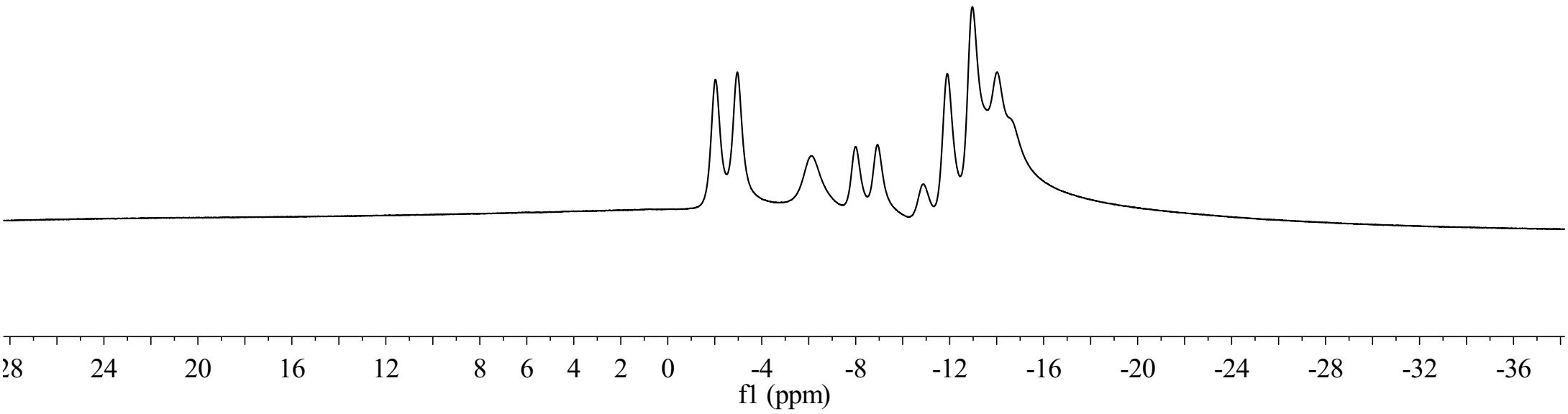
^{13}C, $CDCl_3$, 125MHz, 298K

ZCY-1671-B

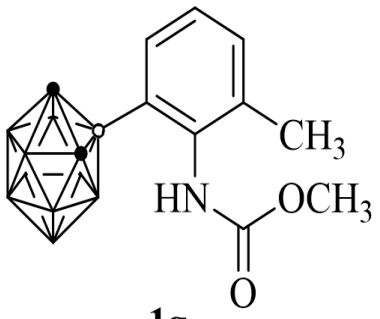


1g

^{11}B, $CDCl_3$, 160MHz, 298K



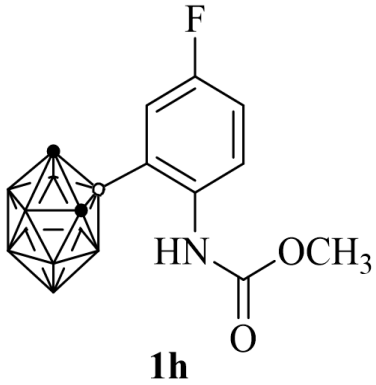
ZCY-1671-B{H}



1g

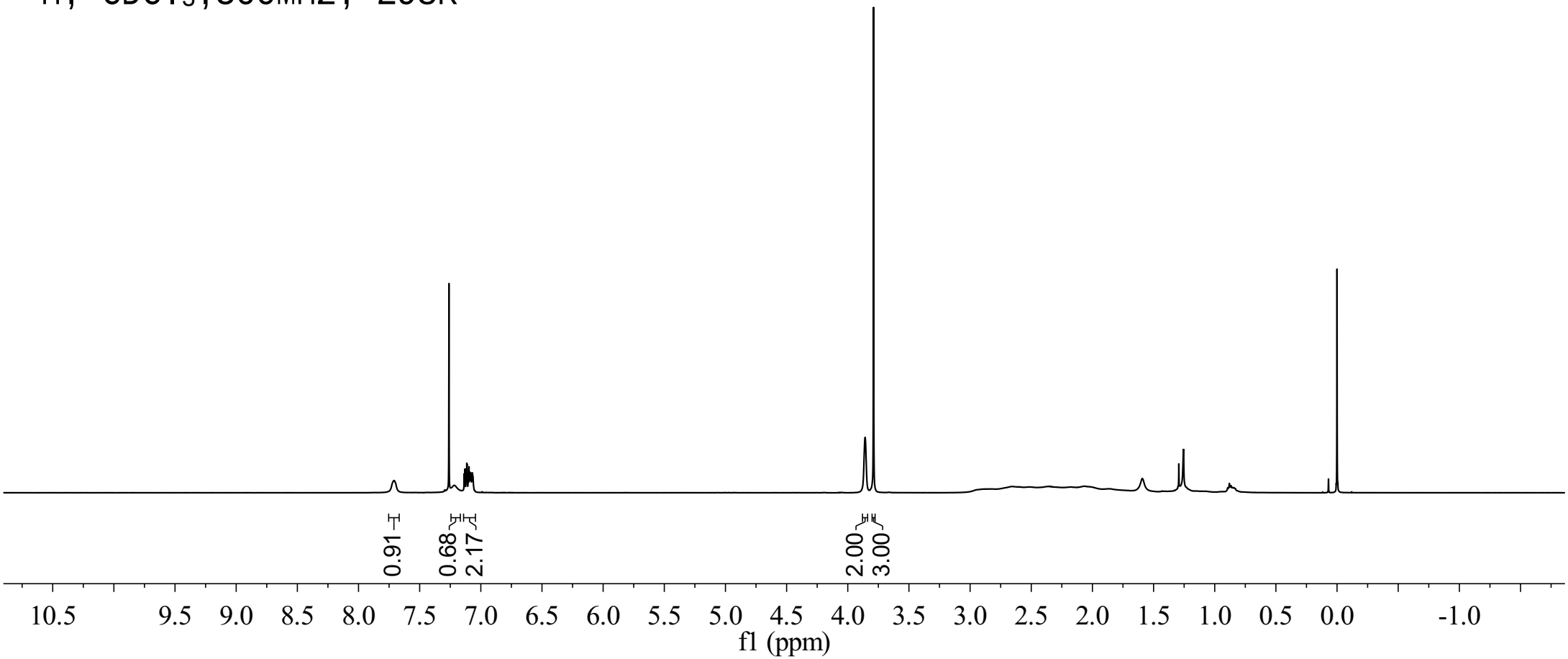
$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

ZCY-1640-H

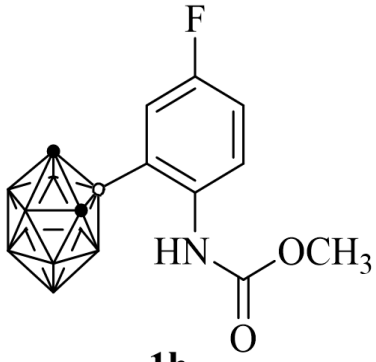


1h

^{1}H, $CDCl_3$, 500MHz, 298K

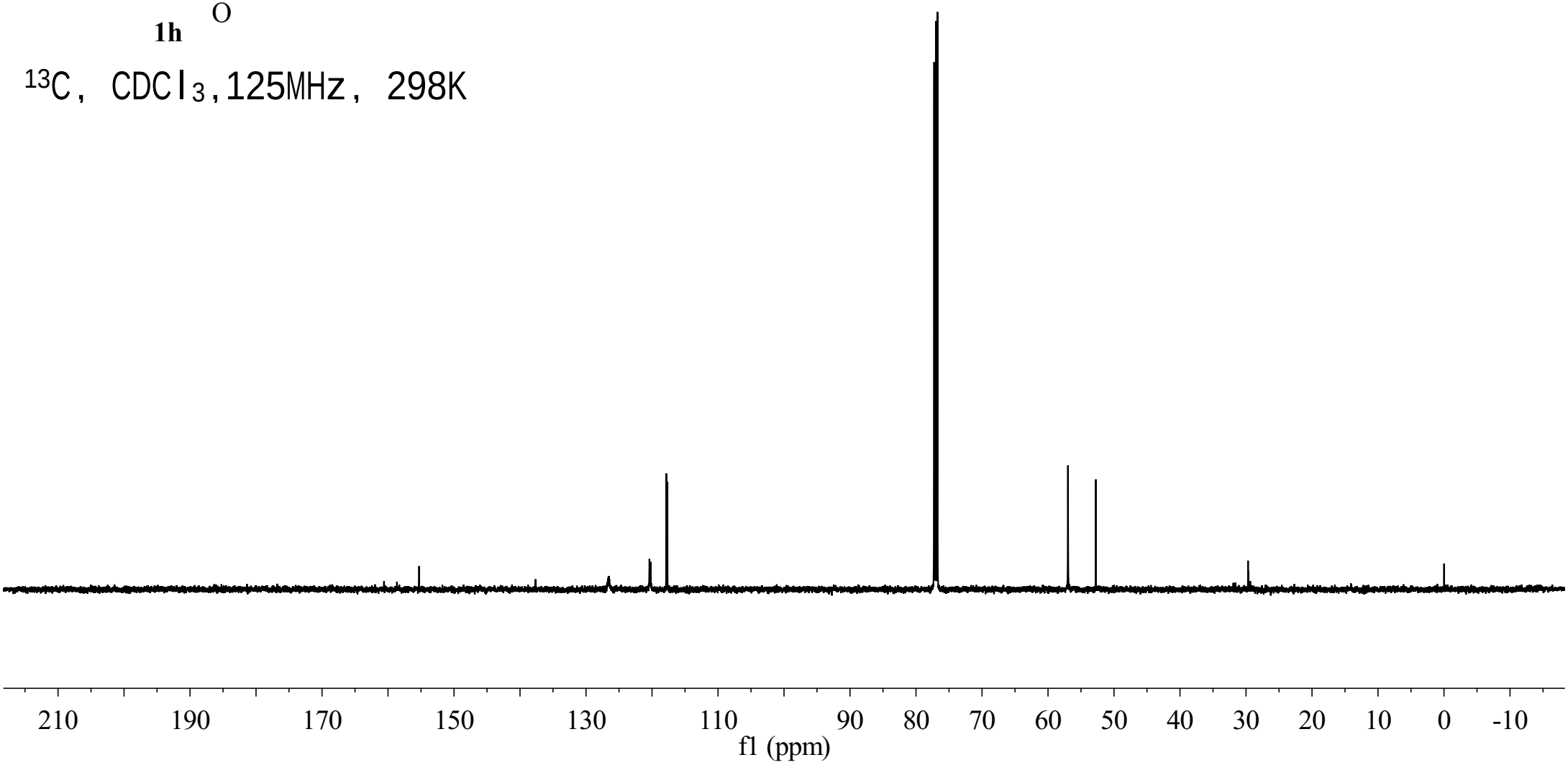


ZCY-1640-C

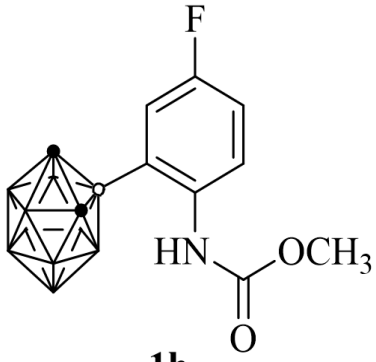


1h

^{13}C, $CDCl_3$, 125MHz, 298K



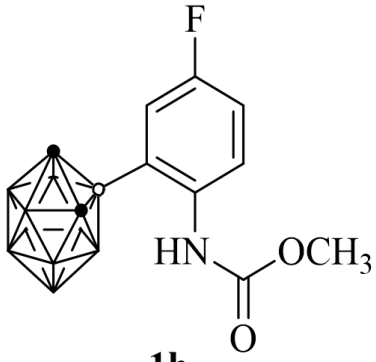
ZCY-1640-B



1h

^{11}B, $CDCl_3$, 160MHz, 298K

ZCY-1640-B{H}

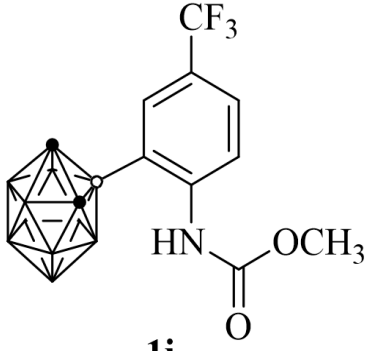


1h

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

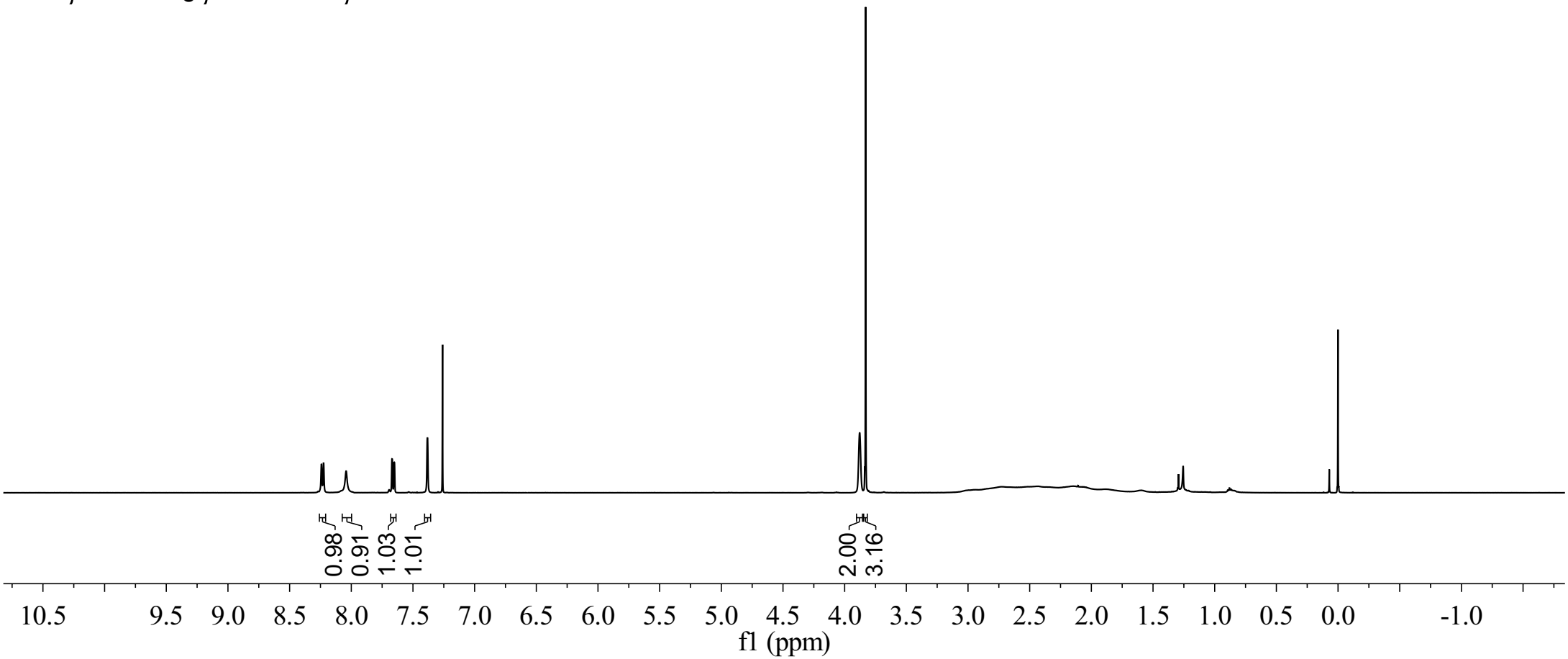
ZCY-1645-H

8.24 8.22 8.04 7.67 7.65 7.38 7.26 3.88 3.83 0.07 0.00

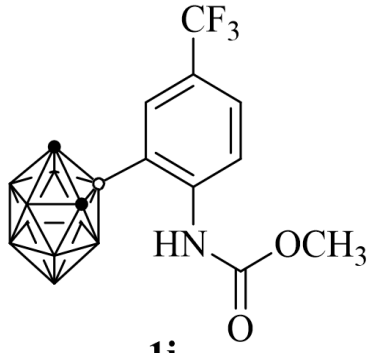


1i

^{1}H, CDCl$_3$,500MHz, 298K



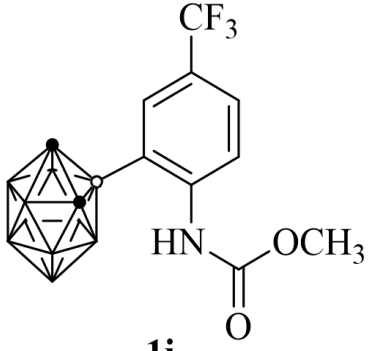
ZCY-1645-C



1i

^{13}C, $CDCl_3$, 125MHz, 298K

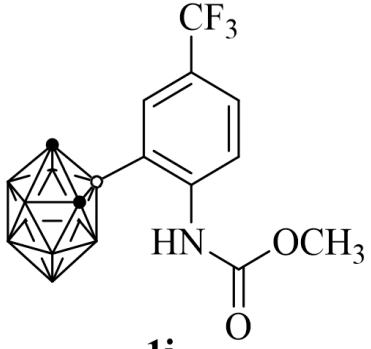
ZCY-1645-B



1i

^{11}B, $CDCl_3$, 160MHz, 298K

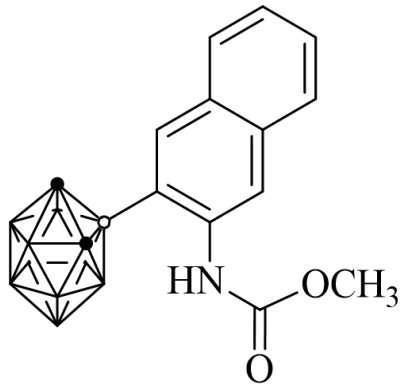
ZCY-1645-B{H}



1i

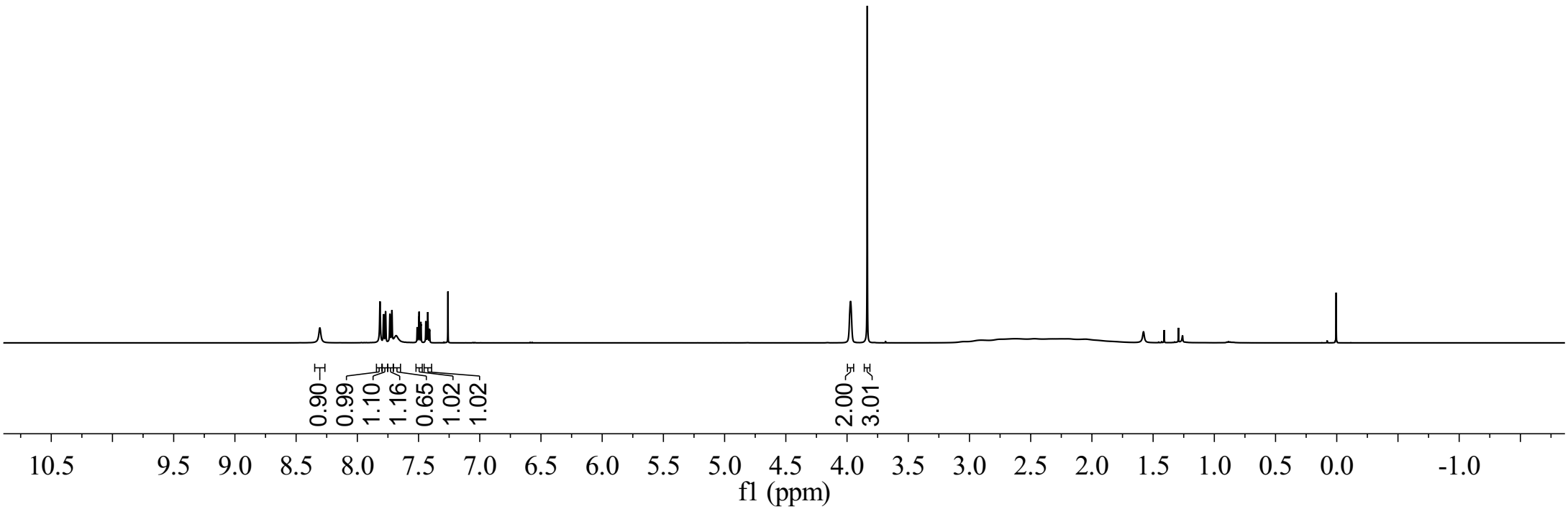
$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

ZCY-1647-H



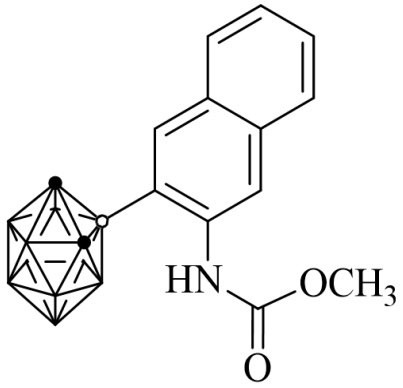
1j

^{1}H, $CDCl_3$, 500MHz, 298K



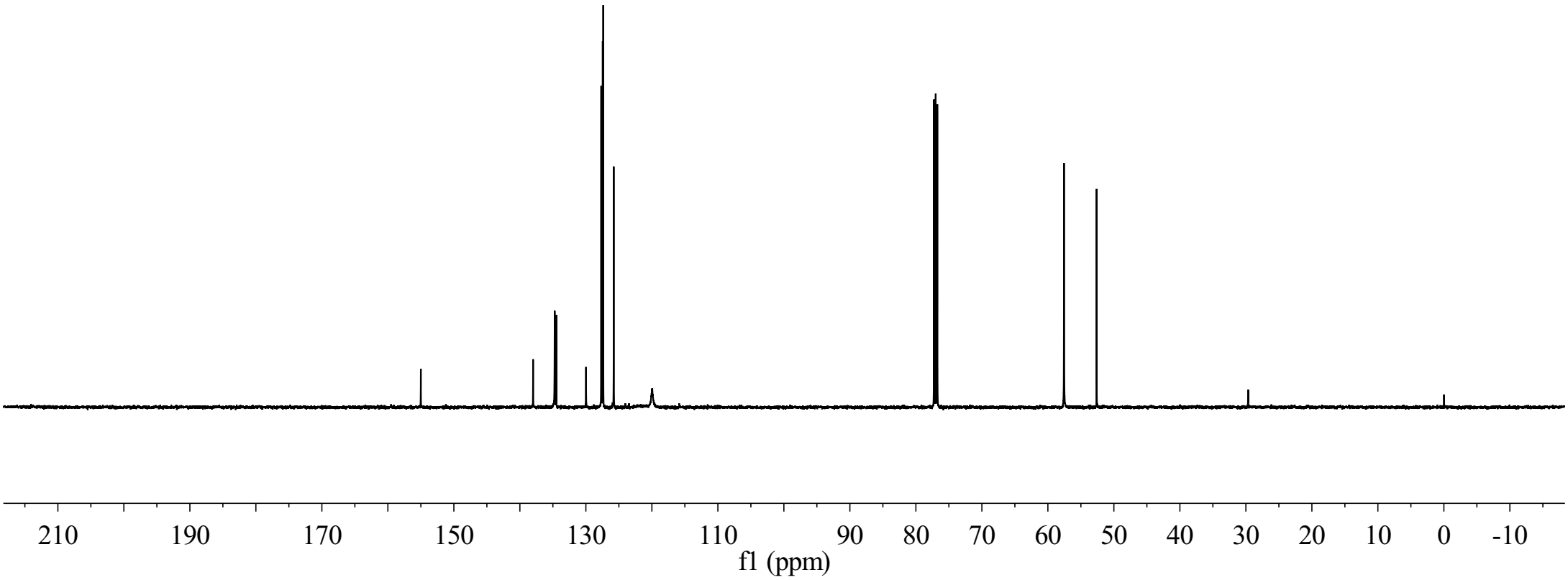
ZCY-1647-C

155.01
137.99
134.72
134.48
129.98
127.68
127.45
127.37
125.78
119.95
77.25
77.00
76.75
57.56
52.62
-0.02

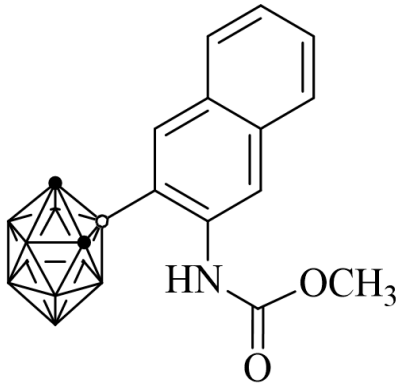


1j

^{13}C, $CDCl_3$, 125MHz, 298K

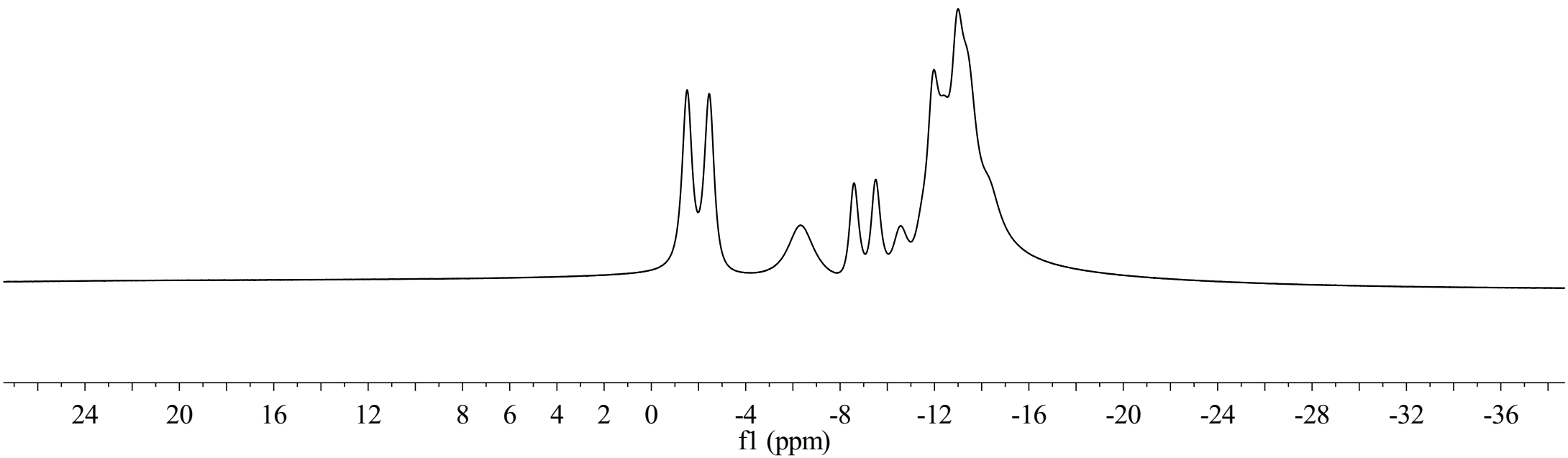


ZCY-1647-B

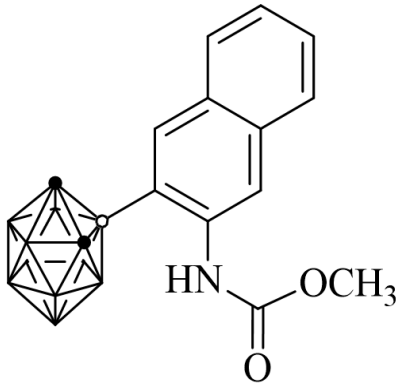


1j

^{11}B, $CDCl_3$, 160MHz, 298K



ZCY-1647-B{H}



1j

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

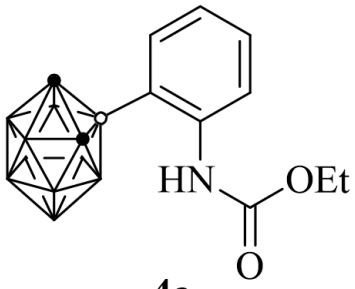
ZCY-1655-H

7.81 7.46 7.42 7.41 7.40 7.38 7.34 7.32 7.26 7.13 7.12 7.10

4.26 4.25 4.24 4.24 4.23 4.22 4.21 4.21 3.88

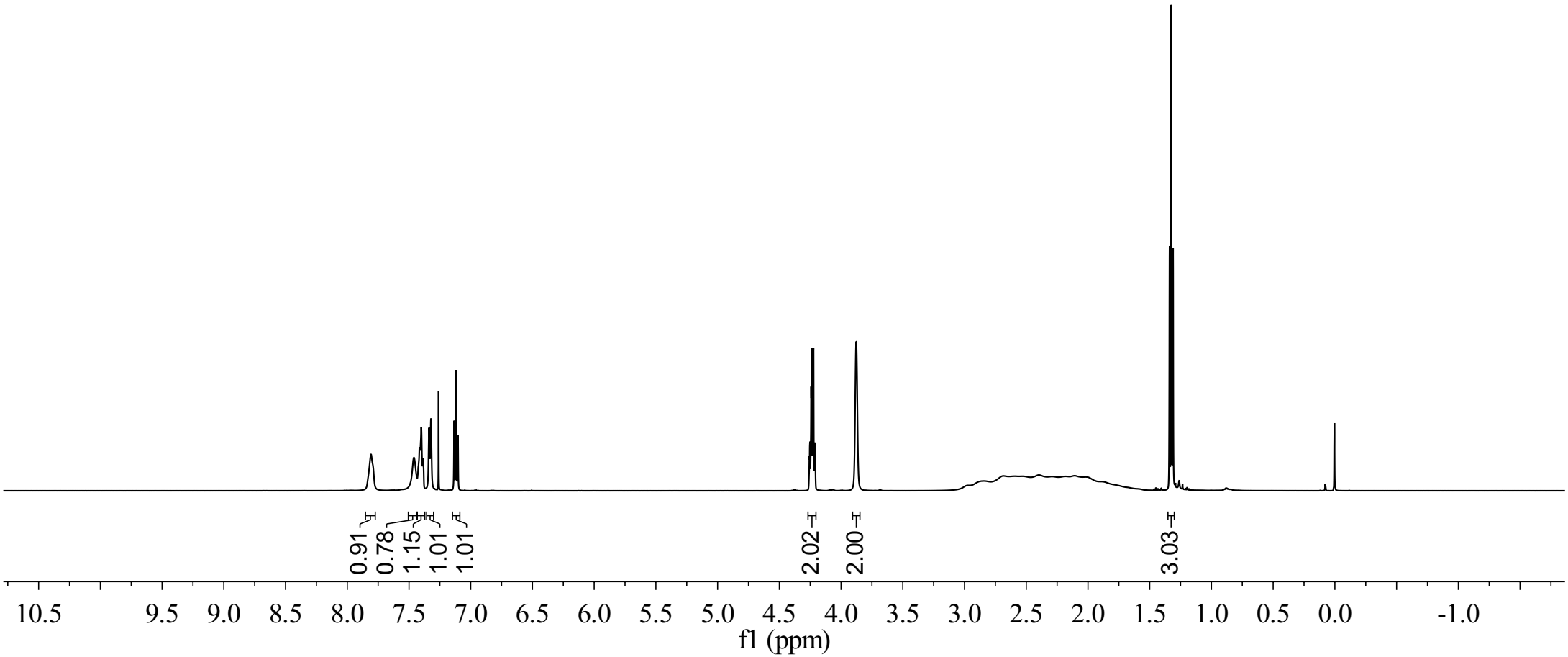
1.34 1.32 1.31

0.00

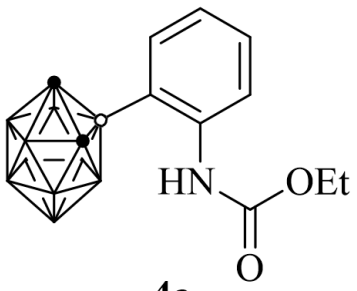


4a

^{1}H, $CDCl_3$, 500MHz, 298K

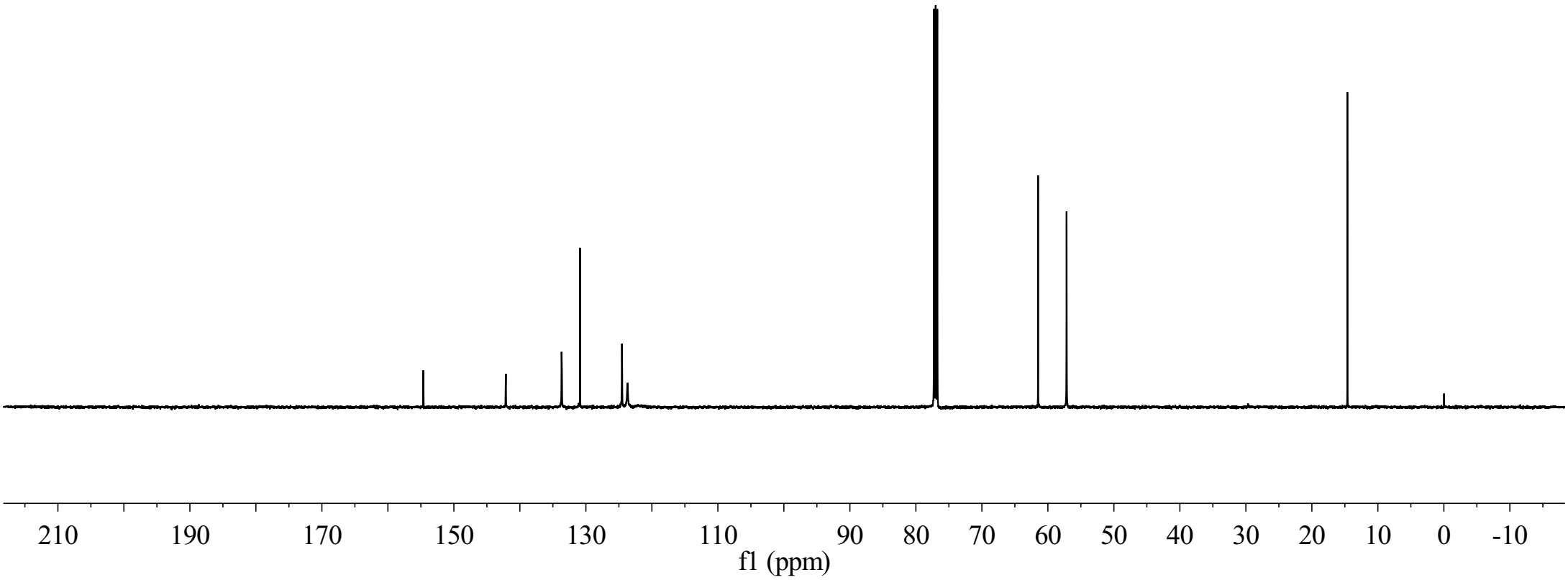


ZCY-1655-C

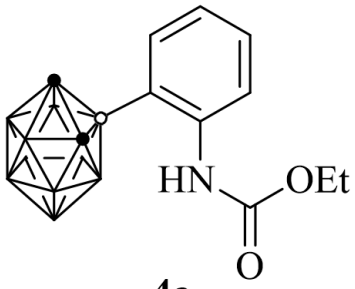


4a

^{13}C, $CDCl_3$, 125MHz, 298K



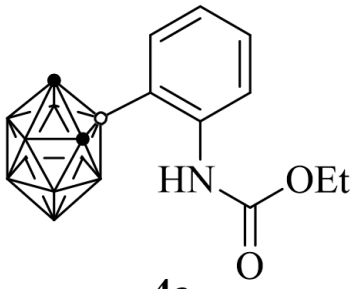
ZCY-1655-B



4a

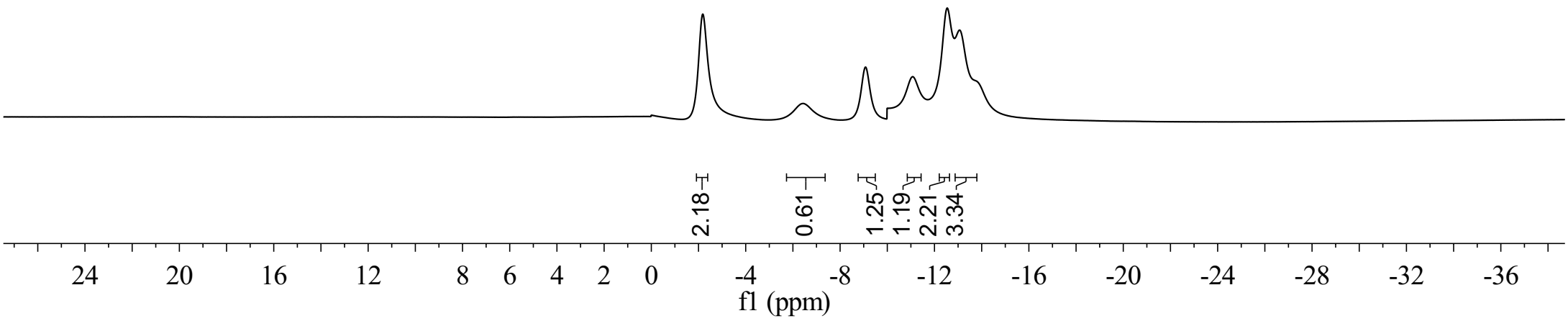
^{11}B, $CDCl_3$, 160MHz, 298K

ZCY-1655-B{H}

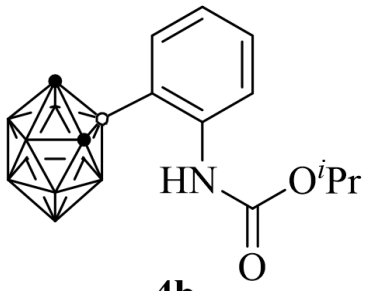


4a

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K



ZCY-1658-H

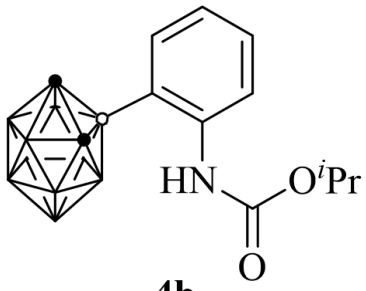


4b

^{1}H, CDCl$_{3}$,500MHz, 298K

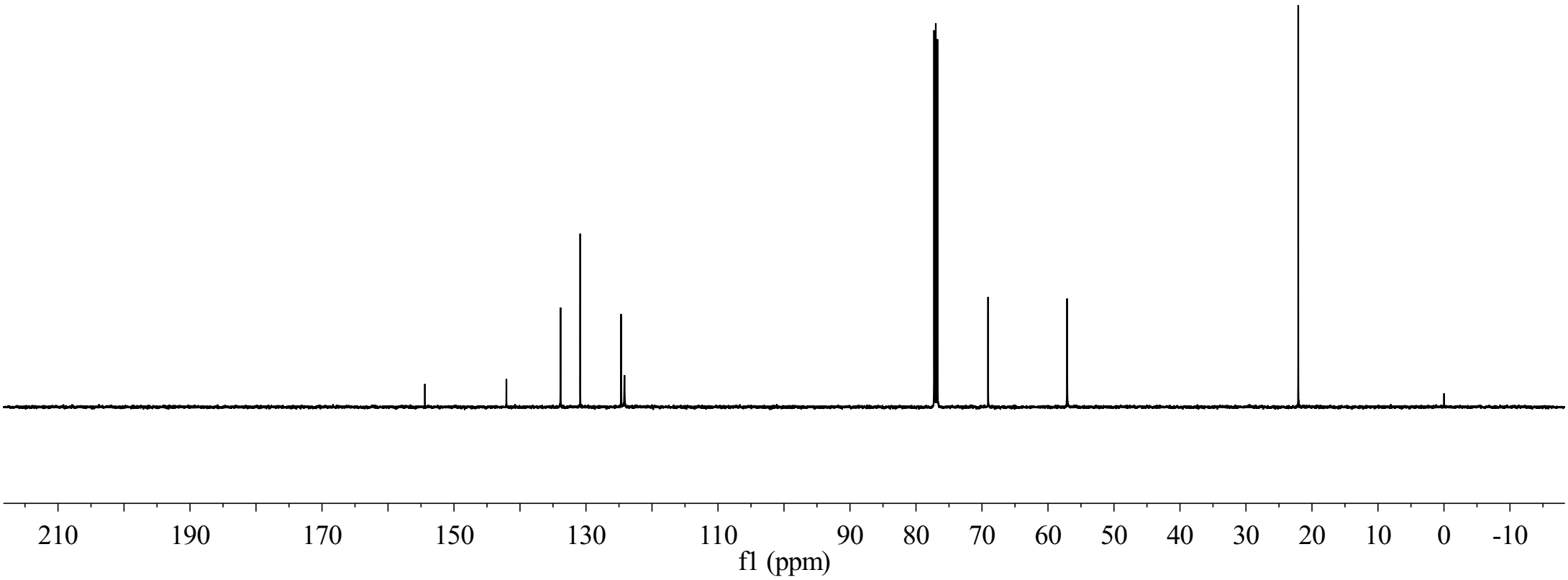
ZCY-1658-C

154.41
142.06
133.86
130.87
124.68
124.17
77.25
77.00
76.75
69.07
57.10
22.08
-0.02

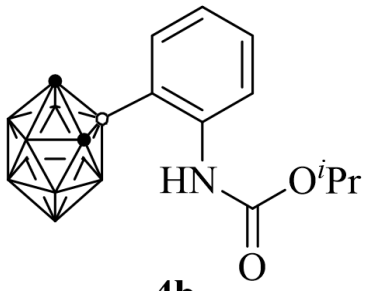


4b

^{13}C, $CDCl_3$, 125MHz, 298K



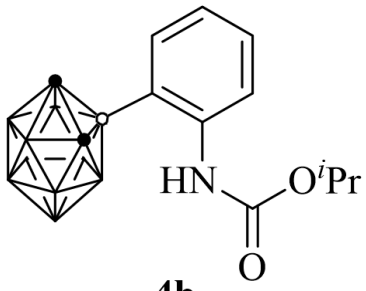
ZCY-1658-B



4b

^{11}B, CDCl$_3$,160MHz, 298K

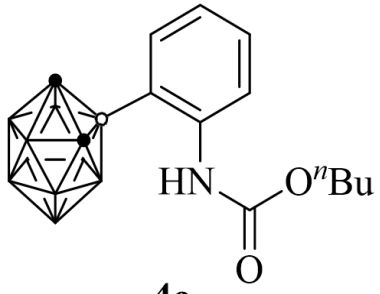
ZCY-1658-B{H}



4b

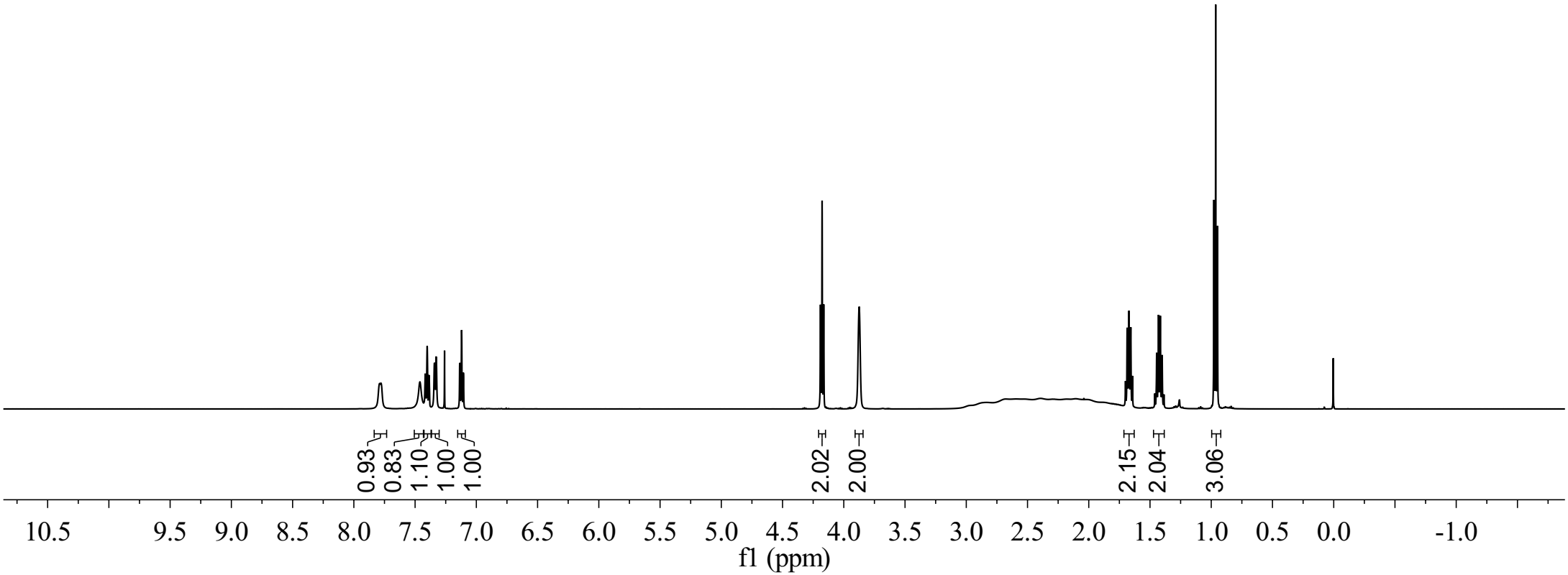
$^{11}B\{^1H\}$, $CDCl_3$, 160MHz, 298K

ZCY-1657-H



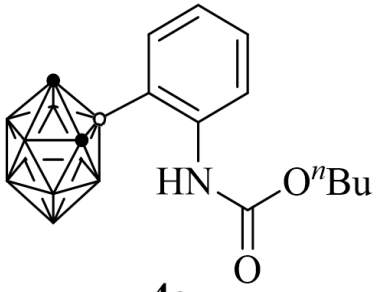
4c

^{1}H, CDCl$_3$,500MHz, 298K



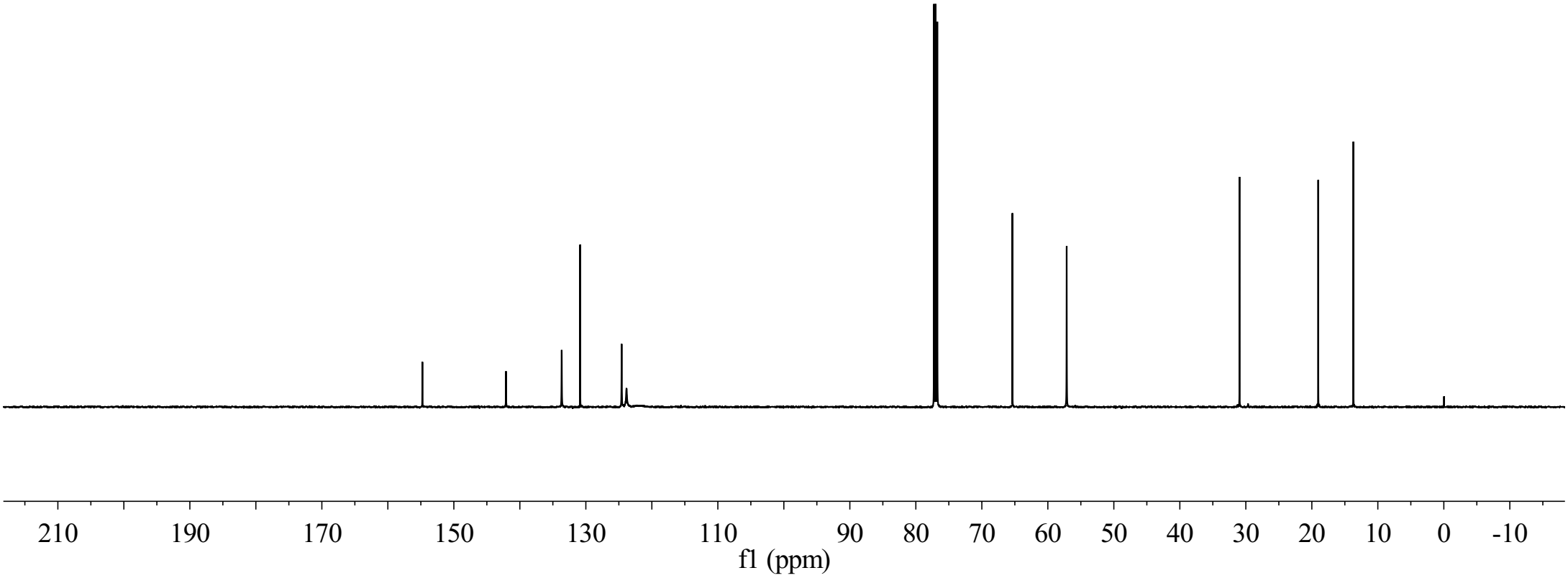
ZCY-1657-C

154.76
142.10
133.66
130.87
124.58
123.83
77.25
77.00
76.75
65.37
57.15
30.96
19.03
13.70
-0.03

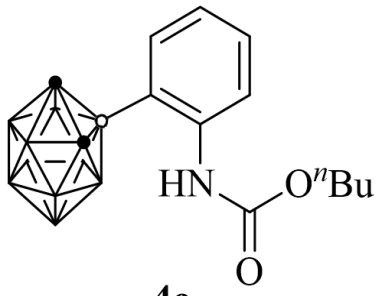


4c

^{13}C, CDCl$_3$, 125MHz, 298K

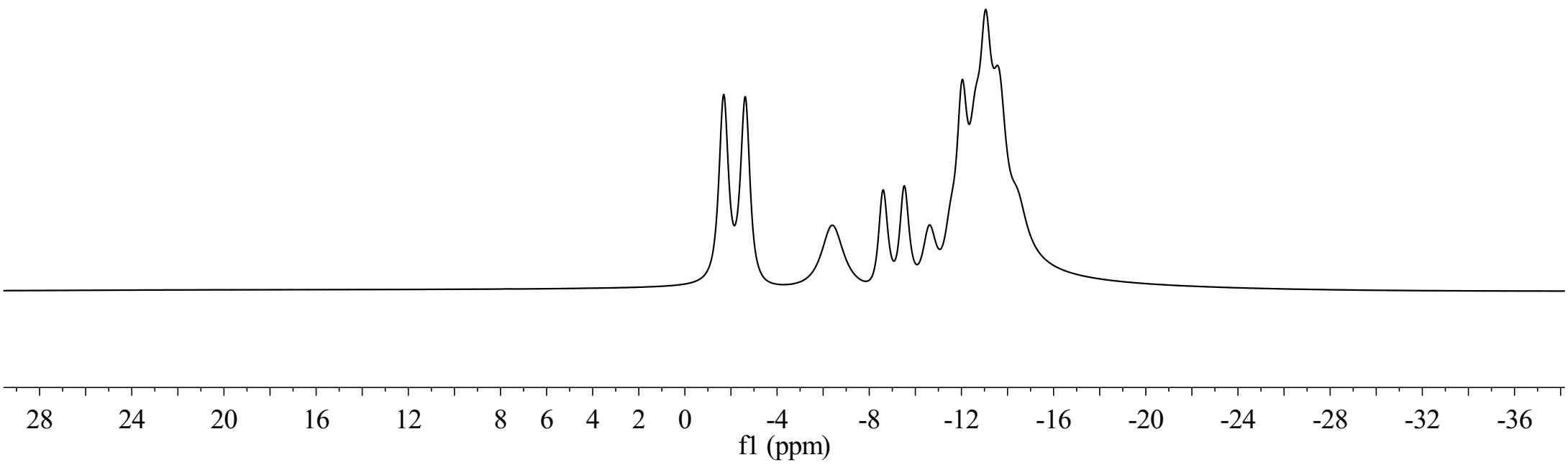


ZCY-1657-B

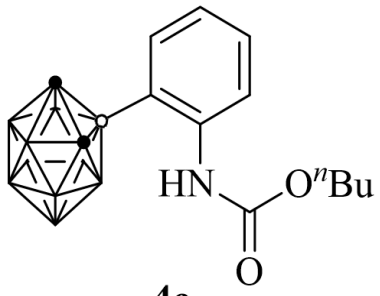


4c

^{11}B, CDCl$_3$,160MHz, 298K



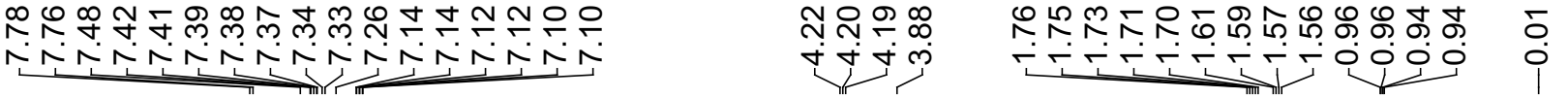
ZCY-1657-B{H}

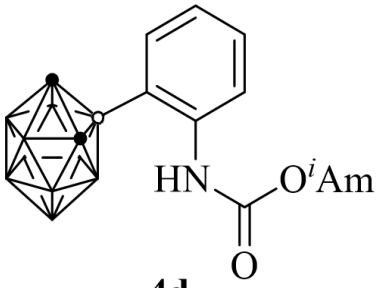


4c

$^{11}B\{^1H\}$, $CDCl_3$, 160MHz, 298K

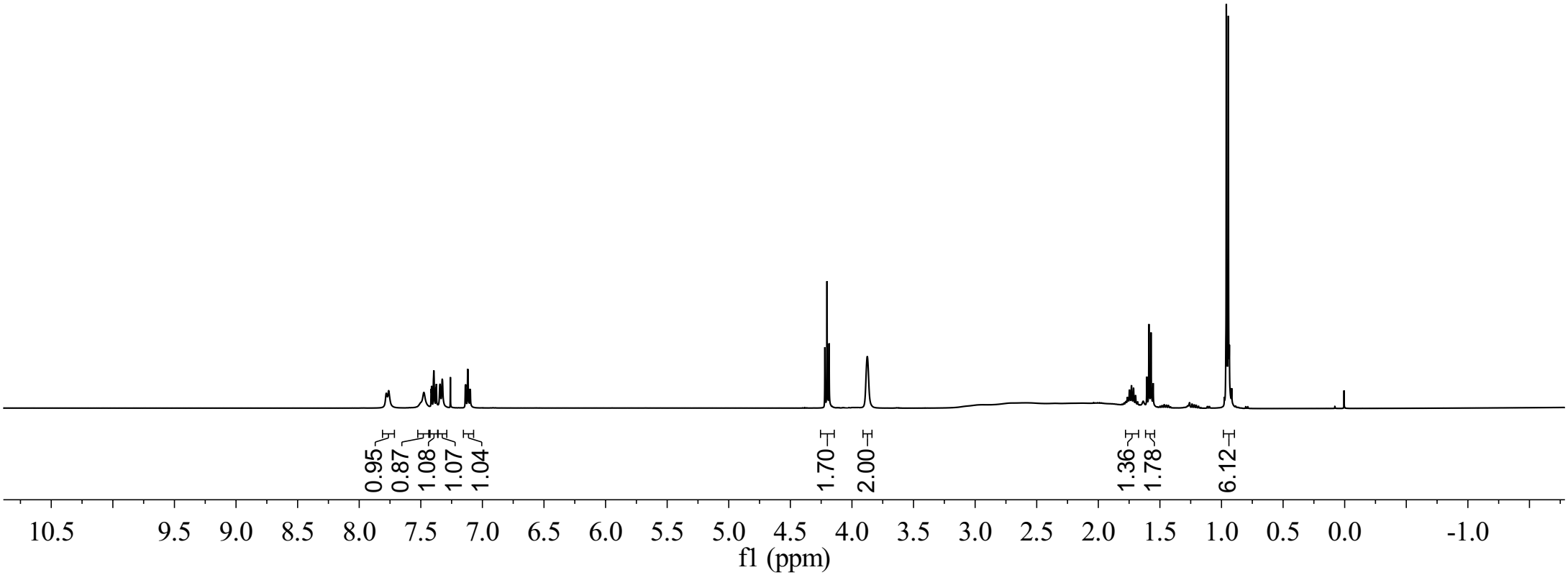
ZCY-1753-H



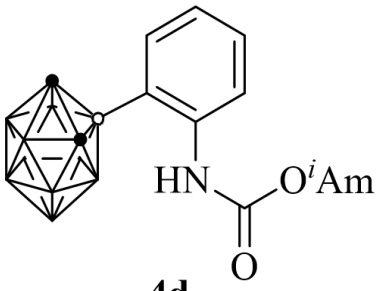


4d

^{1}H, CDCl$_{3}$,600MHz, 298K



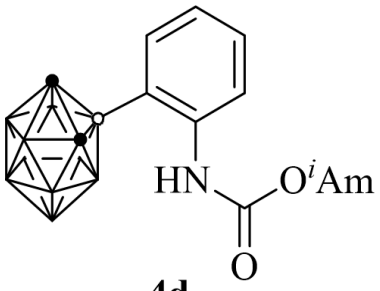
ZCY-1753-C



4d

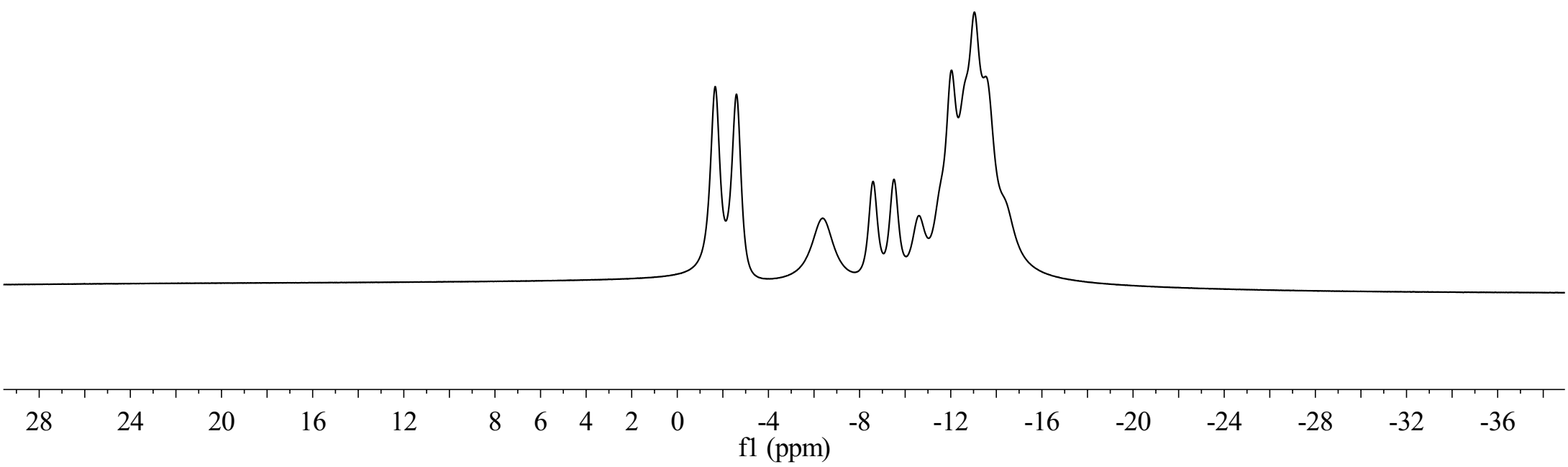
^{13}C, $CDCl_3$, 150MHz, 298K

ZCY-1753-B

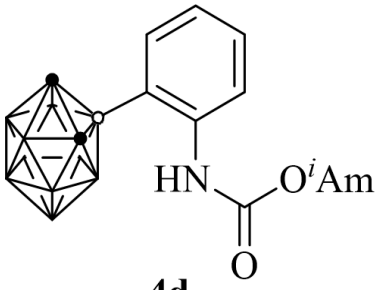


4d

^{11}B, CDCl$_3$,160MHz, 298K

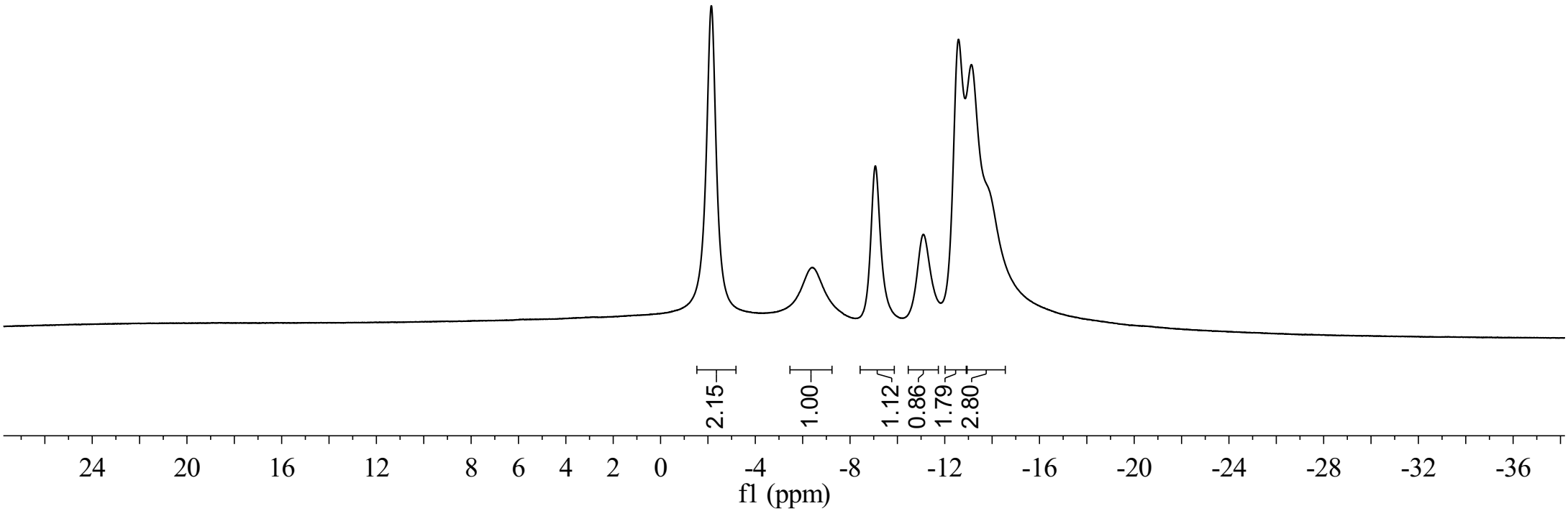


ZCY-1753-B{H}

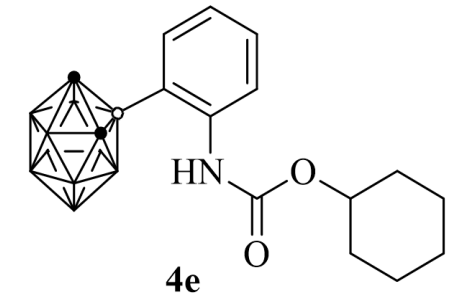


4d

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

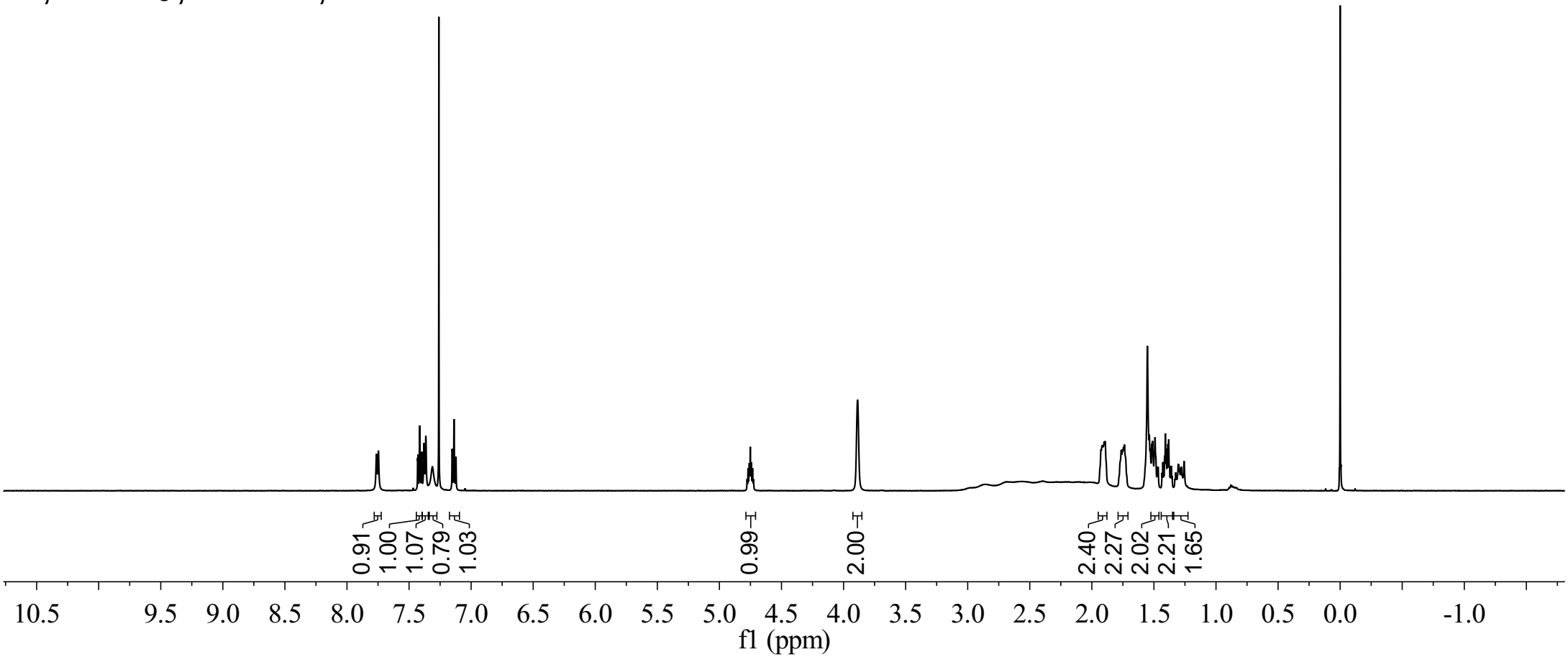


ZCY-1693-H

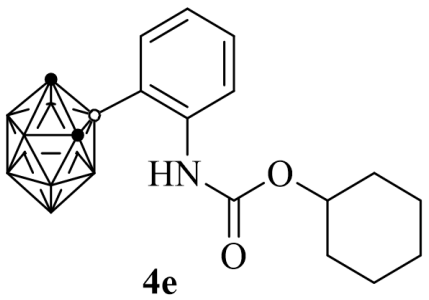


4e

^{1}H, $CDCl_3$, 500MHz, 298K



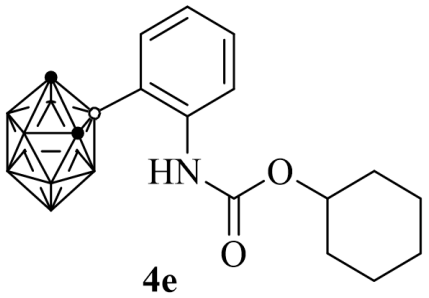
ZCY-1693-C



4e

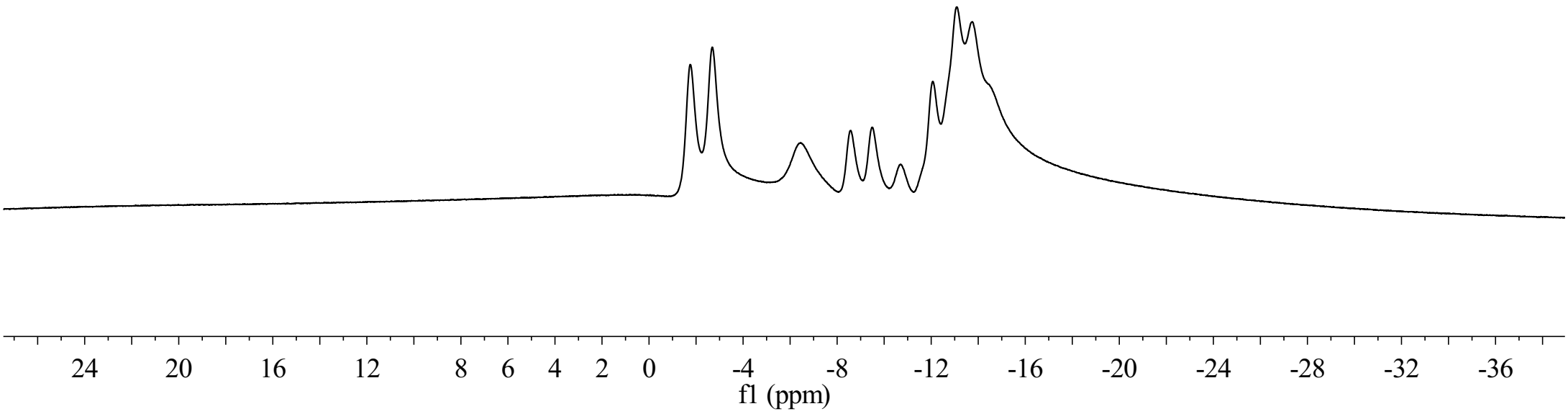
^{13}C, $CDCl_3$, 125MHz, 298K

ZCY-1693-B

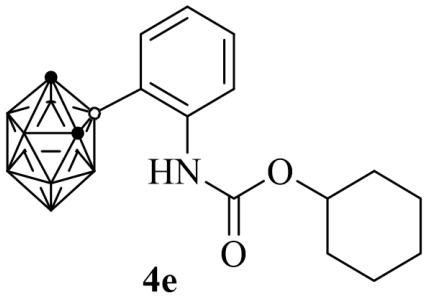


4e

^{11}B, $CDCl_3$, 160MHz, 298K



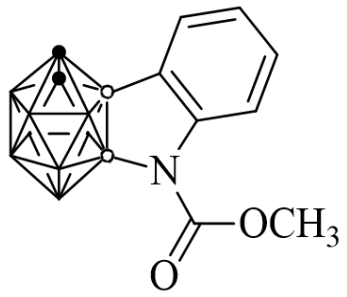
ZCY-1693-B{H}



4e

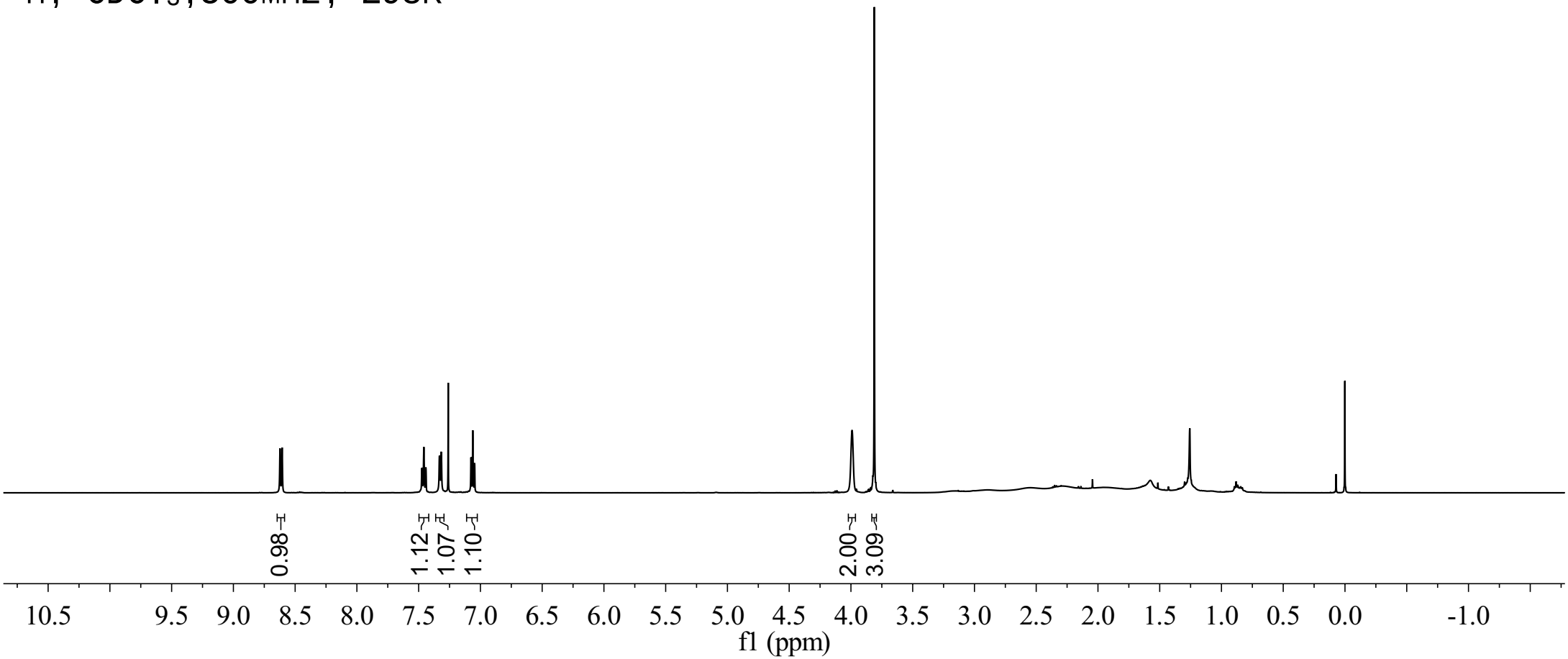
$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

ZCY-B3-B8-H



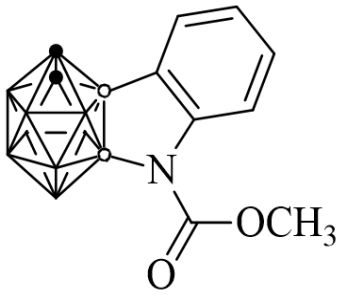
2a

^{1}H, CDCl$_3$,500MHz, 298K



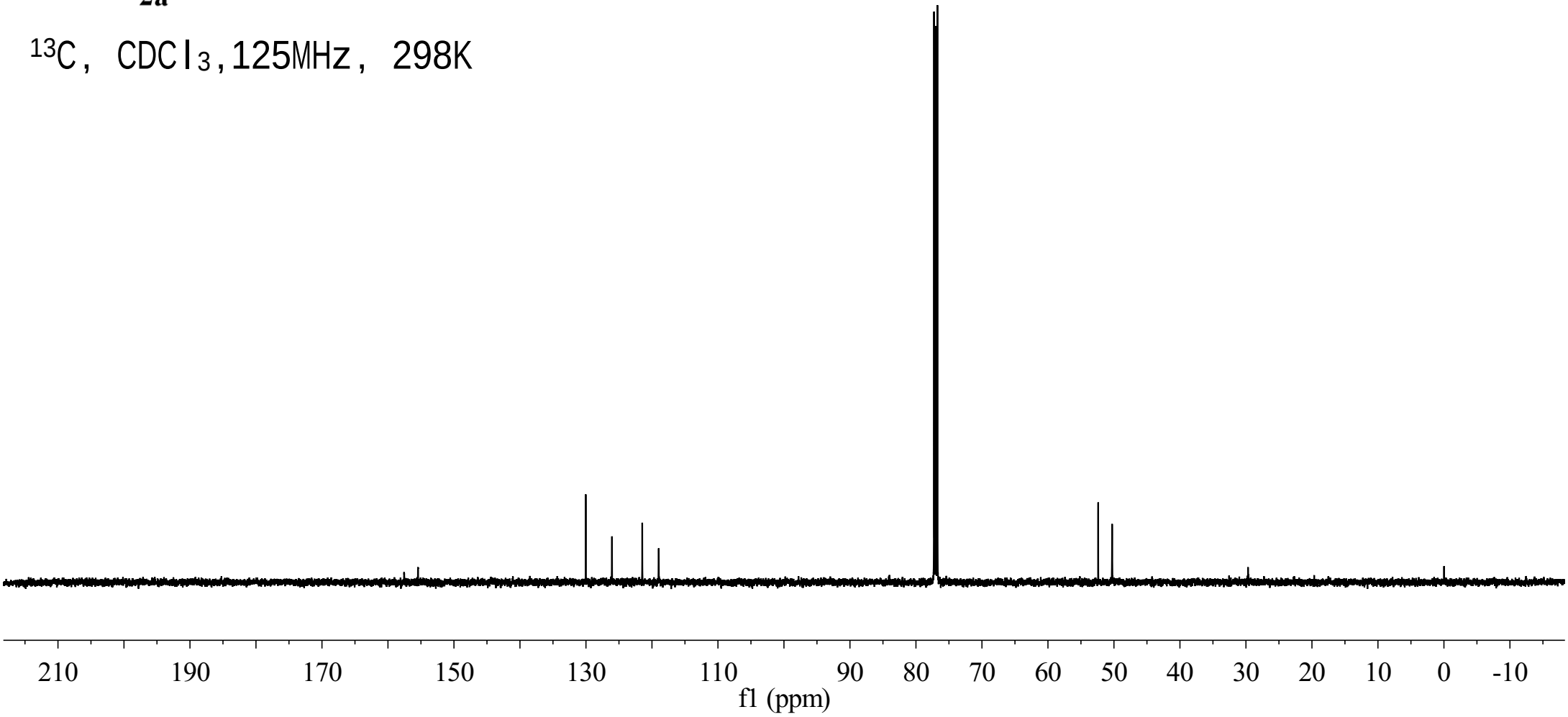
ZCY-B3-B8-C

157.55
155.45
130.03
126.06
121.47
118.98
77.25
77.00
76.75
52.38
50.28
43.97
-0.02

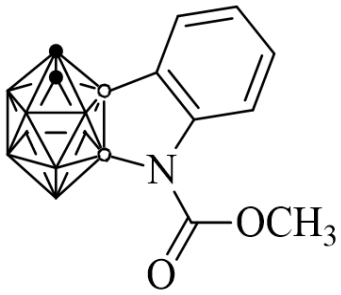


2a

^{13}C, $CDCl_3$, 125MHz, 298K

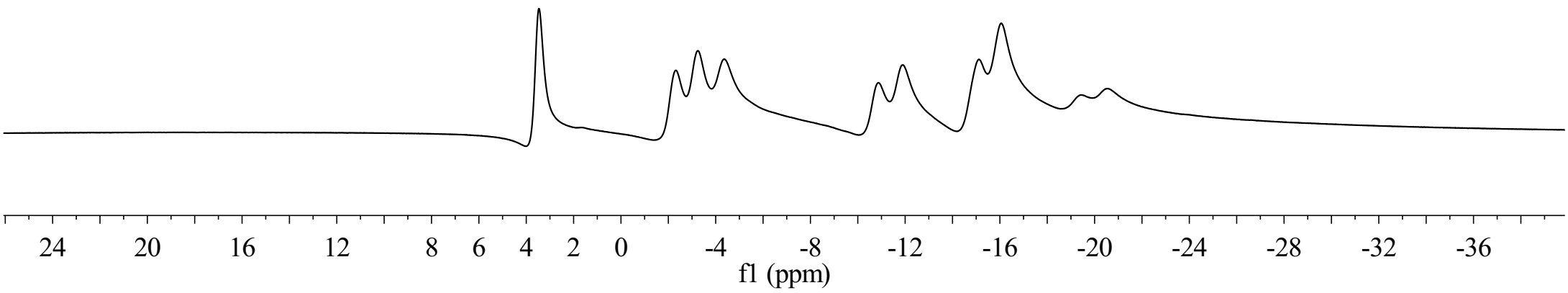


ZCY-B3-B8-B

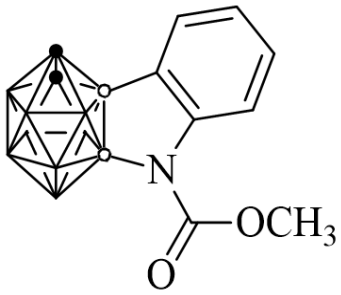


2a

^{11}B, $CDCl_3$, 160MHz, 298K



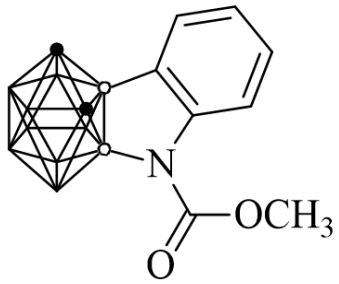
ZCY-B3-B8-B{H}



2a

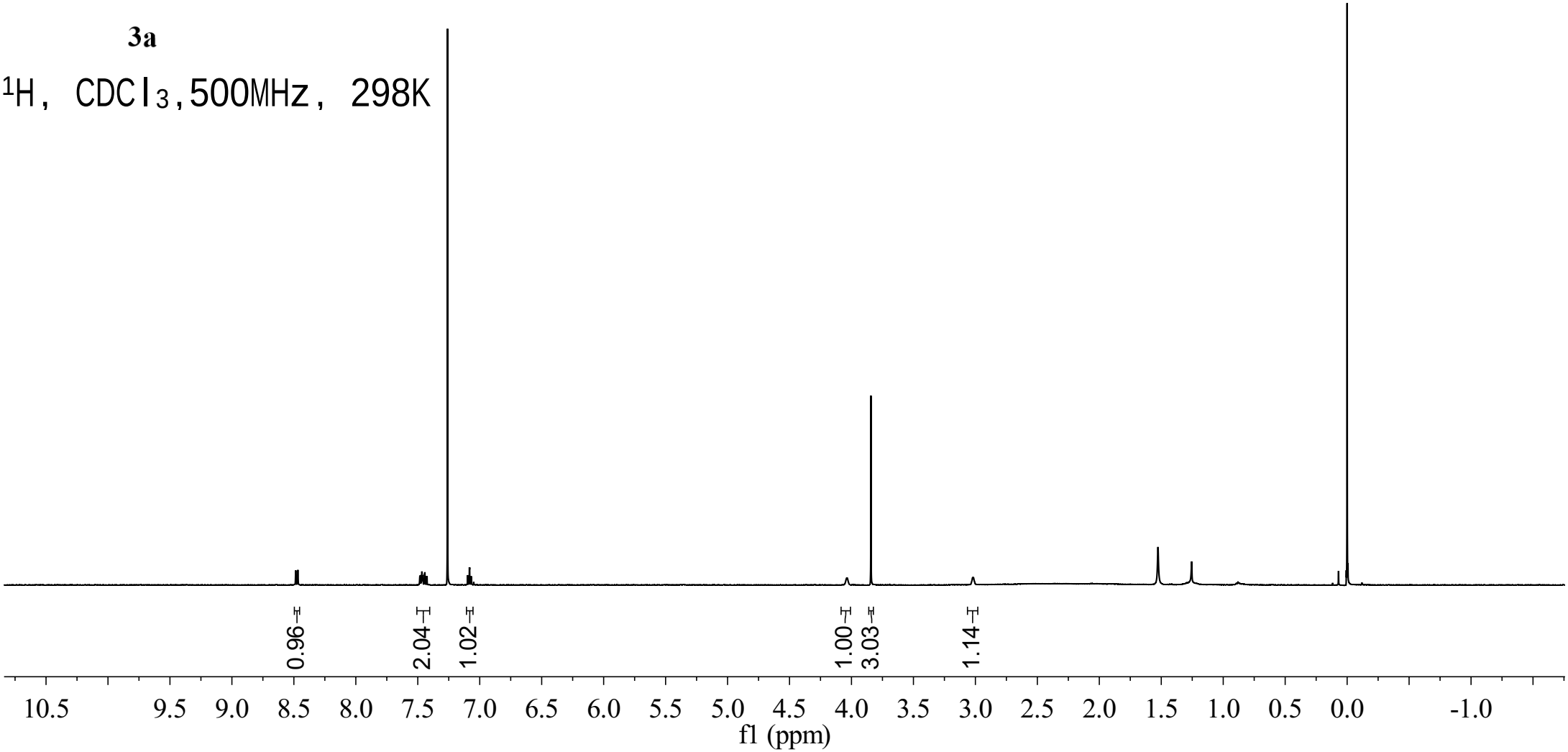
$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

ZCY-1653-H

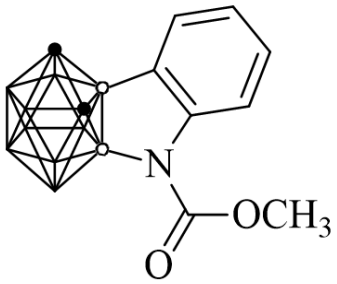


3a

^{1}H, CDCl$_3$,500MHz, 298K



ZCY-1653-C

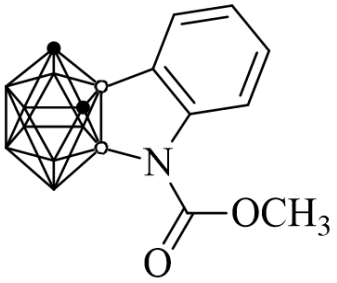


3a

^{13}C, $CDCl_3$, 125MHz, 298K

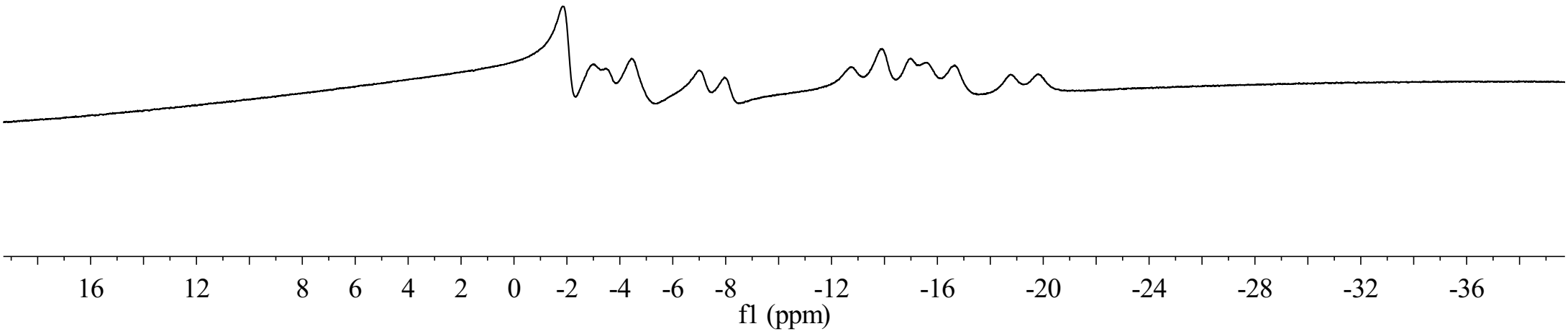
ZCY-1653-B

-1.84
-3.02
-4.45
-6.98
-7.95
-12.76
-13.90
-14.99
-16.65
-18.77
-19.81

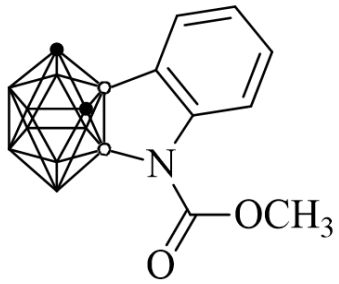


3a

^{11}B, $CDCl_3$, 160MHz, 298K



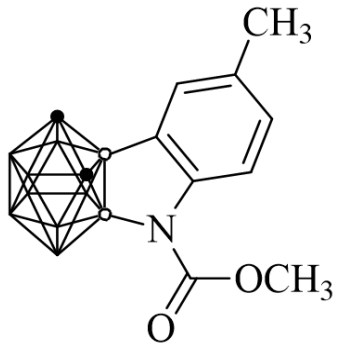
ZCY-1653-B{H}



3a

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

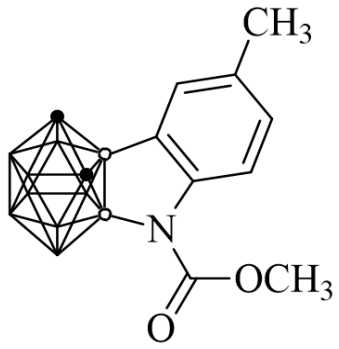
ZCY-1643-H



3b

^{1}H, CDCl$_3$,500MHz, 298K

ZCY-1643-C



3b

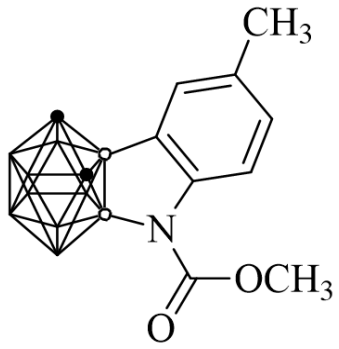
^{13}C, $CDCl_3$, 125MHz, 298K

155.13
153.78
131.59
131.17
128.77
118.43
77.25
77.00
76.75
58.33
52.58
51.90
20.61
1.01
-0.02

210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10

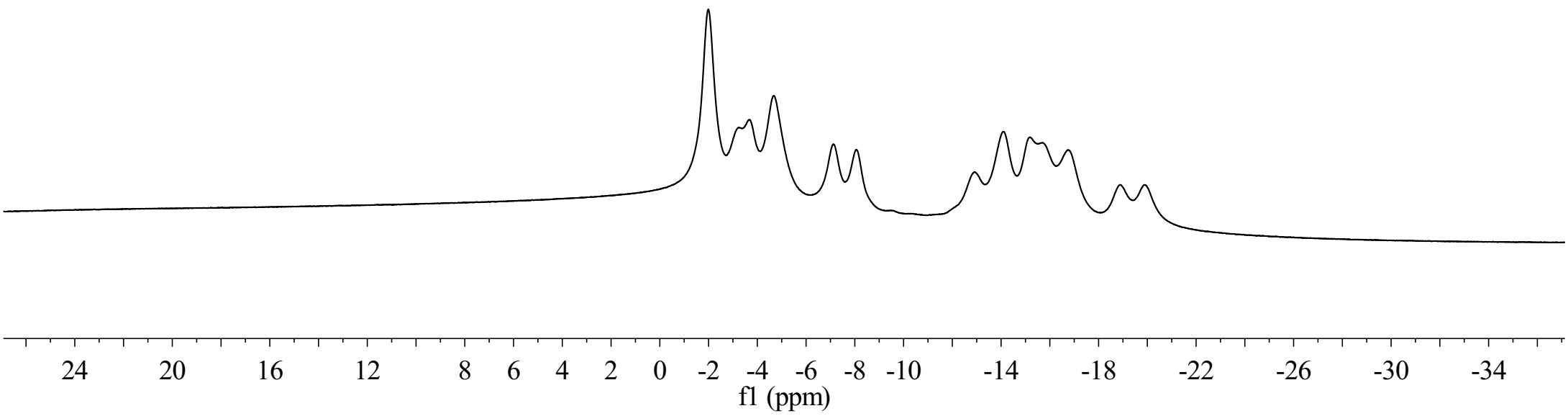
f1 (ppm)

ZCY-1643-B

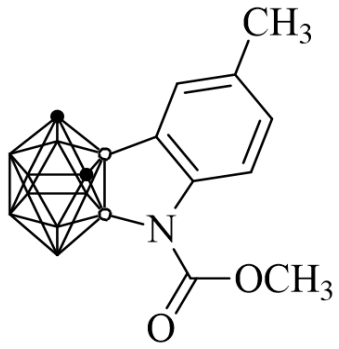


3b

^{11}B, $CDCl_3$, 160MHz, 298K



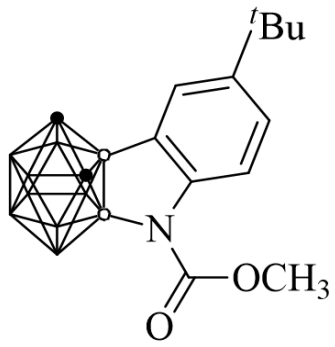
ZCY-1643-B{H}



3b

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

ZCY-1684-H

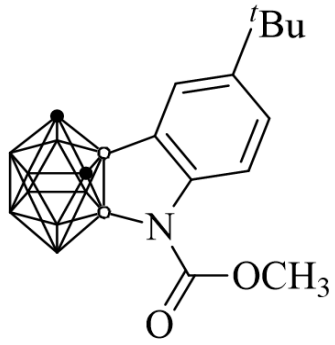


3c

^{1}H, CDCl$_3$,500MHz, 298K

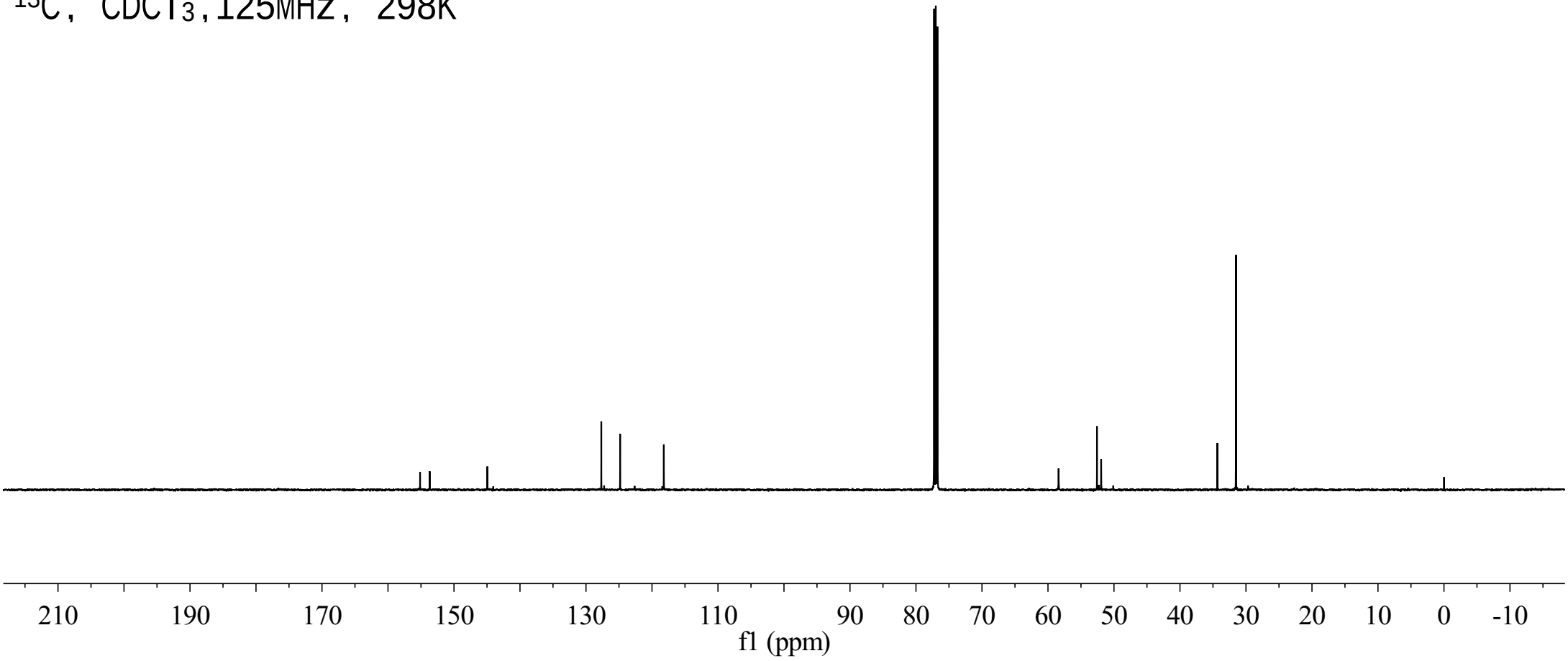
ZCY-1684-C

155.14
153.69
144.94
127.68
124.83
118.21
77.25
77.00
76.75
58.39
52.58
51.94
34.33
31.49
-0.02

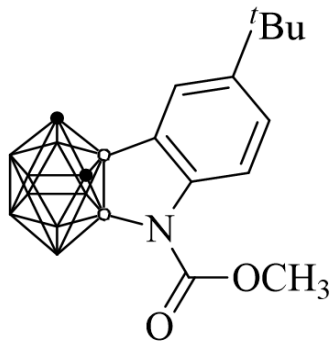


3c

^{13}C, $CDCl_3$, 125MHz, 298K



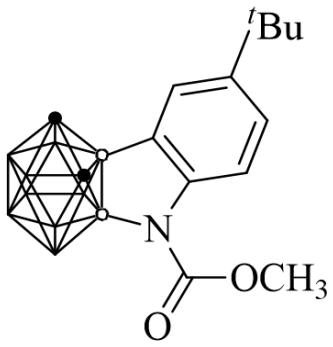
ZCY-1684-B



3c

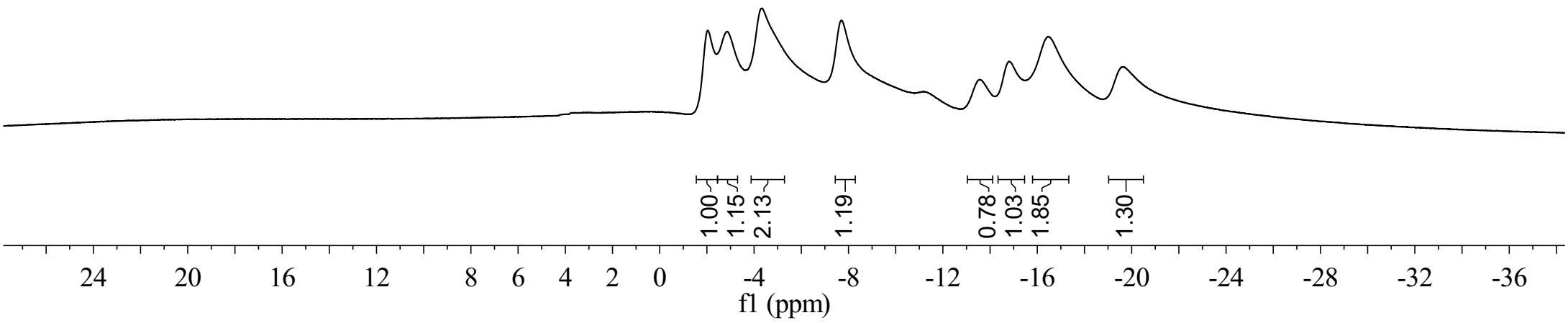
^{11}B, $CDCl_3$, 160MHz, 298K

ZCY-1684-B{H}

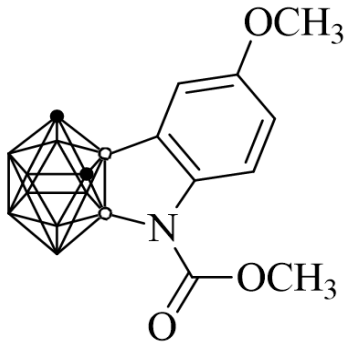


3c

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

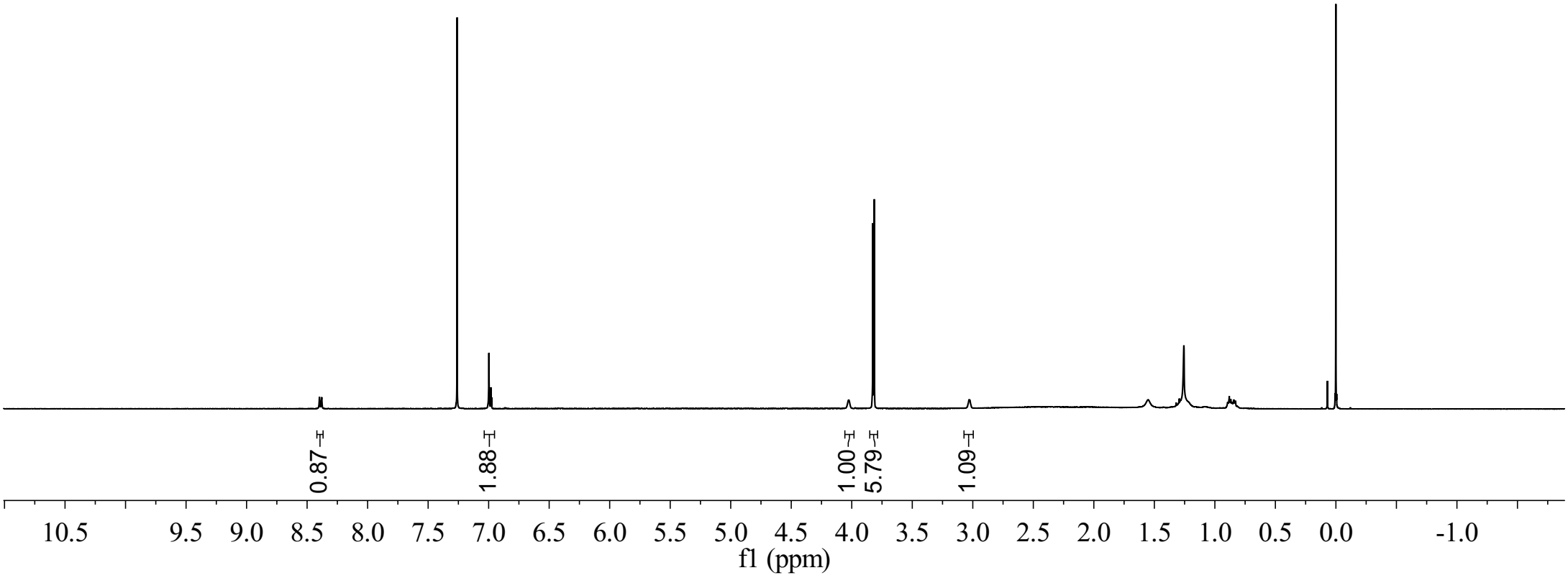


ZCY-1662-H

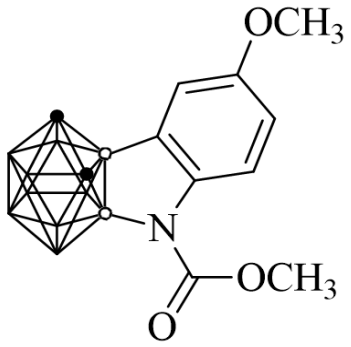


3d

^{1}H, $CDCl_3$, 500MHz, 298K



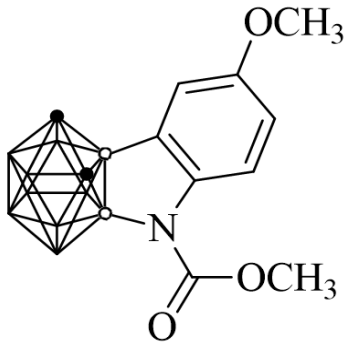
ZCY-1662-C



3d

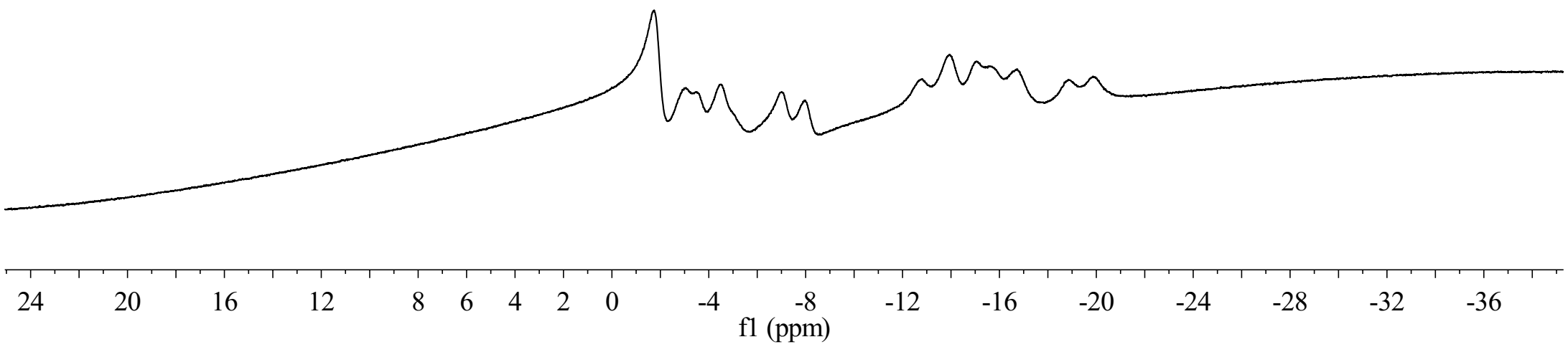
^{13}C, $CDCl_3$, 125MHz, 298K

ZCY-1662-B

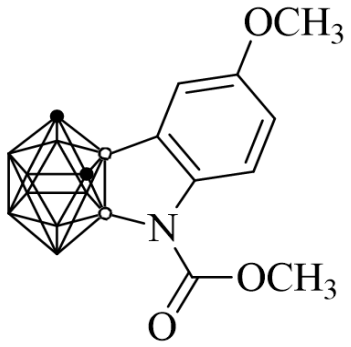


3d

^{11}B, $CDCl_3$, 160MHz, 298K



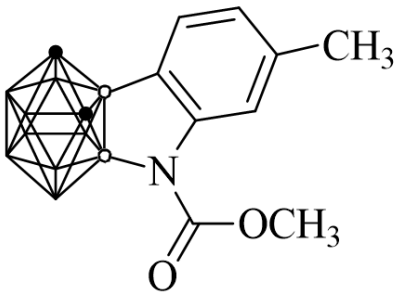
ZCY-1662-B{H}



3d

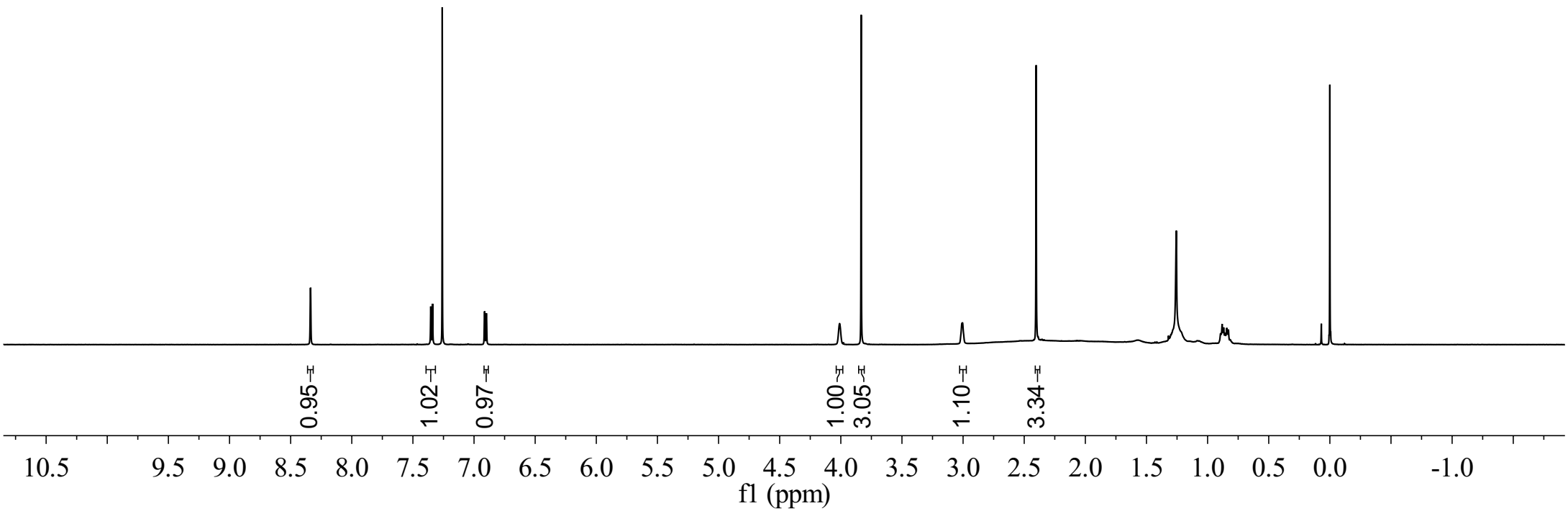
$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

ZCY-1663-H

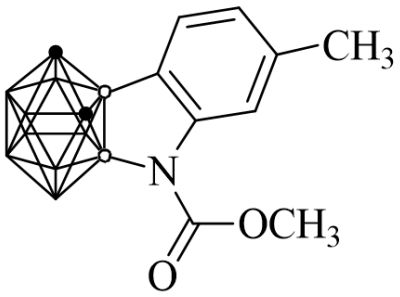


3e

^{1}H, $CDCl_3$, 500MHz, 298K



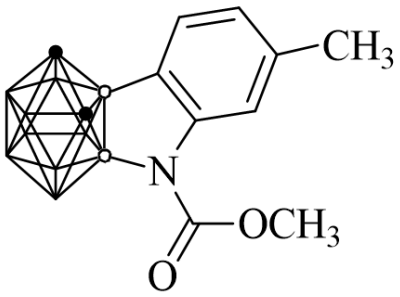
ZCY-1663-C



3e

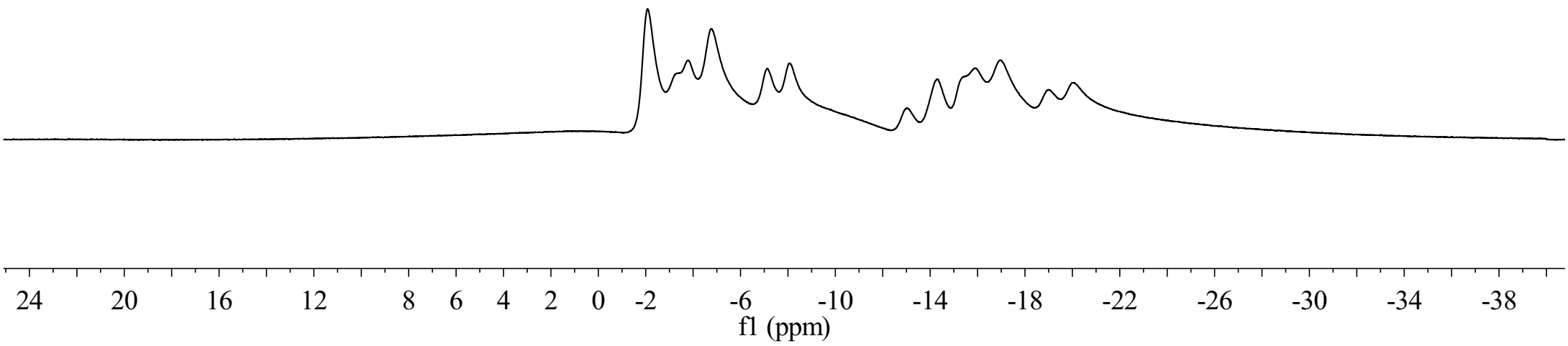
^{13}C, $CDCl_3$, 125MHz, 298K

ZCY-1663-B

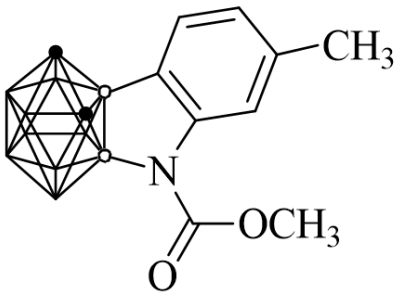


3e

^{11}B, $CDCl_3$, 160MHz, 298K

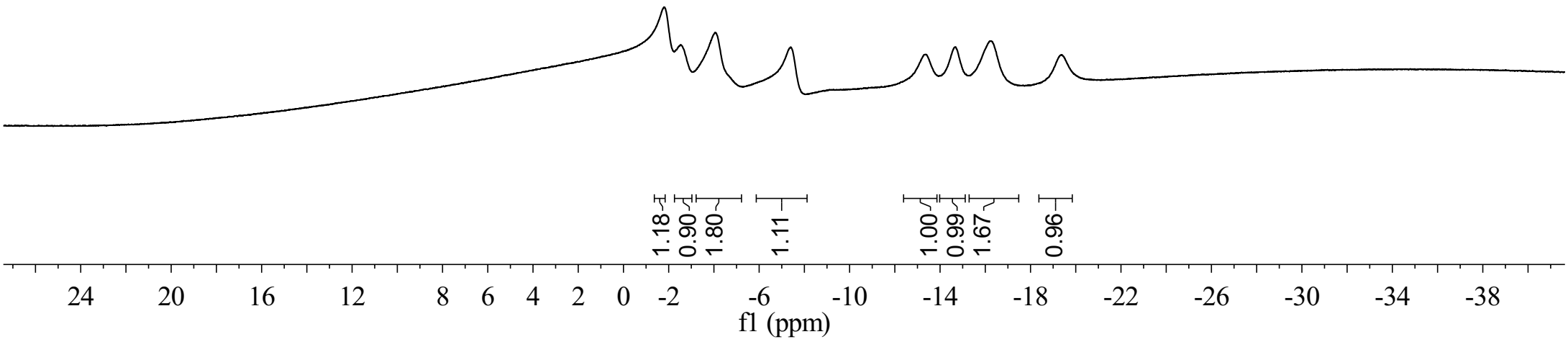


ZCY-1663-B{H}

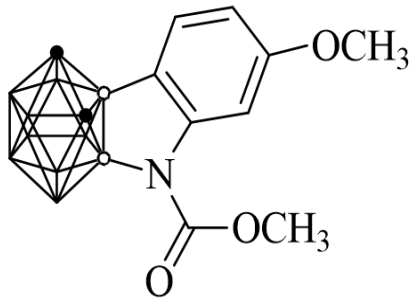


3e

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

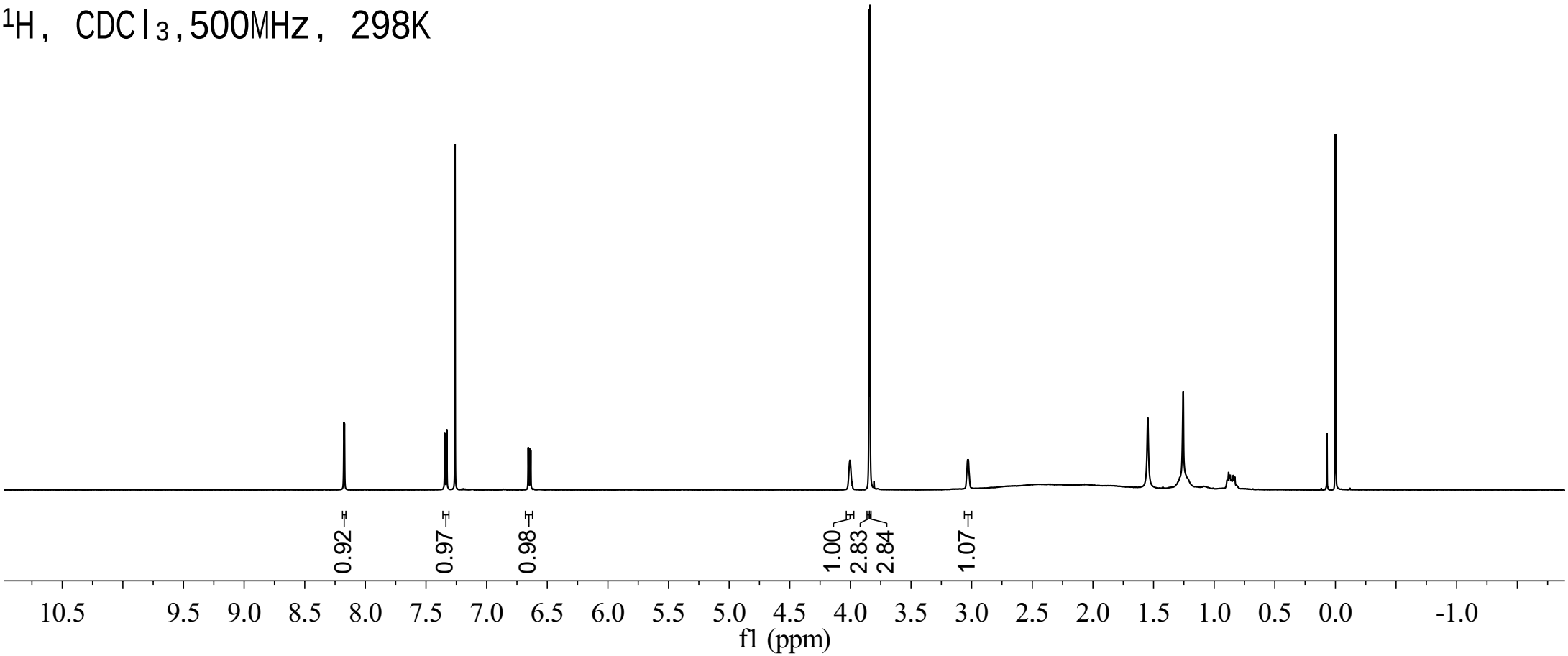


ZCY-1677-H

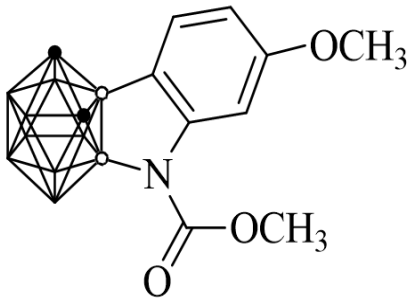


3f

^{1}H, $CDCl_3$, 500MHz, 298K



ZCY-1677-C

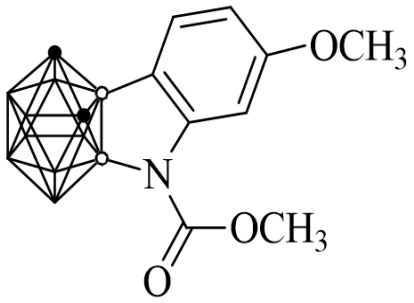


3f

^{13}C, $CDCl_3$, 125MHz, 298K

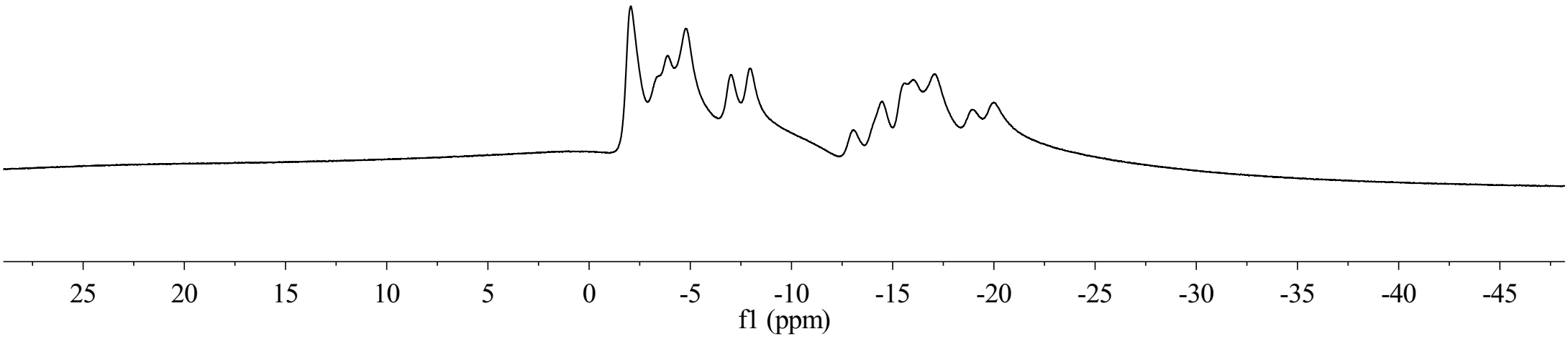
ZCY-1677-B

-2.07
-3.90
-4.77
-7.00
-7.95
-14.48
-16.01
-17.09
-18.97
-20.00

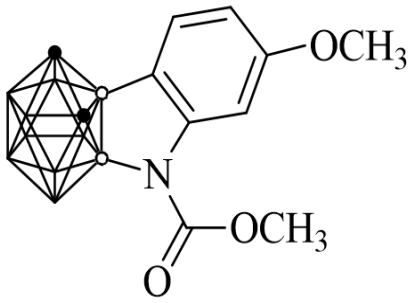


3f

^{11}B, $CDCl_3$, 160MHz, 298K

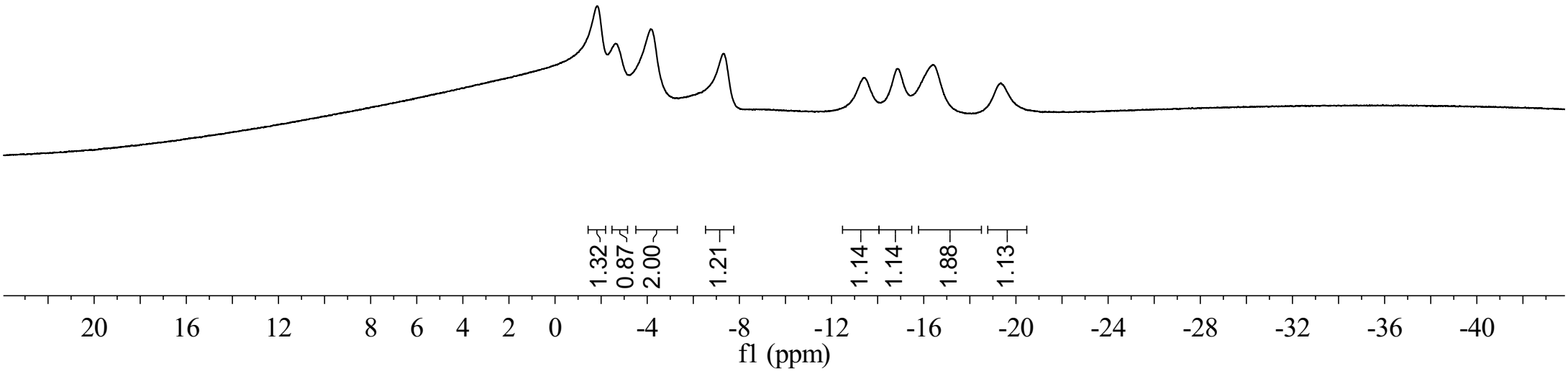


ZCY-1677-B{H}

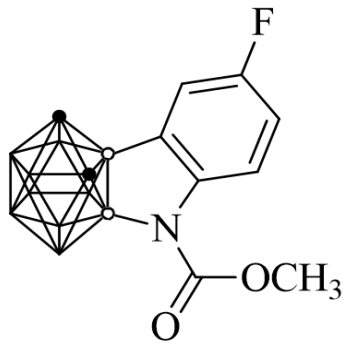


3f

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

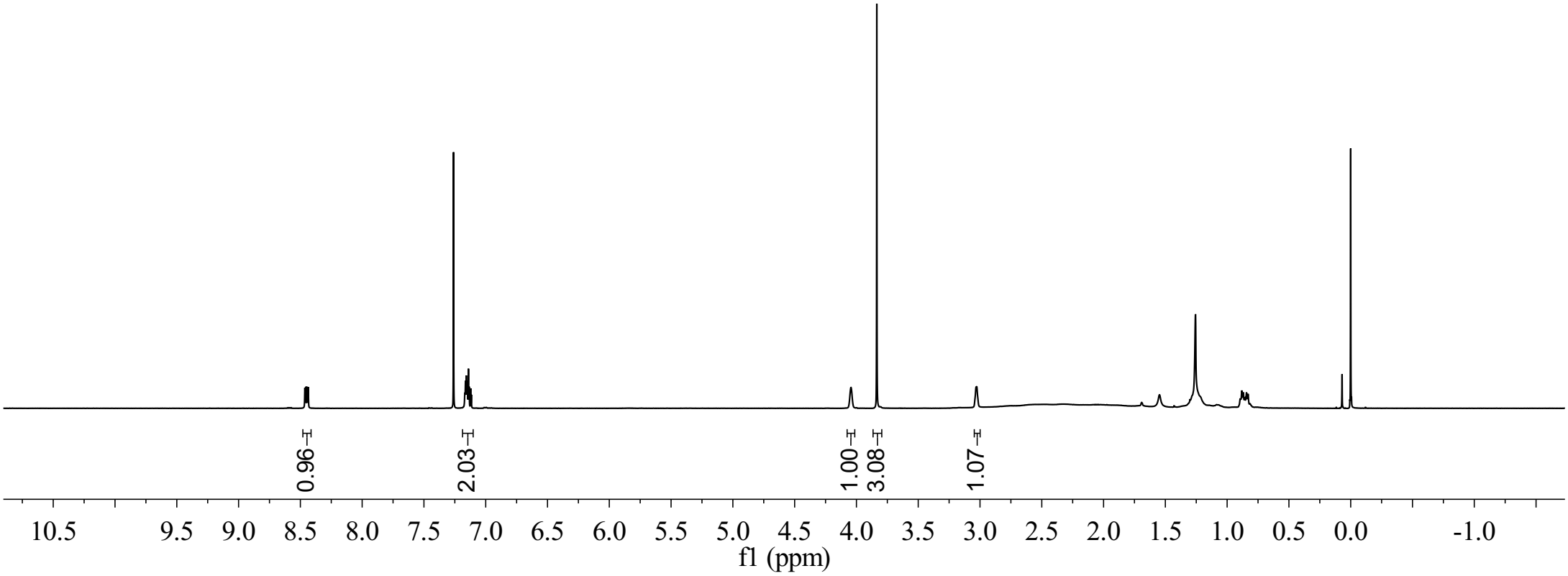


ZCY-1666-H

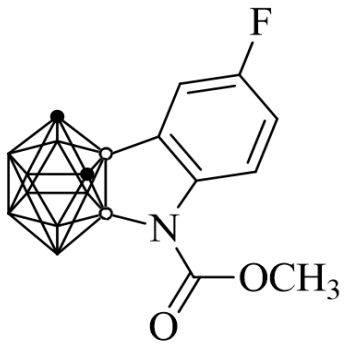


3h

^{1}H, $CDCl_3$, 500MHz, 298K



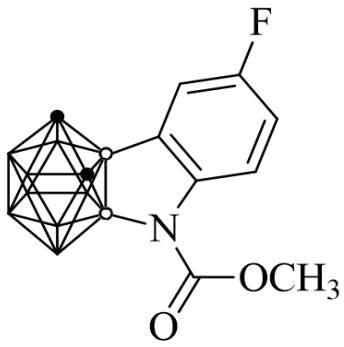
ZCY-1666-C



3h

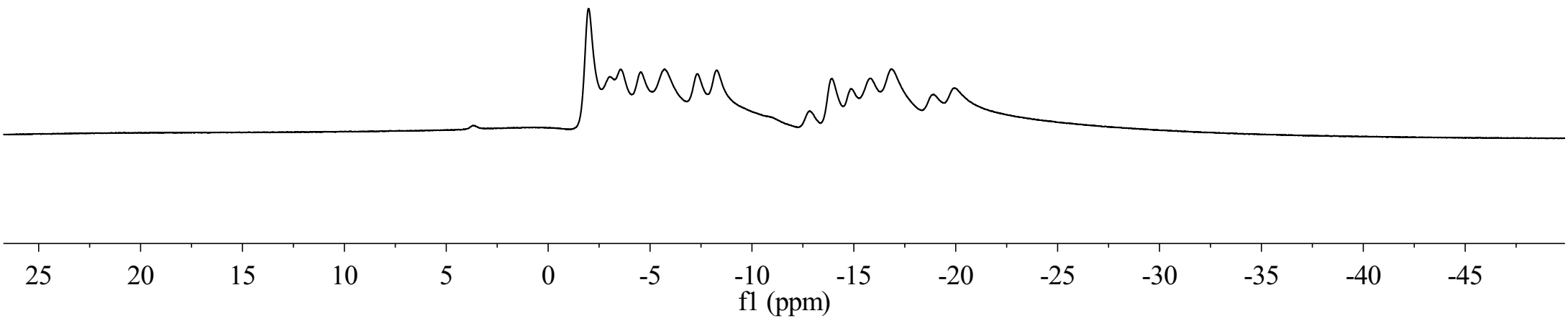
^{13}C, $CDCl_3$, 125MHz, 298K

ZCY-1666-B

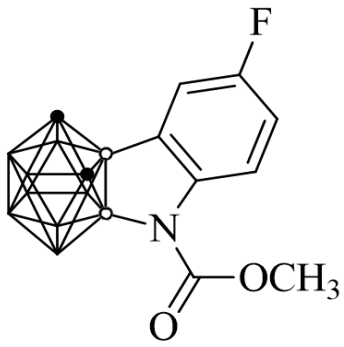


3h

^{11}B, $CDCl_3$, 160MHz, 298K

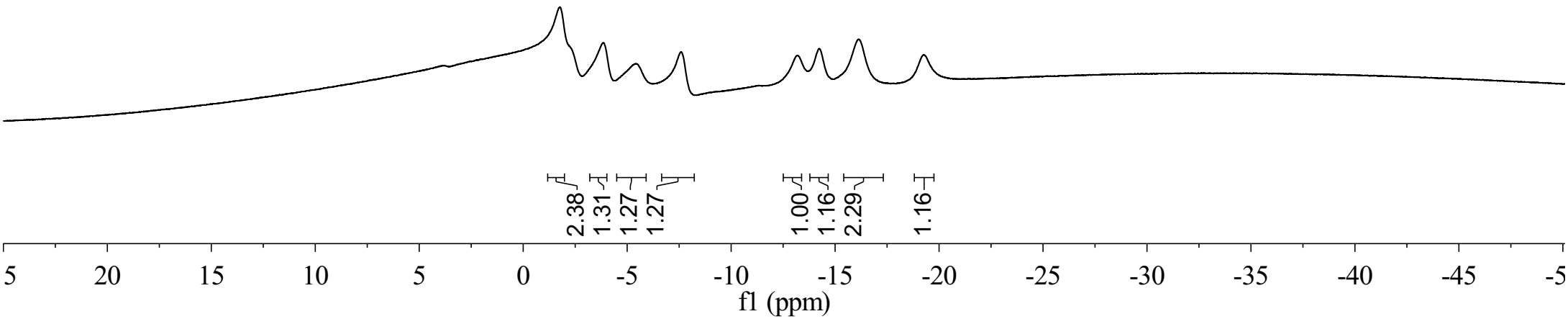


ZCY-1666-B{H}

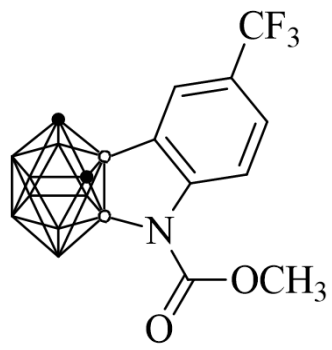


3h

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

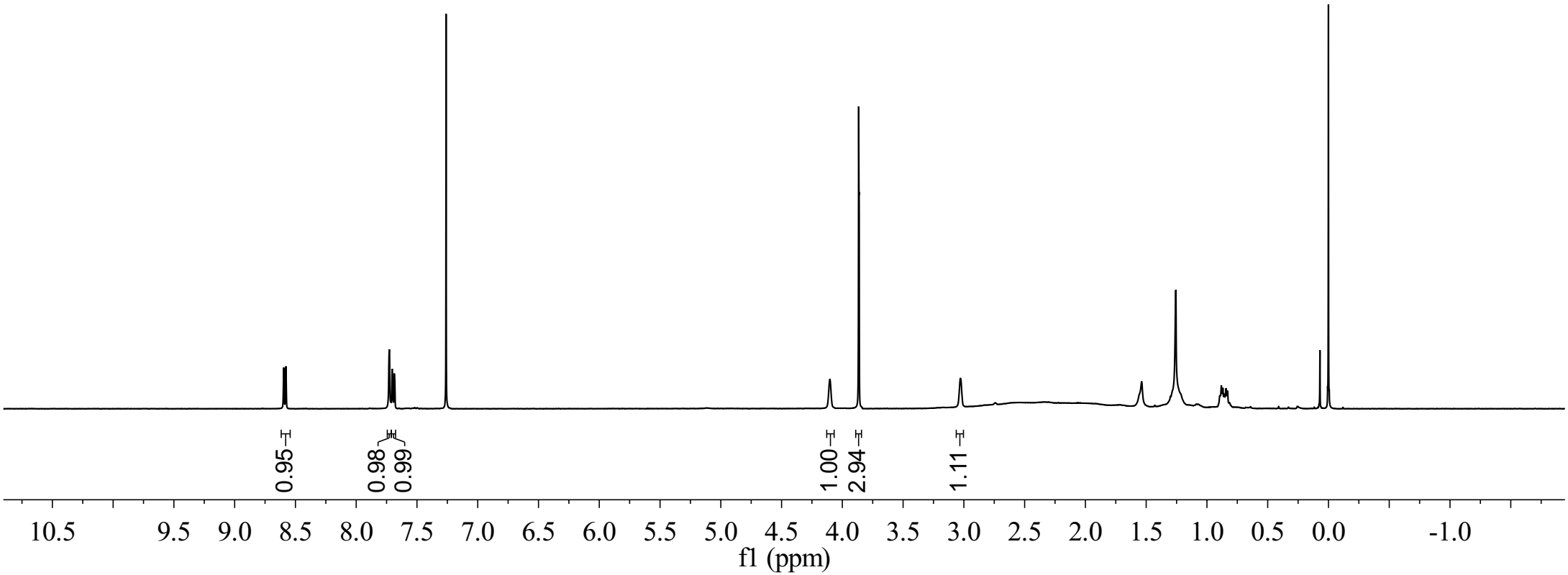


ZCY-1668-H

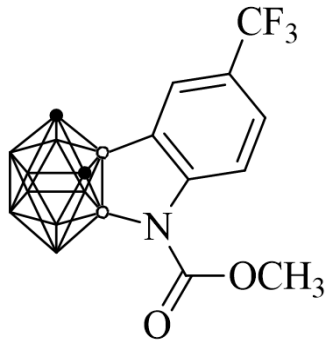


3i

^{1}H, $CDCl_3$, 500MHz, 298K



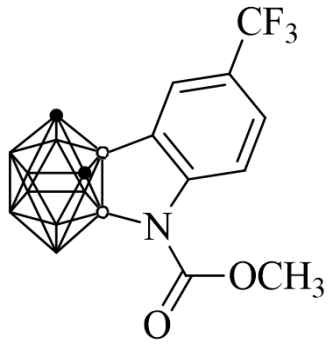
ZCY-1668-C



3i

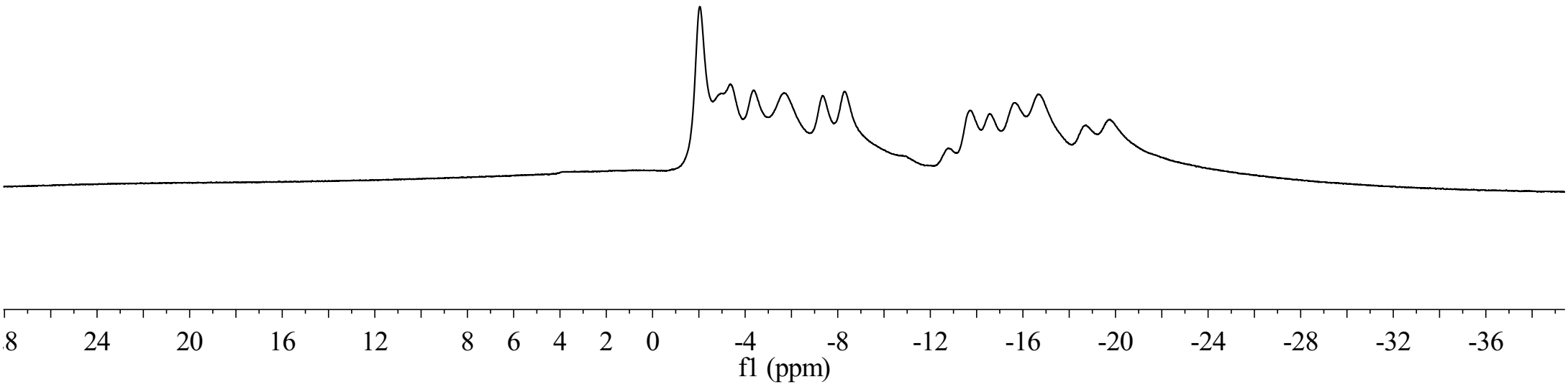
^{13}C, $CDCl_3$, 125MHz, 298K

ZCY-1668-B

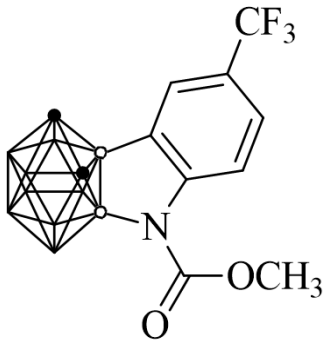


3i

^{11}B, $CDCl_3$, 160MHz, 298K

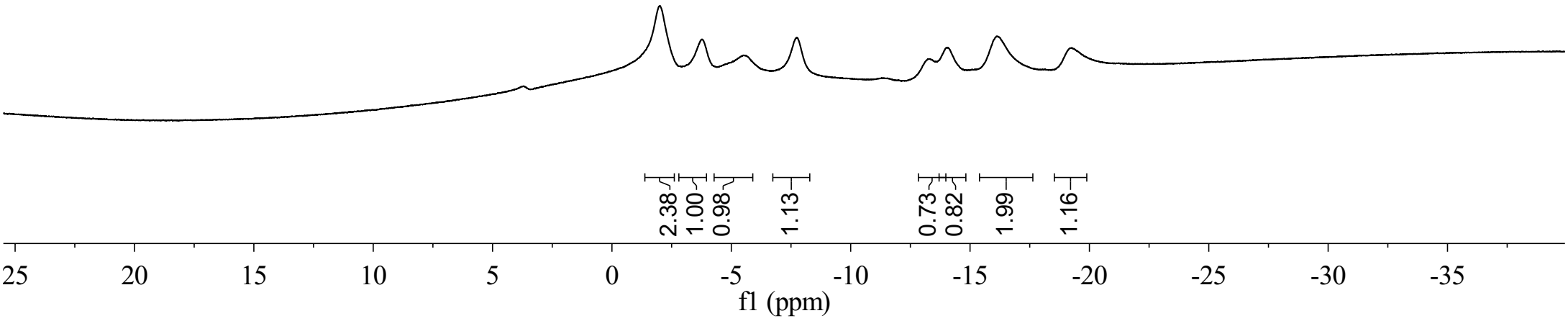


ZCY-1668-B{H}

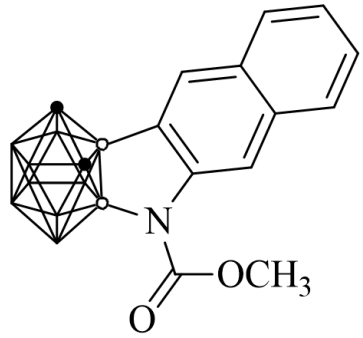


3i

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K

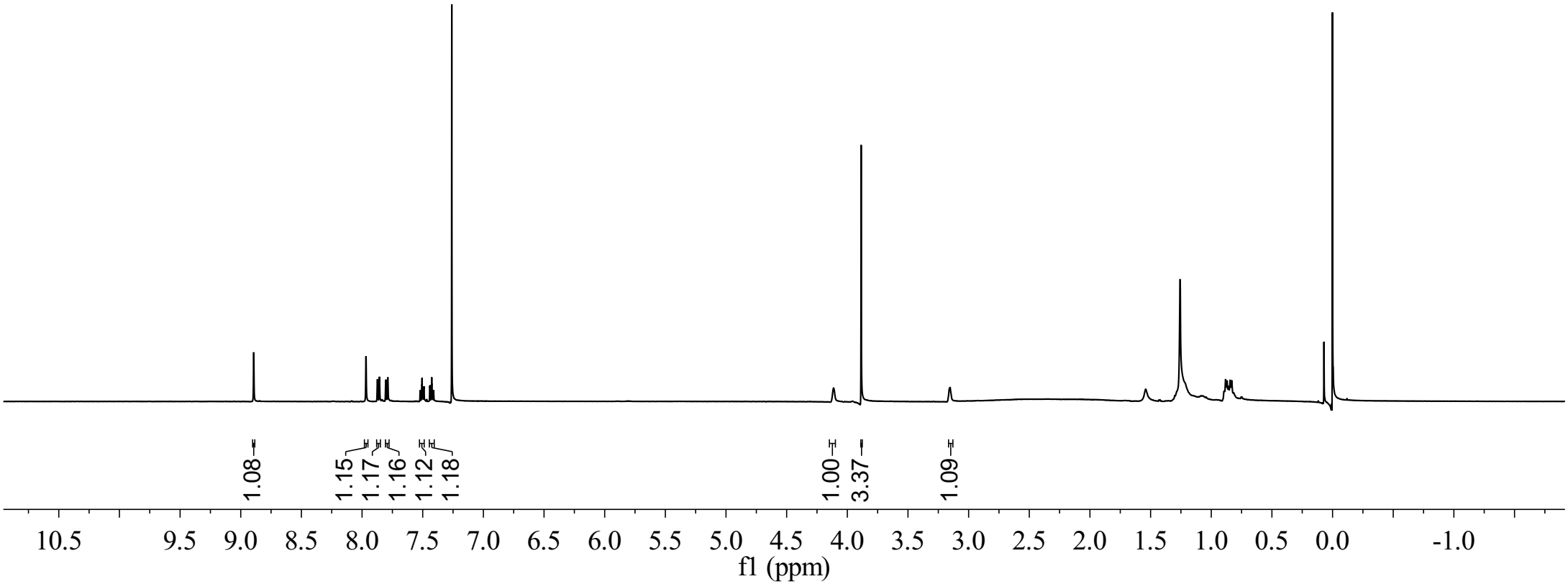


ZCY-1669-H

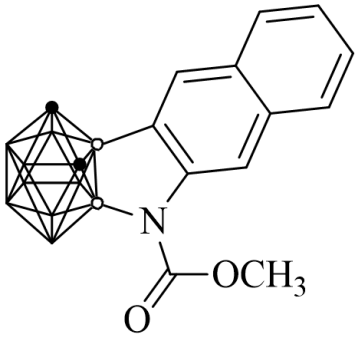


3j

^{1}H, $CDCl_3$, 500MHz, 298K



ZCY-1669-C

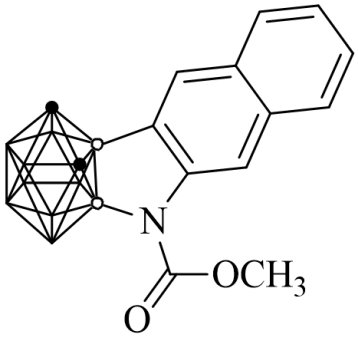


3j

^{13}C, $CDCl_3$, 125MHz, 298K

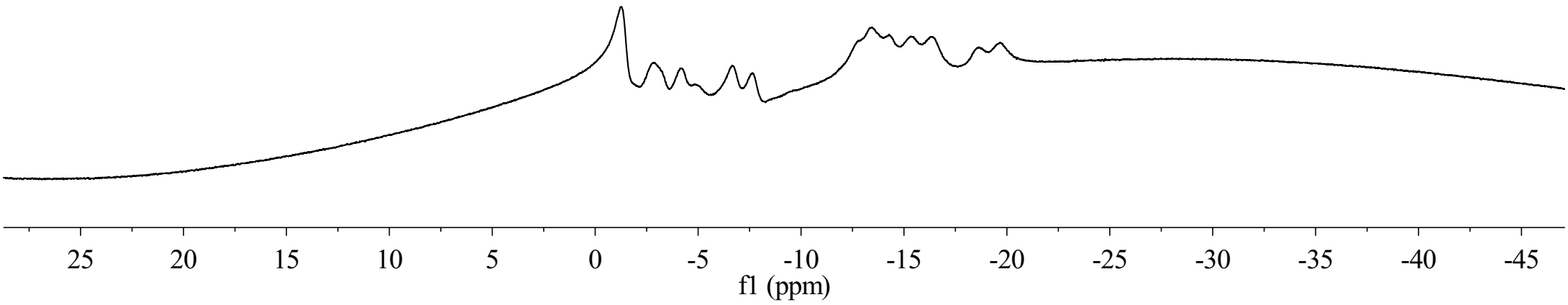
ZCY-1669-B

-1.28
-2.82
-4.13
-6.68
-7.62
-13.46
-15.33
-16.37
-18.66
-19.64

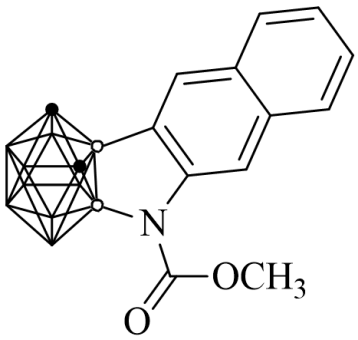


3j

^{11}B, $CDCl_3$, 160MHz, 298K

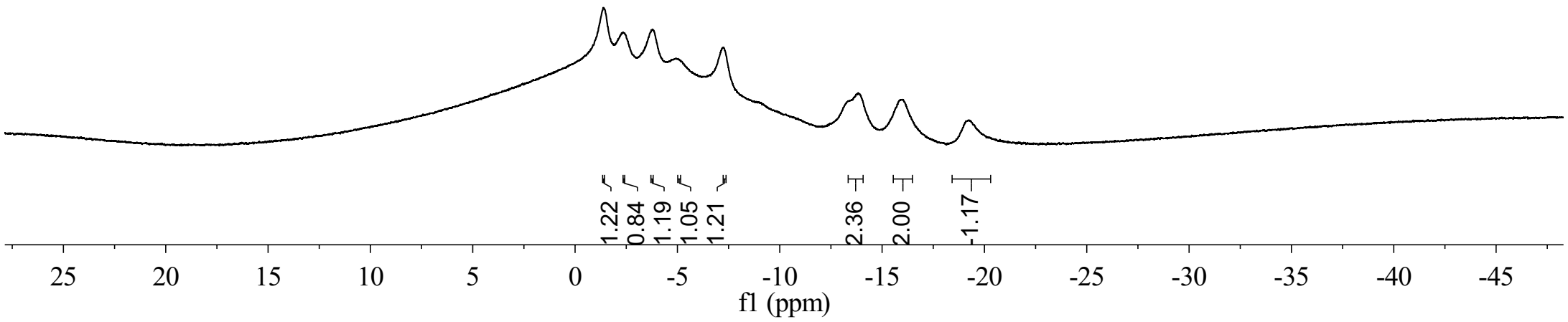


ZCY-1669-B{H}



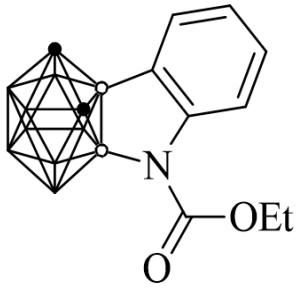
3j

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K



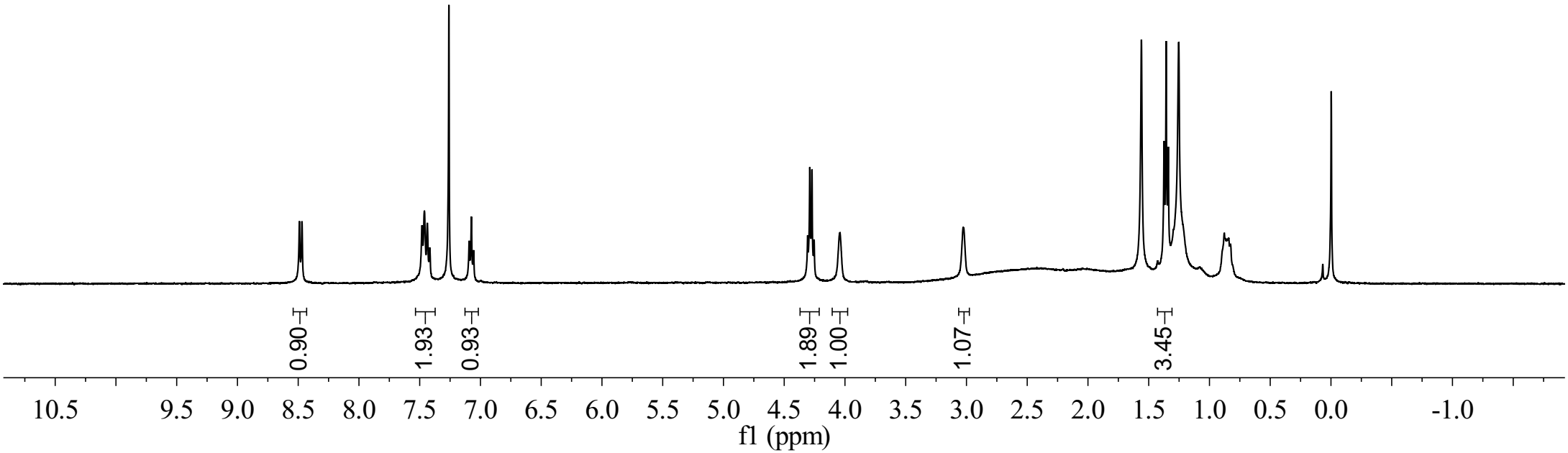
ZCY-1673-H

8.49 8.47 7.48 7.46 7.44 7.42 7.26 7.09 7.07 7.06 4.31 4.29 4.27 4.25 4.04 3.03 1.37 1.36 1.34 0.07 -0.00

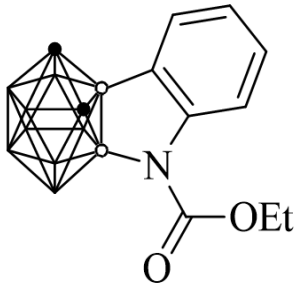


5a

^{1}H, $CDCl_3$, 500MHz, 298K



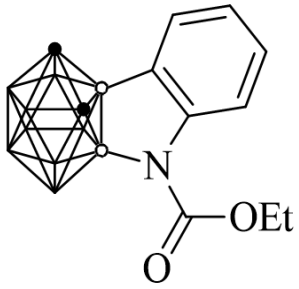
ZCY-1673-C



5a

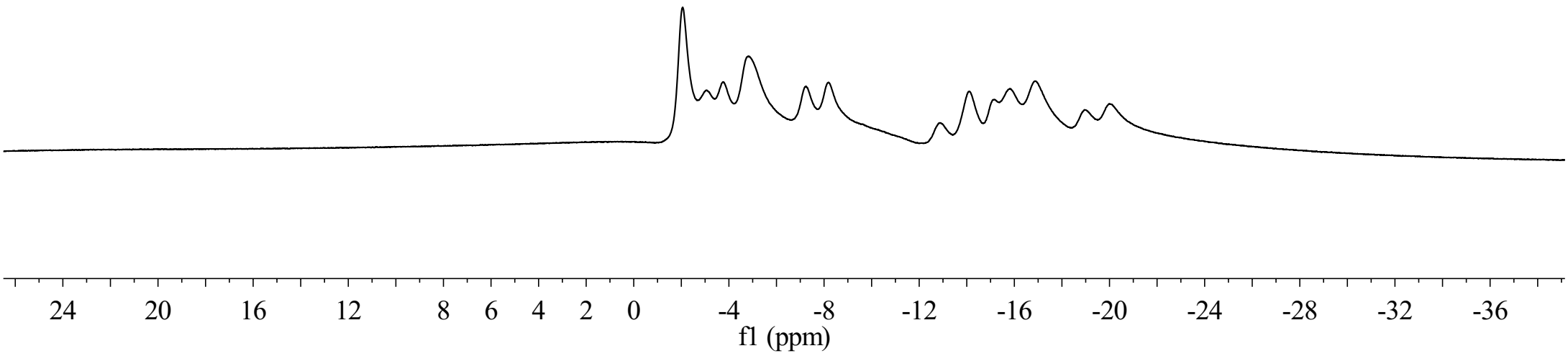
^{13}C, $CDCl_3$, 125MHz, 298K

ZCY-1673-B

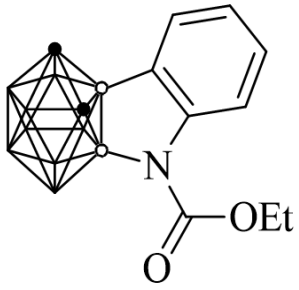


5a

^{11}B, $CDCl_3$, 160MHz, 298K

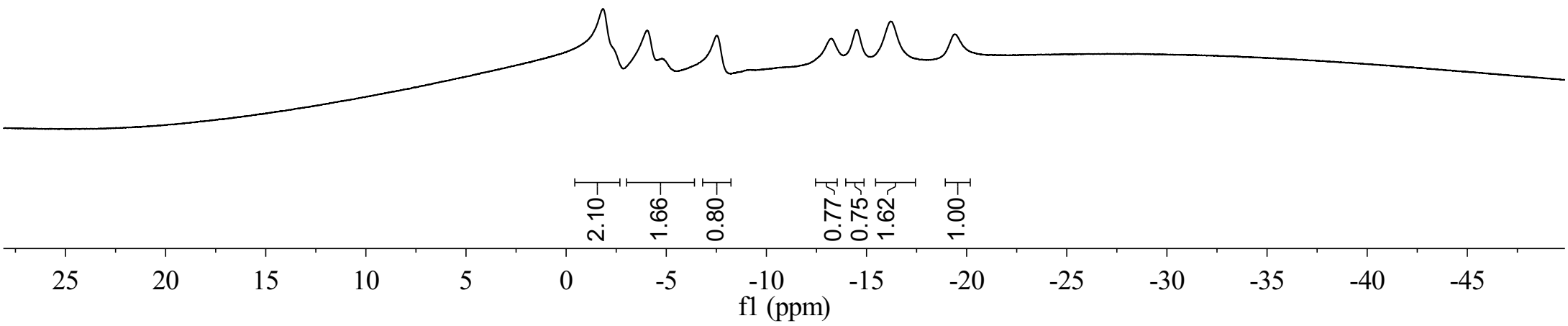


ZCY-1673-B{H}



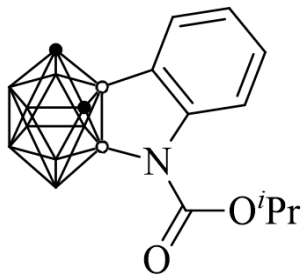
5a

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K



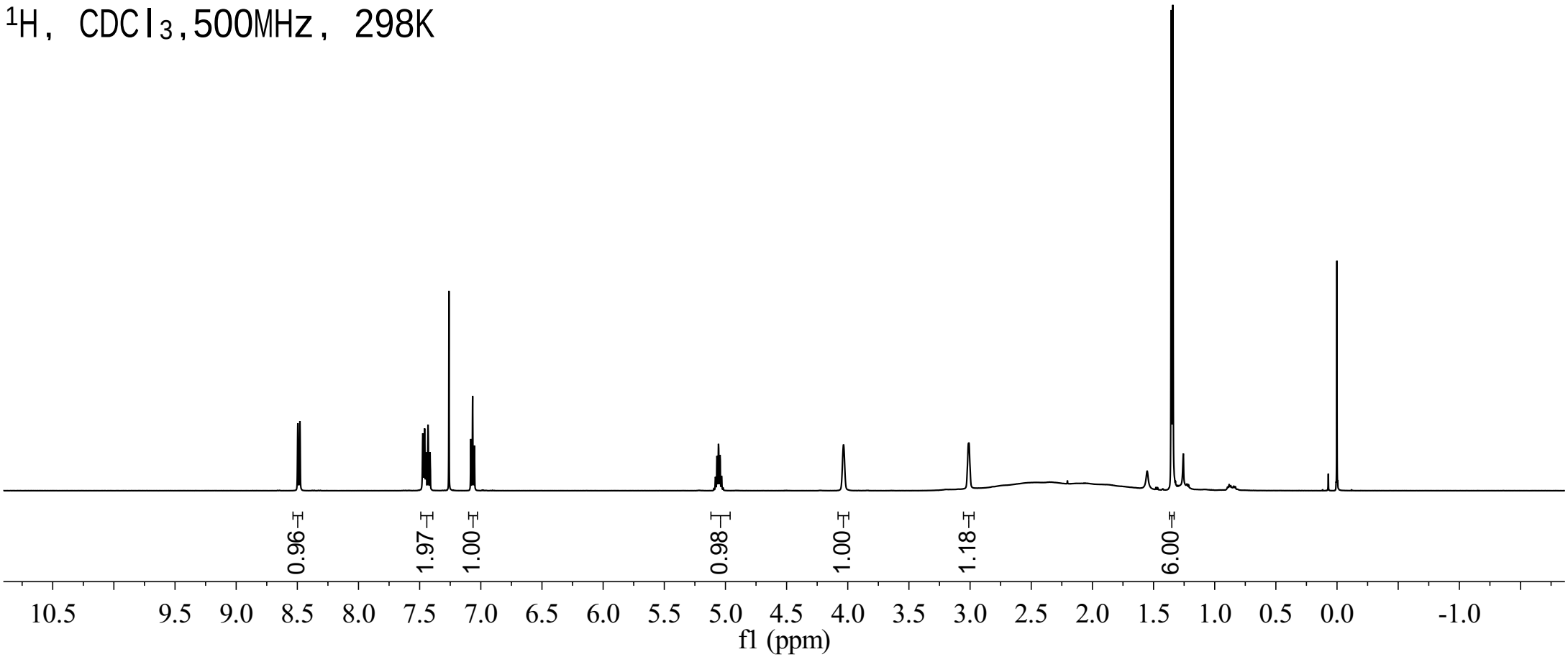
ZCY-1679-H

8.50 8.48 7.47 7.46 7.45 7.43 7.41 7.26 7.08 7.07 7.05 5.08 5.07 5.06 5.04 5.03 4.03 3.01 1.35 1.34 0.07 0.00



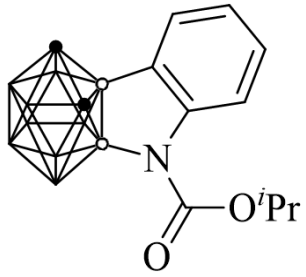
5b

^{1}H, CDCl$_{3}$, 500MHz, 298K



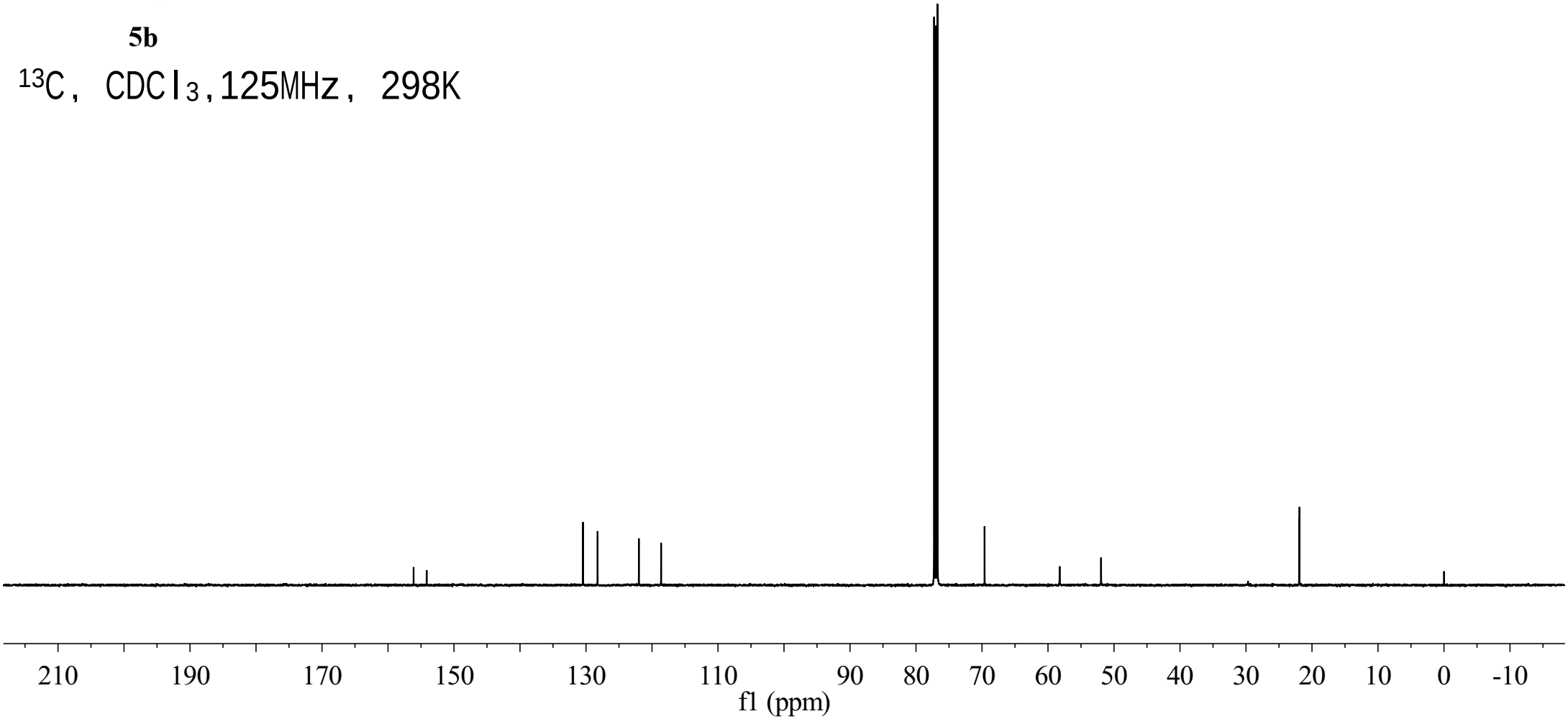
ZCY-1679-C

156.12
154.14
130.47
128.25
121.99
118.62
77.25
77.00
76.75
69.61
58.22
51.96
21.95
21.89
-0.02

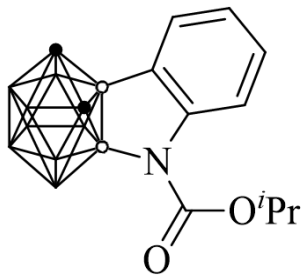


5b

^{13}C, CDCl$_3$, 125MHz, 298K

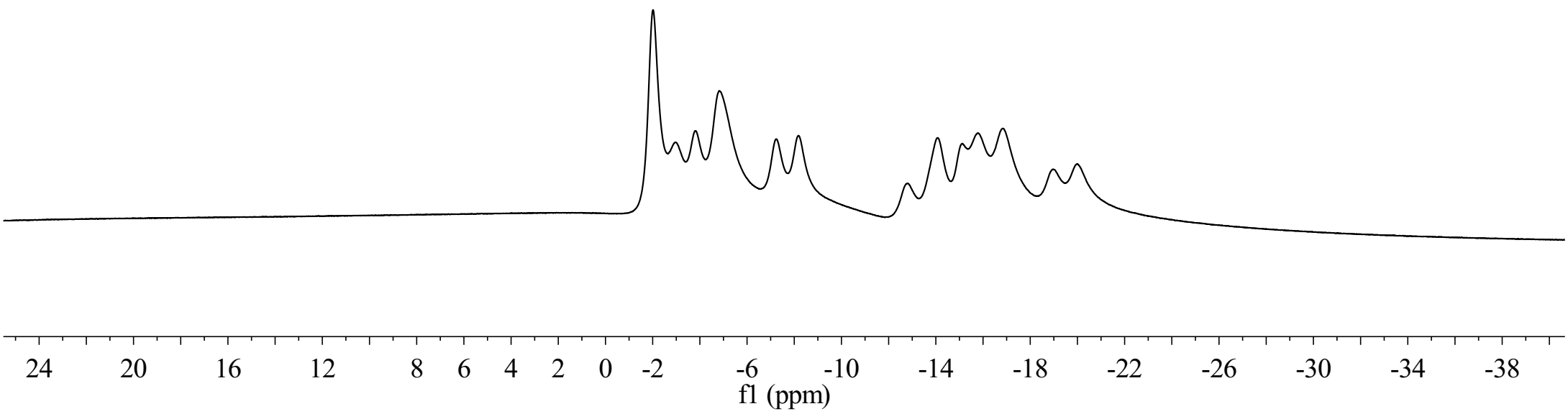


ZCY-1679-B

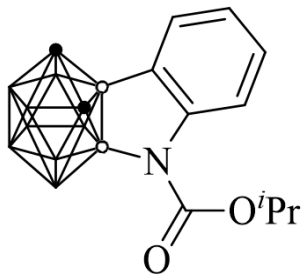


5b

^{11}B, CDCl$_3$,160MHz, 298K

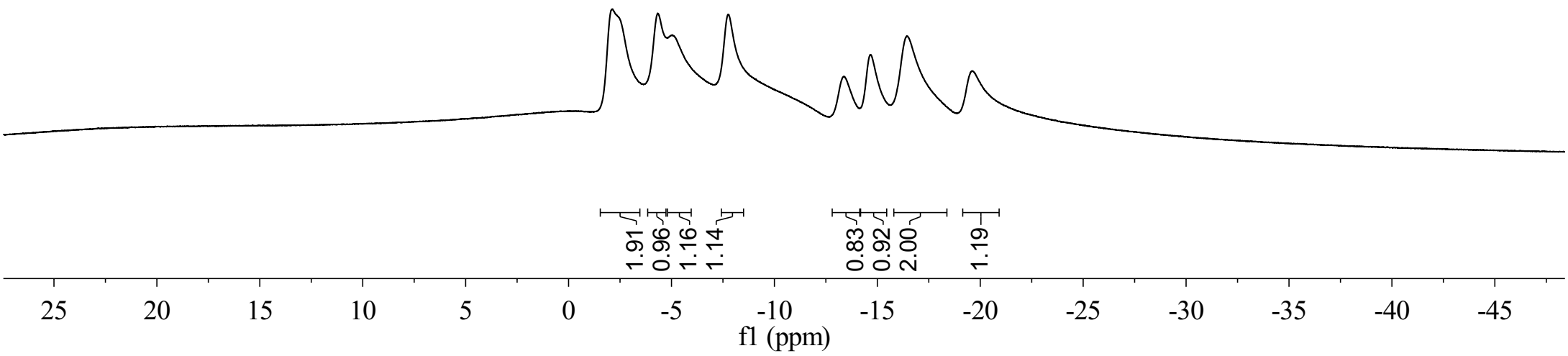


ZCY-1679-B{H}

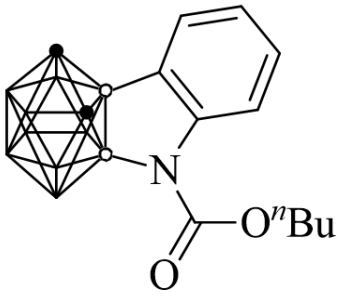


5b

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K



ZCY-1674-H

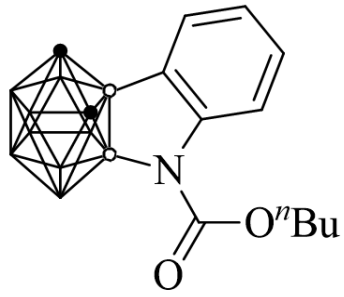


5c

^{1}H, CDCl$_3$,500MHz, 298K

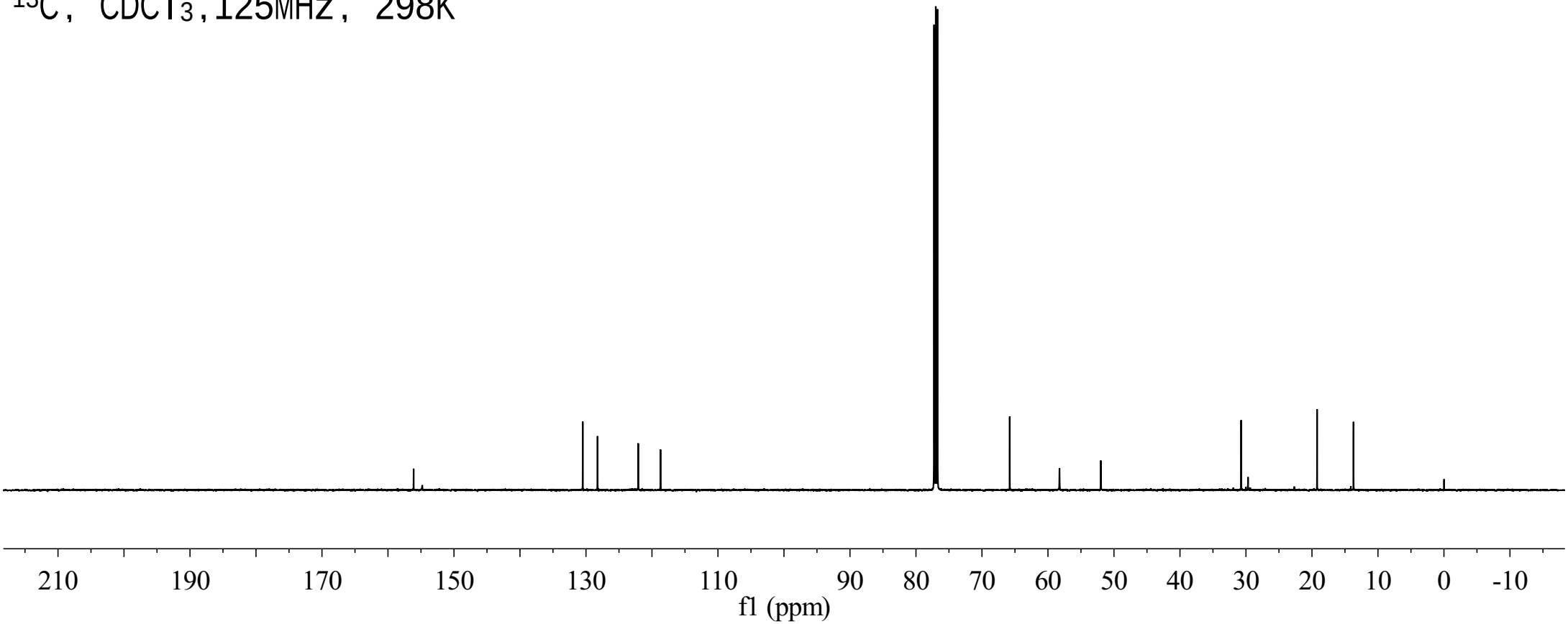
ZCY-1674-C

156.11
154.80
130.49
128.25
122.08
118.71
77.25
77.00
76.75
65.79
58.25
51.99
30.73
19.23
13.70
-0.02



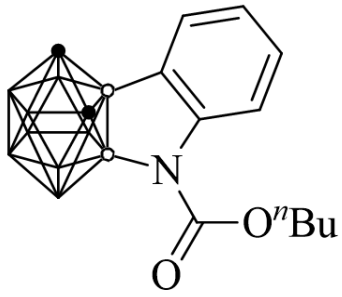
5c

^{13}C, CDCl$_3$, 125MHz, 298K



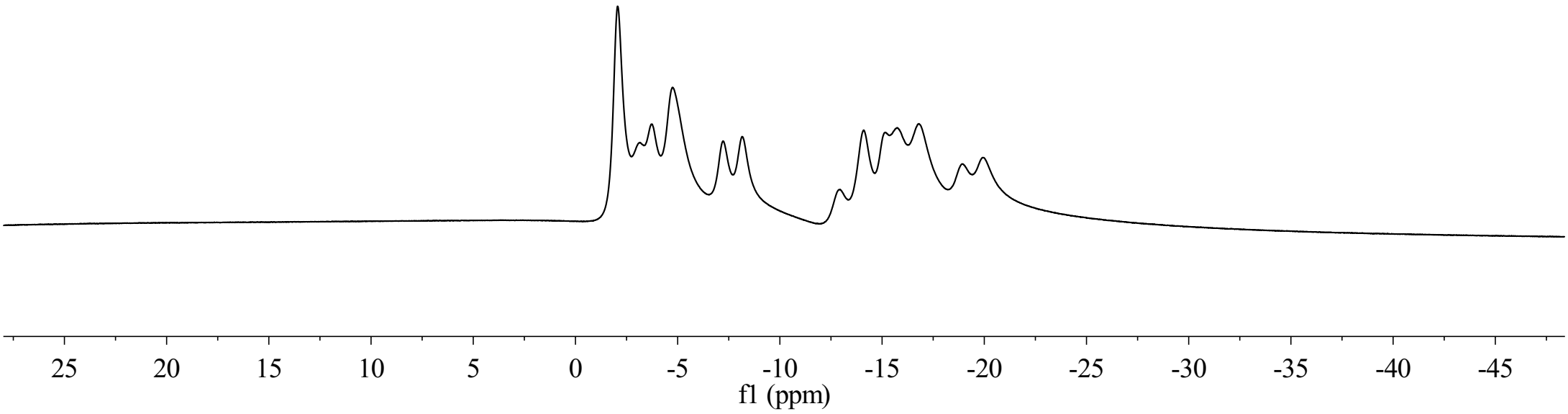
ZCY-1674-B

-2.07
-3.13
-3.74
-4.74
-7.22
-8.17
-12.93
-14.10
-15.15
-15.76
-16.80
-18.92
-19.92

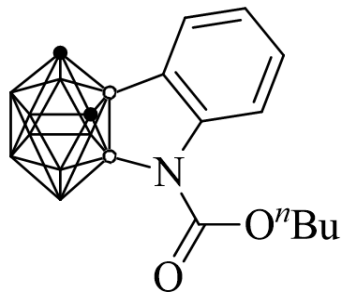


5c

^{11}B, CDCl$_3$,160MHz, 298K

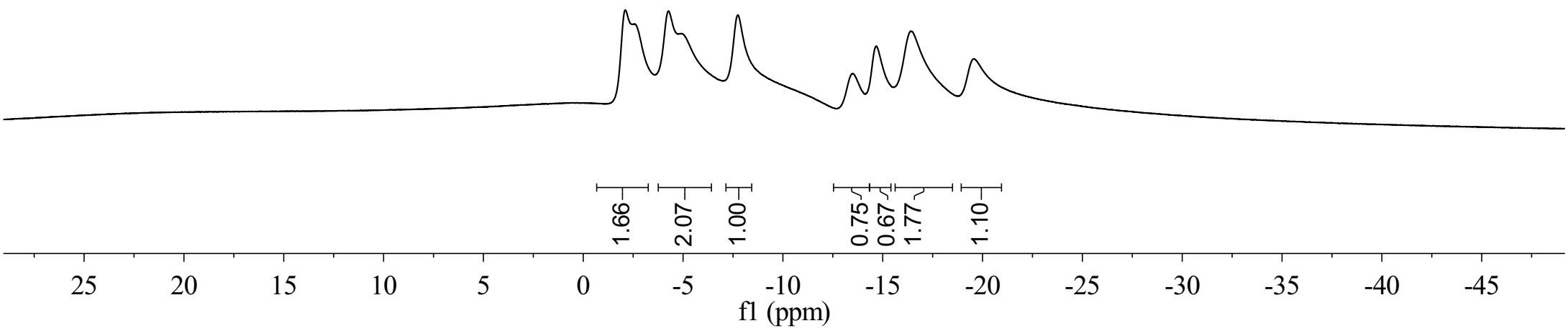


ZCY-1674-B{H}

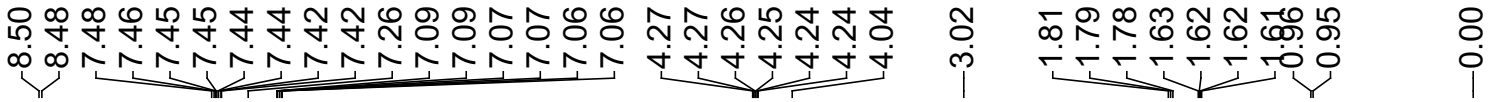


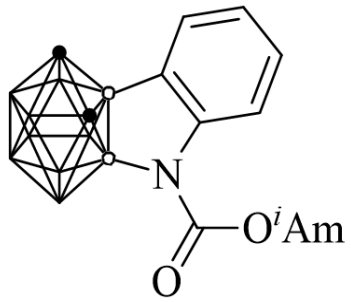
5c

$^{11}B\{^1H\}$, $CDCl_3$, 160MHz, 298K



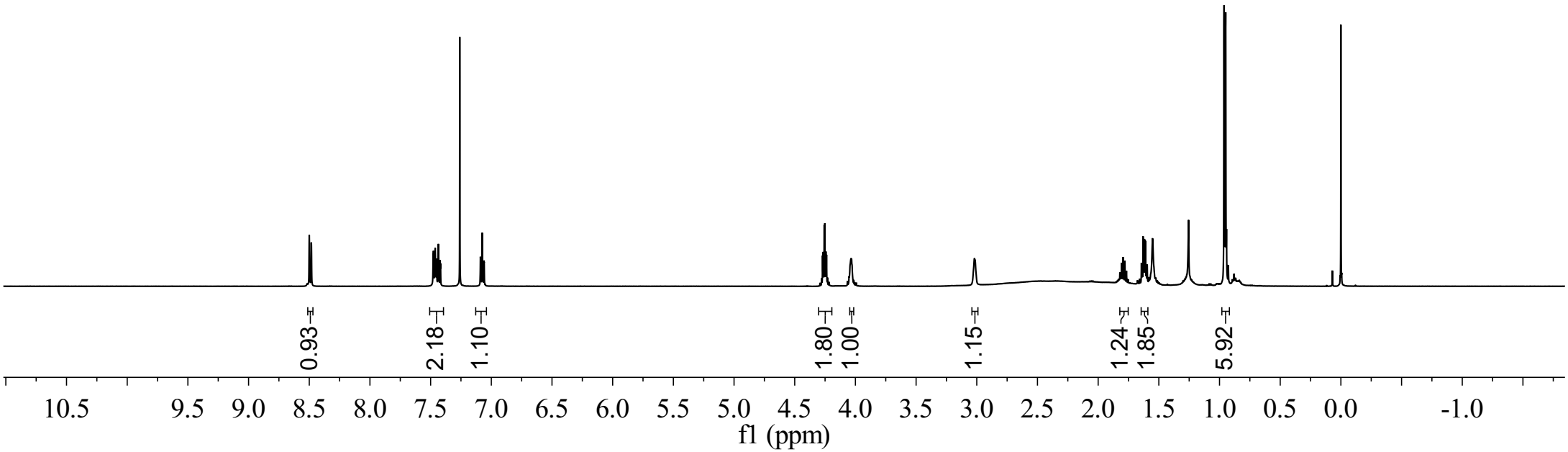
ZCY-1771-H



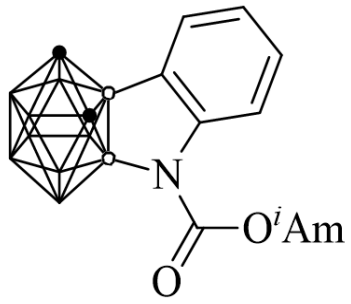


5d

^{1}H, CDCl$_{3}$,600MHz, 298K



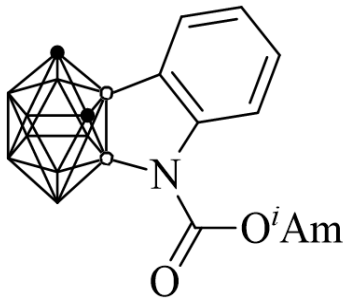
ZCY-1771-C



5d

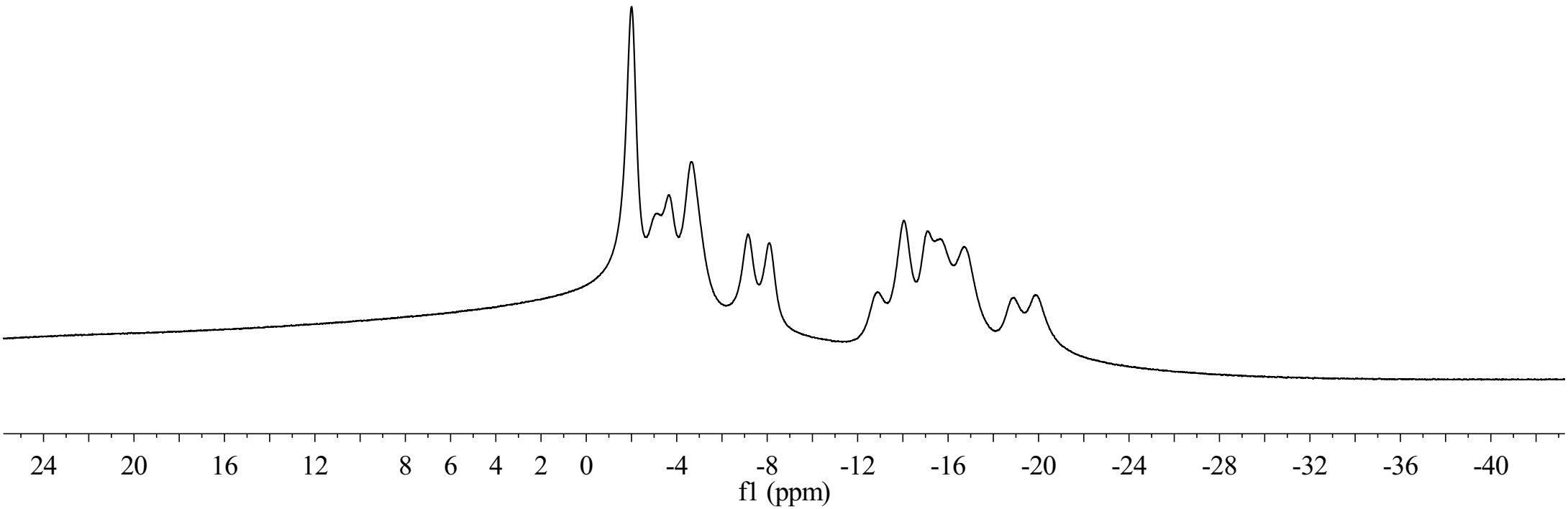
^{13}C, CDCl$_3$,150MHz, 298K

ZCY-1771-B

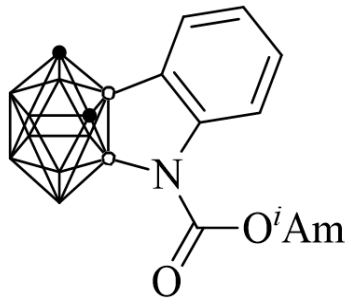


5d

^{11}B, CDCl$_3$,160MHz, 298K

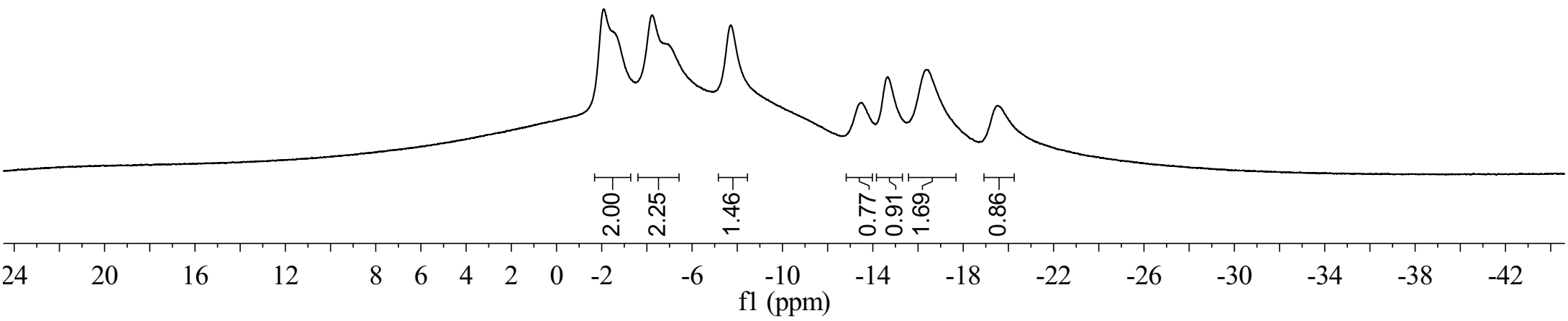


ZCY-1771-B{H}

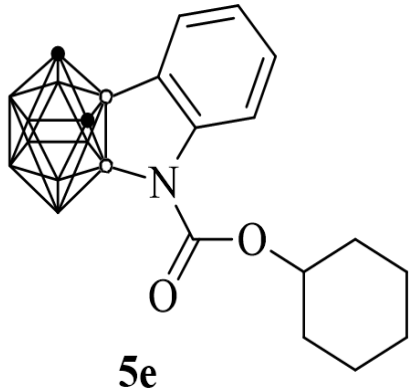


5d

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K



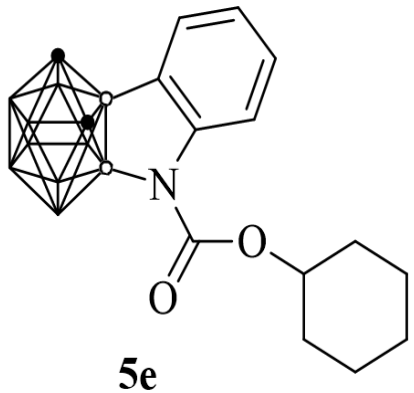
ZCY-1702-H



5e

^{1}H, CDCl$_3$, 500MHz, 298K

ZCY-1702-C

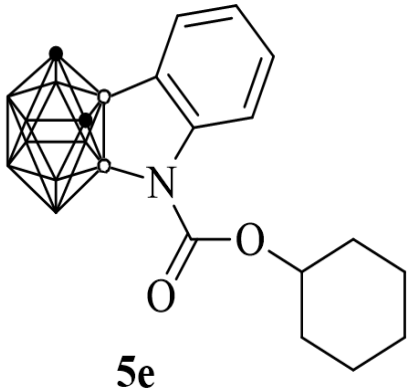


5e

^{13}C, $CDCl_3$, 125MHz, 298K

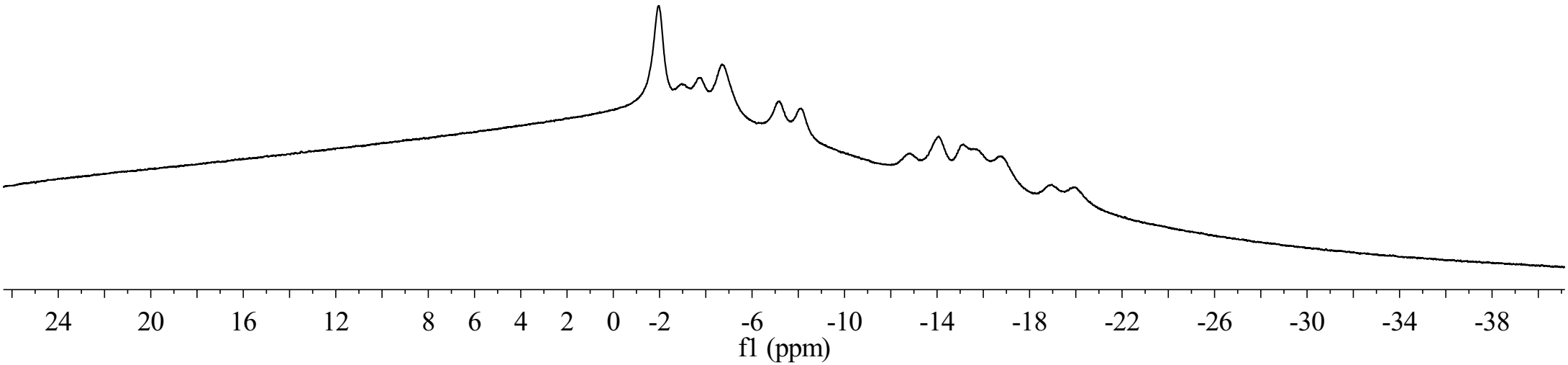
ZCY-1702-B

-1.97
-2.95
-3.73
-4.69
-7.18
-8.11
-12.85
-14.06
-15.14
-16.82
-18.96
-19.95

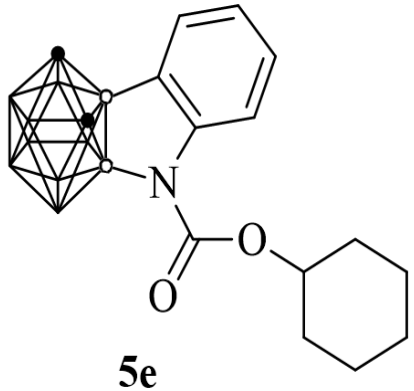


5e

^{11}B, $CDCl_3$, 160MHz, 298K



ZCY-1702-B{H}



5e

$^{11}B\{^{1}H\}$, $CDCl_3$, 160MHz, 298K