

Supporting Information

Organoaluminum Hydrides Catalyzed Hydroboration of Carbonates, Esters, Carboxylic Acids, and Carbon Dioxide

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General Information.

All operations during the experiment were performed in a pure N₂ atmosphere using Schlenk techniques or inside a Mbraun MB 150-GI glove box. Commercially available chemicals were purchased from J&K chemical reagents company or Aldrich reagents company, and stored and used according to the instructions. The NMR spectra were provided using the Bruker Ascend II 400 spectrometer.

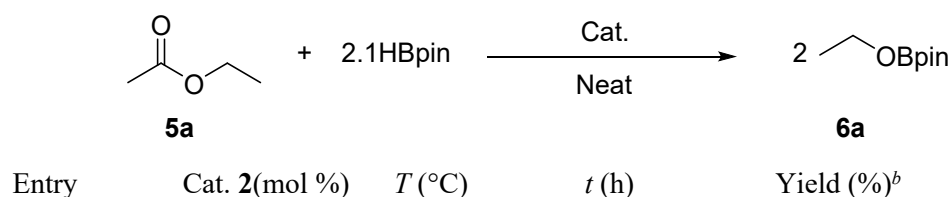
Method for preparation of LAIH₂:

LH (L = HC(CMeNAr)₂ Ar = 2,6 - *i*Pr₂C₆H₃) (0.418g, 1 mmol) in toluene (10 mL) was added under cooling with an ice bath to a solution of AlH₃·NMe₃ (0.089 g, 1 mmol) in toluene (2 mL) under nitrogen atmosphere, and the reaction mixture was stirred for additional 24 h, concentrated to 5 mL and stored overnight at -30 °C. The crude product was crystallized from toluene to afford colorless crystals of **1** and dried in vacuo.

Method for preparation of L'AlH₂:

A solution of LH (L' = HC(CMeNAr)₂, Ar = 2,6 - Et₂C₆H₃) (0.362g, 1 mmol) in toluene (10 mL) was added under cooling with an ice bath to a solution of AlH₃·NMe₃ (0.089 g, 1 mmol) in toluene (2 mL) under nitrogen atmosphere, and the reaction mixture was stirred for additional 24 h, concentrated to 5 mL and stored overnight at -30 °C. The crude product was crystallized from toluene to afford colorless crystals of **2** and dried in vacuo. [S1]

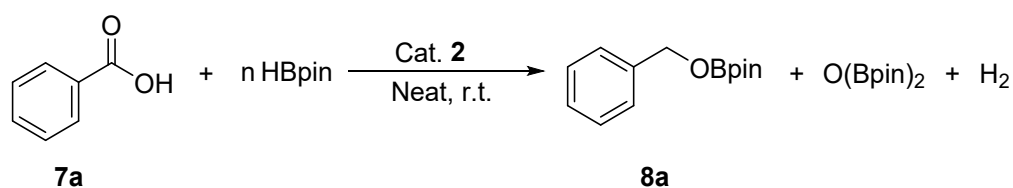
Table S1. Optimization of Al-Catalyzed Hydroboration of Ethylacetate^a



| | | | | |
|---|----------|-----------|-----------|-----------|
| 1 | - | 23 | 8 | 0 |
| 2 | - | 60 | 8 | 0 |
| 3 | 5 | 23 | 8 | 21 |
| 4 | 5 | 40 | 8 | 35 |
| 5 | 5 | 60 | 8 | 55 |
| 6 | 5 | 60 | 10 | 83 |
| 7 | 5 | 60 | 12 | 99 |

^aEthylacetate (**5a**) (1 mmol), HBpin (2.1 equiv), **2** (5 mol %). ^bThe reaction was monitored by ¹H NMR spectroscopy.

Table S2. Optimization of Al-Catalyzed Hydroboration of Benzoic Acid^a



| Entry | n | Cat. 2 (mol %) | <i>t</i> (h) | Yield (%) ^b |
|----------|------------|-----------------------|--------------|------------------------|
| 1 | 3.1 | 2 | 1 | 57 |
| 2 | 3.3 | 2 | 1 | 63 |
| 3 | 3.1 | 2 | 2 | 91 |
| 4 | 3.3 | 2 | 2 | 99 |
| 5 | 3.3 | 1 | 2 | 78 |
| 6 | 3.3 | - | 1 | 17 |
| 7 | 3.3 | - | 2 | 36 |

^aReaction conditions: benzoic acid (**7a**) (1 mmol) and HBpin (3.3 mmol, 3.3 equiv). ^bThe reaction was monitored by ¹H NMR spectroscopy with mesitylene as an internal standard.

In the NMR spectra we used the following marks:

* - MeOBPin: ¹H NMR (400 MHz, CDCl₃) δ: 3.32 (s, 3H), 1.18 (s, 12H). ¹³C NMR (101 MHz, CDCl₃) δ: 81.72, 51.54, 23.59.

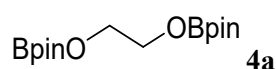
■ - EtOBPin: ¹H NMR (400 MHz, CDCl₃) δ 3.89 (q, *J* = 7.1 Hz, 2H). 1.18 (t, *J* = 6.6 Hz, 12H), 1.13 (s, 3H). ¹³C NMR (101 MHz, CDCl₃): δ 81.54, 59.60, 23.58, 16.18.

▼ - Mesitylene: ¹H NMR (400 MHz, CDCl₃) δ: 6.65 (s, 3H), 2.13 (s, 9H). ¹³C NMR

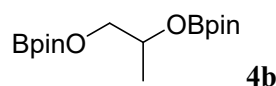
(101 MHz, CDCl₃): 136.82, 125.88, 21.13.

General Procedure for Hydroboration of Carbonates.

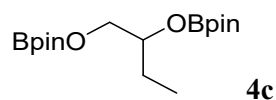
Carbonate (1.0 mmol), HBpin (3.1 mmol) and catalyst **2** (5 mol%) were placed in a 10 ml Schlenk flask equipped with a magnetic stir bar inside the glove box. The reaction mixture was stirred for 10 h at 100 °C, and then subjected to NMR analysis. The progress of the reaction was monitored by ¹H NMR, ¹³C NMR, and ¹¹B NMR spectra, respectively which indicated the progress of the reaction by the disappearance of the carbonate proton and appearance of new products and CH₃OBpin and there is no need to separate the products.



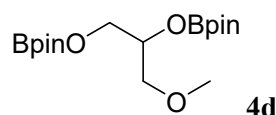
¹H NMR (400 MHz, CDCl₃): δ 3.86 (s, 4H, OCH₂), 1.18 (s, 24H, BOCMe₂). ¹³C {1H} NMR (101 MHz, CDCl₃): δ 81.74, 64.03, 51.58. ¹¹B {1H} NMR (128 MHz, CDCl₃): δ 22.43.



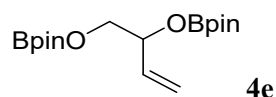
¹H NMR (400 MHz, CDCl₃): δ 4.22-4.18 (q, *J* = 6.0 Hz, 1H, CH), 3.67 (d, *J* = 5.7 Hz, 2H, OCH₂), 1.17 (s, 24H, BOCMe₂), 1.09 (d, *J* = 6.3 Hz, 3H, Me). ¹³C {1H} NMR (101 MHz, CDCl₃): δ 81.68, 81.55, 69.33, 68.13, 23.60, 23.54, 17.47. ¹¹B {1H} NMR (128 MHz, CDCl₃): δ 22.24.



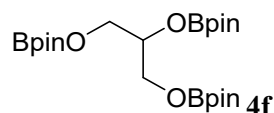
¹H NMR (400 MHz, CDCl₃): δ 4.10-4.04 (m, 1H, CH), 3.78 (dd, *J* = 14.0, 5.6 Hz, 2H, OCH₂), 1.56-1.44 (m, 2H, CH₂), 1.26 (s, 24H, BOCMe₂), 0.92 (t, *J* = 7.5 Hz, 3H, Me). ¹³C {1H} NMR (101 MHz, CDCl₃): δ 82.77, 82.55, 75.39, 67.72, 25.28, 24.62, 24.56, 9.48. ¹¹B {1H} NMR (128 MHz, CDCl₃): δ 22.24.



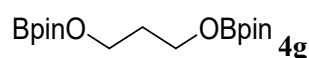
¹H NMR (400 MHz, CDCl₃): δ 4.31 (s, 1H, CH), 3.95-3.82 (m, 2H, OCH₂), 3.49-3.44 (m, 2H, CH₂), 3.36 (d, *J* = 11.1 Hz, CH₃), 1.26 (s, 24H, BOCMe₂). ¹³C {1H} NMR (101 MHz, CDCl₃): δ 82.71, 82.66, 72.81, 65.42, 59.02, 52.49, 24.55, 24.48. ¹¹B {1H} NMR (128 MHz, CDCl₃): δ 22.31.



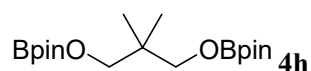
^1H NMR (400 MHz, CDCl_3): δ 5.78-5.69 (m, 1H, $\text{CH}=\text{CH}_2$), 5.28-5.24 (m, 1H, $\text{CH}=\text{CH}_2$), 5.09-5.07 (m, 1H, $\text{CH}=\text{CH}_2$), 4.45 (q, $J = 4.1$ Hz, 1H, CH), 3.51 (d, 2H, OCH_2), 1.17 (s, 24H, BOCMe_2). ^{13}C {1H} NMR (101 MHz, CDCl_3): δ 134.44, 115.37, 81.70, 81.68, 73.85, 66.84, 23.61, 23.55. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.19.



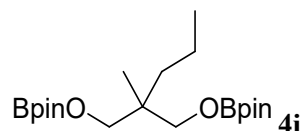
^1H NMR (400 MHz, CDCl_3): δ 4.18 (d, $J = 4.6$ Hz, 1H, CH), 3.83 (d, $J = 4.5$ Hz, 2H, OCH_2), 3.75 (d, $J = 6.3$ Hz, 2H, CH_2), 1.17 (s, 36H, BOCMe_2). ^{13}C {1H} NMR (101 MHz, CDCl_3): δ 82.73, 82.69, 73.62, 65.06, 24.54, 24.52. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.37.



^1H NMR (400 MHz, CDCl_3): δ 3.93(m, 4H, OCH_2), 1.85-1.84 (m, 2H, CH_2), 1.25 (s, 24H, BOCMe_2). ^{13}C {1H} NMR (101 MHz, CDCl_3): δ 82.66, 82.58, 61.46, 33.23, 24.54. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.20.



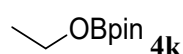
^1H NMR (400 MHz, CDCl_3): δ 3.56 (s, 4H, OCH_2), 1.17 (s, 24H, BOCMe_2), 0.80 (s, 6H, Me). ^{13}C {1H} NMR (101 MHz, CDCl_3): δ 81.74, 81.59, 69.28, 35.65, 23.60, 19.82. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.37.



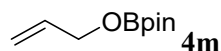
^1H NMR (400 MHz, CDCl_3): δ 3.66 (d, $J = 4.0$ Hz, 4H, OCH_2), 1.27 (s, 4H, CH_2), 1.26-1.24 (24H, BOCMe_2 , CH_2), 0.88 (d, $J = 6.3$ Hz, 3H, CH_2Me), 0.83 (s, 3H, CMe). ^{13}C {1H} NMR (101 MHz, CDCl_3): δ 81.73, 81.56, 68.78, 38.05, 34.97, 23.59, 17.28, 15.38, 13.90. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.24.



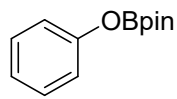
^1H NMR (400 MHz, CDCl_3): δ 352 (s, 3H, Me), 1.18 (s, 12H, BOCMe_2). {1H} NMR (101 MHz, CDCl_3): δ 81.72, 51.54, 23.59. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.22.



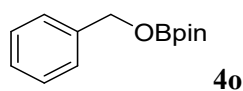
^1H NMR (400 MHz, CDCl_3): δ 3.82 (q, $J = 7.0$ Hz, 2H, OCH_2), 1.17 (s, 12H, BOCMe_2), 1.16 (t, $J = 7.0$ Hz, 3H, Me). {1H} NMR (101 MHz, CDCl_3): δ 81.72, 81.55, 59.50, 23.57, 16.18. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.11.



^1H NMR (400 MHz, CDCl_3): δ 5.82 (d, $J = 10.5$ Hz, 1H, $\text{CH}=\text{CH}_2$), 5.20 (d, $J = 18.9$ Hz, 2H, $\text{CH}=\text{CH}_2$), 5.04 (d, $J = 12.0$ Hz, 2H, CH_2), 4.29 (d, $J = 4.8$ Hz, 3H, OCH_3), 1.18 (s, 24H, BOCMe_2). $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 135.35, 114.91, 82.76, 65.46, 24.56, 24.53. ^{11}B $\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 22.32.



^1H NMR (400 MHz, CDCl_3): δ 7.18-7.14 (m, 2H, Ar- H), 7.00-6.91 (m, 3H, Ar- H), 1.15 (s, 12H, BOCMe_2). $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 152.44, 128.23, 122.00, 118.46, 82.41, 81.67, 23.56. ^{11}B $\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 22.25.



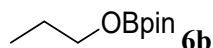
^1H NMR (400 MHz, CDCl_3): δ 7.29-7.17 (m, 5H, Ar- H), 4.84 (s, 2H, OCH_2), 1.17 (s, 12H, BOCMe_2). $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 138.20, 127.24, 126.33, 126.68, 81.91, 65.63, 23.58. ^{11}B $\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 22.35.

General Procedure for Hydroboration of Esters.

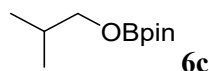
Ester (1.0 mmol), HBpin (2.1 mmol) and catalyst **2** (5 mol%) were placed in a 10 ml Schlenk flask equipped with a magnetic stir bar inside the glove box. The reaction mixture was stirred for 12 h at 60 °C. The progress of the reaction was monitored by ^1H NMR, ^{13}C NMR, and ^{11}B NMR, which indicated the completion of the reaction by the disappearance of the ester proton and appearance of new products and there is no need to separate the products.



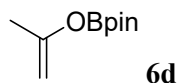
^1H NMR (400 MHz, CDCl_3): δ 3.89 (q, $J = 7.1$ Hz, 2H, BOCMe_2), 1.18 (t, $J = 6.6$ Hz, 12H, BOCMe_2), 1.13 (s, 3H, $\text{MeCH}_2\text{OBpin}$). ^{13}C NMR (101 MHz, CDCl_3): δ 81.54, 59.60, 23.58, 16.18. ^{11}B $\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 22.13.



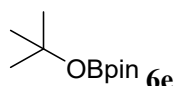
^1H NMR (400 MHz, CDCl_3): δ 3.76-3.67 (m, 2H, MeCH_2CH_2), 1.52 (q, $J = 7.4$ Hz, 2H, MeCH_2CH_2), 1.19-1.16 (m, 12H, BOCMe_2), 0.84 (t, 3H, $J = 8$ Hz, MeCH_2CH_2). ^{13}C NMR (101 MHz, CDCl_3) δ 81.56, 65.54, 23.65, 23.57, 9.07. ^{11}B $\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ 22.24.



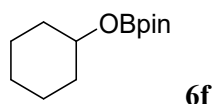
^1H NMR (400 MHz, CDCl_3): δ 3.54 (d, $J = 6.5$ Hz, 2H, CH_2OBpin), 1.74 (s, 1H, CHMe_2), 1.18 (s, 12H, BOCMe_2), 0.82 (d, $J = 6.8$ Hz, 6H, CHMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 81.56, 70.35, 28.80, 23.56, 17.73. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.05.



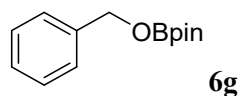
^1H NMR (400 MHz, CDCl_3): δ 4.89 (s, 1H, $\text{C}=\text{CH}_2$), 4.75 (s, 1H, $\text{C}=\text{CH}_2$), 4.17 (s, 2H, CH_2OBpin), 1.64 (s, 3H, $\text{MeC}=\text{CH}_2$), 1.18 (s, 12H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 141.63, 109.00, 81.74, 67.24, 23.56. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.21.



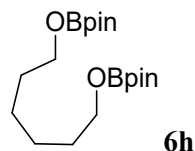
^1H NMR (400 MHz, CDCl_3): δ 1.26 (s, 9H, $(\text{CH}_3)_3\text{COBpin}$), 1.18 (s, 12H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 81.54, 80.95, 72.81, 28.93, 23.51. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.29.



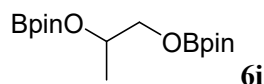
^1H NMR (400 MHz, CDCl_3): δ 3.92 (dt, $J = 9.0, 4.7$ Hz, 1H, $\text{C}_\gamma\text{OBpin}$), 1.84-1.71 (m, 2H, $\text{C}_\gamma\text{OBpin}$), 1.69-1.60 (m, 2H, $\text{C}_\gamma\text{OBpin}$), 1.49-1.38 (m, 2H, $\text{C}_\gamma\text{OBpin}$), 1.30 (dd, $J = 19.9, 10.0$ Hz, 4H, $\text{C}_\gamma\text{OBpin}$), 1.18 (s, 12H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 81.55, 81.38, 71.55, 33.23, 24.44, 23.58, 23.55, 22.78. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.01.



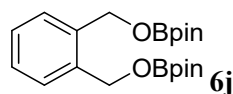
^1H NMR (400 MHz, CDCl_3): δ 7.25 (s, 3H, Ar-H), 7.17 (dd, $J = 8.6, 4.3$ Hz, 1H, Ar-H), 4.85 (s, 2H, OCH_2), 1.18 (d, $J = 1.4$ Hz, 12H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 138.22, 127.24, 126.32, 125.68, 81.87, 65.63, 23.51. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.42.



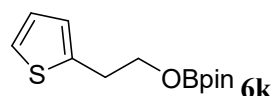
^1H NMR (400 MHz, CDCl_3): δ 3.81-3.69 (m, 4H, $\text{pinBOCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OBpin}$), 1.49 (s, 4H, $\text{pinBOCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OBpin}$), 1.29 (s, 4H, $\text{pinBOCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OBpin}$), 1.24-1.11 (m, 24H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 82.53, 64.80, 31.38, 25.26, 24.56. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.03.



^1H NMR (400 MHz, CDCl_3): δ 4.21 (q, $J = 6.0$ Hz, 1H, MeCH), 3.67 (d, $J = 5.7$ Hz, 2H, CH_2OBpin), 1.21-1.16 (m, 24H, BOCMe_2), 1.10 (d, $J = 6.4$ Hz, 3H, MeCH). ^{13}C NMR (101 MHz, CDCl_3) δ 82.52, 82.39, 70.19, 69.00, 24.52, 24.45, 18.34. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.36.

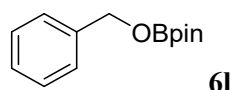


^1H NMR (400 MHz, CDCl_3): δ 7.37 (dd, $J = 5.5, 3.5$ Hz, 2H, Ar-*H*), 7.19 (dd, $J = 5.7, 3.4$ Hz, 2H, Ar-*H*), 4.91 (s, 4H, CH_2OBpin), 1.19 (d, $J = 3.6$ Hz, 24H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 136.42, 127.49, 127.22, 82.96, 64.09, 24.63. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.39.

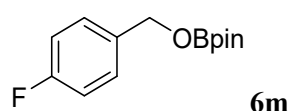


^1H NMR (400 MHz, CDCl_3): δ 6.84-6.79 (m, 1H, $\text{C}_4\text{H}_3\text{S}$), 6.77 (d, $J = 2.7$ Hz, 1H, $\text{C}_4\text{H}_3\text{S}$), 3.98 (t, $J = 6.7$ Hz, 1H, $\text{C}_4\text{H}_3\text{S}$), 3.81 (q, $J = 7.0$ Hz, 2H, $\text{CH}_2\text{CH}_2\text{OBpin}$), 3.00 (t, $J = 6.7$ Hz, 2H, $\text{CH}_2\text{CH}_2\text{OBpin}$), 1.17 (s, 12H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 139.48, 125.68, 124.38, 122.61, 81.70, 81.51, 64.36, 23.57, 23.54.

^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.06.

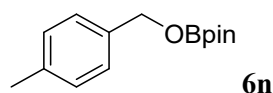


^1H NMR (400 MHz, CDCl_3): δ 7.24 (d, $J = 6.9$ Hz, 4H, Ar-*H*), 7.17 (d, $J = 8.5$ Hz, 1H, Ar-*H*), 4.83 (s, 2H, CH_2OBpin), 1.16 (d, $J = 3.9$ Hz, 12H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 138.22, 127.24, 126.32, 125.68, 81.87, 81.67, 65.63, 23.57, 23.51. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.30.

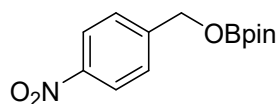


^1H NMR (400 MHz, CDCl_3): δ 7.36-7.11 (m, 2H, Ar-*H*), 6.92 (d, $J = 17.1$ Hz, 2H, Ar-*H*), 4.79 (s, 2H, CH_2OBpin), 1.17 (s, 12H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 162.40, 159.97, 133.99, 131.14, 127.65, 114.17, 81.98, 81.72, 65.02, 23.58.

^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.28.



^1H NMR (400 MHz, CDCl_3): δ 7.13 (d, $J = 7.9$ Hz, 2H, Ar-*H*), 7.03 (d, $J = 7.9$ Hz, 2H, Ar-*H*), 4.78 (s, 2H, CH_2OBpin), 2.23 (s, 3H, Ar- CH_3), 1.15 (d, $J = 2.7$ Hz, 12H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 135.88, 135.26, 127.90, 125.82, 81.79, 81.66, 65.53, 23.57, 23.50, 20.06. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.42.

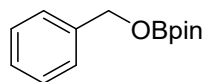


60

^1H NMR (400 MHz, CDCl_3): δ 8.11 (d, $J = 8.8$ Hz, 2H, Ar- H), 7.43 (d, $J = 8.8$ Hz, 2H, Ar- H), 4.95 (s, 2H, CH_2OBpin), 1.22-1.11 (m, 12H, BOCMe_2). ^{13}C NMR (101 MHz, CDCl_3) δ 146.24, 129.70, 125.85, 122.56, 82.35, 81.73, 64.53, 23.58, 23.52. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.28.

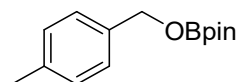
General Procedure for Hydroboration of carboxylic acids.

Carboxylic acid (1.0 mmol), HBpin (3.3 mmol), mesitylene (1.0 mmol) and catalyst **2** (2 mol%) were placed in a 10 ml Schlenk flask equipped with a magnetic stir bar inside the glove box. After the reaction was completed, the aliquot of the crude reaction mixture was analyzed by NMR spectroscopy and there is no need to separate the products.



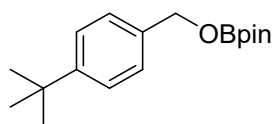
8a

^1H NMR (400 MHz, CDCl_3): δ 7.24-7.13 (m, 5H, Ar- H), 4.83 (s, 2H, OCH_2), 1.16 (s, 36H, CH_3 , OBpin & pinBOBPIn). {1H} NMR (101 MHz, CDCl_3): δ 138.18, 127.24, 125.87, 125.70, 82.03, 81.97, 65.63, 23.52, 23.58. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.35.



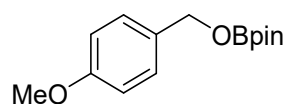
8b

^1H NMR (400 MHz, CDCl_3): δ 7.15 (d, $J = 7.7$ Hz, 2H, Ar- H), 7.05 (d, $J = 7.8$ Hz, 2H, Ar- H), 4.80 (s, 2H, OCH_2), 2.25 (s, 3H, CH_3), 1.18 (s, 36H, CH_3 , OBpin & pinBOBPIn). {1H} NMR (101 MHz, CDCl_3): δ 136.69, 136.29, 128.97, 126.93, 83.27, 82.90, 66.61, 24.57, 23.58, 21.15. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 22.31.



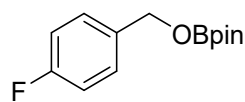
8c

^1H NMR (400 MHz, CDCl_3): δ 7.26 (d, $J = 8.3$ Hz, 2H, Ar- H), 7.19 (d, $J = 8.2$ Hz, 2H, Ar- H), 4.81 (s, 2H, OCH_2), 1.22 (s, 9H, $\text{C}(\text{CH}_3)_3$). 1.15 (s, 36H, OBpin & pinBOBPIn). ^{13}C NMR (101 MHz, CDCl_3) δ 149.23, 135.26, 125.87, 124.14, 82.00, 81.81, 65.47, 33.44, 30.33, 23.58, 23.51. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.14.



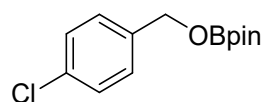
8d

^1H NMR (400 MHz, CDCl_3): δ 7.14 (d, $J = 8.5$ Hz, 2H, Ar-*H*), 6.73 (d, $J = 8.5$ Hz, 2H, Ar-*H*), 4.72 (s, 2H, OCH_2), 3.63 (s, 3H, OCH_3), 1.12 (s, 36H, OBpin & pinBOBpin). ^{13}C NMR (101 MHz, CDCl_3) δ 158.08, 130.42, 127.46, 112.63, 81.92, 81.71, 65.38, 54.02, 23.81, 23.55. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.23.



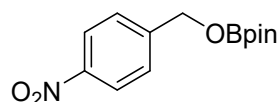
8e

^1H NMR (400 MHz, CDCl_3): δ 7.23-7.15 (m, 2H, Ar-*H*), 6.88 (d, $J = 8.7$ Hz, 2H, Ar-*H*), 4.75 (s, 2H, OCH_2), 1.14 (s, 36H, CH_3 , OBpin & pinBOBpin). ^{13}C NMR (101 MHz, CDCl_3) δ 162.38, 159.95, 127.58, 114.14, 81.99, 81.93, 64.96, 23.51, 23.45. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.24.



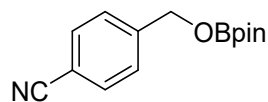
8f

^1H NMR (400 MHz, CDCl_3): δ 7.20 (d, $J = 1.9$ Hz, 4H, Ar-*H*), 4.80 (s, 2H, OCH_2), 1.18 (s, 36H, CH_3 , OBpin & pinBOBpin). ^{13}C NMR (101 MHz, CDCl_3) δ 136.71, 132.08, 127.40, 127.07, 82.22, 82.04, 64.91, 23.86, 23.58. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.15.



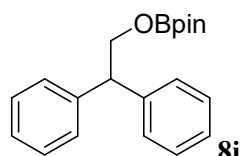
8g

^1H NMR (400 MHz, CDCl_3): δ 8.11 (d, $J = 8.6$ Hz, 2H, Ar-*H*), 7.42 (d, $J = 8.5$ Hz, 2H, Ar-*H*), 4.94 (s, 2H, OCH_2), 1.19 (s, 36H, CH_3 , OBpin & pinBOBpin). ^{13}C NMR (101 MHz, CDCl_3) δ 147.27, 146.63, 126.91, 123.59, 83.37, 83.26, 65.56, 24.89, 24.55. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.12.



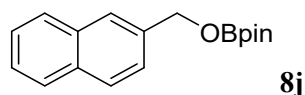
8h

^1H NMR (400 MHz, CDCl_3): δ 8.11 (d, $J = 8.6$ Hz, 2H, Ar-*H*), 7.42 (d, $J = 8.5$ Hz, 2H, Ar-*H*), 4.94 (s, 2H, OCH_2), 1.19 (s, 36H, CH_3 , OBpin & pinBOBpin). ^{13}C NMR (101 MHz, CDCl_3) δ 147.27, 146.63, 126.91, 126.87, 123.59, 83.37, 83.08, 65.56, 24.89, 24.62. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.12.

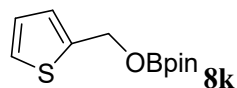


8i

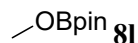
^1H NMR (400 MHz, CDCl_3): δ 7.16 (d, $J = 3.8$ Hz, 8H, Ar- H), 7.09 (d, $J = 4.7$ Hz, 2H, Ar- H), 4.32 (d, $J = 7.2$ Hz, 2H, OCH_2), 4.14 (t, $J = 7.1$ Hz, 1H, CH), 1.17 (s, 24H, CH_3 , CH_3 , pinBOBpin), 1.05 (s, 12H, CH_3 , OBpin). ^{13}C NMR (101 MHz, CDCl_3) δ 140.70, 127.44, 127.32, 125.42, 82.01, 81.62, 66.76, 51.49, 23.85, 23.46. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.21.



^1H NMR (400 MHz, CDCl_3): δ 7.71 (d, $J = 4.0$ Hz, 4H, Ar- H), 7.42-7.25 (m, 3H, Ar- H), 4.99 (s, 2H, OCH_2), 1.19 (s, 36H, CH_3 , OBpin & pinBOBpin). ^{13}C NMR (101 MHz, CDCl_3) δ 135.68, 132.31, 131.80, 126.94, 126.85, 126.62, 124.97, 124.67, 124.10, 123.81, 82.19, 81.96, 65.70, 23.58, 23.50. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.20.



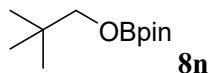
^1H NMR (400 MHz, CDCl_3): δ 7.16 (dd, $J = 5.1, 1.0$ Hz, 1H, Ar- H), 6.93 (d, $J = 2.9$ Hz, 1H, Ar- H), 6.86 (dd, $J = 5.0, 3.5$ Hz, 1H, Ar- H), 4.96 (s, 2H, OCH_2), 1.18 (s, 36H, CH_3 , OBpin & pinBOBpin). ^{13}C NMR (101 MHz, CDCl_3) δ 140.97, 125.88, 124.84, 124.47, 82.23, 82.08, 60.60, 23.86, 23.59. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.15.



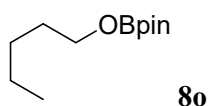
^1H NMR (400 MHz, CDCl_3): δ 3.51 (s, 3H, CH_3), 1.17 (s, 36H, CH_3 , OBpin & pinBOBpin). ^{13}C NMR (101 MHz, CDCl_3) δ 82.03, 81.70, 51.52, 23.57, 23.51. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.15.



^1H NMR (400 MHz, CDCl_3): δ 3.78 (q, $J = 7.0$ Hz, 2H, OCH_2), 1.13 (s, 36H, CH_3 , OBpin & pinBOBpin), 1.09 (d, $J = 7.0$ Hz, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl_3) δ 81.87, 81.39, 59.46, 23.54, 23.49, 16.20. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.18.

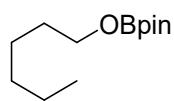


^1H NMR (400 MHz, CDCl_3): δ 3.44 (s, 2H, OCH_2), 1.18 (s, 36H, CH_3 , OBpin & pinBOBpin), 0.82 (s, 9H, $\text{C}(\text{CH}_3)_3$). ^{13}C NMR (101 MHz, CDCl_3) δ 82.23, 82.06, 73.89, 31.31, 24.98, 23.87, 23.53. ^{11}B {1H} NMR (128 MHz, CDCl_3): δ 21.14.



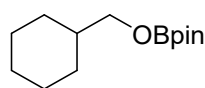
^1H NMR (400 MHz, CDCl_3): δ 3.71 (t, $J = 6.5$ Hz, 2H, OCH_2), 1.44 (s, 2H, CH_2), 1.29-1.19 (m,

4H, CH_2), 1.18 (s, 36H, CH_3 , OBpin & pinBOBpin), 0.90-0.65 (m, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 82.03, 81.78, 81.31, 63.72, 30.25, 26.86, 23.82, 23.53, 23.48, 21.40, 13.01. ^{11}B {1H} NMR (128 MHz, $CDCl_3$): δ 21.19.



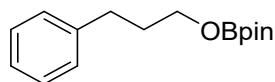
8p

1H NMR (400 MHz, $CDCl_3$): δ 3.71 (t, $J = 6.5$ Hz, 2H, OCH_2), 1.51-1.34 (m, 2H, CH_2), 1.30-1.18 (m, 6H, CH_2), 1.12 (s, 36H, CH_3 , OBpin & pinBOBpin), 0.79 (t, $J = 6.8$ Hz, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 82.04, 81.81, 63.76, 30.58, 30.52, 24.36, 23.83, 23.53, 23.48, 21.67, 13.01. ^{11}B {1H} NMR (128 MHz, $CDCl_3$): δ 21.25.



8q

1H NMR (400 MHz, $CDCl_3$): δ 3.71-3.44 (m, 2H, OCH_2), 1.70-1.27 (m, 8H, CH_2), 1.15 (s, 36H, CH_3 , OBpin & pinBOBpin), 1.10-0.89 (m, 2H, CH_2), 0.86-0.81 (m, 2H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 82.94, 82.44, 70.29, 39.35, 29.34, 26.55, 25.79, 24.85, 24.51. ^{11}B {1H} NMR (128 MHz, $CDCl_3$): δ 21.18.



8r

1H NMR (400 MHz, $CDCl_3$): δ 7.16 (t, $J = 7.4$ Hz, 2H, Ar- H), 7.10-7.05 (m, 3H, Ar- H), 3.77 (t, $J = 6.3$ Hz, 2H, OCH_2), 2.65-2.49 (m, 2H, CH_2), 1.87-1.65 (m, 2H, CH_2), 1.14 (s, 36H, CH_3 , OBpin & pinBOBpin). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.79, 127.44, 127.28, 124.73, 81.97, 81.59, 63.07, 32.12, 30.85, 23.50. ^{11}B {1H} NMR (128 MHz, $CDCl_3$): δ 21.21.

General Procedure for Hydroboration of CO_2 .

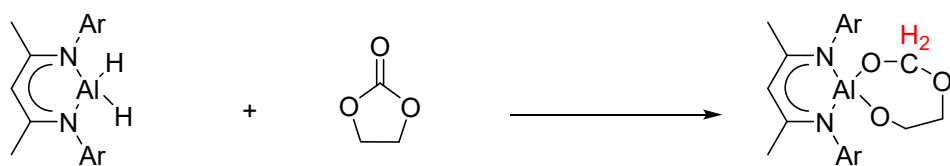
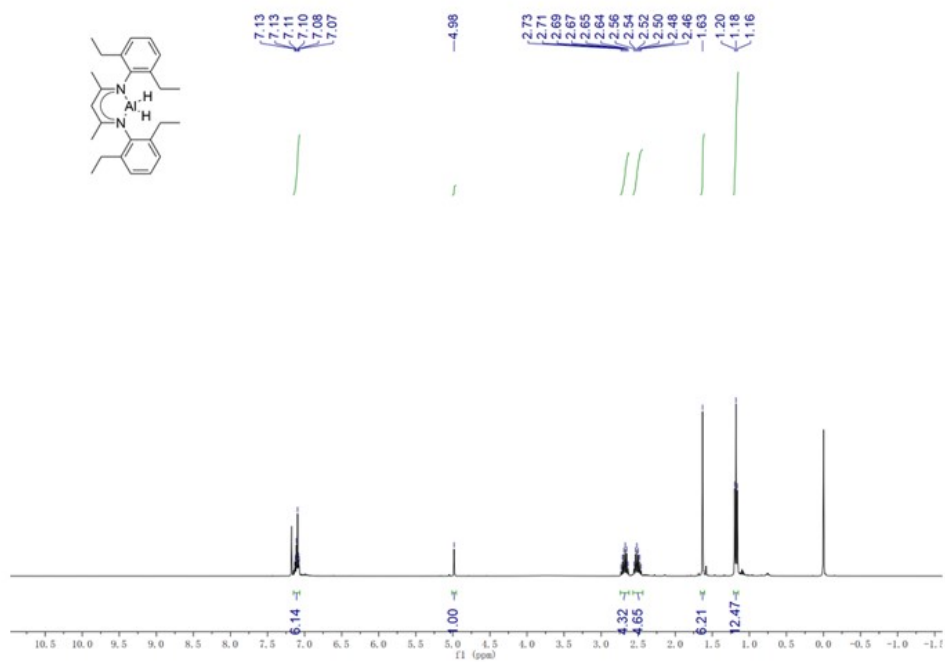
In a glove box, an oven-dried 10 ml Schlenk flask charged with mesitylene (0.50 mmol), HBpin (0.50 mmol) and catalyst **1** (10% mmol) was evacuated and refilled with CO_2 gas (1 atm) for three cycles. The resulting mixture was stirring at 100 °C for 48 h, and then subjected to NMR analysis.

Mechanism Experiment

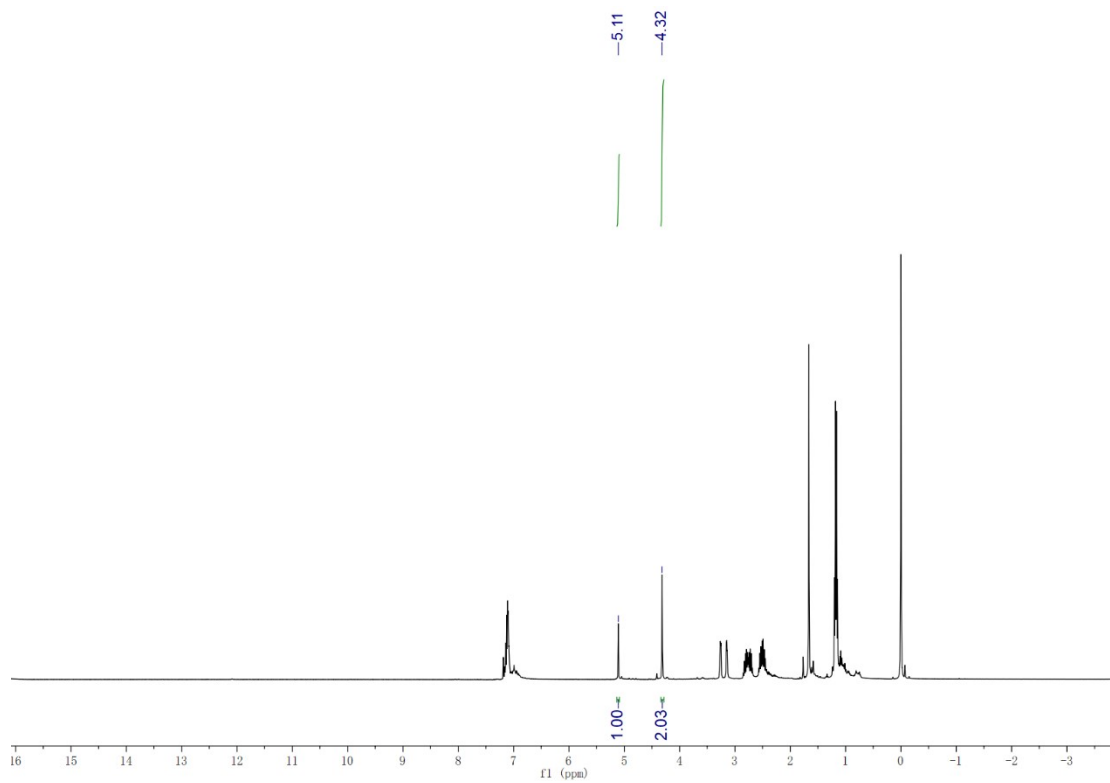
The stoichiometric reaction of **2** with ethylene carbonate (1:1) was performed at room temperature for 24 h under nitrogen atmosphere, solvent toluene was removed in vacuo resulting in a solid containing a mixture of products and then subjected to NMR

analysis.

Scheme S1. ^1H NMR (400 MHz, CDCl_3 , 298 K). Top spectrum, starting material of **2**, bottom spectrum of the crude product from the reaction of **2** with ethylene carbonate.



$\text{Ar} = 2,6\text{-Et}_2\text{C}_6\text{H}_3$



¹H, ¹³C and ¹¹B NMR Spectra of Hydroboration Products of Carbonates.

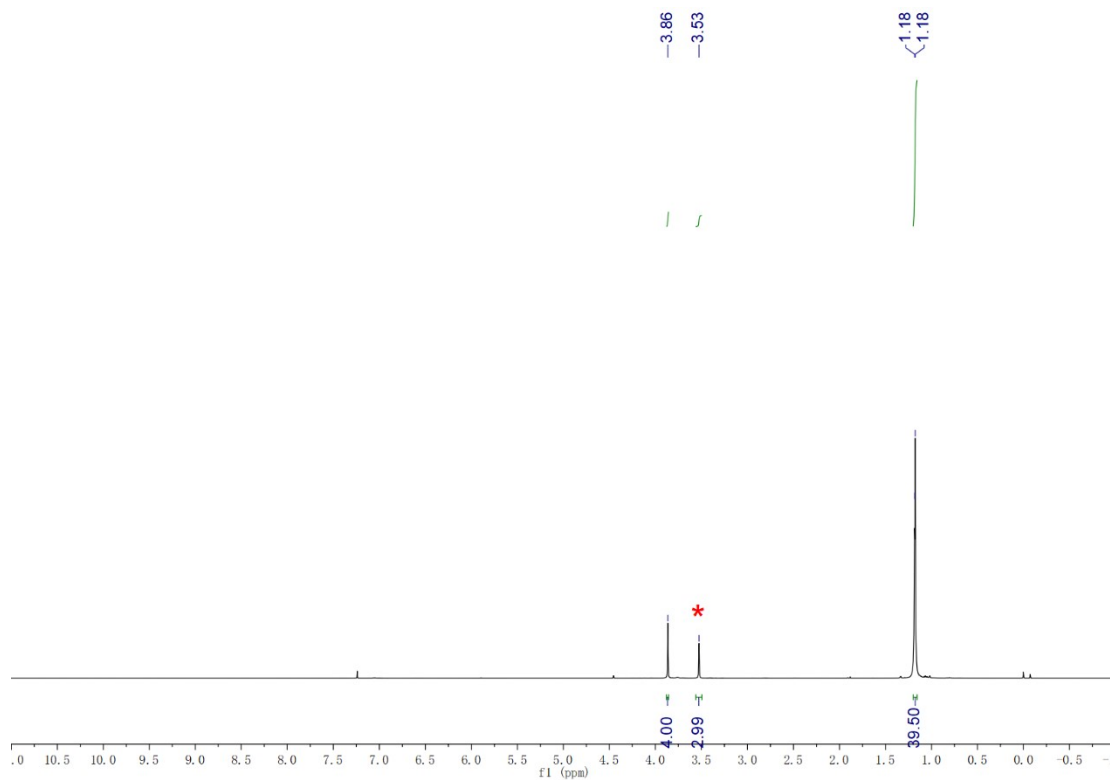


Figure S1.1.1 ^1H NMR spectrum of compound **4a** in CDCl_3

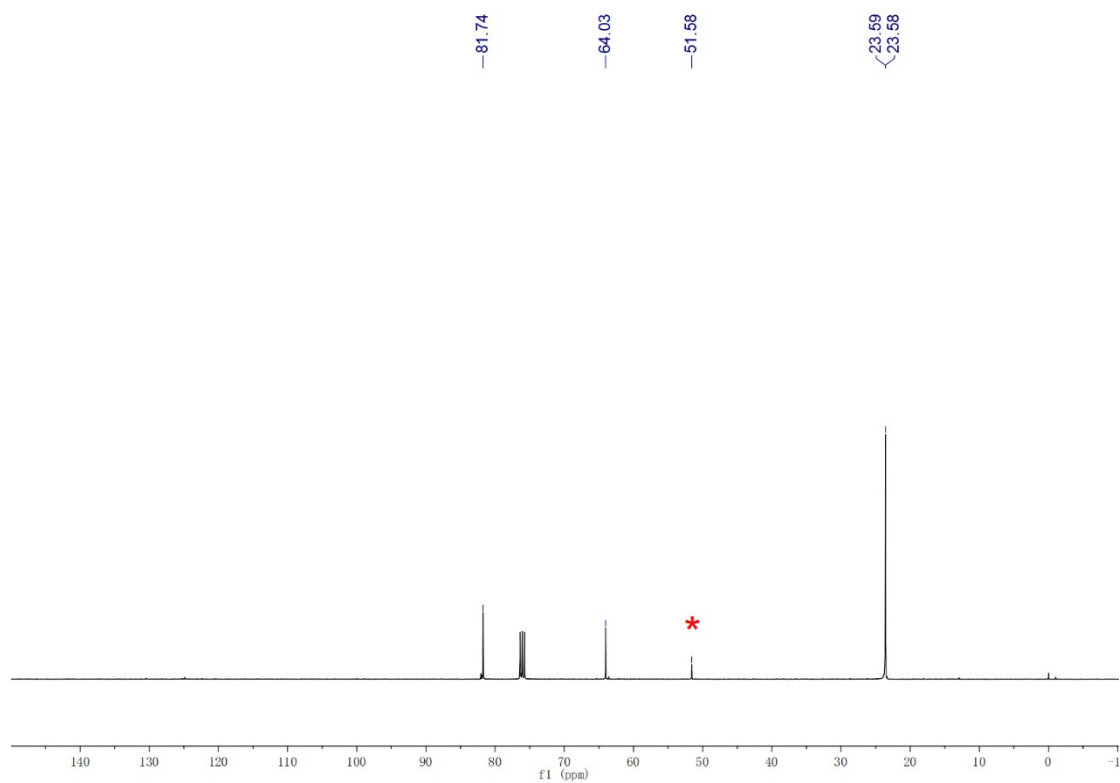


Figure S1.1.2 ^{13}C NMR spectrum of compound **4a** in CDCl_3

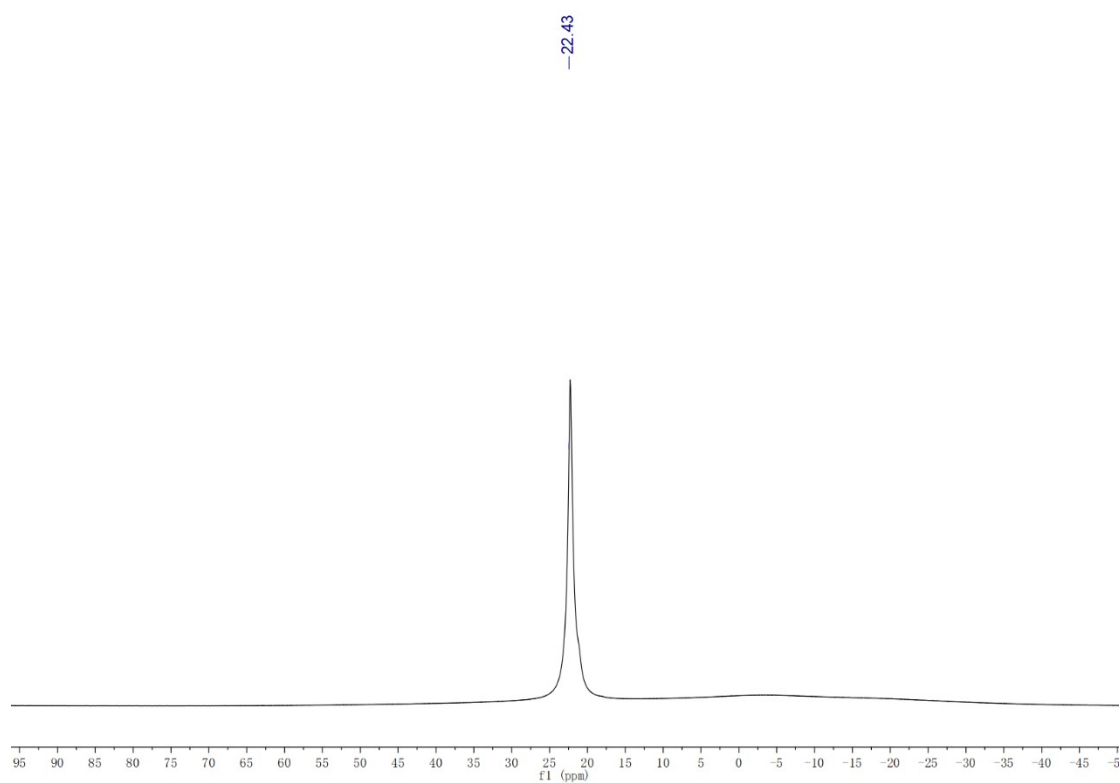


Figure S1.1.3 ^{11}B NMR spectrum of compound **4a** in CDCl_3

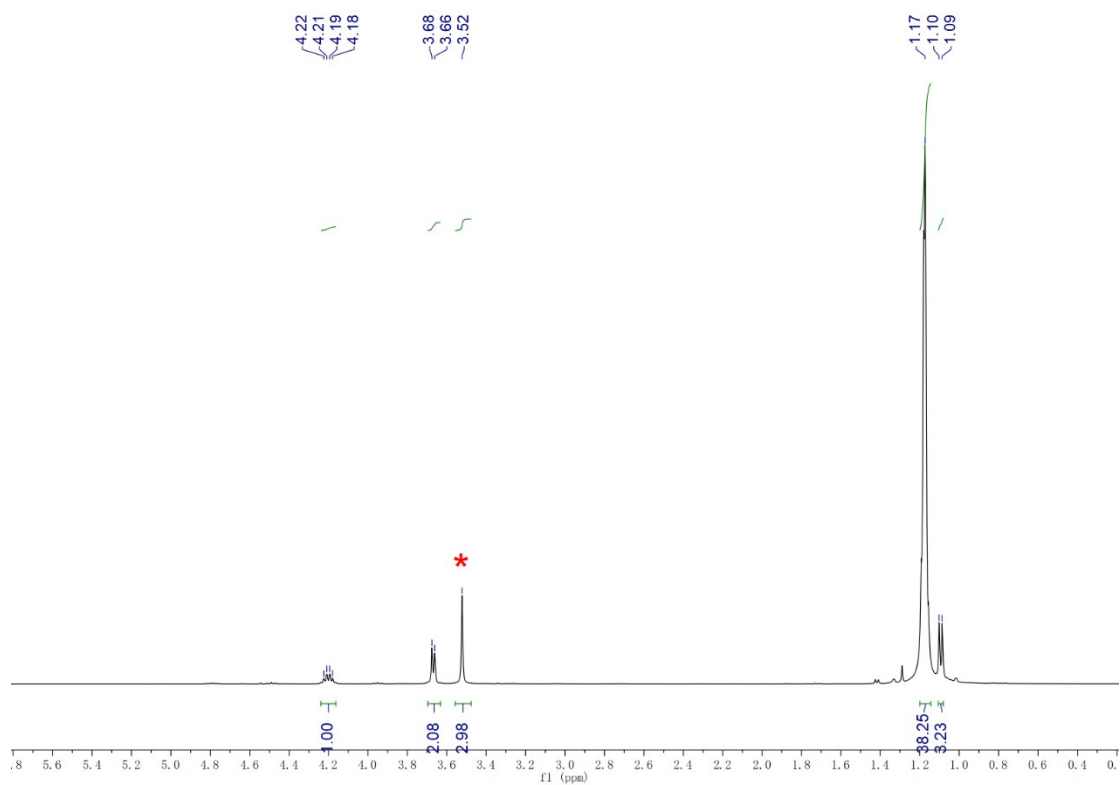


Figure S1.2.1 ^1H NMR spectrum of compound **4b** in CDCl_3

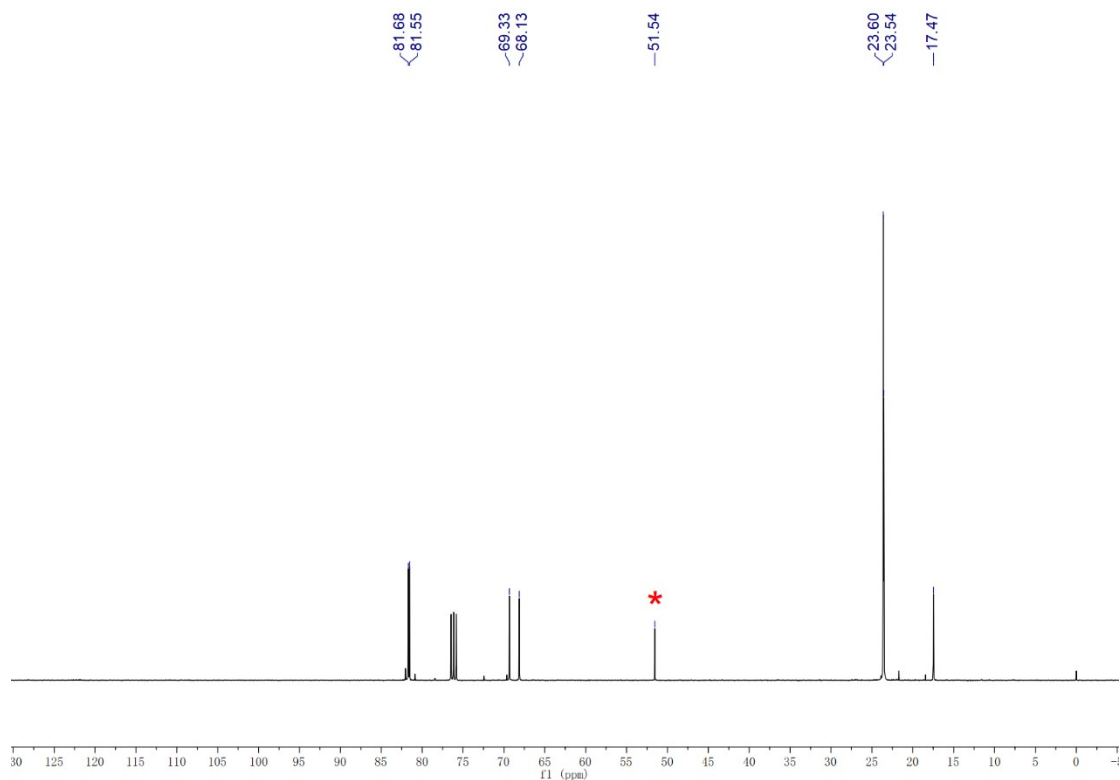


Figure S1.2.2 ^{13}C NMR spectrum of compound **4b** in CDCl_3

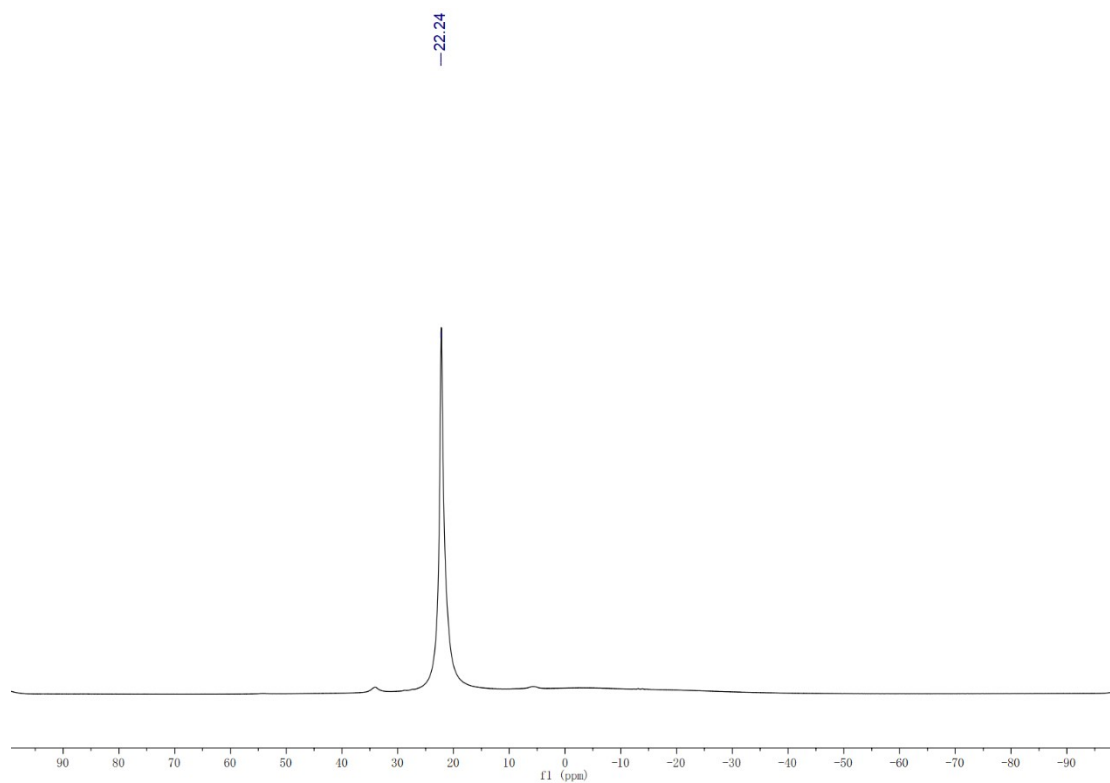


Figure S1.2.3 ^{11}B NMR spectrum of compound **4b** in CDCl_3

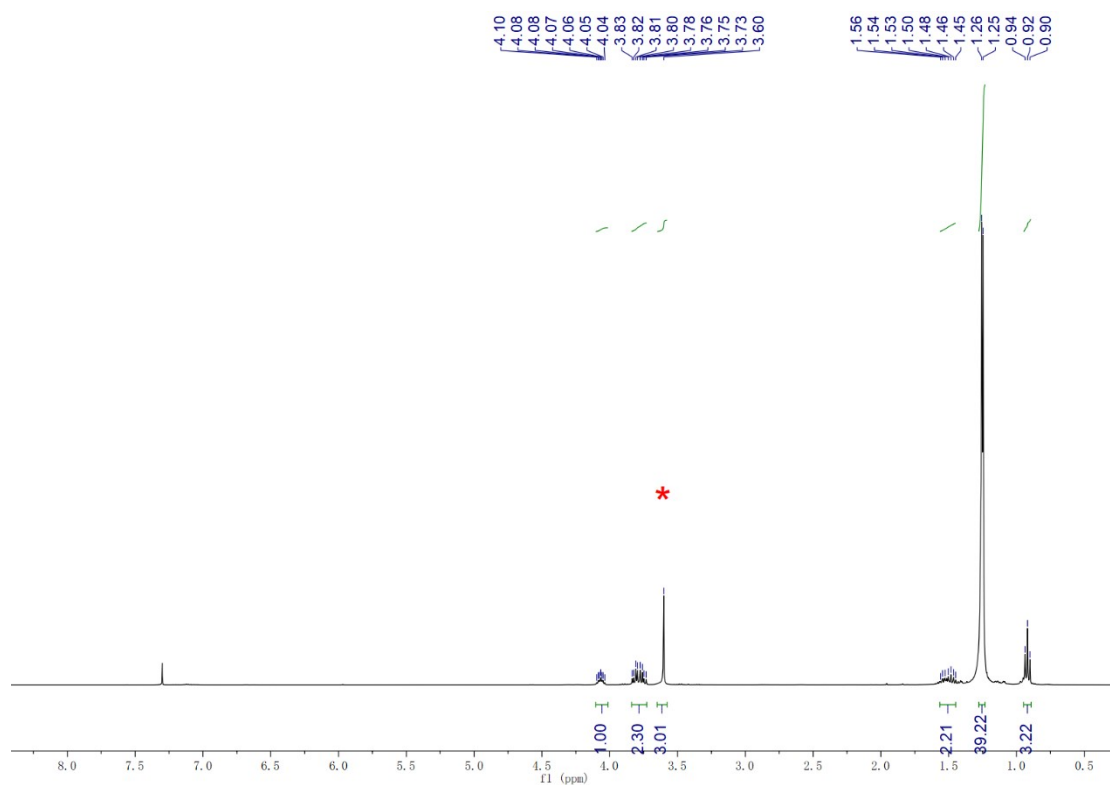


Figure S1.3.1 ^1H NMR spectrum of compound **4c** in CDCl_3

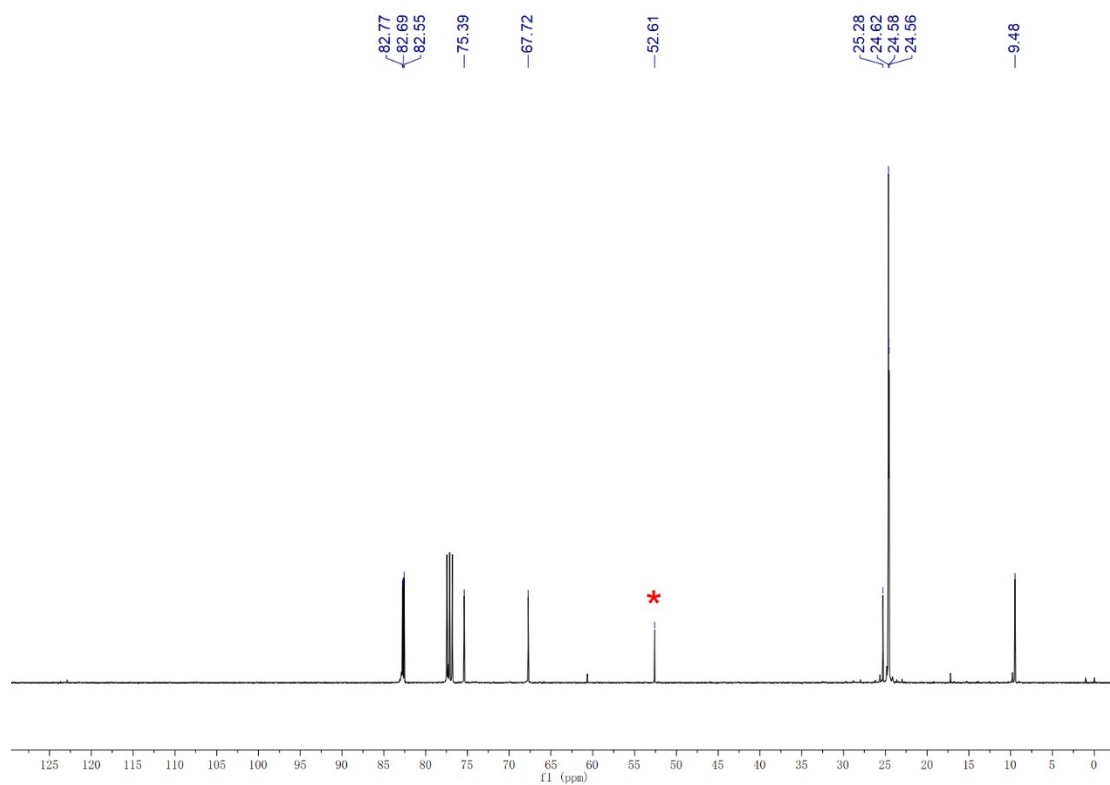


Figure S1.3.2 ^{13}C NMR spectrum of compound **4c** in CDCl_3

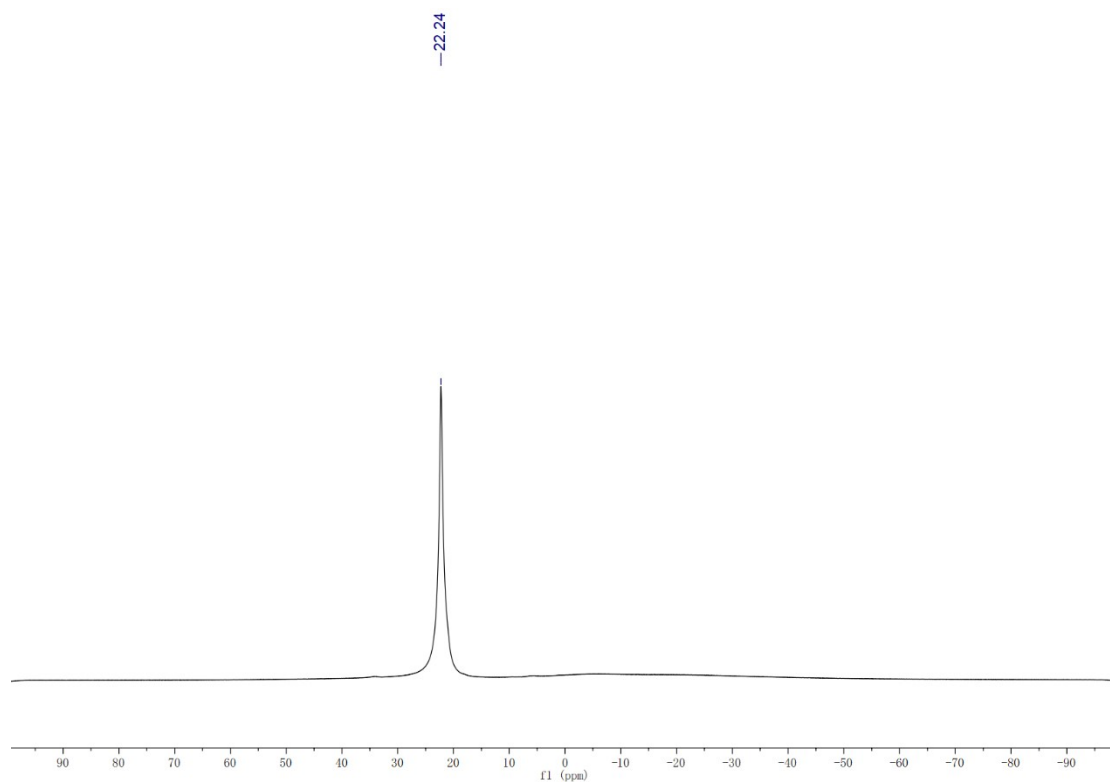


Figure S1.3.3 ^{11}B NMR spectrum of compound **4c** in CDCl_3

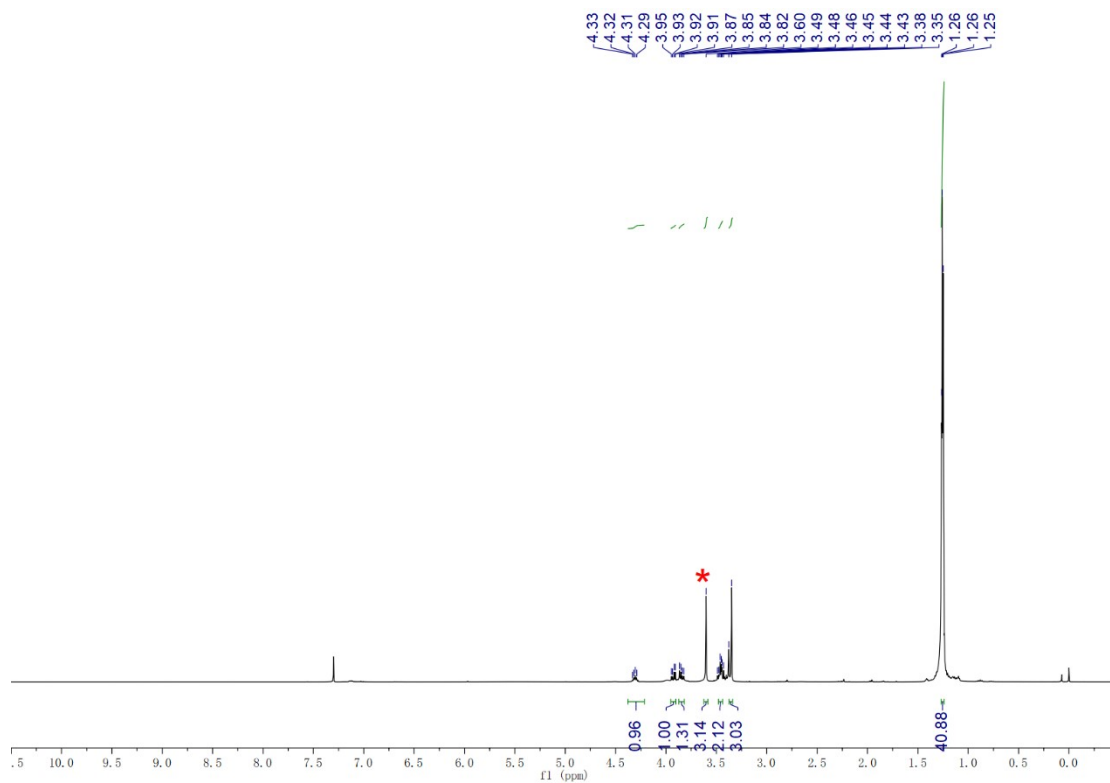


Figure S1.4.1 ^1H NMR spectrum of compound **4d** in CDCl_3

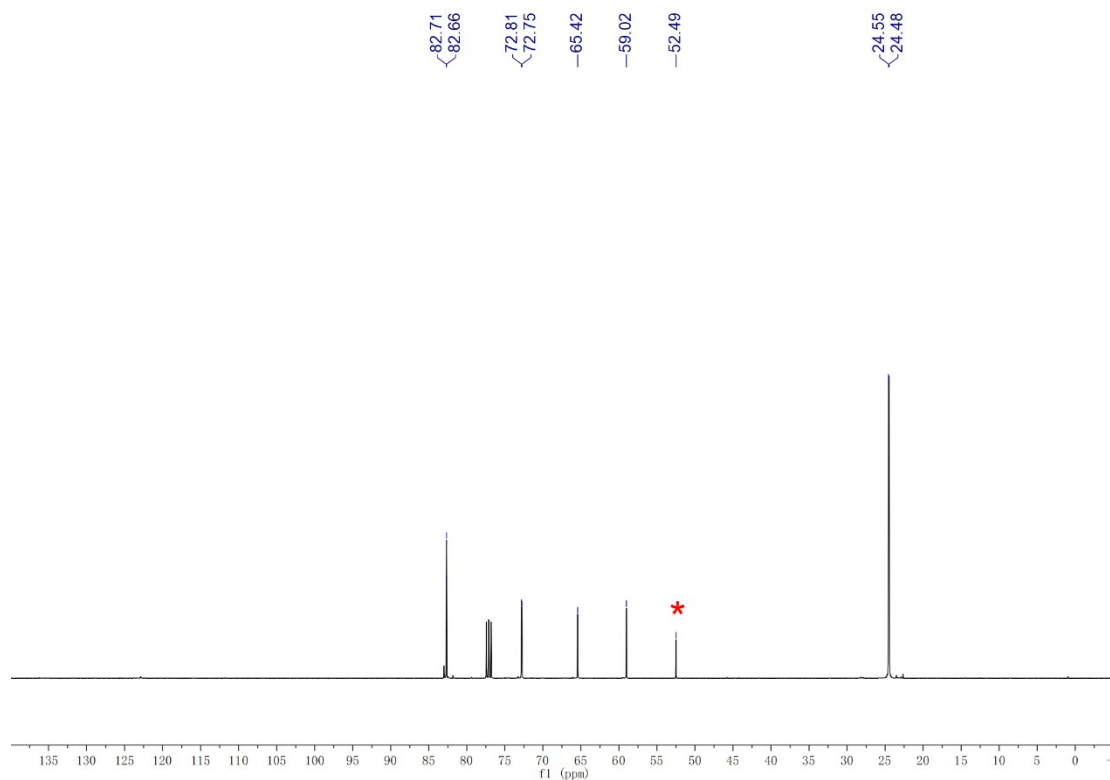


Figure S1.4.2 ^{13}C NMR spectrum of compound **4d** in CDCl_3

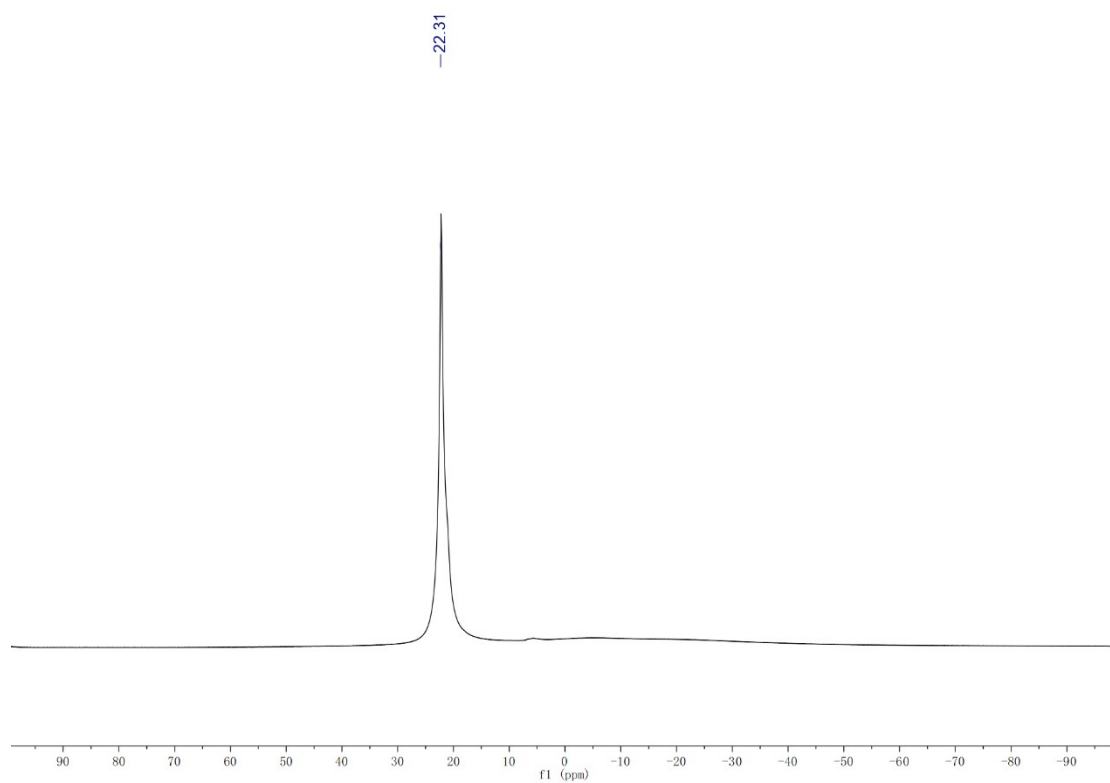


Figure S1.4.3 ^{11}B NMR spectrum of compound **4d** in CDCl_3

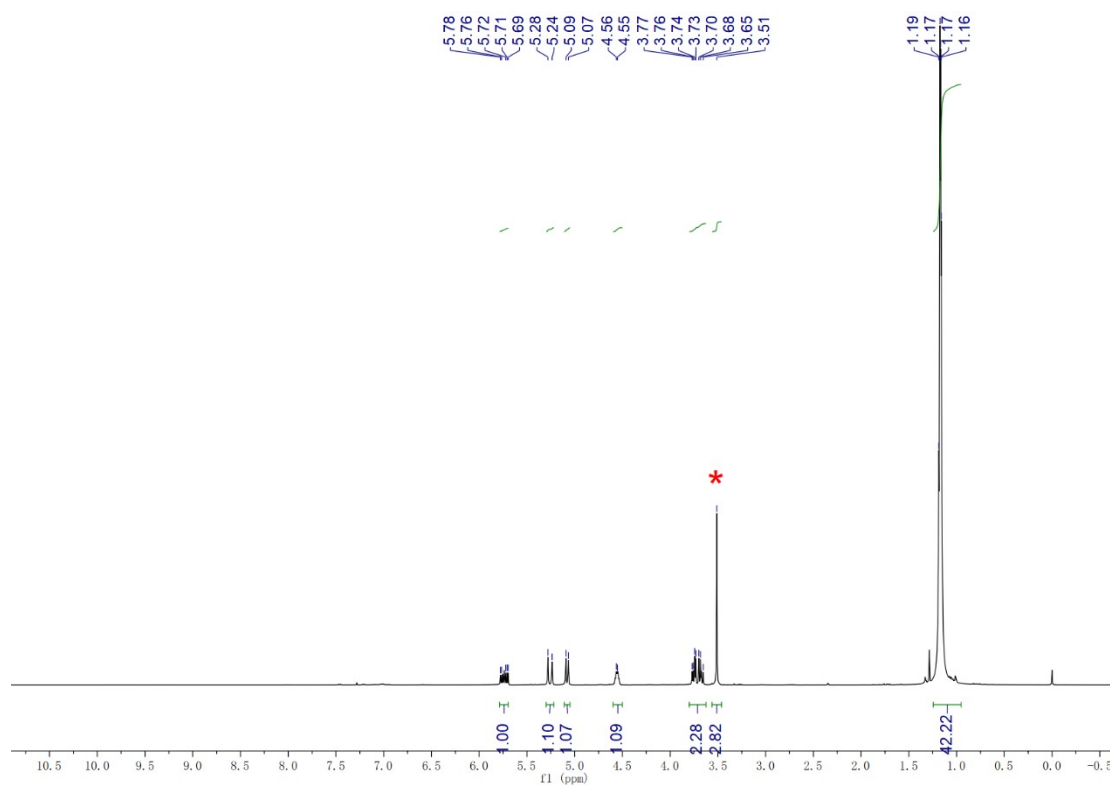


Figure S1.5.1 ^1H NMR spectrum of compound **4e** in CDCl_3

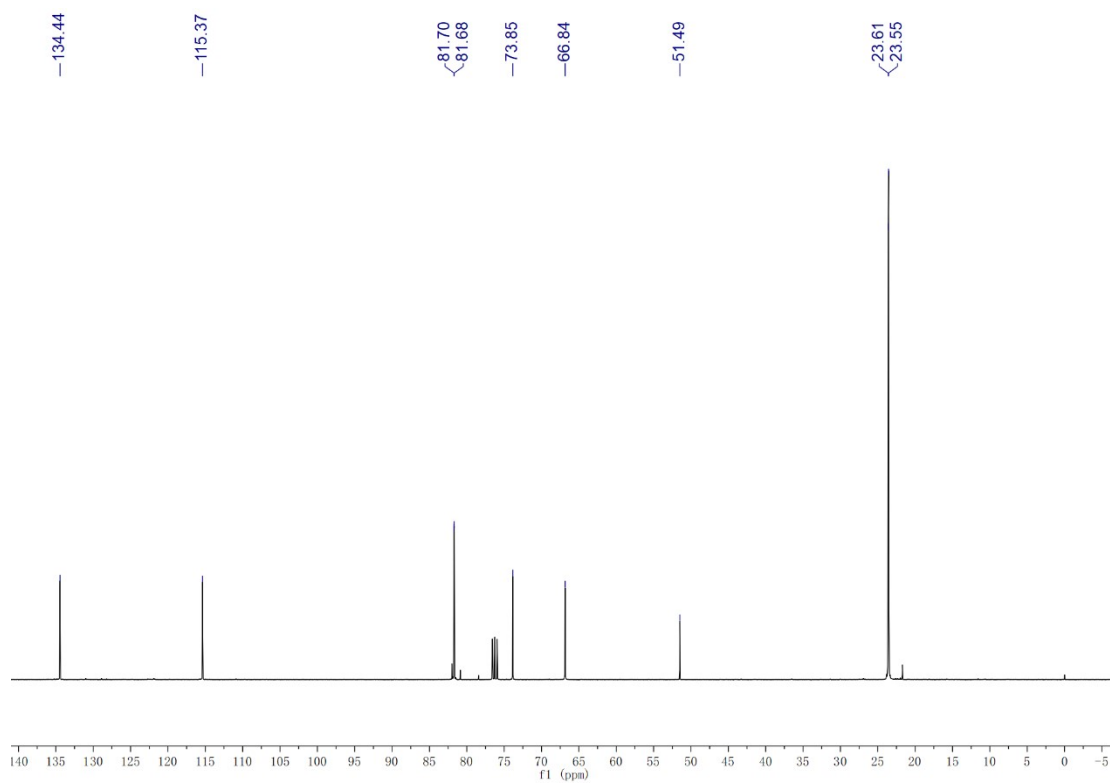


Figure S1.5.2 ^{13}C NMR spectrum of compound **4e** in CDCl_3

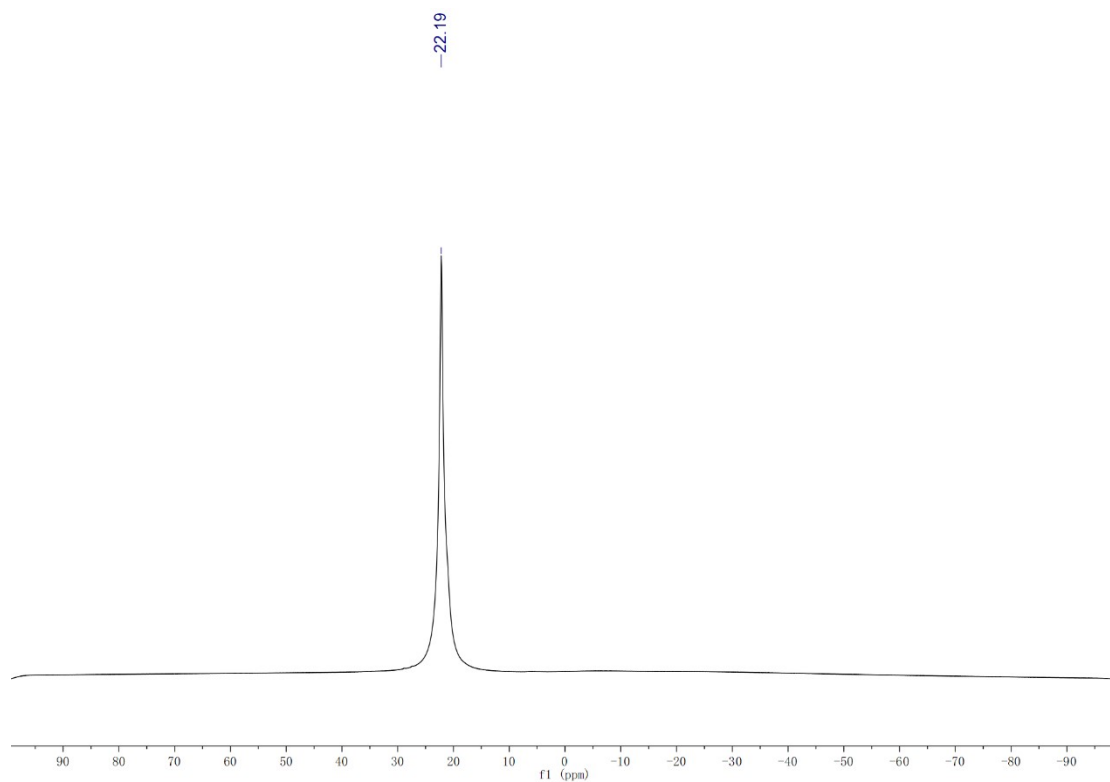


Figure S1.5.3 ^{11}B NMR spectrum of compound **4e** in CDCl_3

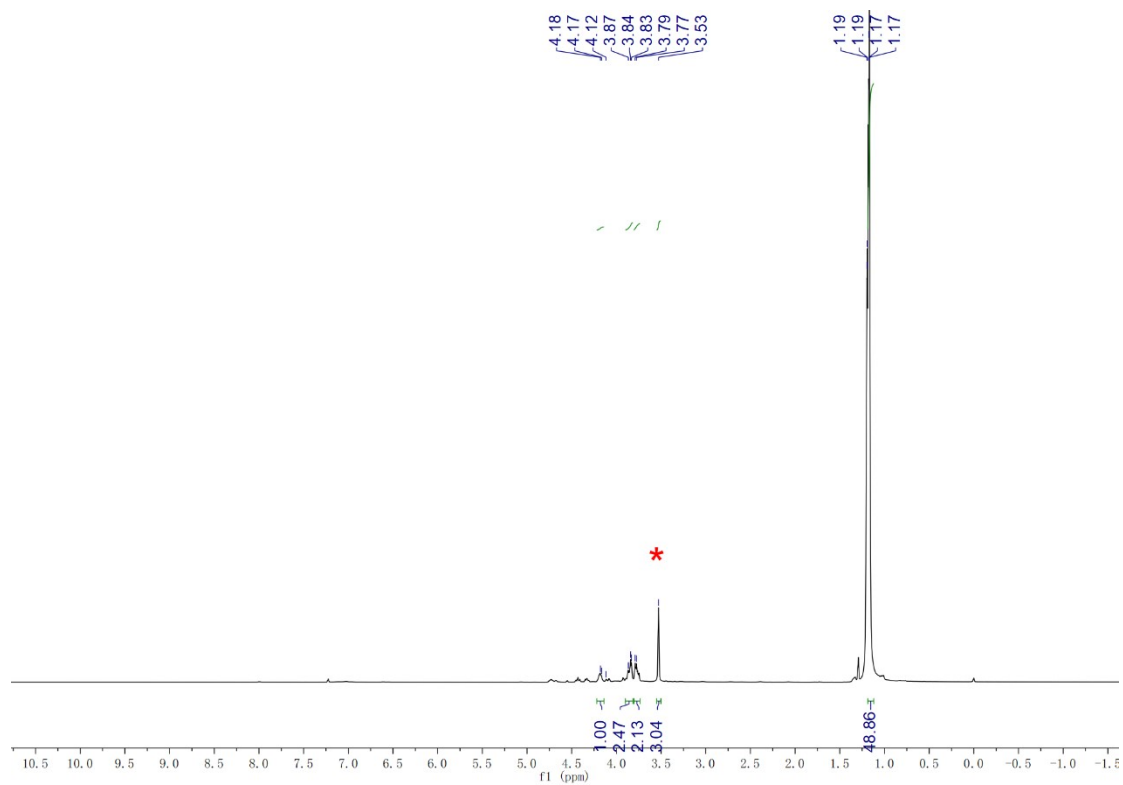


Figure S1.6.1 ^1H NMR spectrum of compound **4f** in CDCl_3

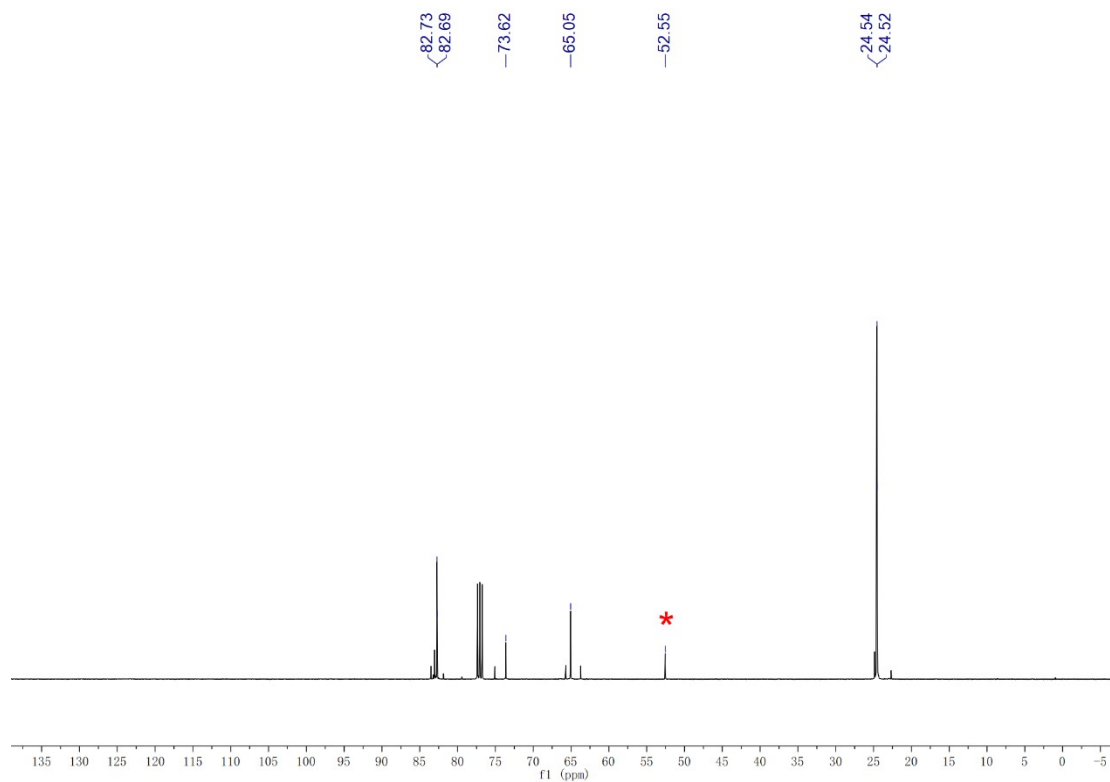


Figure S1.6.2 ^{13}C NMR spectrum of compound **4f** in CDCl_3

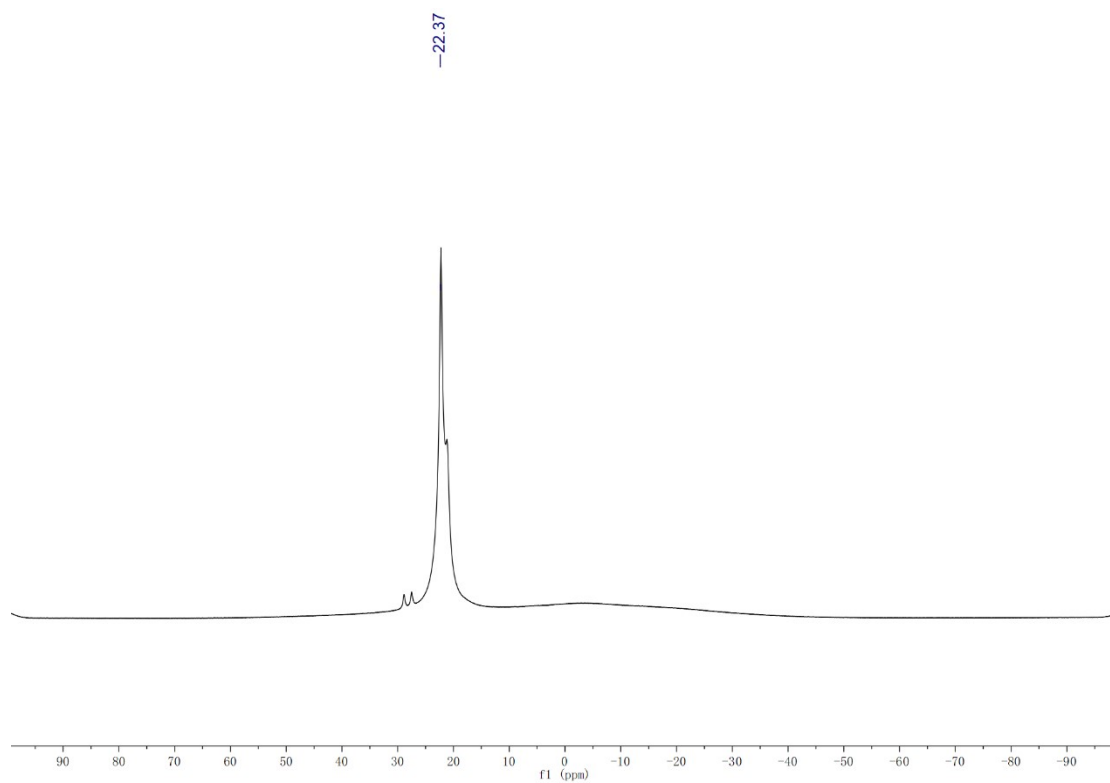


Figure S1.6.3 ^{11}B NMR spectrum of compound **4f** in CDCl_3

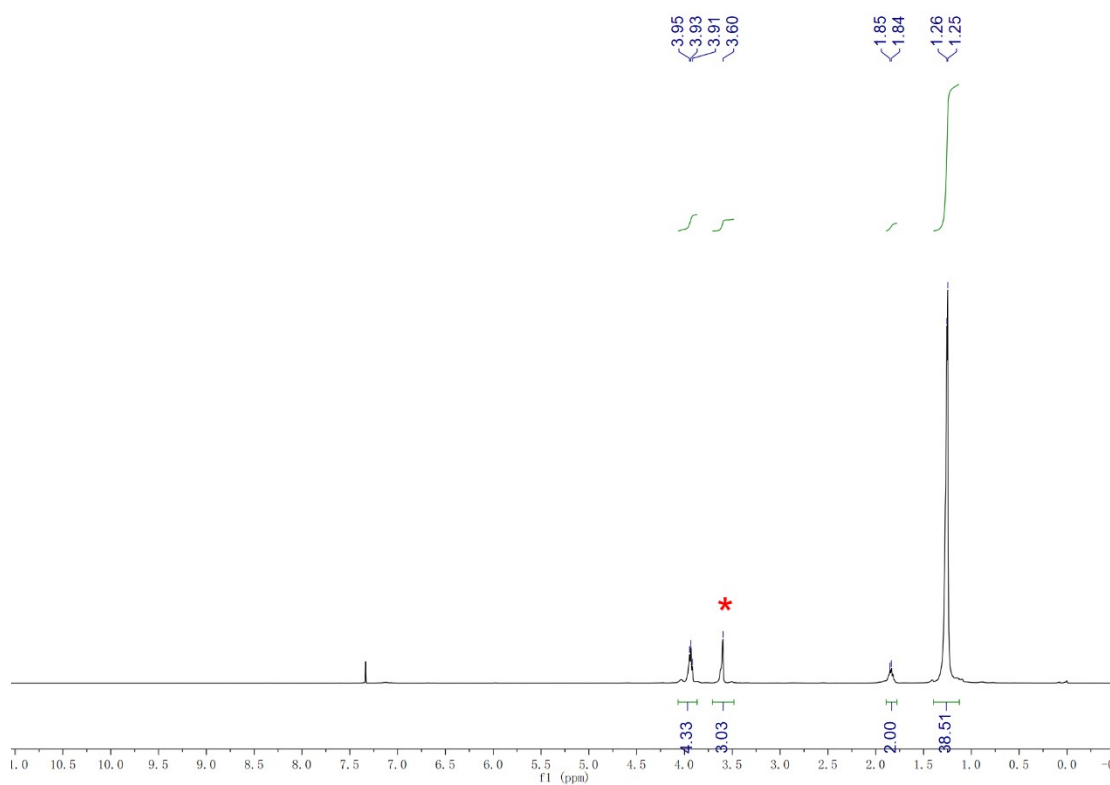


Figure S1.7.1 ^1H NMR spectrum of compound **4g** in CDCl_3

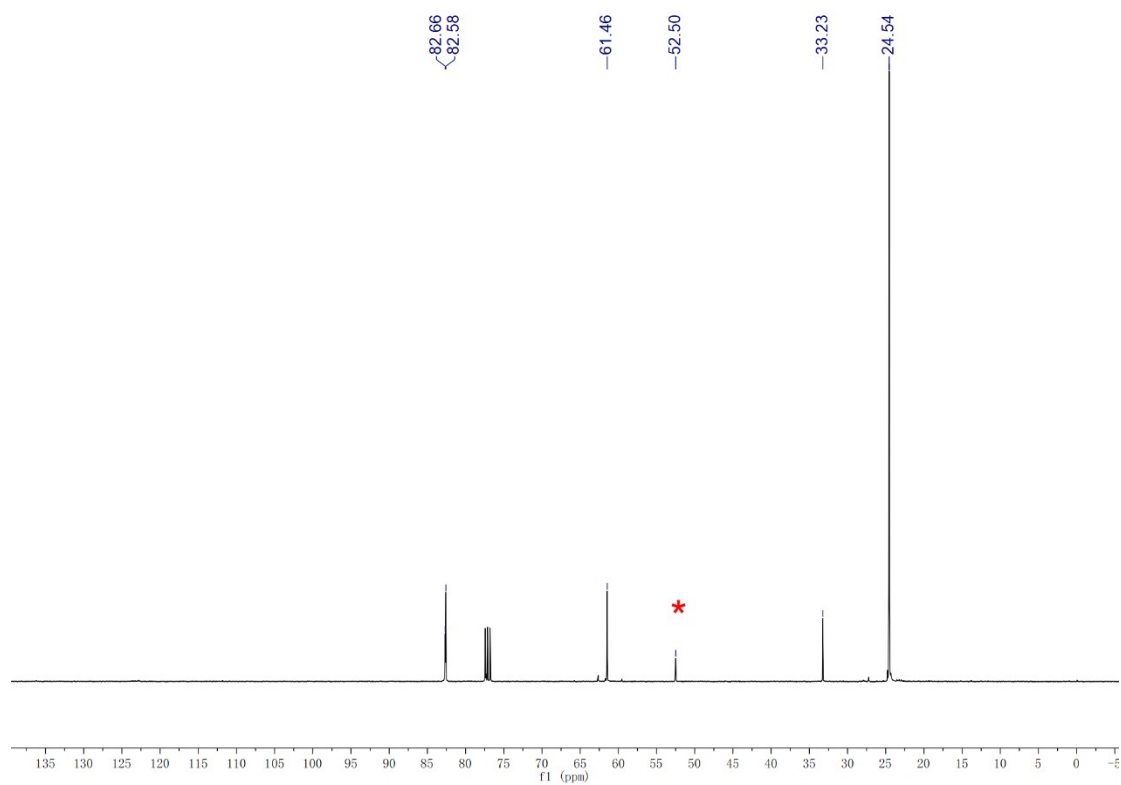


Figure S1.7.2 ¹³C NMR spectrum of compound **4g** in CDCl₃

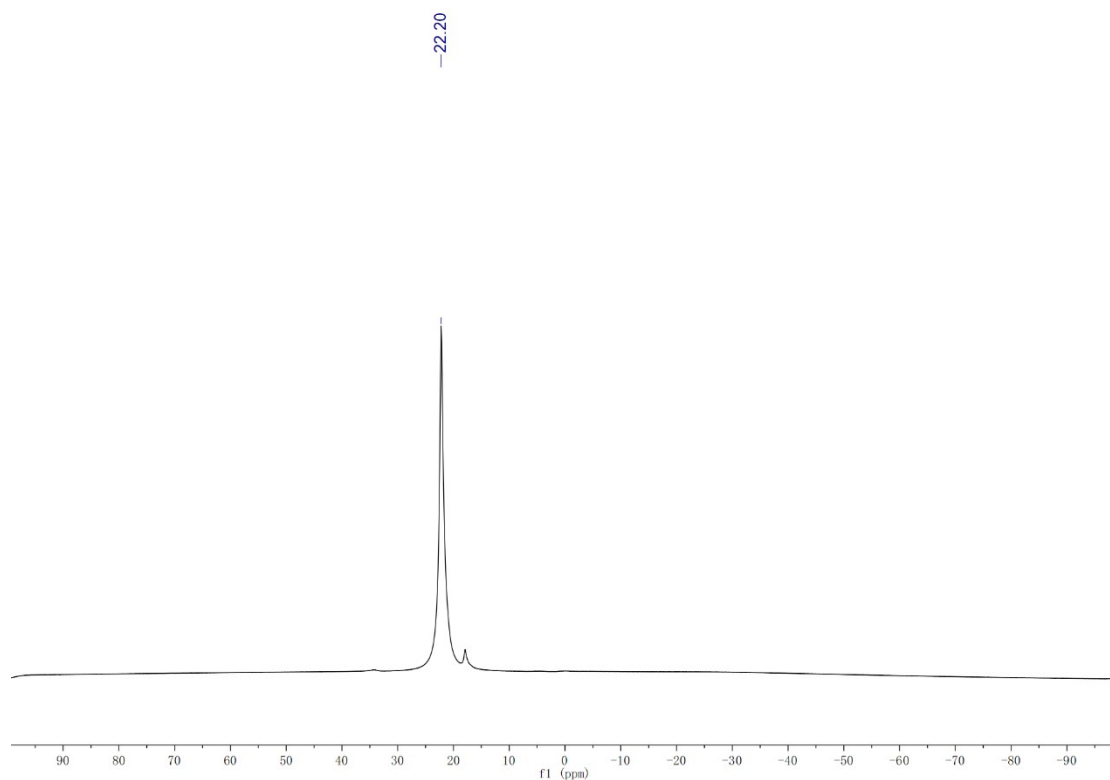


Figure S1.7.3 ¹¹B NMR spectrum of compound **4g** in CDCl₃

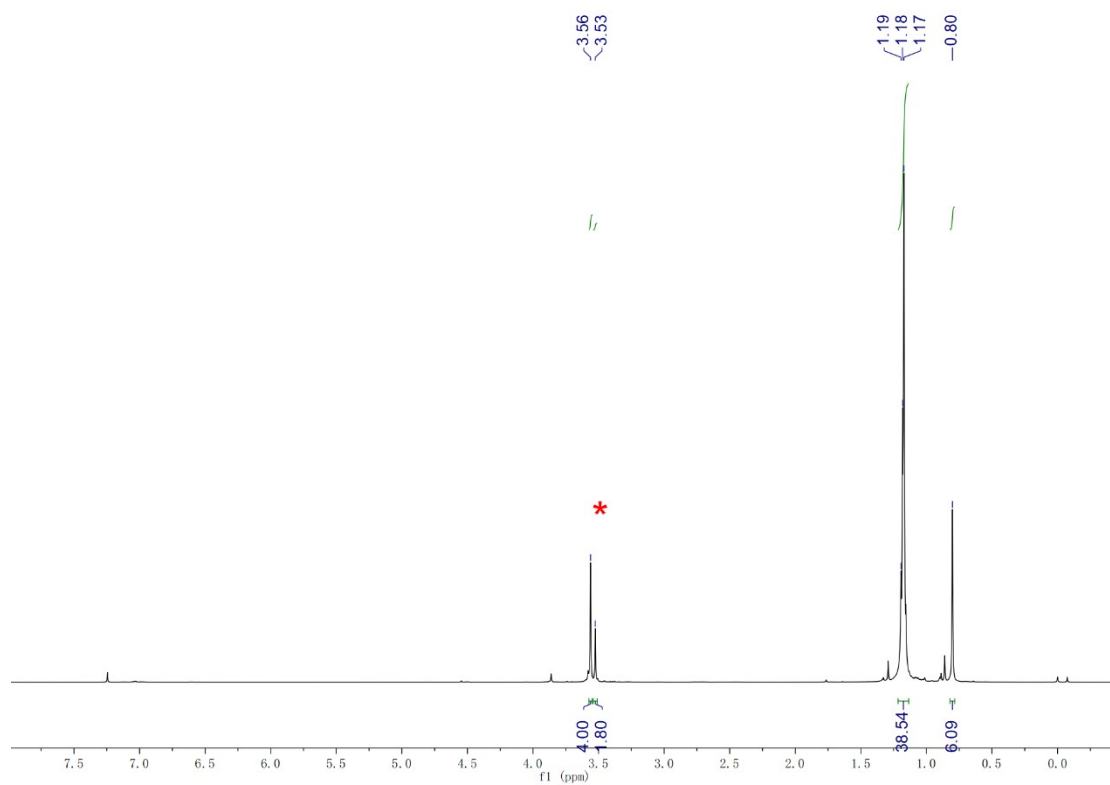


Figure S1.8.1 ^1H NMR spectrum of compound **4h** in CDCl_3

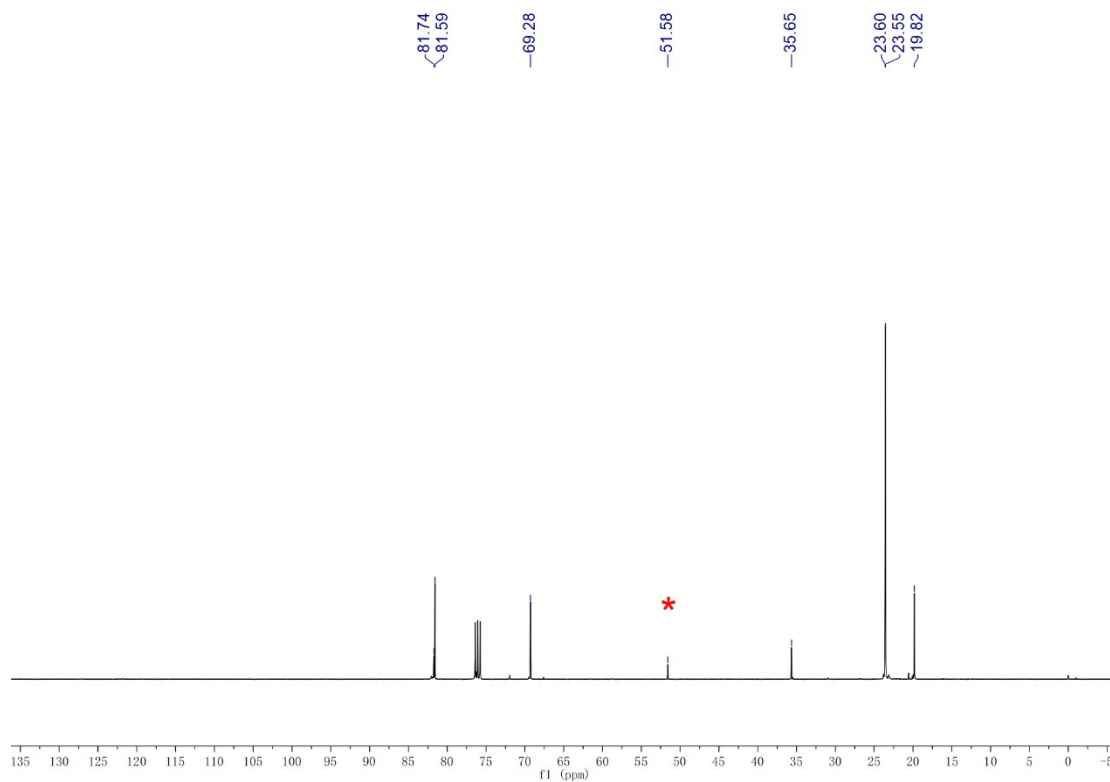


Figure S1.8.2 ^{13}C NMR spectrum of compound **4h** in CDCl_3

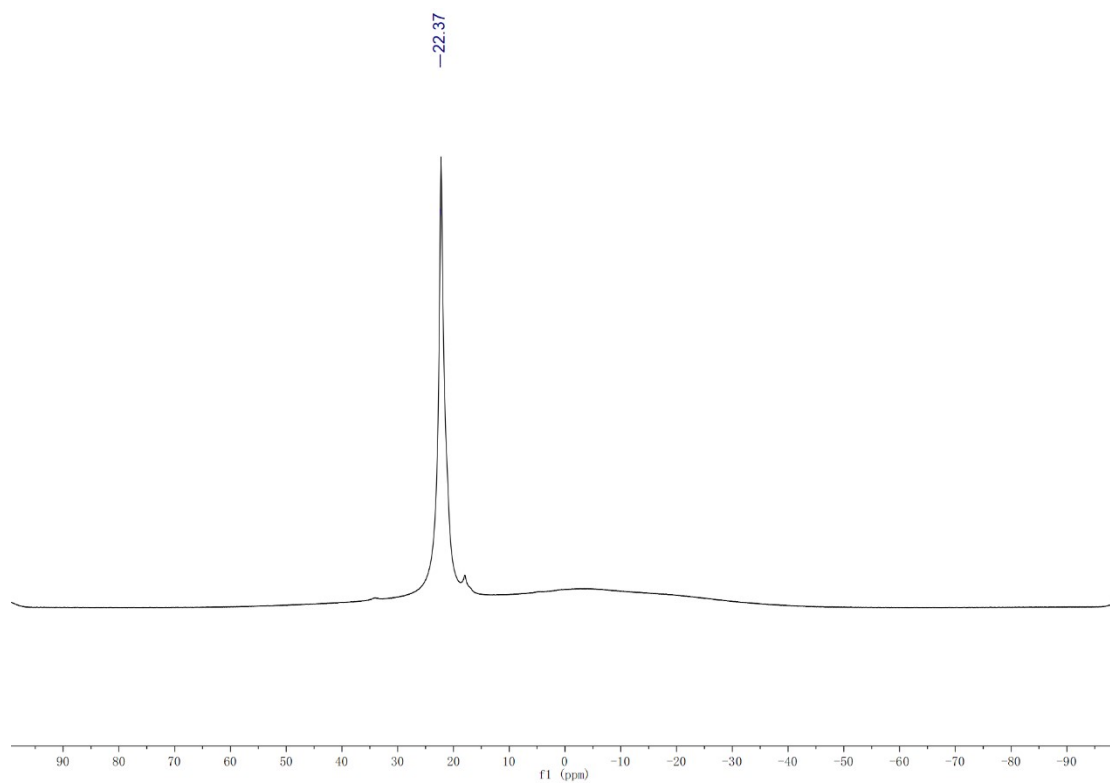


Figure S1.8.3 ^{11}B NMR spectrum of compound **4h** in CDCl_3

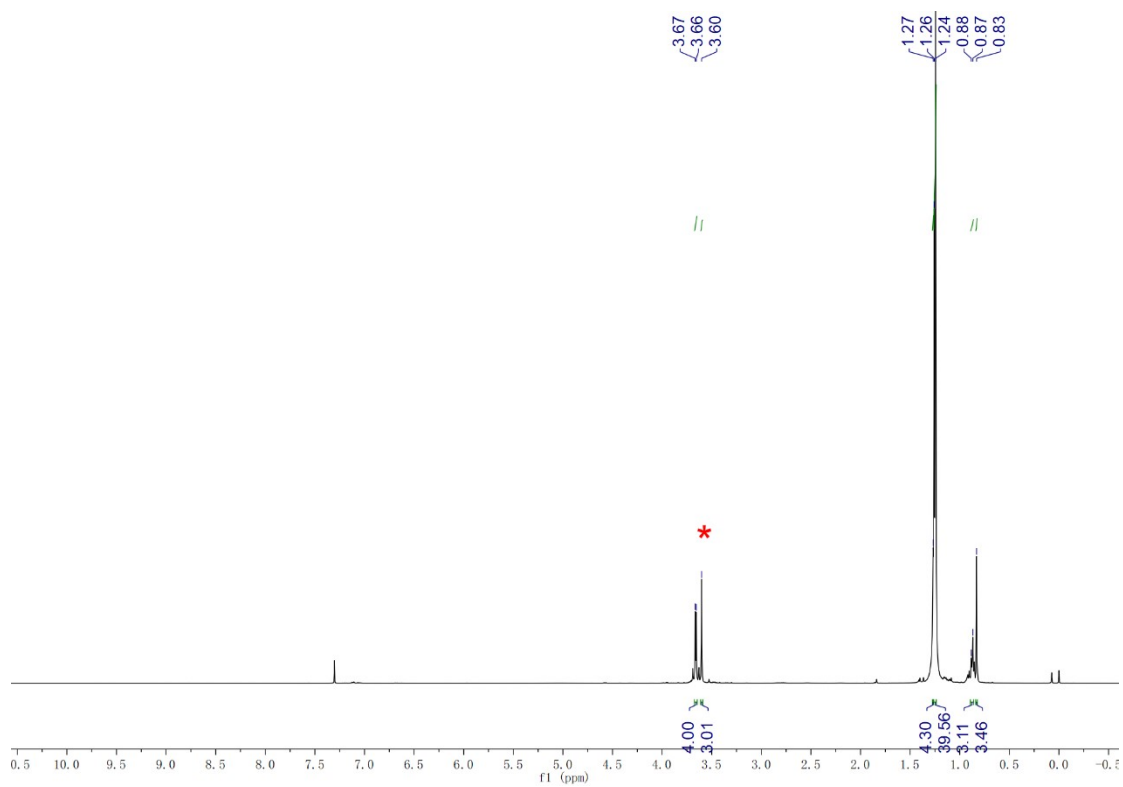


Figure S1.9.1 ^1H NMR spectrum of compound **4i** in CDCl_3

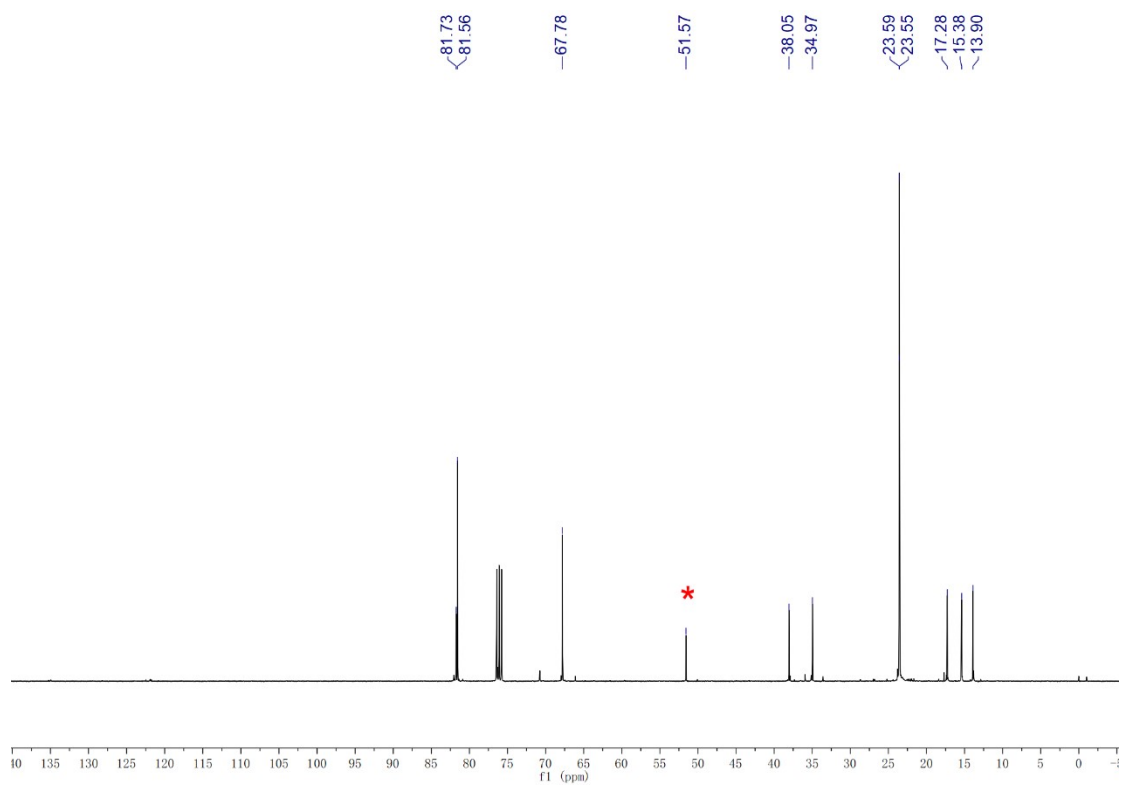


Figure S1.9.2 ^{13}C NMR spectrum of compound **4i** in CDCl_3

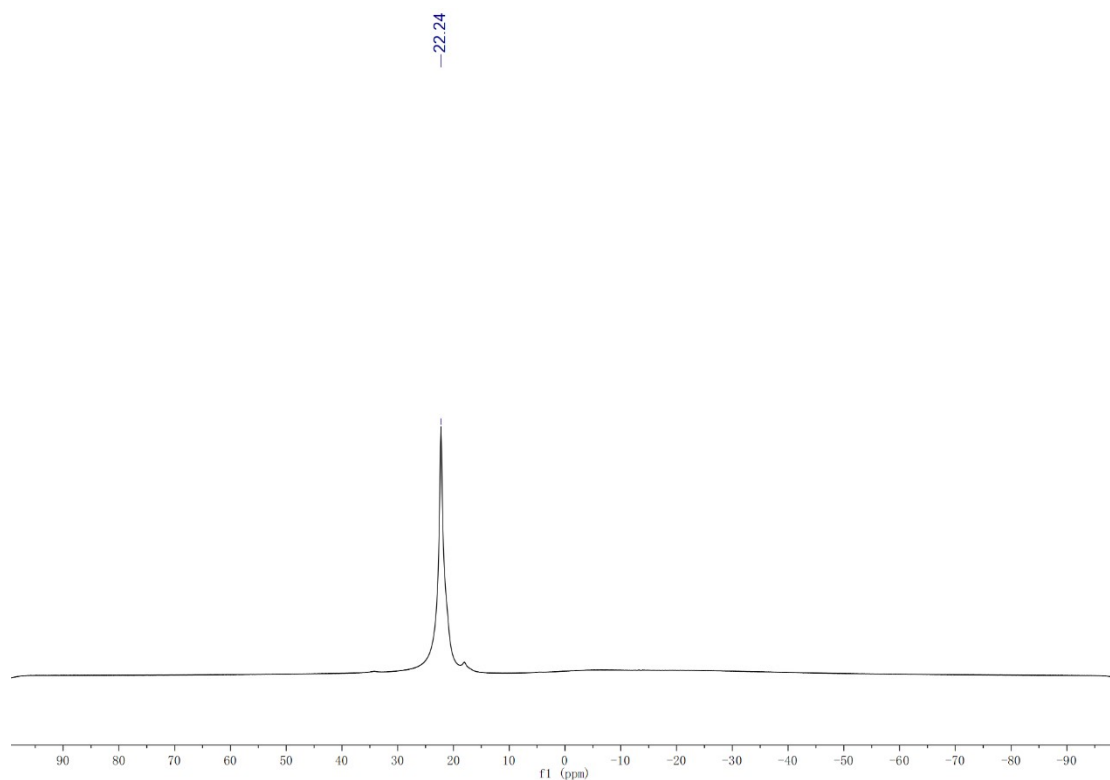


Figure S1.9.3 ^{11}B NMR spectrum of compound **4i** in CDCl_3

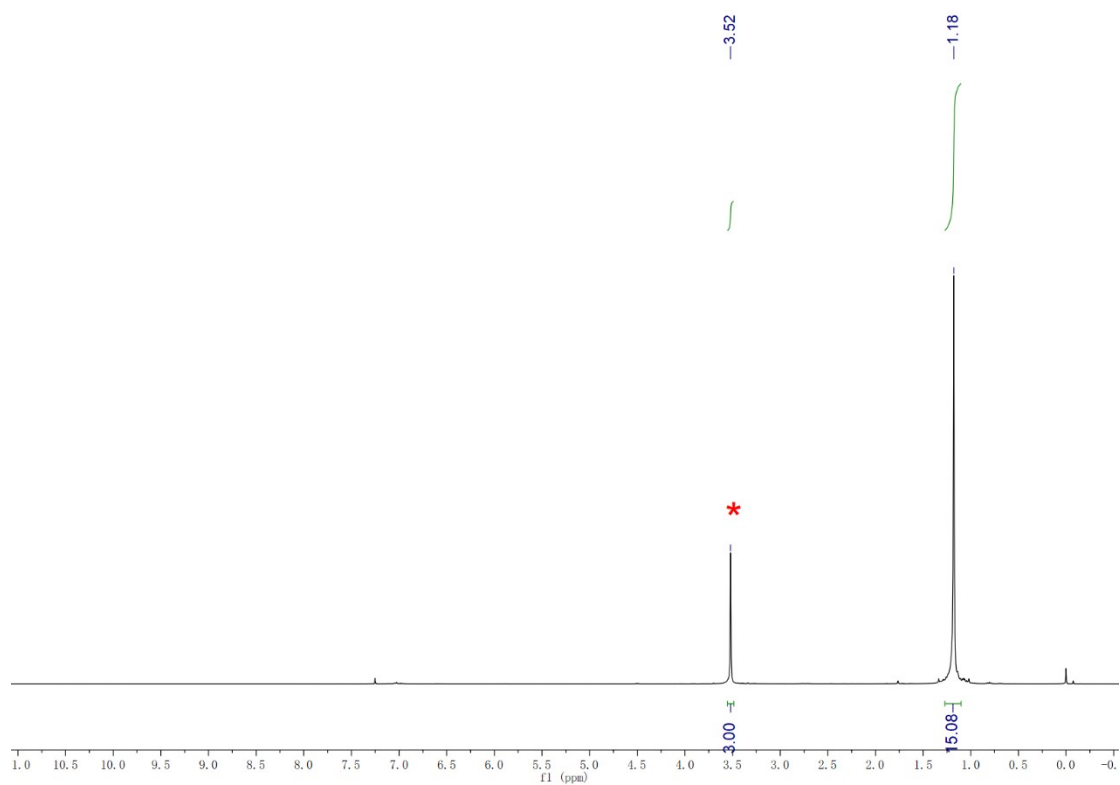


Figure S1.10.1 ^1H NMR spectrum of compound **4j** in CDCl_3

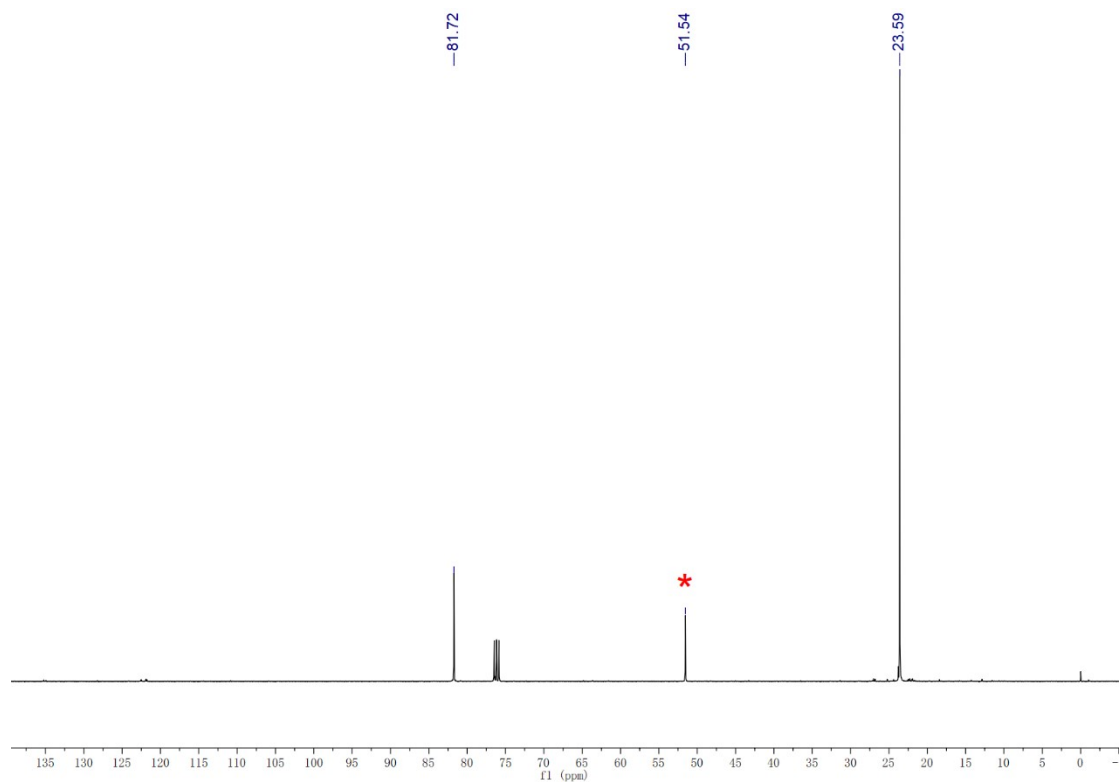


Figure S1.10.2 ^{13}C NMR spectrum of compound **4j** in CDCl_3

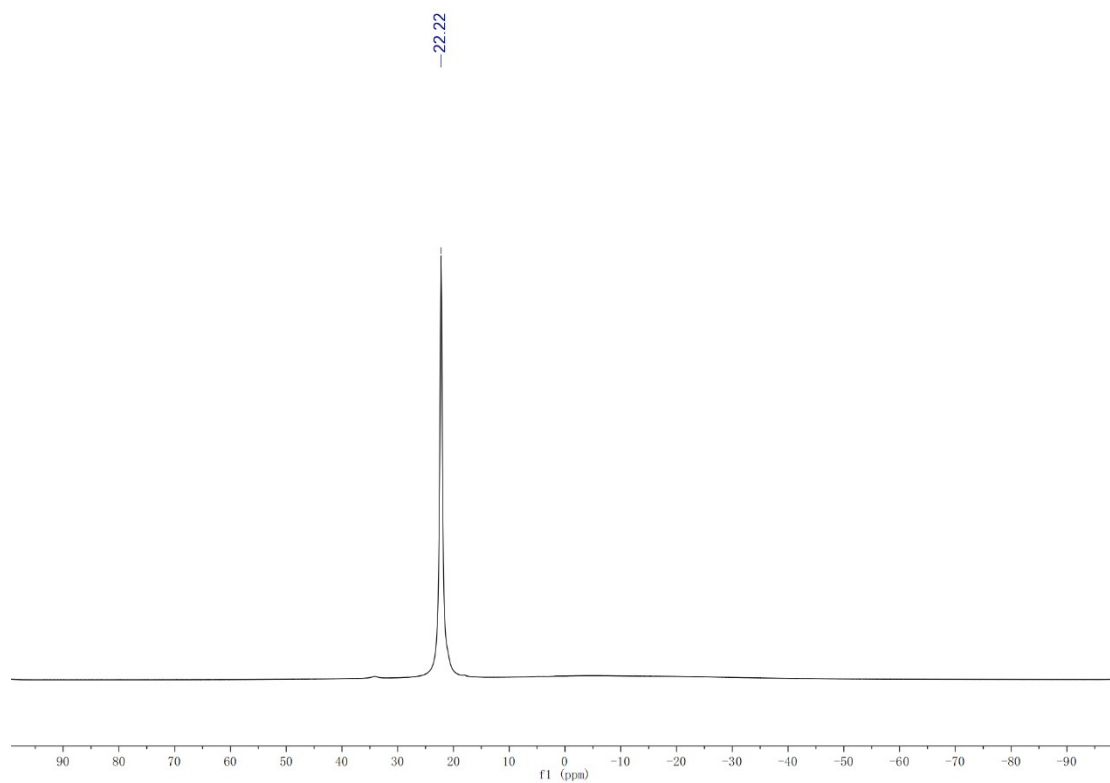


Figure S1.10.3 ^{11}B NMR spectrum of compound **4j** in CDCl_3

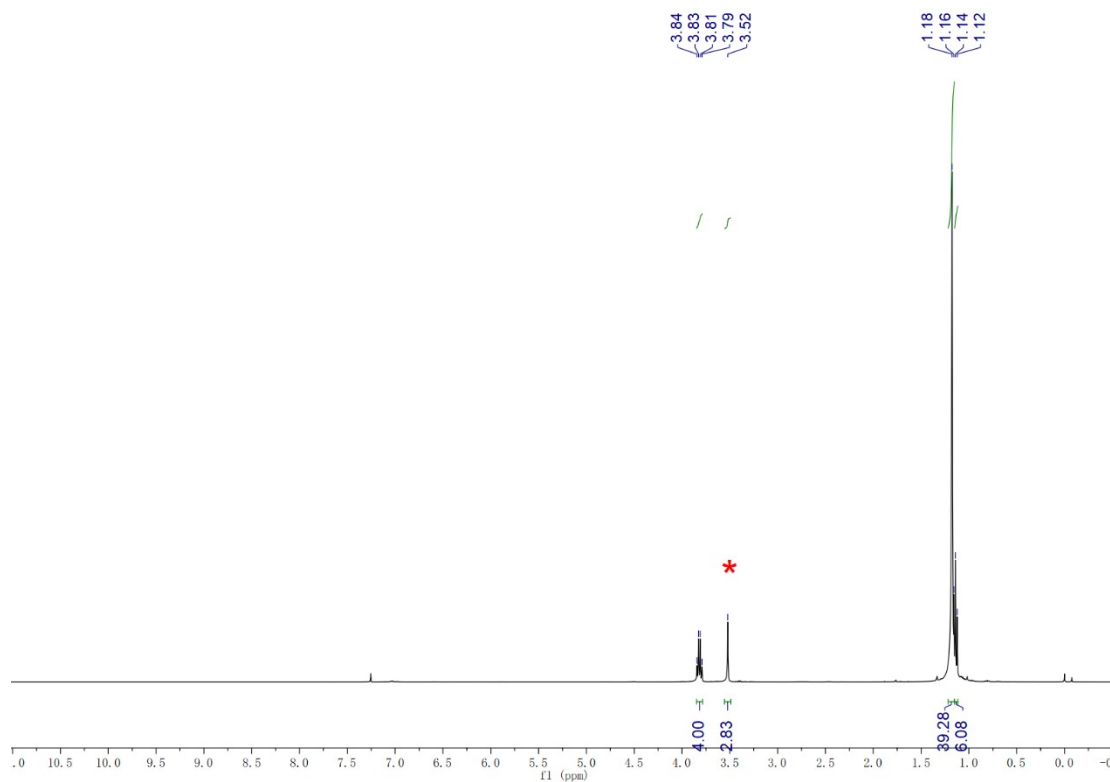


Figure S1.11.1 ^1H NMR spectrum of compound **4k** in CDCl_3

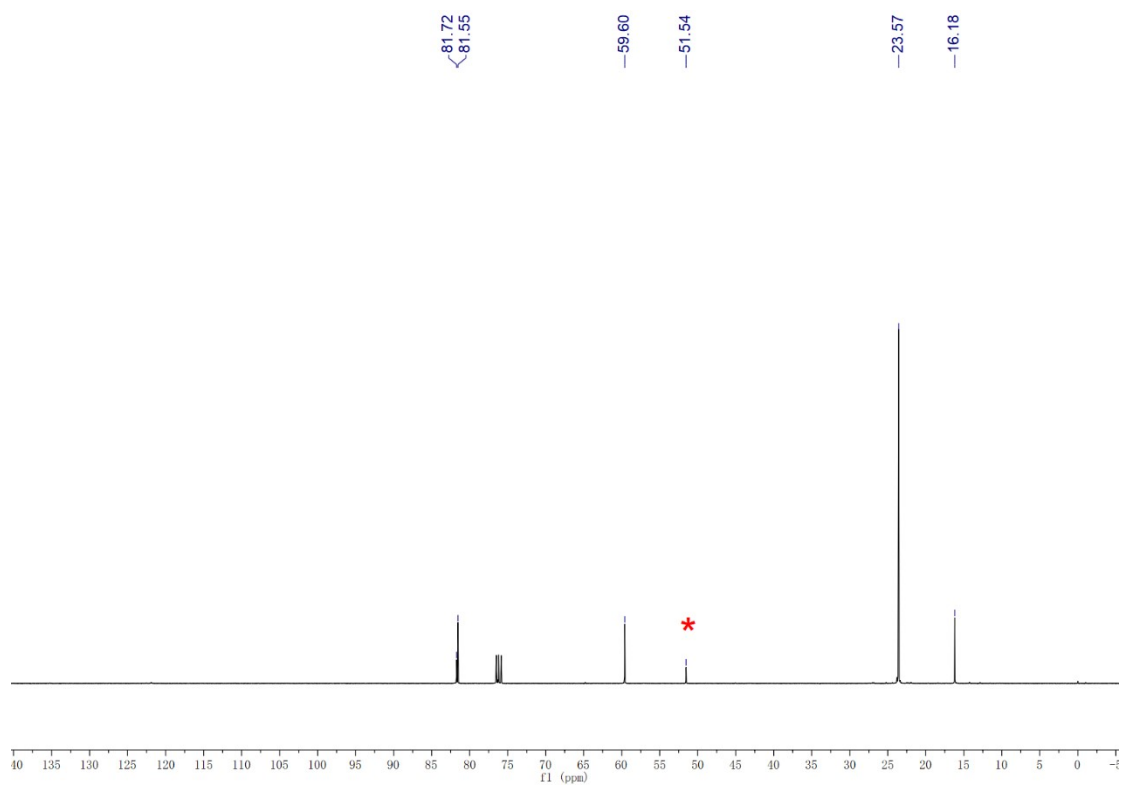


Figure S1.11.2 ¹³C NMR spectrum of compound **4k** in CDCl₃

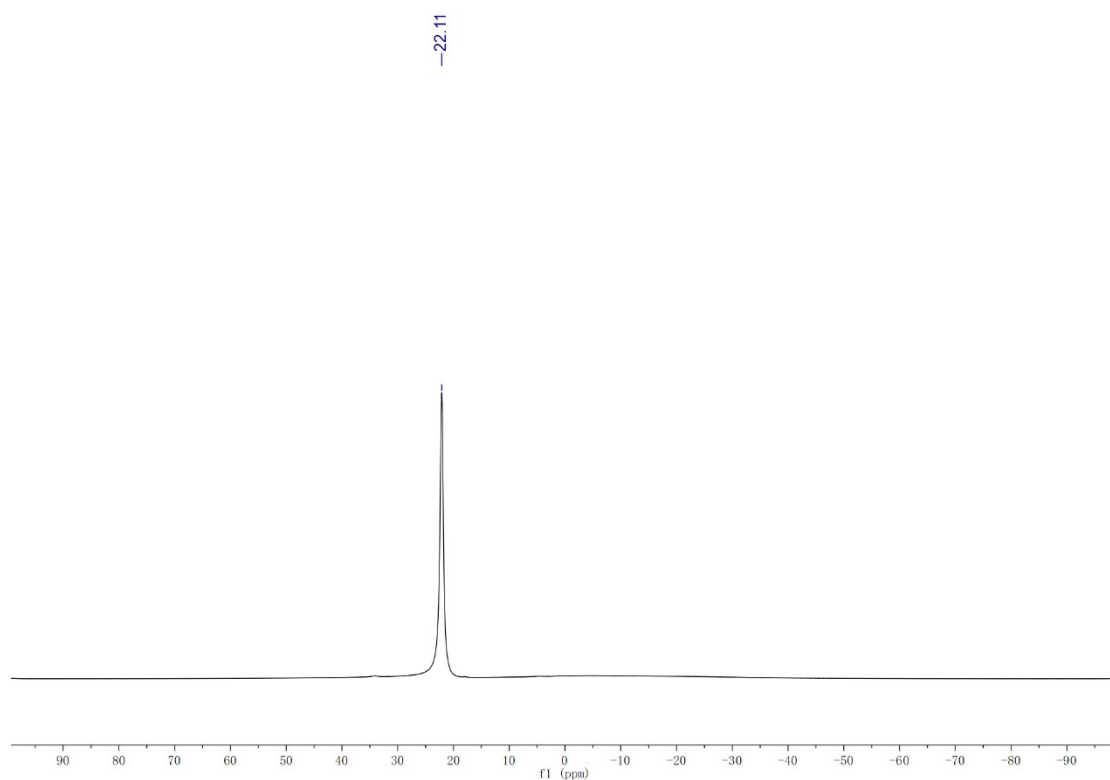


Figure S1.11.3 ¹¹B NMR spectrum of compound **4k** in CDCl₃

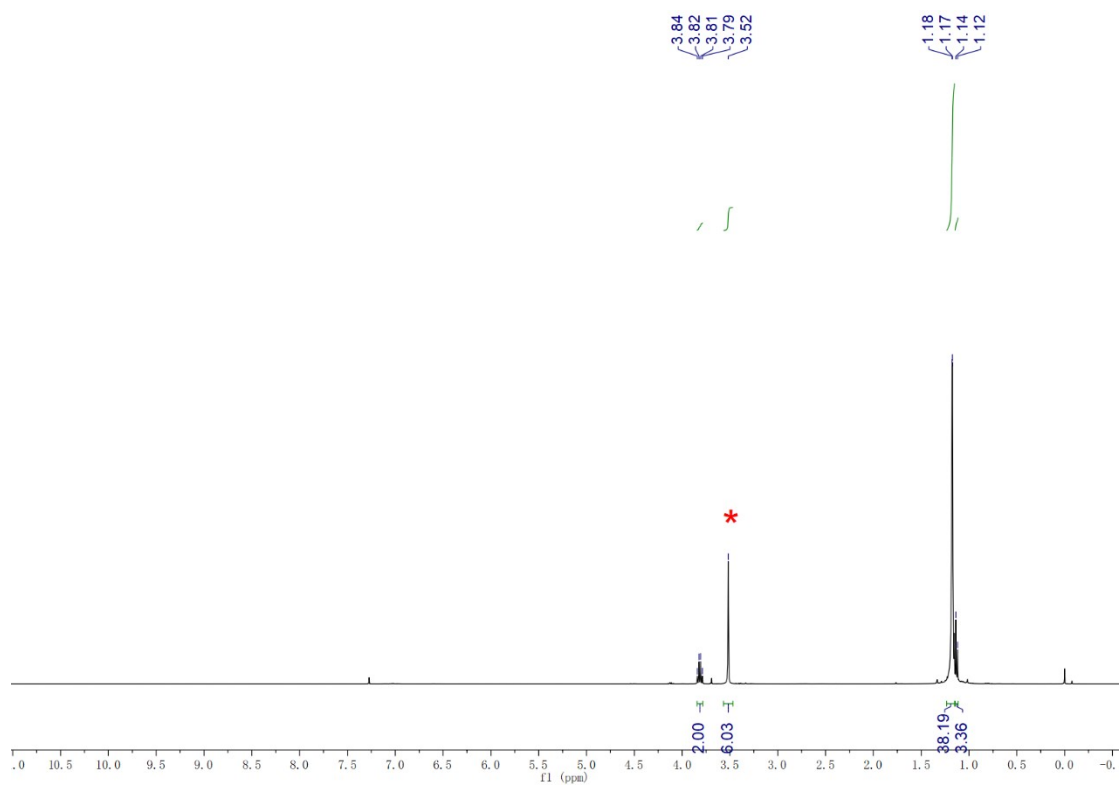


Figure S1.12.1 ^1H NMR spectrum of compound **4I** in CDCl_3

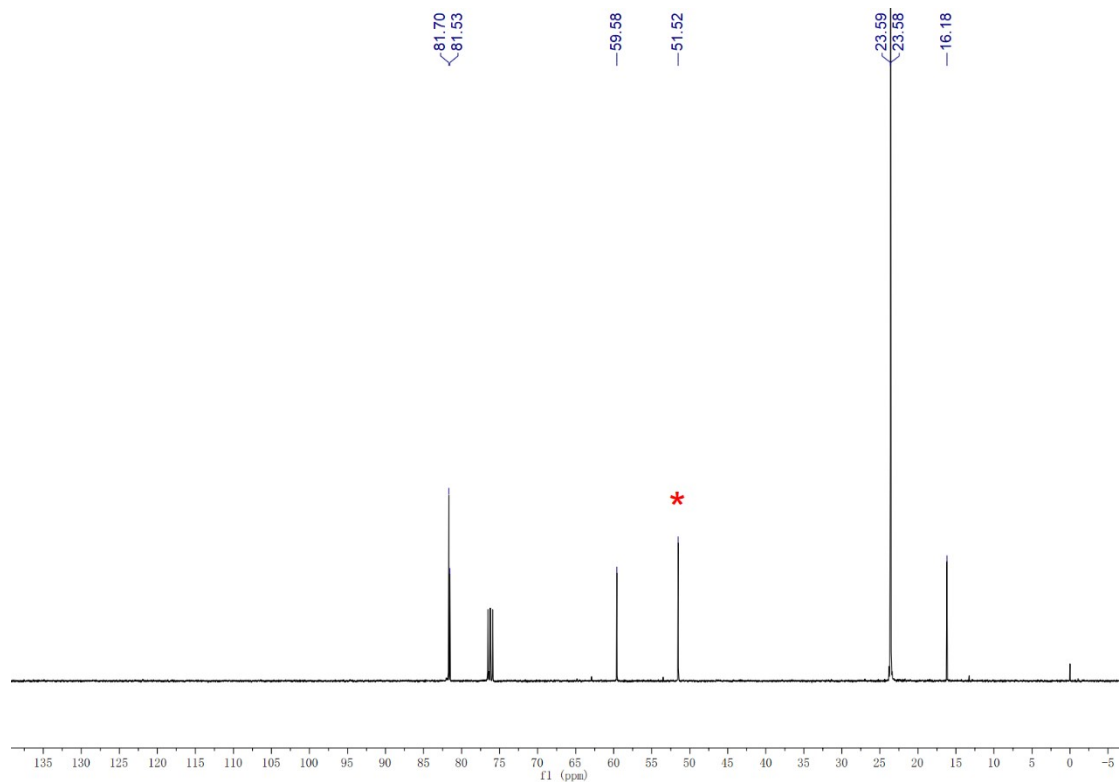


Figure S1.12.2 ^{13}C NMR spectrum of compound **4I** in CDCl_3



Figure S1.12.3 ^{11}B NMR spectrum of compound **4l** in CDCl_3

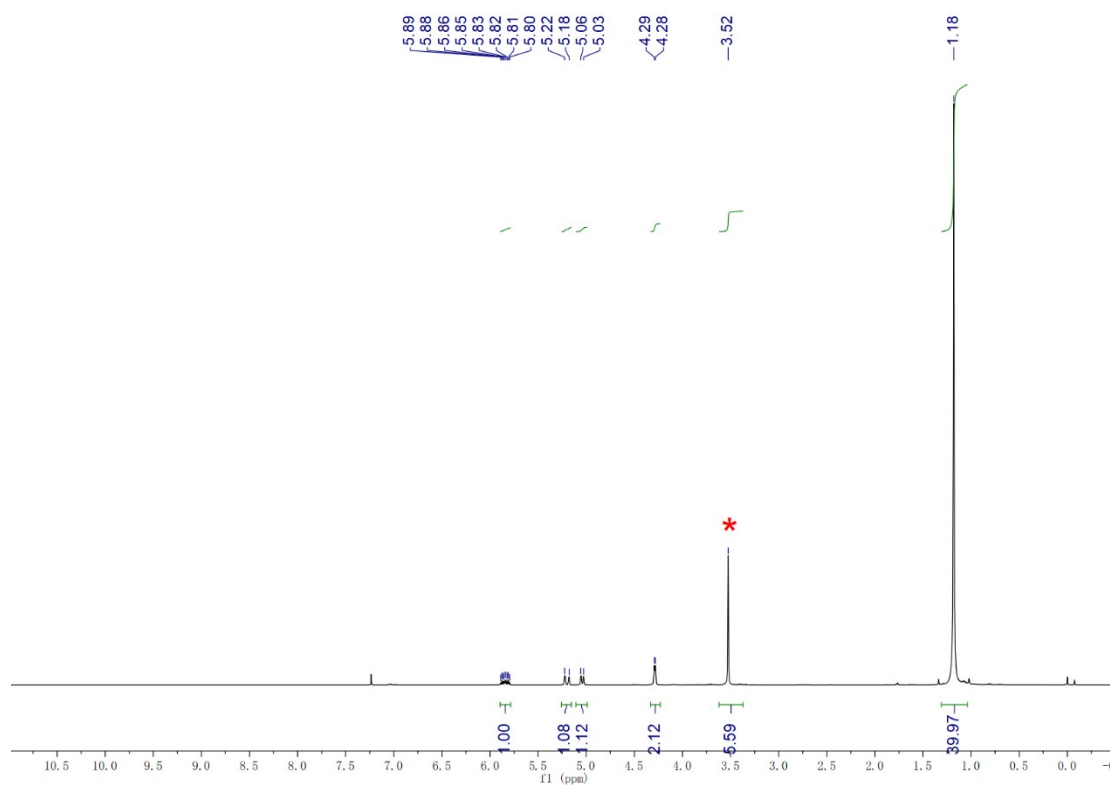


Figure S1.13.1 ^1H NMR spectrum of compound **4m** in CDCl_3

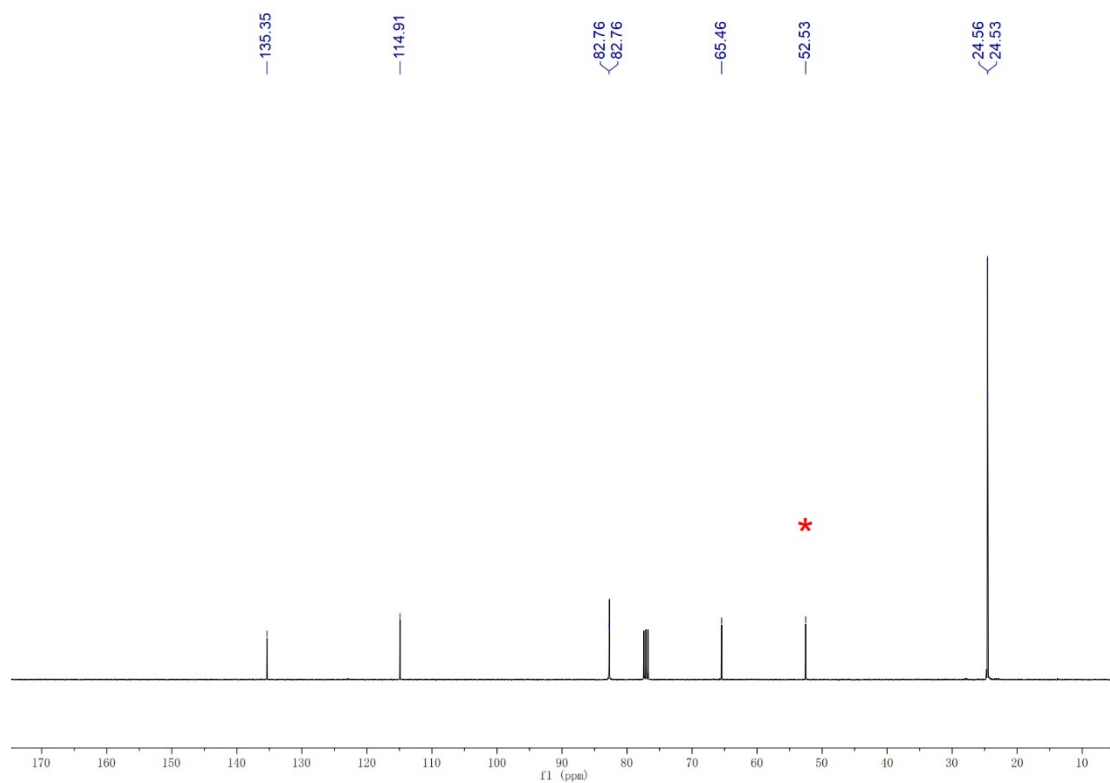


Figure S1.13.2 ^{13}C NMR spectrum of compound **4m** in CDCl_3

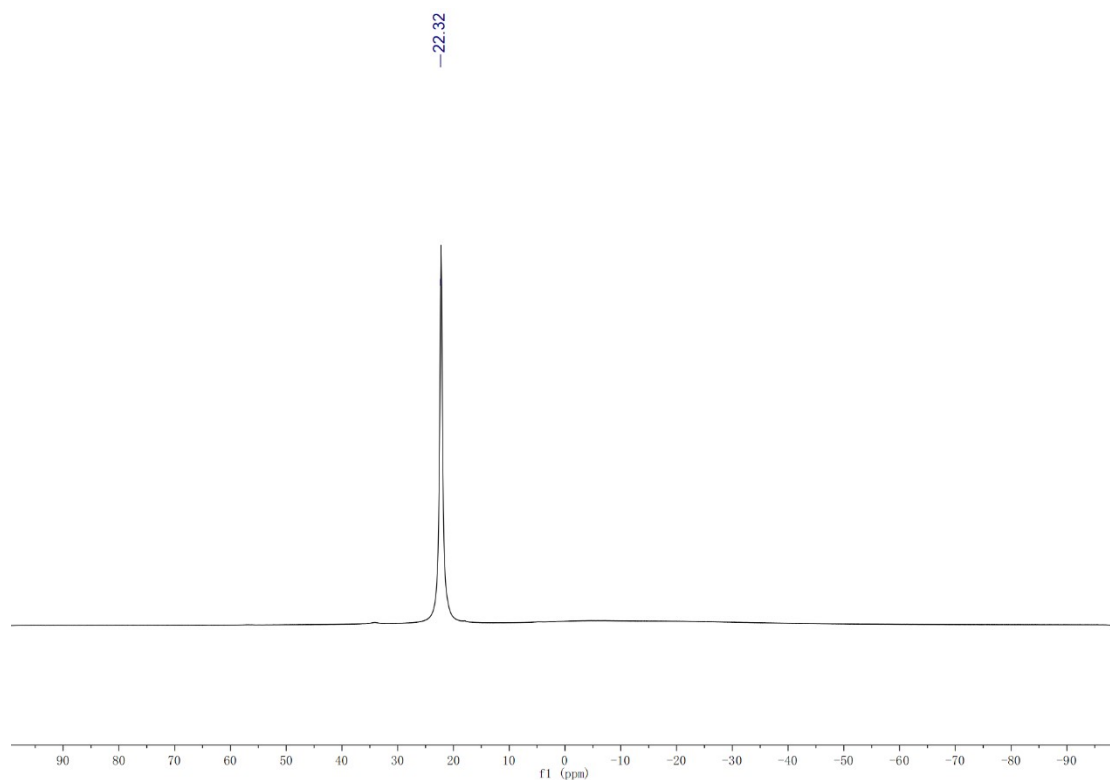


Figure S1.14.3 ^{11}B NMR spectrum of compound **4m** in CDCl_3

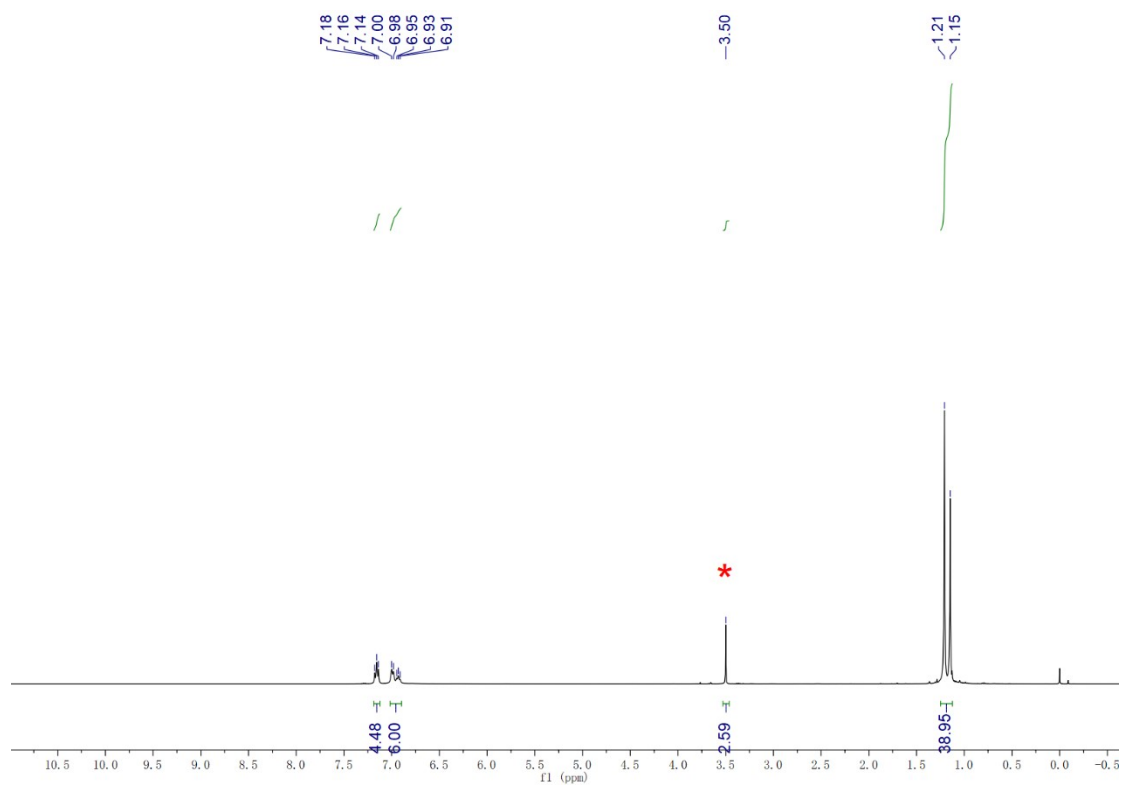


Figure S1.14.1 ^1H NMR spectrum of compound **4n** in CDCl_3

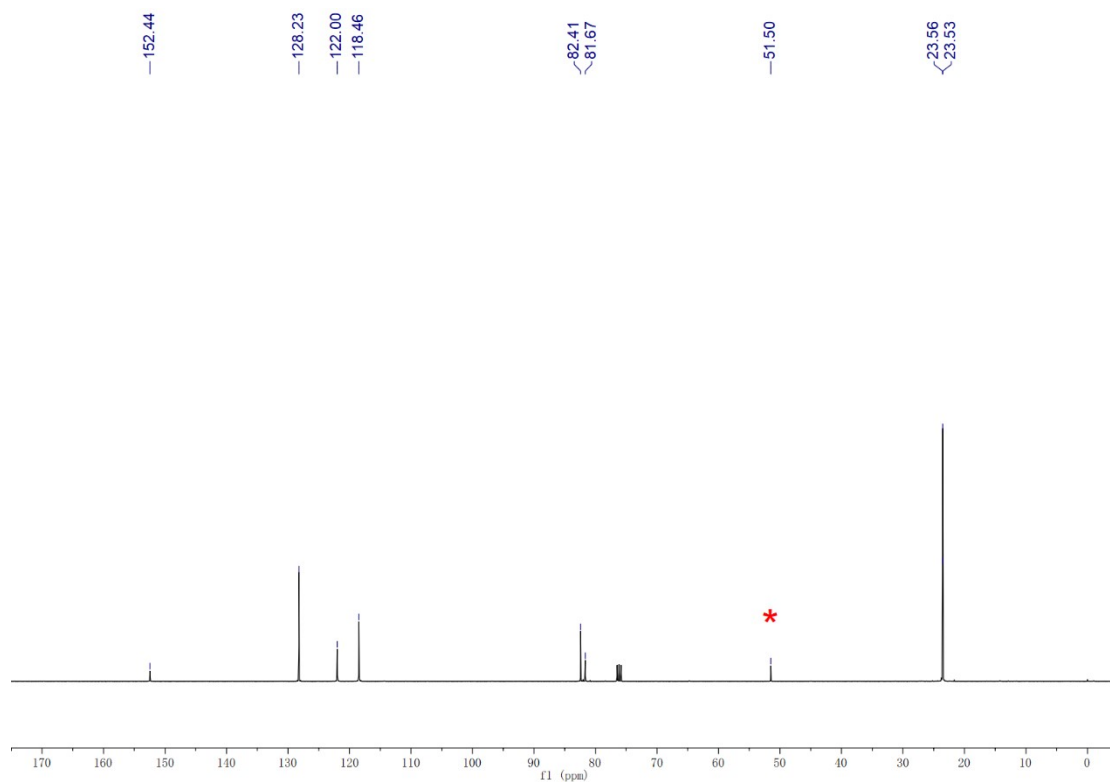


Figure S1.14.2 ^{13}C NMR spectrum of compound **4n** in CDCl_3

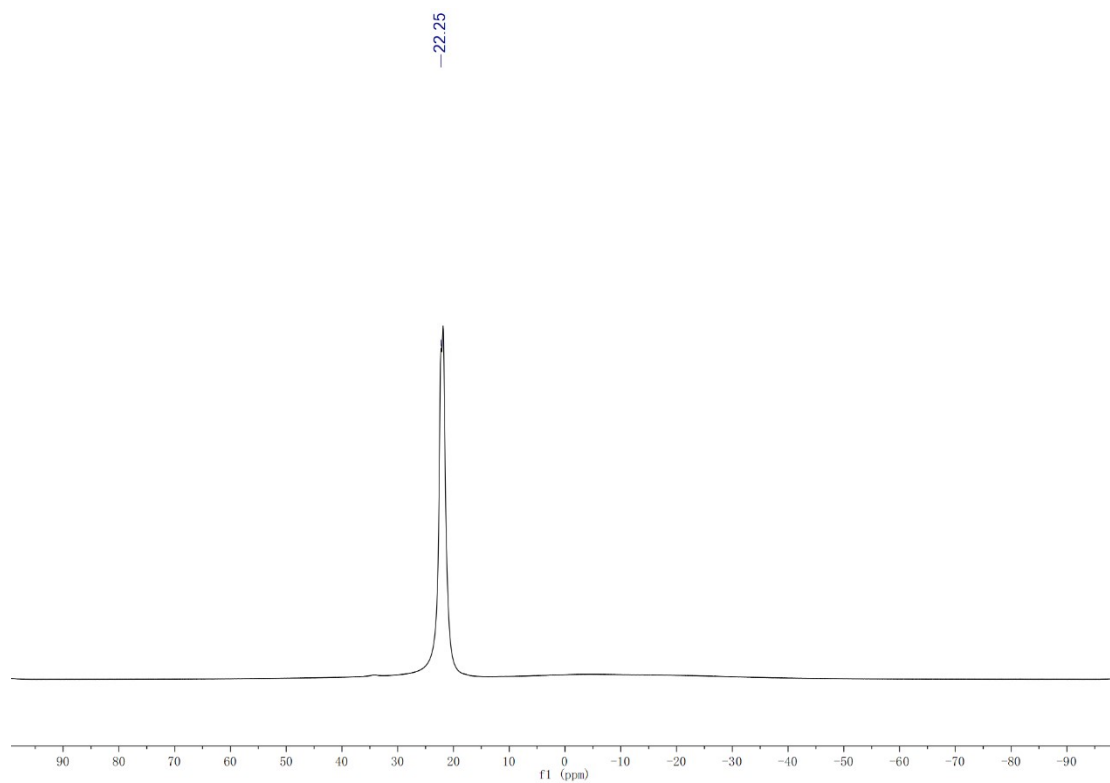


Figure S1.14.3 ^{11}B NMR spectrum of compound **4n** in CDCl_3

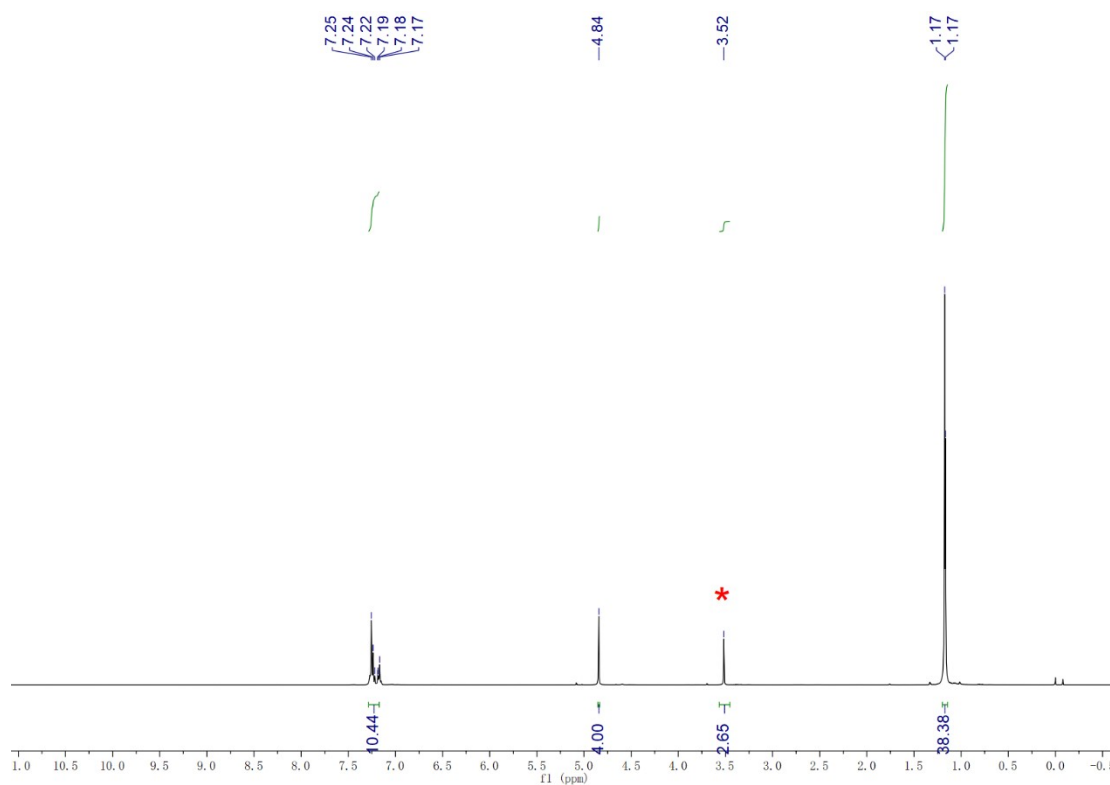


Figure S1.15.1 ^1H NMR spectrum of compound **4o** in CDCl_3

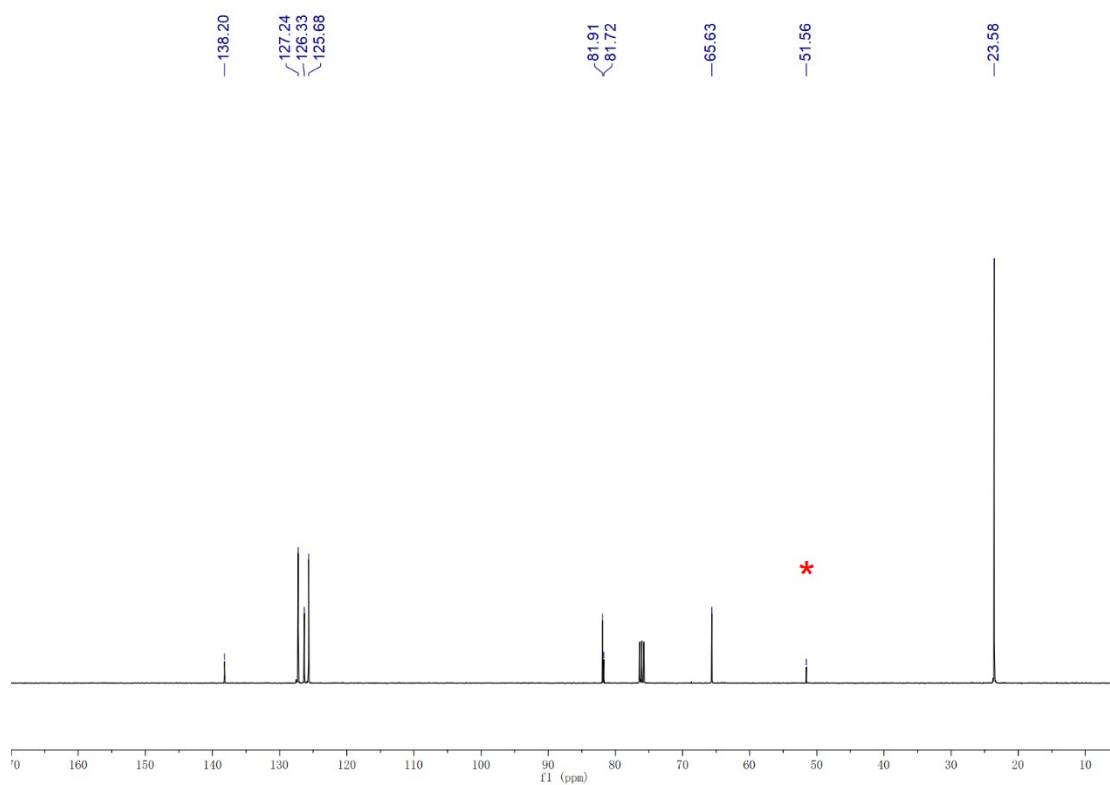


Figure S1.15.2 ^{13}C NMR spectrum of compound **4o** in CDCl_3

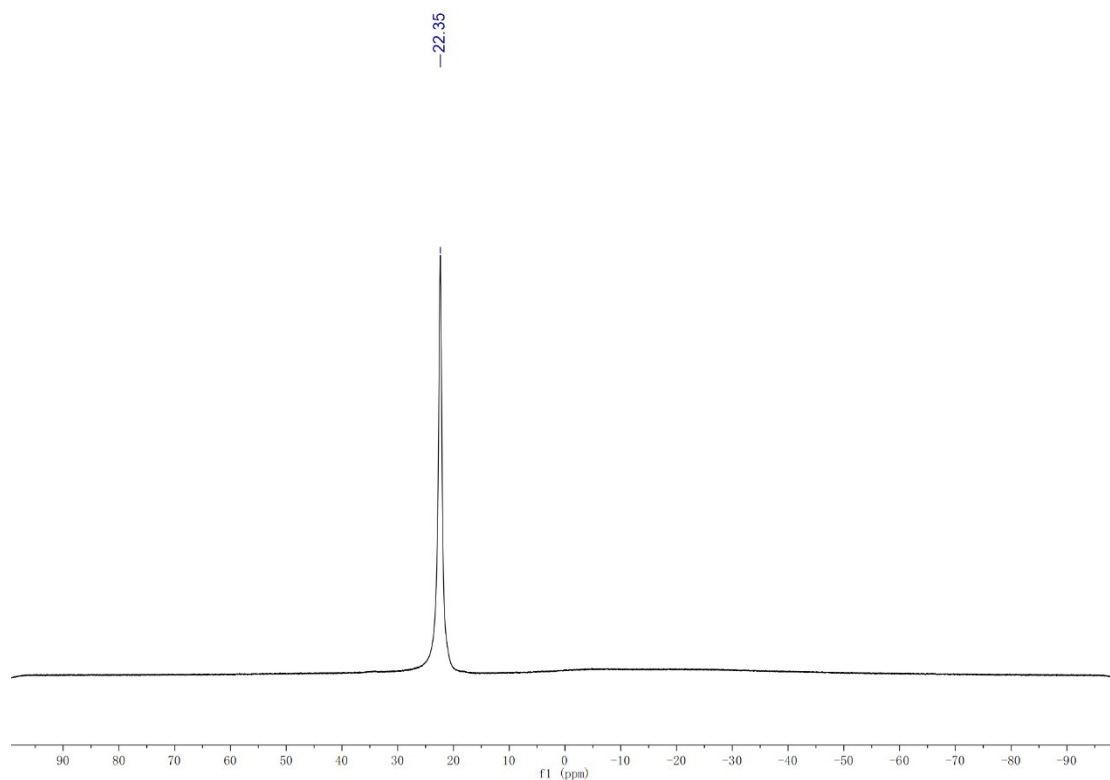


Figure S1.15.3 ^{11}B NMR spectrum of compound **4o** in CDCl_3

^1H , ^{13}C and ^{11}B NMR Spectra of Hydroboration Products of Esters.

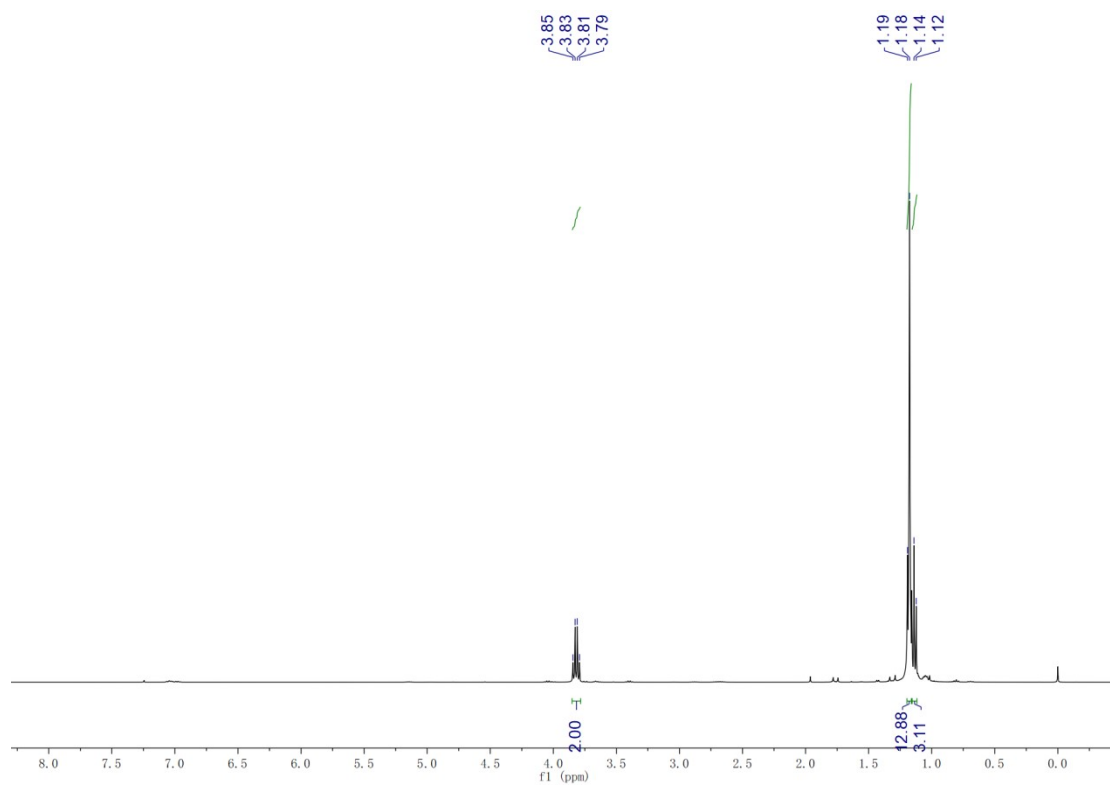


Figure S2.1.1 ^1H NMR spectrum of compound **6a** in CDCl_3

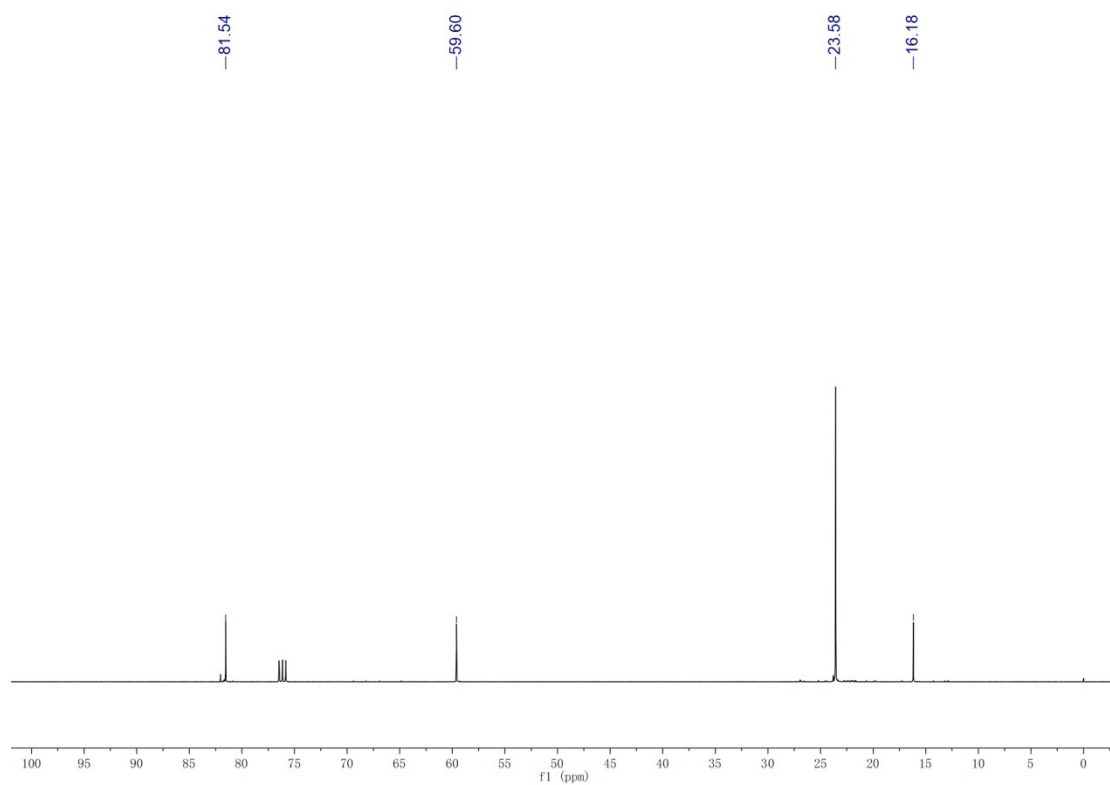


Figure S2.1.2 ¹³C NMR spectrum of compound **6a** in CDCl₃

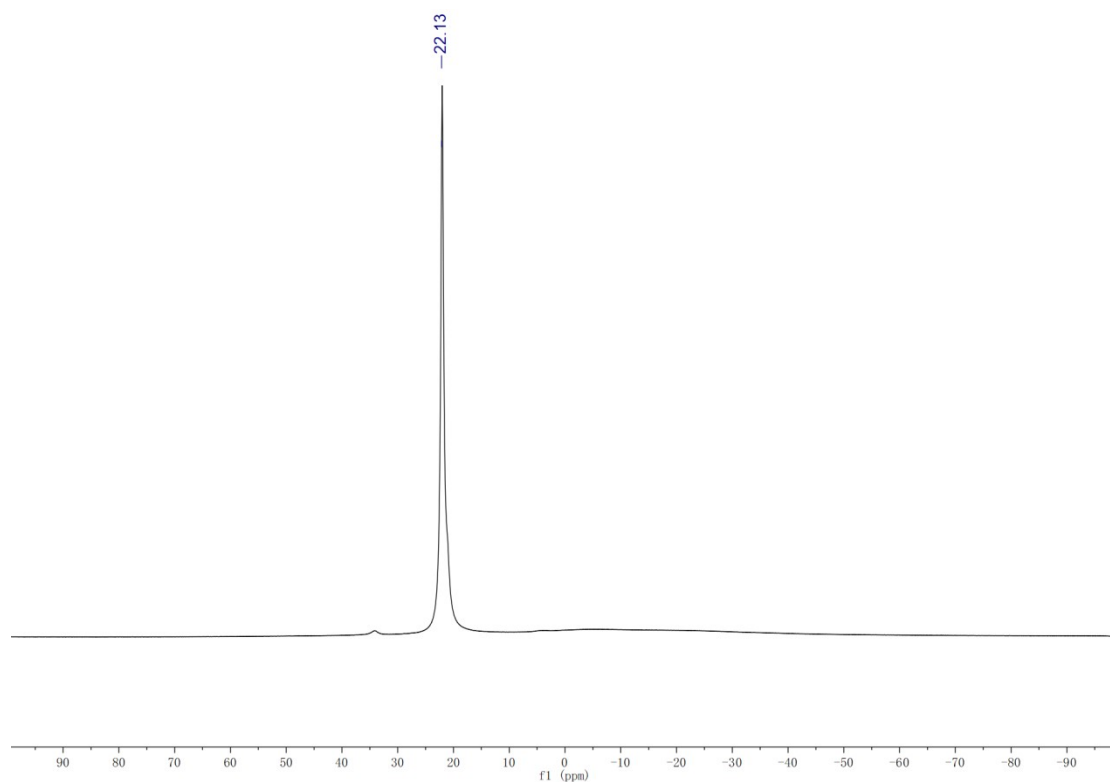


Figure S2.1.3 ¹¹B NMR spectrum of compound **6a** in CDCl₃

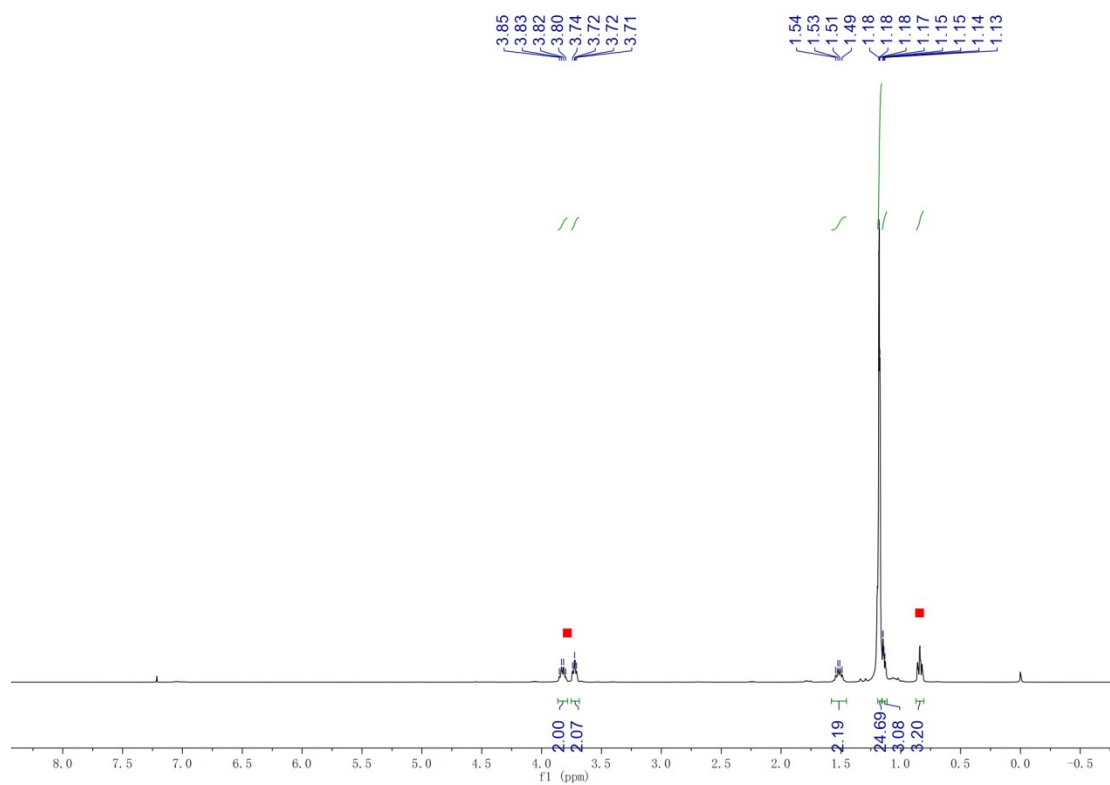


Figure S2.2.1 ^1H NMR spectrum of compound **6b** in CDCl_3

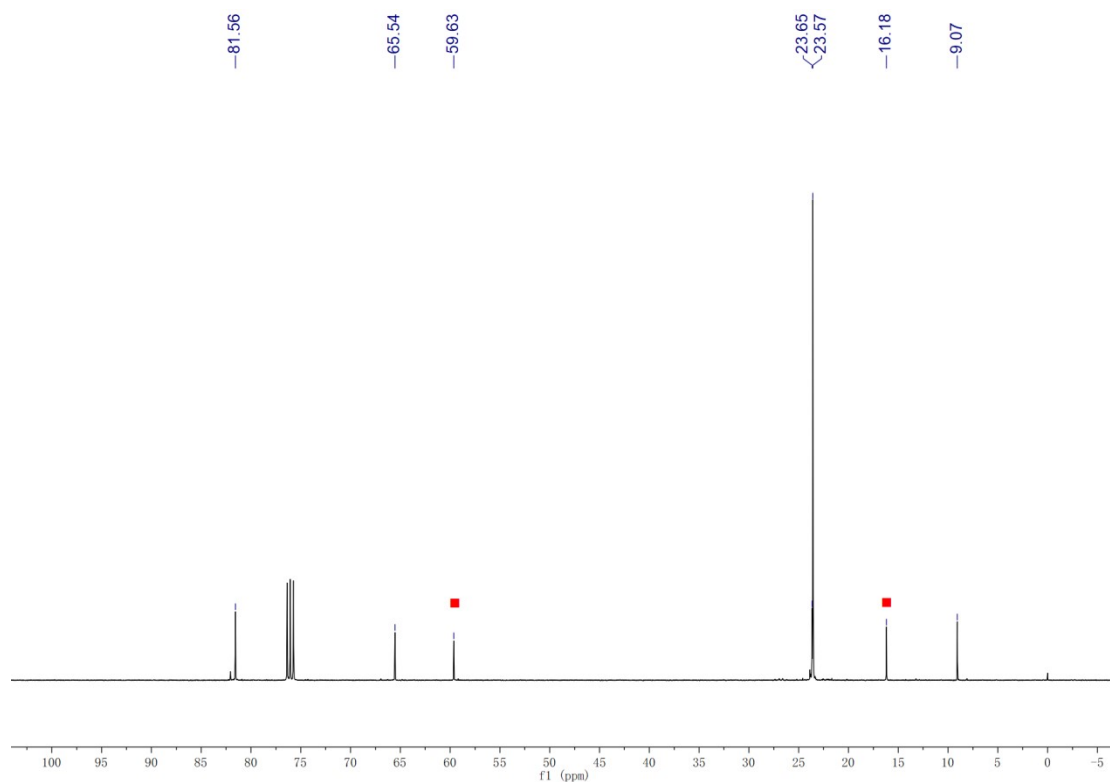


Figure S2.2.2 ^{13}C NMR spectrum of compound **6b** in CDCl_3

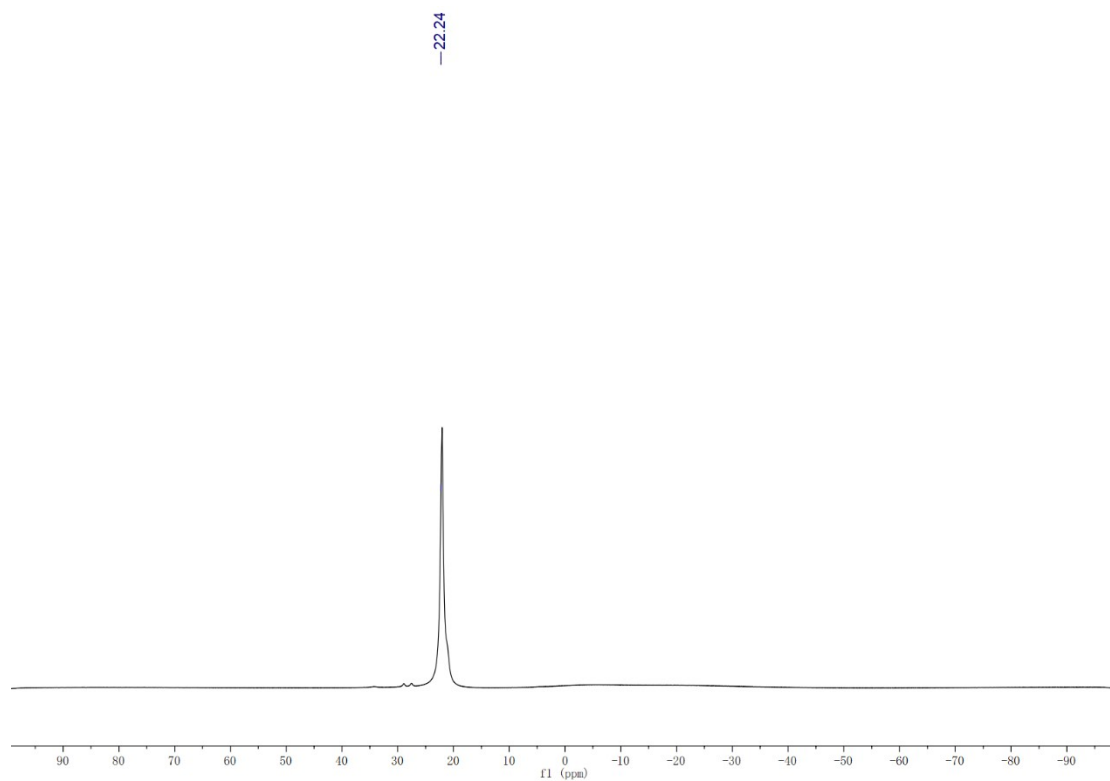


Figure S2.2.3 ¹¹B NMR spectrum of compound **6b** in CDCl₃

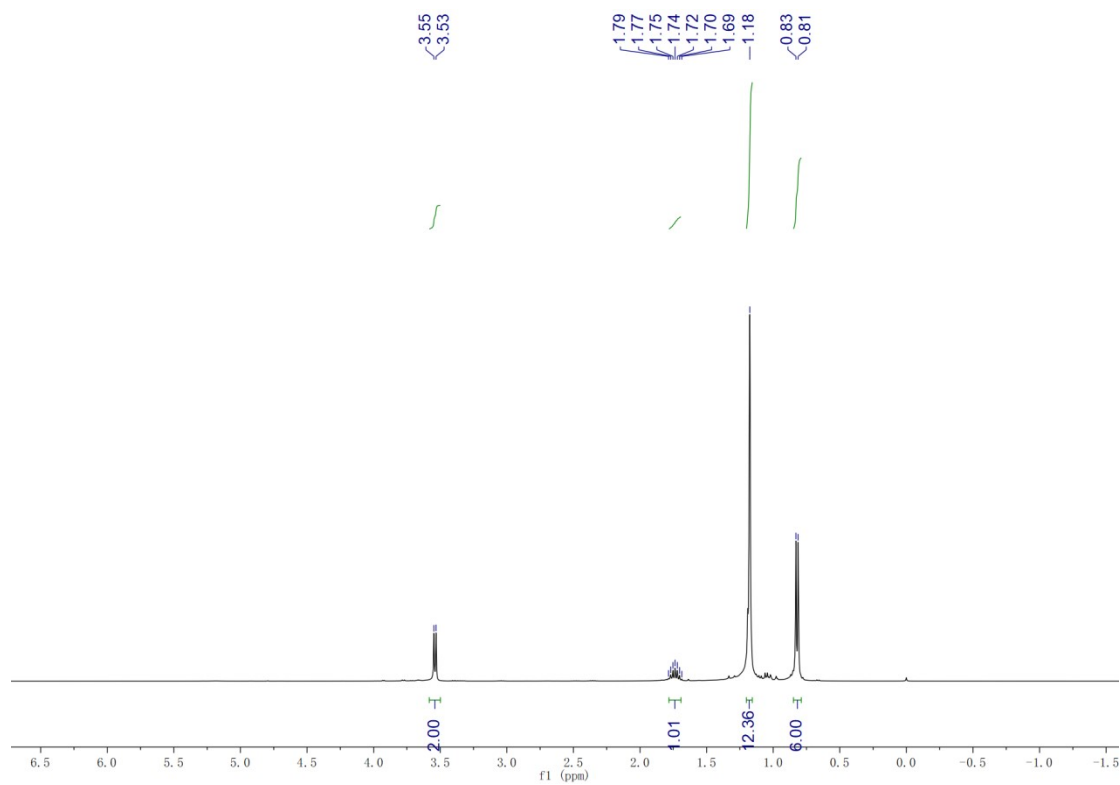


Figure S2.3.1 ¹H NMR spectrum of compound **6c** in CDCl₃

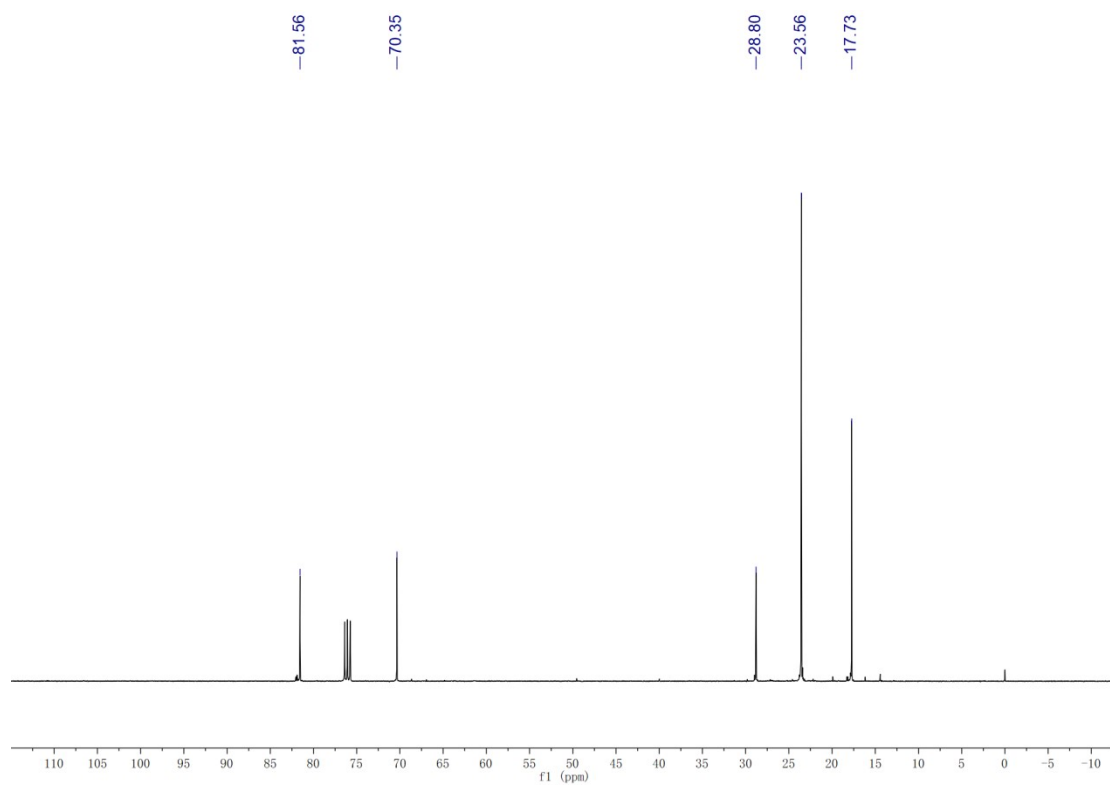


Figure S2.3.2 ^{13}C NMR spectrum of compound **6c** in CDCl_3

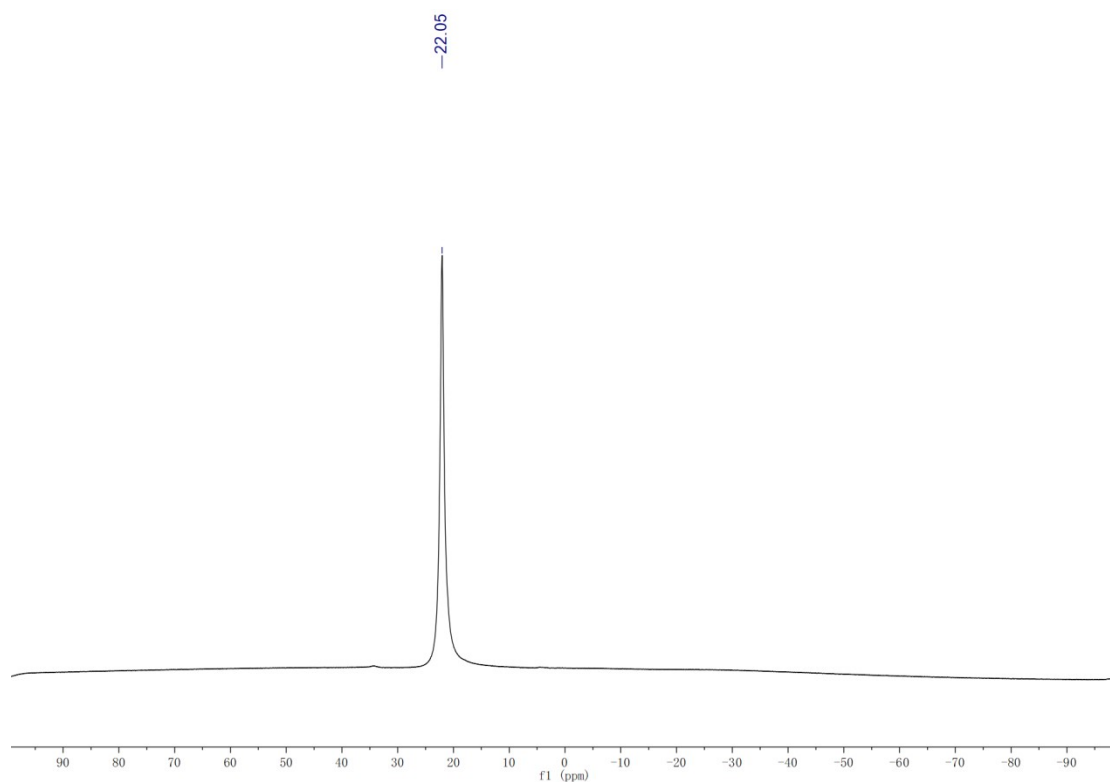


Figure S2.3.3 ^{11}B NMR spectrum of compound **6c** in CDCl_3

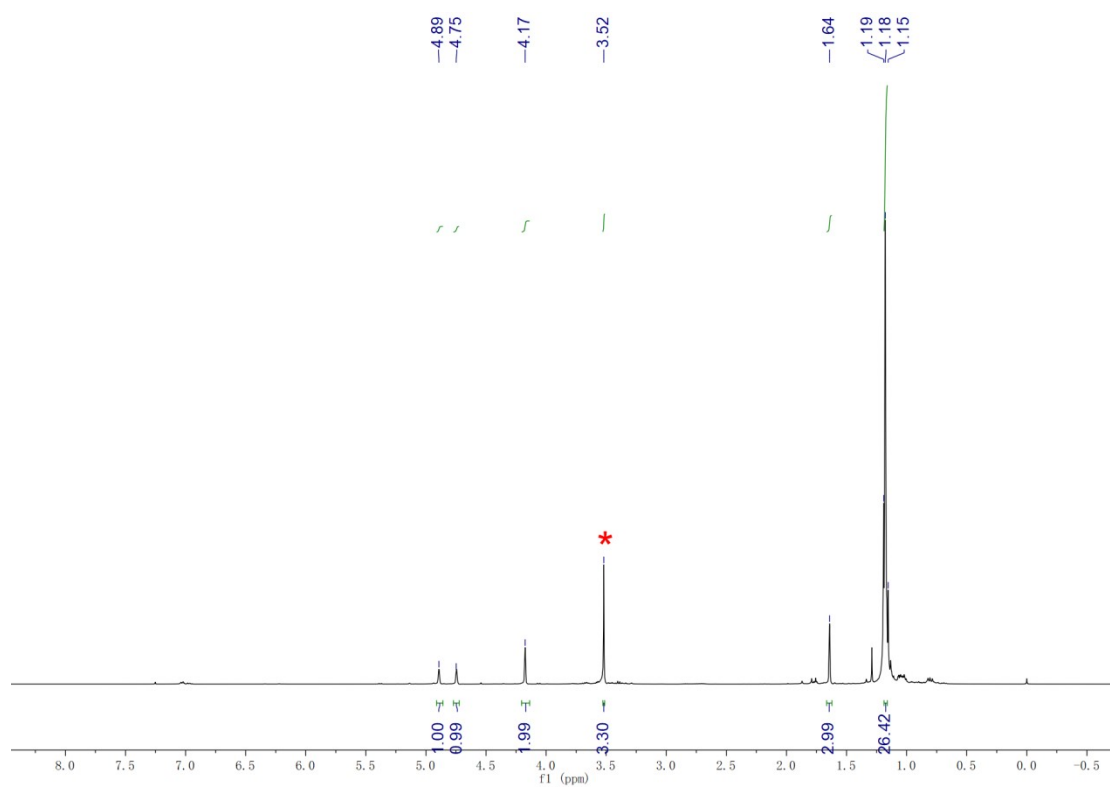


Figure S2.4.1 ^1H NMR spectrum of compound **6d** in CDCl_3

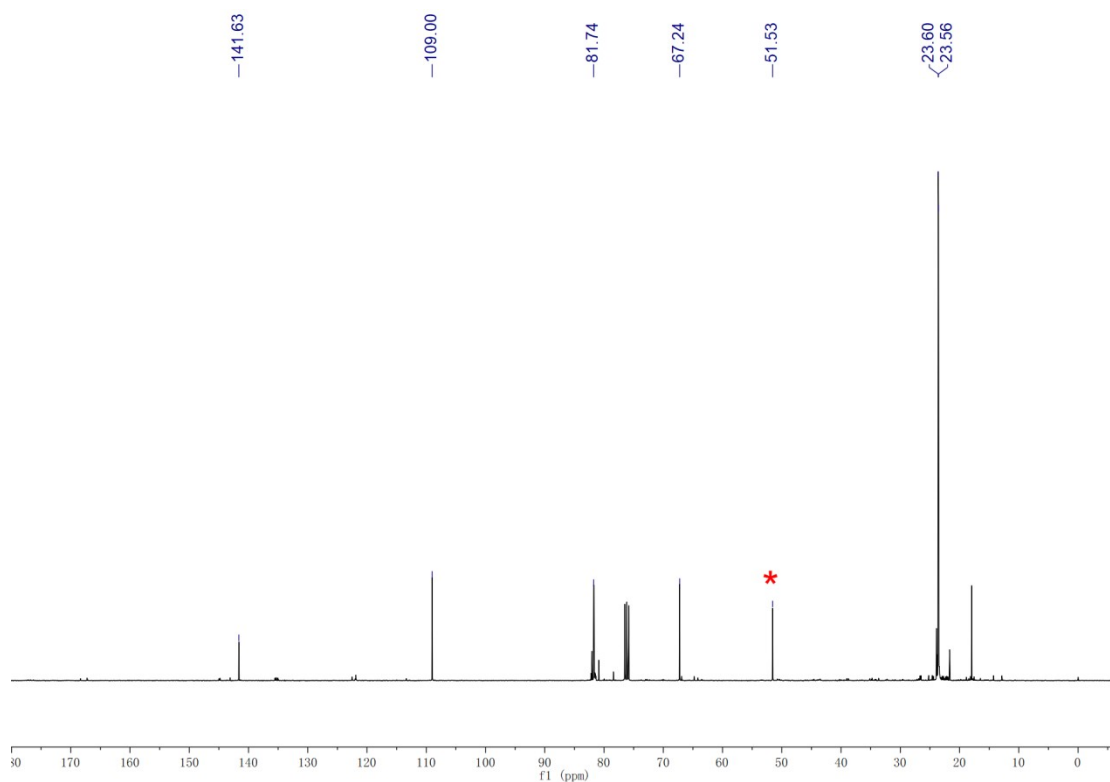


Figure S2.4.2 ^{13}C NMR spectrum of compound **6d** in CDCl_3

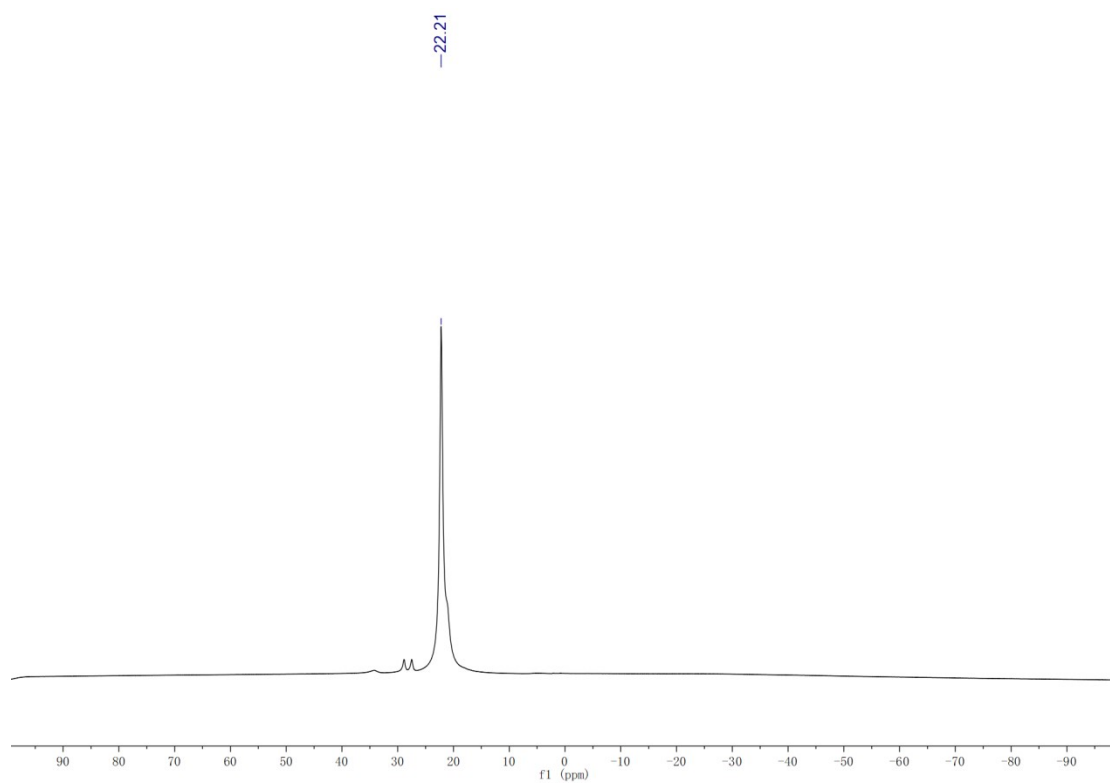


Figure S2.4.3 ^{11}B NMR spectrum of compound **6d** in CDCl_3

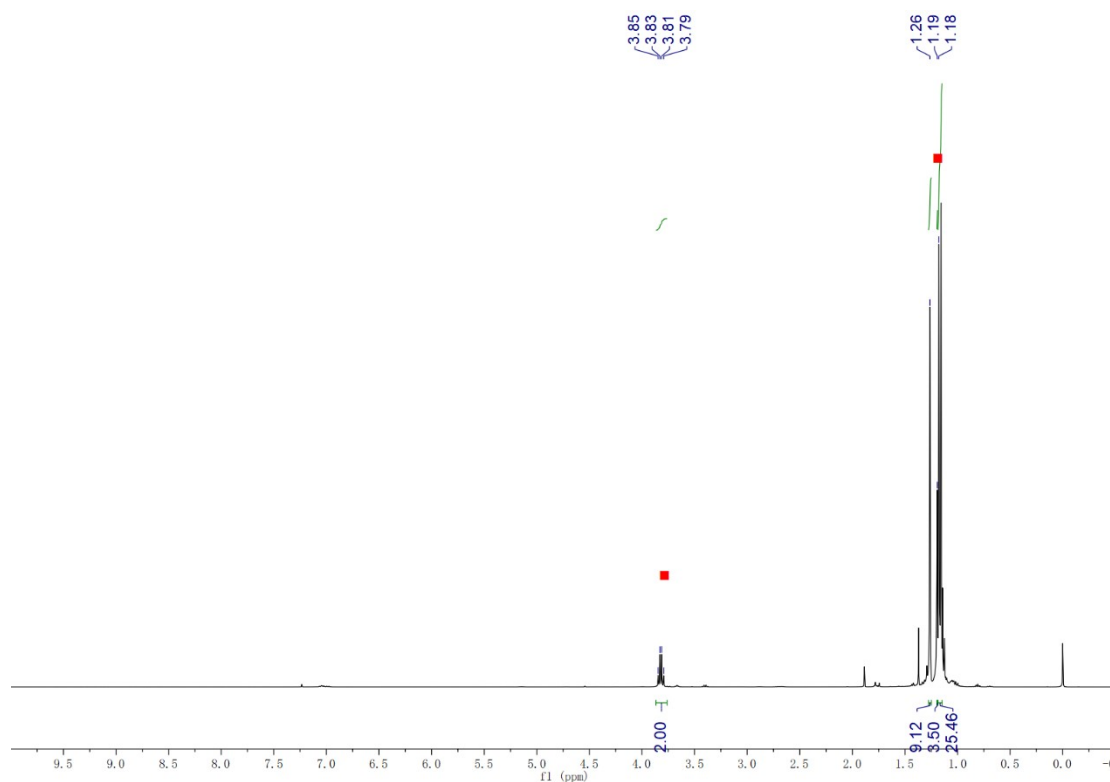


Figure S2.5.1 ^1H NMR spectrum of compound **6e** in CDCl_3

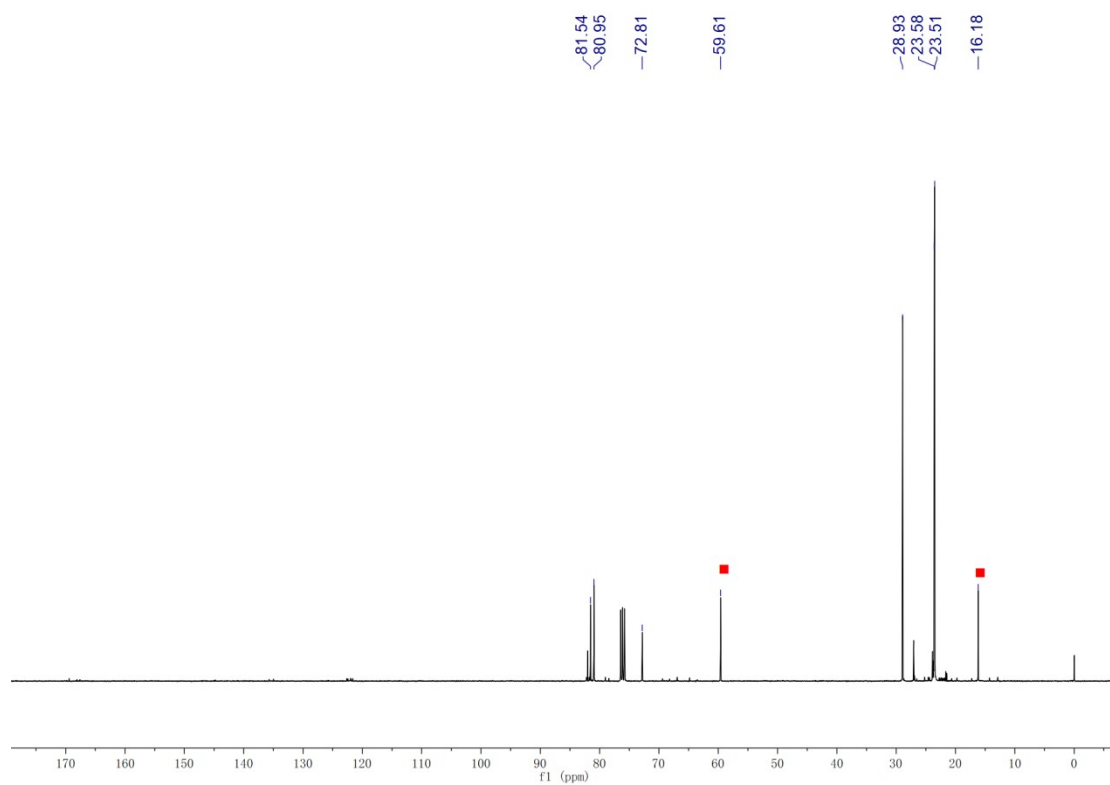


Figure S2.5.2 ^{13}C NMR spectrum of compound **6e** in CDCl_3

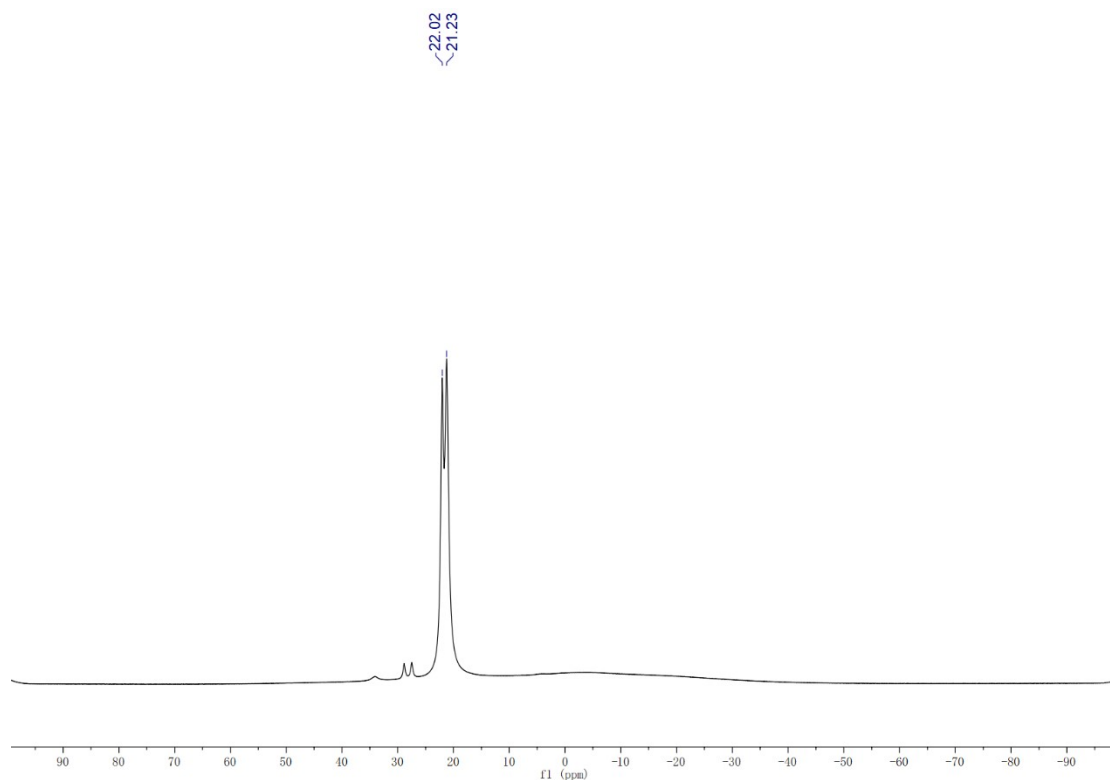


Figure S2.5.3 ^{11}B NMR spectrum of compound **6e** in CDCl_3

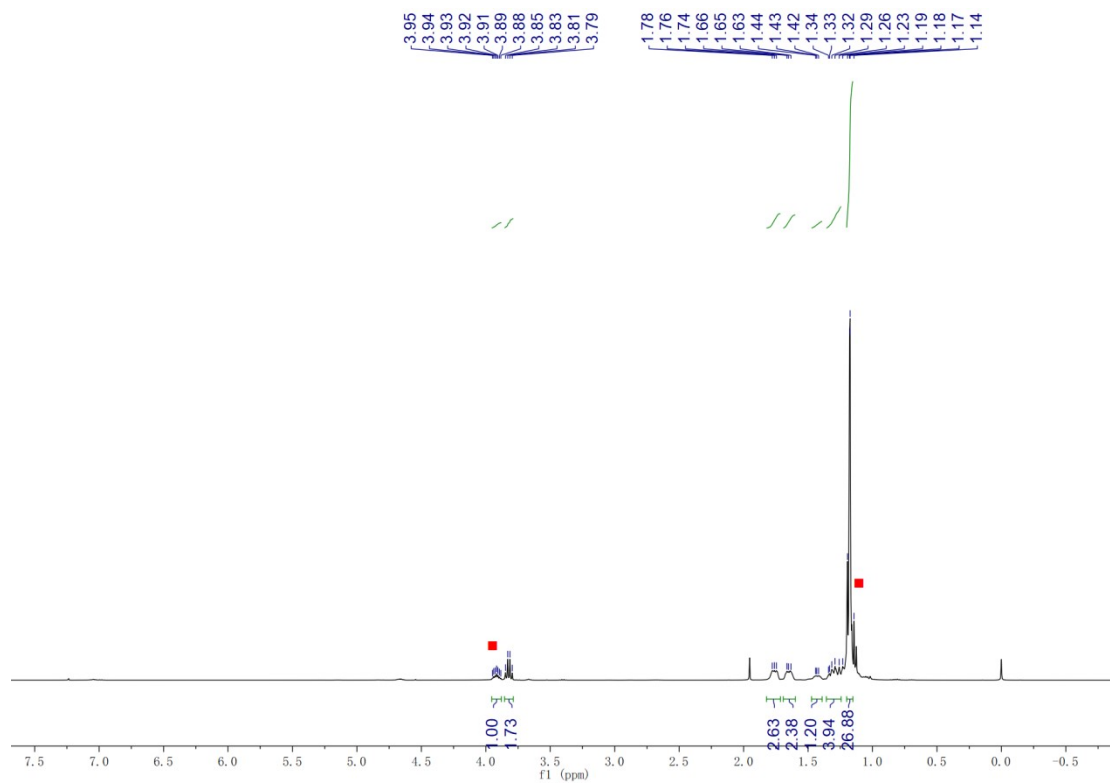


Figure S2.6.1 ^1H NMR spectrum of compound **6f** in CDCl_3

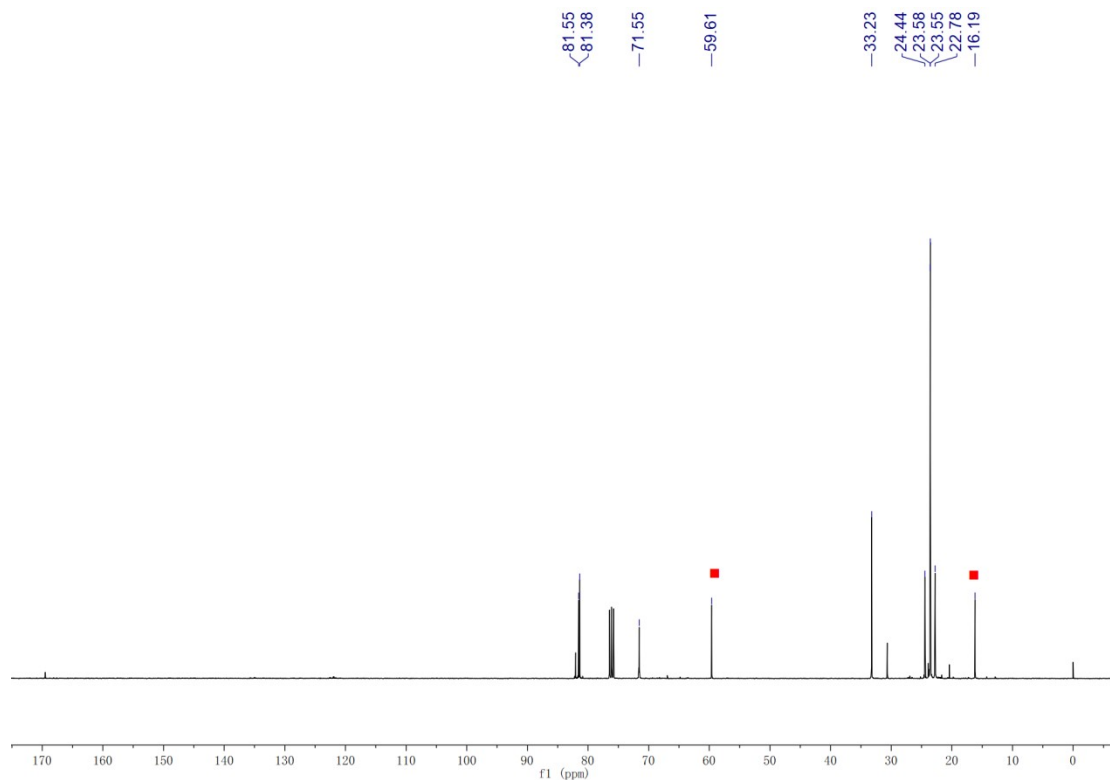


Figure S2.6.2 ^{13}C NMR spectrum of compound **6f** in CDCl_3

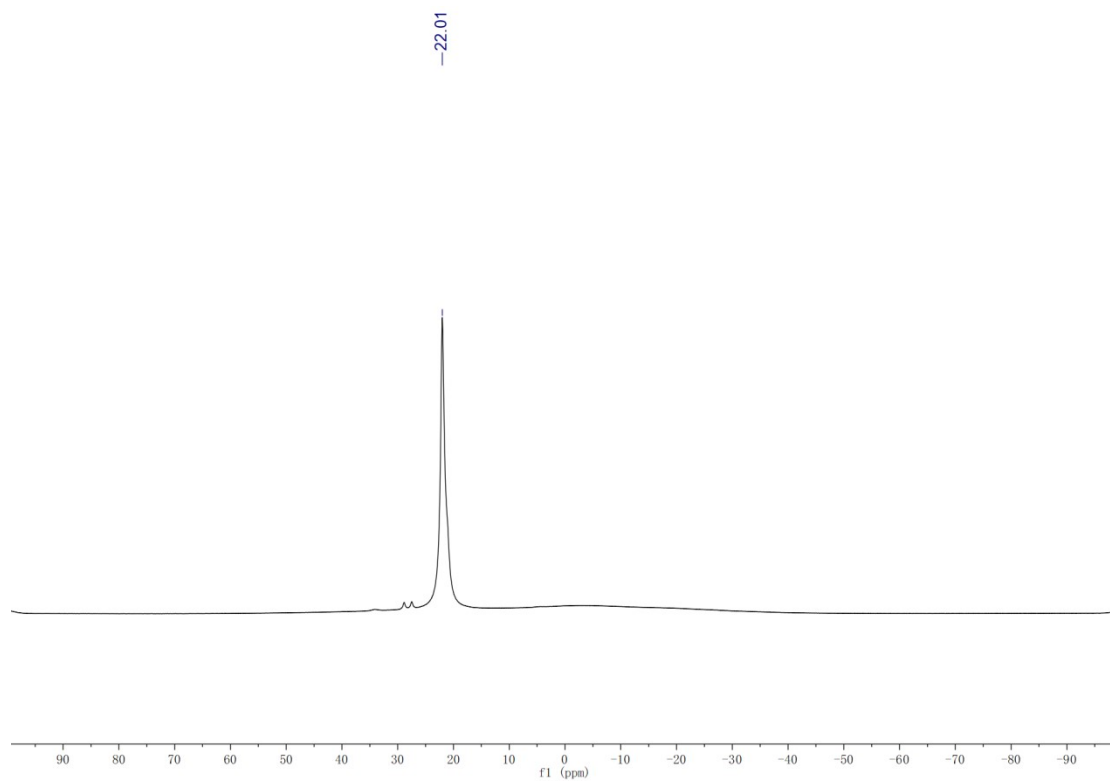


Figure S2.6.3 ^{11}B NMR spectrum of compound **6f** in CDCl_3

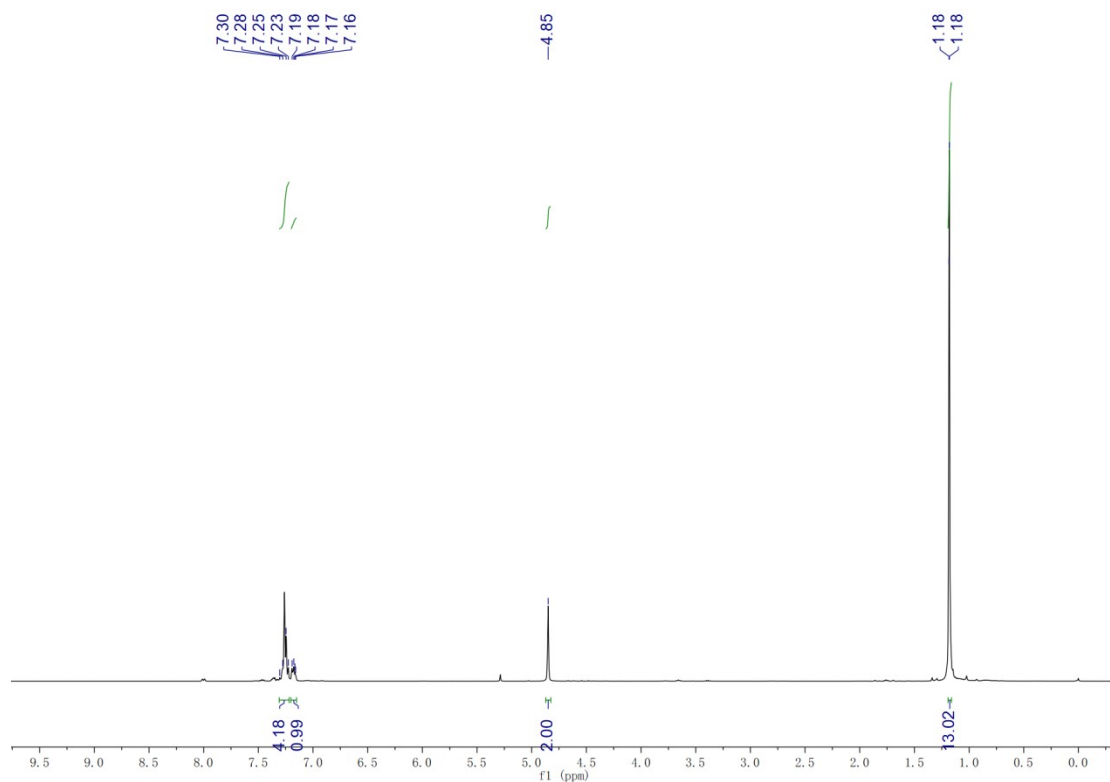


Figure S2.7.1 ^1H NMR spectrum of compound **6g** in CDCl_3

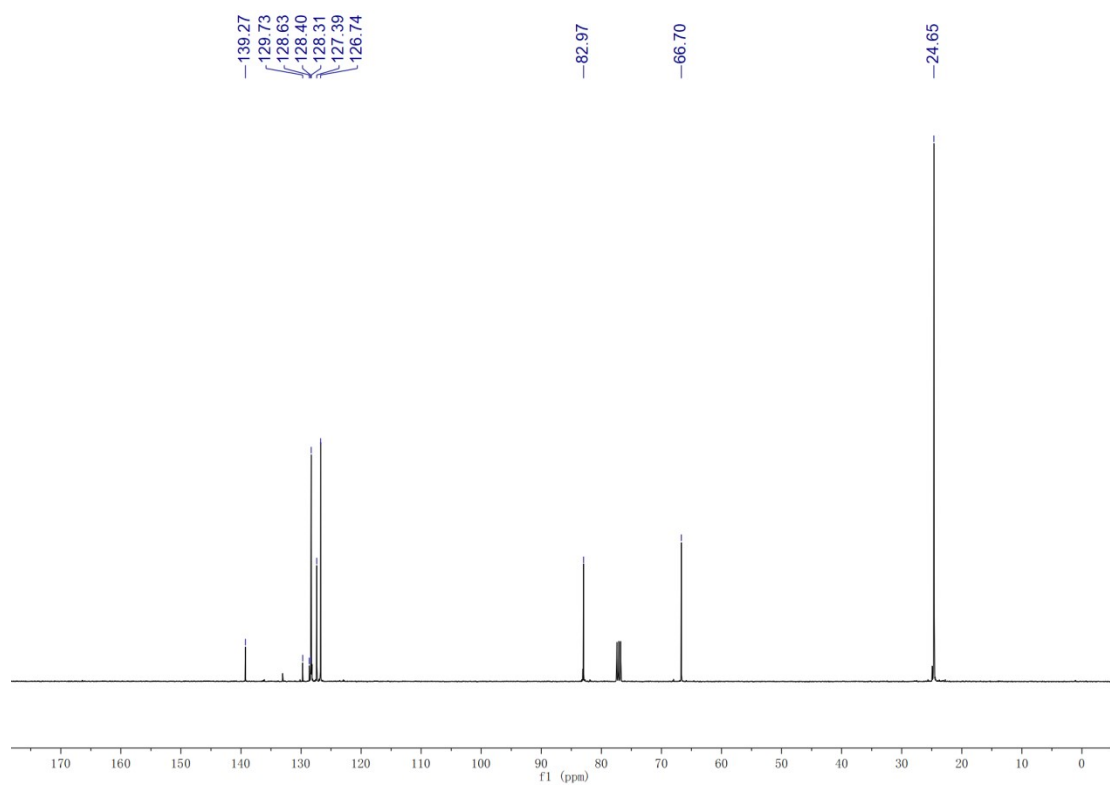


Figure S2.7.2 ^{13}C NMR spectrum of compound **6g** in CDCl_3

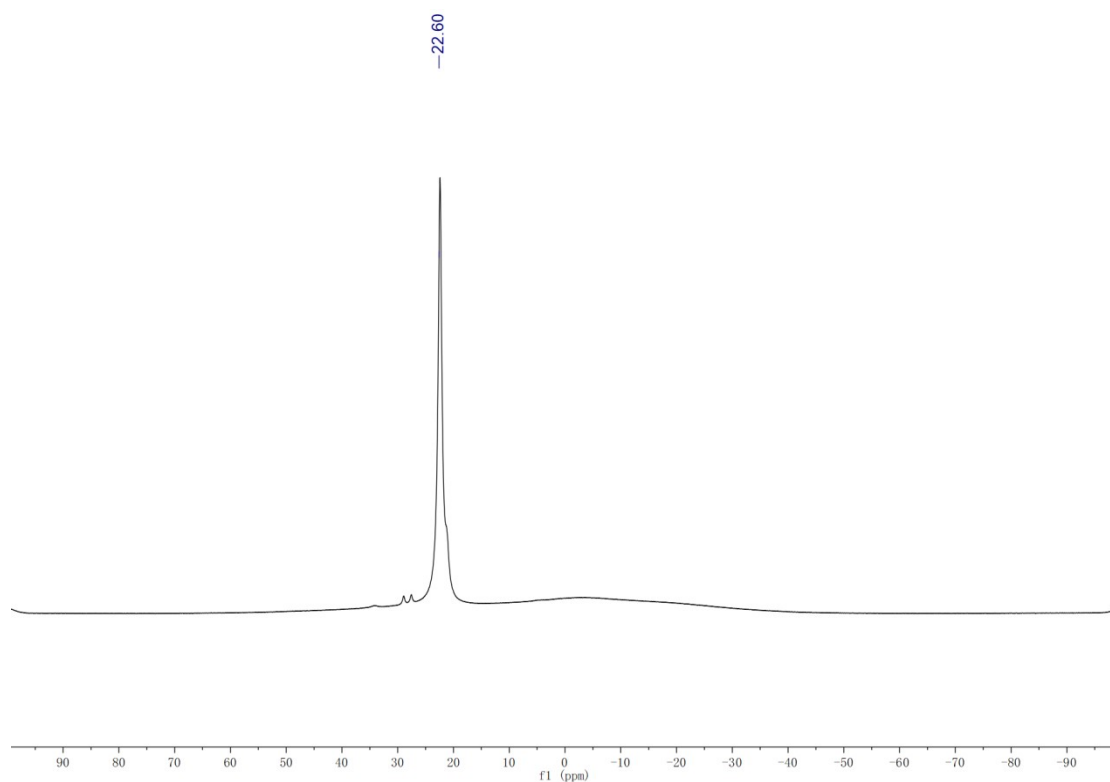


Figure S2.7.3 ^{11}B NMR spectrum of compound **6g** in CDCl_3

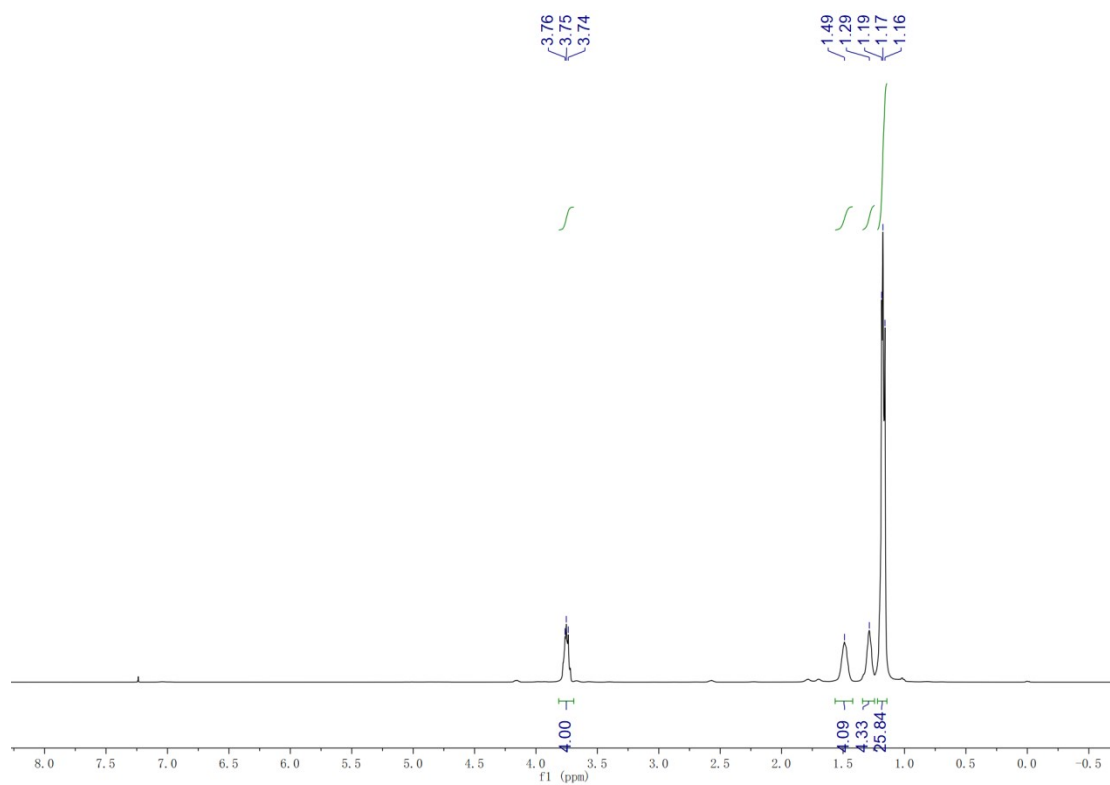


Figure S2.8.1 ^1H NMR spectrum of compound **6h** in CDCl_3

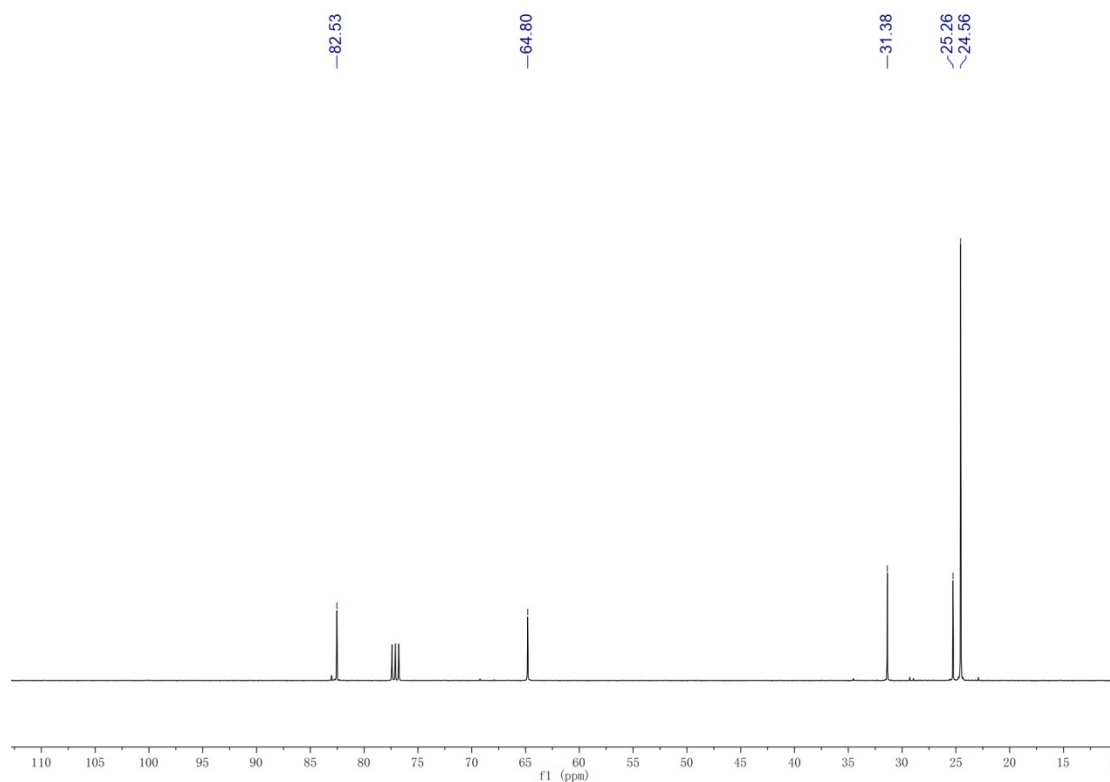


Figure S2.8.2 ^{13}C NMR spectrum of compound **6h** in CDCl_3

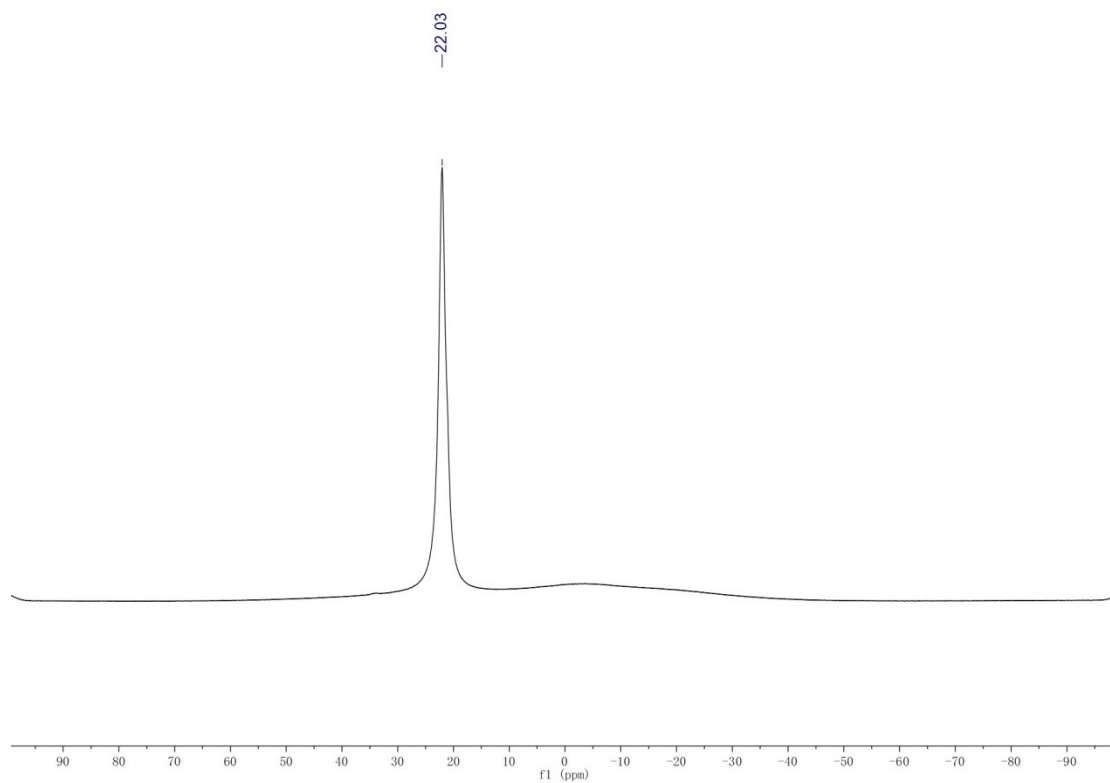


Figure S2.8.3 ^{11}B NMR spectrum of compound **6h** in CDCl_3

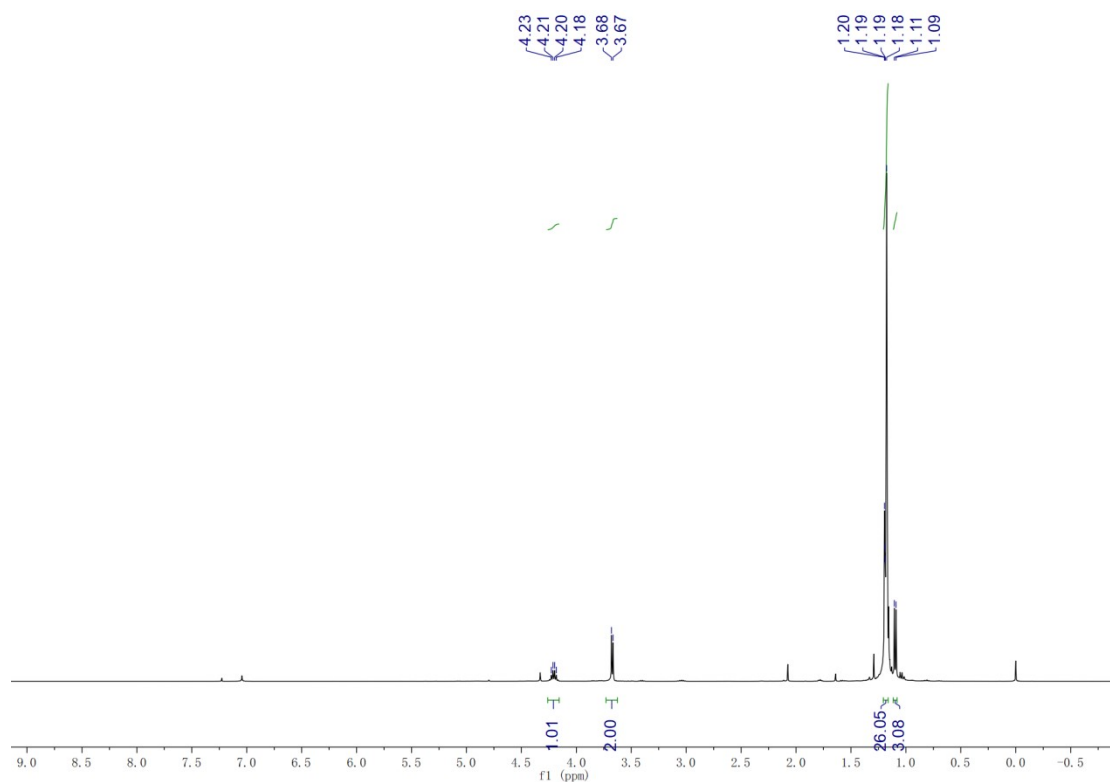


Figure S2.9.1 ^1H NMR spectrum of compound **6i** in CDCl_3

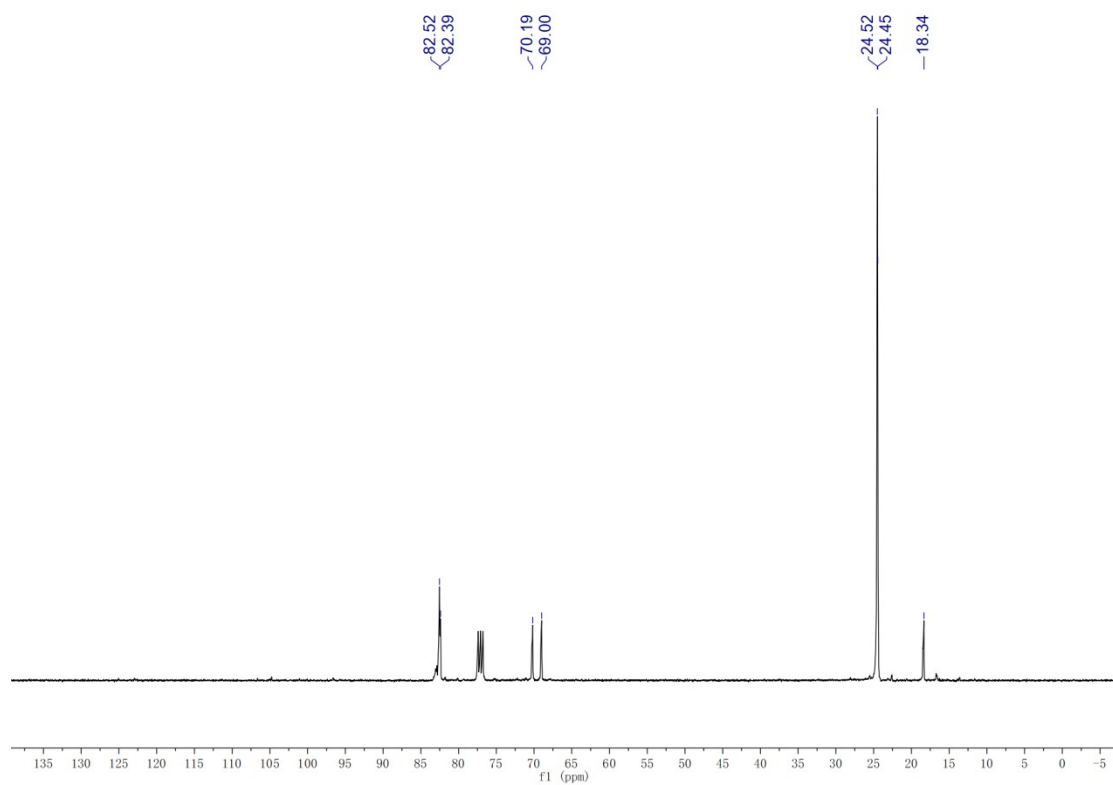


Figure S2.9.2 ¹³C NMR spectrum of compound **6i** in CDCl₃

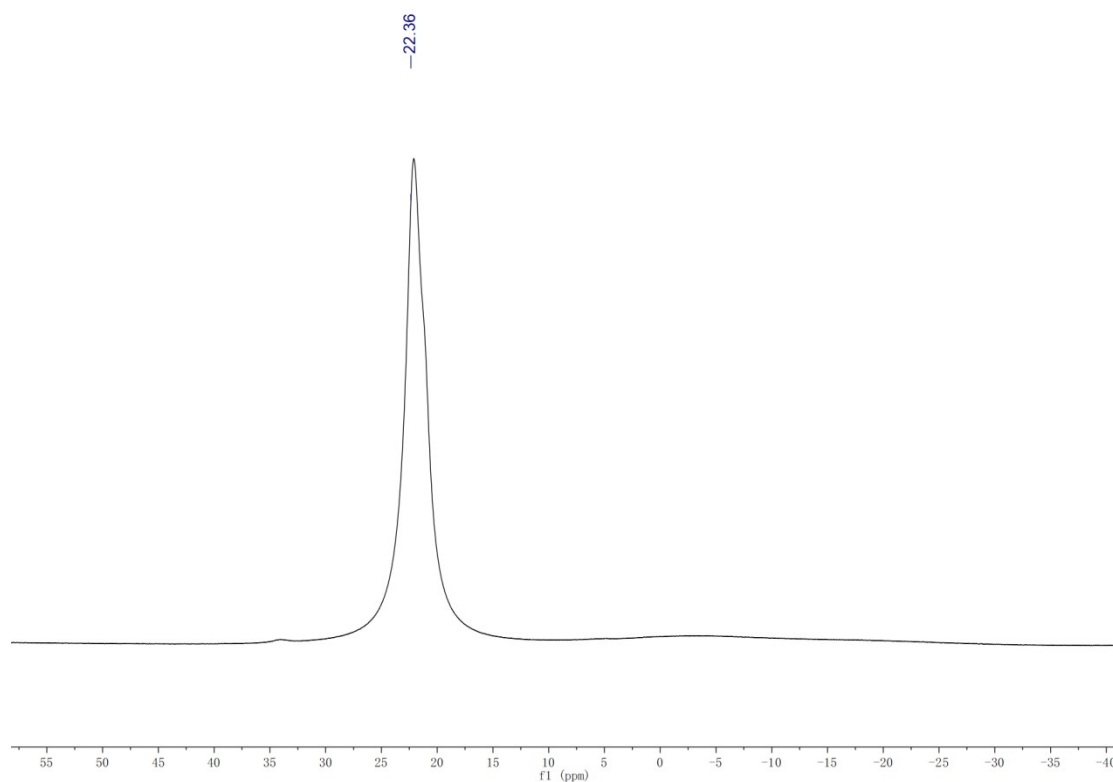


Figure S2.9.3 ¹¹B NMR spectrum of compound **6i** in CDCl₃

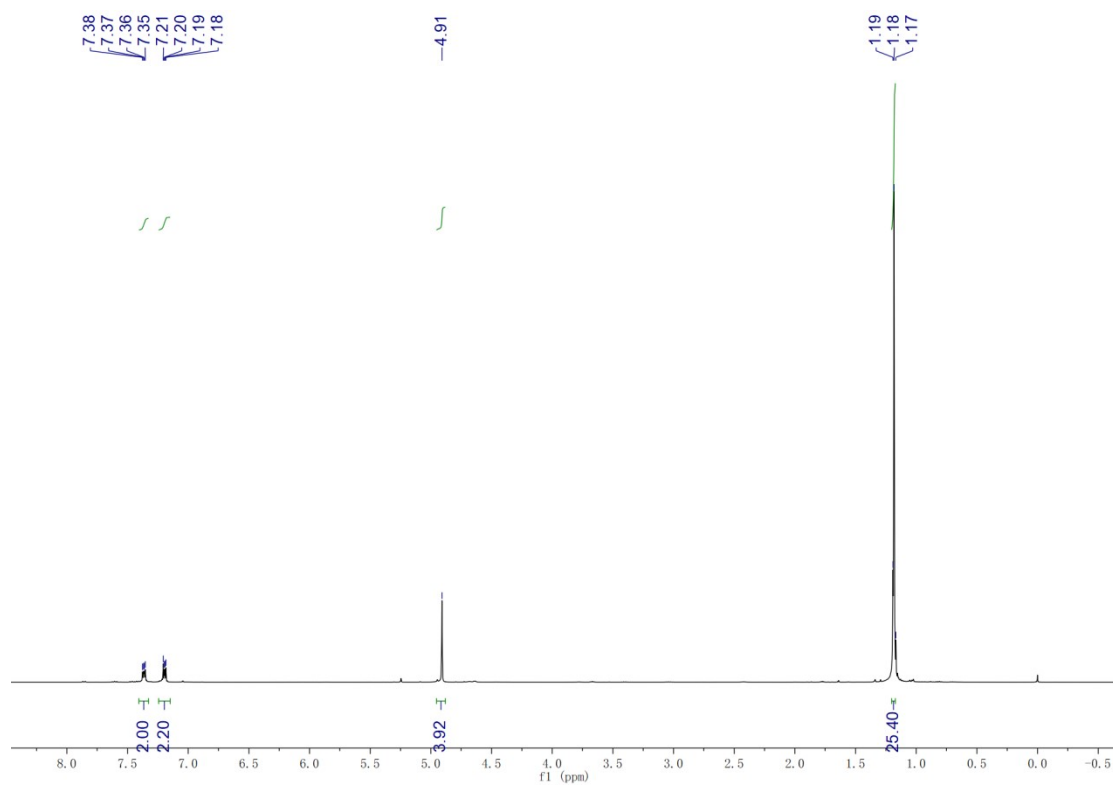


Figure S2.10.1 ^1H NMR spectrum of compound **6j** in CDCl_3

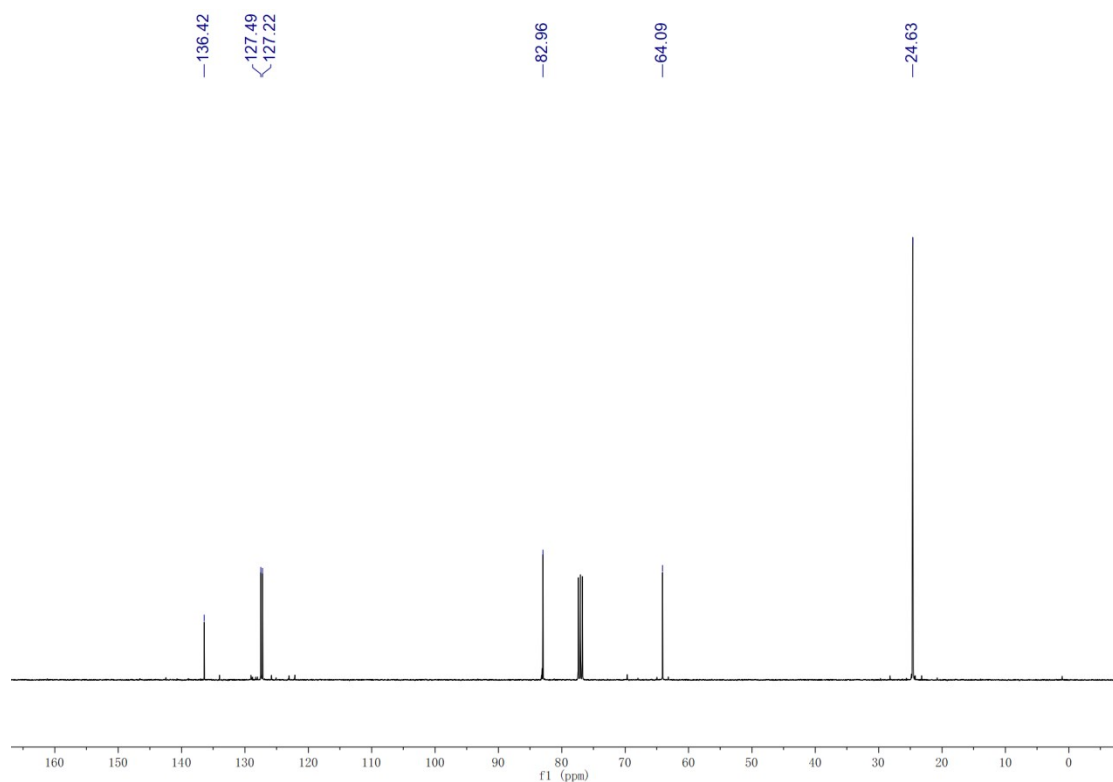


Figure S2.10.2 ^{13}C NMR spectrum of compound **6j** in CDCl_3

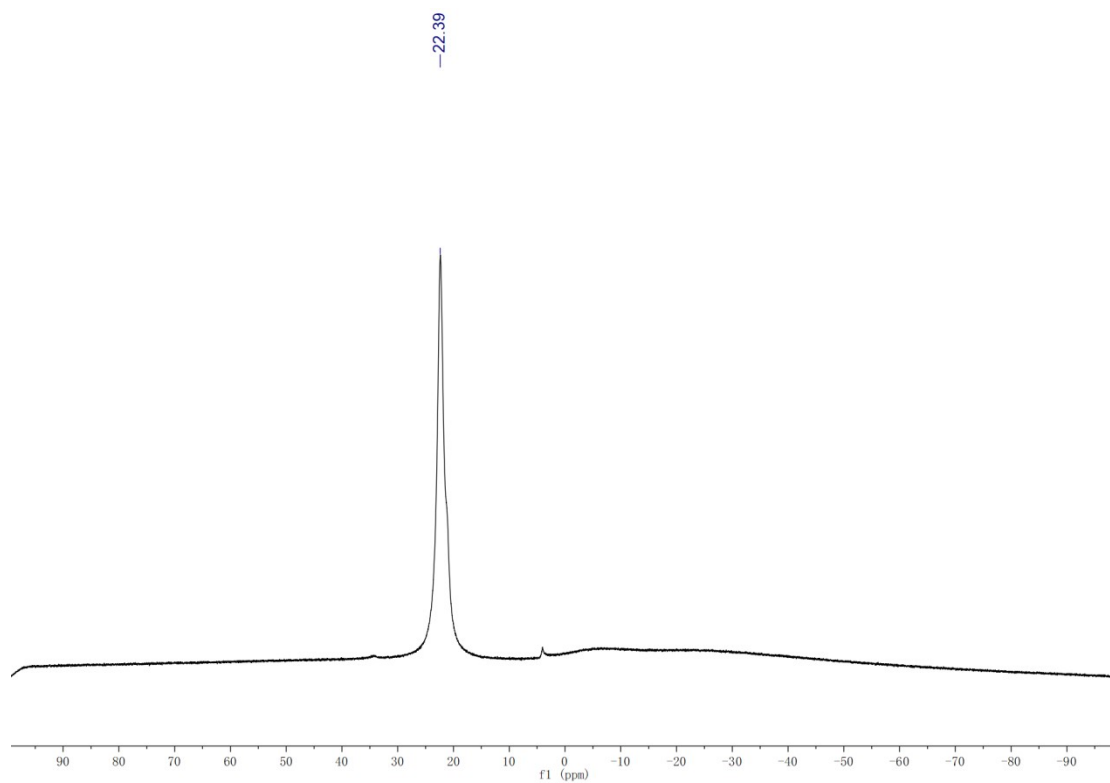


Figure S2.10.3 ^{11}B NMR spectrum of compound **6j** in CDCl_3

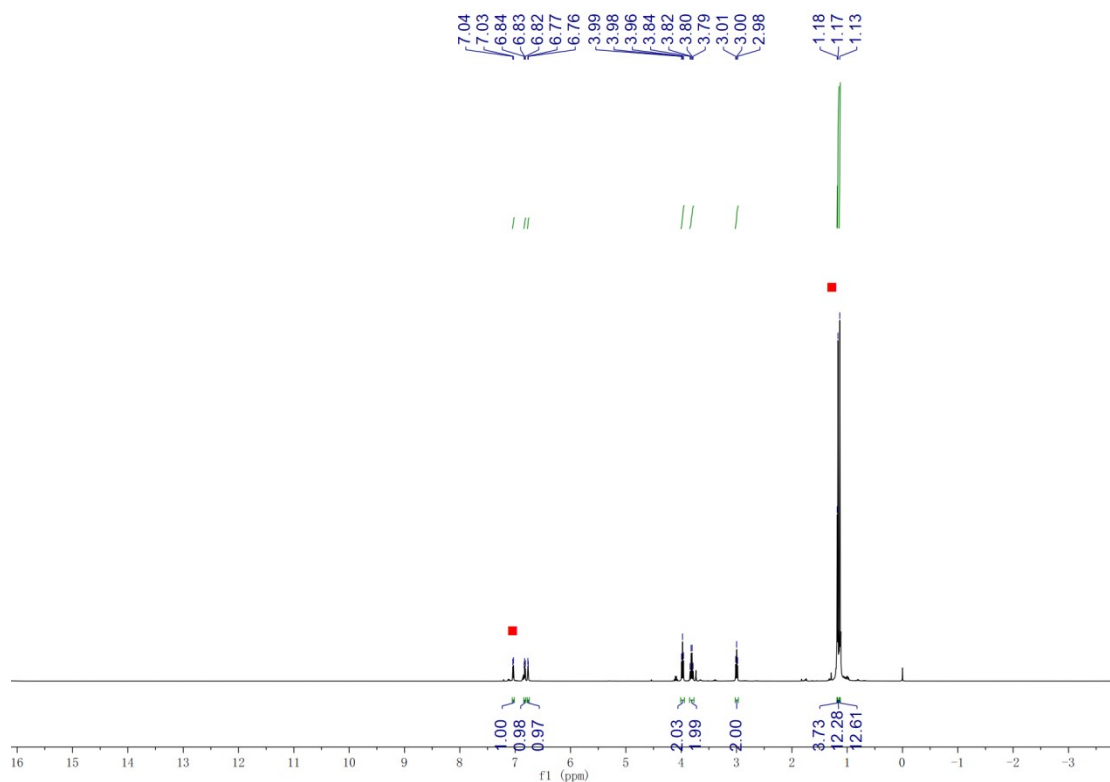


Figure S2.11.1 ^1H NMR spectrum of compound **6k** in CDCl_3

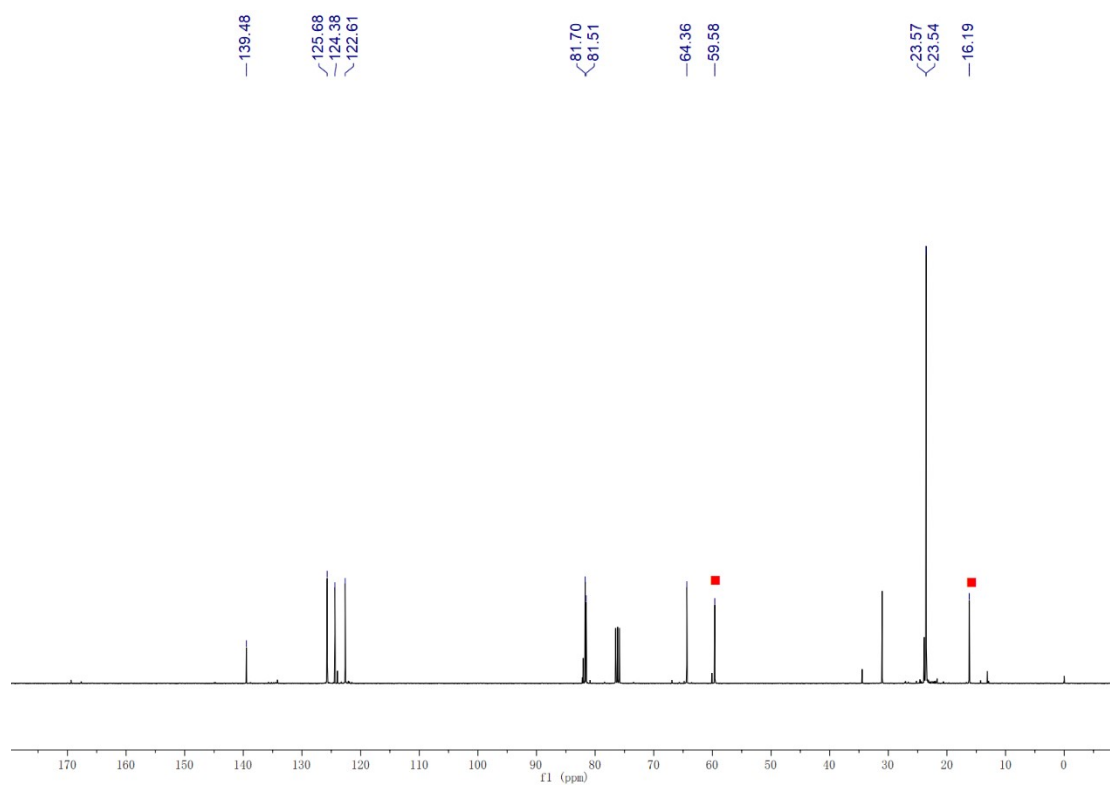


Figure S2.11.2 ^{13}C NMR spectrum of compound **6k** in CDCl_3

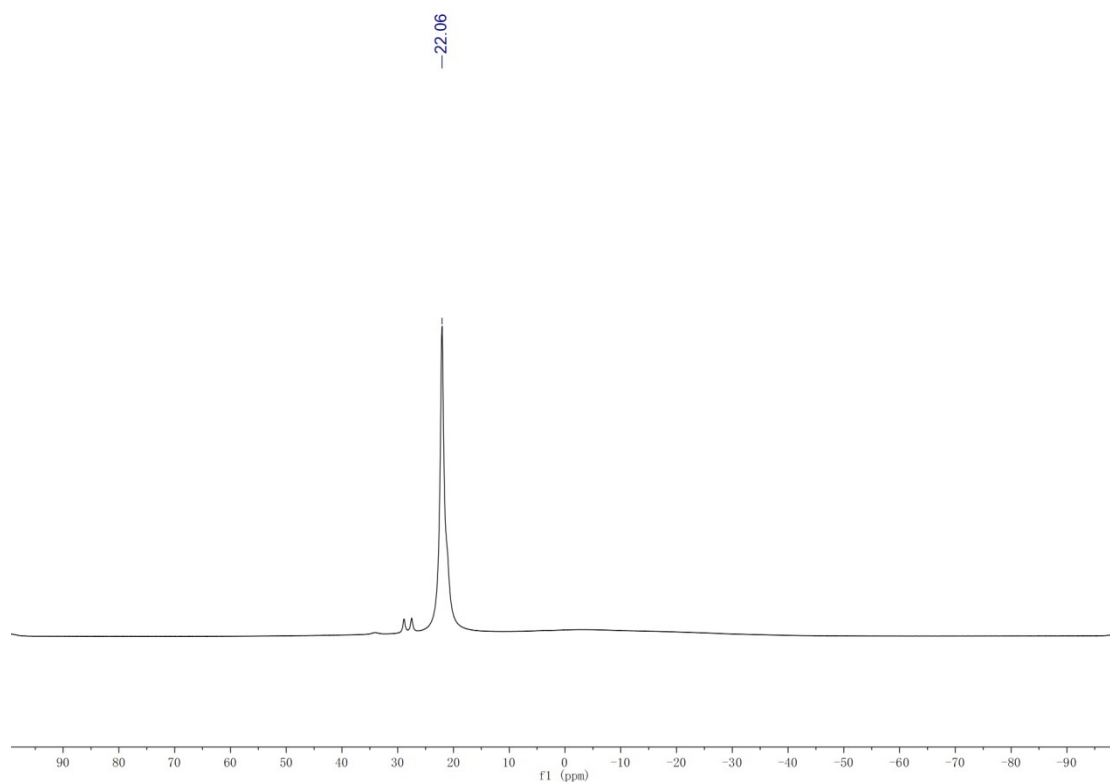


Figure S2.11.3 ^{11}B NMR spectrum of compound **6k** in CDCl_3

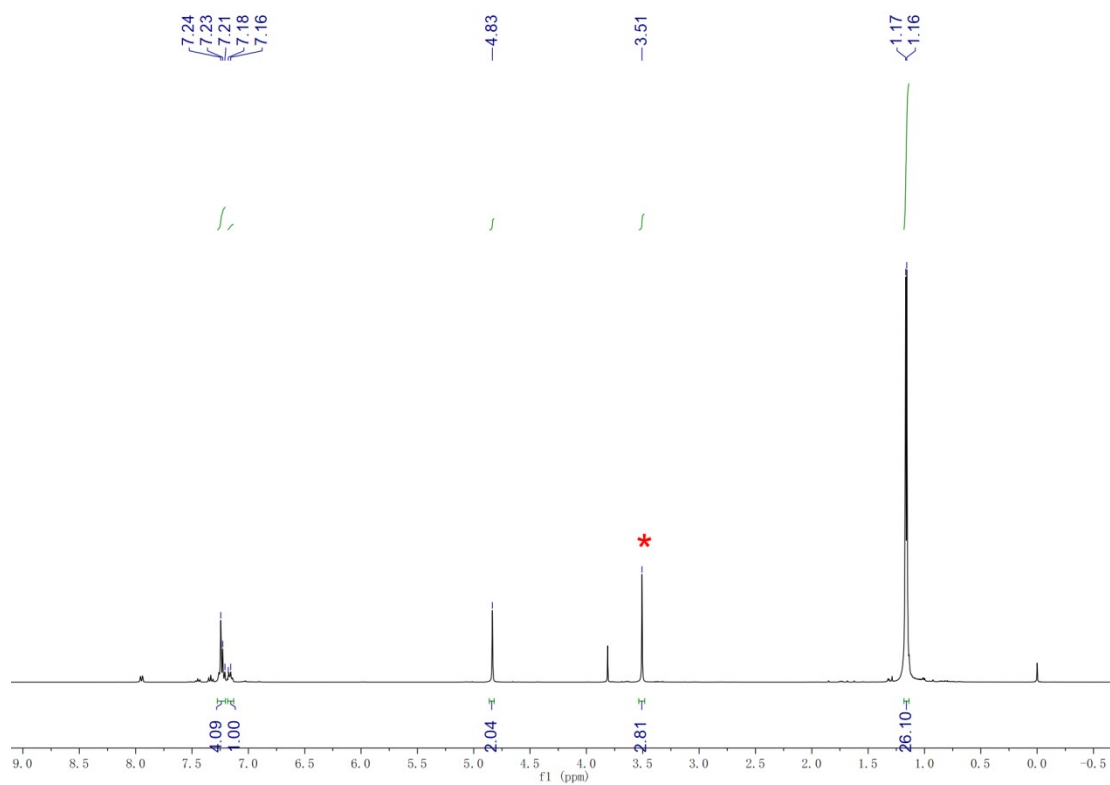


Figure S2.12.1 ^1H NMR spectrum of compound **6I** in CDCl_3

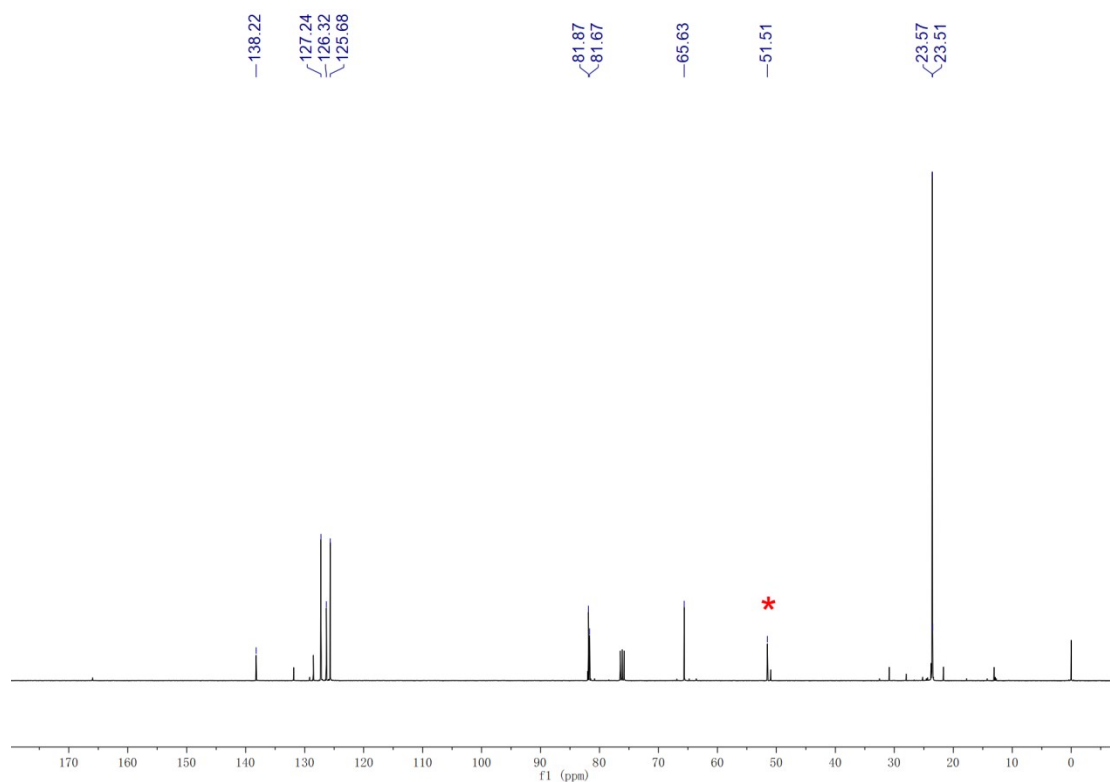


Figure S2.12.2 ^{13}C NMR spectrum of compound **6I** in CDCl_3

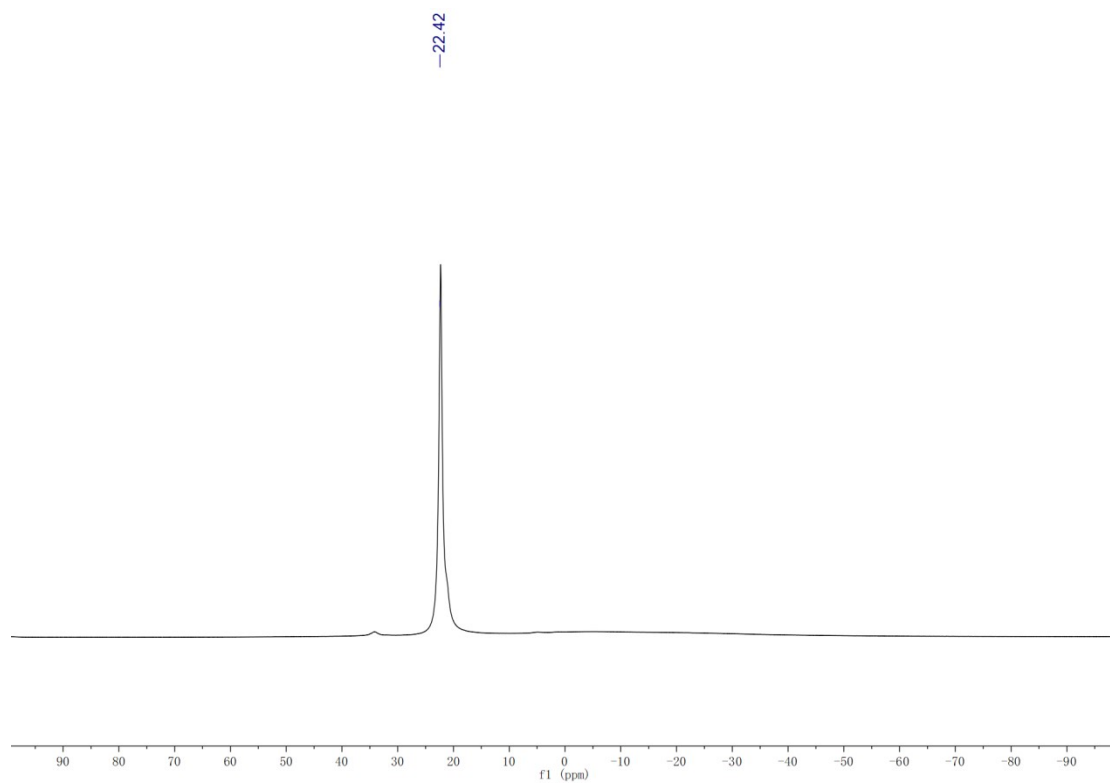


Figure S2.12.3 ^{11}B NMR spectrum of compound **6l** in CDCl_3

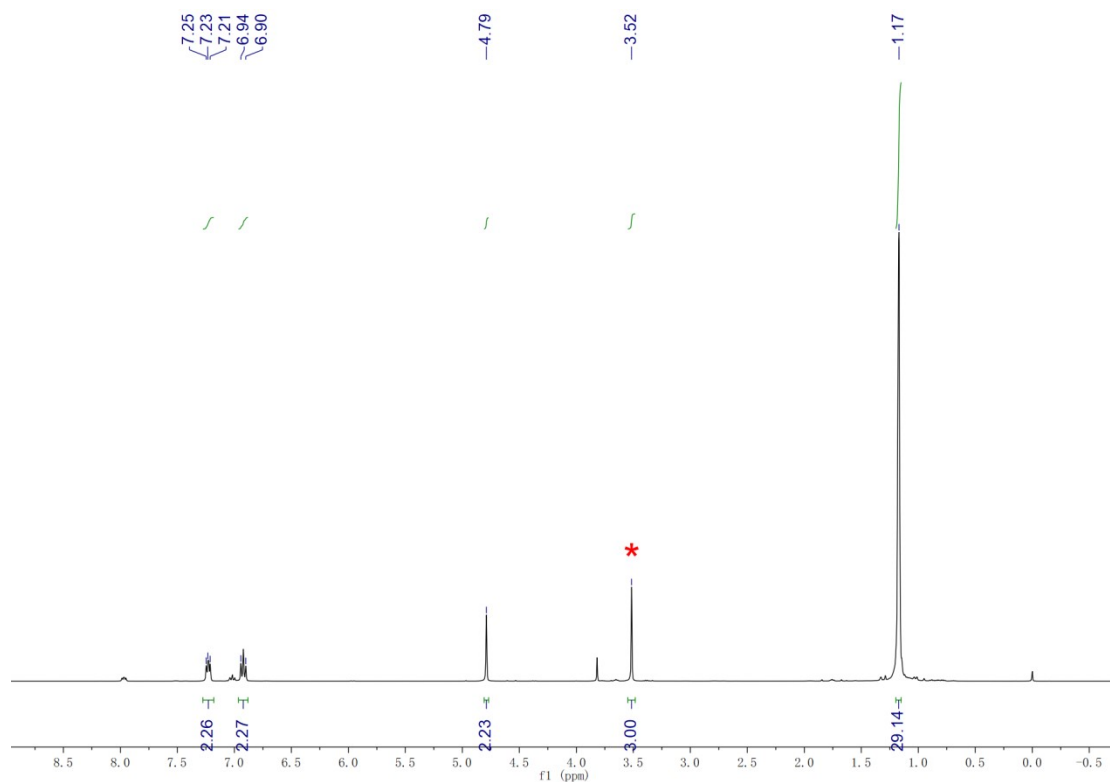


Figure S2.13.1 ^1H NMR spectrum of compound **6m** in CDCl_3

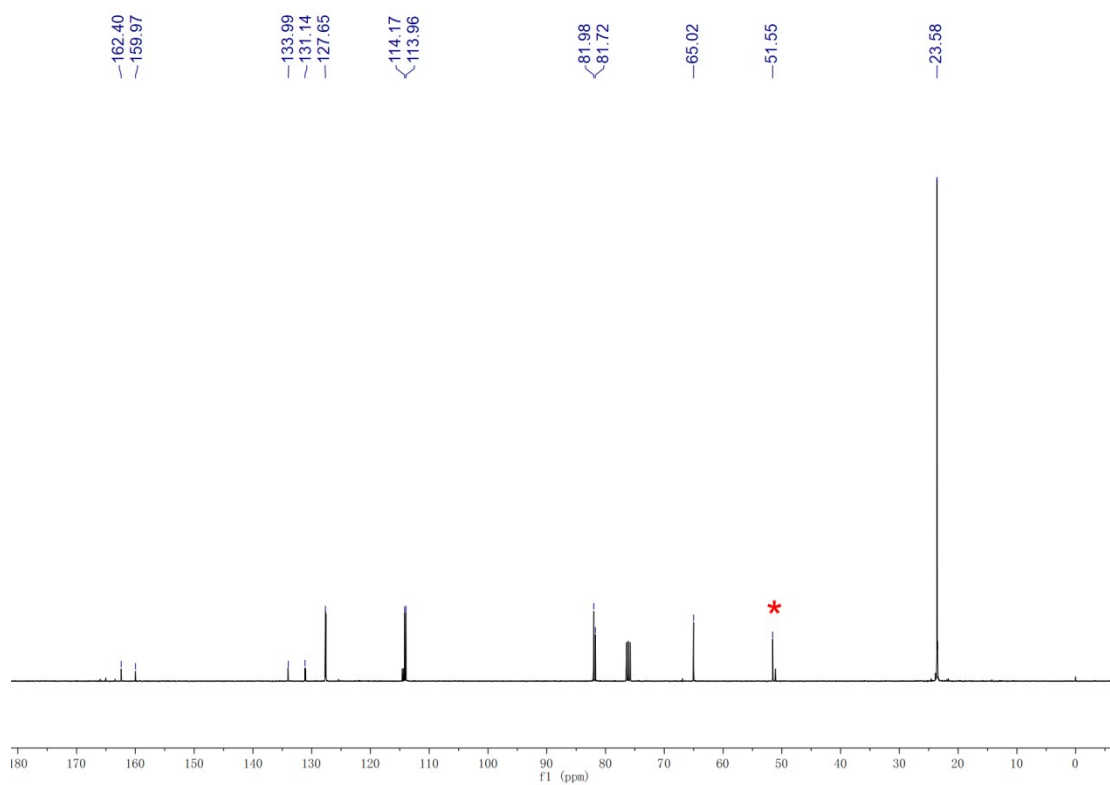


Figure S2.13.2 ^{13}C NMR spectrum of compound **6m** in CDCl_3

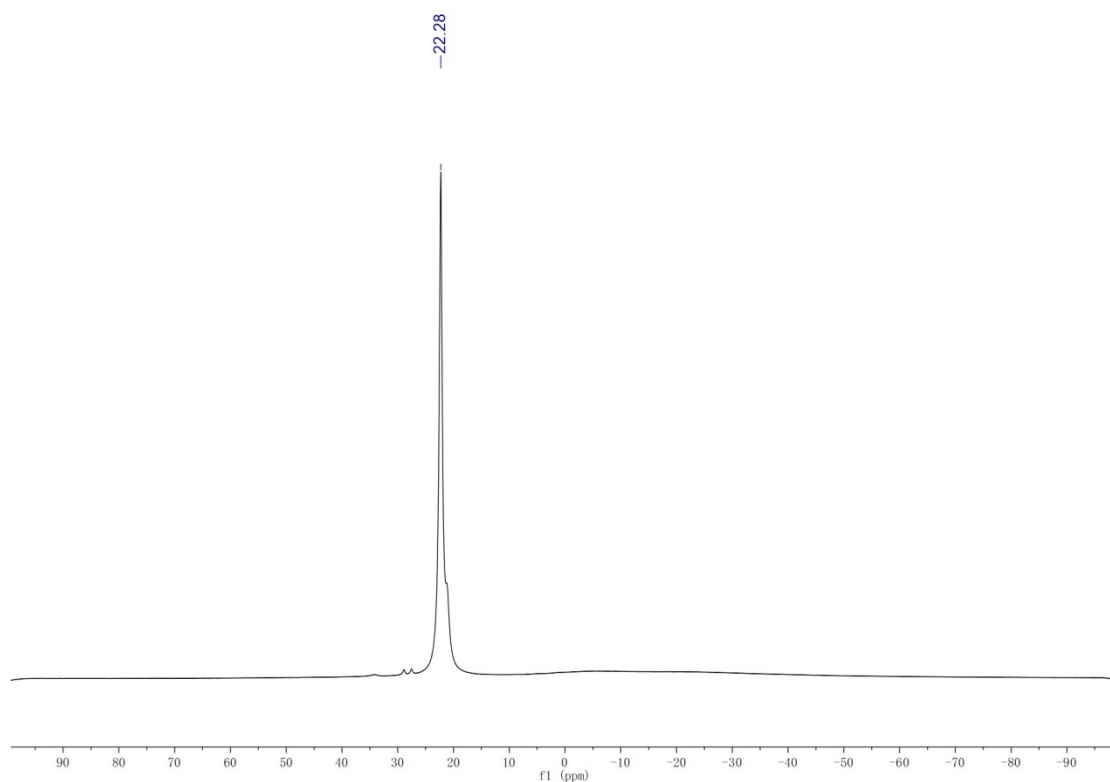


Figure S2.13.3 ^{11}B NMR spectrum of compound **6m** in CDCl_3

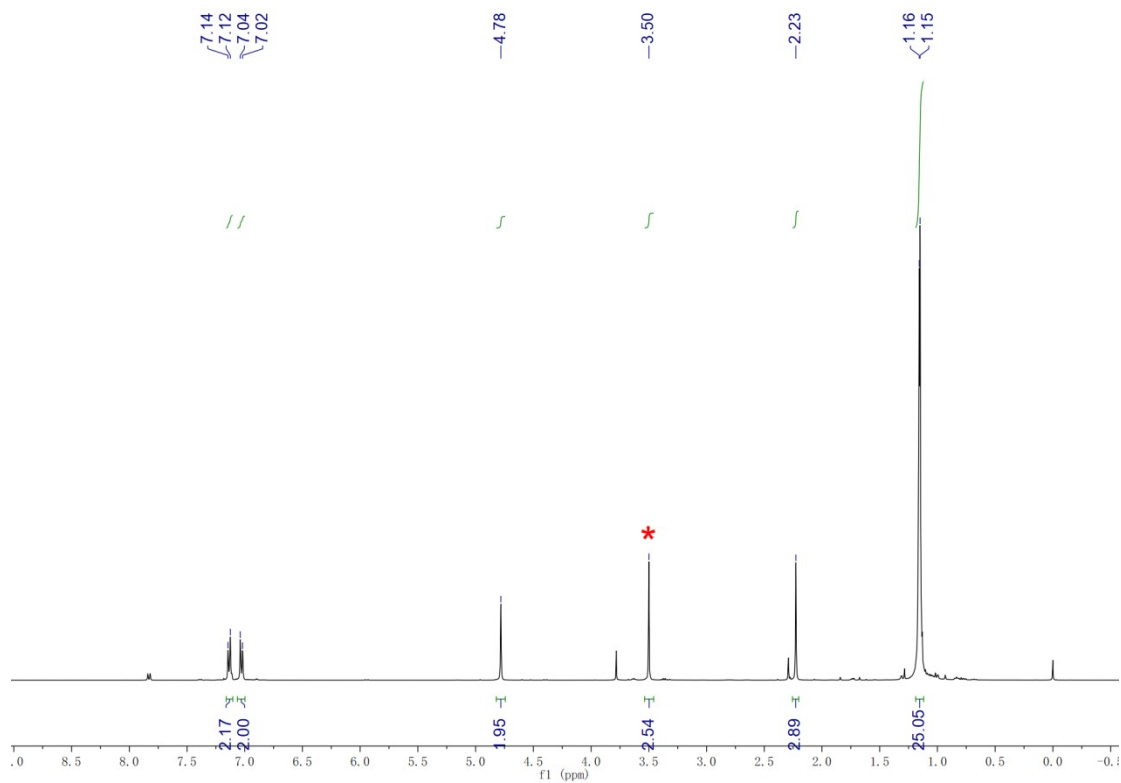


Figure S2.14.1 ^1H NMR spectrum of compound **6n** in CDCl_3

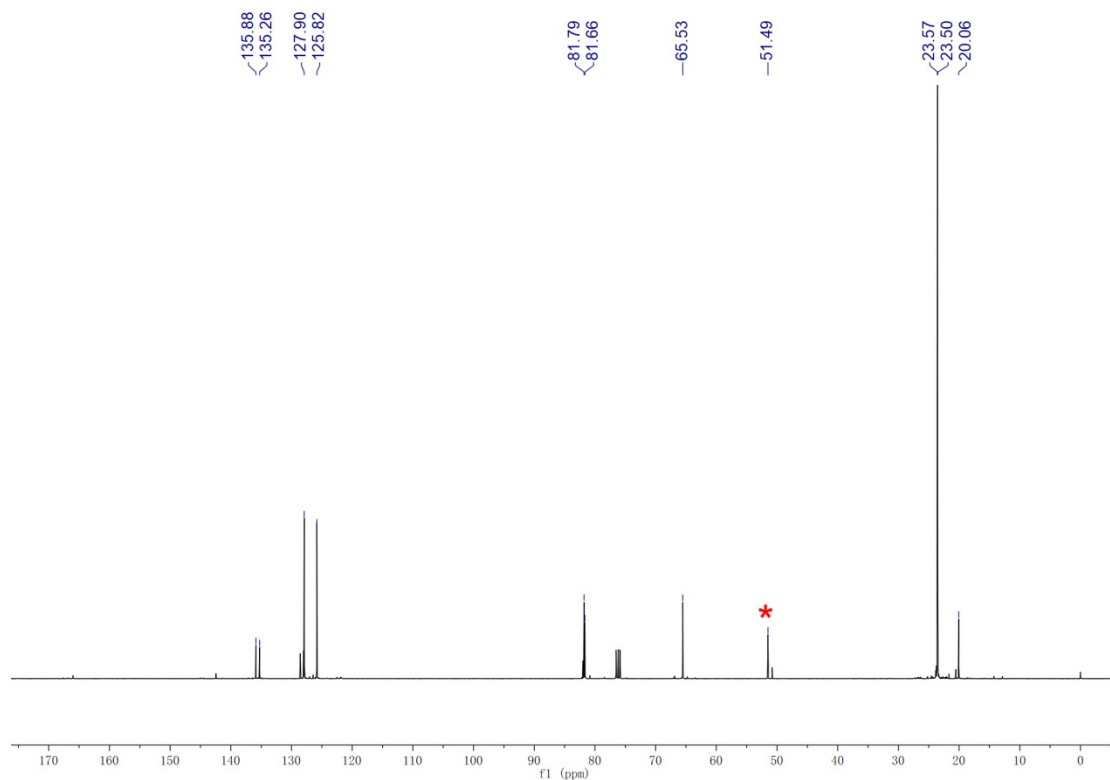


Figure S2.14.2 ^{13}C NMR spectrum of compound **6n** in CDCl_3



Figure S2.14.3 ^{11}B NMR spectrum of compound **6n** in CDCl_3

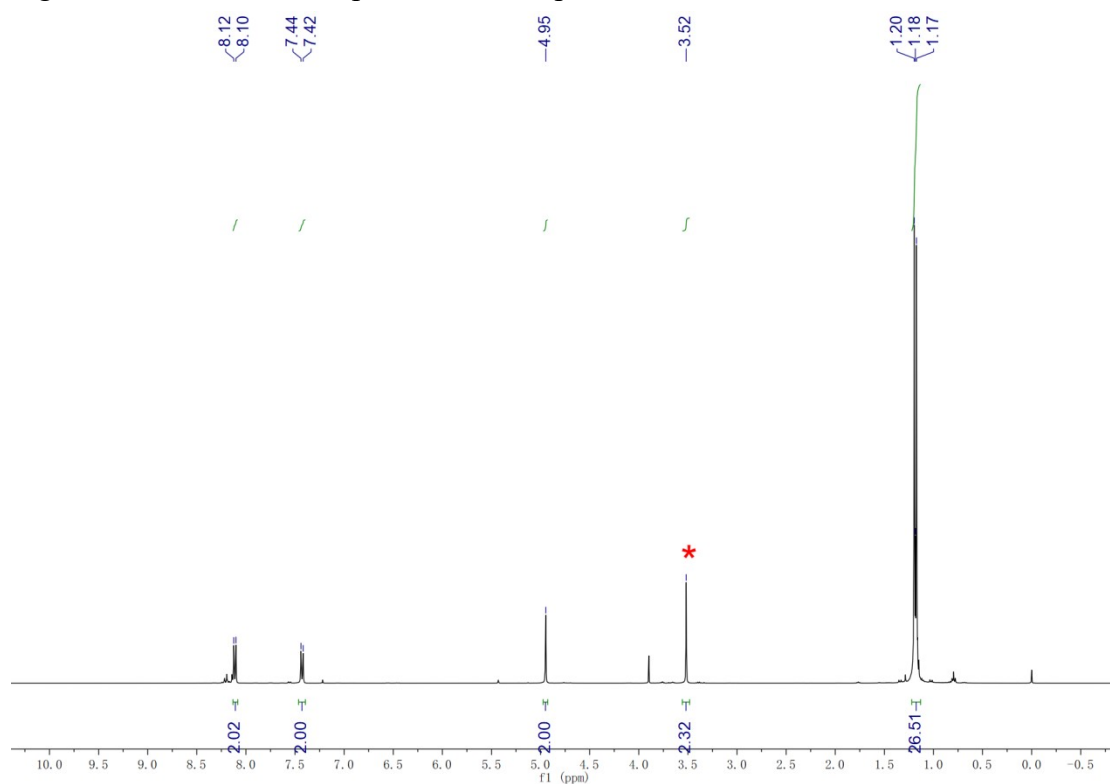


Figure S2.15.1 ^1H NMR spectrum of compound **6o** in CDCl_3

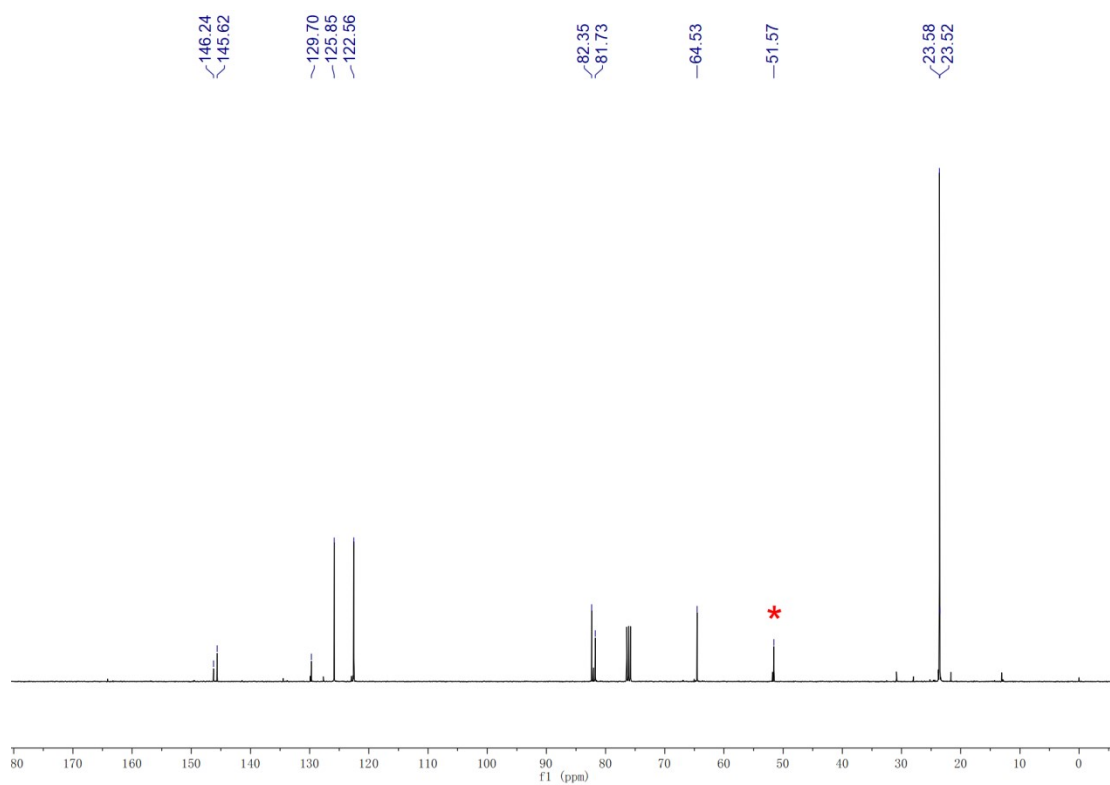


Figure S2.15.2 ^{13}C NMR spectrum of compound **60** in CDCl_3

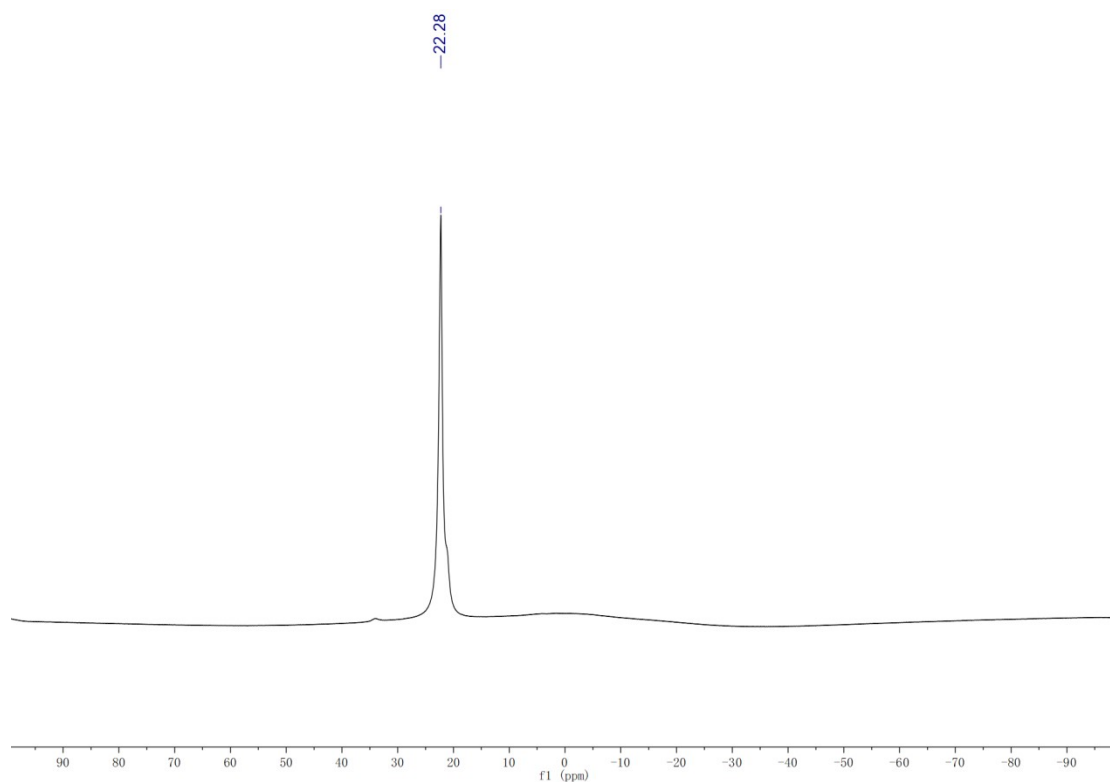


Figure S2.15.3 ^{11}B NMR spectrum of compound **60** in CDCl_3

^1H , ^{13}C and ^{11}B NMR Spectra of Hydroboration Products of Carboxylic Acids.

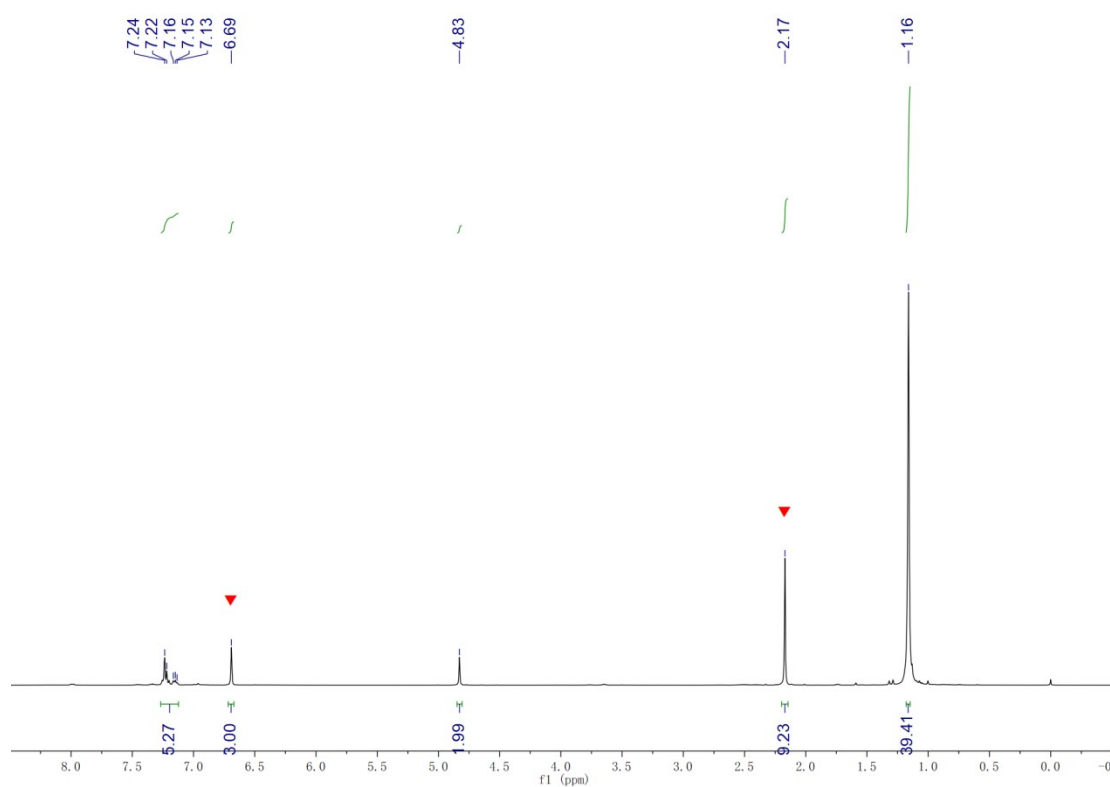


Figure S3.1.1 ^1H NMR spectrum of compound **8a** in CDCl_3

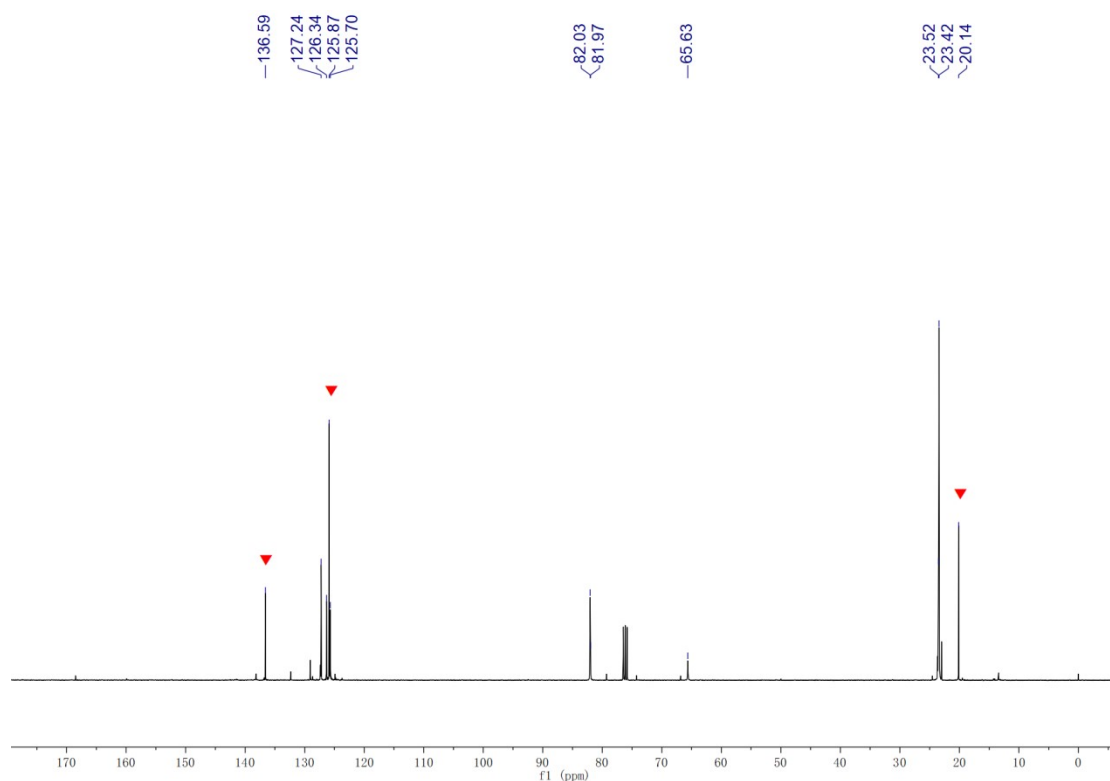


Figure S3.1.2 ^{13}C NMR spectrum of compound **8a** in CDCl_3

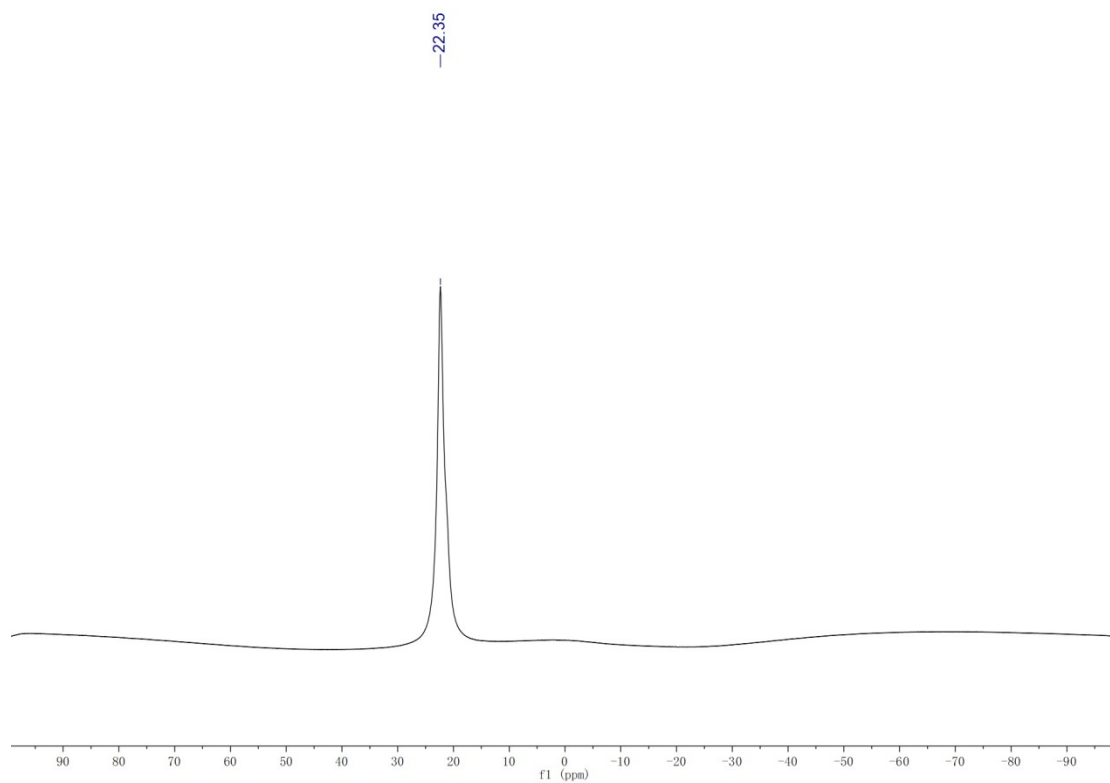


Figure S3.1.3 ^{11}B NMR spectrum of compound **8a** in CDCl_3

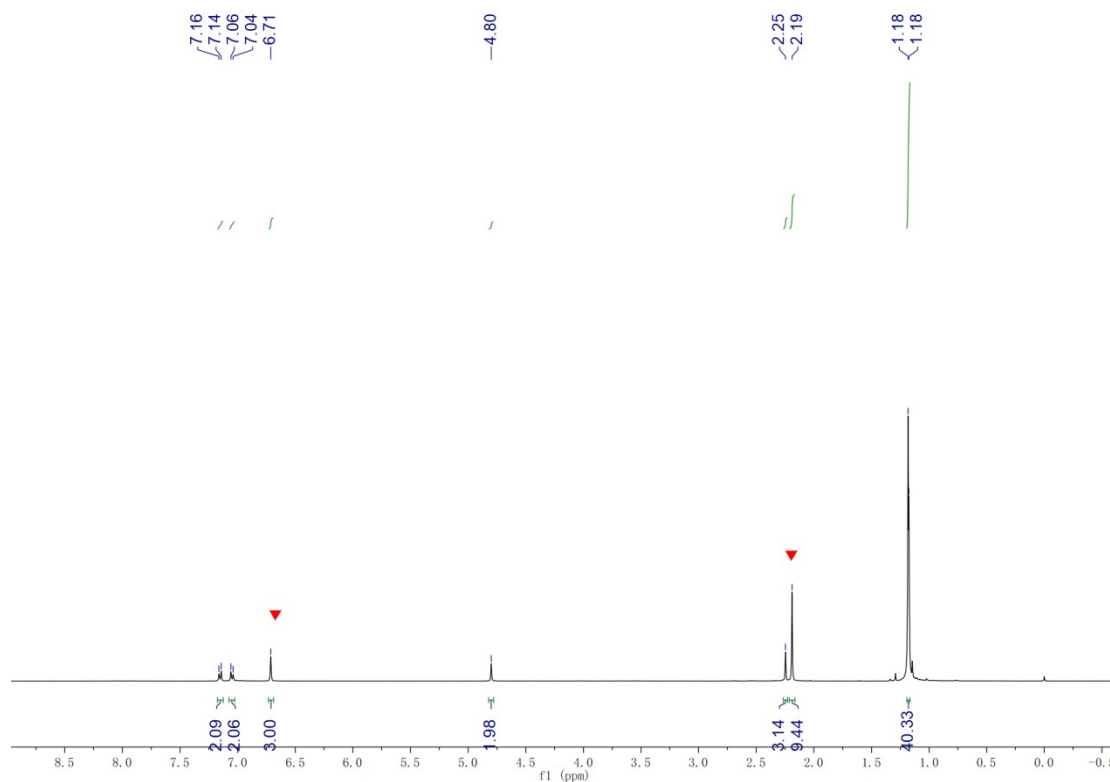


Figure S3.2.1 ^1H NMR spectrum of compound **8b** in CDCl_3

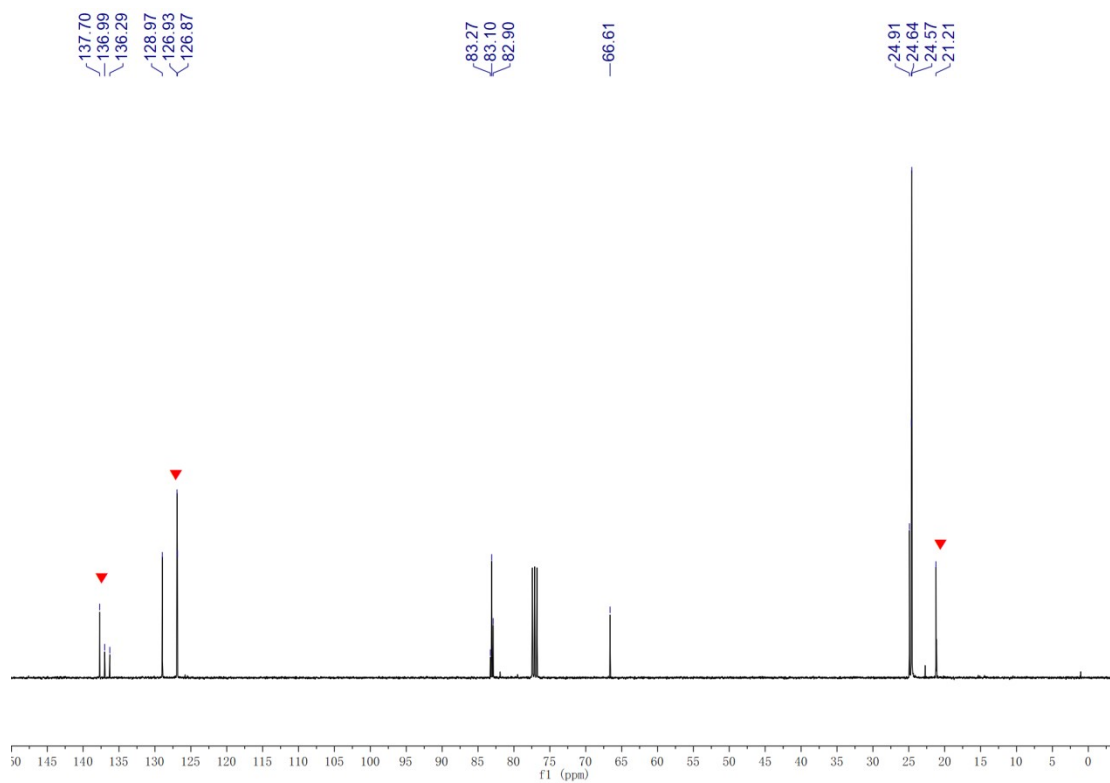


Figure S3.2.2 ^{13}C NMR spectrum of compound **8b** in CDCl_3

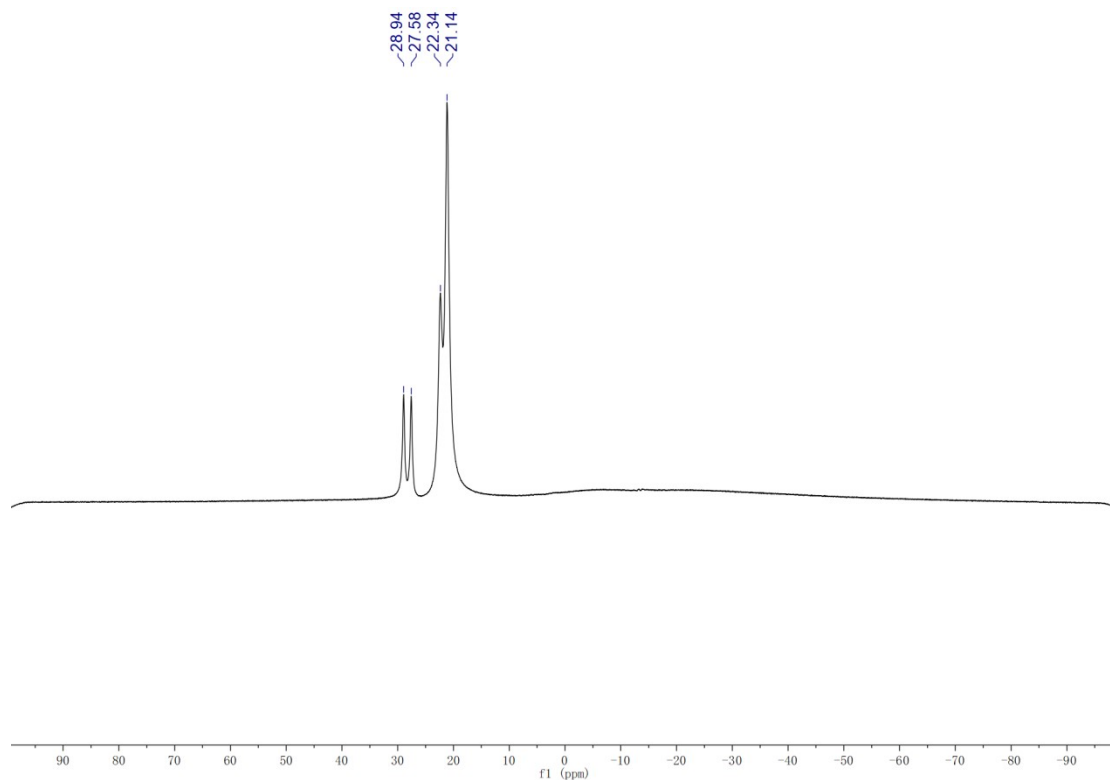


Figure S3.2.3 ^{11}B NMR spectrum of compound **8b** in CDCl_3

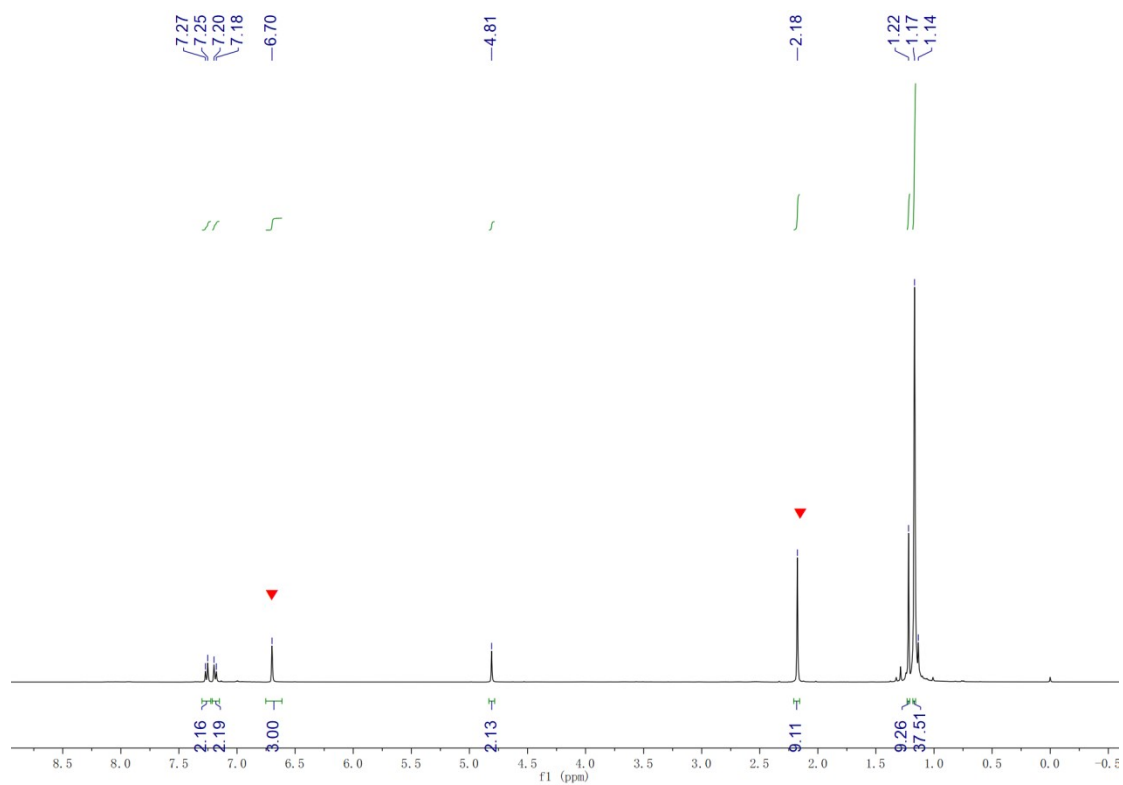


Figure S3.3.1 ^1H NMR spectrum of compound **8c** in CDCl_3

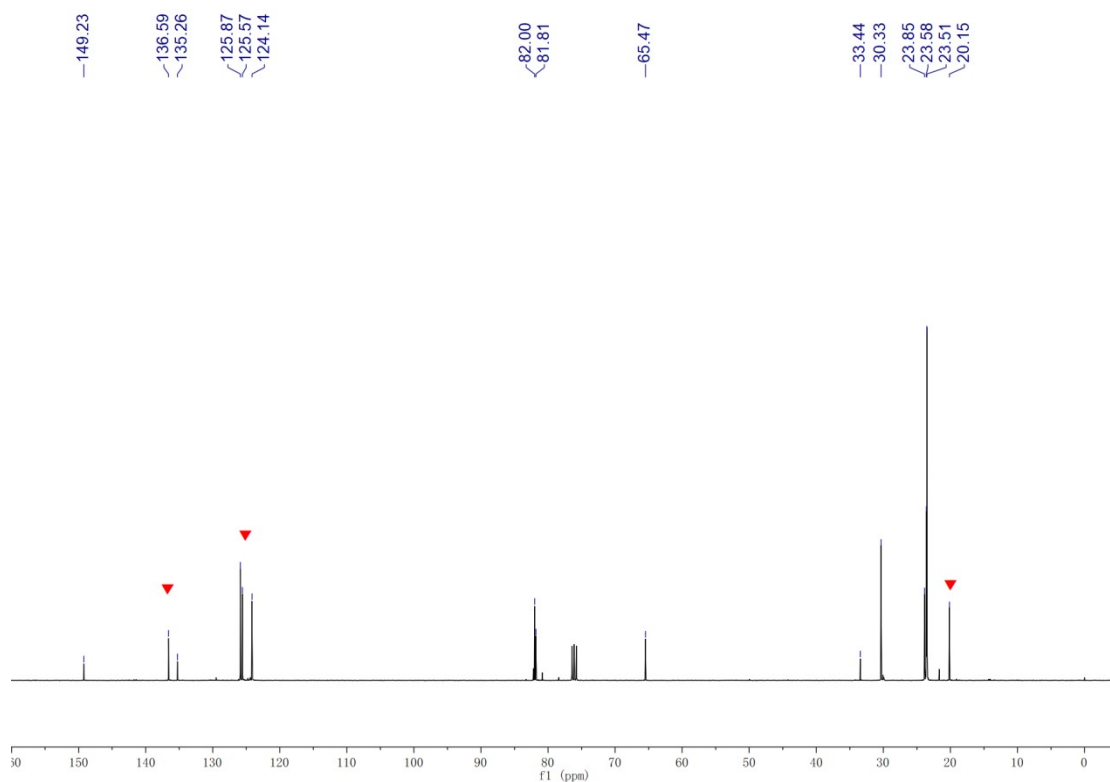


Figure S3.3.2 ^{13}C NMR spectrum of compound **8c** in CDCl_3

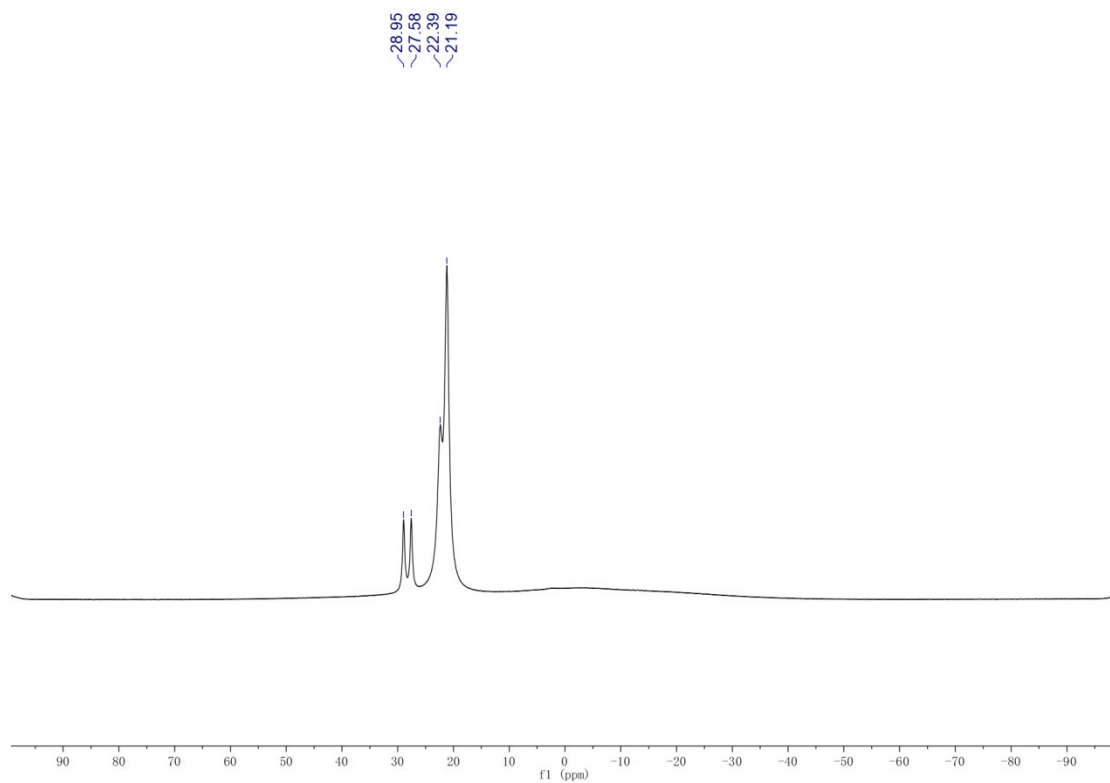


Figure S3.3.3 ^{11}B NMR spectrum of compound **8c** in CDCl_3

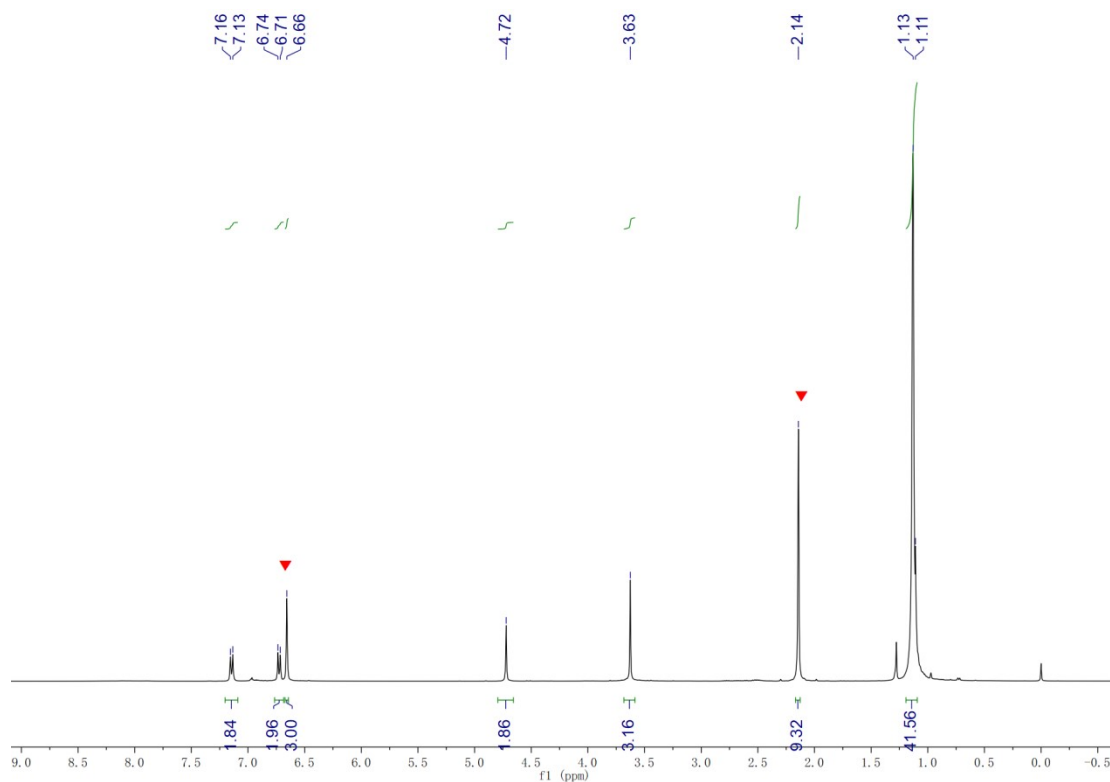


Figure S3.4.1 ^1H NMR spectrum of compound **8d** in CDCl_3

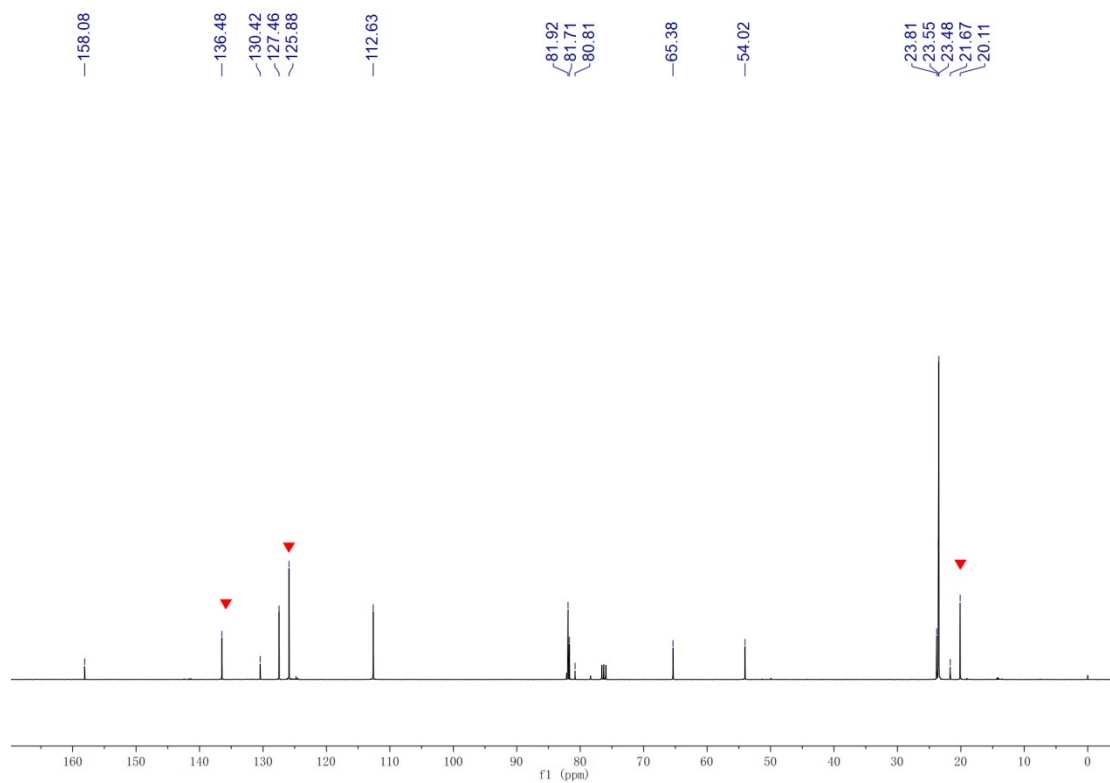


Figure S3.4.2 ^{13}C NMR spectrum of compound **8d** in CDCl_3

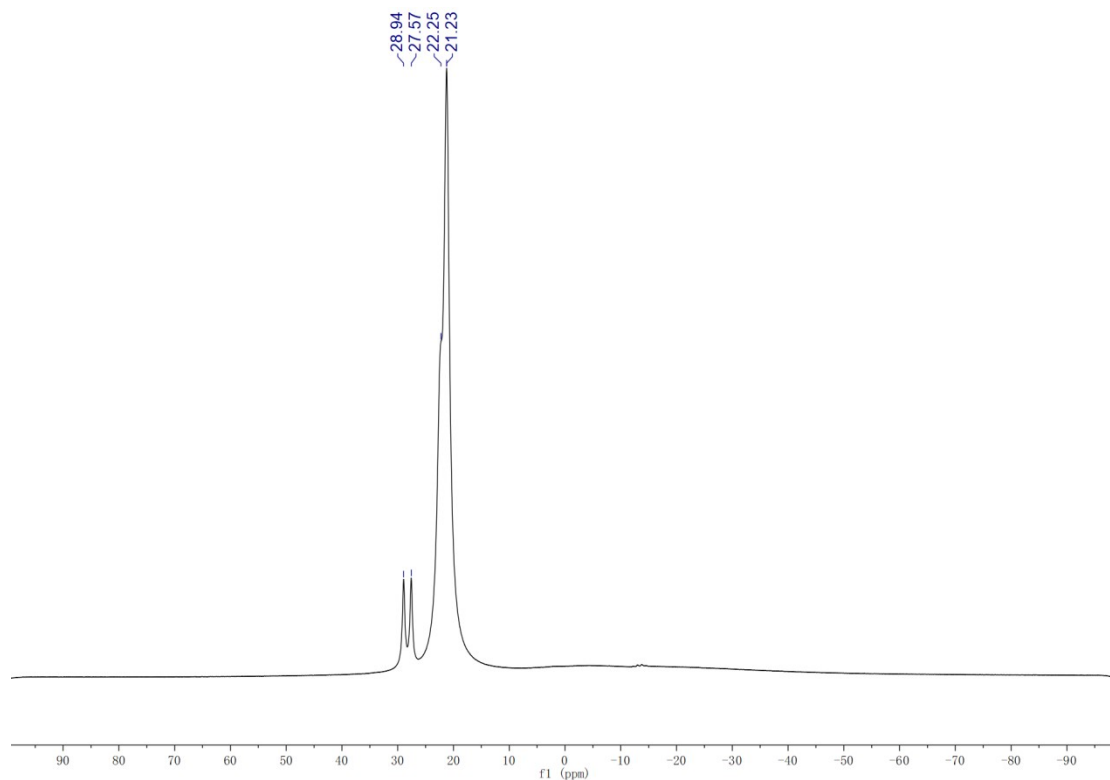


Figure S3.4.3 ^{11}B NMR spectrum of compound **8d** in CDCl_3

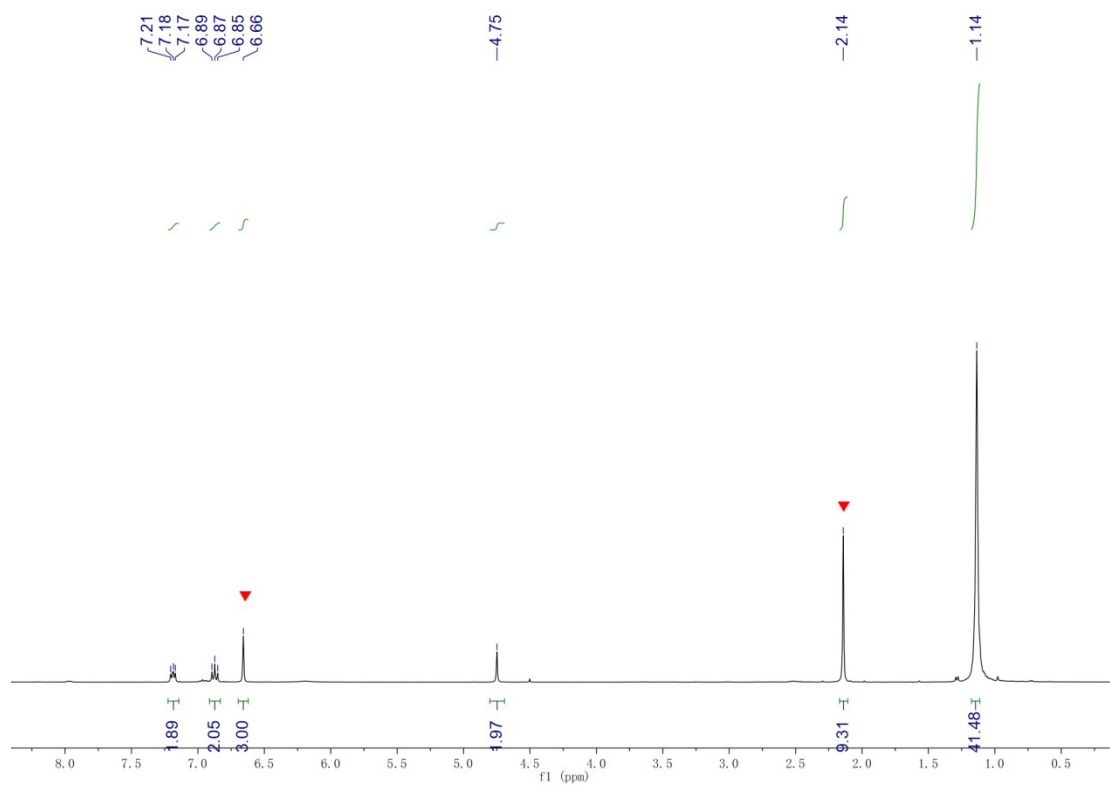


Figure S3.5.1 ^1H NMR spectrum of compound **8e** in CDCl_3

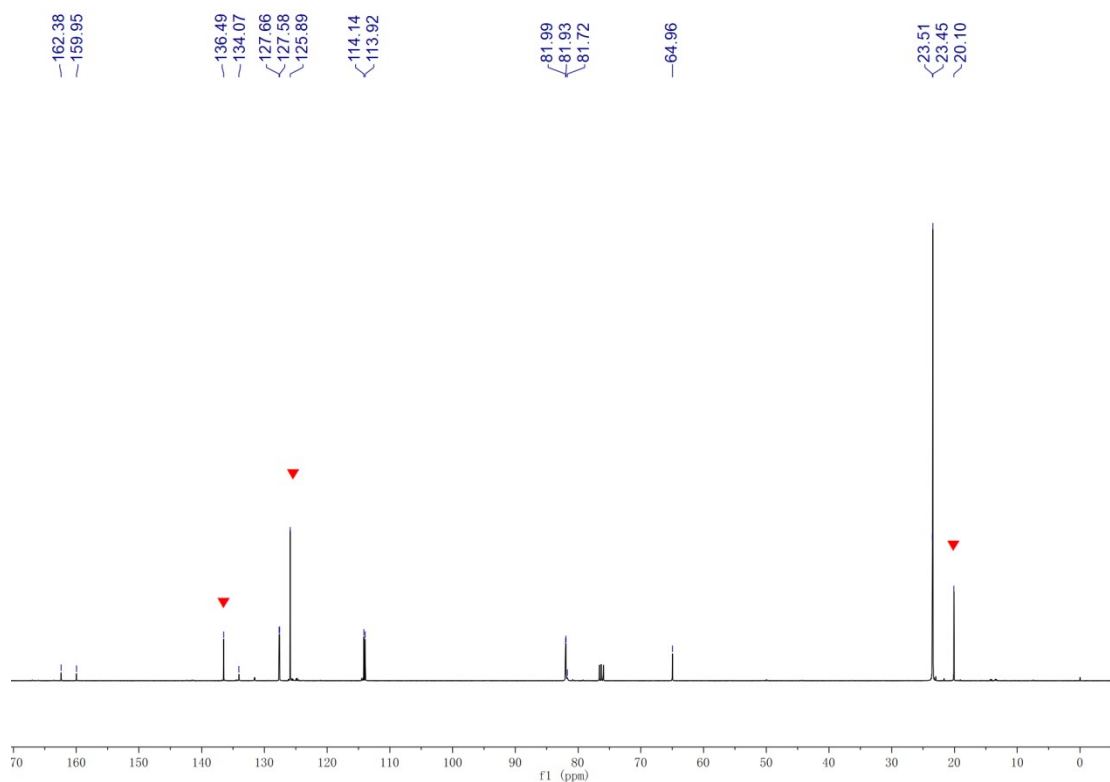


Figure S3.5.2 ^{13}C NMR spectrum of compound **8e** in CDCl_3

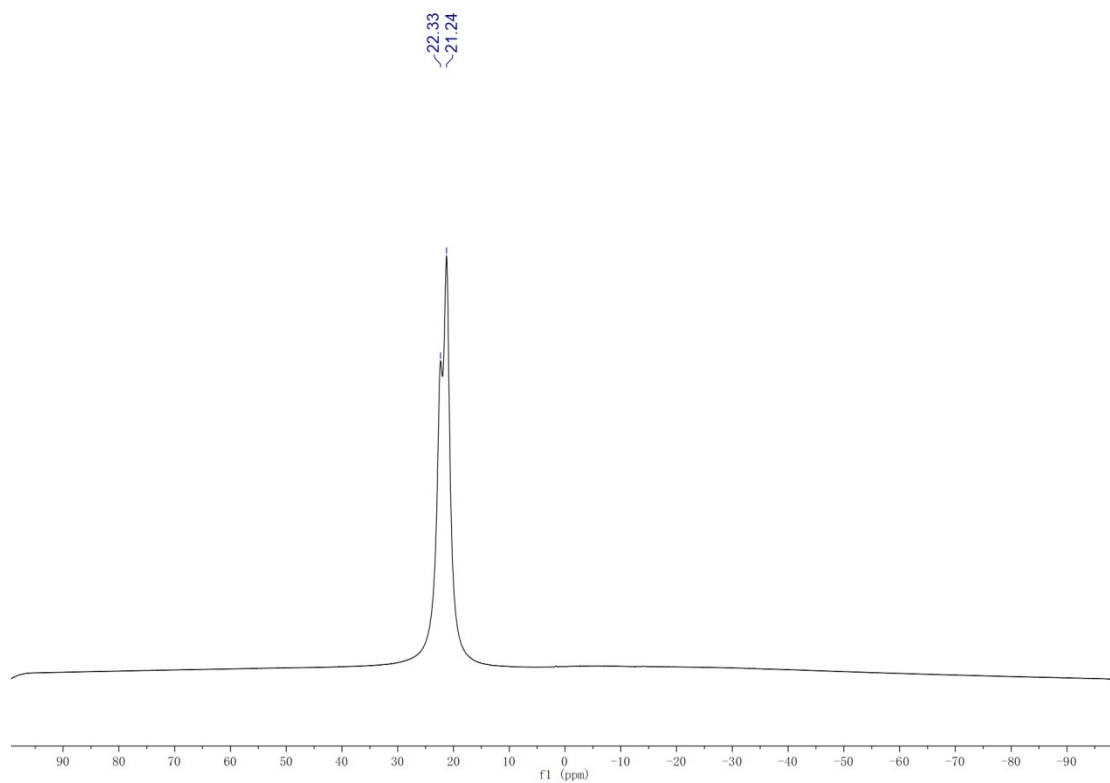


Figure S3.5.3 ^{11}B NMR spectrum of compound **8e** in CDCl_3

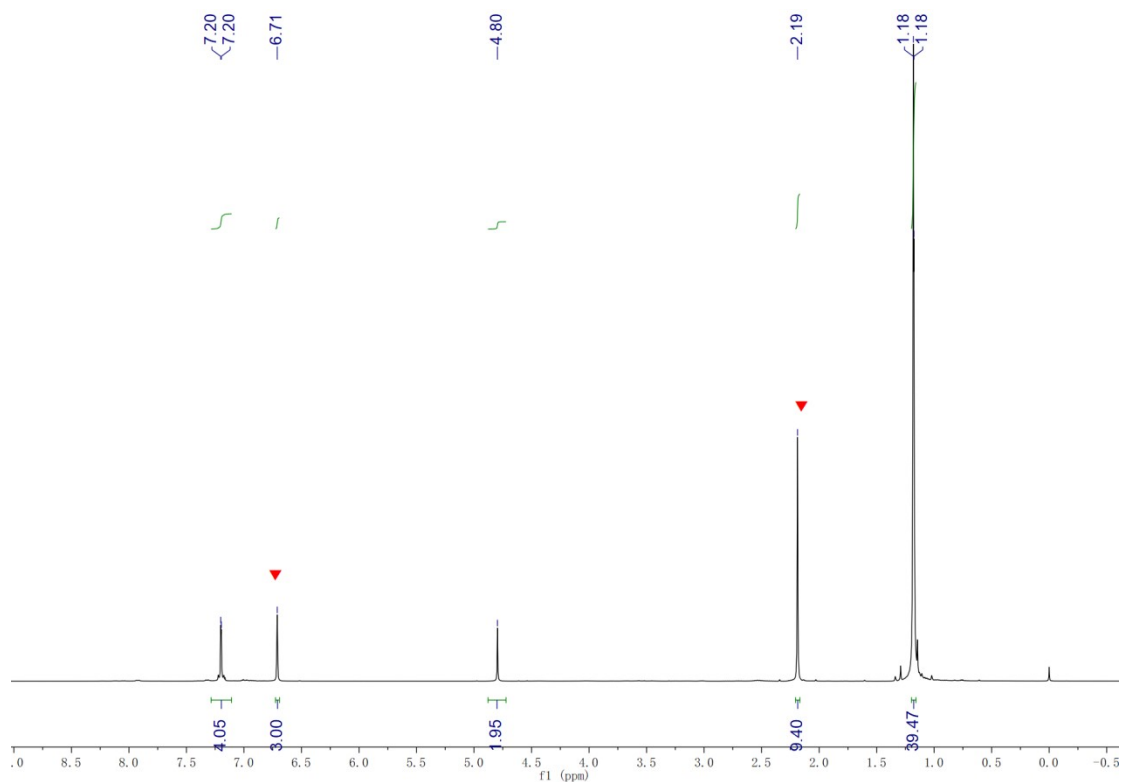


Figure S3.6.1 ^1H NMR spectrum of compound **8f** in CDCl_3

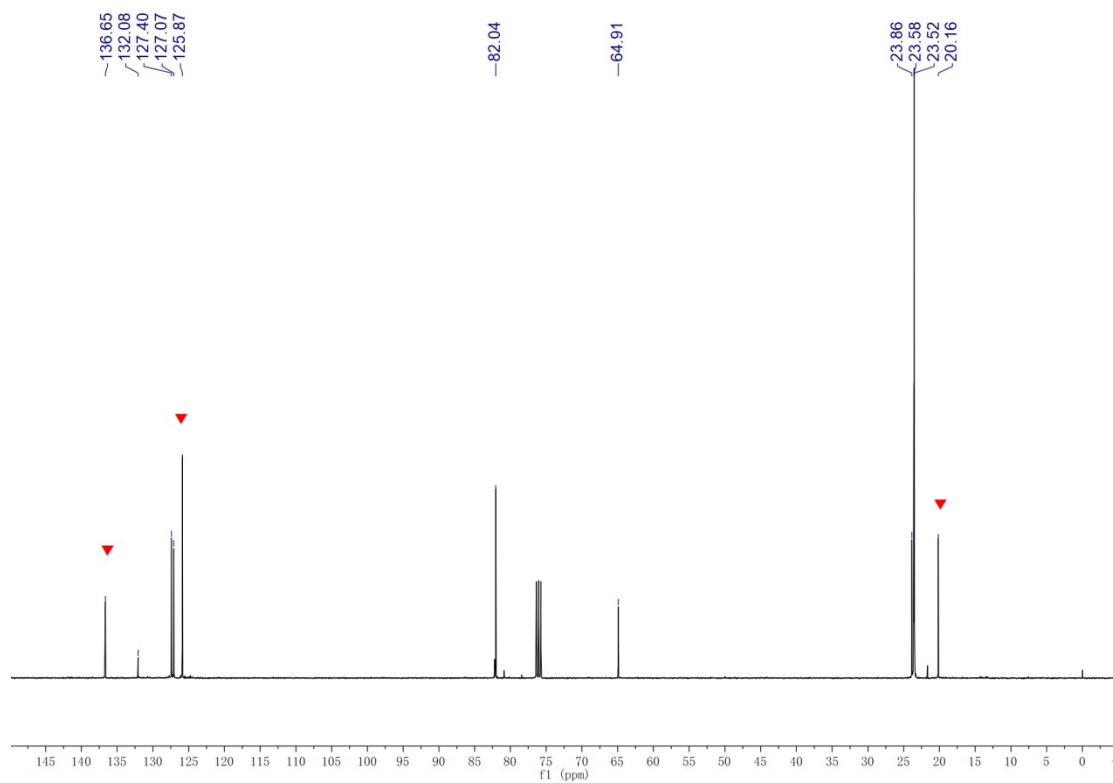


Figure S3.6.2 ^{13}C NMR spectrum of compound **8f** in CDCl_3

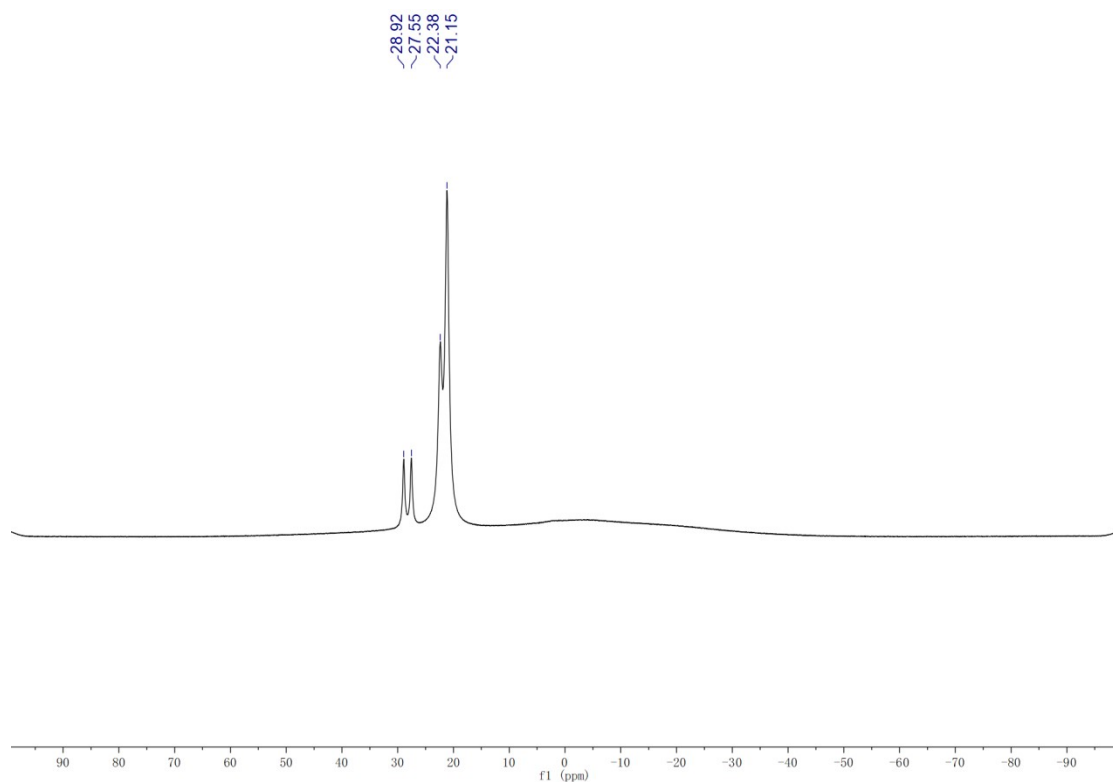


Figure S3.6.3 ^{11}B NMR spectrum of compound **8f** in CDCl_3

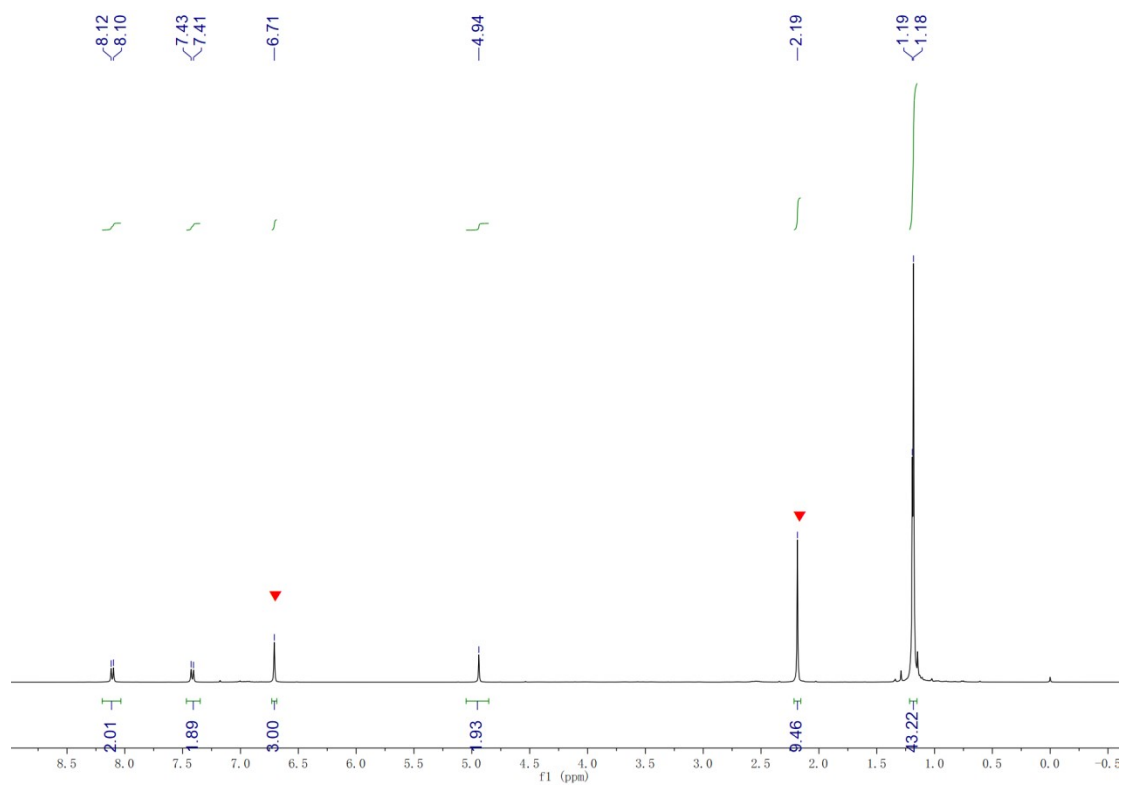


Figure S3.7.1 ^1H NMR spectrum of compound **8g** in CDCl_3

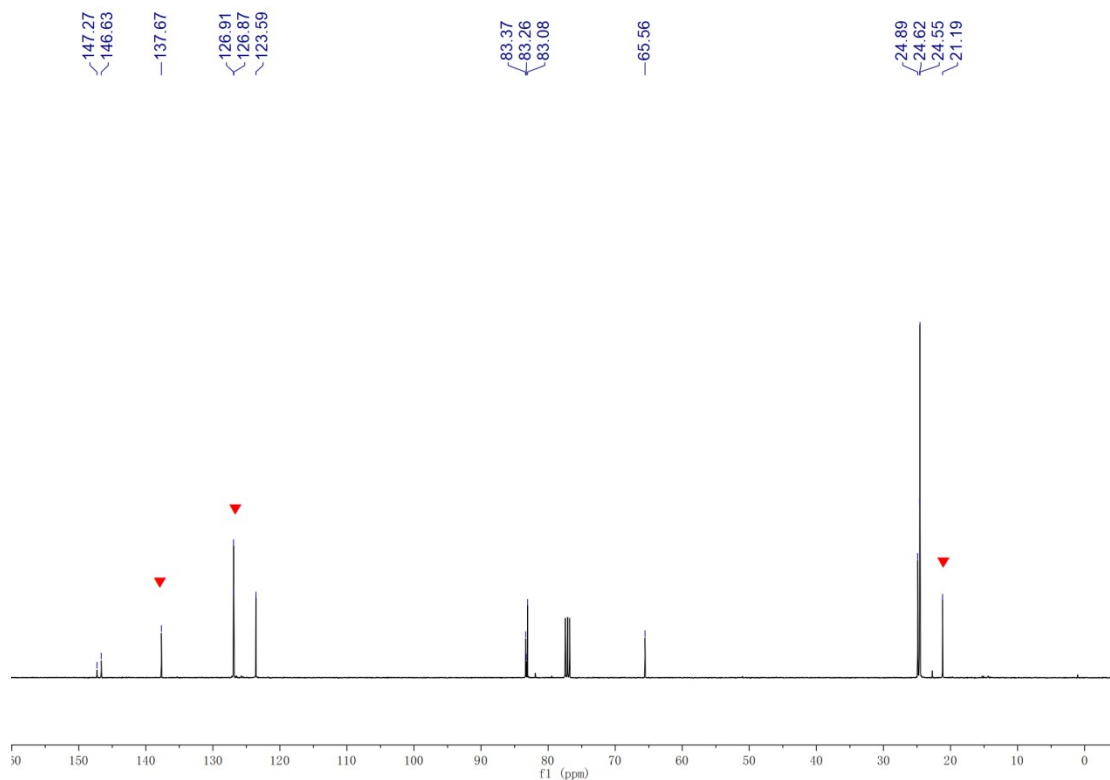


Figure S3.7.2 ^{13}C NMR spectrum of compound **8g** in CDCl_3

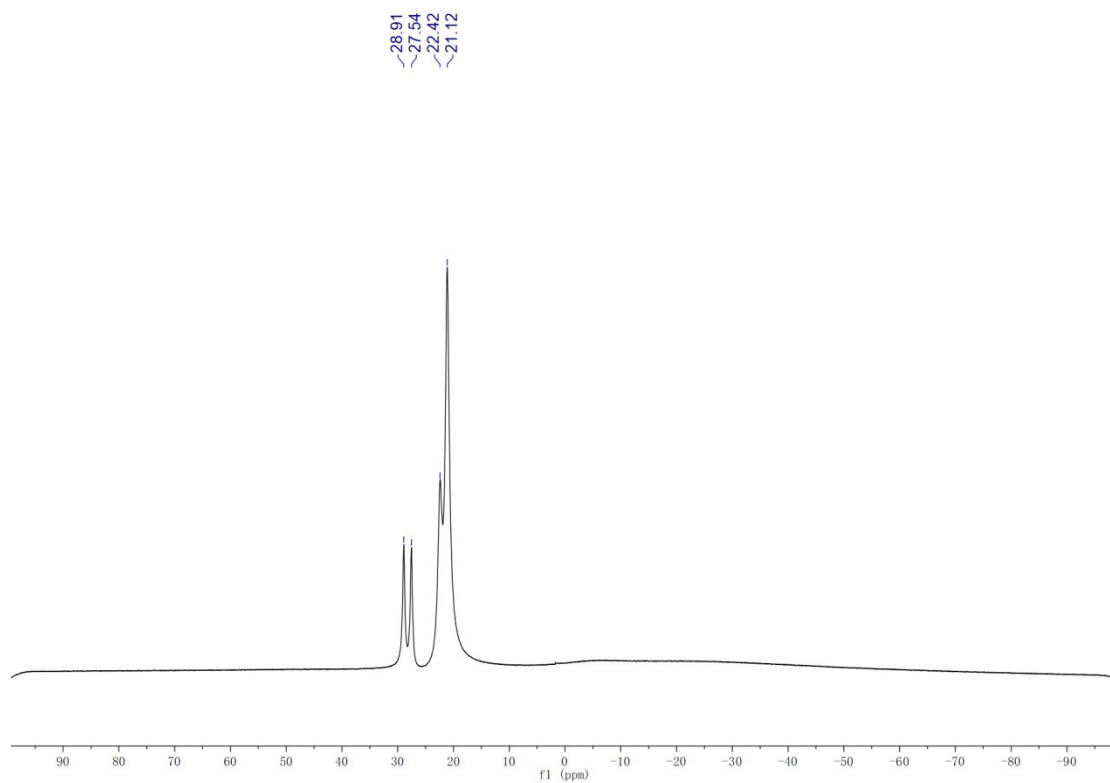


Figure S3.7.3 ^{11}B NMR spectrum of compound **8g** in CDCl_3

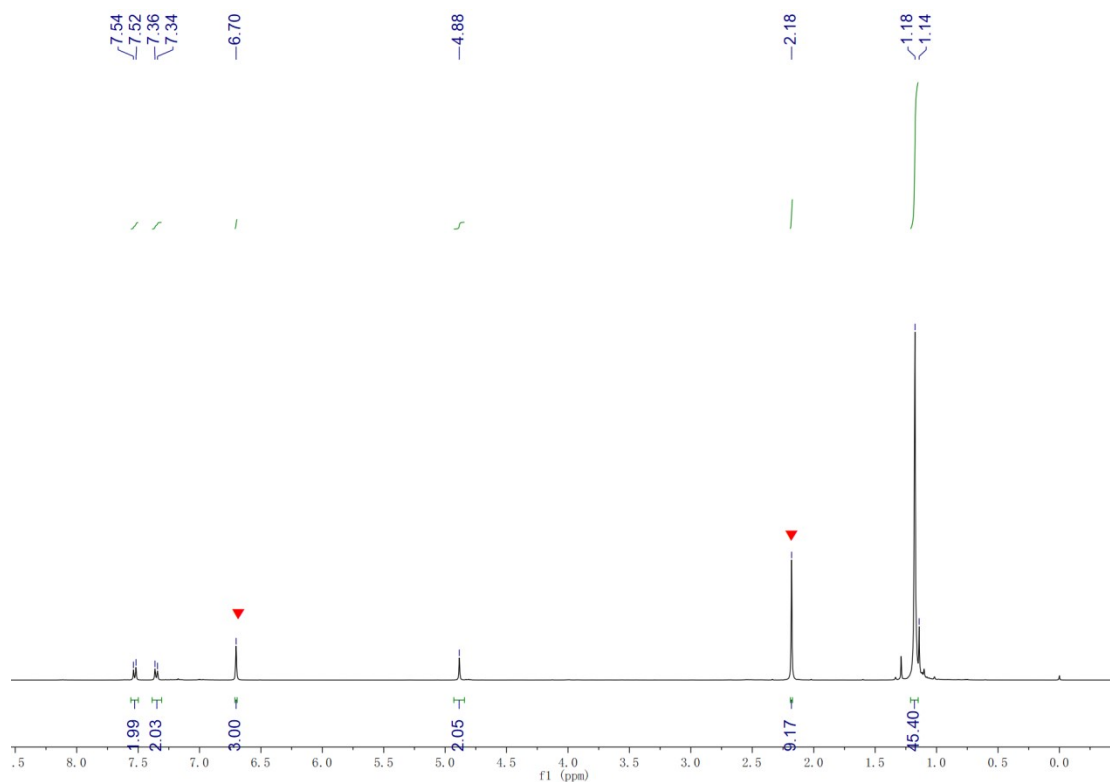


Figure S3.8.1 ^1H NMR spectrum of compound **8h** in CDCl_3

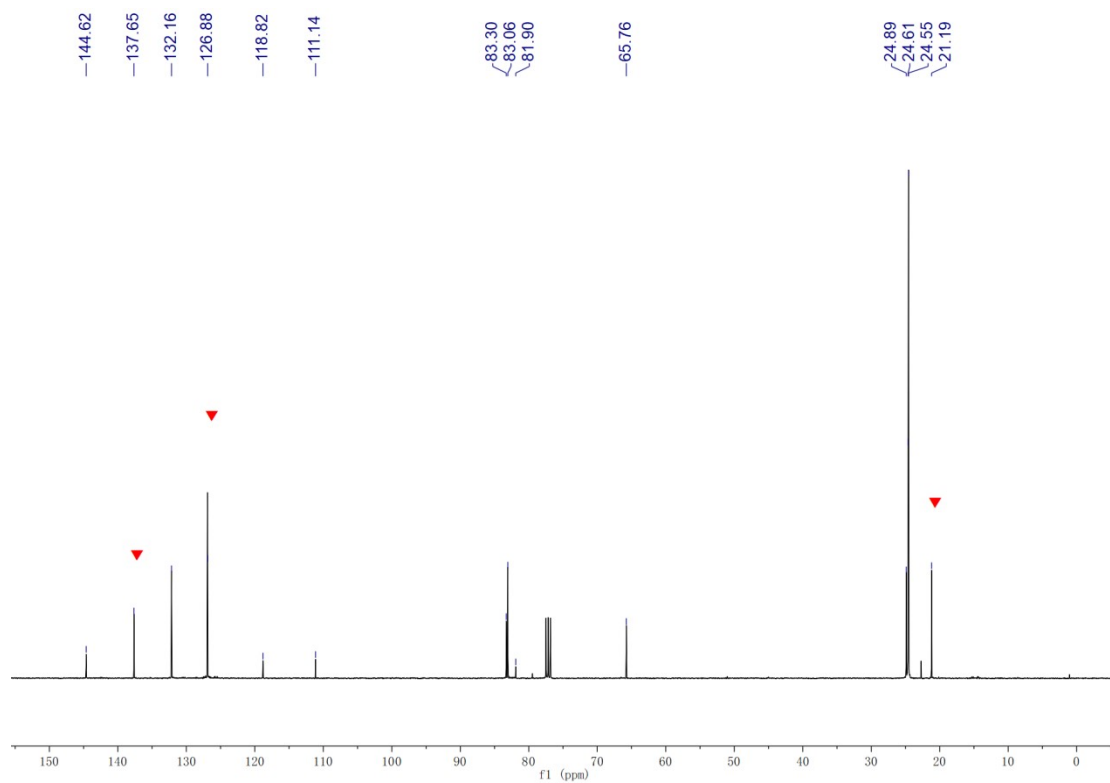


Figure S3.8.2 ^{13}C NMR spectrum of compound **8h** in CDCl_3

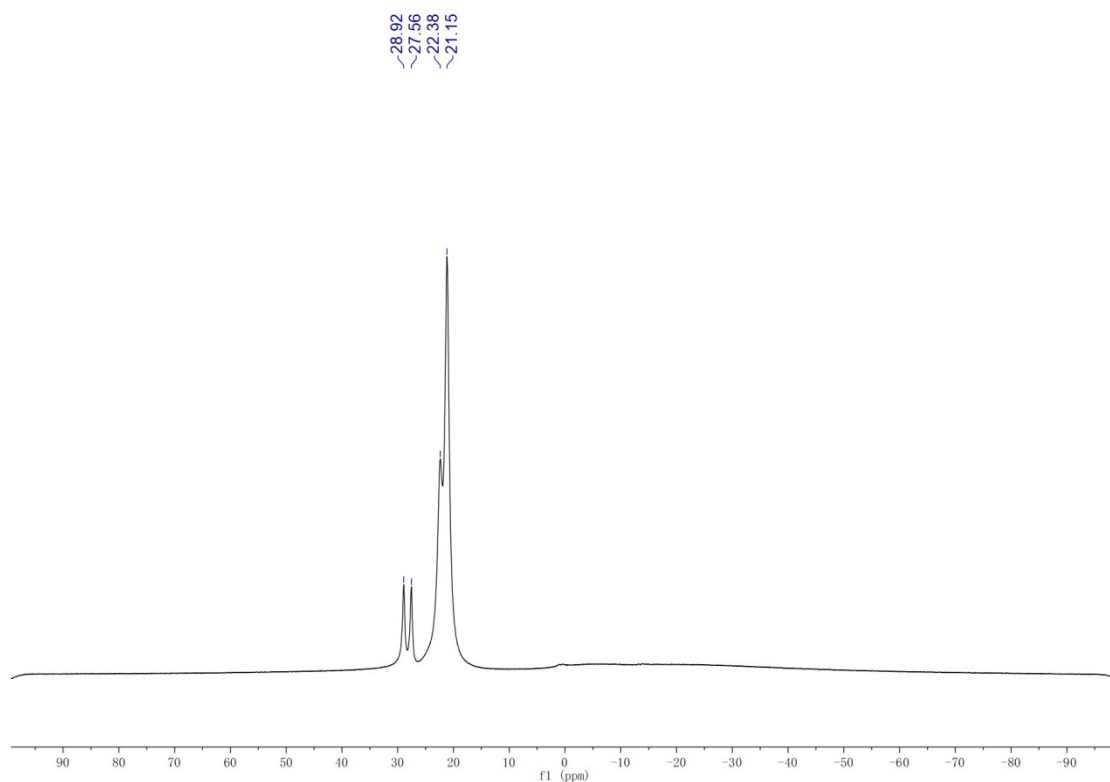


Figure S3.8.3 ^{11}B NMR spectrum of compound **8h** in CDCl_3

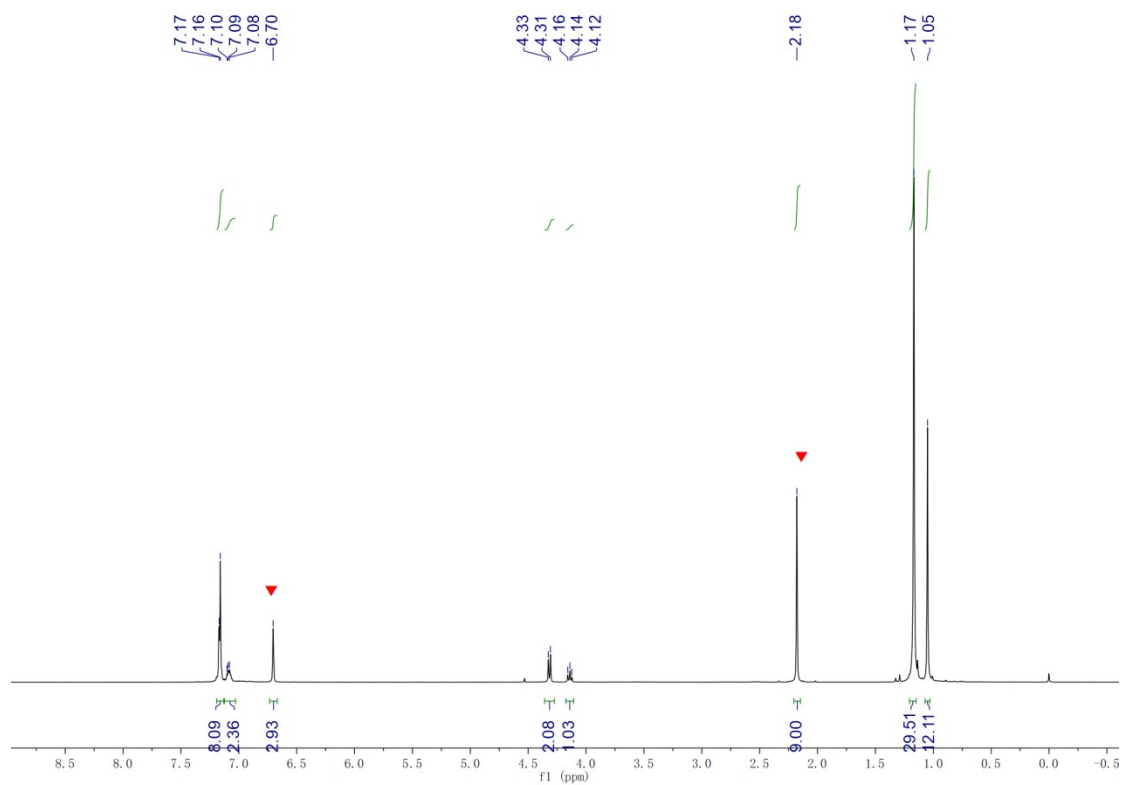


Figure S3.9.1 ^1H NMR spectrum of compound **8i** in CDCl_3

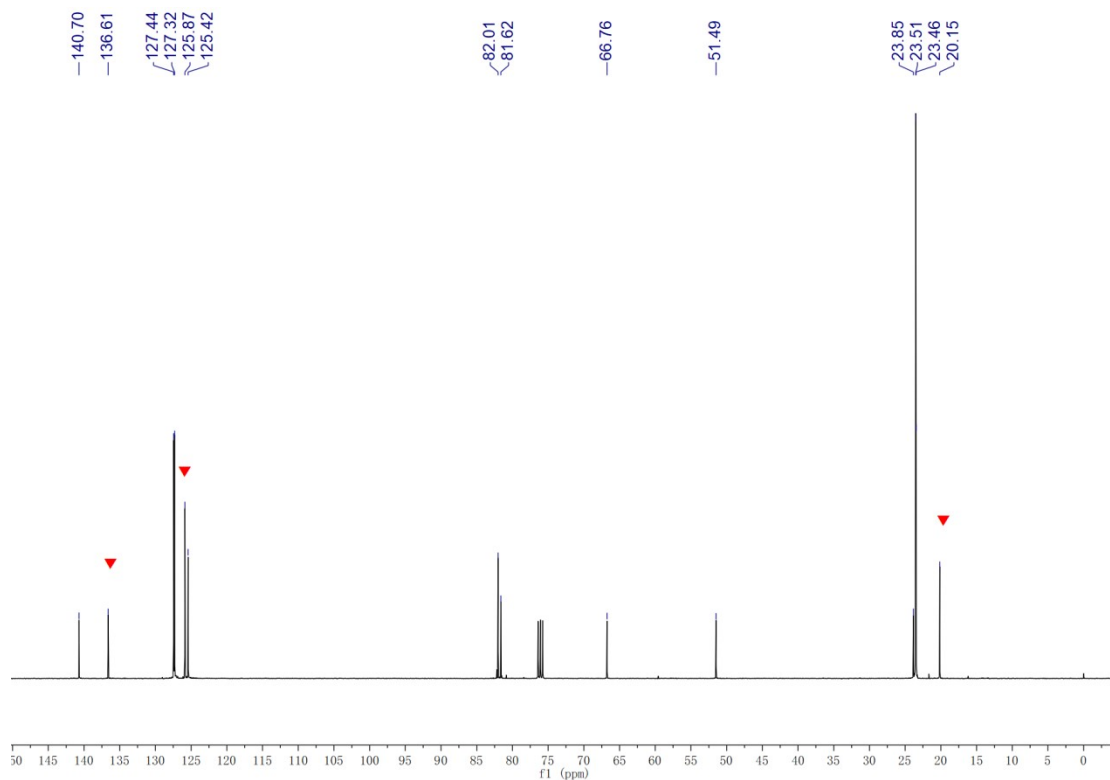


Figure S3.9.2 ^{13}C NMR spectrum of compound **8i** in CDCl_3

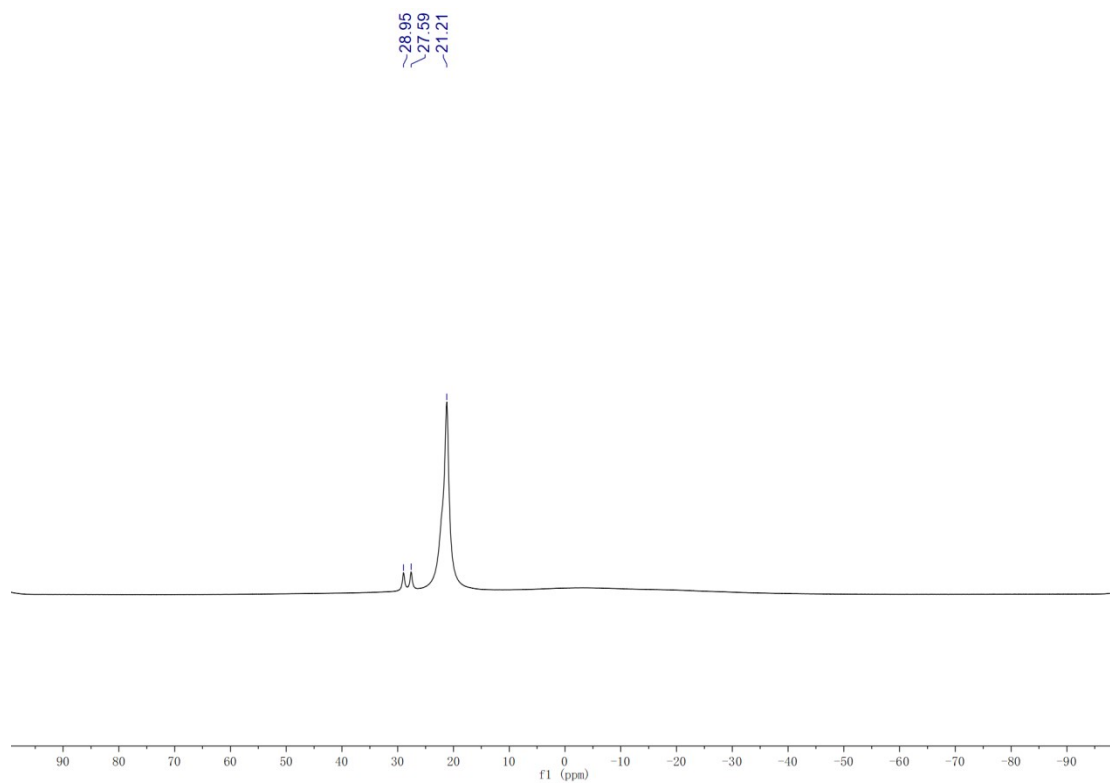


Figure S3.9.3 ¹¹B NMR spectrum of compound **8i** in CDCl₃

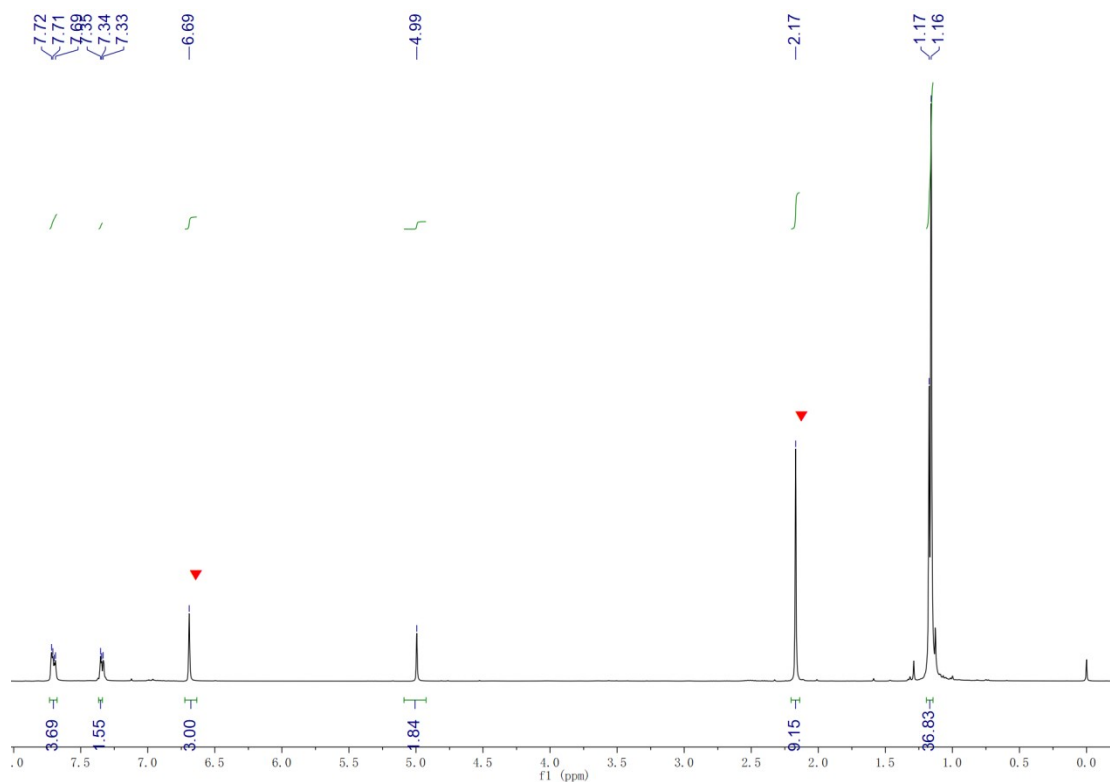


Figure S3.10.1 ¹H NMR spectrum of compound **8j** in CDCl₃

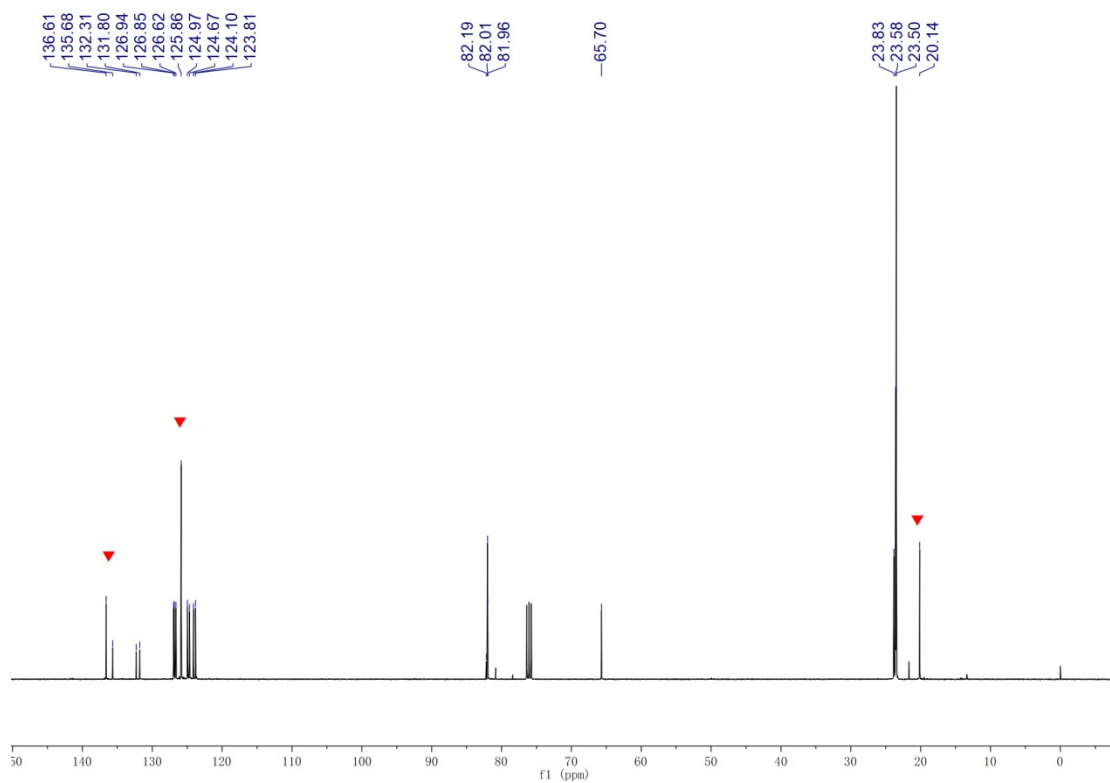


Figure S3.10.2 ^{13}C NMR spectrum of compound **8j** in CDCl_3

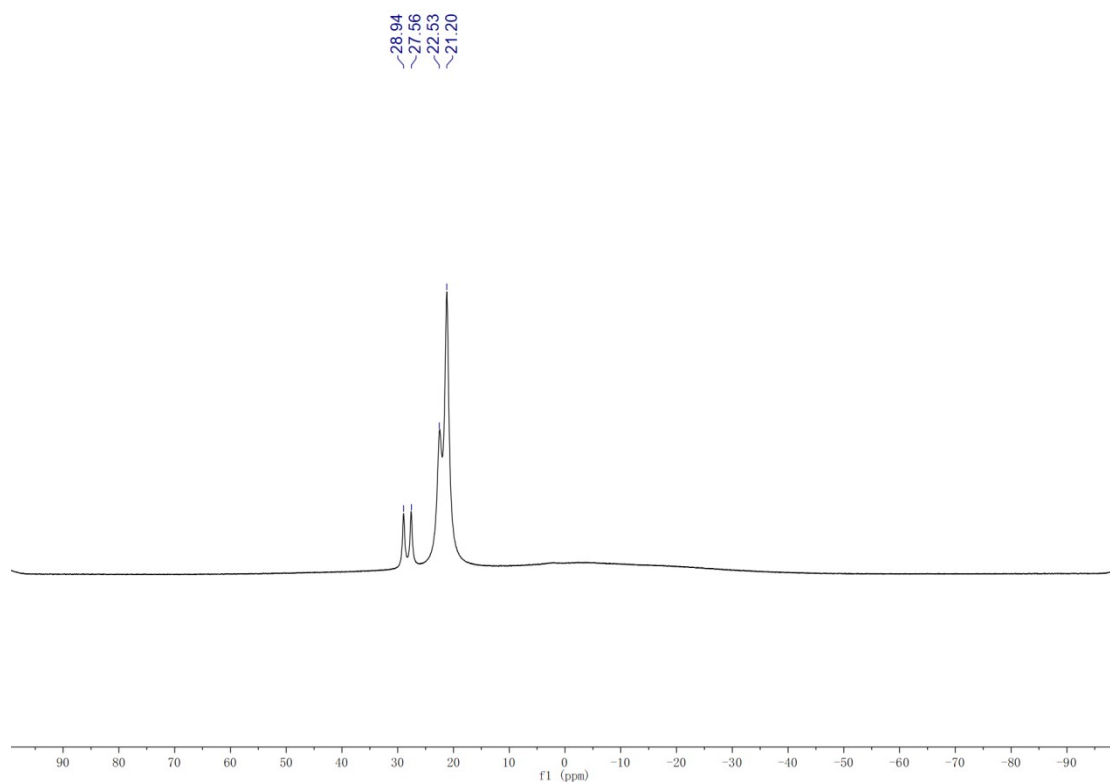


Figure S3.10.3 ^{11}B NMR spectrum of compound **8j** in CDCl_3

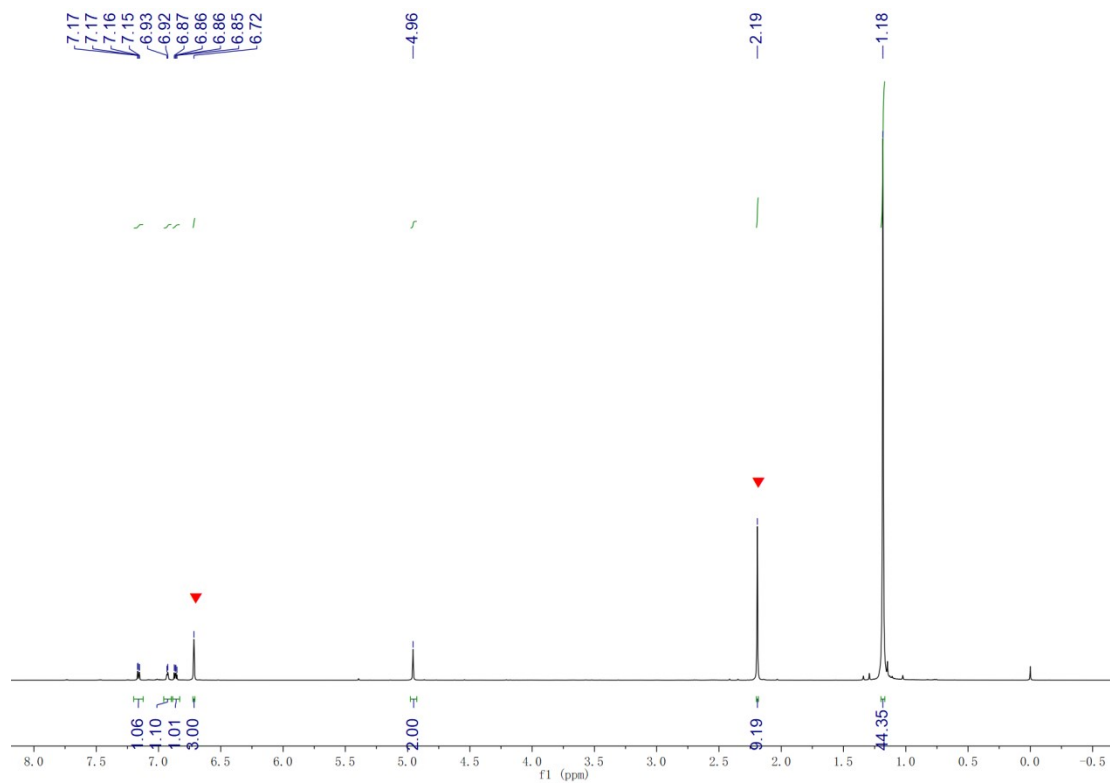


Figure S3.11.1 ^1H NMR spectrum of compound **8k** in CDCl_3

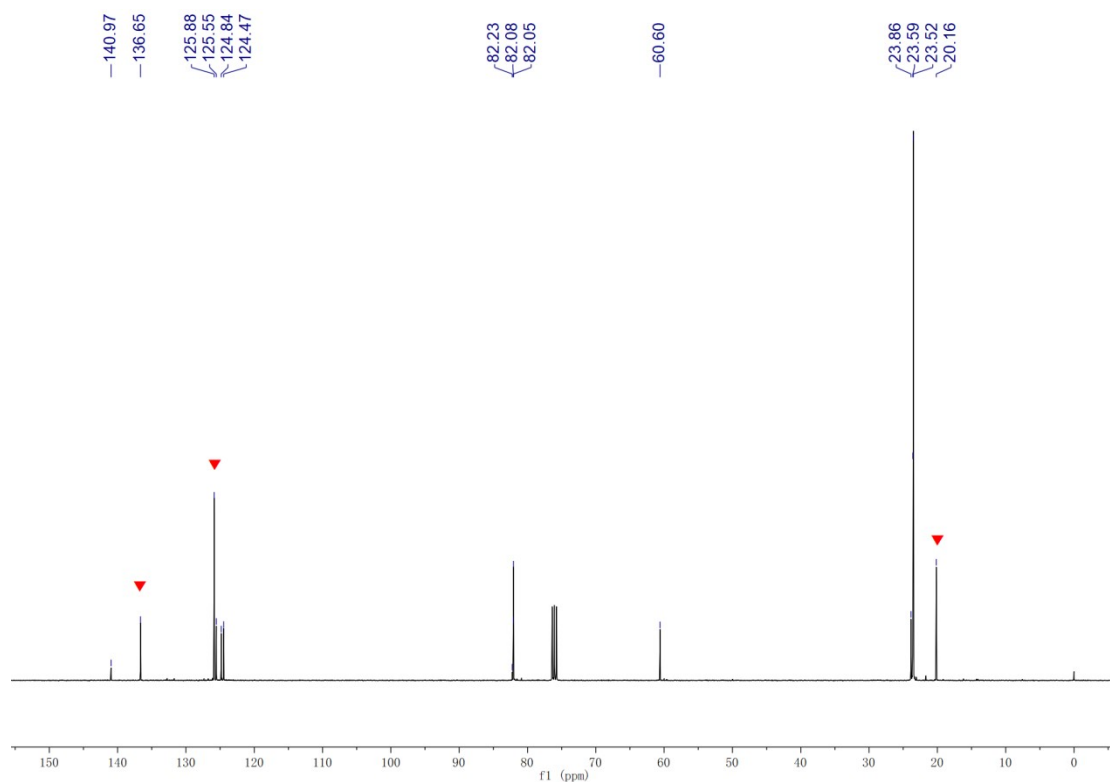


Figure S3.11.2 ^{13}C NMR spectrum of compound **8k** in CDCl_3

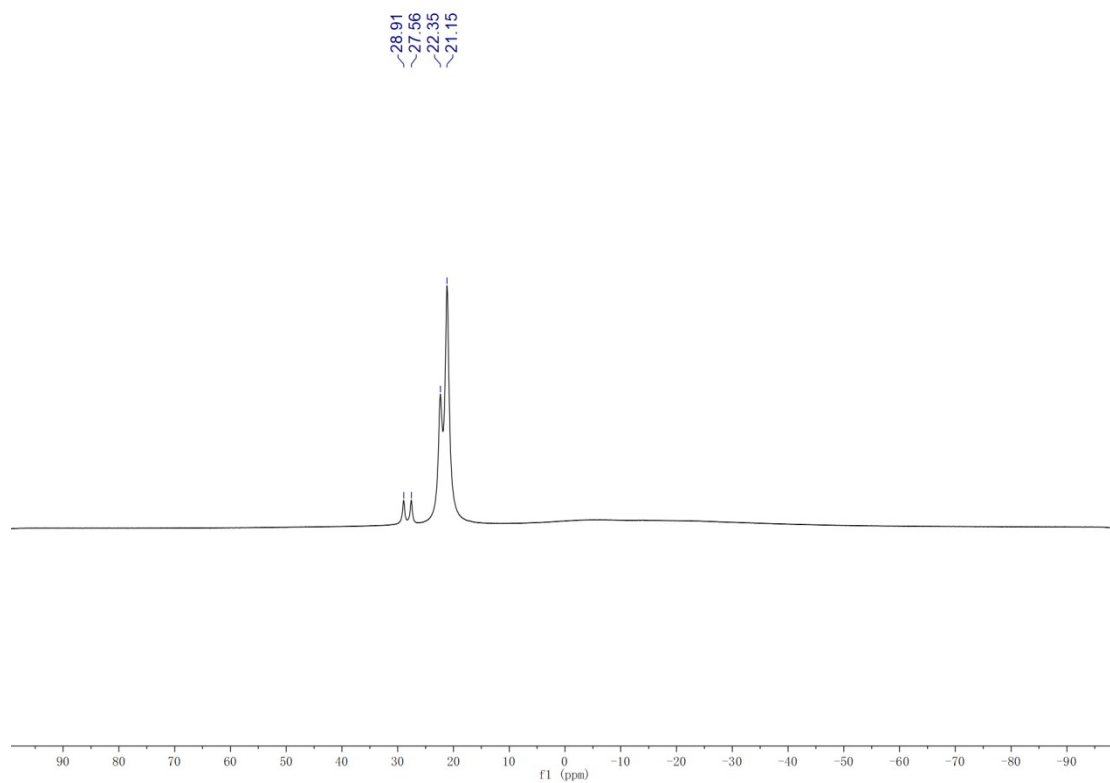


Figure S3.11.3 ^{11}B NMR spectrum of compound **8k** in CDCl_3

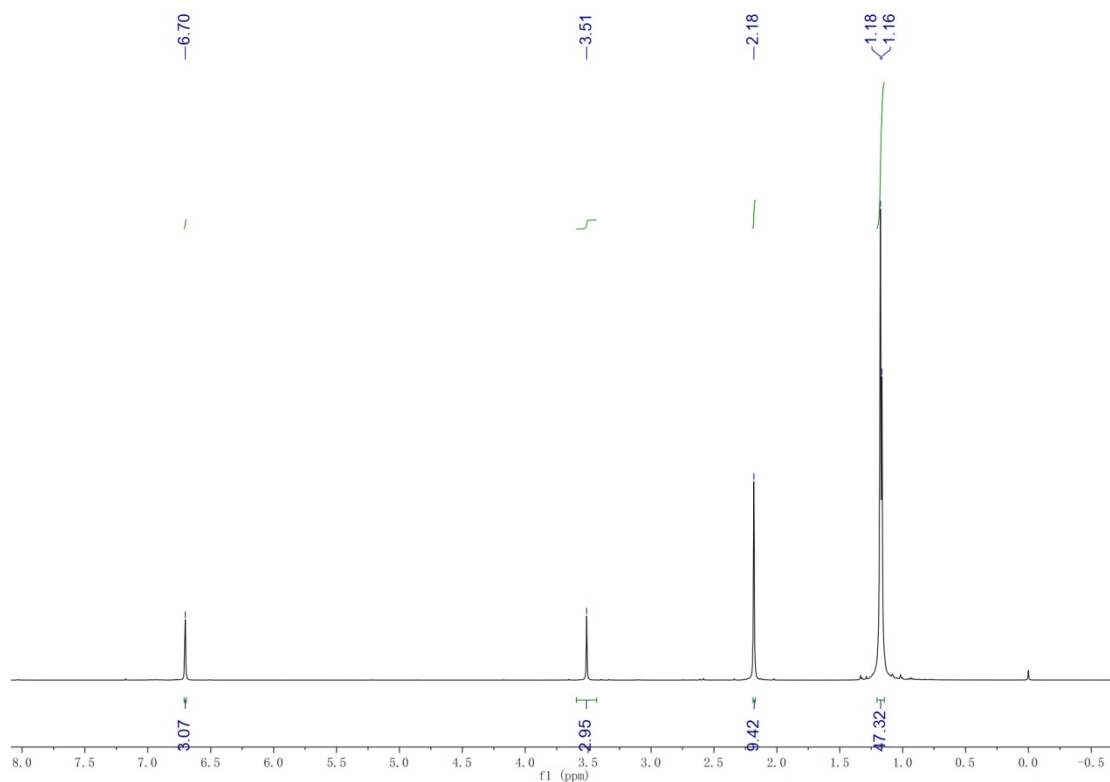


Figure S3.12.1 ^1H NMR spectrum of compound **8l** in CDCl_3

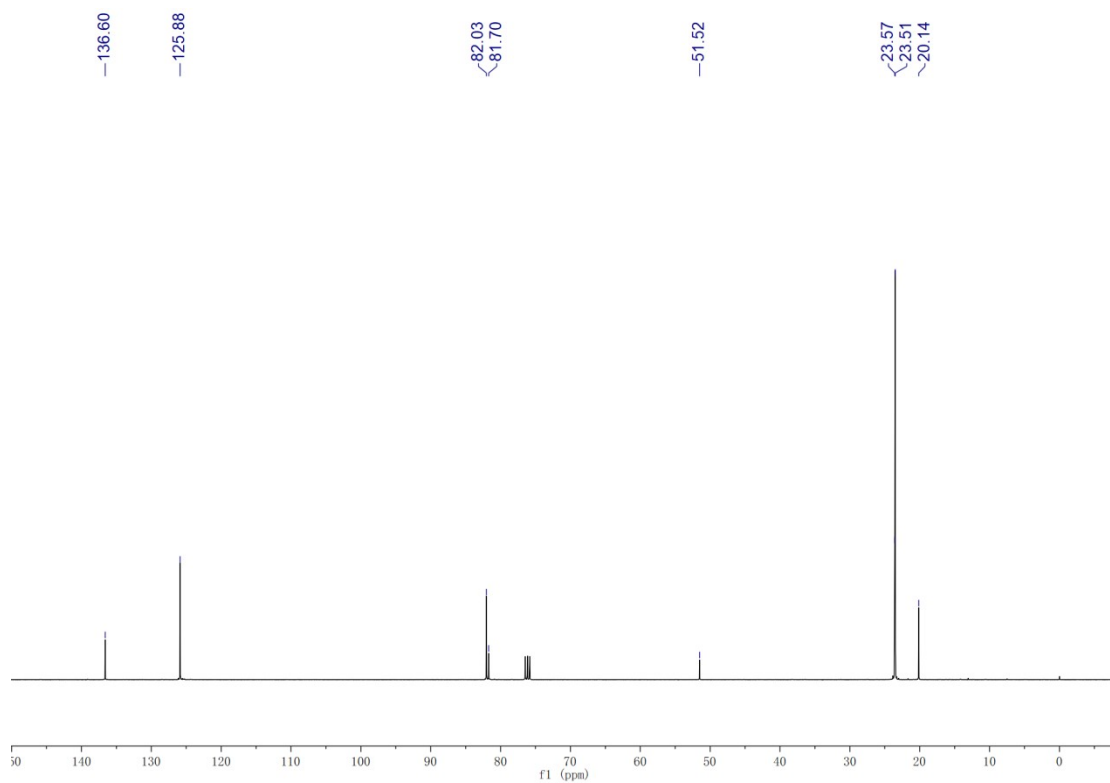


Figure S3.12.2 ^{13}C NMR spectrum of compound **8I** in CDCl_3

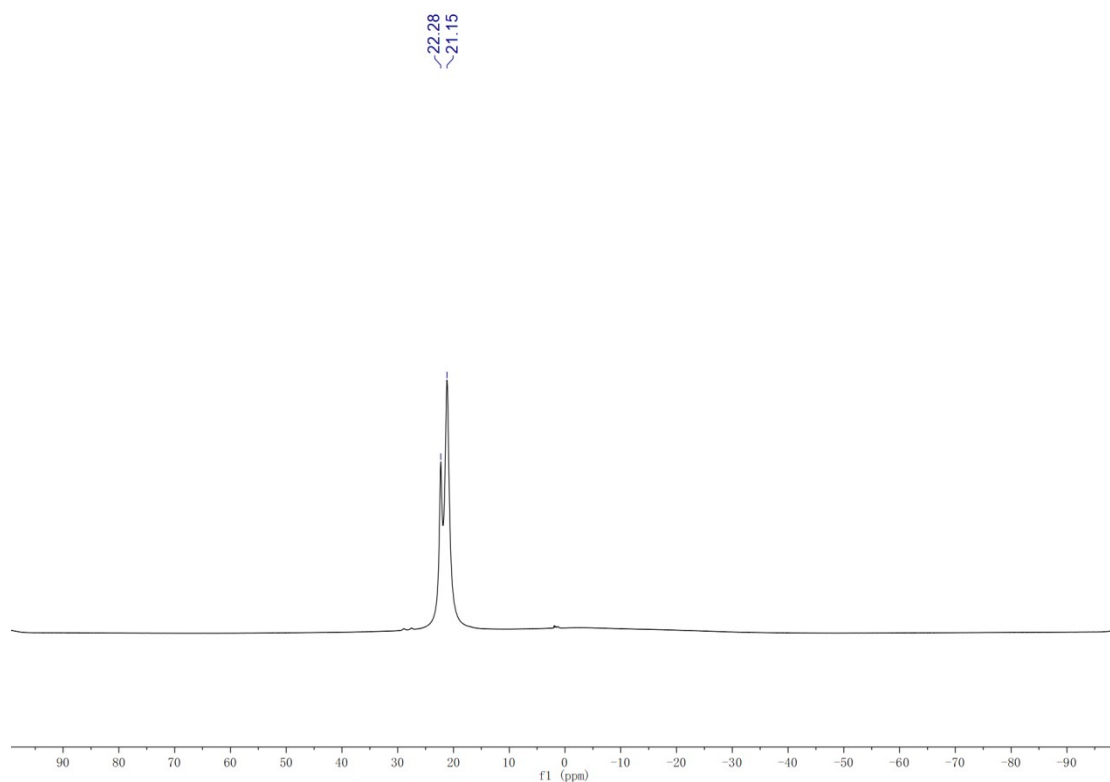


Figure S3.12.3 ^{11}B NMR spectrum of compound **8I** in CDCl_3

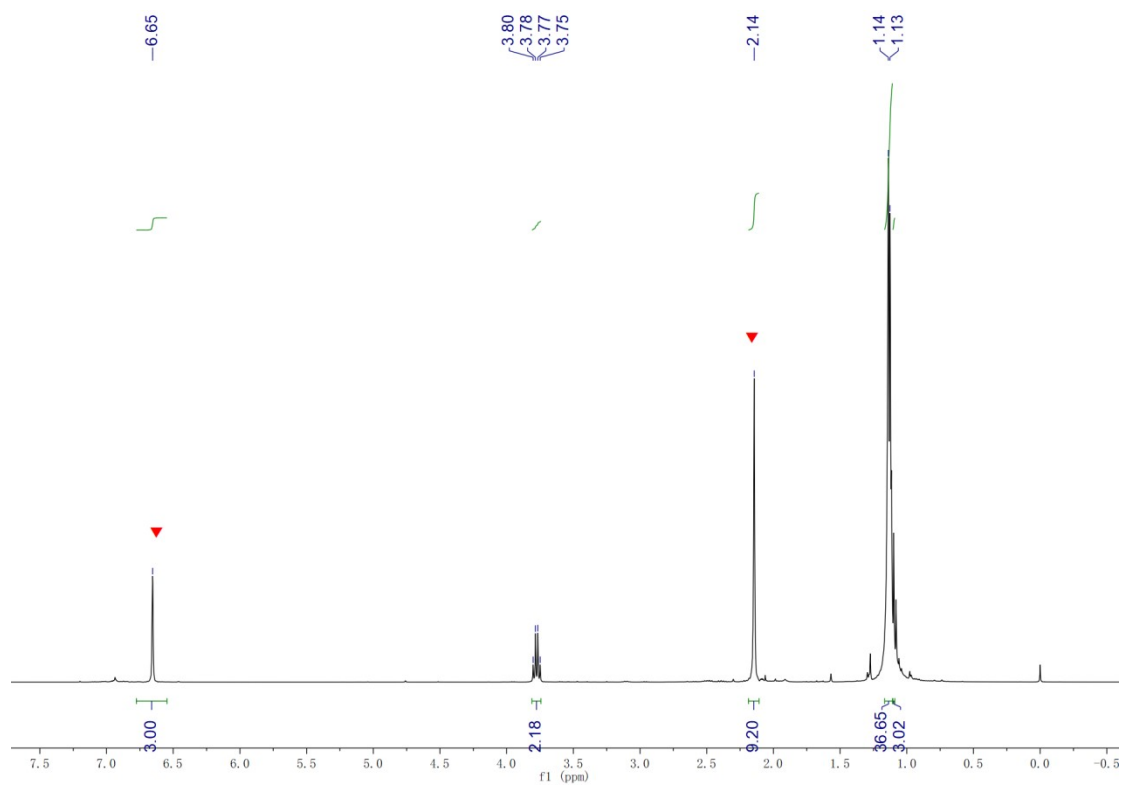


Figure S3.13.1 ^1H NMR spectrum of compound **8m** in CDCl_3

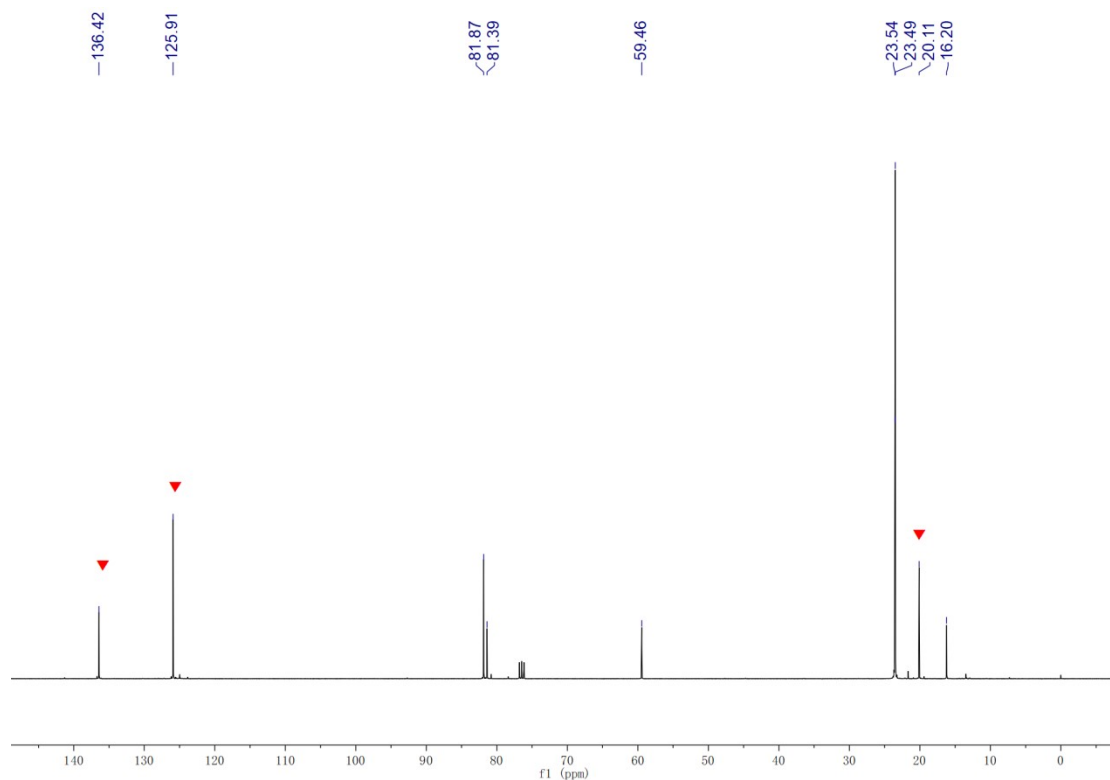


Figure S3.13.2 ^{13}C NMR spectrum of compound **8m** in CDCl_3

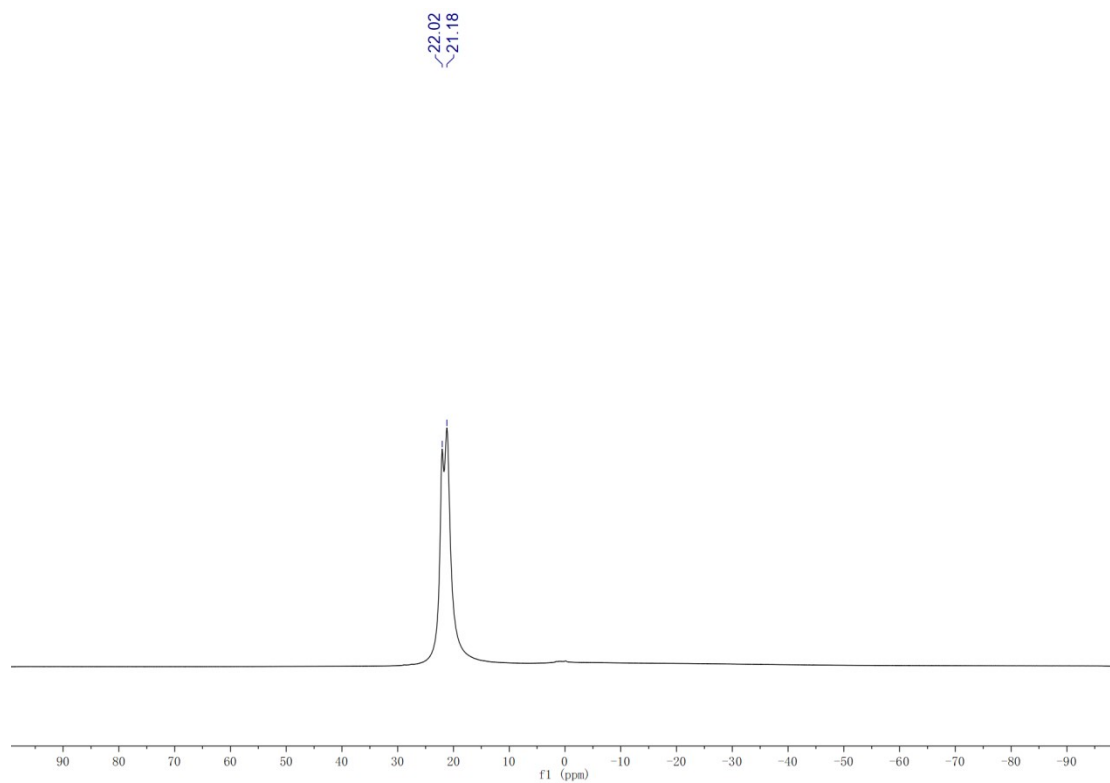


Figure S3.13.3 ^{11}B NMR spectrum of compound **8m** in CDCl_3

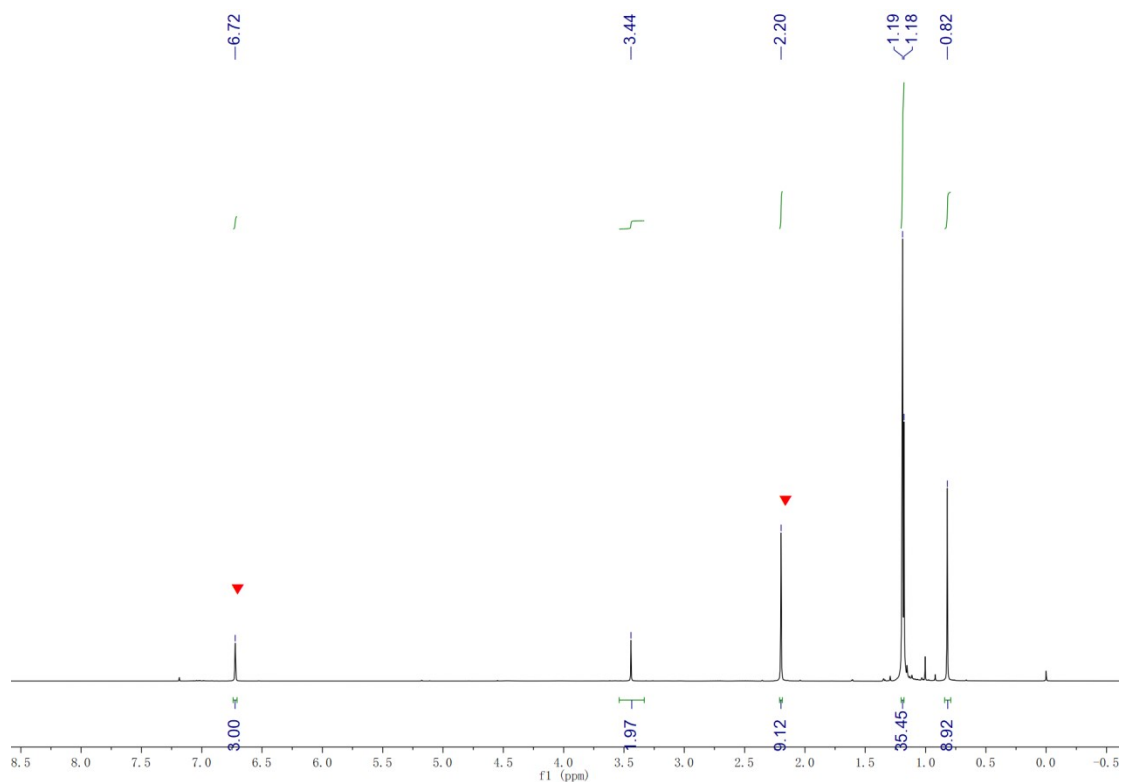


Figure S3.14.1 ^1H NMR spectrum of compound **8n** in CDCl_3

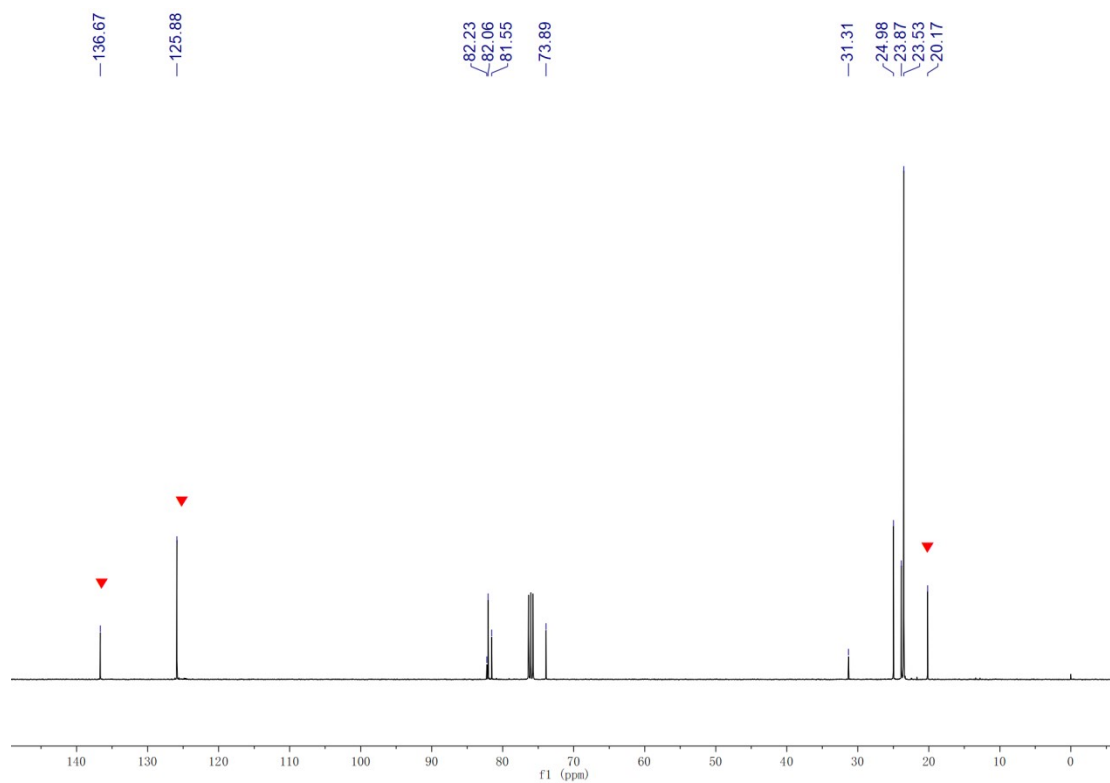


Figure S3.14.2 ^{13}C NMR spectrum of compound **8n** in CDCl_3

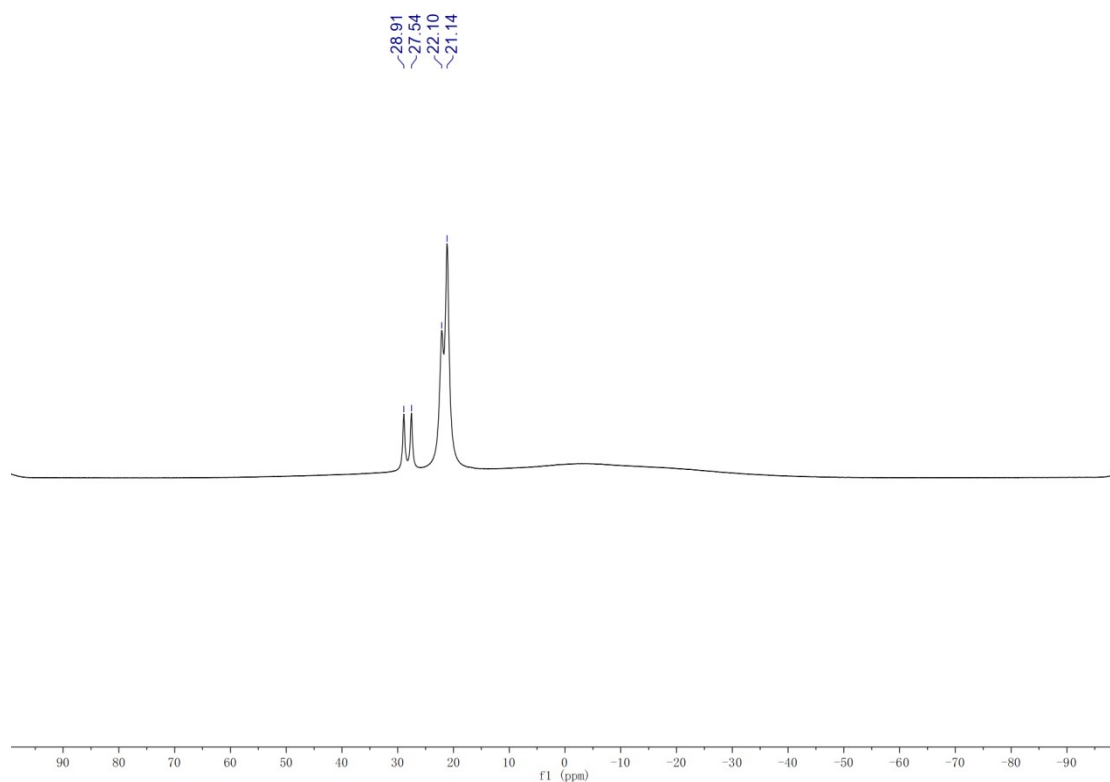


Figure S3.14.3 ^{11}B NMR spectrum of compound **8n** in CDCl_3

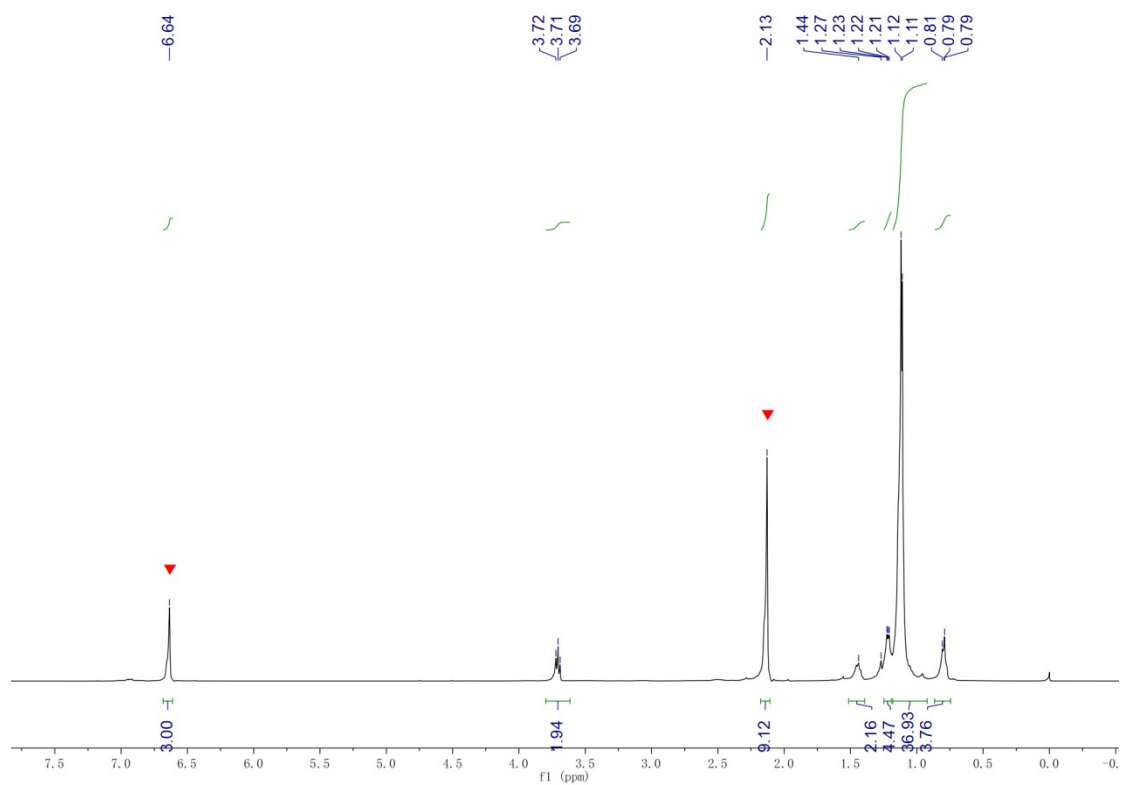


Figure S3.15.1 ^1H NMR spectrum of compound **8o** in CDCl_3

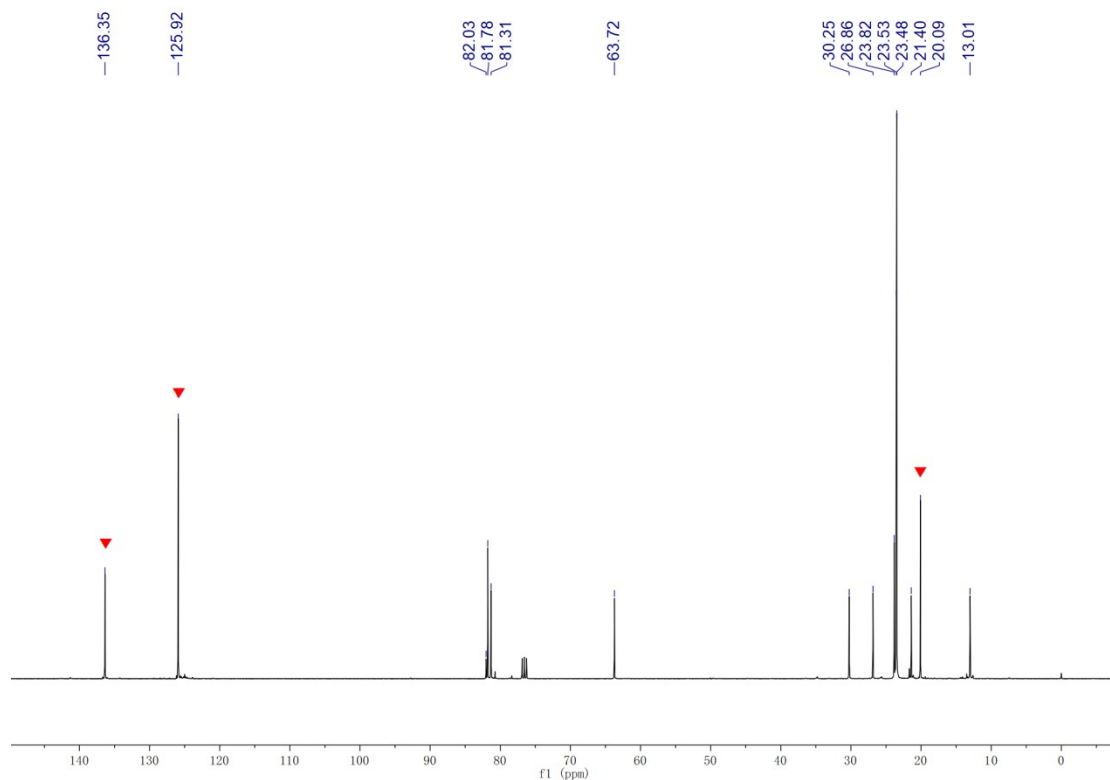


Figure S3.15.2 ^{13}C NMR spectrum of compound **8o** in CDCl_3

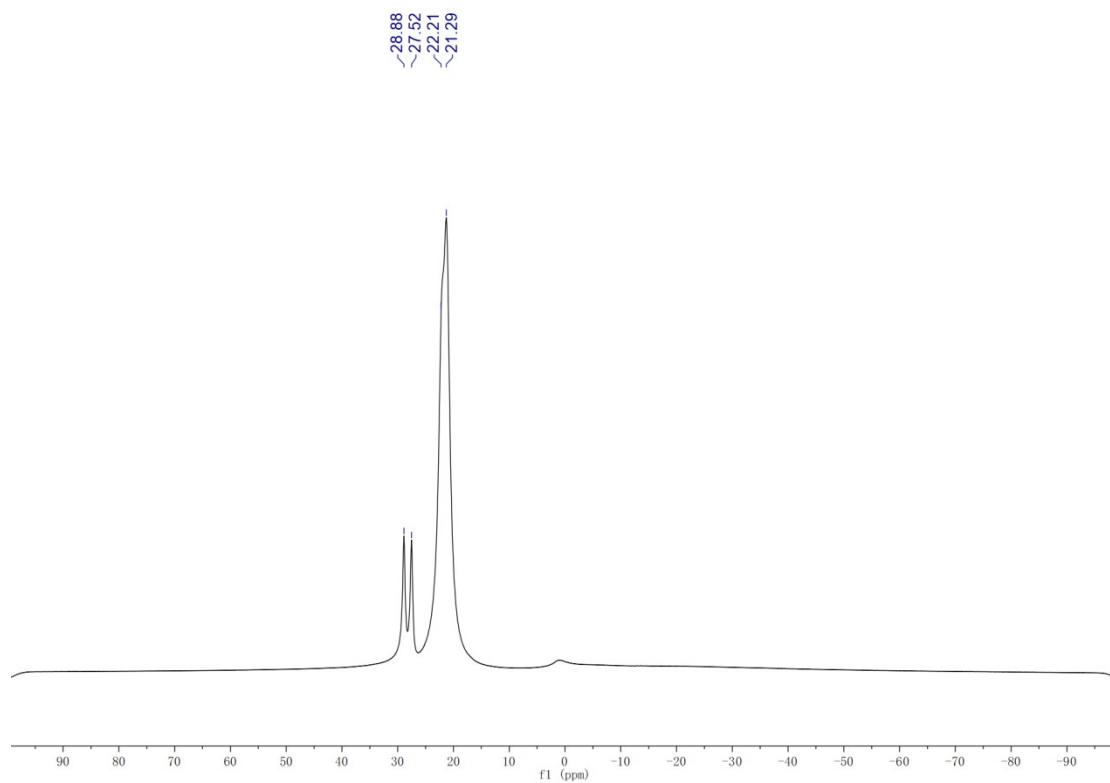


Figure S3.15.3 ¹¹B NMR spectrum of compound **8o** in CDCl₃

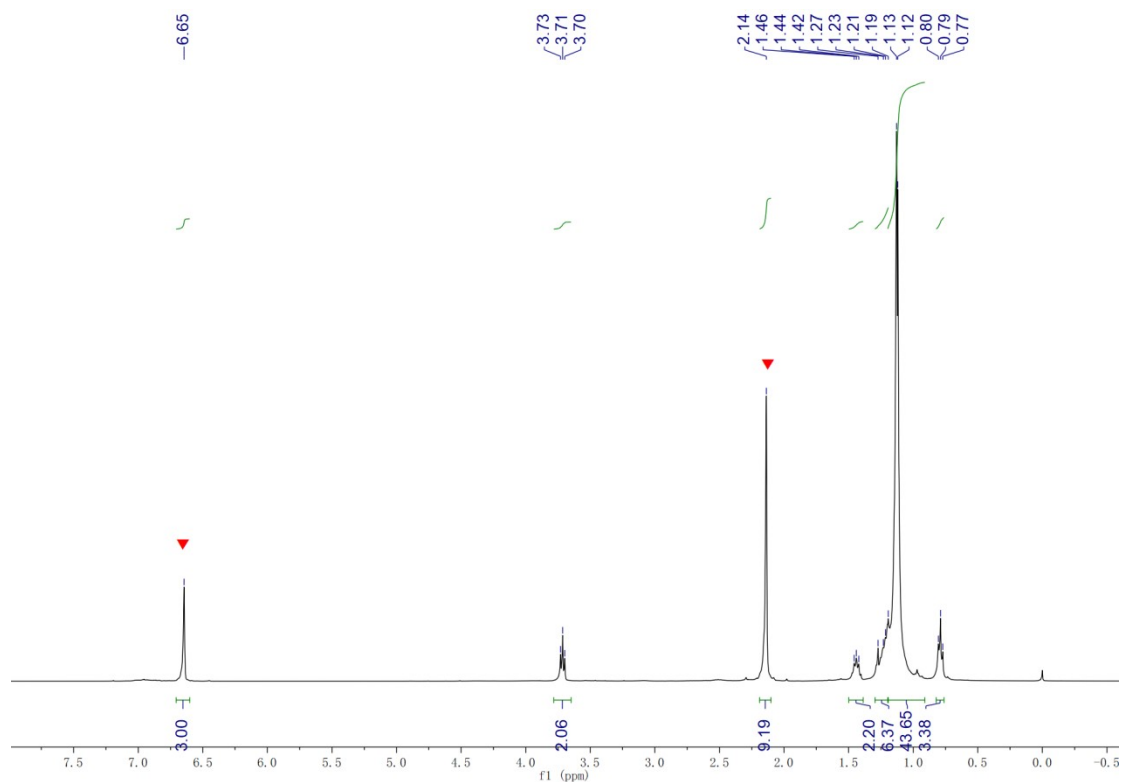


Figure S3.16.1 ¹H NMR spectrum of compound **8p** in CDCl₃

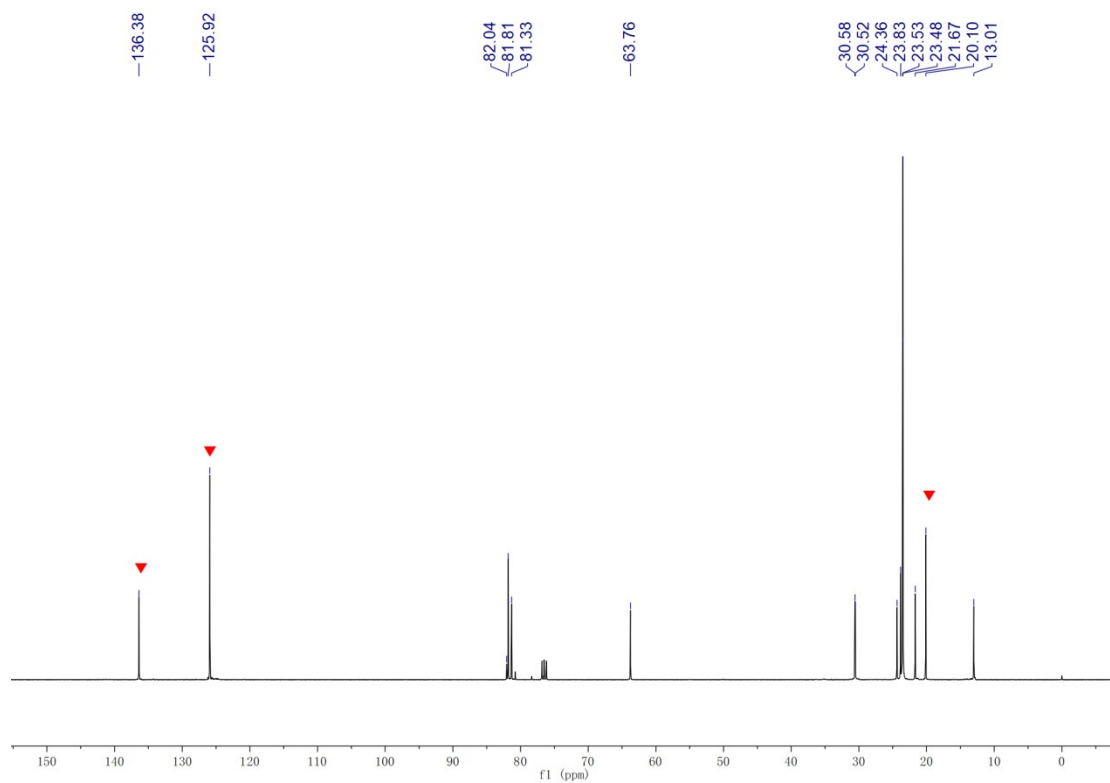


Figure S3.16.2 ^{13}C NMR spectrum of compound **8p** in CDCl_3

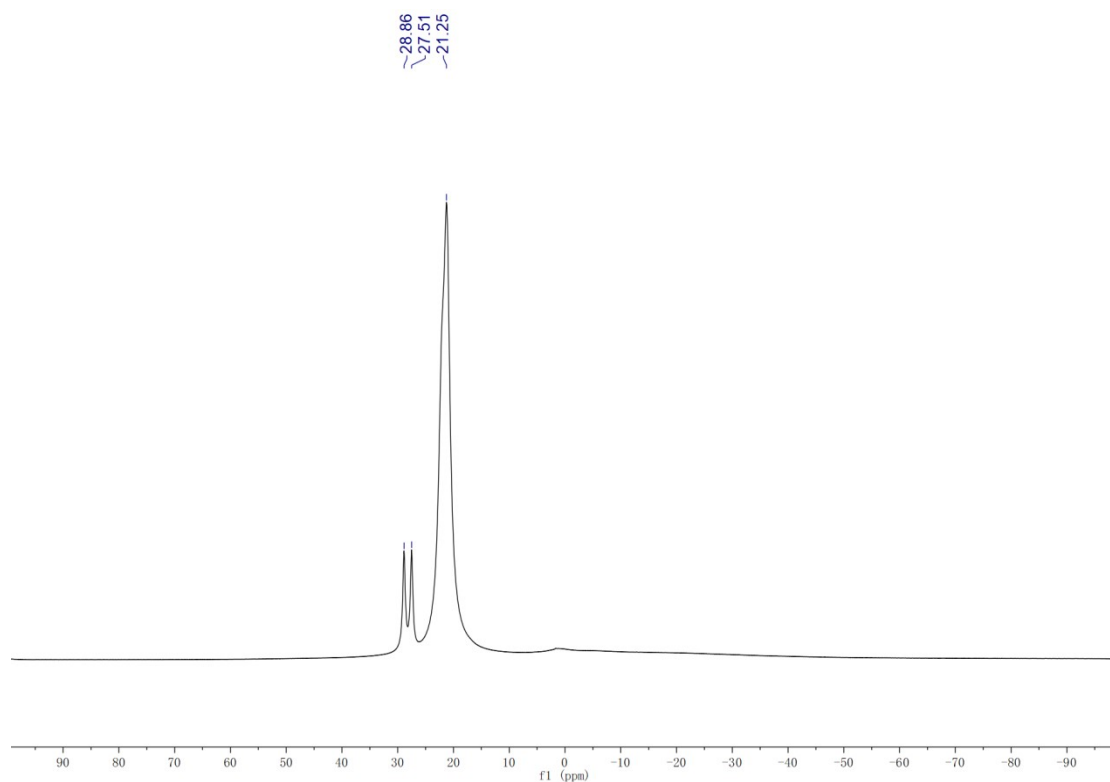


Figure S3.16.3 ^{11}B NMR spectrum of compound **8p** in CDCl_3

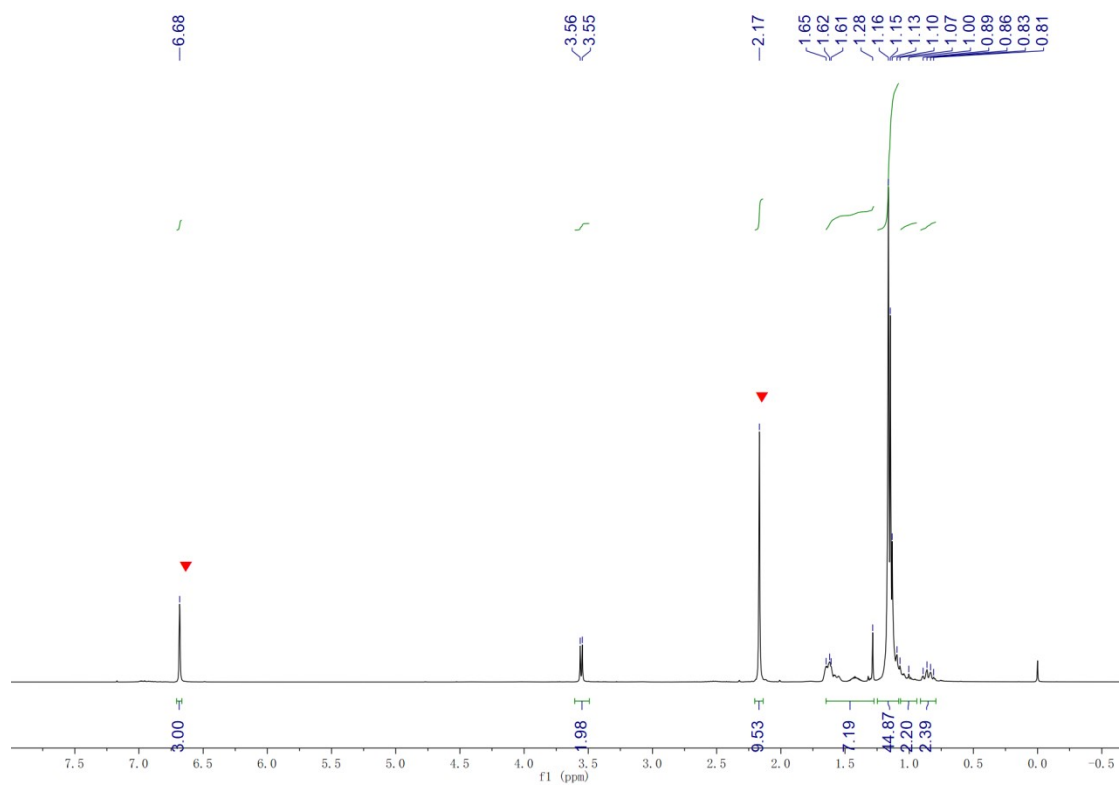


Figure S3.17.1 ^1H NMR spectrum of compound **8q** in CDCl_3

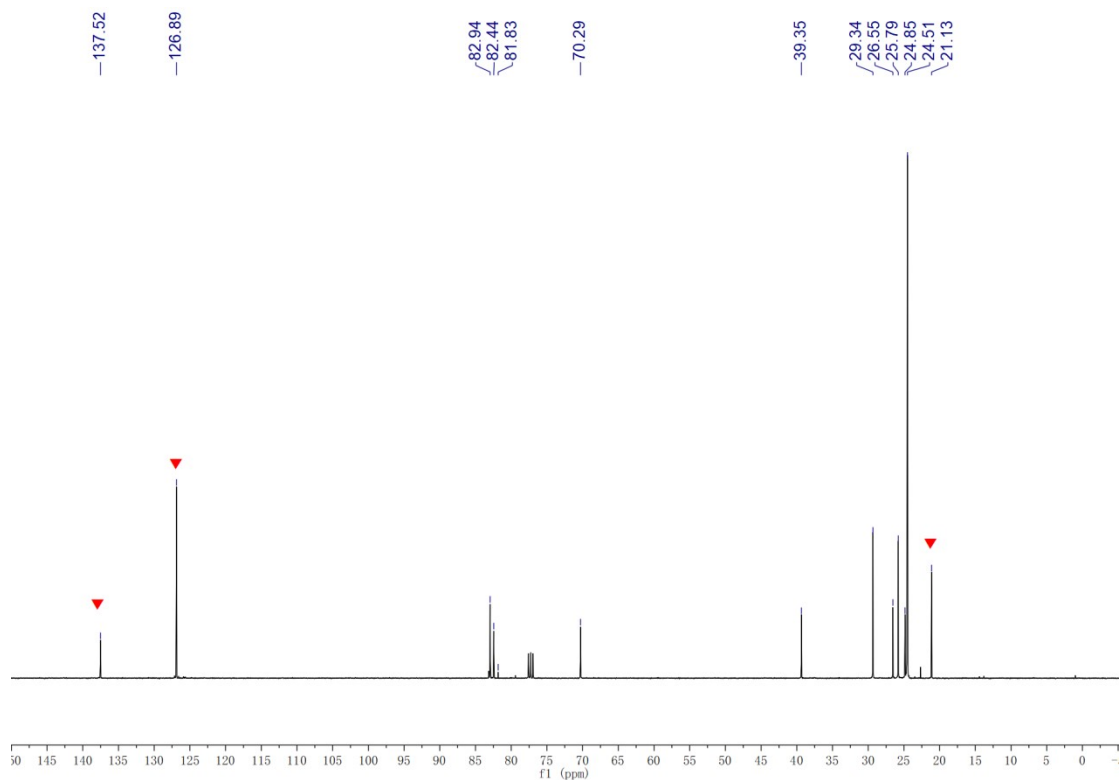


Figure S3.17.2 ^{13}C NMR spectrum of compound **8q** in CDCl_3

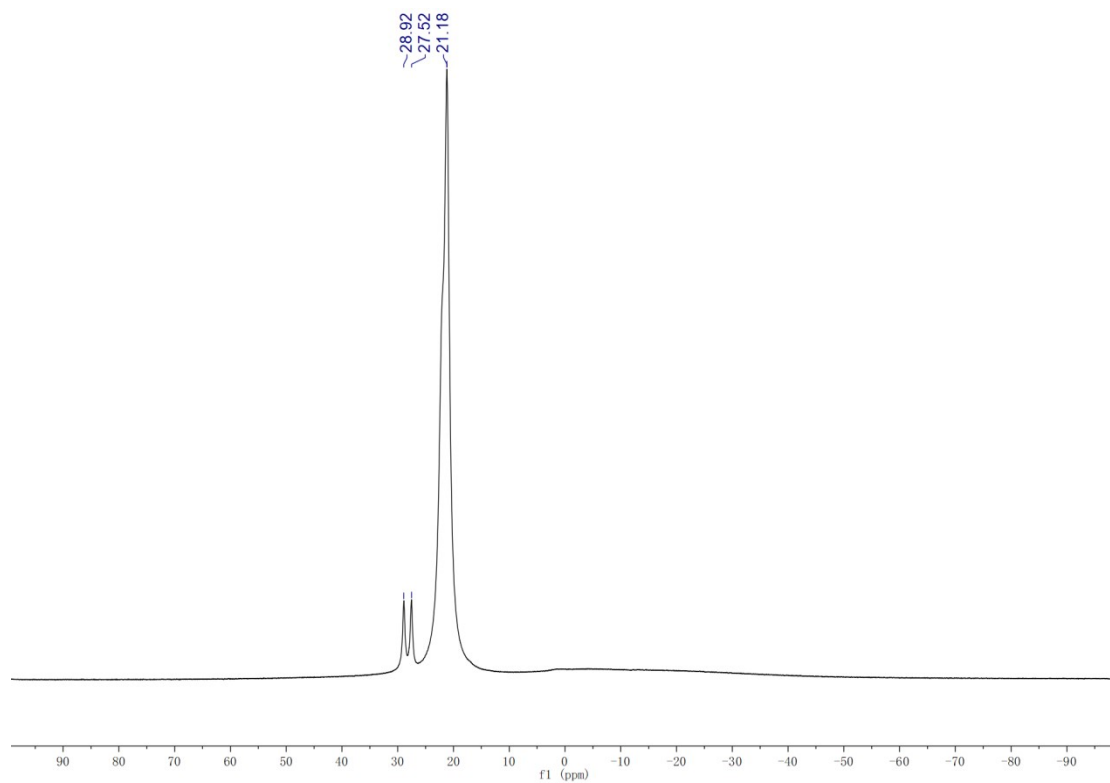


Figure S3.17.3 ^{11}B NMR spectrum of compound **8q** in CDCl_3

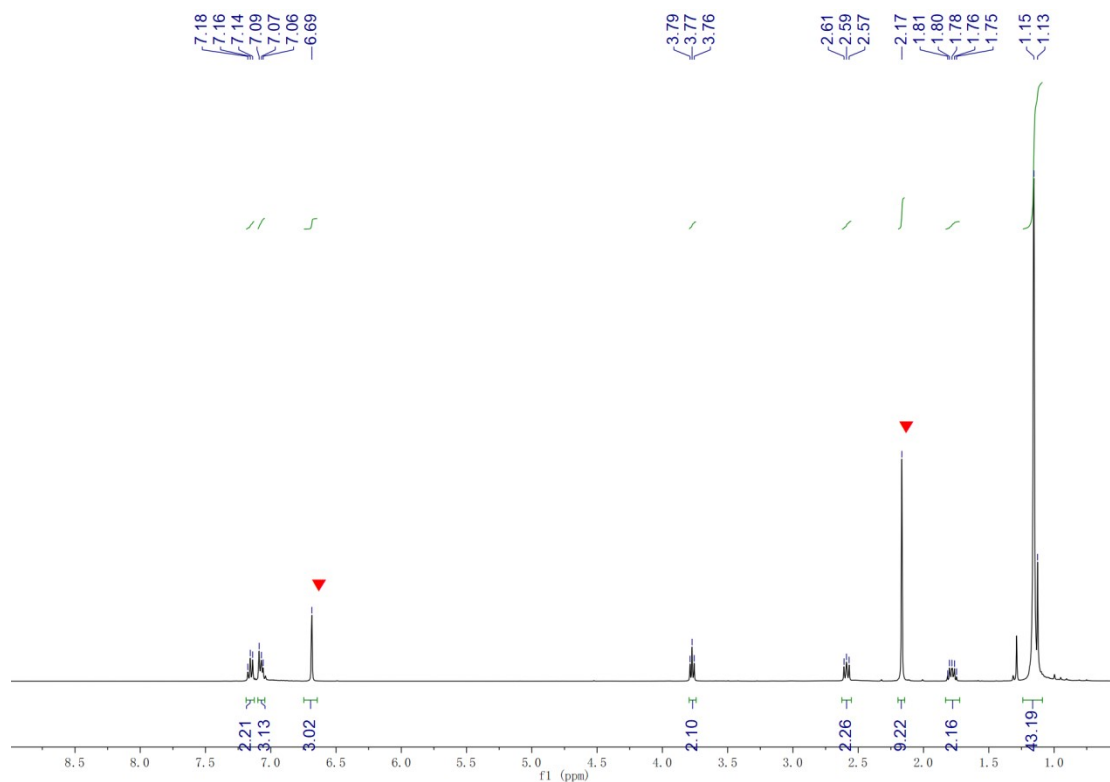


Figure S3.18.1 ^1H NMR spectrum of compound **8r** in CDCl_3

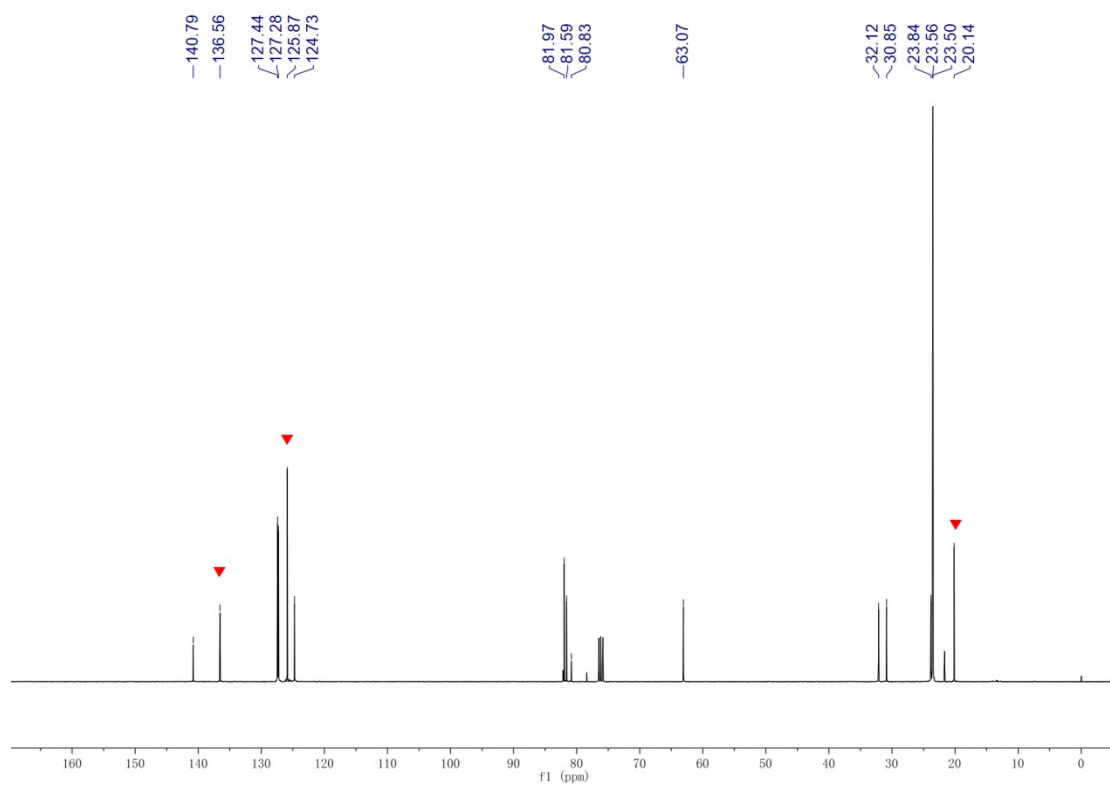


Figure S3.18.2 ^{13}C NMR spectrum of compound **8r** in CDCl_3

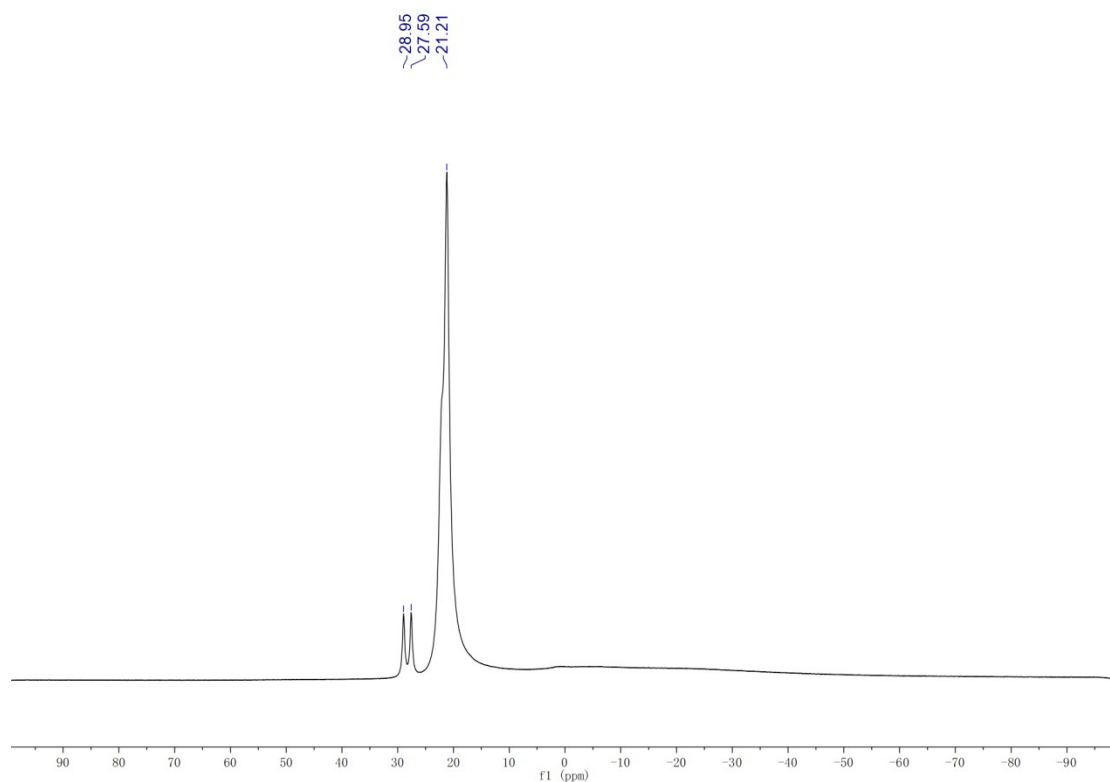


Figure S3.18.3 ^{11}B NMR spectrum of compound **8r** in CDCl_3

^1H , ^{13}C and ^{11}B NMR Spectra of Hydroboration Products of CO_2 .

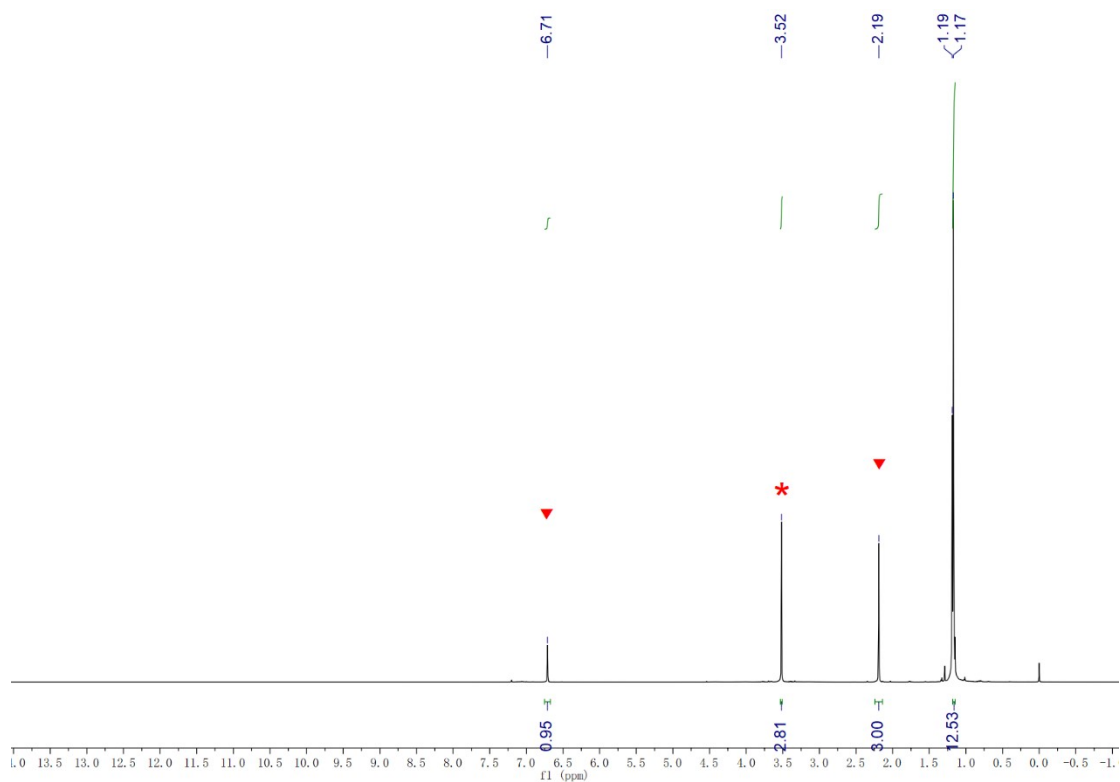


Figure S4.1.1 ^1H NMR spectrum of **4j** in CDCl_3

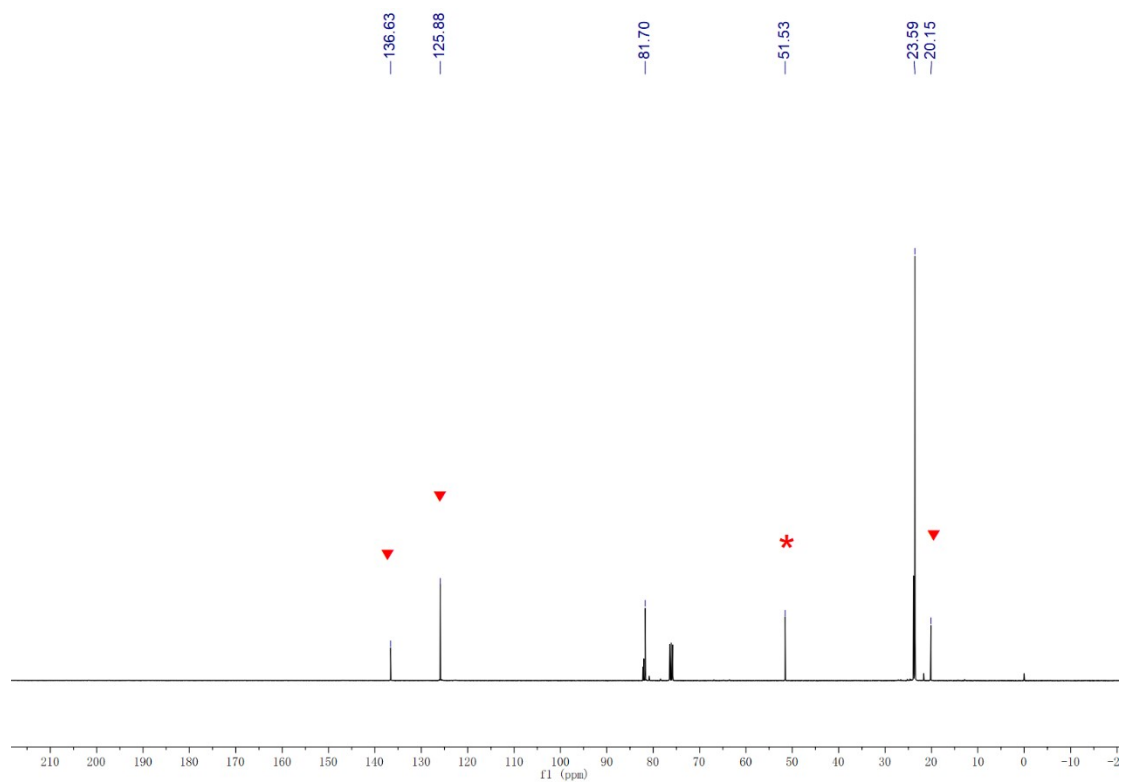


Figure S4.1.2 ^{13}C NMR spectrum NMR of **4j** in CDCl_3

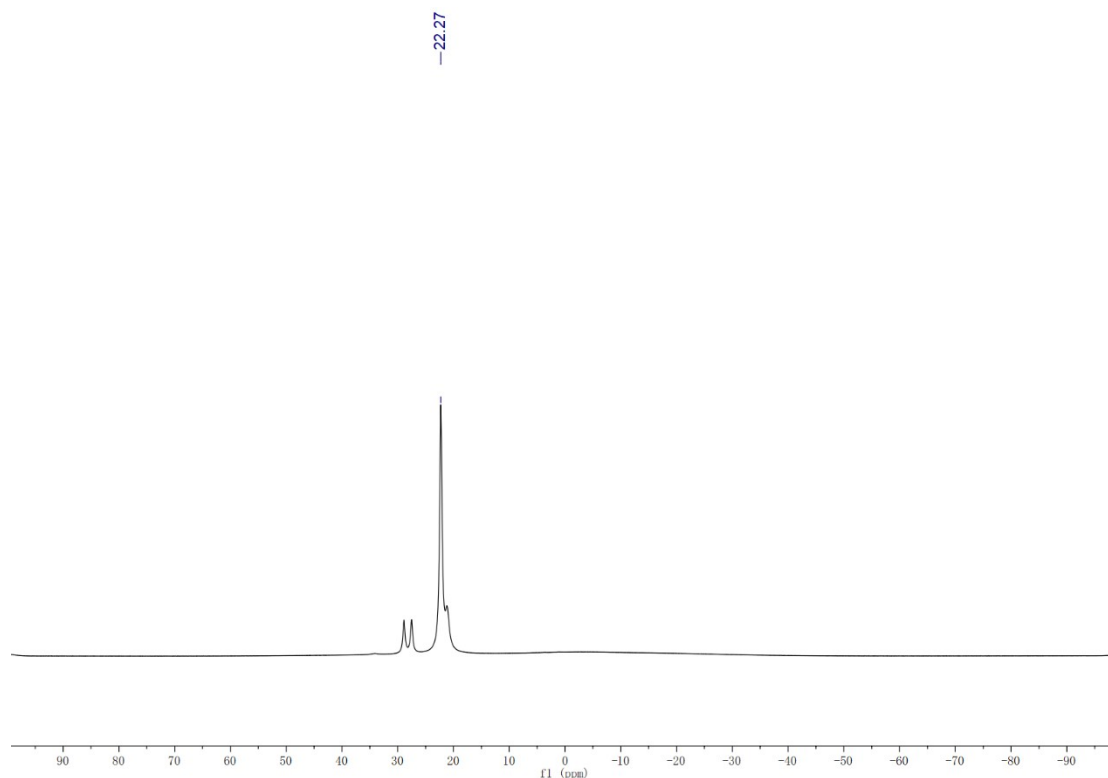


Figure S4.1.3 ^{11}B NMR spectrum of compound **4j** in CDCl_3

DFT Calculations

Computational Details

All computations reported in this article were performed employing a DFT method implemented in the Gaussian 09 suite of programs.^[S2] Geometry optimizations were carried out using gradient-corrected BP86 functional^[S3,S4] in conjunction with Ahlrichs' split valence plus polarization basis set (def2-SVP)^[S5,S6] for all the atoms. BP86 is composed of Becke's 1988 exchange and Perdew's 1986 correlation functionals. No symmetry constraints were imposed during structural optimizations. The frequency analyses were executed on the optimized geometries at the same level to ascertain the nature of stationary points and also to obtain the thermochemical energy values. The stationary points were characterized as either real minimum (no imaginary frequency) or transition state which is the first-order saddle point (one imaginary frequency) on the potential energy surface. The transition states were searched using the linear synchronous transit (LST) method,^[S7] and subsequent optimizations were performed

by utilizing the default Berny algorithm, implemented in the Gaussian 09 code. Intrinsic reaction coordinate (IRC) calculations were enforced to ensure that the transition state connects the corresponding real minima.^[S8,S9] Furthermore, to improve the accuracy of the energies obtained at the R-BP86/def2-SVP level, single-point calculations were performed on the optimized geometries employing the triple- ζ valence plus polarization basis set (def2-TZVP)^[S5,S6] for all the atoms. Tight wave function convergence criteria and “ultrafine” (99,950) grid were used in numerical integration during single-point calculations. Additionally, to incorporate the London dispersion effects, we used Grimme's D3 empirical corrections.^[S10] All the energy values (ΔG_L) reported in this article were obtained at the R-BP86-D3/def2-TZVP//R-BP86/def2-SVP level.

Moreover, to enrich our understanding towards the origin of activation barriers, distortion–interaction analysis was performed on the optimized geometries of selected transition states.^[S11,S12] The distortion–interaction model allows for partitioning the activation barrier of a transition state ($\Delta^\ddagger E$) into two physically meaningful terms:

$$\Delta^\ddagger E = \Delta^\ddagger E_{\text{dist}} + \Delta^\ddagger E_{\text{int}} \quad (\text{Eq. 1})$$

In Eq. 1, the destabilizing distortion energy term $\Delta^\ddagger E_{\text{dist}}$ accounts for the energy required to promote the reactants from their equilibrium geometries to the geometries in the transition state. In contrast, the stabilizing interaction energy term $\Delta^\ddagger E_{\text{int}}$ corresponds to the energy change upon interaction of the two distorted fragments. Optimized geometries were rendered using CYLview^[S13] visualization software.

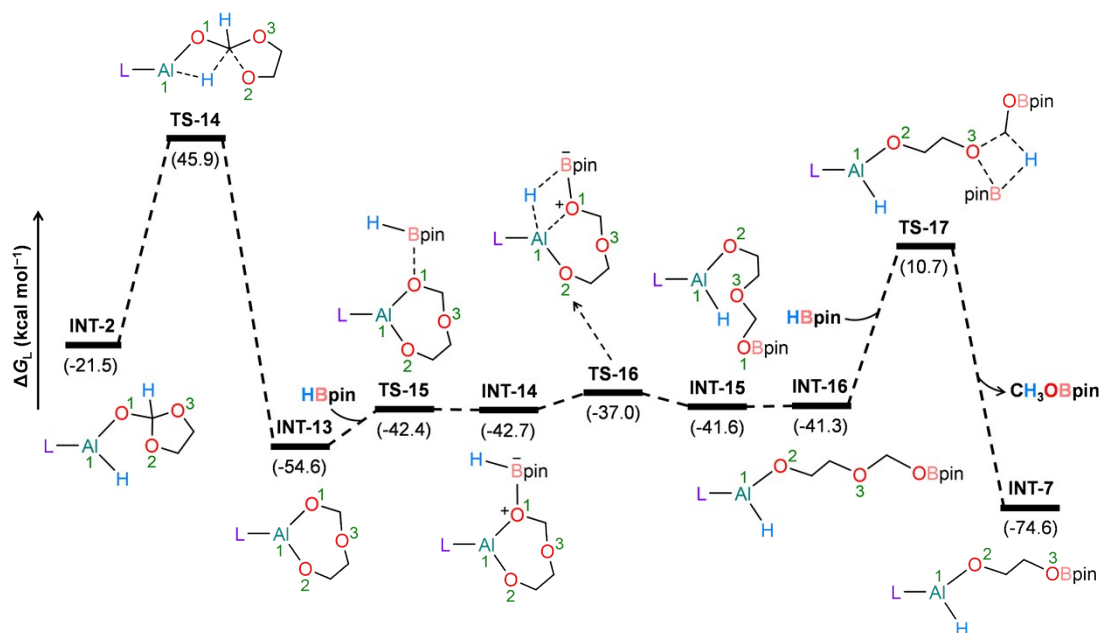


Figure S5. Energy profile for the formation of the intermediate **INT-7** and **CH₃OBpin** following unfavorable pathway. L = HC(CMeNAr)₂, Ar = 2,6 - Et₂C₆H₃.

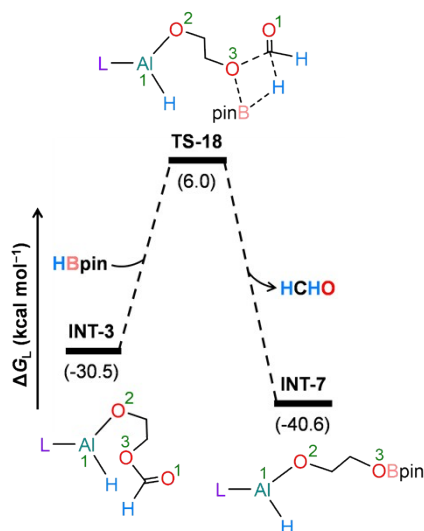


Figure S6. Energy profile for the formation of the intermediate **INT-7** and formaldehyde following unfavorable pathway. L = HC(CMeNAr)₂, Ar = 2,6 - Et₂C₆H₃.

Table S3. Distortion–interaction analysis of the transition state **TS-8**.^[a]

| $\Delta^\ddagger E$ | $\Delta^\ddagger E_{\text{dist}}$ | $\Delta^\ddagger E_{\text{dist-INT-3}}^{\text{[b]}}$ | $\Delta^\ddagger E_{\text{dist-2}}^{\text{[b]}}$ | $\Delta^\ddagger E_{\text{int}}$ |
|---------------------|-----------------------------------|--|--|----------------------------------|
| 12.7 | 36.3 | 27.7 | 8.6 | -23.6 |

^[a]Energy values are given in kcal mol⁻¹. ^[b] $\Delta^\ddagger E_{\text{dist-INT-3}}$ and $\Delta^\ddagger E_{\text{dist-2}}$ are distortion

energies of the **INT-3** and catalyst (**2**) fragments, respectively.

Table S4. Distortion–interaction analysis of the transition state **TS-18**.^[a]

| $\Delta^\ddagger E$ | $\Delta^\ddagger E_{\text{dist}}$ | $\Delta^\ddagger E_{\text{dist-INT-3}}^{[b]}$ | $\Delta^\ddagger E_{\text{dist-HBpin}}^{[b]}$ | $\Delta^\ddagger E_{\text{int}}$ |
|---------------------|-----------------------------------|---|---|----------------------------------|
| 22.6 | 50.5 | 22.7 | 27.8 | -27.9 |

^[a]Energy values are given in kcal mol⁻¹. ^[b] $\Delta^\ddagger E_{\text{dist-INT-3}}$ and $\Delta^\ddagger E_{\text{dist-HBpin}}$ are distortion energies of the **INT-3** and pinacolborane (**HBpin**) fragments, respectively.

Table S5. Absolute energies (in hartree) of the optimized geometries. E_e = Electronic energy at the R-BP86/def2-SVP level, G_{298} = Gibbs free energy at the R-BP86/def2-SVP level, and E^L = Electronic energy at the R-BP86-D3/def2-TZVP//R-BP86/def2-SVP level at 298 K.

| Species | E_e | G_{298} | E^L | No. of imaginary frequency |
|----------------------------|--------------|--------------|--------------|----------------------------|
| 3a | -342.1561788 | -342.11215 | -342.5564047 | 0 |
| 2 | -1324.899002 | -1324.439135 | -1326.218975 | 0 |
| HBpin | -411.5507017 | -411.400246 | -412.031617 | 0 |
| 4a | -1050.909046 | -1050.55018 | -1052.136061 | 0 |
| CH₃OBpin | -526.0486084 | -525.869773 | -526.6633053 | 0 |
| HCHO | -114.4165947 | -114.412687 | -114.5528376 | 0 |
| INT-1 | -1667.103246 | -1666.575679 | -1668.833084 | 0 |
| INT-2 | -1667.104076 | -1666.574595 | -1668.835191 | 0 |
| INT-3 | -1667.112781 | -1666.586744 | -1668.846007 | 0 |
| INT-4 | -1552.705351 | -1552.198718 | -1554.300882 | 0 |
| INT-5 | -1964.255127 | -1963.576647 | -1966.34447 | 0 |
| INT-6 | -1964.262757 | -1963.589797 | -1966.34233 | 0 |
| INT-7 | -1964.264152 | -1963.592807 | -1966.339563 | 0 |
| INT-8 | -2375.806976 | -2374.963255 | -2378.379093 | 0 |
| INT-9 | -2877.618125 | -2876.636057 | -2880.544391 | 0 |
| INT-10 | -3289.160672 | -3288.002453 | -3292.588431 | 0 |
| INT-11 | -1439.403552 | -1438.913046 | -1440.863673 | 0 |
| INT-12 | -1850.947852 | -1850.284246 | -1852.904334 | 0 |
| INT-13 | -1667.162048 | -1666.625917 | -1668.89461 | 0 |
| INT-14 | -2078.699904 | -2077.99118 | -2080.929407 | 0 |
| INT-15 | -2078.704241 | -2078.002329 | -2080.920785 | 0 |
| INT-16 | -2078.706123 | -2078.007449 | -2080.917125 | 0 |
| TS-1 | -1667.036911 | -1666.511016 | -1668.767348 | 1 |
| TS-2 | -1667.084377 | -1666.553598 | -1668.819722 | 1 |

| | | | | |
|--------------|--------------|--------------|--------------|---|
| TS-3 | -1667.079884 | -1666.548587 | -1668.815637 | 1 |
| TS-4 | -1964.250025 | -1963.570157 | -1966.343602 | 1 |
| TS-5 | -1964.247194 | -1963.568976 | -1966.334864 | 1 |
| TS-6 | -2375.803244 | -2374.958764 | -2378.379493 | 1 |
| TS-7 | -2375.78778 | -2374.943732 | -2378.360658 | 1 |
| TS-8 | -2991.96978 | -2990.962803 | -2995.044785 | 1 |
| TS-9 | -3289.157426 | -3288.000586 | -3292.588217 | 1 |
| TS-10 | -3289.150185 | -3287.994036 | -3292.575942 | 1 |
| TS-11 | -1439.305874 | -1438.820701 | -1440.771491 | 1 |
| TS-12 | -1850.944701 | -1850.281245 | -1852.904641 | 1 |
| TS-13 | -1850.93714 | -1850.275487 | -1852.891451 | 1 |
| TS-14 | -1666.98463 | -1666.461009 | -1668.721887 | 1 |
| TS-15 | -2078.699119 | -2077.989379 | -2080.930022 | 1 |
| TS-16 | -2078.69122 | -2077.983197 | -2080.919635 | 1 |
| TS-17 | -2490.178292 | -2489.309632 | -2492.88541 | 1 |
| TS-18 | -2078.618548 | -2077.919978 | -2080.841583 | 1 |

Table S6. Cartesian coordinates (Å) of the optimized geometries at the R-BP86/def2-SVP level.

| HBpin | | | |
|--------------|-------------|-------------|-------------|
| H | -0.00061600 | 3.16340700 | -0.00024600 |
| B | -0.00017500 | 1.95414200 | -0.00025700 |
| O | -1.09415900 | 1.20770100 | -0.36256100 |
| O | 1.09392100 | 1.20806700 | 0.36208400 |
| C | -0.79486200 | -0.19061800 | -0.04567000 |
| C | 0.79490800 | -0.19038700 | 0.04580200 |
| C | -1.48402100 | -0.49254200 | 1.29540500 |
| C | -1.37896400 | -1.07409600 | -1.15084700 |
| C | 1.37940100 | -1.07340200 | 1.15117200 |
| C | 1.48391200 | -0.49277300 | -1.29523300 |
| H | -2.56500100 | -0.26528100 | 1.20234900 |
| H | -1.37605800 | -1.55770400 | 1.58378500 |
| H | -1.07536900 | 0.13599900 | 2.11201500 |
| H | -1.11916200 | -2.14005900 | -0.98474100 |
| H | -2.48442300 | -0.98831000 | -1.15178400 |
| H | -1.01646900 | -0.77405200 | -2.15211300 |
| H | 1.11978300 | -2.13944700 | 0.98541000 |
| H | 2.48484300 | -0.98735300 | 1.15177700 |
| H | 1.01716300 | -0.77311900 | 2.15244300 |
| H | 1.37645900 | -1.55819200 | -1.58279800 |
| H | 1.07459300 | 0.13496200 | -2.11212700 |
| H | 2.56478600 | -0.26479600 | -1.20264600 |

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| | | | |
|----|-------------|-------------|-------------|
| N | 1.44875300 | -0.00006800 | 0.43976800 |
| C | 3.40481100 | -1.24347000 | -0.41989700 |
| Al | -0.00003600 | -0.00005200 | -0.86880500 |
| C | 4.68300100 | -1.21597500 | -1.01491300 |
| H | 5.18971800 | -2.16163300 | -1.25820900 |
| C | 1.27465200 | -0.00015100 | 1.77623000 |
| C | 0.00001600 | -0.00015500 | 2.39428300 |
| H | 0.00003300 | -0.00028900 | 3.49239600 |
| C | 2.77969300 | -0.00001500 | -0.11982600 |
| C | 4.68293300 | 1.21613600 | -1.01479600 |
| H | 5.18959600 | 2.16184300 | -1.25801000 |
| C | 5.31744800 | 0.00011200 | -1.30782600 |
| H | 6.31501300 | 0.00016400 | -1.77559200 |
| C | 3.40474600 | 1.24350500 | -0.41976300 |
| C | 2.49323500 | -0.00020400 | 2.67723400 |
| H | 3.13159400 | -0.88657200 | 2.48167700 |
| H | 2.20302300 | -0.00023500 | 3.74407400 |
| H | 3.13159200 | 0.88619500 | 2.48175800 |
| N | -1.44878500 | -0.00005400 | 0.43981400 |
| C | -3.40488600 | -1.24342600 | -0.41979200 |
| C | -4.68307300 | -1.21591000 | -1.01481400 |
| H | -5.18981100 | -2.16156000 | -1.25810000 |
| C | -1.27464200 | -0.00013800 | 1.77627200 |
| C | -2.77973700 | 0.00002000 | -0.11974700 |
| C | -4.68292800 | 1.21620100 | -1.01477800 |
| H | -5.18954900 | 2.16191700 | -1.25805000 |
| C | -5.31748400 | 0.00018700 | -1.30776200 |
| H | -6.31504400 | 0.00025500 | -1.77554100 |
| C | -3.40474200 | 1.24354900 | -0.41974100 |
| C | -2.49318900 | -0.00017600 | 2.67732700 |
| H | -3.13158200 | -0.88652100 | 2.48178000 |
| H | -2.20293100 | -0.00023700 | 3.74415500 |
| H | -3.13152700 | 0.88624700 | 2.48189900 |
| H | -0.00006500 | 1.36825100 | -1.71967300 |
| H | -0.00005500 | -1.36829800 | -1.71975800 |
| C | -2.68796300 | -2.54789200 | -0.10276800 |
| C | -3.41390800 | -3.83802900 | -0.49612100 |
| H | -2.45596900 | -2.57697300 | 0.98645200 |
| H | -1.69066900 | -2.51785800 | -0.59707700 |
| H | -2.79873900 | -4.72170500 | -0.22983900 |
| H | -4.38990300 | -3.94627200 | 0.02264700 |
| H | -3.60561300 | -3.88694600 | -1.58847300 |
| C | -2.68764300 | 2.54791600 | -0.10269800 |

| | | | |
|-----------|-------------|-------------|-------------|
| C | -3.41337200 | 3.83816500 | -0.49608000 |
| H | -1.69033200 | 2.51773100 | -0.59696300 |
| H | -2.45568700 | 2.57696400 | 0.98653100 |
| H | -2.79805800 | 4.72174600 | -0.22981900 |
| H | -3.60506400 | 3.88709500 | -1.58843500 |
| H | -4.38935300 | 3.94657600 | 0.02267800 |
| C | 2.68772000 | 2.54788900 | -0.10262100 |
| C | 3.41359500 | 3.83813100 | -0.49575500 |
| H | 2.45564600 | 2.57681100 | 0.98658600 |
| H | 1.69045800 | 2.51784800 | -0.59699600 |
| H | 2.79833600 | 4.72172700 | -0.22941600 |
| H | 4.38954500 | 3.94637500 | 0.02309600 |
| H | 3.60537700 | 3.88721100 | -1.58808800 |
| C | 2.68787100 | -2.54792500 | -0.10287400 |
| C | 3.41387000 | -3.83807300 | -0.49608800 |
| H | 1.69062700 | -2.51792200 | -0.59728700 |
| H | 2.45576400 | -2.57695300 | 0.98632300 |
| H | 2.79870000 | -4.72174300 | -0.22978900 |
| H | 3.60565100 | -3.88706600 | -1.58842400 |
| H | 4.38983300 | -3.94625700 | 0.02275400 |
| 3a | | | |
| C | 1.30240500 | 0.76100400 | -0.11758200 |
| C | 1.30246400 | -0.76097700 | 0.11760700 |
| H | 1.94600400 | 1.32166400 | 0.58846600 |
| H | 1.58546600 | 1.03181500 | -1.15897000 |
| H | 1.58544900 | -1.03181600 | 1.15900300 |
| H | 1.94611400 | -1.32158900 | -0.58843500 |
| O | -0.06852700 | -1.11887300 | -0.10671800 |
| O | -0.06860100 | 1.11888900 | 0.10668200 |
| C | -0.85744600 | -0.00000500 | -0.00000800 |
| O | -2.05631700 | -0.00004200 | 0.00001600 |
| 4a | | | |
| O | -1.42663100 | -0.98178200 | -0.16245100 |
| O | 1.51953400 | 1.04306800 | 0.67918600 |
| C | -0.35038700 | -0.07496400 | -0.39584200 |
| C | 0.43956200 | 0.13764200 | 0.90101500 |
| H | -0.71523000 | 0.90225400 | -0.77926500 |
| H | 0.31721800 | -0.52710500 | -1.16129900 |
| H | 0.80158800 | -0.84229500 | 1.28126400 |
| H | -0.22486500 | 0.58879000 | 1.66922200 |
| B | 2.76378400 | 0.57358200 | 0.37068800 |
| O | 3.83455700 | 1.42682300 | 0.18605000 |
| O | 3.07893500 | -0.76747500 | 0.21657000 |
| C | 4.92381500 | 0.62023300 | -0.34882900 |

| | | | |
|----------------------------|-------------|-------------|-------------|
| C | 4.53381700 | -0.84733200 | 0.13438100 |
| C | 4.89191700 | 0.77680400 | -1.87898900 |
| C | 6.24569300 | 1.15203700 | 0.21043400 |
| C | 4.90841900 | -1.96924600 | -0.83666000 |
| C | 5.04643600 | -1.17119500 | 1.54788300 |
| H | 4.94941900 | 1.85518300 | -2.12924800 |
| H | 5.74267400 | 0.25974200 | -2.36729600 |
| H | 3.94866300 | 0.37960300 | -2.30583100 |
| H | 7.09748900 | 0.51832700 | -0.11252800 |
| H | 6.42309400 | 2.17995800 | -0.16576000 |
| H | 6.23471700 | 1.19542700 | 1.31592900 |
| H | 6.00686000 | -2.01193700 | -0.98812300 |
| H | 4.58296700 | -2.94586000 | -0.42418300 |
| H | 4.42023400 | -1.83921400 | -1.82099100 |
| H | 6.14401500 | -1.32778900 | 1.56450900 |
| H | 4.79741300 | -0.36072000 | 2.26258500 |
| H | 4.55780500 | -2.10086500 | 1.90298500 |
| B | -2.71701200 | -0.54011600 | -0.11077800 |
| O | -3.76170700 | -1.39455600 | 0.18537100 |
| O | -3.11023000 | 0.76735800 | -0.35067800 |
| C | -4.99033900 | -0.66313400 | -0.09417300 |
| C | -4.51879700 | 0.85472800 | 0.01845300 |
| C | -5.43216500 | -1.04996200 | -1.51629800 |
| C | -6.05290800 | -1.08480300 | 0.92375500 |
| C | -5.21714500 | 1.82214200 | -0.93990500 |
| C | -4.57400500 | 1.39584300 | 1.45716500 |
| H | -5.52785500 | -2.15289800 | -1.57311100 |
| H | -6.41001700 | -0.60093500 | -1.78428100 |
| H | -4.68292500 | -0.73550900 | -2.27096600 |
| H | -6.98353500 | -0.49428600 | 0.79449900 |
| H | -6.30464700 | -2.15493400 | 0.77862400 |
| H | -5.69565200 | -0.96110100 | 1.96357400 |
| H | -6.30854300 | 1.85682400 | -0.74245400 |
| H | -4.81281900 | 2.84527200 | -0.79989000 |
| H | -5.05741600 | 1.53776500 | -1.99713400 |
| H | -5.61593900 | 1.56982400 | 1.79419100 |
| H | -4.08816200 | 0.69819400 | 2.16918800 |
| H | -4.02956600 | 2.36070500 | 1.49952000 |
| CH₃OBpin | | | |
| O | 2.50323500 | -0.71789600 | 0.18897100 |
| B | 1.18409700 | -0.38975400 | 0.10418000 |
| O | 0.19138900 | -1.28948500 | 0.44621500 |
| O | 0.70293000 | 0.84106400 | -0.31964100 |
| C | -1.06957500 | -0.70437500 | 0.01367400 |

| | | | |
|--------------|-------------|-------------|-------------|
| C | -0.72700300 | 0.85056100 | -0.03329000 |
| C | -1.38800200 | -1.28986400 | -1.37331200 |
| C | -2.15931800 | -1.09398900 | 1.01567400 |
| C | -1.44202300 | 1.63796800 | -1.13372600 |
| C | -0.91025700 | 1.54667700 | 1.32621300 |
| H | -1.39113900 | -2.39608400 | -1.30174900 |
| H | -2.37958800 | -0.96174700 | -1.74589400 |
| H | -0.61955500 | -1.00078500 | -2.11880300 |
| H | -3.12332200 | -0.60443500 | 0.76550200 |
| H | -2.31636800 | -2.19135400 | 0.98785100 |
| H | -1.88016800 | -0.82042500 | 2.05077600 |
| H | -2.54257700 | 1.60097600 | -0.99660700 |
| H | -1.12991000 | 2.70160100 | -1.09703100 |
| H | -1.19737100 | 1.24888500 | -2.14017800 |
| H | -1.98074900 | 1.66868600 | 1.58830400 |
| H | -0.41317600 | 0.97943300 | 2.13913400 |
| H | -0.44737500 | 2.55313100 | 1.28016900 |
| C | 3.51547700 | 0.23104100 | -0.12220900 |
| H | 4.28578300 | 0.21317300 | 0.67762200 |
| H | 4.00901000 | -0.04088600 | -1.08091600 |
| H | 3.10979000 | 1.26102600 | -0.21157700 |
| HCHO | | | |
| C | -0.52829900 | -0.00000600 | 0.00000000 |
| O | 0.68134100 | -0.00001700 | 0.00000000 |
| H | -1.14032600 | 0.95312700 | 0.00000100 |
| H | -1.14060800 | -0.95295600 | 0.00000100 |
| INT-1 | | | |
| N | -1.40777000 | -0.82059100 | 0.69337500 |
| C | -3.52472000 | 0.43037800 | 0.36405700 |
| Al | 0.01758200 | -0.15182700 | -0.42270900 |
| C | -4.80374100 | 0.48807700 | -0.22841900 |
| H | -5.43156400 | 1.37796900 | -0.07453600 |
| C | -1.22251700 | -1.35346300 | 1.92024500 |
| C | 0.05626600 | -1.54265200 | 2.49740200 |
| H | 0.06803100 | -1.97355900 | 3.50737100 |
| C | -2.74242500 | -0.73712100 | 0.13907000 |
| C | -4.49791100 | -1.70416200 | -1.23492200 |
| H | -4.88714700 | -2.52000200 | -1.86181500 |
| C | -5.28701700 | -0.56543700 | -1.01743300 |
| H | -6.28783000 | -0.49588700 | -1.47298600 |
| C | -3.21277400 | -1.81319500 | -0.66555000 |
| C | -2.42932100 | -1.80026100 | 2.71899600 |
| H | -3.14235500 | -0.96355300 | 2.86739900 |
| H | -2.13089800 | -2.19561500 | 3.70740200 |

| | | | |
|---|-------------|-------------|-------------|
| H | -2.99084000 | -2.58860100 | 2.17572800 |
| N | 1.47691300 | -0.76504500 | 0.68340100 |
| C | 3.53787200 | 0.57030600 | 0.33133400 |
| C | 4.80482600 | 0.68203300 | -0.27918500 |
| H | 5.39616900 | 1.59793900 | -0.13372000 |
| C | 1.32268300 | -1.30435500 | 1.91137100 |
| C | 2.80131100 | -0.62851500 | 0.11587400 |
| C | 4.57808100 | -1.52222400 | -1.28037800 |
| H | 4.99319800 | -2.32171000 | -1.91171800 |
| C | 5.32132100 | -0.35089200 | -1.07434000 |
| H | 6.31201600 | -0.23968900 | -1.54353900 |
| C | 3.30600900 | -1.68460300 | -0.69461500 |
| C | 2.55205700 | -1.70441400 | 2.70036800 |
| H | 3.23501000 | -0.84167100 | 2.84075800 |
| H | 2.27724400 | -2.10823400 | 3.69220200 |
| H | 3.13731100 | -2.47296800 | 2.15375700 |
| H | 0.03258900 | -0.76546600 | -1.90104400 |
| C | 2.95667700 | 1.68410300 | 1.18919800 |
| C | 3.81020600 | 2.94798600 | 1.32667600 |
| H | 2.73283600 | 1.27929900 | 2.20296100 |
| H | 1.96583200 | 1.95891000 | 0.76598600 |
| H | 3.29535100 | 3.68781400 | 1.97327900 |
| H | 4.80297300 | 2.74591500 | 1.78246200 |
| H | 3.97632000 | 3.43195800 | 0.34201600 |
| C | 2.47212900 | -2.93918900 | -0.91241200 |
| C | 3.09628900 | -4.03017500 | -1.78807800 |
| H | 1.49643300 | -2.62914500 | -1.35104000 |
| H | 2.20531900 | -3.37313600 | 0.07795000 |
| H | 2.40561000 | -4.89331600 | -1.87877300 |
| H | 3.30564900 | -3.66638600 | -2.81568000 |
| H | 4.04950700 | -4.41170700 | -1.36503200 |
| C | -2.33006200 | -3.03196100 | -0.89447000 |
| C | -2.91761900 | -4.14622600 | -1.76613800 |
| H | -2.03544100 | -3.45632500 | 0.09220000 |
| H | -1.37248100 | -2.68145000 | -1.34243200 |
| H | -2.19243500 | -4.97945500 | -1.86679000 |
| H | -3.84924600 | -4.56837700 | -1.33369200 |
| H | -3.15347600 | -3.78905700 | -2.79031400 |
| C | -2.97671900 | 1.56993100 | 1.20951100 |
| C | -3.89807500 | 2.77931300 | 1.39310800 |
| H | -2.02136500 | 1.90574700 | 0.74920400 |
| H | -2.68882700 | 1.17248200 | 2.20964200 |
| H | -3.40505500 | 3.54236000 | 2.02983800 |
| H | -4.13127600 | 3.26187200 | 0.42121900 |

| | | | |
|--------------|-------------|-------------|-------------|
| H | -4.86002900 | 2.51367600 | 1.88137700 |
| O | -0.01990800 | 1.62445500 | -0.42014100 |
| C | -0.00219800 | 2.53793500 | -1.43790500 |
| O | 1.02409800 | 3.51636600 | -1.26760400 |
| O | -1.24346300 | 3.25770000 | -1.45923200 |
| C | 0.41377400 | 4.66610700 | -0.68164800 |
| C | -0.97199300 | 4.65059900 | -1.33173100 |
| H | 0.34412700 | 4.57218100 | 0.42869700 |
| H | 1.02396500 | 5.55779300 | -0.93092600 |
| H | -1.76219800 | 5.12319400 | -0.71137900 |
| H | -0.95676800 | 5.14950700 | -2.33166900 |
| H | 0.17090000 | 2.05416900 | -2.43068100 |
| INT-2 | | | |
| N | 1.27712900 | 0.80670800 | -0.84973800 |
| C | 3.16653300 | 1.59120500 | 0.53017700 |
| Al | -0.07485600 | -0.01544600 | 0.26759200 |
| C | 4.47246200 | 1.38601700 | 1.02040900 |
| H | 4.90666300 | 2.10521600 | 1.73068400 |
| C | 1.02022800 | 1.49915000 | -1.97747600 |
| C | -0.29216300 | 1.74317500 | -2.45019300 |
| H | -0.36748300 | 2.31971300 | -3.38172700 |
| C | 2.63827100 | 0.64059700 | -0.39019700 |
| C | 4.68722600 | -0.65562100 | -0.28329000 |
| H | 5.28701900 | -1.52740100 | -0.58366800 |
| C | 5.22603100 | 0.27296200 | 0.61860000 |
| H | 6.24308300 | 0.12605100 | 1.01634300 |
| C | 3.38769900 | -0.49522000 | -0.80917700 |
| C | 2.17641400 | 2.06595700 | -2.77507400 |
| H | 2.77536100 | 2.76782600 | -2.15825200 |
| H | 1.81921000 | 2.60078700 | -3.67436000 |
| H | 2.87307100 | 1.26231300 | -3.09060900 |
| N | -1.60200500 | 0.64594000 | -0.71529000 |
| C | -3.46230300 | 1.18467800 | 0.81780500 |
| C | -4.70894800 | 0.83298700 | 1.37486500 |
| H | -5.16739200 | 1.48118100 | 2.13631200 |
| C | -1.51969600 | 1.36471800 | -1.85636100 |
| C | -2.89991600 | 0.32139700 | -0.16397800 |
| C | -4.79994900 | -1.17866200 | 0.01183700 |
| H | -5.32922100 | -2.09614000 | -0.28507000 |
| C | -5.37268800 | -0.33591000 | 0.97532000 |
| H | -6.34467600 | -0.59608500 | 1.42418100 |
| C | -3.55488900 | -0.87342200 | -0.57621400 |
| C | -2.79698400 | 1.81296700 | -2.53658500 |
| H | -3.40590900 | 2.44286600 | -1.85521600 |

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| H | -2.57981500 | 2.39010800 | -3.45419900 |
| H | -3.43467500 | 0.94519100 | -2.80300000 |
| C | -2.71630500 | 2.44313300 | 1.23799100 |
| C | -3.39546100 | 3.31771300 | 2.29643300 |
| H | -2.50837900 | 3.05835500 | 0.33303400 |
| H | -1.70920600 | 2.13832500 | 1.60266000 |
| H | -2.76589400 | 4.20118400 | 2.52762500 |
| H | -4.38339600 | 3.69474100 | 1.95723100 |
| H | -3.55361500 | 2.76764900 | 3.24757100 |
| C | -2.90876900 | -1.77981200 | -1.61376700 |
| C | -3.65564000 | -3.07592400 | -1.94418100 |
| H | -1.87967100 | -2.01690900 | -1.26297900 |
| H | -2.75522200 | -1.20113900 | -2.55368600 |
| H | -3.08933400 | -3.66354200 | -2.69543900 |
| H | -3.78060400 | -3.71959800 | -1.04824900 |
| H | -4.66565000 | -2.88730600 | -2.36625100 |
| C | 2.79224800 | -1.48655000 | -1.79744300 |
| C | 3.56734000 | -2.79259200 | -1.99556700 |
| H | 2.66870200 | -0.97792200 | -2.78259400 |
| H | 1.76093200 | -1.72486700 | -1.46115700 |
| H | 3.03418100 | -3.44687200 | -2.71544300 |
| H | 4.59031300 | -2.63020100 | -2.39673300 |
| H | 3.65080100 | -3.35028600 | -1.04012100 |
| C | 2.32268600 | 2.78345500 | 0.95824500 |
| C | 2.96723800 | 3.75447600 | 1.95231300 |
| H | 1.37244400 | 2.39250500 | 1.38719100 |
| H | 2.00604900 | 3.34638800 | 0.05088700 |
| H | 2.26548500 | 4.57822000 | 2.19578600 |
| H | 3.23173600 | 3.25395700 | 2.90727000 |
| H | 3.89220100 | 4.21659500 | 1.54723300 |
| O | 0.02363600 | -1.77694600 | 0.03795200 |
| C | 0.19303500 | -2.81984900 | 0.91151900 |
| O | 1.55907800 | -3.10262500 | 1.19903500 |
| O | -0.43384900 | -2.54531300 | 2.16987900 |
| C | 1.87487200 | -2.39874700 | 2.40275900 |
| C | 0.56345200 | -2.50438200 | 3.19186400 |
| H | 2.73817800 | -2.89790900 | 2.88639500 |
| H | 2.14703400 | -1.33559200 | 2.19743600 |
| H | 0.52594100 | -3.43516600 | 3.80727500 |
| H | 0.37932900 | -1.62976100 | 3.85116200 |
| H | 0.01771700 | 0.51716500 | 1.77353700 |
| H | -0.24111400 | -3.74566700 | 0.46670900 |
| INT-3 | | | |
| N | -1.08066200 | -0.66783800 | -1.04390500 |

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| C | -3.08112800 | -1.56145300 | 0.09538300 |
| Al | 0.17804900 | 0.08591800 | 0.22325300 |
| C | -4.43510100 | -1.40470900 | 0.45835100 |
| H | -4.92794300 | -2.17622000 | 1.06843300 |
| C | -0.72936300 | -1.28294100 | -2.19386500 |
| C | 0.61481000 | -1.48731100 | -2.58548100 |
| H | 0.76239000 | -2.00110100 | -3.54466400 |
| C | -2.47939800 | -0.54528300 | -0.69868400 |
| C | -4.55049800 | 0.72033700 | -0.72023900 |
| H | -5.13302800 | 1.60297800 | -1.02321400 |
| C | -5.16437300 | -0.27652800 | 0.05269300 |
| H | -6.22166600 | -0.17200600 | 0.34485000 |
| C | -3.19941200 | 0.61106800 | -1.10920000 |
| C | -1.81576700 | -1.80154300 | -3.11394200 |
| H | -2.45075900 | -2.54909300 | -2.59470900 |
| H | -1.38437100 | -2.26994600 | -4.01770600 |
| H | -2.49796700 | -0.98431600 | -3.42631100 |
| N | 1.78138000 | -0.49547900 | -0.69680600 |
| C | 3.53735000 | -1.11166900 | 0.92830900 |
| C | 4.73174500 | -0.77830700 | 1.60004100 |
| H | 5.14640700 | -1.47028800 | 2.34791700 |
| C | 1.79331000 | -1.13768500 | -1.88307900 |
| C | 3.02973700 | -0.19173900 | -0.03199900 |
| C | 4.88171800 | 1.32227400 | 0.38428300 |
| H | 5.41412700 | 2.26463600 | 0.18724300 |
| C | 5.39866000 | 0.42554500 | 1.33079300 |
| H | 6.32975500 | 0.66930400 | 1.86711700 |
| C | 3.68954700 | 1.03824000 | -0.31412800 |
| C | 3.12154200 | -1.52687200 | -2.49915100 |
| H | 3.69165900 | -2.19226600 | -1.81801800 |
| H | 2.97799700 | -2.04623800 | -3.46453400 |
| H | 3.76221700 | -0.63639500 | -2.66469600 |
| C | 2.79186900 | -2.40970300 | 1.20403800 |
| C | 3.40956600 | -3.34294300 | 2.24987200 |
| H | 2.66817100 | -2.96418000 | 0.24591400 |
| H | 1.75329900 | -2.14874200 | 1.50914800 |
| H | 2.78492500 | -4.25138300 | 2.37144100 |
| H | 4.42889900 | -3.67787200 | 1.96339300 |
| H | 3.48173500 | -2.85770800 | 3.24566600 |
| C | 3.10165900 | 2.00238000 | -1.33353100 |
| C | 3.85833400 | 3.31790500 | -1.54204800 |
| H | 2.05124200 | 2.21117700 | -1.02842200 |
| H | 3.00867600 | 1.47962000 | -2.31305200 |
| H | 3.33683900 | 3.94515000 | -2.29376500 |

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| H | 3.92189000 | 3.91183000 | -0.60600800 |
| H | 4.89487300 | 3.15768800 | -1.90799800 |
| C | -2.50615500 | 1.68308300 | -1.93632500 |
| C | -3.32864600 | 2.93636400 | -2.25161900 |
| H | -2.15598700 | 1.22923600 | -2.89215000 |
| H | -1.56867100 | 1.96766700 | -1.40789500 |
| H | -2.72160000 | 3.65706900 | -2.83677500 |
| H | -4.23594000 | 2.70807000 | -2.85031000 |
| H | -3.65792200 | 3.45508900 | -1.32688800 |
| C | -2.26271200 | -2.76874400 | 0.53040400 |
| C | -2.98481800 | -3.80815800 | 1.39327800 |
| H | -1.36587900 | -2.39478700 | 1.07415000 |
| H | -1.84840500 | -3.26885600 | -0.37452900 |
| H | -2.29546200 | -4.63677600 | 1.65462500 |
| H | -3.35134500 | -3.37242400 | 2.34618400 |
| H | -3.85612900 | -4.25537100 | 0.86977700 |
| O | -2.48137300 | 1.47406700 | 4.25512700 |
| C | -2.75819300 | 1.30979900 | 3.08644600 |
| O | -2.04591500 | 1.76896900 | 2.03422700 |
| O | 0.16732800 | 1.84647200 | 0.17706000 |
| C | -0.82293300 | 2.48292700 | 2.34272400 |
| C | -0.18691700 | 2.90179600 | 1.02286500 |
| H | -1.05895500 | 3.36971700 | 2.97107400 |
| H | -0.15686500 | 1.81541200 | 2.93064800 |
| H | -0.89887700 | 3.58620200 | 0.49697000 |
| H | 0.70947900 | 3.52093800 | 1.27841100 |
| H | 0.04609500 | -0.56874200 | 1.67953700 |
| H | -3.64949600 | 0.75638000 | 2.69340500 |
| INT-4 | | | |
| N | 1.43731700 | -0.00714700 | 0.78157100 |
| C | 3.39811800 | -1.23942800 | -0.08707400 |
| Al | 0.00002900 | -0.00004600 | -0.46919400 |
| C | 4.69333300 | -1.20180900 | -0.64415400 |
| H | 5.20907900 | -2.14376800 | -0.88277000 |
| C | 1.27296400 | -0.00478600 | 2.12315500 |
| C | 0.00019300 | -0.00007100 | 2.74286700 |
| H | 0.00032500 | -0.00020800 | 3.84098700 |
| C | 2.76995600 | 0.00025100 | 0.21578400 |
| C | 4.67826500 | 1.23109000 | -0.63882000 |
| H | 5.18202100 | 2.18058800 | -0.87314300 |
| C | 5.33115500 | 0.01919100 | -0.90849500 |
| H | 6.34383000 | 0.02639700 | -1.34267700 |
| C | 3.38322900 | 1.24929000 | -0.08047700 |
| C | 2.49710700 | -0.00666500 | 3.01265000 |

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| H | 3.13432500 | -0.89144700 | 2.80626900 |
| H | 2.21577400 | -0.01013500 | 4.08177200 |
| H | 3.13261900 | 0.88075900 | 2.81224100 |
| N | -1.43710500 | 0.00739400 | 0.78178100 |
| C | -3.38302300 | -1.24914900 | -0.08019100 |
| C | -4.67807200 | -1.23096500 | -0.63852000 |
| H | -5.18178000 | -2.18047400 | -0.87291100 |
| C | -1.27267600 | 0.00473100 | 2.12336000 |
| C | -2.76977300 | -0.00010700 | 0.21605800 |
| C | -4.69322900 | 1.20193200 | -0.64377900 |
| H | -5.20901900 | 2.14388300 | -0.88231900 |
| C | -5.33101500 | -0.01909200 | -0.90814600 |
| H | -6.34368400 | -0.02634800 | -1.34233900 |
| C | -3.39798900 | 1.23956100 | -0.08677200 |
| C | -2.49670000 | 0.00634500 | 3.01298500 |
| H | -3.13175600 | -0.88150000 | 2.81296700 |
| H | -2.21523100 | 0.01027500 | 4.08207300 |
| H | -3.13439700 | 0.89071400 | 2.80638000 |
| C | -2.62358800 | -2.54451200 | 0.16634200 |
| C | -3.37653800 | -3.84375400 | -0.13547700 |
| H | -2.26701900 | -2.56447500 | 1.22100000 |
| H | -1.69426400 | -2.50036000 | -0.44887200 |
| H | -2.73175000 | -4.71983800 | 0.08112800 |
| H | -4.29749700 | -3.94894200 | 0.47669800 |
| H | -3.67237100 | -3.91220700 | -1.20321900 |
| C | -2.65517400 | 2.54576100 | 0.15021400 |
| C | -3.43939400 | 3.83376400 | -0.11943100 |
| H | -1.74431900 | 2.52337900 | -0.49294600 |
| H | -2.26912400 | 2.56311700 | 1.19419800 |
| H | -2.80724300 | 4.71965400 | 0.09465000 |
| H | -3.75867700 | 3.91005800 | -1.17986100 |
| H | -4.34934400 | 3.91310400 | 0.51283700 |
| C | 2.62381300 | 2.54465200 | 0.16613500 |
| C | 3.37680000 | 3.84389300 | -0.13560000 |
| H | 2.26722100 | 2.56455800 | 1.22078100 |
| H | 1.69451800 | 2.50055100 | -0.44912300 |
| H | 2.73204000 | 4.71998800 | 0.08103900 |
| H | 4.29774700 | 3.94902800 | 0.47660800 |
| H | 3.67266900 | 3.91238900 | -1.20332900 |
| C | 2.65529400 | -2.54562300 | 0.14984300 |
| C | 3.43966500 | -3.83360800 | -0.11944000 |
| H | 1.74460200 | -2.52335400 | -0.49356400 |
| H | 2.26889300 | -2.56288600 | 1.19369400 |
| H | 2.80753600 | -4.71951600 | 0.09462300 |

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| H | 3.75917600 | -3.91004400 | -1.17979300 |
| H | 4.34949200 | -3.91275500 | 0.51302900 |
| O | 0.03469100 | -1.31951400 | -1.65213400 |
| O | -0.03515900 | 1.31918800 | -1.65232600 |
| C | -0.20941600 | -0.75207600 | -2.93730600 |
| C | 0.20723600 | 0.75159200 | -2.93769500 |
| H | 0.35600900 | -1.30718400 | -3.72282200 |
| H | -1.29546600 | -0.84053400 | -3.19260000 |
| H | 1.29294100 | 0.84003200 | -3.19447200 |
| H | -0.35924700 | 1.30652300 | -3.72257900 |
| INT-5 | | | |
| N | 1.97323800 | 0.08838600 | 0.83227300 |
| C | 2.82292800 | -2.23590000 | 0.53532800 |
| Al | 0.51558900 | 0.59211600 | -0.27605300 |
| C | 3.76234000 | -3.09665100 | -0.07654600 |
| H | 3.68309900 | -4.18151000 | 0.09530500 |
| C | 2.15693300 | 0.60114500 | 2.07086500 |
| C | 1.30542000 | 1.58055400 | 2.63510800 |
| H | 1.56050500 | 1.90339700 | 3.65301000 |
| C | 2.94397000 | -0.84216700 | 0.28136300 |
| C | 4.89237900 | -1.21984100 | -1.12389200 |
| H | 5.70191800 | -0.84021700 | -1.76454300 |
| C | 4.78199700 | -2.60084500 | -0.89661200 |
| H | 5.50003800 | -3.29384300 | -1.36379000 |
| C | 3.98008800 | -0.31503600 | -0.54687500 |
| C | 3.33534600 | 0.12888400 | 2.89153800 |
| H | 3.26304000 | -0.95978800 | 3.09255000 |
| H | 3.39267000 | 0.66632400 | 3.85571100 |
| H | 4.28585200 | 0.27673700 | 2.33834400 |
| N | -0.25006700 | 1.95964600 | 0.79489600 |
| C | -2.67753400 | 2.43037700 | 0.48890200 |
| C | -3.67545900 | 3.23454100 | -0.10585400 |
| H | -4.73437400 | 2.99768800 | 0.07720600 |
| C | 0.21088300 | 2.24791700 | 2.03680600 |
| C | -1.31956400 | 2.76610000 | 0.22812700 |
| C | -1.99982500 | 4.63987900 | -1.16248500 |
| H | -1.75259400 | 5.50018200 | -1.80170400 |
| C | -3.34518300 | 4.32237200 | -0.92304000 |
| H | -4.14305800 | 4.93229000 | -1.37639300 |
| C | -0.96191700 | 3.87308000 | -0.59655500 |
| C | -0.45282000 | 3.35560100 | 2.82389600 |
| H | -1.52619800 | 3.13335900 | 2.99373600 |
| H | 0.04150500 | 3.50145900 | 3.80170900 |
| H | -0.42339600 | 4.31051600 | 2.25923700 |

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| C | -3.05801100 | 1.24095400 | 1.35484000 |
| C | -4.36075700 | 1.38925000 | 2.15528700 |
| H | -2.22568500 | 1.00567000 | 2.04886300 |
| H | -3.13454300 | 0.33859200 | 0.70232100 |
| H | -4.50717900 | 0.50655500 | 2.81103400 |
| H | -4.35647800 | 2.29378700 | 2.80124300 |
| H | -5.25569400 | 1.45268100 | 1.50194700 |
| C | 0.50175700 | 4.19482700 | -0.85907400 |
| C | 0.78930600 | 5.50174600 | -1.60562600 |
| H | 0.92882300 | 3.34063600 | -1.43318900 |
| H | 1.05124300 | 4.19857900 | 0.10890600 |
| H | 1.88343000 | 5.64761700 | -1.71520600 |
| H | 0.35803100 | 5.50011200 | -2.62846800 |
| H | 0.38612600 | 6.38868000 | -1.07206000 |
| C | 4.07270900 | 1.18338300 | -0.79677000 |
| C | 5.28803700 | 1.66822100 | -1.59357200 |
| H | 4.04101900 | 1.71506700 | 0.18087300 |
| H | 3.13945100 | 1.49036200 | -1.32268200 |
| H | 5.26248100 | 2.77220300 | -1.69756200 |
| H | 6.24738400 | 1.40213400 | -1.10104100 |
| H | 5.30799900 | 1.24486200 | -2.61955200 |
| C | 1.72670400 | -2.81279300 | 1.41531400 |
| C | 2.19511600 | -3.86884000 | 2.43136200 |
| H | 0.93868400 | -3.25365900 | 0.76269100 |
| H | 1.20647400 | -1.99342400 | 1.94903500 |
| H | 1.34061900 | -4.20752400 | 3.05257800 |
| H | 2.61543900 | -4.77188400 | 1.94194200 |
| H | 2.97612100 | -3.47368400 | 3.11668700 |
| O | 0.91979200 | 1.12652400 | -1.91491400 |
| C | -0.63269100 | -0.67433700 | -2.38947900 |
| C | 0.57650400 | 0.14892500 | -2.88363600 |
| H | -0.65310000 | -1.68833400 | -2.83621100 |
| H | -1.60109500 | -0.16947600 | -2.59224500 |
| H | 1.44197600 | -0.53336800 | -3.07184800 |
| H | 0.32247600 | 0.63103400 | -3.85603100 |
| O | -0.47760400 | -0.79518300 | -0.95108700 |
| B | -1.39259200 | -1.71801800 | -0.02415700 |
| O | -2.77382800 | -1.52557100 | -0.42409200 |
| O | -1.09448800 | -3.12337300 | -0.19283100 |
| H | -1.04531200 | -1.24757300 | 1.08599200 |
| C | -3.43751400 | -2.79458500 | -0.32570000 |
| C | -2.26317300 | -3.82324100 | -0.65253000 |
| C | -3.97788700 | -2.95729900 | 1.11188500 |
| C | -4.60904400 | -2.82034100 | -1.31611700 |

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| C | -2.35922700 | -5.16137900 | 0.09724500 |
| C | -2.12214900 | -4.10913600 | -2.16200000 |
| H | -4.64637500 | -2.10230000 | 1.34144300 |
| H | -4.56076700 | -3.89258700 | 1.24101100 |
| H | -3.15341800 | -2.95237300 | 1.85295400 |
| H | -5.09763200 | -3.81706200 | -1.33766000 |
| H | -5.37255200 | -2.07423200 | -1.01322200 |
| H | -4.28072100 | -2.56548200 | -2.34188200 |
| H | -3.29888100 | -5.69929300 | -0.14989000 |
| H | -1.50959600 | -5.81408800 | -0.19248100 |
| H | -2.31141600 | -5.01599400 | 1.19320300 |
| H | -2.92852600 | -4.77086200 | -2.54144000 |
| H | -2.13915300 | -3.17473400 | -2.75689300 |
| H | -1.14948900 | -4.61222400 | -2.33985300 |
| INT-6 | | | |
| N | -0.91010000 | 1.97508500 | 0.83895000 |
| C | 1.36984500 | 2.86952000 | 1.18859900 |
| Al | -0.82561400 | 0.21546500 | 0.02242900 |
| C | 2.39135100 | 3.75475300 | 0.78675500 |
| H | 3.35374000 | 3.75041500 | 1.31905800 |
| C | -1.90221100 | 2.38957500 | 1.65413300 |
| C | -3.03008600 | 1.59504900 | 1.97189300 |
| H | -3.76053900 | 2.05008500 | 2.65402900 |
| C | 0.14207500 | 2.89762300 | 0.47285800 |
| C | 0.98877800 | 4.64001700 | -0.99137100 |
| H | 0.86026900 | 5.32720600 | -1.84092600 |
| C | 2.20252500 | 4.63471200 | -0.28806000 |
| H | 3.01389100 | 5.31711600 | -0.58813900 |
| C | -0.06248400 | 3.77177200 | -0.63252400 |
| C | -1.82435400 | 3.77388000 | 2.26607500 |
| H | -0.86854500 | 3.91072700 | 2.81249800 |
| H | -2.66455400 | 3.95010500 | 2.96293000 |
| H | -1.84447900 | 4.55941700 | 1.48256900 |
| N | -2.55294200 | -0.40051800 | 0.66451800 |
| C | -2.55089100 | -2.84472100 | 1.03069500 |
| C | -2.91470100 | -4.13246700 | 0.58504700 |
| H | -2.61943500 | -5.01472700 | 1.17219200 |
| C | -3.35353000 | 0.30320000 | 1.49190800 |
| C | -2.94948600 | -1.72624700 | 0.24492800 |
| C | -4.02537900 | -3.19368900 | -1.36354800 |
| H | -4.59480100 | -3.34603300 | -2.29250000 |
| C | -3.64607300 | -4.30657800 | -0.59882200 |
| H | -3.92016600 | -5.32080200 | -0.93104700 |
| C | -3.68473700 | -1.88473100 | -0.96356100 |

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|---|-------------|-------------|-------------|
| C | -4.66928400 | -0.30218300 | 1.93780400 |
| H | -4.50988700 | -1.27106200 | 2.45433600 |
| H | -5.21273600 | 0.37905300 | 2.61824700 |
| H | -5.31708800 | -0.52391200 | 1.06434300 |
| C | -1.75354100 | -2.62941200 | 2.30924800 |
| C | -1.34987200 | -3.88864500 | 3.08237400 |
| H | -2.32856200 | -1.95624700 | 2.98523500 |
| H | -0.84310700 | -2.04444500 | 2.04775500 |
| H | -0.76965900 | -3.61479400 | 3.98725500 |
| H | -2.23058100 | -4.47529000 | 3.41954400 |
| H | -0.71161000 | -4.56172800 | 2.47242400 |
| C | -4.06486700 | -0.66307300 | -1.78554300 |
| C | -4.86904100 | -0.92418700 | -3.06277200 |
| H | -3.12043300 | -0.12648300 | -2.03277800 |
| H | -4.62866200 | 0.04635500 | -1.13775200 |
| H | -5.08790600 | 0.03201300 | -3.58081900 |
| H | -4.31257500 | -1.56469700 | -3.77905400 |
| H | -5.84220700 | -1.41904000 | -2.85697300 |
| C | -1.37778600 | 3.73459100 | -1.39747900 |
| C | -1.48394400 | 4.65737000 | -2.61573600 |
| H | -2.21363400 | 3.96476300 | -0.69772000 |
| H | -1.55584400 | 2.67942500 | -1.70431300 |
| H | -2.47198300 | 4.53567600 | -3.10514500 |
| H | -1.38030000 | 5.72931700 | -2.34372000 |
| H | -0.70871100 | 4.42854300 | -3.37689800 |
| C | 1.54899400 | 1.89984700 | 2.34714400 |
| C | 2.92928900 | 1.88454700 | 3.00946000 |
| H | 1.31222300 | 0.87760800 | 1.97664000 |
| H | 0.76868700 | 2.10798200 | 3.11532900 |
| H | 2.95187000 | 1.14268900 | 3.83398900 |
| H | 3.71623600 | 1.59871300 | 2.28174000 |
| H | 3.20026200 | 2.86978000 | 3.44479600 |
| O | -0.92692300 | 0.36689500 | -1.72450100 |
| C | 1.15534300 | -0.50563900 | -2.72347800 |
| C | -0.07611000 | 0.38703600 | -2.83538300 |
| H | 1.67457900 | -0.52723600 | -3.71055500 |
| H | 0.85633100 | -1.54838700 | -2.47492700 |
| H | 0.27467600 | 1.42886900 | -3.04595900 |
| H | -0.63841700 | 0.05162400 | -3.74201200 |
| O | 2.04355100 | 0.01031200 | -1.72564600 |
| B | 2.96060100 | -0.81086800 | -1.13941700 |
| O | 3.16945200 | -2.13257000 | -1.50534900 |
| O | 3.79665400 | -0.37643300 | -0.12298400 |
| H | 0.32494400 | -0.73029200 | 0.61306100 |

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| C | 4.06342500 | -2.70787200 | -0.50913100 |
| C | 4.79693200 | -1.41754700 | 0.06767000 |
| C | 3.17974400 | -3.41334600 | 0.53372000 |
| C | 4.98212100 | -3.71857500 | -1.20009300 |
| C | 5.15366000 | -1.49637900 | 1.55417800 |
| C | 6.03355700 | -1.01232600 | -0.75398300 |
| H | 2.54061600 | -4.15688700 | 0.01627500 |
| H | 3.78294700 | -3.94474400 | 1.29767000 |
| H | 2.51141200 | -2.69171600 | 1.04546000 |
| H | 5.73238500 | -4.12353900 | -0.48966700 |
| H | 4.38159600 | -4.56889400 | -1.58260700 |
| H | 5.51468400 | -3.26817900 | -2.05911200 |
| H | 5.84755300 | -2.34005800 | 1.75048900 |
| H | 5.65904500 | -0.56112900 | 1.87008500 |
| H | 4.25307200 | -1.62436900 | 2.18375600 |
| H | 6.88152600 | -1.71050600 | -0.60099700 |
| H | 5.80254000 | -0.97268200 | -1.83785200 |
| H | 6.35517700 | 0.00083300 | -0.43919400 |
| INT-7 | | | |
| Al | -1.30348200 | 0.12873200 | 0.20046700 |
| N | -1.93015700 | 1.93702100 | -0.08422200 |
| N | -3.03225100 | -0.72564800 | 0.01287200 |
| O | -0.23144000 | -0.34401900 | -1.11946200 |
| O | 3.28100300 | -1.15322100 | -1.80174200 |
| C | -3.21421300 | 2.27294600 | -0.33484700 |
| C | -0.91991100 | 2.97029100 | -0.02164500 |
| C | -4.18486000 | -0.07869400 | -0.25665600 |
| C | -3.03056500 | -2.16411900 | 0.16052700 |
| C | 0.95808700 | -1.09758700 | -1.05924700 |
| C | 2.11725900 | -0.32660500 | -1.70630000 |
| C | -4.26275000 | 1.32603700 | -0.41439500 |
| C | -3.56772800 | 3.73235200 | -0.53529300 |
| C | -0.59817000 | 3.54279900 | 1.24077100 |
| C | -0.23859900 | 3.34814000 | -1.21319100 |
| C | -5.46521500 | -0.87666900 | -0.39269900 |
| C | -3.18546900 | -2.72181200 | 1.46079100 |
| C | -2.81623900 | -2.98056100 | -0.98614900 |
| H | 0.83721800 | -2.06494900 | -1.60528700 |
| H | 1.24333700 | -1.35404700 | -0.00835400 |
| H | 2.32863400 | 0.59873300 | -1.12669000 |
| H | 1.82824200 | -0.03532800 | -2.73915600 |
| H | -5.26125800 | 1.73146200 | -0.62517800 |
| H | -3.28250400 | 4.33412500 | 0.35237800 |
| H | -4.65050900 | 3.85991600 | -0.71861100 |

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| H | -3.00810400 | 4.16423500 | -1.39054700 |
| C | 0.41775800 | 4.51995600 | 1.28580300 |
| C | -1.34241500 | 3.09283700 | 2.48996000 |
| C | 0.76823200 | 4.33090000 | -1.11355100 |
| C | -0.59548000 | 2.68566600 | -2.53524700 |
| H | -5.66997000 | -1.45813000 | 0.52997500 |
| H | -6.32854400 | -0.21683500 | -0.59675200 |
| H | -5.38425900 | -1.62066600 | -1.21198500 |
| C | -3.13732200 | -4.12525600 | 1.59006100 |
| C | -3.39149000 | -1.80627200 | 2.65915900 |
| C | -2.77767400 | -4.37846800 | -0.80202900 |
| C | -2.62379900 | -2.33895000 | -2.35231800 |
| H | 0.68787300 | 4.97996400 | 2.24787200 |
| C | 1.09294100 | 4.91236200 | 0.12096500 |
| C | -0.92515000 | 3.75287900 | 3.80776700 |
| H | -1.22796500 | 1.98868400 | 2.57774100 |
| H | -2.43466700 | 3.24611400 | 2.33383100 |
| H | 1.31194700 | 4.64402100 | -2.01719800 |
| C | 0.19832900 | 3.14409100 | -3.76236700 |
| H | -1.68264500 | 2.82964000 | -2.73078900 |
| H | -0.47782300 | 1.58635800 | -2.39952900 |
| H | -3.25413000 | -4.58459300 | 2.58279500 |
| C | -2.93802200 | -4.94611600 | 0.47048100 |
| C | -3.53005600 | -2.48879800 | 4.02345900 |
| H | -4.28659900 | -1.16878700 | 2.47678300 |
| H | -2.54174200 | -1.08734800 | 2.69012300 |
| H | -2.61409700 | -5.03526400 | -1.66923600 |
| C | -2.38136100 | -3.29388300 | -3.52528400 |
| H | -1.77784700 | -1.61866400 | -2.26892500 |
| H | -3.50922500 | -1.70207000 | -2.57955600 |
| H | 1.88488100 | 5.67639900 | 0.17649000 |
| H | -1.52550200 | 3.34785600 | 4.64788000 |
| H | 0.14274800 | 3.56349700 | 4.04451000 |
| H | -1.07694200 | 4.85288100 | 3.79253200 |
| H | -0.14038900 | 2.59558600 | -4.66499200 |
| H | 0.07208100 | 4.22849100 | -3.96758600 |
| H | 1.28523800 | 2.94822200 | -3.64835300 |
| H | -2.90148400 | -6.04060100 | 0.59184900 |
| H | -3.66776400 | -1.73021800 | 4.82086700 |
| H | -4.40369200 | -3.17319800 | 4.06343900 |
| H | -2.62700400 | -3.07986900 | 4.28316600 |
| H | -2.24738500 | -2.72006300 | -4.46496700 |
| H | -1.46468900 | -3.90312200 | -3.38027500 |
| H | -3.22923400 | -3.99401200 | -3.68327600 |

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| H | -0.64751300 | -0.11175500 | 1.64495900 |
| B | 4.25635900 | -1.09885600 | -0.85277200 |
| O | 5.39529100 | -1.88123600 | -0.93859100 |
| O | 4.22654500 | -0.27820200 | 0.26566200 |
| C | 6.09086000 | -1.74782300 | 0.33266100 |
| C | 5.54704900 | -0.35255200 | 0.87632600 |
| C | 5.66512600 | -2.93910600 | 1.20884400 |
| C | 7.59890800 | -1.79484100 | 0.07271500 |
| C | 5.38936100 | -0.26717600 | 2.39648300 |
| C | 6.35297500 | 0.85009000 | 0.35565500 |
| H | 5.87881600 | -3.87924600 | 0.66161500 |
| H | 6.21346300 | -2.96380800 | 2.17246000 |
| H | 4.57771200 | -2.91211900 | 1.42431000 |
| H | 8.16974400 | -1.62116300 | 1.00848500 |
| H | 7.87899700 | -2.79438600 | -0.31752800 |
| H | 7.90854700 | -1.04223400 | -0.67694700 |
| H | 6.36673200 | -0.39919700 | 2.90536700 |
| H | 4.99065100 | 0.72933900 | 2.67560500 |
| H | 4.68473200 | -1.03021300 | 2.77773600 |
| H | 7.35175100 | 0.91827000 | 0.83271300 |
| H | 6.49218200 | 0.79557600 | -0.74315500 |
| H | 5.79471200 | 1.78074900 | 0.58244600 |
| INT-8 | | | |
| Al | -1.07897100 | -0.73991800 | 0.03816800 |
| N | -1.60303000 | -1.27031400 | 1.81237000 |
| N | -2.77365600 | -0.98202600 | -0.83775500 |
| O | -0.32067900 | 0.93457900 | -0.14931400 |
| O | 3.26757800 | 1.62919600 | -0.62579800 |
| C | -2.89882200 | -1.44004100 | 2.16388800 |
| C | -0.55631700 | -1.59699900 | 2.76496000 |
| C | -3.92468900 | -1.17051400 | -0.15282100 |
| C | -2.78254900 | -1.07004900 | -2.28731200 |
| C | 0.91962700 | 1.14636000 | -0.86679700 |
| C | 2.10786800 | 1.20581200 | 0.09663700 |
| C | -3.97557400 | -1.30235400 | 1.25543100 |
| C | -3.23030200 | -1.85719100 | 3.58102300 |
| C | 0.01886800 | -2.90060500 | 2.70905700 |
| C | -0.11638000 | -0.62673500 | 3.71029400 |
| C | -5.22364900 | -1.30880600 | -0.91758400 |
| C | -2.50762000 | -2.33617900 | -2.88240600 |
| C | -3.03884800 | 0.08637200 | -3.07699800 |
| H | 0.82142500 | 2.09699200 | -1.42500900 |
| H | 1.04774300 | 0.31904800 | -1.59586200 |
| H | 2.27170700 | 0.21454600 | 0.57337900 |

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| H | 1.88816800 | 1.95377500 | 0.88501500 |
| H | -4.97839900 | -1.42708700 | 1.68495800 |
| H | -2.76252300 | -2.83592900 | 3.81726600 |
| H | -4.32288700 | -1.94408000 | 3.72490900 |
| H | -2.82643200 | -1.13657400 | 4.32026300 |
| C | 1.07022500 | -3.20592400 | 3.59635300 |
| C | -0.51296000 | -3.92908400 | 1.72167500 |
| C | 0.93657500 | -0.98989700 | 4.57926300 |
| C | -0.75399400 | 0.74945200 | 3.79397100 |
| H | -5.18541500 | -2.18487300 | -1.59835600 |
| H | -6.08013500 | -1.43275400 | -0.22974500 |
| H | -5.40474700 | -0.42536000 | -1.56271700 |
| C | -2.47031400 | -2.41930300 | -4.28872200 |
| C | -2.27299200 | -3.55717000 | -2.00507200 |
| C | -2.99604500 | -0.05629300 | -4.48161600 |
| C | -3.34523200 | 1.42807700 | -2.43581900 |
| H | 1.53289400 | -4.20336500 | 3.56916600 |
| C | 1.53123200 | -2.25649500 | 4.51949100 |
| C | 0.10589900 | -5.32869500 | 1.79227700 |
| H | -0.37808500 | -3.52093800 | 0.69464800 |
| H | -1.61639600 | -4.00982200 | 1.84741200 |
| H | 1.29637000 | -0.26048800 | 5.31998500 |
| C | -0.61210500 | 1.47187100 | 5.14062800 |
| H | -1.82969200 | 0.67281100 | 3.53160400 |
| H | -0.34179900 | 1.40828200 | 2.99526300 |
| H | -2.25635000 | -3.38409800 | -4.77160800 |
| C | -2.70788700 | -1.28811600 | -5.08285300 |
| C | -2.05155200 | -4.88812700 | -2.73061900 |
| H | -3.12777500 | -3.66325500 | -1.29938800 |
| H | -1.39685200 | -3.34643300 | -1.35110400 |
| H | -3.19369000 | 0.82043500 | -5.11605400 |
| C | -4.08815300 | 2.44398500 | -3.31246500 |
| H | -2.40280800 | 1.90104100 | -2.07956100 |
| H | -3.91759200 | 1.26571000 | -1.49850300 |
| H | 2.35525100 | -2.51052000 | 5.20541000 |
| H | -0.36424700 | -5.99548900 | 1.04089700 |
| H | 1.19529700 | -5.31161700 | 1.58014400 |
| H | -0.03608100 | -5.79896800 | 2.78816800 |
| H | -1.18110500 | 2.42371800 | 5.12135500 |
| H | -0.99730600 | 0.86489400 | 5.98826300 |
| H | 0.44149500 | 1.73529500 | 5.37031600 |
| H | -2.67507000 | -1.37023100 | -6.18112700 |
| H | -1.90218400 | -5.70632700 | -1.99681100 |
| H | -2.91848600 | -5.16696400 | -3.36600100 |

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| H | -1.15243600 | -4.86146500 | -3.38099200 |
| H | -4.30953200 | 3.35573900 | -2.72192700 |
| H | -3.48506200 | 2.76855600 | -4.18619800 |
| H | -5.05038300 | 2.04478400 | -3.69976100 |
| H | 0.05525600 | -1.68097300 | -0.57866600 |
| B | 4.28857100 | 0.76737900 | -0.89904000 |
| O | 5.42943000 | 1.18611200 | -1.55888200 |
| O | 4.29998000 | -0.57605400 | -0.55694800 |
| C | 6.18633300 | -0.01373200 | -1.88684500 |
| C | 5.65066000 | -1.06125200 | -0.81233100 |
| C | 5.82181300 | -0.39732500 | -3.33170900 |
| C | 7.67972600 | 0.30709600 | -1.78513600 |
| C | 5.56649800 | -2.50781600 | -1.30514100 |
| C | 6.41237100 | -0.99572800 | 0.52253000 |
| H | 6.02098100 | 0.47006800 | -3.99267400 |
| H | 6.41836300 | -1.25799000 | -3.69660800 |
| H | 4.74641600 | -0.65238100 | -3.42208200 |
| H | 8.29414100 | -0.60157500 | -1.95365000 |
| H | 7.95433000 | 1.05318600 | -2.55822400 |
| H | 7.94027700 | 0.73388900 | -0.79814500 |
| H | 6.56948200 | -2.88959900 | -1.58757200 |
| H | 5.16959300 | -3.15561200 | -0.49725600 |
| H | 4.89181600 | -2.60439400 | -2.17668300 |
| H | 7.43216600 | -1.42326200 | 0.43932500 |
| H | 6.49859400 | 0.04831800 | 0.88610800 |
| H | 5.85269100 | -1.57590400 | 1.28364100 |
| B | -1.14420800 | 2.18993000 | 0.41887200 |
| O | -0.32907300 | 2.87042800 | 1.41191500 |
| O | -1.41148000 | 3.15751000 | -0.62306900 |
| H | -2.14967000 | 1.56716600 | 0.83353500 |
| C | -0.61137900 | 4.27534500 | 1.31025300 |
| C | -0.90378500 | 4.45308800 | -0.24800800 |
| C | -1.84540700 | 4.59285900 | 2.18312800 |
| C | 0.59576200 | 5.06601600 | 1.83074500 |
| C | -1.97169900 | 5.50845300 | -0.57740800 |
| C | 0.36646600 | 4.76181600 | -1.06574600 |
| H | -1.63767000 | 4.27108600 | 3.22415300 |
| H | -2.08310300 | 5.67638900 | 2.19965100 |
| H | -2.74069000 | 4.04218000 | 1.83114400 |
| H | 0.44650000 | 6.15818800 | 1.69915200 |
| H | 0.73245600 | 4.87103900 | 2.91449000 |
| H | 1.53089200 | 4.77546300 | 1.31511200 |
| H | -1.67132200 | 6.51552900 | -0.21844900 |
| H | -2.10996900 | 5.56958300 | -1.67683100 |

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| H | -2.94994700 | 5.24990400 | -0.12936000 |
| H | 0.71403700 | 5.80477500 | -0.91343800 |
| H | 1.20475500 | 4.08442900 | -0.81049700 |
| H | 0.13829600 | 4.63307100 | -2.14393600 |
| INT-9 | | | |
| Al | -3.35096100 | 0.24038000 | 0.18939600 |
| N | -4.11298100 | 1.84104800 | -0.59055300 |
| N | -4.66104400 | -0.98831400 | -0.54232400 |
| O | -1.76381900 | -0.07522100 | -0.50455900 |
| O | 1.76323100 | 0.07191200 | 0.50157400 |
| C | -5.19230900 | 1.86206400 | -1.40146800 |
| C | -3.43994300 | 3.07864400 | -0.26389400 |
| C | -5.67192800 | -0.63700700 | -1.36340100 |
| C | -4.48215500 | -2.37478400 | -0.17398800 |
| C | -0.57726100 | -0.48800900 | 0.14244800 |
| C | 0.57691700 | 0.48481600 | -0.14577400 |
| C | -5.91417900 | 0.69947800 | -1.76222700 |
| C | -5.67354200 | 3.18841100 | -1.95342100 |
| C | -3.82271300 | 3.77828400 | 0.91485000 |
| C | -2.38022000 | 3.53502300 | -1.09783000 |
| C | -6.60613700 | -1.70946300 | -1.88533700 |
| C | -5.09287900 | -2.85233400 | 1.01966600 |
| C | -3.65535900 | -3.20822300 | -0.97978200 |
| H | -0.27823500 | -1.50470300 | -0.21328500 |
| H | -0.70754100 | -0.56264500 | 1.25113600 |
| H | 0.27782600 | 1.50157500 | 0.20975100 |
| H | 0.70751100 | 0.55934000 | -1.25443300 |
| H | -6.77143400 | 0.85402800 | -2.43089000 |
| H | -5.92168200 | 3.89248700 | -1.13233700 |
| H | -6.56736400 | 3.05576400 | -2.59051600 |
| H | -4.87971900 | 3.68239200 | -2.55090600 |
| C | -3.12869900 | 4.96266500 | 1.23778600 |
| C | -4.94865000 | 3.23862300 | 1.78531700 |
| C | -1.71874500 | 4.72555300 | -0.73032700 |
| C | -1.98456100 | 2.73674200 | -2.33048000 |
| H | -7.09358700 | -2.25210300 | -1.04905200 |
| H | -7.39022600 | -1.27649400 | -2.53355300 |
| H | -6.04833100 | -2.47486600 | -2.46354900 |
| C | -4.87350500 | -4.19648700 | 1.38537200 |
| C | -5.94835300 | -1.91508100 | 1.86010900 |
| C | -3.46902500 | -4.54503700 | -0.56967300 |
| C | -2.99521400 | -2.64611100 | -2.22975900 |
| H | -3.40316200 | 5.52506200 | 2.14257100 |
| C | -2.08895900 | 5.43371000 | 0.42264100 |

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|----|-------------|-------------|-------------|
| C | -5.29014900 | 4.04942000 | 3.03930800 |
| H | -4.68449800 | 2.19747000 | 2.07902700 |
| H | -5.86484500 | 3.12602700 | 1.16188100 |
| H | -0.89515700 | 5.10236500 | -1.35458000 |
| C | -0.82457600 | 3.29578700 | -3.15971800 |
| H | -2.87760400 | 2.61710200 | -2.98565200 |
| H | -1.74259400 | 1.70248700 | -1.99408500 |
| H | -5.33375700 | -4.59317000 | 2.30248600 |
| C | -4.07215300 | -5.03595000 | 0.59765100 |
| C | -6.55503700 | -2.50528400 | 3.13678800 |
| H | -6.76454400 | -1.50297400 | 1.22388100 |
| H | -5.32724500 | -1.02858100 | 2.12145100 |
| H | -2.83601800 | -5.21280900 | -1.17260600 |
| C | -2.10127600 | -3.60770400 | -3.01881700 |
| H | -2.40984000 | -1.74815700 | -1.92494200 |
| H | -3.78570400 | -2.24636300 | -2.90568500 |
| H | -1.55830900 | 6.36130000 | 0.69126300 |
| H | -6.11665200 | 3.56445100 | 3.59792500 |
| H | -4.42498400 | 4.12502100 | 3.73078500 |
| H | -5.61703300 | 5.08226700 | 2.79487300 |
| H | -0.62160900 | 2.63518100 | -4.02724800 |
| H | -1.03932500 | 4.31015500 | -3.55886500 |
| H | 0.11333100 | 3.35677200 | -2.56917900 |
| H | -3.91163600 | -6.08333500 | 0.90002900 |
| H | -7.15004100 | -1.73665300 | 3.67113300 |
| H | -7.23247200 | -3.35909200 | 2.92361300 |
| H | -5.77290100 | -2.86323000 | 3.83859400 |
| H | -1.66819200 | -3.09096300 | -3.89950200 |
| H | -1.25205700 | -3.97807700 | -2.40744000 |
| H | -2.65859900 | -4.49217700 | -3.39509500 |
| H | -3.34744600 | 0.25646700 | 1.79493500 |
| Al | 3.35194700 | -0.23953000 | -0.19059700 |
| N | 4.65919900 | 0.98842000 | 0.54744400 |
| N | 4.11452600 | -1.84176800 | 0.58559000 |
| H | 3.35125000 | -0.25050500 | -1.79619300 |
| C | 5.66932300 | 0.63562300 | 1.36881800 |
| C | 4.47908900 | 2.37595300 | 0.18369600 |
| C | 5.19272900 | -1.86414800 | 1.39797400 |
| C | 3.44322000 | -3.07908500 | 0.25434500 |
| C | 5.91274300 | -0.70189300 | 1.76346700 |
| C | 6.60125900 | 1.70752300 | 1.89593500 |
| C | 5.09123400 | 2.85859000 | -1.00718300 |
| C | 3.64982100 | 3.20541100 | 0.99104800 |
| C | 5.67464100 | -3.19167700 | 1.94647500 |

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|---|------------|-------------|-------------|
| C | 3.82828000 | -3.77478400 | -0.92598700 |
| C | 2.38295300 | -3.53913500 | 1.08556300 |
| H | 6.76926300 | -0.85759200 | 2.43280600 |
| H | 7.08891000 | 2.25411900 | 1.06235600 |
| H | 7.38518500 | 1.27330700 | 2.54351400 |
| H | 6.04152400 | 2.46984900 | 2.47635500 |
| C | 4.87076700 | 4.20378200 | -1.36838600 |
| C | 5.94929700 | 1.92549100 | -1.84961400 |
| C | 3.46247900 | 4.54346400 | 0.58547000 |
| C | 2.98822200 | 2.63792300 | 2.23782500 |
| H | 5.92413000 | -3.89316100 | 1.12359000 |
| H | 6.56775400 | -3.06008900 | 2.58478400 |
| H | 4.88071600 | -3.68807800 | 2.54182500 |
| C | 3.13602700 | -4.95898100 | -1.25333300 |
| C | 4.95475700 | -3.23127300 | -1.79336000 |
| C | 1.72332300 | -4.72933400 | 0.71368900 |
| C | 1.98474400 | -2.74497700 | 2.32005000 |
| H | 5.33209200 | 4.60437700 | -2.28325900 |
| C | 4.06700100 | 5.03937200 | -0.57901000 |
| C | 6.55777600 | 2.52126400 | -3.12284800 |
| H | 5.32962000 | 1.03935500 | -2.11555700 |
| H | 6.76472100 | 1.51176400 | -1.21346200 |
| H | 2.82754200 | 5.20822000 | 1.18970200 |
| C | 2.09159100 | 3.59548100 | 3.02873500 |
| H | 3.77804700 | 2.23679500 | 2.91371300 |
| H | 2.40459000 | 1.74029600 | 1.92872400 |
| H | 3.41227200 | -5.51836400 | -2.15944300 |
| C | 2.09580700 | -5.43364600 | -0.44090600 |
| C | 5.29867300 | -4.03785900 | -3.04940300 |
| H | 5.87004300 | -3.11964700 | -1.16841000 |
| H | 4.68991100 | -2.18948400 | -2.08417800 |
| H | 0.89941300 | -5.10896400 | 1.33580800 |
| C | 0.82425900 | -3.30780900 | 3.14603800 |
| H | 1.74204300 | -1.71001700 | 1.98637500 |
| H | 2.87676100 | -2.62625500 | 2.97678200 |
| H | 3.90567700 | 6.08764200 | -0.87787500 |
| H | 7.15472700 | 1.75537400 | -3.65895300 |
| H | 5.77660800 | 2.88097600 | -3.82483100 |
| H | 7.23378000 | 3.37504600 | -2.90507300 |
| H | 1.65761900 | 3.07499500 | 3.90677200 |
| H | 2.64706900 | 4.47932600 | 3.40919400 |
| H | 1.24298900 | 3.96693500 | 2.41715600 |
| H | 1.56658700 | -6.36105600 | -0.71295000 |
| H | 6.12533300 | -3.55028900 | -3.60551900 |

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|---------------|-------------|-------------|-------------|
| H | 5.62638200 | -5.07109300 | -2.80772700 |
| H | 4.43443600 | -4.11228100 | -3.74216900 |
| H | 0.61935700 | -2.65001100 | 4.01524300 |
| H | -0.11277600 | -3.36812600 | 2.55404500 |
| H | 1.03964100 | -4.32310700 | 3.54247400 |
| INT-10 | | | |
| Al | 3.55910100 | -0.01341800 | -0.20946500 |
| N | 4.41148800 | -1.46546000 | -1.16520400 |
| N | 4.59338400 | 1.40749500 | -1.02618900 |
| O | 1.86392100 | 0.08849700 | -0.68771800 |
| O | -1.54394800 | -0.52513700 | 0.59252200 |
| C | 5.38714300 | -1.31078300 | -2.08614100 |
| C | 3.93429800 | -2.79333400 | -0.84768800 |
| C | 5.54111300 | 1.22646300 | -1.96903300 |
| C | 4.28485400 | 2.74298000 | -0.56570300 |
| C | 0.71591600 | 0.33817100 | 0.09237400 |
| C | -0.29092700 | -0.80348600 | -0.08849400 |
| C | 5.90848300 | -0.04947700 | -2.45961100 |
| C | 5.97029500 | -2.53860200 | -2.75519000 |
| C | 4.51943600 | -3.49160700 | 0.24548700 |
| C | 2.86023400 | -3.34366000 | -1.60286700 |
| C | 6.26173500 | 2.43362100 | -2.53327800 |
| C | 4.97022200 | 3.25201200 | 0.57318600 |
| C | 3.26949700 | 3.48963800 | -1.22751100 |
| H | 0.22856100 | 1.29027400 | -0.23420000 |
| H | 0.94891000 | 0.44991800 | 1.17766600 |
| H | 0.09185200 | -1.76136100 | 0.31575300 |
| H | -0.50245500 | -0.94023800 | -1.17018500 |
| H | 6.69821400 | -0.06240600 | -3.22248800 |
| H | 6.39347800 | -3.23564000 | -2.00252700 |
| H | 6.76571700 | -2.26325700 | -3.47201400 |
| H | 5.18655600 | -3.10951500 | -3.29450400 |
| C | 4.01267300 | -4.76879900 | 0.56332700 |
| C | 5.65579300 | -2.85392400 | 1.03216500 |
| C | 2.39101200 | -4.62454600 | -1.24426200 |
| C | 2.24835000 | -2.54813400 | -2.74608300 |
| H | 6.76855800 | 3.00509500 | -1.72836000 |
| H | 7.01461200 | 2.13465800 | -3.28573000 |
| H | 5.54622000 | 3.13825800 | -3.00529400 |
| C | 4.62857100 | 4.54143500 | 1.03051100 |
| C | 6.03346300 | 2.40612200 | 1.25915900 |
| C | 2.96626600 | 4.77414300 | -0.73002700 |
| C | 2.54257700 | 2.89272800 | -2.42348700 |
| H | 4.44540100 | -5.33249700 | 1.40302600 |

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|----|-------------|-------------|-------------|
| C | 2.96035200 | -5.33101000 | -0.17425600 |
| C | 6.23023600 | -3.67650600 | 2.18959600 |
| H | 5.29648400 | -1.87334000 | 1.41861000 |
| H | 6.47734400 | -2.58921600 | 0.32811100 |
| H | 1.56129100 | -5.07564800 | -1.80825600 |
| C | 1.09033800 | -3.21387600 | -3.49561900 |
| H | 3.04969700 | -2.28586400 | -3.47405900 |
| H | 1.91660300 | -1.56912300 | -2.33105600 |
| H | 5.14193200 | 4.96122300 | 1.90828900 |
| C | 3.63889200 | 5.29648300 | 0.38434500 |
| C | 6.70605400 | 3.02180100 | 2.48993500 |
| H | 6.81487900 | 2.13350000 | 0.51347500 |
| H | 5.56775200 | 1.43436500 | 1.53957200 |
| H | 2.18451200 | 5.37371800 | -1.21903300 |
| C | 1.45702300 | 3.76320600 | -3.06401200 |
| H | 2.10658900 | 1.91909400 | -2.10233100 |
| H | 3.29290100 | 2.61679500 | -3.19953300 |
| H | 2.57652500 | -6.32919600 | 0.09044900 |
| H | 7.04563600 | -3.11683100 | 2.69175400 |
| H | 5.46195800 | -3.89996400 | 2.95899300 |
| H | 6.65471700 | -4.64368000 | 1.84647100 |
| H | 0.72151500 | -2.54683400 | -4.30132800 |
| H | 1.38973300 | -4.17249800 | -3.97050700 |
| H | 0.22992500 | -3.42445600 | -2.82660800 |
| H | 3.38459100 | 6.30149400 | 0.75761800 |
| H | 7.45351900 | 2.31921300 | 2.91178200 |
| H | 7.23862100 | 3.96605500 | 2.24893200 |
| H | 5.97280100 | 3.24427600 | 3.29316800 |
| H | 0.99201600 | 3.22791100 | -3.91687600 |
| H | 0.64498400 | 4.00507200 | -2.34707600 |
| H | 1.86062800 | 4.72181700 | -3.45455700 |
| H | 3.76209200 | -0.07672600 | 1.37969300 |
| Al | -2.92401900 | 0.40000300 | -0.20742500 |
| N | -4.56033600 | -0.57982200 | -0.49919400 |
| N | -3.65681800 | 1.86586800 | 0.80382900 |
| H | -2.28179700 | 0.87919500 | -1.59108700 |
| C | -5.67960300 | -0.33075300 | 0.21759200 |
| C | -4.60860200 | -1.53986600 | -1.58766400 |
| C | -4.88557500 | 1.80018400 | 1.36676000 |
| C | -2.90909900 | 3.10834900 | 0.88032400 |
| C | -5.77930900 | 0.72231400 | 1.15909900 |
| C | -6.91902900 | -1.16415800 | -0.03183200 |
| C | -4.89356300 | -1.05687800 | -2.89821700 |
| C | -4.35913100 | -2.92032700 | -1.34127100 |

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| C | -5.37288400 | 2.95803800 | 2.21212600 |
| C | -3.07373900 | 4.05672100 | -0.17050100 |
| C | -2.03021500 | 3.35213900 | 1.97343200 |
| H | -6.72978900 | 0.78191700 | 1.70587100 |
| H | -7.27483600 | -1.02779900 | -1.07477800 |
| H | -7.73517900 | -0.87994400 | 0.65761300 |
| H | -6.70949900 | -2.24647000 | 0.08363100 |
| C | -4.89879600 | -1.97754100 | -3.96543700 |
| C | -5.18977800 | 0.41843500 | -3.12026900 |
| C | -4.38272200 | -3.79949400 | -2.44658300 |
| C | -4.08353800 | -3.43363200 | 0.06056000 |
| H | -5.45020600 | 3.88216400 | 1.60161200 |
| H | -6.36499100 | 2.74157800 | 2.64929100 |
| H | -4.66005200 | 3.18723500 | 3.02969100 |
| C | -2.33002900 | 5.25297100 | -0.11497900 |
| C | -4.03726400 | 3.76997600 | -1.31219800 |
| C | -1.31335400 | 4.56874100 | 1.98167800 |
| C | -1.87179800 | 2.33830700 | 3.09123000 |
| H | -5.11244300 | -1.62678500 | -4.98579600 |
| C | -4.64016100 | -3.33744600 | -3.74365800 |
| C | -5.57698500 | 0.83226600 | -4.54352800 |
| H | -4.29412400 | 0.99749800 | -2.80088900 |
| H | -5.99150100 | 0.73524200 | -2.41575000 |
| H | -4.19662000 | -4.87129200 | -2.28375400 |
| C | -4.23384800 | -4.94522200 | 0.26851200 |
| H | -4.73847200 | -2.89964000 | 0.78155100 |
| H | -3.06029600 | -3.13786800 | 0.38413200 |
| H | -2.44060600 | 6.00026200 | -0.91453200 |
| C | -1.45469600 | 5.50673600 | 0.95086700 |
| C | -4.20719100 | 4.87596700 | -2.35848000 |
| H | -5.03375100 | 3.51183200 | -0.88800600 |
| H | -3.70068400 | 2.83617800 | -1.81640800 |
| H | -0.62910400 | 4.78291300 | 2.81565500 |
| C | -1.19641700 | 2.83513700 | 4.37373900 |
| H | -1.30514200 | 1.45517600 | 2.72321700 |
| H | -2.86576500 | 1.91069900 | 3.34333300 |
| H | -4.64774600 | -4.04442500 | -4.58879100 |
| H | -5.78409000 | 1.92117000 | -4.58487900 |
| H | -4.76552800 | 0.62474700 | -5.27194300 |
| H | -6.48933800 | 0.30735900 | -4.89747700 |
| H | -4.07201400 | -5.19553900 | 1.33653500 |
| H | -5.24252800 | -5.31451700 | -0.01687000 |
| H | -3.48727700 | -5.52640700 | -0.31245300 |
| H | -0.88176000 | 6.44736500 | 0.98069100 |

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| H | -4.93719800 | 4.56441600 | -3.13329900 |
| H | -4.58235500 | 5.82023400 | -1.91040300 |
| H | -3.25398900 | 5.10596700 | -2.87861900 |
| H | -1.17606300 | 2.01753500 | 5.12175800 |
| H | -0.14283600 | 3.14044200 | 4.20223200 |
| H | -1.72811800 | 3.70019200 | 4.82572400 |
| B | -1.88280900 | -1.17817700 | 2.02117200 |
| O | -1.65254600 | -2.60531100 | 1.92150800 |
| O | -1.02089100 | -0.69065700 | 3.07646700 |
| H | -3.07240700 | -0.78674500 | 2.10654000 |
| C | -1.14501500 | -3.05681100 | 3.18558900 |
| C | -0.32966700 | -1.78681400 | 3.70305800 |
| C | -2.34369300 | -3.40206600 | 4.09680500 |
| C | -0.29740500 | -4.31545100 | 2.96090500 |
| C | -0.37252100 | -1.58436000 | 5.22659900 |
| C | 1.14173600 | -1.78890400 | 3.24588300 |
| H | -2.97305200 | -4.15917400 | 3.58551700 |
| H | -2.02597300 | -3.82176000 | 5.07354600 |
| H | -2.97470200 | -2.51041800 | 4.28558300 |
| H | 0.18303400 | -4.64973300 | 3.90436900 |
| H | -0.94325900 | -5.14184400 | 2.59812900 |
| H | 0.49186400 | -4.14760400 | 2.20361500 |
| H | 0.06615000 | -2.45175000 | 5.76403700 |
| H | 0.21778300 | -0.68509300 | 5.49950400 |
| H | -1.40720700 | -1.43014500 | 5.58768800 |
| H | 1.74363200 | -2.55145400 | 3.78257300 |
| H | 1.23911600 | -1.98058600 | 2.15950200 |
| H | 1.58749600 | -0.79490000 | 3.45274000 |
| INT-11 | | | |
| N | 1.44099600 | 0.17216300 | 0.59263600 |
| C | 3.43279900 | -1.12548700 | -0.10184800 |
| Al | 0.00007100 | -0.01192900 | -0.68732700 |
| C | 4.71771300 | -1.13561100 | -0.68378200 |
| H | 5.25156500 | -2.09020700 | -0.80230000 |
| C | 1.27265900 | 0.30982900 | 1.92466000 |
| C | 0.00001100 | 0.36953500 | 2.54142700 |
| H | -0.00000600 | 0.48292100 | 3.63368800 |
| C | 2.77525500 | 0.12982600 | 0.03664900 |
| C | 4.65653600 | 1.27664400 | -0.98735400 |
| H | 5.14194300 | 2.19811800 | -1.34152700 |
| C | 5.32503700 | 0.05093300 | -1.12029200 |
| H | 6.32841700 | 0.01935100 | -1.57446900 |
| C | 3.37135200 | 1.34239800 | -0.41053200 |
| C | 2.49369500 | 0.41611600 | 2.81501200 |

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| H | 3.13495000 | -0.48441600 | 2.71953400 |
| H | 2.20641100 | 0.53675200 | 3.87581000 |
| H | 3.12766100 | 1.27663500 | 2.51659200 |
| N | -1.44099900 | 0.17208900 | 0.59263700 |
| C | -3.43283500 | -1.12547500 | -0.10189300 |
| C | -4.71774800 | -1.13553900 | -0.68383200 |
| H | -5.25161200 | -2.09011900 | -0.80242600 |
| C | -1.27265100 | 0.30976900 | 1.92463700 |
| C | -2.77527100 | 0.12981600 | 0.03669000 |
| C | -4.65653000 | 1.27673800 | -0.98722300 |
| H | -5.14192000 | 2.19824400 | -1.34133600 |
| C | -5.32505700 | 0.05104900 | -1.12024200 |
| H | -6.32844000 | 0.01952100 | -1.57441600 |
| C | -3.37134100 | 1.34243000 | -0.41040500 |
| C | -2.49366300 | 0.41607800 | 2.81503200 |
| H | -3.13491200 | -0.48446200 | 2.71958600 |
| H | -2.20634500 | 0.53673200 | 3.87581700 |
| H | -3.12765400 | 1.27658200 | 2.51662000 |
| H | -0.00008700 | 1.13351900 | -1.81227600 |
| C | -2.74236300 | -2.40109700 | 0.35666400 |
| C | -3.52028500 | -3.70563300 | 0.15812600 |
| H | -2.47324900 | -2.29919500 | 1.43293300 |
| H | -1.76221600 | -2.45885800 | -0.17076200 |
| H | -2.92176100 | -4.56709400 | 0.51870400 |
| H | -4.48182300 | -3.71487000 | 0.71452000 |
| H | -3.75023500 | -3.89175500 | -0.91205100 |
| C | -2.61787700 | 2.65667600 | -0.26298500 |
| C | -3.32860100 | 3.91219900 | -0.77768900 |
| H | -1.63804000 | 2.54836400 | -0.78089000 |
| H | -2.34985700 | 2.80110500 | 0.80846400 |
| H | -2.68957200 | 4.80590900 | -0.62539000 |
| H | -3.54934900 | 3.84620600 | -1.86361200 |
| H | -4.28784500 | 4.09716500 | -0.24958400 |
| C | 2.61794000 | 2.65668000 | -0.26315200 |
| C | 3.32867700 | 3.91214200 | -0.77798700 |
| H | 2.35000600 | 2.80118600 | 0.80831000 |
| H | 1.63806400 | 2.54837900 | -0.78098100 |
| H | 2.68967800 | 4.80588100 | -0.62573200 |
| H | 4.28794800 | 4.09712800 | -0.24993900 |
| H | 3.54937500 | 3.84605000 | -1.86391500 |
| C | 2.74230900 | -2.40106500 | 0.35679700 |
| C | 3.52028000 | -3.70560900 | 0.15852200 |
| H | 1.76222800 | -2.45891400 | -0.17074800 |
| H | 2.47304700 | -2.29903000 | 1.43301500 |

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|---------------|-------------|-------------|-------------|
| H | 2.92175400 | -4.56702900 | 0.51919600 |
| H | 3.75030600 | -3.89190300 | -0.91160800 |
| H | 4.48177900 | -3.71472700 | 0.71498500 |
| O | 0.00001800 | -1.63924200 | -1.35732200 |
| C | -0.00014800 | -2.06042500 | -2.69919100 |
| H | -0.00032000 | -1.21091000 | -3.42506200 |
| H | 0.89750800 | -2.68520400 | -2.92348300 |
| H | -0.89779900 | -2.68531400 | -2.92321000 |
| INT-12 | | | |
| N | -1.34358500 | 1.32948700 | 0.64379700 |
| C | -0.74584000 | 3.67253800 | 0.02892000 |
| Al | -0.71671800 | -0.05448800 | -0.53338100 |
| C | -1.13948800 | 4.88869000 | -0.57158200 |
| H | -0.42496400 | 5.72415800 | -0.61031300 |
| C | -1.55634000 | 1.11158400 | 1.96244100 |
| C | -1.44736800 | -0.16430000 | 2.56535200 |
| H | -1.61565400 | -0.19313800 | 3.65008400 |
| C | -1.69778000 | 2.61489700 | 0.06766000 |
| C | -3.34668000 | 4.00316000 | -1.06271000 |
| H | -4.35144300 | 4.14627400 | -1.48665400 |
| C | -2.41915500 | 5.05333200 | -1.11726100 |
| H | -2.69933100 | 6.01103600 | -1.58452500 |
| C | -3.00926000 | 2.77046900 | -0.46847700 |
| C | -1.99230800 | 2.26597000 | 2.83922400 |
| H | -1.27727200 | 3.11088600 | 2.77505900 |
| H | -2.08428600 | 1.95179600 | 3.89512500 |
| H | -2.97215300 | 2.66449900 | 2.50211300 |
| N | -1.03861000 | -1.56446100 | 0.61475000 |
| C | 0.06797400 | -3.71690700 | 0.00537700 |
| C | -0.03114100 | -4.97152300 | -0.63642300 |
| H | 0.84595300 | -5.63536500 | -0.65426200 |
| C | -1.30054000 | -1.42326200 | 1.93433100 |
| C | -1.08746700 | -2.88458100 | 0.01107500 |
| C | -2.35243900 | -4.56277000 | -1.21808500 |
| H | -3.28494100 | -4.90601500 | -1.68961700 |
| C | -1.21948500 | -5.38854300 | -1.24885100 |
| H | -1.26706200 | -6.36990200 | -1.74753000 |
| C | -2.31233600 | -3.30353200 | -0.58690300 |
| C | -1.50695900 | -2.66006100 | 2.78236200 |
| H | -0.62716600 | -3.33299200 | 2.73423300 |
| H | -1.69656400 | -2.39237800 | 3.83802100 |
| H | -2.36816000 | -3.25098500 | 2.40605100 |
| H | -1.55629500 | -0.13153700 | -1.89165000 |
| C | 1.36469500 | -3.28089200 | 0.66460200 |

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|---|-------------|-------------|-------------|
| C | 2.30962100 | -4.41001700 | 1.09732800 |
| H | 1.13472000 | -2.63987500 | 1.54082800 |
| H | 1.92333600 | -2.59430500 | -0.01171300 |
| H | 3.18127900 | -3.98693200 | 1.63690600 |
| H | 1.81375500 | -5.13940800 | 1.77362000 |
| H | 2.71460400 | -4.97774300 | 0.23363100 |
| C | -3.53878600 | -2.40523600 | -0.52550200 |
| C | -4.83262000 | -2.97227900 | -1.11819100 |
| H | -3.28935200 | -1.44935900 | -1.03916400 |
| H | -3.71830600 | -2.11347800 | 0.53391100 |
| H | -5.65951200 | -2.24148300 | -1.00686000 |
| H | -4.73182100 | -3.19149800 | -2.20161000 |
| H | -5.14786700 | -3.90944000 | -0.61283400 |
| C | -4.00786500 | 1.62547100 | -0.38653900 |
| C | -5.41241000 | 1.90244700 | -0.93187900 |
| H | -4.08634900 | 1.28981000 | 0.67222700 |
| H | -3.57267600 | 0.75213500 | -0.92277200 |
| H | -6.05530000 | 1.00649600 | -0.81282500 |
| H | -5.90953900 | 2.74010500 | -0.39878100 |
| H | -5.39569500 | 2.15411600 | -2.01281400 |
| C | 0.64481900 | 3.49784200 | 0.61139500 |
| C | 1.43369100 | 4.78215100 | 0.88991700 |
| H | 1.25754700 | 2.85442900 | -0.05810300 |
| H | 0.57992800 | 2.89964600 | 1.54508900 |
| H | 2.40668000 | 4.52666900 | 1.35536500 |
| H | 1.66084800 | 5.34668000 | -0.03879500 |
| H | 0.89506100 | 5.46990600 | 1.57693600 |
| O | 1.01032200 | 0.15117800 | -1.14830600 |
| C | 1.35016200 | 0.18847600 | -2.54893300 |
| H | 0.43871300 | -0.01476900 | -3.14435300 |
| H | 1.74968100 | 1.18916200 | -2.80744100 |
| H | 2.11817800 | -0.58390200 | -2.74842900 |
| B | 2.19373900 | 0.21262800 | -0.06191200 |
| O | 3.13514800 | -0.84139600 | -0.38788700 |
| O | 2.92638600 | 1.45929900 | -0.13484500 |
| H | 1.49845100 | 0.07944400 | 0.97059200 |
| C | 4.45664600 | -0.35228200 | -0.11811500 |
| C | 4.31516800 | 1.20989300 | -0.41355000 |
| C | 4.79390600 | -0.64538200 | 1.36040100 |
| C | 5.45404000 | -1.08824600 | -1.02234100 |
| C | 5.16588900 | 2.10840200 | 0.49889900 |
| C | 4.61354200 | 1.57542600 | -1.88204700 |
| H | 4.69126900 | -1.73527900 | 1.53942400 |
| H | 5.82984200 | -0.34944500 | 1.62539700 |

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|---------------|-------------|-------------|-------------|
| H | 4.09355600 | -0.12329500 | 2.04284600 |
| H | 6.48044700 | -0.68174000 | -0.90527200 |
| H | 5.48221400 | -2.16406200 | -0.75202300 |
| H | 5.16722200 | -1.01756500 | -2.08907500 |
| H | 6.24880500 | 1.88553800 | 0.39398400 |
| H | 5.01215700 | 3.17257000 | 0.22392300 |
| H | 4.88127000 | 1.99179200 | 1.56180800 |
| H | 5.69837100 | 1.52708000 | -2.11170800 |
| H | 4.08337300 | 0.90935100 | -2.58947600 |
| H | 4.27027800 | 2.61406900 | -2.06793600 |
| INT-13 | | | |
| N | 1.41635700 | -0.02336100 | 0.97865400 |
| C | 3.40262200 | -1.23888600 | 0.14166200 |
| Al | -0.01134600 | -0.00105800 | -0.30531500 |
| C | 4.70067100 | -1.19067000 | -0.40775800 |
| H | 5.22169300 | -2.12803300 | -0.65282200 |
| C | 1.23043300 | -0.04061300 | 2.31641100 |
| C | -0.04983600 | -0.04481700 | 2.91957900 |
| H | -0.06280200 | -0.05913000 | 4.01748300 |
| C | 2.76211000 | -0.00511000 | 0.44473200 |
| C | 4.68469100 | 1.24097800 | -0.35757200 |
| H | 5.19340800 | 2.19456100 | -0.56284900 |
| C | 5.33665500 | 0.03492300 | -0.65331000 |
| H | 6.34992000 | 0.05044000 | -1.08584400 |
| C | 3.38647200 | 1.24880500 | 0.19361400 |
| C | 2.43952500 | -0.05613900 | 3.22811300 |
| H | 3.07964300 | -0.93898000 | 3.02292800 |
| H | 2.13781800 | -0.07458400 | 4.29154600 |
| H | 3.07978400 | 0.83327700 | 3.05422100 |
| N | -1.47033300 | -0.01465000 | 0.94433500 |
| C | -3.43436000 | -1.25129900 | 0.08576200 |
| C | -4.71956600 | -1.21847200 | -0.49487800 |
| H | -5.23154500 | -2.16246700 | -0.73362000 |
| C | -1.31528900 | -0.03123600 | 2.28654200 |
| C | -2.80462400 | -0.00926600 | 0.38105400 |
| C | -4.71586300 | 1.21333800 | -0.48368800 |
| H | -5.22514200 | 2.16105400 | -0.71337200 |
| C | -5.35509600 | -0.00028100 | -0.77614500 |
| H | -6.35874500 | 0.00330800 | -1.23096900 |
| C | -3.43031600 | 1.23727500 | 0.09670400 |
| C | -2.54513600 | -0.03459900 | 3.17018800 |
| H | -3.18510400 | -0.91576900 | 2.95762800 |
| H | -2.26817400 | -0.04606900 | 4.24042600 |
| H | -3.17637700 | 0.85671100 | 2.97413200 |

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| C | -2.71790000 | -2.55946200 | 0.38677000 |
| C | -3.47508900 | -3.84583600 | 0.04254400 |
| H | -2.44003700 | -2.57900400 | 1.46532600 |
| H | -1.74466300 | -2.53985600 | -0.15379100 |
| H | -2.86086800 | -4.73289300 | 0.30002200 |
| H | -4.43326000 | -3.93427900 | 0.59754500 |
| H | -3.70791700 | -3.91204400 | -1.04107100 |
| C | -2.70827700 | 2.53987500 | 0.40646500 |
| C | -3.46655100 | 3.83198100 | 0.08731700 |
| H | -1.74105800 | 2.52221100 | -0.14598500 |
| H | -2.41765500 | 2.54451600 | 1.48178400 |
| H | -2.84845300 | 4.71446500 | 0.35122200 |
| H | -3.70943300 | 3.91392700 | -0.99304400 |
| H | -4.41952700 | 3.91428300 | 0.65226600 |
| C | 2.64835900 | 2.54163000 | 0.50937300 |
| C | 3.38240700 | 3.84413800 | 0.17622400 |
| H | 2.37430500 | 2.54603600 | 1.58937700 |
| H | 1.67186800 | 2.51077100 | -0.02526700 |
| H | 2.75052600 | 4.71800500 | 0.43600300 |
| H | 4.33576300 | 3.94721800 | 0.73688600 |
| H | 3.61967400 | 3.92020900 | -0.90571500 |
| C | 2.68112400 | -2.55322600 | 0.40029200 |
| C | 3.44249300 | -3.83152500 | 0.03605700 |
| H | 1.71432300 | -2.51865800 | -0.15168900 |
| H | 2.38743400 | -2.59843800 | 1.47405600 |
| H | 2.82259500 | -4.72408800 | 0.25856900 |
| H | 3.69595400 | -3.86851600 | -1.04421400 |
| H | 4.38974100 | -3.93612100 | 0.60675400 |
| O | -0.03353200 | -1.46429700 | -1.28324600 |
| C | 0.10063400 | -1.63419600 | -2.65951600 |
| O | 0.69436200 | -0.54098000 | -3.33444600 |
| O | -0.04635400 | 1.48048900 | -1.24227300 |
| C | -0.14162400 | 0.59669400 | -3.54449600 |
| C | 0.19659100 | 1.75229100 | -2.59839700 |
| H | 0.01090300 | 0.94189100 | -4.59397600 |
| H | -1.21809000 | 0.31761500 | -3.43273400 |
| H | 1.26954200 | 2.02469200 | -2.75830500 |
| H | -0.40811600 | 2.63699600 | -2.91785300 |
| H | 0.77511100 | -2.49693200 | -2.86678200 |
| H | -0.90509100 | -1.84594300 | -3.11223900 |
| INT-14 | | | |
| H | 1.61718600 | 0.02377200 | -1.33331000 |
| B | 2.25965300 | 0.18528500 | -0.27665000 |
| O | 3.04207300 | -0.95973800 | 0.10773500 |

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| O | 3.10225000 | 1.35043200 | -0.13744000 |
| C | 4.34169400 | -0.54730000 | 0.56867900 |
| C | 4.47197500 | 0.91875600 | -0.04521600 |
| C | 4.36434300 | -0.58009100 | 2.11073900 |
| C | 5.38527600 | -1.54523800 | 0.04182500 |
| C | 5.24881800 | 1.91000700 | 0.83067500 |
| C | 5.06354200 | 0.91925800 | -1.47072600 |
| H | 4.07273600 | -1.59649600 | 2.44523000 |
| H | 5.37346300 | -0.35953800 | 2.51704100 |
| H | 3.64121100 | 0.12549900 | 2.56217900 |
| H | 6.41717600 | -1.21977500 | 0.29165300 |
| H | 5.22221600 | -2.53799600 | 0.50981100 |
| H | 5.31034400 | -1.67338800 | -1.05465000 |
| H | 6.30045500 | 1.58261000 | 0.96976300 |
| H | 5.26514500 | 2.90785500 | 0.34555300 |
| H | 4.78630400 | 2.02646200 | 1.82986500 |
| H | 6.14417500 | 0.66810000 | -1.48270600 |
| H | 4.52776900 | 0.20227300 | -2.12475400 |
| H | 4.93870000 | 1.93178900 | -1.90600300 |
| O | 0.96386200 | 0.43017800 | 0.73010000 |
| Al | -0.71214500 | -0.04345300 | 0.15832400 |
| C | 1.13780300 | 1.15044700 | 1.98053700 |
| N | -1.08417000 | -1.54149200 | -0.97574200 |
| N | -1.40721000 | 1.34971700 | -0.94679300 |
| O | -1.58729900 | -0.20552100 | 1.66790600 |
| O | 1.04834500 | 0.34519600 | 3.11078700 |
| H | 2.16031400 | 1.56696700 | 1.92189900 |
| H | 0.38468500 | 1.97212700 | 2.01026000 |
| C | -1.51066300 | -1.38812900 | -2.25312500 |
| C | -1.09013700 | -2.87703900 | -0.39673200 |
| C | -1.78256700 | 1.14469200 | -2.22960100 |
| C | -1.47363400 | 2.68302300 | -0.37787200 |
| C | -1.18834600 | -0.73083600 | 2.91341200 |
| C | -0.25286600 | 0.19982300 | 3.68568700 |
| C | -1.77140900 | -0.12967300 | -2.84389300 |
| C | -1.77063100 | -2.61999500 | -3.09307000 |
| C | 0.06749500 | -3.70026500 | -0.47684600 |
| C | -2.28701400 | -3.32495200 | 0.23863400 |
| C | -2.26125500 | 2.32002700 | -3.05220400 |
| C | -0.39958400 | 3.59578400 | -0.57541900 |
| C | -2.61245600 | 3.02430200 | 0.41172900 |
| H | -0.69313900 | -1.72642200 | 2.80412200 |
| H | -2.09251500 | -0.89227400 | 3.54958500 |
| H | -0.08691400 | -0.20769500 | 4.70599900 |

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| H | -0.73603500 | 1.20264200 | 3.78683200 |
| H | -2.08307100 | -0.15314800 | -3.89639600 |
| H | -0.87275000 | -3.26911200 | -3.13676000 |
| H | -2.06636100 | -2.34401300 | -4.12185200 |
| H | -2.57668000 | -3.23877600 | -2.64655200 |
| C | 0.01160200 | -4.97175700 | 0.13739300 |
| C | 1.31921200 | -3.24198800 | -1.20260200 |
| C | -2.28380900 | -4.60106100 | 0.83675400 |
| C | -3.52789000 | -2.44359900 | 0.25225200 |
| H | -1.44965700 | 3.06341900 | -3.19095200 |
| H | -2.61535400 | 1.99326300 | -4.04701900 |
| H | -3.08366400 | 2.85467500 | -2.53356800 |
| C | -0.47898100 | 4.85155900 | 0.06870900 |
| C | 0.80771800 | 3.26333800 | -1.43770100 |
| C | -2.64147500 | 4.29377200 | 1.02166100 |
| C | -3.75123000 | 2.02967300 | 0.57789700 |
| H | 0.89348900 | -5.62797900 | 0.09221900 |
| C | -1.14168000 | -5.41457000 | 0.79610800 |
| C | 2.21543200 | -4.35555700 | -1.76218900 |
| H | 1.93063600 | -2.60393900 | -0.52307900 |
| H | 1.03351800 | -2.55226900 | -2.02400900 |
| H | -3.19130900 | -4.96802900 | 1.33836000 |
| C | -4.78675300 | -3.04632300 | 0.88434400 |
| H | -3.76072000 | -2.13322500 | -0.79160600 |
| H | -3.26120400 | -1.49962700 | 0.77753100 |
| H | 0.34647000 | 5.56972900 | -0.05782400 |
| C | -1.57930800 | 5.19783900 | 0.86133800 |
| C | 1.21610500 | 4.36509700 | -2.43154000 |
| H | 0.62743700 | 2.32021300 | -1.98896300 |
| H | 1.67662300 | 3.02582900 | -0.78435100 |
| H | -3.50843100 | 4.58194100 | 1.63432000 |
| C | -4.99389000 | 2.53415000 | 1.31845600 |
| H | -3.34037200 | 1.13778400 | 1.10367000 |
| H | -4.04951900 | 1.65661400 | -0.42767200 |
| H | -1.15695900 | -6.40842700 | 1.27169900 |
| H | 3.05183300 | -3.91212100 | -2.33986500 |
| H | 2.67474500 | -4.97195900 | -0.96134700 |
| H | 1.66274900 | -5.04409600 | -2.43752200 |
| H | -5.62741300 | -2.32484900 | 0.82718100 |
| H | -5.11265700 | -3.97602100 | 0.37140500 |
| H | -4.63771100 | -3.29030600 | 1.95710400 |
| H | -1.61558500 | 6.18224300 | 1.35498300 |
| H | 2.07921400 | 4.02851300 | -3.04177000 |
| H | 0.39075800 | 4.62745200 | -3.12836600 |

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| H | 1.52451900 | 5.30217400 | -1.92317300 |
| H | -5.76559100 | 1.73843000 | 1.35920700 |
| H | -4.76607400 | 2.82061500 | 2.36664500 |
| H | -5.45138300 | 3.41595200 | 0.82149800 |
| INT-15 | | | |
| B | 4.02088000 | -0.19472600 | -0.05951300 |
| O | 4.50134600 | 0.54028600 | -1.12584100 |
| O | 4.64830200 | 0.09064100 | 1.14523200 |
| C | 5.69772200 | 1.22686900 | -0.65927500 |
| C | 5.47515900 | 1.27152300 | 0.91738800 |
| C | 6.90314600 | 0.36359100 | -1.07090600 |
| C | 5.77150300 | 2.59666000 | -1.33884700 |
| C | 6.74982300 | 1.14516300 | 1.75498300 |
| C | 4.65560100 | 2.49057900 | 1.37298100 |
| H | 6.86470200 | 0.19518400 | -2.16589600 |
| H | 7.86766700 | 0.85347100 | -0.82715300 |
| H | 6.87760300 | -0.62779800 | -0.57461000 |
| H | 6.62981800 | 3.18575700 | -0.95438900 |
| H | 5.91062600 | 2.46346800 | -2.43087700 |
| H | 4.84356900 | 3.17959000 | -1.18672700 |
| H | 7.44282400 | 1.98763500 | 1.55158100 |
| H | 6.49313100 | 1.16853200 | 2.83366000 |
| H | 7.27963800 | 0.19481800 | 1.55421000 |
| H | 5.23858800 | 3.43100400 | 1.30109900 |
| H | 3.73218600 | 2.60408600 | 0.76969800 |
| H | 4.35678600 | 2.34914900 | 2.43121400 |
| O | 3.03107800 | -1.12331100 | -0.21860700 |
| Al | -1.27133300 | -0.00841500 | 0.01432700 |
| C | 2.51934800 | -1.86325300 | 0.89023700 |
| N | -2.03951600 | -1.68895400 | -0.59112900 |
| N | -2.79913400 | 1.10150500 | -0.45520600 |
| O | -1.14798600 | 0.05795400 | 1.77284400 |
| O | 1.27764800 | -1.40444300 | 1.32885500 |
| H | 2.34690800 | -2.89873800 | 0.53476000 |
| H | 3.26406600 | -1.84729900 | 1.72332100 |
| C | -3.27236300 | -1.81014500 | -1.13045900 |
| C | -1.23274300 | -2.87729200 | -0.42059400 |
| C | -3.93941100 | 0.64438800 | -1.00958500 |
| C | -2.64779700 | 2.51571000 | -0.19596900 |
| C | -0.10222300 | -0.01695900 | 2.69998800 |
| C | 1.28290000 | -0.19021200 | 2.08112400 |
| C | -4.15353300 | -0.71968500 | -1.32157400 |
| C | -3.75314100 | -3.17887300 | -1.57040500 |
| C | -0.30388100 | -3.23280000 | -1.43641200 |

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|---|-------------|-------------|-------------|
| C | -1.35566300 | -3.62904000 | 0.78066900 |
| C | -5.05038500 | 1.62291000 | -1.33312000 |
| C | -2.04928600 | 3.33678400 | -1.19325000 |
| C | -3.05453300 | 3.04267900 | 1.06272000 |
| H | -0.27343900 | -0.87593600 | 3.39686800 |
| H | -0.07274000 | 0.90470600 | 3.33397100 |
| H | 2.05754500 | -0.23348000 | 2.88547900 |
| H | 1.52153200 | 0.67656100 | 1.42064200 |
| H | -5.12456300 | -0.96187000 | -1.77354900 |
| H | -3.06125300 | -3.61944900 | -2.31773600 |
| H | -4.76543100 | -3.12299100 | -2.01154500 |
| H | -3.77511300 | -3.88896000 | -0.71820000 |
| C | 0.48074300 | -4.38883200 | -1.24124600 |
| C | -0.17495000 | -2.36837000 | -2.68175000 |
| C | -0.54890300 | -4.77576900 | 0.92843100 |
| C | -2.32493500 | -3.17524500 | 1.86171600 |
| H | -4.69788300 | 2.40250300 | -2.03993200 |
| H | -5.92071900 | 1.10698900 | -1.77905300 |
| H | -5.38334300 | 2.16274800 | -0.42275200 |
| C | -1.87211300 | 4.70648300 | -0.90708100 |
| C | -1.62021900 | 2.72803300 | -2.52045900 |
| C | -2.85661300 | 4.41940700 | 1.29758600 |
| C | -3.66923800 | 2.12459000 | 2.10771400 |
| H | 1.20442000 | -4.69045900 | -2.01300100 |
| C | 0.35519500 | -5.15774200 | -0.07435600 |
| C | 0.91710300 | -2.76949600 | -3.67763900 |
| H | 0.00144400 | -1.32086300 | -2.35003800 |
| H | -1.15961400 | -2.33599500 | -3.20293400 |
| H | -0.62409600 | -5.37891700 | 1.84555600 |
| C | -2.32828700 | -3.99065400 | 3.15853700 |
| H | -3.35679800 | -3.16042300 | 1.44111100 |
| H | -2.10464200 | -2.10695000 | 2.08527700 |
| H | -1.41183200 | 5.36384400 | -1.65965800 |
| C | -2.27241500 | 5.24394800 | 0.32484700 |
| C | -0.97694700 | 3.68074300 | -3.53268500 |
| H | -2.50009900 | 2.23365000 | -2.99185700 |
| H | -0.91846200 | 1.89239300 | -2.29947100 |
| H | -3.16222100 | 4.85449500 | 2.26082600 |
| C | -4.05995500 | 2.77316100 | 3.43920600 |
| H | -2.94652800 | 1.29559700 | 2.28427300 |
| H | -4.56466500 | 1.62726700 | 1.66943700 |
| H | 0.97455200 | -6.05950700 | 0.05877800 |
| H | 0.93249400 | -2.06559700 | -4.53467200 |
| H | 1.92222300 | -2.73959300 | -3.20828500 |

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| H | 0.75991200 | -3.78885300 | -4.08990300 |
| H | -3.05192200 | -3.56086400 | 3.88114900 |
| H | -2.61897900 | -5.04969100 | 2.99146600 |
| H | -1.33189700 | -3.98968200 | 3.64841600 |
| H | -2.12500600 | 6.31651000 | 0.53021300 |
| H | -0.69957400 | 3.13093200 | -4.45520600 |
| H | -1.66139600 | 4.50335400 | -3.83017900 |
| H | -0.04931800 | 4.14221000 | -3.13383800 |
| H | -4.48861900 | 2.01355100 | 4.12469500 |
| H | -3.18414600 | 3.22180100 | 3.95381000 |
| H | -4.82110600 | 3.57290300 | 3.31493500 |
| H | 0.01129700 | 0.46223800 | -0.81427800 |
| INT-16 | | | |
| B | -5.56636900 | 0.47355700 | -0.35586900 |
| O | -6.26604000 | 0.51498800 | 0.83479300 |
| O | -6.12334400 | -0.36684900 | -1.30568800 |
| C | -7.25536600 | -0.55294300 | 0.77491700 |
| C | -7.42655400 | -0.77387000 | -0.79352600 |
| C | -6.64580400 | -1.77176600 | 1.48896000 |
| C | -8.52000300 | -0.08981100 | 1.50247600 |
| C | -7.68859000 | -2.22077600 | -1.21825200 |
| C | -8.47062500 | 0.16444200 | -1.42256700 |
| H | -6.34958400 | -1.47363800 | 2.51477900 |
| H | -7.36576600 | -2.61179400 | 1.56416700 |
| H | -5.73765300 | -2.13268800 | 0.96503900 |
| H | -9.32748800 | -0.84623400 | 1.41662000 |
| H | -8.29926800 | 0.05296700 | 2.57979900 |
| H | -8.89224000 | 0.87323900 | 1.10468500 |
| H | -8.63614400 | -2.59744900 | -0.78039700 |
| H | -7.77712800 | -2.27653100 | -2.32230500 |
| H | -6.86431500 | -2.89223900 | -0.91219700 |
| H | -9.50552300 | -0.12373400 | -1.14770600 |
| H | -8.30584100 | 1.21639700 | -1.11280900 |
| H | -8.37842800 | 0.11571300 | -2.52637600 |
| O | -4.44129300 | 1.22815100 | -0.55080300 |
| Al | 2.22877300 | 0.02373700 | -0.39523200 |
| C | -3.69271800 | 1.08931800 | -1.76130600 |
| N | 2.86252800 | 1.56462700 | 0.58954000 |
| N | 3.36854200 | -1.27162700 | 0.48379500 |
| O | 0.53717000 | -0.28437600 | -0.00238700 |
| O | -2.68243400 | 0.13846500 | -1.65486600 |
| C | 3.80214400 | 1.52296100 | 1.55820900 |
| C | 2.25073500 | 2.82696900 | 0.23732900 |
| C | 4.24523200 | -0.98183700 | 1.46784600 |

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| C | 3.22100900 | -2.63693500 | 0.03048800 |
| C | -0.53212100 | -0.58066100 | -0.87100900 |
| C | -1.59477100 | 0.51903400 | -0.80912600 |
| C | 4.44535100 | 0.32904000 | 1.96310900 |
| C | 4.20488800 | 2.80924400 | 2.24968400 |
| C | 2.80726200 | 3.58658700 | -0.82980600 |
| C | 1.07880800 | 3.24796400 | 0.92774800 |
| C | 5.06611200 | -2.09958200 | 2.07732300 |
| C | 4.00192500 | -3.08295600 | -1.07262700 |
| C | 2.26067800 | -3.47890400 | 0.65983100 |
| H | -1.01211500 | -1.54608300 | -0.58044000 |
| H | -0.20171700 | -0.69646400 | -1.93277100 |
| H | -1.16048800 | 1.49250400 | -1.14809100 |
| H | -1.93775900 | 0.65298600 | 0.24251200 |
| H | 5.19185600 | 0.43244800 | 2.76177800 |
| H | 4.57953700 | 3.55262700 | 1.51589600 |
| H | 4.99103300 | 2.62789700 | 3.00560100 |
| H | 3.33400200 | 3.28288200 | 2.74813500 |
| C | 2.17022800 | 4.79295300 | -1.18739200 |
| C | 4.05245700 | 3.08636300 | -1.54844800 |
| C | 0.48065700 | 4.46234300 | 0.53087000 |
| C | 0.50222100 | 2.38946800 | 2.04352200 |
| H | 5.66423600 | -2.62079800 | 1.30150100 |
| H | 5.75034200 | -1.71509500 | 2.85601800 |
| H | 4.41073900 | -2.87258300 | 2.52934900 |
| C | 3.81381800 | -4.40473900 | -1.52677500 |
| C | 4.99998700 | -2.13804400 | -1.72672800 |
| C | 2.11289200 | -4.79250100 | 0.16781700 |
| C | 1.42311200 | -2.94801500 | 1.81364700 |
| H | 2.57819000 | 5.40119100 | -2.00823000 |
| C | 1.01977300 | 5.22806000 | -0.51349900 |
| C | 4.58322000 | 3.96469700 | -2.68562900 |
| H | 3.83597000 | 2.06659500 | -1.93997300 |
| H | 4.86188800 | 2.92858000 | -0.79962200 |
| H | -0.42640300 | 4.81306000 | 1.04505700 |
| C | -0.77583200 | 2.90772100 | 2.71020900 |
| H | 1.28368200 | 2.23651600 | 2.82267800 |
| H | 0.32185800 | 1.37369200 | 1.62366600 |
| H | 4.40354000 | -4.77687500 | -2.37758600 |
| C | 2.88112200 | -5.25250500 | -0.91175500 |
| C | 5.78874900 | -2.69511400 | -2.91580000 |
| H | 5.71358700 | -1.77415100 | -0.95263700 |
| H | 4.44803100 | -1.22478800 | -2.04494900 |
| H | 1.37951700 | -5.46688500 | 0.63430000 |

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| C | 0.40576400 | -3.91934700 | 2.42019400 |
| H | 0.90323400 | -2.03012500 | 1.45493100 |
| H | 2.10401100 | -2.58626100 | 2.61778600 |
| H | 0.53484800 | 6.17237600 | -0.80868400 |
| H | 5.48515900 | 3.50445800 | -3.13832900 |
| H | 3.83474400 | 4.08859800 | -3.49602700 |
| H | 4.86972500 | 4.97828600 | -2.33376800 |
| H | -1.10587100 | 2.20553400 | 3.50276200 |
| H | -0.63203100 | 3.90056600 | 3.18723700 |
| H | -1.61278300 | 2.99928700 | 1.98659800 |
| H | 2.74713700 | -6.28160500 | -1.28186900 |
| H | 6.47739300 | -1.92326200 | -3.31613000 |
| H | 6.40519200 | -3.57510600 | -2.63497000 |
| H | 5.12038100 | -3.00336700 | -3.74678600 |
| H | -0.15033100 | -3.42651700 | 3.24369800 |
| H | -0.34400800 | -4.25319600 | 1.67251600 |
| H | 0.88680000 | -4.82728100 | 2.84253300 |
| H | 2.48764700 | 0.11814300 | -1.97646600 |
| H | -3.27393800 | 2.10199100 | -1.97669500 |
| H | -4.35415900 | 0.75463500 | -2.58779300 |
| TS-1 | | | |
| N | -1.42482100 | -0.80967700 | 0.60557600 |
| C | -3.40098500 | 0.67432000 | 0.76648300 |
| Al | 0.04182600 | -0.24174200 | -0.59459500 |
| C | -4.72533300 | 0.96549700 | 0.38194600 |
| H | -5.22646000 | 1.85786600 | 0.78597200 |
| C | -1.27228000 | -1.56378300 | 1.72301200 |
| C | -0.02676000 | -1.95498700 | 2.25885200 |
| H | -0.06623700 | -2.56914800 | 3.16825300 |
| C | -2.78505300 | -0.48646100 | 0.22512000 |
| C | -4.78448300 | -0.99265900 | -1.05670900 |
| H | -5.33145200 | -1.62642300 | -1.77060300 |
| C | -5.41358200 | 0.13922900 | -0.51894300 |
| H | -6.44769700 | 0.38426800 | -0.81012600 |
| C | -3.46165400 | -1.32688700 | -0.69902600 |
| C | -2.50661900 | -2.03714600 | 2.46968600 |
| H | -3.11199200 | -1.18167000 | 2.83324200 |
| H | -2.22663700 | -2.66553900 | 3.33539800 |
| H | -3.17562700 | -2.62120700 | 1.80492500 |
| N | 1.46106200 | -0.89897800 | 0.67380600 |
| C | 3.37502700 | 0.65789900 | 0.80487200 |
| C | 4.67620100 | 1.00906300 | 0.38956100 |
| H | 5.13878300 | 1.93280900 | 0.76875000 |
| C | 1.26552300 | -1.61881100 | 1.78958300 |

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| C | 2.80693700 | -0.54632600 | 0.29781100 |
| C | 4.82236500 | -0.98767700 | -0.98839700 |
| H | 5.39706400 | -1.61742700 | -1.68381800 |
| C | 5.39396800 | 0.19635800 | -0.50065100 |
| H | 6.40896000 | 0.48774400 | -0.81552700 |
| C | 3.52521700 | -1.38465100 | -0.60129200 |
| C | 2.45490500 | -2.09911100 | 2.59952300 |
| H | 3.05452000 | -1.24332600 | 2.97343800 |
| H | 2.13016700 | -2.70629400 | 3.46499600 |
| H | 3.14291000 | -2.70582400 | 1.97547000 |
| H | 0.25864100 | -1.14756200 | -1.90076600 |
| C | 2.57355900 | 1.52577500 | 1.76339000 |
| C | 3.25363500 | 2.80486000 | 2.26136800 |
| H | 2.26623800 | 0.91327600 | 2.64071600 |
| H | 1.61490900 | 1.78290700 | 1.25735500 |
| H | 2.57985900 | 3.35917900 | 2.94654000 |
| H | 4.18996200 | 2.59235700 | 2.81947800 |
| H | 3.51396200 | 3.49014000 | 1.42683500 |
| C | 2.89338200 | -2.67391900 | -1.10511600 |
| C | 3.70441500 | -3.47890800 | -2.12479300 |
| H | 1.89873300 | -2.41886800 | -1.53398300 |
| H | 2.65994600 | -3.32325400 | -0.22992400 |
| H | 3.14250100 | -4.38415400 | -2.43332800 |
| H | 3.91087000 | -2.89058300 | -3.04357700 |
| H | 4.67982800 | -3.81953400 | -1.71670500 |
| C | -2.75402900 | -2.54658400 | -1.27150500 |
| C | -3.53864500 | -3.37337700 | -2.29470400 |
| H | -2.43933200 | -3.20801400 | -0.43150700 |
| H | -1.79461500 | -2.21084400 | -1.72632200 |
| H | -2.92498200 | -4.22516600 | -2.65294600 |
| H | -4.47294100 | -3.79538600 | -1.86718200 |
| H | -3.81799300 | -2.77072700 | -3.18427400 |
| C | -2.61805500 | 1.57444000 | 1.70961100 |
| C | -3.36374700 | 2.78974500 | 2.27001500 |
| H | -1.71157800 | 1.92453400 | 1.16723100 |
| H | -2.22272000 | 0.96688300 | 2.55457200 |
| H | -2.70244800 | 3.37089300 | 2.94518300 |
| H | -3.69711700 | 3.47635700 | 1.46402500 |
| H | -4.26098200 | 2.49754200 | 2.85583500 |
| O | -1.26188800 | 1.08452700 | -1.50026200 |
| C | -0.42342800 | 2.00909000 | -1.58319100 |
| O | -0.52007000 | 3.14298600 | -0.81541300 |
| O | 0.24580000 | 2.28228300 | -2.74019400 |
| C | 0.31418900 | 4.17030200 | -1.38158000 |

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| C | 1.07522300 | 3.42676900 | -2.49941500 |
| H | -0.34094600 | 4.98235900 | -1.76430500 |
| H | 0.98150900 | 4.58032100 | -0.59727900 |
| H | 1.16974200 | 3.99971500 | -3.44145900 |
| H | 2.07914000 | 3.08358000 | -2.16666300 |
| H | 0.88596800 | 1.24069200 | -0.70997000 |
| TS-2 | | | |
| N | -1.48256500 | -0.37268800 | -0.84988600 |
| C | -3.63317300 | -1.16690100 | 0.09160600 |
| Al | -0.03927600 | -0.53729300 | 0.49226500 |
| C | -4.93855300 | -0.86806800 | 0.53143700 |
| H | -5.58333800 | -1.67531600 | 0.90978800 |
| C | -1.33140400 | -0.58091600 | -2.18202900 |
| C | -0.08242300 | -0.71552400 | -2.81926700 |
| H | -0.10889500 | -0.89813600 | -3.90167900 |
| C | -2.82838200 | -0.10058700 | -0.39050700 |
| C | -4.61429600 | 1.49040800 | 0.03926000 |
| H | -5.00679700 | 2.51838700 | 0.03361400 |
| C | -5.42787300 | 0.44638800 | 0.50376200 |
| H | -6.45025600 | 0.66035700 | 0.85434200 |
| C | -3.30291600 | 1.23863900 | -0.41407900 |
| C | -2.56104900 | -0.65548600 | -3.06849700 |
| H | -3.28090400 | -1.41204200 | -2.69527000 |
| H | -2.28153700 | -0.90753700 | -4.10837100 |
| H | -3.11018100 | 0.30874100 | -3.07626600 |
| N | 1.39310800 | -0.34135200 | -0.93179700 |
| C | 3.56180500 | -1.20997400 | -0.10548300 |
| C | 4.86081600 | -0.94286000 | 0.37842200 |
| H | 5.50823800 | -1.77885700 | 0.68245900 |
| C | 1.20019400 | -0.53070400 | -2.24811700 |
| C | 2.74566700 | -0.10437700 | -0.48432800 |
| C | 4.53712900 | 1.44546400 | 0.07113800 |
| H | 4.93230700 | 2.47012900 | 0.13819000 |
| C | 5.34462100 | 0.37015800 | 0.47070500 |
| H | 6.36185800 | 0.55684300 | 0.85084700 |
| C | 3.22919200 | 1.23379800 | -0.41183300 |
| C | 2.38285300 | -0.51930000 | -3.19936800 |
| H | 3.15605000 | -1.25385300 | -2.89595500 |
| H | 2.06247200 | -0.74464600 | -4.23351700 |
| H | 2.88280900 | 0.47172800 | -3.19539300 |
| C | 3.04122500 | -2.63335600 | -0.25176300 |
| C | 3.93672100 | -3.74879900 | 0.29639800 |
| H | 2.84055700 | -2.82880900 | -1.33078000 |
| H | 2.03905600 | -2.68605600 | 0.22739300 |

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| H | 3.44775500 | -4.73473200 | 0.15790700 |
| H | 4.92093100 | -3.79529800 | -0.21629600 |
| H | 4.13017600 | -3.62682800 | 1.38319300 |
| C | 2.33419600 | 2.38889300 | -0.83454200 |
| C | 2.96077600 | 3.78665100 | -0.80446200 |
| H | 1.44080600 | 2.36417300 | -0.17260000 |
| H | 1.93940800 | 2.18703500 | -1.85530700 |
| H | 2.22565200 | 4.54531200 | -1.14306900 |
| H | 3.28273500 | 4.07724300 | 0.21761000 |
| H | 3.84690600 | 3.86456500 | -1.46965400 |
| C | -2.39207000 | 2.35409800 | -0.90939000 |
| C | -2.94523600 | 3.78006100 | -0.81878800 |
| H | -2.09918800 | 2.14591200 | -1.96385900 |
| H | -1.42905000 | 2.29509000 | -0.35273100 |
| H | -2.19578000 | 4.51048600 | -1.18645400 |
| H | -3.86132400 | 3.91050700 | -1.43232900 |
| H | -3.19975000 | 4.06114500 | 0.22475700 |
| C | -3.06583700 | -2.57716200 | 0.13522400 |
| C | -3.98768100 | -3.66735300 | 0.69018600 |
| H | -2.12503800 | -2.55441800 | 0.73066000 |
| H | -2.73257900 | -2.86534500 | -0.88806400 |
| H | -3.47116600 | -4.64892600 | 0.68278500 |
| H | -4.28716300 | -3.45970200 | 1.73879100 |
| H | -4.91592700 | -3.77707400 | 0.09021000 |
| O | -1.34506800 | -0.08848500 | 1.91087800 |
| C | -0.84428300 | 0.94992300 | 2.46664800 |
| O | -0.33326100 | 0.93439600 | 3.73103900 |
| O | 0.77966500 | 0.88734200 | 1.56057900 |
| C | 0.80081700 | 0.05032700 | 3.77793600 |
| C | 1.67934600 | 0.55936400 | 2.61417900 |
| H | 1.27131000 | 0.16053300 | 4.77363400 |
| H | 0.48826400 | -1.00532500 | 3.62100500 |
| H | 2.23915300 | 1.47306700 | 2.91387400 |
| H | 2.40820600 | -0.21469800 | 2.29108900 |
| H | 0.32705200 | -1.99851700 | 1.06306000 |
| H | -1.24782900 | 1.96509800 | 2.23807000 |
| TS-3 | | | |
| N | 1.30062500 | -0.03226300 | 0.87592100 |
| C | 3.48146700 | -1.02407700 | 0.20490600 |
| Al | -0.10852600 | -0.08662100 | -0.45509200 |
| C | 4.79625000 | -0.81944500 | -0.26508600 |
| H | 5.44714800 | -1.68809000 | -0.44375000 |
| C | 1.07382300 | 0.02022800 | 2.21366100 |
| C | -0.21006600 | 0.05376500 | 2.79821800 |

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| H | -0.23493300 | 0.08398200 | 3.89548800 |
| C | 2.67033200 | 0.12304100 | 0.42322300 |
| C | 4.47886600 | 1.59068500 | -0.27246400 |
| H | 4.88220600 | 2.59774000 | -0.45563300 |
| C | 5.28840300 | 0.47013700 | -0.51031600 |
| H | 6.31676400 | 0.60427600 | -0.88274700 |
| C | 3.15983800 | 1.44275700 | 0.20457900 |
| C | 2.25915700 | 0.06457100 | 3.15778900 |
| H | 2.93893400 | -0.79457900 | 2.98545200 |
| H | 1.92550800 | 0.05154000 | 4.21170600 |
| H | 2.87008200 | 0.97575200 | 2.99177900 |
| N | -1.60102800 | 0.05741400 | 0.81163400 |
| C | -3.57276400 | -1.24481600 | 0.07342500 |
| C | -4.84621000 | -1.26396000 | -0.53340800 |
| H | -5.36446800 | -2.22356800 | -0.67668600 |
| C | -1.46893900 | 0.09219600 | 2.15027600 |
| C | -2.92868400 | 0.01644600 | 0.23649600 |
| C | -4.82208000 | 1.15418600 | -0.77422400 |
| H | -5.32224000 | 2.07705000 | -1.10343400 |
| C | -5.46462200 | -0.07874300 | -0.95603400 |
| H | -6.45920900 | -0.11626500 | -1.42881300 |
| C | -3.54628200 | 1.23075700 | -0.17755400 |
| C | -2.70477200 | 0.18915000 | 3.02181500 |
| H | -3.37939100 | -0.67666900 | 2.86163100 |
| H | -2.43524800 | 0.23520400 | 4.09312300 |
| H | -3.29697800 | 1.09117800 | 2.76297400 |
| C | -2.90203100 | -2.52411600 | 0.55687500 |
| C | -3.65455400 | -3.83248000 | 0.29501400 |
| H | -2.69893300 | -2.43666200 | 1.64864000 |
| H | -1.89164000 | -2.58133100 | 0.09345600 |
| H | -3.06839300 | -4.69359400 | 0.67558000 |
| H | -4.64442600 | -3.85734300 | 0.79788600 |
| H | -3.82289500 | -4.00261900 | -0.78898500 |
| C | -2.83298100 | 2.55794700 | 0.02715400 |
| C | -3.60503300 | 3.81656400 | -0.38078800 |
| H | -1.87135000 | 2.50687600 | -0.53156900 |
| H | -2.53499000 | 2.64263700 | 1.09703800 |
| H | -2.99663300 | 4.72180700 | -0.17808100 |
| H | -3.84602800 | 3.82195000 | -1.46472600 |
| H | -4.56024000 | 3.92810300 | 0.17556900 |
| C | 2.27625000 | 2.64638800 | 0.50886000 |
| C | 2.85860700 | 4.02288000 | 0.17124900 |
| H | 2.00806900 | 2.62719800 | 1.59045400 |
| H | 1.30200300 | 2.51455500 | -0.01250700 |

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|-------------|-------------|-------------|-------------|
| H | 2.12778700 | 4.81996300 | 0.41784800 |
| H | 3.78724800 | 4.23884600 | 0.74059500 |
| H | 3.09867400 | 4.11828800 | -0.90879100 |
| C | 2.93710300 | -2.41736800 | 0.46999800 |
| C | 3.96556000 | -3.55397400 | 0.49764300 |
| H | 2.17643800 | -2.65218900 | -0.31026400 |
| H | 2.37232000 | -2.40869400 | 1.42807600 |
| H | 3.46718500 | -4.51251500 | 0.74833800 |
| H | 4.45434900 | -3.69544700 | -0.48876400 |
| H | 4.76517500 | -3.38254800 | 1.24998900 |
| O | 0.84168800 | -3.06375300 | -1.99526800 |
| C | 0.32343100 | -1.99928100 | -2.25595100 |
| O | 1.12456700 | -0.72507100 | -2.09811200 |
| O | -0.25428300 | 1.38268800 | -1.45930400 |
| C | 0.97620000 | 0.22063100 | -3.17418900 |
| C | 0.62010000 | 1.57749400 | -2.53983800 |
| H | 1.91296700 | 0.25683300 | -3.77203100 |
| H | 0.14682200 | -0.12339300 | -3.83678000 |
| H | 1.56109800 | 2.08451500 | -2.20989200 |
| H | 0.15747100 | 2.23283100 | -3.31563400 |
| H | -0.67743500 | -1.54999900 | -1.09289100 |
| H | -0.43314700 | -1.82589900 | -3.06684100 |
| TS-4 | | | |
| N | -0.07953300 | -1.97385900 | 0.67358900 |
| C | -2.48380900 | -1.85349000 | 1.22691000 |
| Al | 0.71068000 | -0.52328000 | -0.27718100 |
| C | -3.81459700 | -2.18651000 | 0.90161800 |
| H | -4.63364200 | -1.82720500 | 1.54147200 |
| C | 0.60810400 | -2.72455200 | 1.57072400 |
| C | 1.91961100 | -2.42101500 | 2.00007800 |
| H | 2.35113100 | -3.10666300 | 2.74111500 |
| C | -1.45349800 | -2.33232700 | 0.37108300 |
| C | -3.07835900 | -3.42870800 | -1.05652800 |
| H | -3.32610300 | -4.04134000 | -1.93584500 |
| C | -4.11024300 | -2.96220700 | -0.22890100 |
| H | -5.15759200 | -3.20821600 | -0.46711100 |
| C | -1.72862100 | -3.12825900 | -0.77609100 |
| C | -0.04523700 | -3.96529000 | 2.14137800 |
| H | -0.97364500 | -3.71673300 | 2.69442600 |
| H | 0.64275900 | -4.49763900 | 2.82343400 |
| H | -0.34900100 | -4.65547300 | 1.32727800 |
| N | 2.36993600 | -0.43830000 | 0.67114200 |
| C | 3.24064800 | 1.86056400 | 0.94935700 |
| C | 4.12857600 | 2.87295000 | 0.52968400 |

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|---|-------------|-------------|-------------|
| H | 4.10788600 | 3.85298300 | 1.02848600 |
| C | 2.74579200 | -1.34366100 | 1.60057500 |
| C | 3.29567100 | 0.60725800 | 0.27918100 |
| C | 5.07110400 | 1.40763100 | -1.16737200 |
| H | 5.78595400 | 1.24910900 | -1.98827400 |
| C | 5.03529200 | 2.64944200 | -0.51641500 |
| H | 5.72040100 | 3.45333800 | -0.83008200 |
| C | 4.20372700 | 0.36100800 | -0.78970500 |
| C | 4.10943200 | -1.21925600 | 2.24415200 |
| H | 4.22126300 | -0.23434000 | 2.74256400 |
| H | 4.27319200 | -2.01782000 | 2.99080400 |
| H | 4.91466700 | -1.27022300 | 1.48245800 |
| C | 2.23937600 | 2.08030100 | 2.07196100 |
| C | 2.27858400 | 3.44551900 | 2.76456200 |
| H | 2.36748300 | 1.27826100 | 2.83393300 |
| H | 1.21913500 | 1.91606300 | 1.65818600 |
| H | 1.50833900 | 3.49102700 | 3.56090600 |
| H | 3.26238700 | 3.64945900 | 3.23832500 |
| H | 2.06359600 | 4.27256400 | 2.05648300 |
| C | 4.21013500 | -0.98487600 | -1.49927600 |
| C | 5.26741400 | -1.17379000 | -2.59168000 |
| H | 3.19362400 | -1.13816700 | -1.93037200 |
| H | 4.32196500 | -1.79384900 | -0.74198500 |
| H | 5.18420400 | -2.18802600 | -3.03287600 |
| H | 5.14122400 | -0.44646300 | -3.42090900 |
| H | 6.30241400 | -1.06426400 | -2.20325200 |
| C | -0.59153800 | -3.64042400 | -1.64851200 |
| C | -0.98928800 | -4.52177400 | -2.83669300 |
| H | 0.12503800 | -4.20070600 | -1.00440900 |
| H | -0.00822600 | -2.76424400 | -2.01523000 |
| H | -0.08577600 | -4.83883500 | -3.39644900 |
| H | -1.52499000 | -5.44241600 | -2.52140200 |
| H | -1.64356100 | -3.98060100 | -3.55207300 |
| C | -2.13873000 | -1.01639200 | 2.44868400 |
| C | -3.31919800 | -0.52227700 | 3.28779000 |
| H | -1.55452500 | -0.13589100 | 2.10615800 |
| H | -1.44181700 | -1.59177900 | 3.09987700 |
| H | -2.95242900 | 0.07216500 | 4.14932400 |
| H | -3.97881800 | 0.13692100 | 2.68891300 |
| H | -3.92806400 | -1.35713300 | 3.69563900 |
| O | 0.97409300 | -0.76915300 | -2.01682000 |
| C | 0.26723100 | 1.53031700 | -1.80764600 |
| C | 0.39833700 | 0.31169000 | -2.74243000 |
| H | -0.46844600 | 2.27818100 | -2.16868400 |

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|-------------|-------------|-------------|-------------|
| H | 1.25002300 | 2.04992400 | -1.71089000 |
| H | -0.60712400 | 0.01831000 | -3.13478000 |
| H | 1.03014200 | 0.57462900 | -3.62330300 |
| O | -0.14886000 | 1.05600100 | -0.50669000 |
| B | -1.48456800 | 2.13146300 | 0.49256700 |
| O | -1.59412400 | 3.27749200 | -0.31975900 |
| O | -2.69696200 | 1.41688600 | 0.50963100 |
| H | -0.80697800 | 2.12073900 | 1.50823600 |
| C | -2.98452500 | 3.43586600 | -0.69255200 |
| C | -3.57484100 | 1.96939900 | -0.50153100 |
| C | -3.59690500 | 4.46209800 | 0.28137900 |
| C | -3.06453500 | 3.97878400 | -2.12424100 |
| C | -5.01347400 | 1.92640700 | 0.03094800 |
| C | -3.47937000 | 1.09517400 | -1.76537600 |
| H | -2.99630400 | 5.39329400 | 0.23882400 |
| H | -4.64706700 | 4.71256300 | 0.02597300 |
| H | -3.56611400 | 4.08868000 | 1.32467100 |
| H | -4.11989600 | 4.08404200 | -2.45219900 |
| H | -2.59153100 | 4.98113400 | -2.17059800 |
| H | -2.54102200 | 3.32398700 | -2.84702200 |
| H | -5.71467400 | 2.42657100 | -0.66959000 |
| H | -5.33838700 | 0.87131700 | 0.13897900 |
| H | -5.09867200 | 2.41187800 | 1.02170500 |
| H | -4.21152200 | 1.40495700 | -2.53958600 |
| H | -2.46636500 | 1.12593100 | -2.20956700 |
| H | -3.69013900 | 0.04301900 | -1.48588000 |
| TS-5 | | | |
| N | -1.42316000 | -1.32425300 | 0.86014300 |
| C | -3.46643600 | 0.07933400 | 0.96977200 |
| Al | 0.03891300 | -0.59046100 | -0.20812800 |
| C | -4.77370400 | 0.33619100 | 0.50676500 |
| H | -5.32435500 | 1.20714700 | 0.89202300 |
| C | -1.24678500 | -2.20377400 | 1.87785400 |
| C | 0.00779300 | -2.69991300 | 2.29145400 |
| H | -0.01208000 | -3.40976100 | 3.12891200 |
| C | -2.78430500 | -1.05194300 | 0.44562400 |
| C | -4.70606500 | -1.62738000 | -0.92509400 |
| H | -5.20367700 | -2.28399500 | -1.65439000 |
| C | -5.38461700 | -0.50044500 | -0.43842800 |
| H | -6.40380100 | -0.27711100 | -0.79287800 |
| C | -3.39977000 | -1.93274400 | -0.48898300 |
| C | -2.46251100 | -2.70991500 | 2.63187200 |
| H | -3.06335300 | -1.86679300 | 3.02967300 |
| H | -2.16178900 | -3.36173500 | 3.47278800 |

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| H | -3.14172700 | -3.28295100 | 1.96798500 |
| N | 1.47869800 | -1.55177600 | 0.74071900 |
| C | 3.50846600 | -0.18147100 | 1.04945100 |
| C | 4.81189200 | 0.16148600 | 0.63434500 |
| H | 5.35424600 | 0.96597700 | 1.15291500 |
| C | 1.28730200 | -2.41209800 | 1.75629100 |
| C | 2.83334600 | -1.22541000 | 0.35237700 |
| C | 4.75858100 | -1.54688700 | -1.09301100 |
| H | 5.26025300 | -2.07276700 | -1.91886600 |
| C | 5.42976200 | -0.50913000 | -0.43113100 |
| H | 6.44713900 | -0.22420900 | -0.74417000 |
| C | 3.45388300 | -1.93113500 | -0.71723900 |
| C | 2.47788600 | -3.11639100 | 2.37737700 |
| H | 3.19469300 | -2.39008100 | 2.81253800 |
| H | 2.15778400 | -3.81637100 | 3.17124100 |
| H | 3.04387400 | -3.68212600 | 1.60880600 |
| C | 2.82980900 | 0.52182100 | 2.21717200 |
| C | 3.65712100 | 1.58158900 | 2.95189700 |
| H | 2.49183800 | -0.24127300 | 2.95351100 |
| H | 1.88249500 | 0.97244700 | 1.84298200 |
| H | 3.06994300 | 2.01786300 | 3.78589100 |
| H | 4.58629500 | 1.15706900 | 3.38756800 |
| H | 3.95305300 | 2.41779700 | 2.28452300 |
| C | 2.72047300 | -3.06827700 | -1.40990200 |
| C | 3.47818200 | -3.78452500 | -2.53191800 |
| H | 1.75953600 | -2.66061700 | -1.79783900 |
| H | 2.41631200 | -3.81501200 | -0.64062300 |
| H | 2.85163800 | -4.59324500 | -2.96117600 |
| H | 3.73507800 | -3.09458300 | -3.36339300 |
| H | 4.42324900 | -4.25069400 | -2.17936300 |
| C | -2.66489100 | -3.18006900 | -0.96405300 |
| C | -3.33886900 | -3.98504600 | -2.08035500 |
| H | -2.50555100 | -3.85253000 | -0.08925300 |
| H | -1.63549700 | -2.89347400 | -1.27249900 |
| H | -2.70612900 | -4.85032300 | -2.36541200 |
| H | -4.32747800 | -4.38726900 | -1.77350400 |
| H | -3.49552100 | -3.37436300 | -2.99464600 |
| C | -2.79270300 | 0.95967800 | 2.01013900 |
| C | -3.65833200 | 2.06205700 | 2.62797500 |
| H | -1.89985300 | 1.43483900 | 1.54847800 |
| H | -2.38939600 | 0.31136000 | 2.82006200 |
| H | -3.08042700 | 2.61940100 | 3.39343100 |
| H | -3.98772600 | 2.79963400 | 1.86679600 |
| H | -4.56674300 | 1.65862700 | 3.12433300 |

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|---|-------------|-------------|-------------|
| O | 0.11630700 | -1.33074000 | -1.83075900 |
| C | -0.93949000 | 0.60532100 | -2.80704700 |
| C | -0.71086600 | -0.90992400 | -2.88489100 |
| H | -1.84707400 | 0.91619300 | -3.36971900 |
| H | -0.06479300 | 1.16041000 | -3.20180500 |
| H | -1.69760800 | -1.43559200 | -2.85166100 |
| H | -0.25137500 | -1.15639900 | -3.87172600 |
| O | -1.11150500 | 0.93076800 | -1.40869000 |
| B | -0.34028400 | 2.01342600 | -0.87123100 |
| O | 0.58154800 | 2.68038900 | -1.67810200 |
| O | -0.87117500 | 2.84692100 | 0.12272800 |
| H | 0.58626300 | 0.93764000 | 0.13582600 |
| C | 0.91689100 | 3.93060600 | -1.01968100 |
| C | -0.37047200 | 4.19120500 | -0.11619100 |
| C | 2.19821500 | 3.70232900 | -0.20066800 |
| C | 1.17014200 | 4.98959900 | -2.09784300 |
| C | -0.08109100 | 4.86049800 | 1.23082800 |
| C | -1.47903300 | 4.95979300 | -0.85828700 |
| H | 2.98882900 | 3.31420000 | -0.87358100 |
| H | 2.56338200 | 4.64041800 | 0.26453800 |
| H | 2.03717000 | 2.94975300 | 0.59518900 |
| H | 1.34808400 | 5.98575800 | -1.64219700 |
| H | 2.07204700 | 4.71678500 | -2.68270300 |
| H | 0.32105600 | 5.06919700 | -2.80281000 |
| H | 0.36924200 | 5.86472800 | 1.08708800 |
| H | -1.02663300 | 4.99037000 | 1.79577400 |
| H | 0.60361600 | 4.25203200 | 1.85115900 |
| H | -1.21444800 | 6.02577000 | -1.01353700 |
| H | -1.69480700 | 4.50280600 | -1.84483200 |
| H | -2.40871500 | 4.91725300 | -0.25591200 |

TS-6

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|----|-------------|-------------|-------------|
| Al | 1.22691500 | -0.51366600 | 0.08058300 |
| N | 1.98301100 | -1.07454500 | -1.60599900 |
| N | 2.88573900 | -0.00850000 | 0.93414400 |
| O | 0.05150700 | 0.86172800 | -0.06742900 |
| O | -3.61405200 | 0.84193300 | 0.17304200 |
| C | 3.21578100 | -0.68458300 | -2.00372800 |
| C | 1.23249400 | -2.00236000 | -2.43183100 |
| C | 4.00552400 | 0.25719600 | 0.22516200 |
| C | 2.93672000 | 0.02301700 | 2.38390900 |
| C | -1.21725300 | 0.81350100 | 0.58846800 |
| C | -2.34375600 | 0.54675300 | -0.41823200 |
| C | 4.10992600 | 0.02801800 | -1.16860900 |
| C | 3.70400400 | -1.07053700 | -3.38430600 |

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| C | 1.40668200 | -3.39899500 | -2.21309900 |
| C | 0.32738400 | -1.51226400 | -3.41430900 |
| C | 5.23492300 | 0.76832700 | 0.94658500 |
| C | 3.28984300 | -1.17085800 | 3.07584700 |
| C | 2.60789200 | 1.21729800 | 3.08406900 |
| H | -1.39947500 | 1.78749500 | 1.09070700 |
| H | -1.22200800 | 0.02590700 | 1.37721800 |
| H | -2.30513500 | -0.50655900 | -0.77353100 |
| H | -2.20664400 | 1.22079400 | -1.28789000 |
| H | 5.05885400 | 0.32915900 | -1.63217100 |
| H | 3.80377300 | -2.17311400 | -3.46936600 |
| H | 4.68675800 | -0.61283400 | -3.60138100 |
| H | 2.98144400 | -0.76443300 | -4.16744000 |
| C | 0.65775500 | -4.29778500 | -2.99974500 |
| C | 2.37426100 | -3.88776800 | -1.14663900 |
| C | -0.39783800 | -2.45386800 | -4.17554500 |
| C | 0.15858600 | -0.01892700 | -3.62423700 |
| H | 5.61819500 | 0.00493100 | 1.65589400 |
| H | 6.04096900 | 1.01841300 | 0.23231800 |
| H | 4.99971500 | 1.66498200 | 1.55487500 |
| C | 3.31136100 | -1.14560600 | 4.48527100 |
| C | 3.62107800 | -2.43344700 | 2.29558800 |
| C | 2.64524400 | 1.18960500 | 4.49468800 |
| C | 2.23161200 | 2.47421200 | 2.32191000 |
| H | 0.77476600 | -5.38094500 | -2.84820300 |
| C | -0.23723000 | -3.83116000 | -3.97282800 |
| C | 2.53858000 | -5.40507300 | -1.01483000 |
| H | 2.04182800 | -3.46818100 | -0.17031000 |
| H | 3.37193000 | -3.42533900 | -1.32067300 |
| H | -1.10200800 | -2.09894900 | -4.94234800 |
| C | -0.80300400 | 0.41619400 | -4.73206100 |
| H | 1.15570400 | 0.43990900 | -3.80834100 |
| H | -0.16292900 | 0.44550600 | -2.66900100 |
| H | 3.58036200 | -2.05555800 | 5.04163000 |
| C | 2.99196500 | 0.02349500 | 5.19023400 |
| C | 4.05040200 | -3.65299800 | 3.11719600 |
| H | 4.40979300 | -2.20166200 | 1.54490600 |
| H | 2.72830200 | -2.69784100 | 1.68495100 |
| H | 2.39751900 | 2.10132100 | 5.05790500 |
| C | 1.95763700 | 3.72893000 | 3.15372600 |
| H | 1.34540500 | 2.26395200 | 1.68731000 |
| H | 3.02646500 | 2.70125200 | 1.57684700 |
| H | -0.81514600 | -4.54804300 | -4.57791100 |
| H | 3.26890000 | -5.64566600 | -0.21546500 |

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|---|-------------|-------------|-------------|
| H | 1.58364200 | -5.90463400 | -0.74921400 |
| H | 2.91072400 | -5.86742000 | -1.95337700 |
| H | -0.84840100 | 1.52258400 | -4.76427500 |
| H | -0.48696800 | 0.05721900 | -5.73485600 |
| H | -1.83608900 | 0.05012600 | -4.55341500 |
| H | 3.01289900 | 0.02482600 | 6.29186200 |
| H | 4.27455800 | -4.50897000 | 2.44836700 |
| H | 4.96412200 | -3.45192500 | 3.71535600 |
| H | 3.25531200 | -3.98262100 | 3.81804900 |
| H | 1.68880900 | 4.56346100 | 2.47661100 |
| H | 1.10975900 | 3.58640600 | 3.85671900 |
| H | 2.84010200 | 4.04417200 | 3.75062000 |
| H | 0.49847800 | -1.70992900 | 0.85279000 |
| B | -4.38576200 | -0.14699000 | 0.70853600 |
| O | -5.62568000 | 0.12001900 | 1.26022500 |
| O | -4.02796100 | -1.48542900 | 0.75463600 |
| C | -6.05294100 | -1.09785200 | 1.93481600 |
| C | -5.21219400 | -2.22143400 | 1.18006300 |
| C | -5.66523300 | -0.95316700 | 3.41685600 |
| C | -7.57192100 | -1.22683100 | 1.79536100 |
| C | -4.76995000 | -3.39648600 | 2.05540100 |
| C | -5.90417700 | -2.73609100 | -0.09381300 |
| H | -6.11641200 | -0.02209600 | 3.81499300 |
| H | -6.02842800 | -1.80518900 | 4.02667700 |
| H | -4.56588000 | -0.87703800 | 3.54044200 |
| H | -7.93159700 | -2.18155000 | 2.23205200 |
| H | -8.06806600 | -0.39559500 | 2.33633600 |
| H | -7.89134700 | -1.17791500 | 0.73716300 |
| H | -5.64746300 | -3.93815300 | 2.46543200 |
| H | -4.17894600 | -4.11260400 | 1.44905400 |
| H | -4.13376400 | -3.06303400 | 2.89690200 |
| H | -6.77756400 | -3.37824700 | 0.13965500 |
| H | -6.24678100 | -1.89730900 | -0.73319000 |
| H | -5.17804000 | -3.33570000 | -0.67889400 |
| B | 0.63184900 | 2.55536500 | -1.01642900 |
| O | -0.30424600 | 2.73094100 | -2.05921600 |
| O | 0.55227100 | 3.62617900 | -0.11063500 |
| H | 1.71266000 | 2.01949800 | -1.21198400 |
| C | -0.76282600 | 4.10447400 | -2.03911600 |
| C | -0.47196700 | 4.56271100 | -0.53683600 |
| C | 0.07722400 | 4.87331700 | -3.07887800 |
| C | -2.24089700 | 4.14892700 | -2.44640300 |
| C | 0.10925400 | 5.97925100 | -0.40729700 |
| C | -1.69306200 | 4.44552400 | 0.39210900 |

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| H | -0.04214700 | 4.38396800 | -4.06674400 |
| H | -0.24052900 | 5.93141800 | -3.17703600 |
| H | 1.15516400 | 4.85195700 | -2.82158400 |
| H | -2.63305600 | 5.18642000 | -2.40540100 |
| H | -2.35193600 | 3.78685900 | -3.48900100 |
| H | -2.87304200 | 3.51332300 | -1.79796500 |
| H | -0.59086800 | 6.73994500 | -0.81104600 |
| H | 0.28139600 | 6.21440200 | 0.66314900 |
| H | 1.07805000 | 6.07478800 | -0.93283100 |
| H | -2.43701000 | 5.24159300 | 0.18349800 |
| H | -2.20850200 | 3.47111100 | 0.30180900 |
| H | -1.35777500 | 4.55953400 | 1.44314700 |
| TS-7 | | | |
| Al | 2.19148200 | 0.11010300 | 0.15378600 |
| N | 1.82612700 | -1.04686200 | -1.35147500 |
| C | 2.08189000 | -3.50398000 | -0.99063400 |
| C | 2.87678200 | -4.66012600 | -1.15015800 |
| H | 2.51044600 | -5.62226000 | -0.76283300 |
| C | 4.12111000 | -4.60764800 | -1.79129500 |
| H | 4.72434400 | -5.52335900 | -1.89893700 |
| C | 4.59673900 | -3.39120400 | -2.30074000 |
| H | 5.57264000 | -3.36173400 | -2.80727800 |
| C | 3.84123800 | -2.20827100 | -2.17364000 |
| C | 2.58281900 | -2.27593300 | -1.50759400 |
| C | 0.96384600 | -0.67217400 | -2.32377800 |
| C | 0.37048400 | 0.61276000 | -2.38847100 |
| H | -0.35153300 | 0.76170600 | -3.20235600 |
| C | 0.73645300 | -3.56811200 | -0.28841800 |
| H | 0.01706700 | -2.91765000 | -0.82940600 |
| H | 0.82954700 | -3.09625200 | 0.71598200 |
| C | 0.12668100 | -4.96475200 | -0.11761800 |
| H | 0.01146800 | -5.49640800 | -1.08659500 |
| H | -0.87800400 | -4.88637600 | 0.34538000 |
| H | 0.73651700 | -5.61060600 | 0.54822100 |
| H | 3.55903500 | -0.44526900 | -3.38576000 |
| H | 4.41419000 | -0.16895500 | -1.87239900 |
| C | 5.67597400 | -0.91201000 | -3.47539900 |
| H | 5.64228300 | -1.58087200 | -4.36124400 |
| H | 6.50928500 | -1.25415900 | -2.82688100 |
| H | 5.93710100 | 0.10338100 | -3.83747200 |
| C | 0.65311100 | -1.64118100 | -3.44594400 |
| H | -0.12327900 | -1.23424400 | -4.11983400 |
| H | 0.31490000 | -2.62079400 | -3.05218400 |
| H | 1.56442000 | -1.84848100 | -4.04552400 |

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|---|-------------|-------------|-------------|
| N | 1.54543800 | 1.76222200 | -0.59227600 |
| C | 3.20089900 | 3.58533800 | -0.44977600 |
| C | 3.66116900 | 4.76141300 | 0.17240900 |
| H | 4.59973100 | 5.22440300 | -0.16619800 |
| C | 2.94180600 | 5.35088100 | 1.22412000 |
| H | 3.32175800 | 6.26612200 | 1.70571300 |
| C | 1.74274900 | 4.77541000 | 1.65802700 |
| H | 1.18291700 | 5.24383000 | 2.48291700 |
| C | 1.23138300 | 3.59898500 | 1.06456100 |
| C | 1.98014500 | 3.00657700 | 0.01089700 |
| C | 0.70192700 | 1.77373000 | -1.64664100 |
| C | 3.97011900 | 2.92899300 | -1.58569800 |
| H | 3.28106100 | 2.77500600 | -2.44646400 |
| H | 4.24221900 | 1.89898800 | -1.26163600 |
| C | 5.22872500 | 3.65578300 | -2.06933900 |
| H | 5.70003900 | 3.09663100 | -2.90326000 |
| H | 5.98871300 | 3.74938900 | -1.26577400 |
| H | 5.00366800 | 4.67783200 | -2.44080600 |
| C | -0.07488100 | 3.00437200 | 1.56229700 |
| H | -0.39475300 | 2.19096900 | 0.88259600 |
| H | 0.10838300 | 2.48380200 | 2.52836500 |
| C | -1.22198300 | 4.01380100 | 1.74053100 |
| H | -0.99514200 | 4.78559700 | 2.50522600 |
| H | -2.14480500 | 3.49316900 | 2.06965400 |
| H | -1.45525700 | 4.54859400 | 0.79455100 |
| C | 0.10453000 | 3.09013500 | -2.09401000 |
| H | -0.49374500 | 3.54769600 | -1.27957000 |
| H | -0.54255400 | 2.95622300 | -2.98011700 |
| H | 0.90190100 | 3.82204100 | -2.33973400 |
| C | 4.34117800 | -0.88187000 | -2.72448800 |
| H | 3.77466900 | 0.10531000 | 0.41941600 |
| H | 1.62824900 | -0.07674800 | 1.72430900 |
| B | 0.33140600 | -0.60461800 | 2.11283200 |
| O | -0.03562200 | 0.19348100 | 3.24024900 |
| O | 0.54599900 | -1.94690500 | 2.54891100 |
| C | 0.80280600 | -1.91324400 | 3.97010700 |
| C | -0.02302600 | -0.62846500 | 4.43023200 |
| C | -1.48659400 | -0.95430700 | 4.78485700 |
| H | -1.57082100 | -1.51868600 | 5.73634600 |
| H | -2.04785300 | -0.00454600 | 4.89931300 |
| H | -1.97653800 | -1.54407500 | 3.98430500 |
| C | 0.61848800 | 0.16327900 | 5.57726700 |
| H | 0.71286500 | -0.45892400 | 6.49192800 |
| H | 1.62138100 | 0.54132500 | 5.30211700 |

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|-------------|-------------|-------------|-------------|
| H | -0.01553000 | 1.03867000 | 5.82751700 |
| C | 2.32204900 | -1.76076900 | 4.18525200 |
| H | 2.84230900 | -2.58632300 | 3.65824600 |
| H | 2.70208200 | -0.80518800 | 3.77247900 |
| H | 2.59616000 | -1.80973600 | 5.25883900 |
| C | 0.32739900 | -3.23498200 | 4.58430100 |
| H | -0.72337300 | -3.45518000 | 4.31612800 |
| H | 0.95498900 | -4.06933400 | 4.20923000 |
| H | 0.41471300 | -3.21610800 | 5.69063000 |
| O | -0.31863300 | -0.41123900 | 0.84041400 |
| C | -1.61929600 | -0.95021500 | 0.64138200 |
| C | -2.71100800 | 0.05316500 | 1.03891700 |
| H | -1.75655500 | -1.89076400 | 1.22156900 |
| H | -1.72956400 | -1.20018400 | -0.43758000 |
| O | -3.99828600 | -0.56094900 | 0.92353100 |
| H | -2.64462300 | 0.96279100 | 0.40372000 |
| H | -2.56451100 | 0.35184000 | 2.09759400 |
| B | -4.84362600 | -0.25078900 | -0.09768200 |
| O | -6.10525200 | -0.81160300 | -0.18720500 |
| O | -4.55221300 | 0.63423800 | -1.12776200 |
| C | -6.63541600 | -0.44736000 | -1.49232200 |
| C | -5.79965300 | 0.86140000 | -1.84740400 |
| C | -6.34384800 | -1.62134000 | -2.44355500 |
| C | -8.14580500 | -0.23253900 | -1.36487500 |
| C | -5.48345600 | 1.04268500 | -3.33395000 |
| C | -6.42362200 | 2.14552800 | -1.27462700 |
| H | -6.77463700 | -2.54664700 | -2.01105500 |
| H | -6.78983000 | -1.46504200 | -3.44677600 |
| H | -5.25302600 | -1.78025300 | -2.56473400 |
| H | -8.57982400 | 0.12214000 | -2.32269700 |
| H | -8.63762200 | -1.19083200 | -1.10136600 |
| H | -8.38946600 | 0.49948700 | -0.57182500 |
| H | -6.41534900 | 1.13739300 | -3.92892000 |
| H | -4.89060000 | 1.96843300 | -3.48120300 |
| H | -4.89391900 | 0.19560400 | -3.73299000 |
| H | -7.34309600 | 2.43927700 | -1.82039100 |
| H | -6.67631100 | 2.02599500 | -0.20158400 |
| H | -5.68946500 | 2.97182200 | -1.36143400 |
| TS-8 | | | |
| Al | -3.26572700 | -0.17378900 | 0.19437300 |
| C | 1.69066900 | 0.78675100 | -2.63523600 |
| N | -4.51866900 | 1.02769700 | -0.66510000 |
| N | -4.55001600 | -1.56816000 | 0.59864100 |
| O | -2.14038600 | -0.78703500 | -1.00072900 |

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| O | 1.41434200 | 0.19495900 | -1.28068300 |
| C | -5.80021800 | 0.71525400 | -0.94819900 |
| C | -4.00974600 | 2.33760800 | -1.01069900 |
| C | -5.83456800 | -1.56571200 | 0.18250100 |
| C | -4.04293900 | -2.68352100 | 1.36497000 |
| C | -0.77240400 | -0.91606100 | -1.26976500 |
| C | 0.05307400 | 0.30908900 | -0.84022200 |
| C | -6.40346300 | -0.50721400 | -0.56392900 |
| C | -6.65712300 | 1.71844900 | -1.69274900 |
| C | -4.12435900 | 3.38179500 | -0.04851000 |
| C | -3.37063500 | 2.54084800 | -2.26634700 |
| C | -6.72916600 | -2.73464600 | 0.54204600 |
| C | -4.05533500 | -2.60383700 | 2.78615100 |
| C | -3.49306100 | -3.80628800 | 0.68243800 |
| H | -0.62573300 | -1.06036800 | -2.36874100 |
| H | -0.34814000 | -1.82564800 | -0.77623700 |
| H | 0.07175300 | 0.39862000 | 0.26637100 |
| H | -0.39446700 | 1.23728400 | -1.25889800 |
| H | -7.45447500 | -0.63570500 | -0.85503700 |
| H | -6.74330000 | 2.66678600 | -1.12276800 |
| H | -7.67266500 | 1.32076500 | -1.87415600 |
| H | -6.19808600 | 1.98643800 | -2.66647500 |
| C | -3.60781000 | 4.65034300 | -0.38023900 |
| C | -4.78600100 | 3.10573700 | 1.29437000 |
| C | -2.86130100 | 3.82755300 | -2.54388000 |
| C | -3.25960300 | 1.40336300 | -3.27172800 |
| H | -6.79451700 | -2.85523700 | 1.64350600 |
| H | -7.74972000 | -2.59536800 | 0.14028500 |
| H | -6.32015100 | -3.68945400 | 0.15247200 |
| C | -3.51114200 | -3.68029900 | 3.51689300 |
| C | -4.64542500 | -1.37927700 | 3.47046000 |
| C | -2.96133800 | -4.85611100 | 1.46038700 |
| C | -3.48887800 | -3.84551800 | -0.83855500 |
| H | -3.68691700 | 5.47697600 | 0.34130600 |
| C | -2.98513800 | 4.87284300 | -1.61778000 |
| C | -4.85521400 | 4.28052200 | 2.27504600 |
| H | -4.24638300 | 2.25679100 | 1.77227600 |
| H | -5.81443700 | 2.71556700 | 1.11947100 |
| H | -2.35318700 | 4.01138600 | -3.50166000 |
| C | -2.31243400 | 1.63720200 | -4.45507600 |
| H | -4.28039700 | 1.16925900 | -3.65742800 |
| H | -2.94921100 | 0.48831800 | -2.72145600 |
| H | -3.50951300 | -3.64591300 | 4.61651000 |
| C | -2.96991300 | -4.79610200 | 2.86174500 |

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| C | -4.62998700 | -1.37901200 | 5.00214200 |
| H | -5.69114400 | -1.23773400 | 3.11441400 |
| H | -4.10209800 | -0.48293800 | 3.09439100 |
| H | -2.53096000 | -5.73679400 | 0.96070400 |
| C | -2.79913300 | -5.04989000 | -1.48681600 |
| H | -3.02539600 | -2.90005200 | -1.20016500 |
| H | -4.54086700 | -3.79411500 | -1.20242600 |
| H | -2.58440600 | 5.87018400 | -1.85922800 |
| H | -5.34788300 | 3.96688100 | 3.21809900 |
| H | -3.84555900 | 4.65852200 | 2.53971400 |
| H | -5.43678400 | 5.13351400 | 1.86599000 |
| H | -2.28643300 | 0.73658200 | -5.10270900 |
| H | -2.63365900 | 2.48571400 | -5.09588800 |
| H | -1.27333000 | 1.83615400 | -4.11657100 |
| H | -2.54877700 | -5.62739200 | 3.44979500 |
| H | -5.08119200 | -0.44358200 | 5.39152800 |
| H | -5.20738600 | -2.22702000 | 5.42732200 |
| H | -3.59755700 | -1.43928100 | 5.40589500 |
| H | -2.83892300 | -4.96504800 | -2.59202000 |
| H | -1.72848300 | -5.11673600 | -1.20009700 |
| H | -3.28024100 | -6.01294900 | -1.21298300 |
| H | -2.60967000 | 0.45783600 | 1.51560100 |
| Al | 3.81743400 | 0.45345300 | -0.83332800 |
| N | 3.32118300 | 1.37566100 | 0.78251400 |
| N | 3.72252200 | -1.36533900 | -0.18953300 |
| C | 2.62621700 | 0.73122200 | 1.74507700 |
| C | 3.76963200 | 2.73739600 | 0.99899400 |
| C | 2.96777700 | -1.65565500 | 0.89367200 |
| C | 4.47307800 | -2.41448700 | -0.84931100 |
| C | 2.38278300 | -0.66660900 | 1.72428000 |
| C | 2.12008900 | 1.51553600 | 2.93728700 |
| C | 5.00815000 | 2.94038600 | 1.67364300 |
| C | 3.00346800 | 3.82998200 | 0.50501300 |
| C | 2.76237600 | -3.10540700 | 1.27944700 |
| C | 5.80859000 | -2.66365000 | -0.40875600 |
| C | 3.90477500 | -3.15547500 | -1.92144700 |
| H | 1.75582400 | -1.04798300 | 2.54147200 |
| H | 1.47835300 | 0.88943300 | 3.58419400 |
| H | 1.54702500 | 2.40749000 | 2.61243700 |
| H | 2.96760900 | 1.89593500 | 3.54537000 |
| C | 5.46516900 | 4.26178300 | 1.84980600 |
| C | 5.81045100 | 1.74740100 | 2.16940700 |
| C | 3.50781400 | 5.13319600 | 0.70767100 |
| C | 1.68111900 | 3.59776300 | -0.20424900 |

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| H | 2.30109300 | -3.67444500 | 0.44657200 |
| H | 3.73389500 | -3.59888200 | 1.49157400 |
| H | 2.11734600 | -3.19499700 | 2.17268800 |
| C | 6.55309800 | -3.66833300 | -1.05489800 |
| C | 6.39584300 | -1.84481500 | 0.72901600 |
| C | 4.69485600 | -4.15443800 | -2.53437700 |
| C | 2.47811300 | -2.92789600 | -2.39708500 |
| H | 6.41911600 | 4.44353000 | 2.36631000 |
| C | 4.72299900 | 5.35018600 | 1.36981200 |
| C | 7.11441900 | 2.06000900 | 2.91004300 |
| H | 6.03165200 | 1.10104900 | 1.29071500 |
| H | 5.16456800 | 1.11577300 | 2.82019200 |
| H | 2.93334900 | 5.99495000 | 0.33802400 |
| C | 0.84739500 | 4.84494000 | -0.51308400 |
| H | 1.07004600 | 2.89233600 | 0.40110900 |
| H | 1.84362800 | 3.05154700 | -1.16194700 |
| H | 7.58334900 | -3.87479900 | -0.72955900 |
| C | 6.00210500 | -4.41270100 | -2.10996500 |
| C | 7.81436900 | -2.21085400 | 1.17566600 |
| H | 5.70968700 | -1.89556700 | 1.60419600 |
| H | 6.37006500 | -0.77578700 | 0.41856200 |
| H | 4.26646100 | -4.74286600 | -3.36112800 |
| C | 2.31295500 | -2.83536500 | -3.92429400 |
| H | 2.07351500 | -2.00999900 | -1.92542200 |
| H | 1.84083400 | -3.76270700 | -2.02091900 |
| H | 5.09621800 | 6.37691700 | 1.51321800 |
| H | 7.61208400 | 1.12091200 | 3.22760000 |
| H | 7.83267700 | 2.61349800 | 2.26994300 |
| H | 6.94057100 | 2.66705100 | 3.82351000 |
| H | -0.10441600 | 4.54935200 | -0.99709100 |
| H | 0.59643800 | 5.42186900 | 0.40274800 |
| H | 1.37059700 | 5.53011500 | -1.21277000 |
| H | 6.59923500 | -5.19685900 | -2.60220100 |
| H | 8.13617400 | -1.55490400 | 2.01006700 |
| H | 7.88208300 | -3.25976200 | 1.53418900 |
| H | 8.55301700 | -2.08623400 | 0.35655500 |
| H | 1.25649900 | -2.62268700 | -4.18860000 |
| H | 2.94031000 | -2.02435300 | -4.35005200 |
| H | 2.59497900 | -3.77612300 | -4.44124400 |
| H | 3.09003500 | 0.88482600 | -2.34359500 |
| H | 5.34700100 | 0.80006300 | -1.20011300 |
| O | 1.16072500 | 1.85500000 | -2.94644700 |
| H | 1.80429800 | -0.05586400 | -3.36841500 |

TS-9

| | | | |
|----|-------------|-------------|-------------|
| Al | 3.52397000 | 0.16771500 | -0.26307100 |
| N | 4.47403600 | -1.22532200 | -1.21386900 |
| N | 4.45766300 | 1.65482300 | -1.08531400 |
| O | 1.82702300 | 0.14640300 | -0.73670500 |
| O | -1.52030700 | -0.51805000 | 0.66930600 |
| C | 5.43592500 | -1.00539100 | -2.13653700 |
| C | 4.09404800 | -2.58333000 | -0.89268600 |
| C | 5.41575200 | 1.53687300 | -2.02711700 |
| C | 4.04535000 | 2.96704200 | -0.63957300 |
| C | 0.66497100 | 0.41224300 | 0.01809900 |
| C | -0.29129700 | -0.78937300 | -0.01721300 |
| C | 5.87108100 | 0.28733200 | -2.51229500 |
| C | 6.09809400 | -2.19162300 | -2.80734500 |
| C | 4.73718800 | -3.23885600 | 0.19442000 |
| C | 3.05634600 | -3.20911600 | -1.63981100 |
| C | 6.04946000 | 2.78906600 | -2.59740400 |
| C | 4.68180700 | 3.53801100 | 0.49827700 |
| C | 2.97923600 | 3.62693200 | -1.31422500 |
| H | 0.12798300 | 1.29655000 | -0.40617900 |
| H | 0.89676200 | 0.66241100 | 1.08212800 |
| H | 0.17957800 | -1.67897800 | 0.45668900 |
| H | -0.48188400 | -1.05386600 | -1.08417600 |
| H | 6.65985600 | 0.32609000 | -3.27527900 |
| H | 6.56772000 | -2.86052800 | -2.05674500 |
| H | 6.87211000 | -1.86359700 | -3.52541400 |
| H | 5.35237900 | -2.81198700 | -3.34608100 |
| C | 4.32852000 | -4.55065200 | 0.51299800 |
| C | 5.82987800 | -2.52078700 | 0.97380000 |
| C | 2.68635900 | -4.52218700 | -1.28135200 |
| C | 2.37608300 | -2.45715200 | -2.77344500 |
| H | 6.50823700 | 3.40231800 | -1.79445900 |
| H | 6.82636000 | 2.54035500 | -3.34370500 |
| H | 5.28698600 | 3.43564100 | -3.07891800 |
| C | 4.23797400 | 4.80086600 | 0.94184300 |
| C | 5.80364000 | 2.78385300 | 1.19794400 |
| C | 2.57294000 | 4.88754500 | -0.82926100 |
| C | 2.30968900 | 2.96676300 | -2.51049200 |
| H | 4.80874700 | -5.08301000 | 1.34736600 |
| C | 3.31525100 | -5.18759500 | -0.21853300 |
| C | 6.46831700 | -3.29877900 | 2.12857400 |
| H | 5.40433900 | -1.56730300 | 1.36076500 |
| H | 6.62674100 | -2.19948700 | 0.26496200 |
| H | 1.88816300 | -5.03195500 | -1.84087400 |
| C | 1.27514200 | -3.20991500 | -3.52631300 |

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|----|-------------|-------------|-------------|
| H | 3.15031700 | -2.12130100 | -3.50042500 |
| H | 1.96449900 | -1.51384000 | -2.34681700 |
| H | 4.71207000 | 5.26739200 | 1.81810700 |
| C | 3.19577400 | 5.47039400 | 0.28402600 |
| C | 6.42263300 | 3.46404400 | 2.42293000 |
| H | 6.60649100 | 2.56267500 | 0.45808000 |
| H | 5.41238600 | 1.78281000 | 1.48894200 |
| H | 1.74938100 | 5.41984000 | -1.32741700 |
| C | 1.15739700 | 3.74078100 | -3.15828600 |
| H | 1.95575400 | 1.96104200 | -2.18768000 |
| H | 3.08372100 | 2.75251600 | -3.28279900 |
| H | 3.00922400 | -6.21257200 | 0.04537500 |
| H | 7.24376300 | -2.68134100 | 2.62630800 |
| H | 5.72235200 | -3.57719200 | 2.90209500 |
| H | 6.95982200 | -4.23294300 | 1.78352900 |
| H | 0.85203500 | -2.56951000 | -4.32684400 |
| H | 1.65010700 | -4.13842200 | -4.00753000 |
| H | 0.43502200 | -3.49209900 | -2.85794500 |
| H | 2.86096500 | 6.45535300 | 0.64703400 |
| H | 7.22057400 | 2.82620300 | 2.85511500 |
| H | 6.88167700 | 4.44355700 | 2.17165200 |
| H | 5.67183000 | 3.63914700 | 3.22168100 |
| H | 0.74026000 | 3.16386300 | -4.00866500 |
| H | 0.32621700 | 3.91812000 | -2.44459800 |
| H | 1.48095400 | 4.72737300 | -3.55359800 |
| H | 3.73622600 | 0.12378700 | 1.32705000 |
| Al | -2.88738400 | 0.27492500 | -0.21857600 |
| N | -4.42440800 | -0.86845100 | -0.50977600 |
| N | -3.78671300 | 1.61446300 | 0.84287200 |
| H | -2.34842100 | 0.84906300 | -1.61198600 |
| C | -5.51229500 | -0.82077300 | 0.29095400 |
| C | -4.42889300 | -1.75316000 | -1.65898300 |
| C | -4.95247400 | 1.35931000 | 1.47904400 |
| C | -3.22247200 | 2.94946200 | 0.90635300 |
| C | -5.69614900 | 0.16979400 | 1.28627400 |
| C | -6.62264200 | -1.83175500 | 0.09357900 |
| C | -4.95154500 | -1.26282800 | -2.89005800 |
| C | -3.89443200 | -3.06755100 | -1.55173800 |
| C | -5.53408600 | 2.40738200 | 2.40467800 |
| C | -3.62654900 | 3.90375200 | -0.07078600 |
| C | -2.26740700 | 3.27294500 | 1.91012500 |
| H | -6.59829300 | 0.06528800 | 1.90377000 |
| H | -7.09667300 | -1.70474000 | -0.90236100 |
| H | -7.40319000 | -1.72278300 | 0.86908800 |

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|---|-------------|-------------|-------------|
| H | -6.22998200 | -2.86841000 | 0.11894900 |
| C | -4.93443600 | -2.11595700 | -4.01224100 |
| C | -5.49962800 | 0.15303100 | -2.97272000 |
| C | -3.90274600 | -3.88246500 | -2.70428100 |
| C | -3.33602100 | -3.56360200 | -0.23080500 |
| H | -5.80446900 | 3.32393400 | 1.83945300 |
| H | -6.43994600 | 2.03005100 | 2.91408100 |
| H | -4.79433100 | 2.72198200 | 3.16839300 |
| C | -3.06097800 | 5.19421800 | -0.01941500 |
| C | -4.63557700 | 3.51681000 | -1.14067000 |
| C | -1.73060900 | 4.57824500 | 1.91704200 |
| C | -1.85139300 | 2.23370300 | 2.93360500 |
| H | -5.33212700 | -1.75845100 | -4.97349600 |
| C | -4.41550200 | -3.41530000 | -3.92196300 |
| C | -6.08896500 | 0.58174300 | -4.32009400 |
| H | -4.67768600 | 0.84952500 | -2.69184100 |
| H | -6.26491500 | 0.29482000 | -2.17672700 |
| H | -3.49978900 | -4.90418100 | -2.64423200 |
| C | -2.88158300 | -5.02391300 | -0.18038800 |
| H | -4.08623700 | -3.38864700 | 0.57174900 |
| H | -2.48692500 | -2.91665900 | 0.07437100 |
| H | -3.35887600 | 5.94880200 | -0.76234000 |
| C | -2.12132700 | 5.53024500 | 0.96579000 |
| C | -5.05893200 | 4.62136400 | -2.11401500 |
| H | -5.54142100 | 3.09308500 | -0.65165600 |
| H | -4.20853000 | 2.66404700 | -1.71537000 |
| H | -0.99108200 | 4.85189400 | 2.68374600 |
| C | -0.87931800 | 2.69091100 | 4.02315000 |
| H | -1.41688700 | 1.35936300 | 2.40419100 |
| H | -2.76029400 | 1.80928000 | 3.41481200 |
| H | -4.41029400 | -4.06884200 | -4.80907300 |
| H | -6.46240600 | 1.62464400 | -4.26323000 |
| H | -5.33467500 | 0.54634100 | -5.13367500 |
| H | -6.94291500 | -0.05942700 | -4.62486900 |
| H | -2.49135300 | -5.25089800 | 0.83124700 |
| H | -3.70841000 | -5.73394300 | -0.39668500 |
| H | -2.06279600 | -5.23118200 | -0.90133600 |
| H | -1.68937800 | 6.54360900 | 0.99124100 |
| H | -5.79897200 | 4.23094000 | -2.84218700 |
| H | -5.53036800 | 5.47990700 | -1.59069200 |
| H | -4.19953600 | 5.01367500 | -2.69679400 |
| H | -0.66673600 | 1.84084600 | 4.70115200 |
| H | 0.09022600 | 3.03118300 | 3.60194500 |
| H | -1.28995600 | 3.52081000 | 4.63750600 |

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|--------------|-------------|-------------|-------------|
| B | -1.98010800 | -1.43387400 | 2.42769100 |
| O | -1.50826900 | -2.74609100 | 2.21925400 |
| O | -1.29872800 | -0.83337700 | 3.49832900 |
| H | -3.14510100 | -1.12096000 | 2.23724700 |
| C | -0.70970100 | -3.13015600 | 3.36488900 |
| C | -0.25910600 | -1.72701200 | 3.97181600 |
| C | -1.63177000 | -3.92582000 | 4.31077100 |
| C | 0.44192100 | -4.02683200 | 2.89783000 |
| C | -0.25027000 | -1.67122500 | 5.50635800 |
| C | 1.09999600 | -1.23973500 | 3.44389000 |
| H | -2.05739700 | -4.78607700 | 3.75522200 |
| H | -1.08866300 | -4.31978700 | 5.19414900 |
| H | -2.47688900 | -3.30255600 | 4.66610000 |
| H | 1.10684600 | -4.29367400 | 3.74567000 |
| H | 0.03603400 | -4.96931400 | 2.47655700 |
| H | 1.05377100 | -3.54397500 | 2.11297600 |
| H | 0.45927600 | -2.41225800 | 5.93027400 |
| H | 0.07380300 | -0.66449300 | 5.84136700 |
| H | -1.25508800 | -1.85966200 | 5.92944000 |
| H | 1.94023200 | -1.82718400 | 3.86709800 |
| H | 1.16410900 | -1.29796200 | 2.34142500 |
| H | 1.24408400 | -0.17967200 | 3.73458500 |
| TS-10 | | | |
| Al | 3.74280500 | -0.60592800 | 0.04001000 |
| N | 4.06927600 | -2.16186500 | -1.06515300 |
| N | 5.40174000 | 0.29939700 | -0.38407700 |
| O | 2.36509200 | 0.32024400 | -0.56214200 |
| O | -1.19277700 | 0.63848700 | 0.36951300 |
| C | 5.15911700 | -2.33938400 | -1.84158700 |
| C | 3.04431800 | -3.18211300 | -1.02760400 |
| C | 6.33653300 | -0.16584000 | -1.23971600 |
| C | 5.60522700 | 1.56957100 | 0.27635400 |
| C | 1.25692100 | 0.79455100 | 0.17460100 |
| C | -0.03664700 | 0.17253200 | -0.36580900 |
| C | 6.21446000 | -1.39968400 | -1.92162500 |
| C | 5.28013900 | -3.60564800 | -2.66428400 |
| C | 3.11713600 | -4.19241100 | -0.02808600 |
| C | 1.96635400 | -3.11839900 | -1.95473500 |
| C | 7.58574800 | 0.65505300 | -1.48603700 |
| C | 6.21905900 | 1.58759300 | 1.56021800 |
| C | 5.14023200 | 2.76008600 | -0.35039600 |
| H | 1.18244500 | 1.90461100 | 0.09774600 |
| H | 1.34655800 | 0.54834900 | 1.26233300 |
| H | 0.01930100 | -0.93575800 | -0.31897900 |

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|---|-------------|-------------|-------------|
| H | -0.18891000 | 0.46943500 | -1.42238600 |
| H | 7.04436800 | -1.66411200 | -2.59031200 |
| H | 5.25327200 | -4.50426300 | -2.01370100 |
| H | 6.22004000 | -3.61612700 | -3.24637500 |
| H | 4.42543700 | -3.70885600 | -3.36416400 |
| C | 2.08598300 | -5.15318600 | 0.01851700 |
| C | 4.28248400 | -4.20880000 | 0.95105500 |
| C | 0.95905900 | -4.10142500 | -1.86292100 |
| C | 1.92249000 | -2.00896000 | -2.99490400 |
| H | 8.13181300 | 0.83945200 | -0.53774400 |
| H | 8.26509300 | 0.14649200 | -2.19471400 |
| H | 7.33127000 | 1.65578100 | -1.89225900 |
| C | 6.37287700 | 2.83286600 | 2.20404500 |
| C | 6.68380400 | 0.28560700 | 2.19696800 |
| C | 5.32141700 | 3.97964200 | 0.33461000 |
| C | 4.45905700 | 2.68740100 | -1.70855500 |
| H | 2.11539000 | -5.94668400 | 0.77990600 |
| C | 1.01766900 | -5.10891100 | -0.88909700 |
| C | 4.28520200 | -5.33451400 | 1.98993900 |
| H | 4.30551700 | -3.22495200 | 1.47222900 |
| H | 5.23651900 | -4.23982000 | 0.37699900 |
| H | 0.10950400 | -4.07403100 | -2.56085600 |
| C | 0.70384400 | -1.99631300 | -3.92268800 |
| H | 2.85003000 | -2.05509300 | -3.61079500 |
| H | 1.99318700 | -1.03793700 | -2.45401400 |
| H | 6.84367200 | 2.87748400 | 3.19729200 |
| C | 5.93139300 | 4.01760900 | 1.59709200 |
| C | 7.32522000 | 0.39471300 | 3.58369500 |
| H | 7.39368700 | -0.22151800 | 1.50435400 |
| H | 5.80885400 | -0.40125500 | 2.24755900 |
| H | 4.97446600 | 4.91685200 | -0.12526000 |
| C | 4.03745800 | 4.02209700 | -2.32984800 |
| H | 3.57280300 | 2.01976500 | -1.60326300 |
| H | 5.12754700 | 2.15117900 | -2.41966800 |
| H | 0.21752600 | -5.86409200 | -0.83260000 |
| H | 5.17318000 | -5.24802300 | 2.64902000 |
| H | 3.38680200 | -5.29876600 | 2.64091300 |
| H | 4.31922200 | -6.33940700 | 1.51844400 |
| H | 0.77429000 | -1.14922400 | -4.63527300 |
| H | 0.62085100 | -2.92677800 | -4.52380300 |
| H | -0.24332800 | -1.87284200 | -3.35699300 |
| H | 6.05983000 | 4.98105600 | 2.11602700 |
| H | 7.61873700 | -0.60956800 | 3.95189200 |
| H | 8.24003700 | 1.02424500 | 3.57459300 |

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|----|-------------|-------------|-------------|
| H | 6.62607500 | 0.82770800 | 4.32940800 |
| H | 3.56436100 | 3.85200500 | -3.31852800 |
| H | 3.29569700 | 4.55476900 | -1.69893700 |
| H | 4.89863400 | 4.70586600 | -2.48797800 |
| H | 3.60329800 | -0.95398500 | 1.60155200 |
| Al | -3.28538000 | 0.39207700 | -0.44025600 |
| N | -5.23831700 | 0.03105000 | -0.74726400 |
| N | -3.44349400 | 2.30984300 | -0.88230700 |
| H | -2.59798900 | -0.51130200 | -1.58347100 |
| C | -6.14378900 | 0.90654600 | -1.20390400 |
| C | -5.65321900 | -1.30927000 | -0.41954800 |
| C | -4.57787800 | 2.90711100 | -1.32895000 |
| C | -2.25978900 | 3.13833500 | -0.80942100 |
| C | -5.81946800 | 2.25631900 | -1.48958500 |
| C | -7.57771300 | 0.46525600 | -1.42818300 |
| C | -5.54589600 | -2.33565300 | -1.40077100 |
| C | -6.12349600 | -1.58465700 | 0.89687500 |
| C | -4.53974500 | 4.38175700 | -1.68983500 |
| C | -1.40490200 | 3.21480500 | -1.94291000 |
| C | -1.97834100 | 3.84954200 | 0.38893800 |
| H | -6.64132200 | 2.87948000 | -1.86632300 |
| H | -8.19195800 | 1.29040500 | -1.83427000 |
| H | -8.03908100 | 0.11301600 | -0.48238600 |
| H | -7.62372500 | -0.39296200 | -2.12989500 |
| C | -5.90663400 | -3.64837000 | -1.03190300 |
| C | -5.06781000 | -1.99445100 | -2.80425300 |
| C | -6.47414000 | -2.91316700 | 1.21438600 |
| C | -6.24017900 | -0.45566400 | 1.91054100 |
| H | -3.79045800 | 4.58406500 | -2.48241500 |
| H | -5.52961200 | 4.72697100 | -2.04122200 |
| H | -4.23632600 | 4.99984200 | -0.82004900 |
| C | -0.25595800 | 4.02863700 | -1.85591500 |
| C | -1.75466800 | 2.44228600 | -3.20776700 |
| C | -0.82021800 | 4.65264800 | 0.42612400 |
| C | -2.91115400 | 3.72165100 | 1.58267300 |
| H | -5.82986600 | -4.46020500 | -1.77055300 |
| C | -6.36365600 | -3.93708500 | 0.26208000 |
| C | -4.92367100 | -3.16609100 | -3.78006000 |
| H | -4.09551300 | -1.46142900 | -2.70993200 |
| H | -5.75813400 | -1.23773600 | -3.24325000 |
| H | -6.83865800 | -3.15310400 | 2.22440400 |
| C | -6.75777600 | -0.83600000 | 3.30124800 |
| H | -6.89180700 | 0.34294800 | 1.48919400 |
| H | -5.23953000 | 0.02568600 | 1.99718400 |

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| H | 0.42376200 | 4.10740000 | -2.71731700 |
| C | 0.03278500 | 4.74360800 | -0.68393400 |
| C | -0.75151600 | 2.53371900 | -4.36186400 |
| H | -2.75440400 | 2.77702200 | -3.56845500 |
| H | -1.91375300 | 1.37414000 | -2.93595400 |
| H | -0.57735400 | 5.21443600 | 1.34027700 |
| C | -2.57836700 | 4.58926000 | 2.80014600 |
| H | -2.91911700 | 2.65525300 | 1.89980800 |
| H | -3.95345200 | 3.93168600 | 1.25342500 |
| H | -6.63809600 | -4.96987700 | 0.53082800 |
| H | -4.55694000 | -2.80518400 | -4.76287100 |
| H | -4.19650300 | -3.92087200 | -3.41336600 |
| H | -5.88761900 | -3.68816900 | -3.95945100 |
| H | -6.80129100 | 0.05974100 | 3.95418900 |
| H | -7.78021200 | -1.26839000 | 3.26467700 |
| H | -6.09962800 | -1.57734700 | 3.80127500 |
| H | 0.93160200 | 5.37902800 | -0.63468100 |
| H | -1.09851700 | 1.92638300 | -5.22275200 |
| H | -0.62268100 | 3.57580300 | -4.72360400 |
| H | 0.25009600 | 2.15388600 | -4.07007700 |
| H | -3.33016400 | 4.43209900 | 3.60055400 |
| H | -1.58701800 | 4.33117500 | 3.22706800 |
| H | -2.57235300 | 5.67345100 | 2.55757200 |
| B | -1.46742700 | 0.03927200 | 1.62972900 |
| O | -1.05434800 | -1.25616200 | 1.89878900 |
| O | -1.68703900 | 0.79262500 | 2.78293100 |
| H | -3.27199300 | -0.08242200 | 1.13094800 |
| C | -1.29637700 | -1.51050000 | 3.30890400 |
| C | -1.33759700 | -0.03559200 | 3.92759900 |
| C | -2.63554000 | -2.25933300 | 3.41657200 |
| C | -0.16125800 | -2.39320200 | 3.83870700 |
| C | -2.39210600 | 0.16525500 | 5.02129700 |
| C | 0.03336000 | 0.45215400 | 4.42839600 |
| H | -2.57743400 | -3.18258000 | 2.80595100 |
| H | -2.86505900 | -2.54698000 | 4.46270100 |
| H | -3.47130900 | -1.65146100 | 3.01868100 |
| H | -0.26209400 | -2.55748200 | 4.93163100 |
| H | -0.19849400 | -3.38206000 | 3.33857300 |
| H | 0.83184600 | -1.95048200 | 3.63461700 |
| H | -2.19312600 | -0.49363400 | 5.89198100 |
| H | -2.36551300 | 1.21548400 | 5.37685300 |
| H | -3.41290000 | -0.04110100 | 4.64828500 |
| H | 0.35197700 | -0.07883400 | 5.34852700 |
| H | 0.81826300 | 0.31919200 | 3.65727800 |

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|--------------|-------------|-------------|-------------|
| H | -0.03389900 | 1.53470000 | 4.65825900 |
| TS-11 | | | |
| N | 1.32802100 | 0.22208500 | 0.56815700 |
| C | 3.20130500 | -1.28882400 | 0.01768900 |
| Al | -0.11032100 | 0.44183800 | -0.74145600 |
| C | 4.53070900 | -1.45709400 | -0.42574500 |
| H | 4.95173500 | -2.46959400 | -0.51573100 |
| C | 1.12221800 | 0.24278700 | 1.91147300 |
| C | -0.14760400 | 0.24842900 | 2.52738100 |
| H | -0.14749800 | 0.27966000 | 3.62497900 |
| C | 2.69119300 | 0.03503100 | 0.11643400 |
| C | 4.80203000 | 0.94845500 | -0.65536700 |
| H | 5.43387800 | 1.80697300 | -0.92729100 |
| C | 5.32525000 | -0.34986600 | -0.75503100 |
| H | 6.36133000 | -0.50004100 | -1.09845100 |
| C | 3.47862300 | 1.16740600 | -0.22547600 |
| C | 2.32516000 | 0.25163600 | 2.83652100 |
| H | 2.91692400 | -0.68192900 | 2.74114800 |
| H | 2.00994900 | 0.35999100 | 3.89074500 |
| H | 3.01828500 | 1.07885200 | 2.58068400 |
| N | -1.56550500 | 0.14550800 | 0.57444900 |
| C | -3.33619200 | -1.31282300 | -0.34071800 |
| C | -4.60000300 | -1.43829700 | -0.95305000 |
| H | -4.97649800 | -2.43563600 | -1.22484300 |
| C | -1.41792600 | 0.14141800 | 1.90782300 |
| C | -2.87867900 | -0.00719100 | -0.00385200 |
| C | -4.92075300 | 0.97040900 | -0.88594200 |
| H | -5.54723900 | 1.84743300 | -1.10617100 |
| C | -5.38550400 | -0.30863200 | -1.22439900 |
| H | -6.36909700 | -0.42611500 | -1.70674700 |
| C | -3.66399900 | 1.15057200 | -0.27147900 |
| C | -2.63338600 | 0.00034200 | 2.80183100 |
| H | -3.14229700 | -0.96941800 | 2.62062000 |
| H | -2.35441100 | 0.05709800 | 3.87035300 |
| H | -3.38509200 | 0.78646400 | 2.58450500 |
| H | -0.48677200 | 1.84497900 | -1.39590500 |
| C | -2.46438100 | -2.52206800 | -0.03553000 |
| C | -3.01473200 | -3.88661900 | -0.46115900 |
| H | -2.24276100 | -2.54169900 | 1.05592800 |
| H | -1.47344300 | -2.35400500 | -0.51530800 |
| H | -2.29708500 | -4.69090500 | -0.19935200 |
| H | -3.97588000 | -4.12600200 | 0.04092500 |
| H | -3.18580400 | -3.93987400 | -1.55677600 |
| C | -3.14429700 | 2.52966000 | 0.10783800 |

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|--------------|-------------|-------------|-------------|
| C | -4.02581300 | 3.72127600 | -0.27806800 |
| H | -2.13618800 | 2.64859300 | -0.34828900 |
| H | -2.95798200 | 2.55556500 | 1.20617700 |
| H | -3.54352800 | 4.67107100 | 0.03102200 |
| H | -4.18765600 | 3.77564400 | -1.37504600 |
| H | -5.02350400 | 3.68414400 | 0.20861400 |
| C | 2.87371800 | 2.55832300 | -0.13766800 |
| C | 3.79343000 | 3.72776500 | -0.50167600 |
| H | 2.46868500 | 2.71342500 | 0.88829200 |
| H | 1.97930700 | 2.57577100 | -0.79966200 |
| H | 3.24992700 | 4.68953900 | -0.40258600 |
| H | 4.68592000 | 3.78146000 | 0.15737800 |
| H | 4.15090900 | 3.65892700 | -1.55020900 |
| C | 2.32476800 | -2.47649200 | 0.39867100 |
| C | 2.89067700 | -3.86733400 | 0.09273100 |
| H | 1.33606900 | -2.36135500 | -0.09890700 |
| H | 2.08493300 | -2.41777300 | 1.48558500 |
| H | 2.16119200 | -4.65259800 | 0.37830400 |
| H | 3.11239100 | -3.99489200 | -0.98777500 |
| H | 3.82746700 | -4.07059200 | 0.65263700 |
| O | 1.47888900 | 0.63455900 | -2.46348300 |
| C | 1.12666500 | -0.52852200 | -2.75429600 |
| H | -0.31982000 | -0.89020300 | -1.72830600 |
| H | 0.52463900 | -0.75442300 | -3.67765000 |
| H | 1.62960500 | -1.43052100 | -2.30795700 |
| TS-12 | | | |
| N | -1.13126300 | 1.48958800 | 0.56109700 |
| C | -0.27927300 | 3.69880500 | -0.20604800 |
| Al | -0.71010400 | 0.02333000 | -0.61960500 |
| C | -0.55106400 | 4.95033600 | -0.79908700 |
| H | 0.27173900 | 5.66419200 | -0.95187900 |
| C | -1.26211800 | 1.31939200 | 1.89623100 |
| C | -1.26969200 | 0.04622400 | 2.51642500 |
| H | -1.32885800 | 0.04964400 | 3.61302100 |
| C | -1.36528900 | 2.79888800 | -0.01842000 |
| C | -2.90722400 | 4.40011500 | -1.00788400 |
| H | -3.92105400 | 4.68414000 | -1.32629000 |
| C | -1.84870900 | 5.30003100 | -1.19637500 |
| H | -2.03742400 | 6.28221900 | -1.65867300 |
| C | -2.68916500 | 3.13746100 | -0.41979700 |
| C | -1.46633200 | 2.53234100 | 2.77935300 |
| H | -0.67391100 | 3.28944600 | 2.61122000 |
| H | -1.47450900 | 2.25017000 | 3.84832200 |
| H | -2.42828500 | 3.03277900 | 2.54059000 |

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|---|-------------|-------------|-------------|
| N | -1.25945500 | -1.40473600 | 0.56244000 |
| C | -0.63583900 | -3.68267400 | -0.22992800 |
| C | -1.03980500 | -4.90095500 | -0.81709100 |
| H | -0.29257100 | -5.68924700 | -0.99038200 |
| C | -1.36925600 | -1.22391300 | 1.89787400 |
| C | -1.62642200 | -2.68425000 | -0.01430300 |
| C | -3.33710400 | -4.12900700 | -0.96814800 |
| H | -4.38063500 | -4.31415200 | -1.26253200 |
| C | -2.37381200 | -5.12480800 | -1.18316600 |
| H | -2.66584900 | -6.08314500 | -1.64175700 |
| C | -2.98598200 | -2.89515900 | -0.38368700 |
| C | -1.66667000 | -2.41546100 | 2.78384800 |
| H | -0.94228000 | -3.23616900 | 2.60731100 |
| H | -1.63965400 | -2.13402200 | 3.85275000 |
| H | -2.66959900 | -2.83373000 | 2.55604100 |
| H | -1.57574000 | 0.03181800 | -1.96526300 |
| C | 0.80778100 | -3.43006300 | 0.16477500 |
| C | 1.79041700 | -4.58470300 | -0.04200300 |
| H | 0.84372200 | -3.10786000 | 1.22934500 |
| H | 1.18383200 | -2.54012000 | -0.38172700 |
| H | 2.80393400 | -4.26247800 | 0.26796700 |
| H | 1.52003300 | -5.48431200 | 0.55122300 |
| H | 1.85447200 | -4.89092000 | -1.10756400 |
| C | -4.01523000 | -1.79915000 | -0.15553000 |
| C | -5.45997900 | -2.12464600 | -0.54709900 |
| H | -3.67785500 | -0.89631800 | -0.71287600 |
| H | -3.98725900 | -1.48908300 | 0.91339600 |
| H | -6.12116800 | -1.25978300 | -0.33475200 |
| H | -5.55521500 | -2.35429300 | -1.62886000 |
| H | -5.85966500 | -2.99308300 | 0.01783900 |
| C | -3.82240600 | 2.14284500 | -0.22209800 |
| C | -5.22336200 | 2.61200900 | -0.62681600 |
| H | -3.83871200 | 1.81547800 | 0.84177000 |
| H | -3.56569000 | 1.22035200 | -0.79070600 |
| H | -5.96837600 | 1.81351600 | -0.43297800 |
| H | -5.54331400 | 3.50929200 | -0.05619600 |
| H | -5.28204900 | 2.86143100 | -1.70678800 |
| C | 1.12166700 | 3.30661600 | 0.22398500 |
| C | 2.21414400 | 4.36504500 | 0.05836900 |
| H | 1.42215900 | 2.38447100 | -0.31741300 |
| H | 1.09924300 | 2.97630300 | 1.28622500 |
| H | 3.17821400 | 3.95345300 | 0.41714700 |
| H | 2.35247800 | 4.66167900 | -1.00299200 |
| H | 2.00248600 | 5.28791300 | 0.63972600 |

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| O | 1.04741800 | -0.01596700 | -1.05797700 |
| C | 1.45796100 | -0.21845500 | -2.40751700 |
| H | 0.61738600 | -0.57939800 | -3.04140600 |
| H | 1.83774500 | 0.72687300 | -2.85657400 |
| H | 2.26910800 | -0.97816000 | -2.43341100 |
| B | 2.43761600 | -0.18422700 | 0.41752300 |
| O | 3.18483000 | -1.29690300 | -0.02059400 |
| O | 3.24833200 | 0.96182000 | 0.46273800 |
| H | 1.52841700 | -0.28205400 | 1.22549100 |
| C | 4.58902100 | -0.94344200 | -0.00925100 |
| C | 4.56039400 | 0.65115300 | -0.06768600 |
| C | 5.18005800 | -1.48711000 | 1.30669000 |
| C | 5.28509000 | -1.61610000 | -1.19831500 |
| C | 5.60670500 | 1.33802800 | 0.82219800 |
| C | 4.66811300 | 1.21874300 | -1.49414000 |
| H | 4.99837100 | -2.57991600 | 1.35617800 |
| H | 6.27342100 | -1.31518300 | 1.37962500 |
| H | 4.69107100 | -1.02423200 | 2.18713800 |
| H | 6.35662700 | -1.33069900 | -1.24732200 |
| H | 5.23234400 | -2.71858300 | -1.08827900 |
| H | 4.80889900 | -1.34978900 | -2.16107300 |
| H | 6.63730900 | 1.05735400 | 0.52023100 |
| H | 5.51475800 | 2.43926300 | 0.72477000 |
| H | 5.46786300 | 1.08227200 | 1.88951400 |
| H | 5.68886000 | 1.09405900 | -1.91041800 |
| H | 3.95009900 | 0.73861700 | -2.18421700 |
| H | 4.43901500 | 2.30344800 | -1.46751500 |
| TS-13 | | | |
| N | -1.81589500 | -1.29812700 | 0.65547600 |
| C | -3.66862300 | 0.33577200 | 0.78484100 |
| Al | -0.20885700 | -0.51137000 | -0.25699600 |
| C | -4.87595200 | 0.83279900 | 0.25167700 |
| H | -5.35045000 | 1.71378100 | 0.70909500 |
| C | -1.79970600 | -2.20284100 | 1.64362800 |
| C | -0.59629400 | -2.74957300 | 2.15730000 |
| H | -0.70765800 | -3.47354200 | 2.97536600 |
| C | -3.07945700 | -0.80465100 | 0.16704000 |
| C | -4.89640500 | -0.90577000 | -1.44603800 |
| H | -5.38615900 | -1.37825200 | -2.31050200 |
| C | -5.48326100 | 0.22247700 | -0.85532100 |
| H | -6.42394200 | 0.62900800 | -1.26024700 |
| C | -3.69066500 | -1.44309700 | -0.94984600 |
| C | -3.10469800 | -2.70173800 | 2.23482600 |
| H | -3.71656300 | -1.86439500 | 2.62818100 |

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| H | -2.92392600 | -3.42493500 | 3.05171500 |
| H | -3.72401100 | -3.19480600 | 1.45669600 |
| N | 1.06249300 | -1.66620000 | 0.71545700 |
| C | 3.36334800 | -0.76661200 | 0.92874300 |
| C | 4.70365100 | -0.77760900 | 0.49077200 |
| H | 5.43217200 | -0.09732300 | 0.95652100 |
| C | 0.72187400 | -2.52972200 | 1.70561300 |
| C | 2.44828500 | -1.65681700 | 0.30238200 |
| C | 4.20914300 | -2.50972600 | -1.14272000 |
| H | 4.55200500 | -3.18054900 | -1.94473000 |
| C | 5.12509100 | -1.63973800 | -0.53298300 |
| H | 6.17750100 | -1.63242000 | -0.85951600 |
| C | 2.85649900 | -2.53486900 | -0.74036300 |
| C | 1.81085200 | -3.35213500 | 2.37132500 |
| H | 2.60936900 | -2.70650500 | 2.78989100 |
| H | 1.39346800 | -3.97500300 | 3.18393500 |
| H | 2.31070800 | -4.01860900 | 1.63805900 |
| H | -0.48993900 | -0.92635600 | -1.78744900 |
| C | 2.88106700 | 0.16360400 | 2.03005900 |
| C | 3.93754400 | 1.07323400 | 2.66384900 |
| H | 2.39074700 | -0.44165500 | 2.82566000 |
| H | 2.06810600 | 0.79934300 | 1.61617100 |
| H | 3.47859800 | 1.69750000 | 3.45751800 |
| H | 4.76596500 | 0.49892000 | 3.13077800 |
| H | 4.37985800 | 1.76599500 | 1.91826300 |
| C | 1.83937300 | -3.46765800 | -1.38414000 |
| C | 2.35170300 | -4.35587200 | -2.52228600 |
| H | 0.98534700 | -2.85247300 | -1.74855900 |
| H | 1.39068700 | -4.11132500 | -0.59345300 |
| H | 1.52916400 | -4.98459800 | -2.92028000 |
| H | 2.74853700 | -3.75781800 | -3.36958300 |
| H | 3.15962900 | -5.04086700 | -2.18858100 |
| C | -3.04475800 | -2.67537000 | -1.56435000 |
| C | -3.74954200 | -3.28074500 | -2.78201400 |
| H | -2.94003700 | -3.45619600 | -0.77652600 |
| H | -1.99871600 | -2.40545600 | -1.83241600 |
| H | -3.18974000 | -4.16470300 | -3.15069000 |
| H | -4.78170800 | -3.61808200 | -2.54814100 |
| H | -3.81450900 | -2.55805400 | -3.62241100 |
| C | -2.99989600 | 0.97467500 | 1.99322500 |
| C | -3.68469000 | 2.21458300 | 2.57626900 |
| H | -1.95105700 | 1.21763800 | 1.71083000 |
| H | -2.89584000 | 0.20976700 | 2.79593600 |
| H | -3.10952400 | 2.60100900 | 3.44245300 |

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| H | -3.75624800 | 3.03713200 | 1.83385900 |
| H | -4.71359000 | 1.99704100 | 2.93350400 |
| O | 1.45732500 | 0.72789700 | -1.11718800 |
| C | 1.96081600 | 0.53839000 | -2.44948200 |
| H | 2.70829100 | 1.32101400 | -2.69574400 |
| H | 2.45838300 | -0.44979100 | -2.47596500 |
| H | 1.13801700 | 0.56188600 | -3.19349800 |
| B | 0.93111900 | 1.99998300 | -0.77817900 |
| O | 1.48631500 | 2.76183800 | 0.24423900 |
| O | 0.19842500 | 2.75182000 | -1.68322700 |
| H | -0.40053000 | 1.04037300 | 0.25363300 |
| C | 0.83483600 | 4.06336000 | 0.20852600 |
| C | 0.32567500 | 4.15108400 | -1.30379200 |
| C | -0.31171200 | 4.04435700 | 1.23283200 |
| C | 1.86588300 | 5.12698000 | 0.59934000 |
| C | -1.03297400 | 4.83416100 | -1.48582300 |
| C | 1.36132400 | 4.77633800 | -2.25481200 |
| H | 0.10069300 | 3.78084500 | 2.22769000 |
| H | -0.80747000 | 5.03286300 | 1.31341900 |
| H | -1.07236400 | 3.28390600 | 0.97054000 |
| H | 1.43822300 | 6.14688300 | 0.50760800 |
| H | 2.17090400 | 4.97980000 | 1.65529800 |
| H | 2.77622500 | 5.06692300 | -0.02658300 |
| H | -0.99720200 | 5.88964500 | -1.14482600 |
| H | -1.31037300 | 4.83120500 | -2.55951800 |
| H | -1.83207000 | 4.30777200 | -0.93114300 |
| H | 1.46911500 | 5.86796500 | -2.09185600 |
| H | 2.35754200 | 4.30465800 | -2.13474400 |
| H | 1.03123800 | 4.61295200 | -3.30059100 |
| TS-14 | | | |
| N | 1.40868700 | -0.86031000 | 0.74637500 |
| C | 3.39255900 | -1.36213000 | -0.63582400 |
| Al | -0.01298900 | -0.00286500 | -0.14942900 |
| C | 4.68757800 | -1.00567400 | -1.06239400 |
| H | 5.21690400 | -1.64134700 | -1.78730500 |
| C | 1.21199100 | -1.62806700 | 1.84601800 |
| C | -0.07198100 | -1.93485700 | 2.35654000 |
| H | -0.08874000 | -2.55236300 | 3.26430600 |
| C | 2.74647000 | -0.51690900 | 0.30779100 |
| C | 4.63556000 | 0.99963400 | 0.31481100 |
| H | 5.12683600 | 1.92037700 | 0.66216300 |
| C | 5.30707600 | 0.15813300 | -0.58329500 |
| H | 6.32059800 | 0.42037400 | -0.92636600 |
| C | 3.33690100 | 0.69218800 | 0.77376200 |

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| C | 2.42031900 | -2.16200800 | 2.58114600 |
| H | 3.06634300 | -2.75900600 | 1.90512500 |
| H | 2.12200400 | -2.78990900 | 3.44051200 |
| H | 3.05227600 | -1.32695000 | 2.94925200 |
| N | -1.48270400 | -0.77480800 | 0.75259400 |
| C | -3.46523000 | -1.33747500 | -0.60004100 |
| C | -4.73455700 | -0.98082200 | -1.09497700 |
| H | -5.28014700 | -1.67536000 | -1.75048100 |
| C | -1.33932400 | -1.53250300 | 1.86120500 |
| C | -2.79517200 | -0.41314300 | 0.25204500 |
| C | -4.61035500 | 1.17334700 | 0.02797100 |
| H | -5.06173500 | 2.15150800 | 0.25059600 |
| C | -5.30711300 | 0.25985700 | -0.77272500 |
| H | -6.30258000 | 0.52248900 | -1.16526100 |
| C | -3.33146500 | 0.87288600 | 0.55154700 |
| C | -2.57337200 | -1.94750800 | 2.62872200 |
| H | -3.13272100 | -1.04879400 | 2.96329400 |
| H | -3.27335500 | -2.52197500 | 1.98839100 |
| H | -2.31142100 | -2.55778600 | 3.51234200 |
| H | 0.00947300 | 1.65249200 | -0.28177600 |
| C | -2.78545400 | -2.64296200 | -0.99218100 |
| C | -3.57836100 | -3.57397100 | -1.91514100 |
| H | -2.49554200 | -3.20404500 | -0.07547600 |
| H | -1.81762500 | -2.38376300 | -1.47937400 |
| H | -2.98926000 | -4.48648100 | -2.13973400 |
| H | -4.53461300 | -3.90099700 | -1.45530800 |
| H | -3.81848600 | -3.08951200 | -2.88426200 |
| C | -2.54443900 | 1.90433000 | 1.34076700 |
| C | -3.37012200 | 2.98245800 | 2.05560000 |
| H | -1.83363900 | 2.43529400 | 0.64067000 |
| H | -1.89920900 | 1.38466200 | 2.08185800 |
| H | -2.69770500 | 3.63722600 | 2.64566100 |
| H | -3.89841500 | 3.64440100 | 1.33857000 |
| H | -4.12853200 | 2.55357800 | 2.74624300 |
| C | 2.57109400 | 1.63220100 | 1.69598600 |
| C | 3.39049900 | 2.74078200 | 2.36654900 |
| H | 2.05381200 | 1.03460600 | 2.47862500 |
| H | 1.74675300 | 2.10951100 | 1.10930400 |
| H | 2.74345200 | 3.33300100 | 3.04450100 |
| H | 4.23224200 | 2.33558600 | 2.96774500 |
| H | 3.81285300 | 3.45106800 | 1.62606300 |
| C | 2.66589900 | -2.58272500 | -1.18376500 |
| C | 3.45286300 | -3.46290300 | -2.15990200 |
| H | 1.73707200 | -2.22411600 | -1.68432100 |

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|--------------|-------------|-------------|-------------|
| H | 2.30503200 | -3.20794900 | -0.33638800 |
| H | 2.83155600 | -4.31920900 | -2.49249700 |
| H | 3.75552400 | -2.90351500 | -3.06929200 |
| H | 4.37245500 | -3.87889900 | -1.69705600 |
| O | -0.13027300 | -0.04717300 | -1.97372500 |
| C | -0.17453700 | 1.28870200 | -1.96973700 |
| O | 0.84513600 | 1.91615200 | -2.50752400 |
| O | -0.38943500 | 3.48333000 | -0.40124200 |
| C | 0.89137000 | 3.39865000 | -2.45115900 |
| C | -0.25051100 | 4.02704900 | -1.62046300 |
| H | 1.87236700 | 3.59546700 | -1.97155800 |
| H | 0.92341600 | 3.74247600 | -3.50996400 |
| H | 0.01333800 | 5.14080200 | -1.66404500 |
| H | -1.18422700 | 3.97824700 | -2.28808200 |
| H | -1.15191400 | 1.81404600 | -1.96007400 |
| TS-15 | | | |
| H | 1.75756600 | -0.10546800 | 1.57756400 |
| B | 2.49936600 | -0.04484100 | 0.60406700 |
| O | 3.15678700 | 1.18166800 | 0.37570100 |
| O | 3.34836800 | -1.11994800 | 0.24124900 |
| C | 4.38920600 | 0.94712700 | -0.34601300 |
| C | 4.66672900 | -0.59707500 | -0.05263000 |
| C | 4.16270800 | 1.27674400 | -1.83381800 |
| C | 5.45850100 | 1.89575700 | 0.21599600 |
| C | 5.26318900 | -1.37132900 | -1.23454100 |
| C | 5.53051100 | -0.83024800 | 1.20260500 |
| H | 3.83425900 | 2.33333100 | -1.91354600 |
| H | 5.09460700 | 1.16621300 | -2.42600800 |
| H | 3.37034500 | 0.65931400 | -2.29751800 |
| H | 6.44962400 | 1.70088200 | -0.24450400 |
| H | 5.18069400 | 2.94514800 | -0.01169200 |
| H | 5.55399800 | 1.80278700 | 1.31430600 |
| H | 6.26802000 | -0.98067000 | -1.49883100 |
| H | 5.37520900 | -2.44134700 | -0.96365300 |
| H | 4.62297000 | -1.31220700 | -2.13569200 |
| H | 6.58507400 | -0.52044200 | 1.05311700 |
| H | 5.12229500 | -0.28333300 | 2.07600500 |
| H | 5.51821500 | -1.91203800 | 1.44648800 |
| O | 1.03304900 | -0.25874600 | -0.63217000 |
| Al | -0.69866000 | 0.00324300 | -0.16714300 |
| C | 1.27874100 | -0.99014100 | -1.83925100 |
| N | -1.21957700 | 1.44511200 | 0.98133300 |
| N | -1.29971000 | -1.45777000 | 0.91791500 |
| O | -1.57095600 | 0.11204000 | -1.68423700 |

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| O | 1.17505600 | -0.21548600 | -3.00525200 |
| H | 2.32333400 | -1.34994400 | -1.76614300 |
| H | 0.58718100 | -1.86618300 | -1.89938300 |
| C | -1.60439600 | 1.24352700 | 2.26525100 |
| C | -1.40883300 | 2.76525900 | 0.40087100 |
| C | -1.66531500 | -1.30143800 | 2.20955500 |
| C | -1.29733000 | -2.78121500 | 0.32291200 |
| C | -1.16001800 | 0.66022900 | -2.91664100 |
| C | -0.10670700 | -0.18643500 | -3.63435100 |
| C | -1.73503800 | -0.03888100 | 2.84669800 |
| C | -1.97158500 | 2.43826100 | 3.11934100 |
| C | -0.34439100 | 3.70806400 | 0.41120000 |
| C | -2.67766700 | 3.07424200 | -0.17109300 |
| C | -2.04853100 | -2.52015100 | 3.01959800 |
| C | -0.16999900 | -3.63523000 | 0.48218300 |
| C | -2.42695100 | -3.17248600 | -0.45701200 |
| H | -0.76409100 | 1.69845800 | -2.79600800 |
| H | -2.04352800 | 0.73340900 | -3.59671100 |
| H | 0.06539200 | 0.22860600 | -4.65104700 |
| H | -0.49613700 | -1.22826400 | -3.74903700 |
| H | -2.02045700 | -0.05541800 | 3.90683600 |
| H | -1.16907800 | 3.20296100 | 3.10527200 |
| H | -2.16390200 | 2.13426300 | 4.16478400 |
| H | -2.88140600 | 2.93795800 | 2.72558500 |
| C | -0.57309100 | 4.96858200 | -0.18253900 |
| C | 0.98707900 | 3.36104600 | 1.04919400 |
| C | -2.85116100 | 4.34717000 | -0.75204500 |
| C | -3.79811300 | 2.04488000 | -0.15767000 |
| H | -1.18906800 | -3.21314500 | 3.12597700 |
| H | -2.40031900 | -2.23510300 | 4.02797200 |
| H | -2.84739600 | -3.09611900 | 2.50827400 |
| C | -0.18903100 | -4.88171800 | -0.18401800 |
| C | 1.03519600 | -3.25217800 | 1.32675600 |
| C | -2.39535800 | -4.43067300 | -1.08938700 |
| C | -3.61845800 | -2.23759500 | -0.59487300 |
| H | 0.23334500 | 5.71652500 | -0.18575300 |
| C | -1.80860200 | 5.28514700 | -0.76237100 |
| C | 1.97591300 | 4.51448000 | 1.24277200 |
| H | 1.49313800 | 2.57166000 | 0.45138200 |
| H | 0.80309700 | 2.86987800 | 2.02997000 |
| H | -3.81906700 | 4.61034700 | -1.20355200 |
| C | -5.14842500 | 2.49750100 | -0.72250900 |
| H | -3.94475600 | 1.67908700 | 0.88360400 |
| H | -3.43418600 | 1.15842200 | -0.72393500 |

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|--------------|-------------|-------------|-------------|
| H | 0.67915700 | -5.55265300 | -0.08612700 |
| C | -1.28214000 | -5.27677700 | -0.96332700 |
| C | 1.50055900 | -4.33420800 | 2.31749800 |
| H | 0.82630800 | -2.31508400 | 1.87704000 |
| H | 1.88502600 | -2.98835000 | 0.65953000 |
| H | -3.25481300 | -4.75535900 | -1.69429700 |
| C | -4.84631800 | -2.80032600 | -1.31794600 |
| H | -3.26140100 | -1.32351600 | -1.12227000 |
| H | -3.91732000 | -1.88626000 | 0.41813400 |
| H | -1.96362800 | 6.27456000 | -1.22193600 |
| H | 2.89449600 | 4.13700500 | 1.73457800 |
| H | 2.28789100 | 4.96316900 | 0.27617900 |
| H | 1.55991200 | 5.32974800 | 1.87303500 |
| H | -5.88926300 | 1.67496500 | -0.65146500 |
| H | -5.56533800 | 3.36733000 | -0.17177500 |
| H | -5.07708600 | 2.78159100 | -1.79331000 |
| H | -1.27181900 | -6.25271900 | -1.47464500 |
| H | 2.36177000 | -3.96444100 | 2.91091800 |
| H | 0.69711100 | -4.62155200 | 3.02971900 |
| H | 1.83116000 | -5.26253100 | 1.80704700 |
| H | -5.65937300 | -2.04607300 | -1.33730400 |
| H | -4.62323100 | -3.06508900 | -2.37280300 |
| H | -5.24745700 | -3.70934800 | -0.82126300 |
| TS-16 | | | |
| H | 0.34793900 | 1.10074700 | -0.50831300 |
| B | -1.11649800 | 1.97521600 | 0.51772900 |
| O | -0.38779300 | 2.77616300 | 1.37666400 |
| O | -1.78875700 | 2.68901100 | -0.46361500 |
| C | -0.65984200 | 4.16389800 | 1.02979900 |
| C | -1.26290600 | 4.04908400 | -0.44543600 |
| C | -1.67435300 | 4.68504700 | 2.06245800 |
| C | 0.64565500 | 4.95837100 | 1.12884700 |
| C | -2.41390800 | 5.01479500 | -0.74314000 |
| C | -0.19725100 | 4.14631100 | -1.54885700 |
| H | -1.25934700 | 4.53151900 | 3.07859800 |
| H | -1.88448900 | 5.76571000 | 1.92896800 |
| H | -2.63258800 | 4.13069600 | 2.00511400 |
| H | 0.49703900 | 6.01030600 | 0.80813300 |
| H | 0.99579300 | 4.96846700 | 2.18091000 |
| H | 1.44580100 | 4.50795000 | 0.51210800 |
| H | -2.07668800 | 6.06897000 | -0.66355000 |
| H | -2.77986700 | 4.85190000 | -1.77718400 |
| H | -3.26667300 | 4.86399500 | -0.05459700 |
| H | 0.20828800 | 5.17417900 | -1.63902700 |

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|----|-------------|-------------|-------------|
| H | 0.64111500 | 3.44746200 | -1.36204400 |
| H | -0.65803700 | 3.86957900 | -2.51859600 |
| O | -1.48024500 | 0.63381300 | 0.81638500 |
| Al | 0.26860800 | -0.46354000 | -0.03332100 |
| C | -2.32024200 | 0.36332900 | 1.96951800 |
| N | 1.97290400 | -1.06330100 | -0.89859900 |
| N | -0.84967300 | -1.71914200 | -1.03913100 |
| O | 0.55680400 | -1.02354400 | 1.62480400 |
| O | -1.70247000 | 0.59397100 | 3.18612000 |
| H | -3.20045000 | 1.03756300 | 1.92165600 |
| H | -2.63774600 | -0.69570800 | 1.84555500 |
| C | 2.06752900 | -1.92921500 | -1.91761300 |
| C | 3.18402700 | -0.47520000 | -0.37367000 |
| C | -0.40251800 | -2.51276600 | -2.04810000 |
| C | -2.23707000 | -1.87386900 | -0.65976300 |
| C | 0.58683900 | -0.38262600 | 2.87213600 |
| C | -0.75323000 | -0.38852300 | 3.61866800 |
| C | 0.93722400 | -2.57673100 | -2.47841300 |
| C | 3.42558800 | -2.26608500 | -2.50372300 |
| C | 3.65571900 | 0.75102100 | -0.92426200 |
| C | 3.87208600 | -1.12394400 | 0.69228100 |
| C | -1.38769200 | -3.42003600 | -2.76268300 |
| C | -3.22410900 | -1.04870400 | -1.26592300 |
| C | -2.57616600 | -2.84835200 | 0.32125600 |
| H | 0.93469400 | 0.67671300 | 2.80244800 |
| H | 1.31714300 | -0.91311700 | 3.53458000 |
| H | -0.57137400 | -0.15416900 | 4.68935800 |
| H | -1.20543700 | -1.40911000 | 3.55801800 |
| H | 1.13887600 | -3.25437000 | -3.31854300 |
| H | 3.33048600 | -2.96204100 | -3.35785700 |
| H | 4.08015000 | -2.73328400 | -1.73882400 |
| H | 3.95512200 | -1.35281300 | -2.84376800 |
| C | 4.81063700 | 1.33429600 | -0.36216700 |
| C | 2.93392900 | 1.38355200 | -2.10539000 |
| C | 5.02287100 | -0.49938100 | 1.21689900 |
| C | 3.36636600 | -2.45454000 | 1.22662400 |
| H | -2.24666200 | -2.84808200 | -3.16860900 |
| H | -0.89460900 | -3.95965800 | -3.59224200 |
| H | -1.82033700 | -4.16762100 | -2.06588600 |
| C | -4.56545800 | -1.21286900 | -0.86155000 |
| C | -2.81583900 | -0.02888900 | -2.31671800 |
| C | -3.93338200 | -2.97829000 | 0.68751600 |
| C | -1.48485500 | -3.70574400 | 0.94588900 |
| H | 5.19160600 | 2.28401900 | -0.76625600 |

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| C | 5.48519900 | 0.72054600 | 0.70266700 |
| C | 3.49330500 | 2.71532700 | -2.61489300 |
| H | 1.86405300 | 1.50357400 | -1.82435000 |
| H | 2.91494900 | 0.65481900 | -2.94763400 |
| H | 5.56918600 | -0.97730500 | 2.04374100 |
| C | 4.16350400 | -3.07596000 | 2.37769400 |
| H | 3.31805600 | -3.18325800 | 0.38520200 |
| H | 2.30552400 | -2.30081200 | 1.52744300 |
| H | -5.34881800 | -0.58440200 | -1.31083100 |
| C | -4.91878700 | -2.16756200 | 0.10442400 |
| C | -3.94175200 | 0.81498900 | -2.92082900 |
| H | -2.26975200 | -0.55392000 | -3.13294000 |
| H | -2.06305800 | 0.65351700 | -1.86616700 |
| H | -4.22426800 | -3.72395800 | 1.44249800 |
| C | -1.93179200 | -4.69792500 | 2.02412300 |
| H | -0.70931900 | -3.02159200 | 1.35963500 |
| H | -0.95714400 | -4.26154800 | 0.13746400 |
| H | 6.38342700 | 1.19371300 | 1.13108500 |
| H | 2.88869200 | 3.08615400 | -3.46778100 |
| H | 3.47436400 | 3.50070800 | -1.83010600 |
| H | 4.54193200 | 2.62330200 | -2.96911700 |
| H | 3.70217200 | -4.03541000 | 2.69005600 |
| H | 5.21675900 | -3.29264600 | 2.09779200 |
| H | 4.18471700 | -2.41655100 | 3.27103300 |
| H | -5.97281300 | -2.28120100 | 0.40503200 |
| H | -3.53144400 | 1.51404800 | -3.67784800 |
| H | -4.71226200 | 0.19430700 | -3.42586100 |
| H | -4.44940500 | 1.43040100 | -2.14955900 |
| H | -1.05908200 | -5.26169700 | 2.41262000 |
| H | -2.40390700 | -4.18617100 | 2.88957900 |
| H | -2.66058500 | -5.44229400 | 1.63862500 |
| TS-17 | | | |
| B | 4.68149000 | -1.20644400 | -0.95236600 |
| O | 4.60808900 | -1.96889300 | 0.17584600 |
| O | 5.87612800 | -0.59750800 | -1.20272000 |
| C | 5.81405400 | -1.63125900 | 0.95170200 |
| C | 6.80635700 | -1.08543600 | -0.17410700 |
| C | 5.38788100 | -0.54926300 | 1.95392700 |
| C | 6.29282400 | -2.89063100 | 1.67337200 |
| C | 7.68954400 | 0.08343500 | 0.26295800 |
| C | 7.64828800 | -2.18785500 | -0.83337700 |
| H | 4.57603500 | -0.95165600 | 2.59223900 |
| H | 6.22747700 | -0.24854000 | 2.61219700 |
| H | 4.99450800 | 0.34532800 | 1.42922400 |

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| H | 7.23849100 | -2.69266100 | 2.21865300 |
| H | 5.53239500 | -3.20616900 | 2.41553800 |
| H | 6.45697100 | -3.73291400 | 0.97492300 |
| H | 8.34954800 | -0.21452300 | 1.10343800 |
| H | 8.33441200 | 0.40096000 | -0.58119900 |
| H | 7.08265400 | 0.95381700 | 0.57430200 |
| H | 8.43434400 | -2.56513400 | -0.14889800 |
| H | 7.02155100 | -3.04500200 | -1.15286200 |
| H | 8.14441000 | -1.77304200 | -1.73373000 |
| O | 3.57736800 | -1.10509900 | -1.82193400 |
| Al | -2.80672500 | -0.47742800 | -0.35948400 |
| C | 3.54079500 | -0.15776200 | -2.74235900 |
| N | -2.83923900 | -2.15951800 | 0.60164100 |
| N | -4.31470700 | 0.31523300 | 0.56449400 |
| O | -1.33104300 | 0.41450700 | 0.00890000 |
| O | 1.83330900 | 0.91952900 | -1.79330000 |
| C | -3.69620100 | -2.45841600 | 1.60087200 |
| C | -1.85120900 | -3.13067200 | 0.18785600 |
| C | -4.99575300 | -0.27066100 | 1.57096100 |
| C | -4.68716000 | 1.64056000 | 0.12132700 |
| C | -0.43670400 | 1.03668900 | -0.89074200 |
| C | 0.95816000 | 0.38313000 | -0.81581300 |
| C | -4.69873100 | -1.56811400 | 2.05343900 |
| C | -3.60042900 | -3.81268200 | 2.27325500 |
| C | -2.16616000 | -4.02091200 | -0.87707900 |
| C | -0.57262300 | -3.13178200 | 0.81414500 |
| C | -6.14239000 | 0.47737300 | 2.21970300 |
| C | -5.61117100 | 1.77105700 | -0.95318700 |
| C | -4.07930100 | 2.77441400 | 0.73096600 |
| H | -0.33166000 | 2.11997600 | -0.64853600 |
| H | -0.78838000 | 0.97842600 | -1.94998500 |
| H | 0.84740400 | -0.70668900 | -1.02451100 |
| H | 1.38208200 | 0.49053800 | 0.20816700 |
| H | -5.32940100 | -1.93161300 | 2.87564200 |
| H | -3.73678600 | -4.63072300 | 1.53580600 |
| H | -4.36205100 | -3.91991400 | 3.06753900 |
| H | -2.59586400 | -3.96605800 | 2.71868200 |
| C | -1.17252300 | -4.92883500 | -1.29796600 |
| C | -3.54096100 | -3.96845100 | -1.52816800 |
| C | 0.38688700 | -4.05765300 | 0.35338700 |
| C | -0.27232500 | -2.14498300 | 1.93196800 |
| H | -6.91752000 | 0.74065600 | 1.47046700 |
| H | -6.61105200 | -0.12445400 | 3.02008000 |
| H | -5.79581000 | 1.43855500 | 2.65237300 |

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| C | -5.93035600 | 3.07024400 | -1.39906400 |
| C | -6.21683900 | 0.52713000 | -1.58772000 |
| C | -4.43387100 | 4.05135800 | 0.24806400 |
| C | -3.07099300 | 2.58529900 | 1.85414500 |
| H | -1.38790400 | -5.62916500 | -2.11859200 |
| C | 0.09086500 | -4.94803200 | -0.68924000 |
| C | -3.79416300 | -4.95924100 | -2.66862800 |
| H | -3.70466300 | -2.93064800 | -1.89725300 |
| H | -4.31824800 | -4.10851500 | -0.74272000 |
| H | 1.38661900 | -4.07583300 | 0.81166400 |
| C | 1.12619900 | -2.22688700 | 2.55138700 |
| H | -1.03487100 | -2.26600800 | 2.73491500 |
| H | -0.44905200 | -1.12024300 | 1.53181300 |
| H | -6.64096800 | 3.20187100 | -2.22843800 |
| C | -5.34993000 | 4.19956800 | -0.80354500 |
| C | -7.19825100 | 0.75842900 | -2.74086000 |
| H | -6.71807300 | -0.07487600 | -0.79581900 |
| H | -5.38054600 | -0.11906900 | -1.93856900 |
| H | -3.98011900 | 4.94654500 | 0.69848400 |
| C | -2.46682500 | 3.86142000 | 2.44783500 |
| H | -2.26017800 | 1.92513500 | 1.46851100 |
| H | -3.54633900 | 1.99446900 | 2.67034100 |
| H | 0.85617400 | -5.66111300 | -1.03560300 |
| H | -4.82028300 | -4.83038000 | -3.06962300 |
| H | -3.08930400 | -4.80672700 | -3.51259500 |
| H | -3.69848300 | -6.01462700 | -2.33635900 |
| H | 1.23404300 | -1.46441600 | 3.34993900 |
| H | 1.32469900 | -3.21869700 | 3.01144200 |
| H | 1.92343500 | -2.03702300 | 1.80268600 |
| H | -5.60935700 | 5.20657800 | -1.16768900 |
| H | -7.57222800 | -0.21127100 | -3.12840400 |
| H | -8.08222500 | 1.35252500 | -2.42625400 |
| H | -6.72004600 | 1.29020900 | -3.58986300 |
| H | -1.74691600 | 3.60605400 | 3.25198500 |
| H | -1.91239000 | 4.44892200 | 1.68635400 |
| H | -3.23683500 | 4.52792500 | 2.89186900 |
| H | -3.05639200 | -0.65154500 | -1.93543000 |
| B | 2.75948600 | 2.05322700 | -1.47771500 |
| O | 2.09279600 | 3.33166000 | -1.44639500 |
| O | 3.51075700 | 1.93011600 | -0.22595900 |
| H | 3.56078100 | 1.91542500 | -2.48676900 |
| C | 2.80349800 | 4.17660400 | -0.53363600 |
| C | 3.35533700 | 3.13756600 | 0.54227200 |
| C | 3.93463500 | 4.88472700 | -1.31320800 |

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|--------------|-------------|-------------|-------------|
| C | 1.83647800 | 5.22973400 | 0.02395800 |
| C | 4.70953900 | 3.52936300 | 1.15420600 |
| C | 2.34562100 | 2.86924900 | 1.67707400 |
| H | 3.48833500 | 5.40649600 | -2.18406600 |
| H | 4.46949900 | 5.63432000 | -0.69396300 |
| H | 4.67149100 | 4.15312700 | -1.70090100 |
| H | 2.32648500 | 5.85969200 | 0.79602000 |
| H | 1.49902100 | 5.89545500 | -0.79684100 |
| H | 0.93674100 | 4.76155000 | 0.46682400 |
| H | 4.65236700 | 4.51339000 | 1.66605800 |
| H | 5.01601100 | 2.77794100 | 1.91192700 |
| H | 5.50296700 | 3.57960500 | 0.38400000 |
| H | 2.25063700 | 3.73320000 | 2.36774100 |
| H | 1.34084900 | 2.63130000 | 1.27507400 |
| H | 2.69065100 | 1.99534100 | 2.26724000 |
| H | 2.75448900 | -0.24769800 | -3.50190100 |
| H | 4.49474000 | 0.33281800 | -2.98203300 |
| TS-18 | | | |
| N | -1.40914500 | 1.86129600 | -0.75046500 |
| C | -0.27169300 | 3.61613100 | 0.56326200 |
| Al | -1.52135700 | 0.19394700 | 0.22614600 |
| C | 0.88316500 | 4.38986700 | 0.80298300 |
| H | 0.88468600 | 5.12670300 | 1.61957100 |
| C | -2.34923100 | 2.30195400 | -1.61483300 |
| C | -3.54883100 | 1.60039000 | -1.88332700 |
| H | -4.22953700 | 2.07306100 | -2.60372500 |
| C | -0.23727100 | 2.67331700 | -0.50384200 |
| C | 2.05690900 | 3.28036300 | -1.01789800 |
| H | 2.97264900 | 3.14997500 | -1.61257800 |
| C | 2.03468000 | 4.22840600 | 0.01715100 |
| H | 2.92788400 | 4.84089900 | 0.21956300 |
| C | 0.92729800 | 2.48216100 | -1.30049400 |
| C | -2.13092200 | 3.61809200 | -2.33246200 |
| H | -2.01551000 | 4.45109800 | -1.60842700 |
| H | -2.97488500 | 3.84970200 | -3.00793200 |
| H | -1.19407300 | 3.59574100 | -2.92646800 |
| N | -3.26268100 | -0.33184000 | -0.43776100 |
| C | -4.48319800 | -1.60933200 | 1.29076700 |
| C | -4.91648600 | -2.85591800 | 1.78813400 |
| H | -5.47605600 | -2.89907600 | 2.73422500 |
| C | -3.98645300 | 0.37232400 | -1.33256500 |
| C | -3.76205700 | -1.59260400 | 0.06372800 |
| C | -3.92577500 | -4.00933700 | -0.11005300 |
| H | -3.71473300 | -4.95037800 | -0.63940100 |

| | | | |
|---|-------------|-------------|-------------|
| C | -4.64194700 | -4.04405400 | 1.09554700 |
| H | -4.98696000 | -5.00842000 | 1.50161900 |
| C | -3.46894900 | -2.78935400 | -0.65093100 |
| C | -5.33781000 | -0.15552900 | -1.76836400 |
| H | -6.00691200 | -0.29508400 | -0.89406800 |
| H | -5.82506600 | 0.53330000 | -2.48277000 |
| H | -5.24341900 | -1.15315500 | -2.24464200 |
| C | -4.76437800 | -0.30539600 | 2.02364700 |
| C | -5.55393300 | -0.41399600 | 3.33167600 |
| H | -5.29424200 | 0.38825200 | 1.33171800 |
| H | -3.78871600 | 0.19345100 | 2.22150500 |
| H | -5.69797200 | 0.59100100 | 3.77813000 |
| H | -6.56115300 | -0.85590000 | 3.17835700 |
| H | -5.02416600 | -1.03497800 | 4.08399100 |
| C | -2.68052200 | -2.72688200 | -1.95132100 |
| C | -2.34921300 | -4.06874100 | -2.61204400 |
| H | -1.74313900 | -2.16060900 | -1.75173700 |
| H | -3.23676700 | -2.09388800 | -2.68031600 |
| H | -1.76087100 | -3.90514000 | -3.53796600 |
| H | -1.74261900 | -4.71895900 | -1.94716700 |
| H | -3.26024300 | -4.63690700 | -2.89645500 |
| C | 0.93576700 | 1.43937900 | -2.40688600 |
| C | 2.26688800 | 1.24089000 | -3.13882800 |
| H | 0.13850700 | 1.69279000 | -3.14376200 |
| H | 0.60893200 | 0.47549000 | -1.95629400 |
| H | 2.15814600 | 0.45728400 | -3.91677900 |
| H | 2.61083600 | 2.16445500 | -3.65186000 |
| H | 3.06585300 | 0.91117400 | -2.44196600 |
| C | -1.52930300 | 3.76229400 | 1.40772000 |
| C | -1.46543400 | 4.77288400 | 2.55695800 |
| H | -1.78493500 | 2.75761500 | 1.81358900 |
| H | -2.38421800 | 4.01776700 | 0.74074300 |
| H | -2.42760300 | 4.78840100 | 3.10838200 |
| H | -0.67065800 | 4.51556900 | 3.28777000 |
| H | -1.27380700 | 5.80605400 | 2.19771700 |
| O | 2.02694600 | 0.82200800 | 3.01420000 |
| C | 2.38711000 | 0.96241300 | 1.88246500 |
| O | 2.29844700 | -0.29967900 | 0.86526900 |
| O | -0.30067900 | -0.91579300 | -0.38308600 |
| C | 1.46721400 | -1.42530800 | 1.26833100 |
| C | 0.58330700 | -1.88021500 | 0.10922600 |
| H | 2.13930900 | -2.24417900 | 1.59871500 |
| H | 0.87055400 | -1.07975100 | 2.13796900 |
| H | 1.24274500 | -2.22552900 | -0.72276500 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.04410000 | -2.79122900 | 0.47737500 |
| H | -1.49871000 | 0.40221800 | 1.81491600 |
| B | 3.86320800 | -0.36998800 | 0.85473800 |
| O | 4.35048900 | -1.54116500 | 1.48796500 |
| O | 4.47468900 | -0.19001600 | -0.41610700 |
| H | 3.97045300 | 0.72852700 | 1.59540000 |
| C | 5.60033800 | -1.86677400 | 0.83458300 |
| C | 5.36108800 | -1.31550700 | -0.64092100 |
| C | 6.73384900 | -1.12678000 | 1.57122400 |
| C | 5.81907100 | -3.38014900 | 0.93070000 |
| C | 6.62430700 | -0.81309200 | -1.34890200 |
| C | 4.62435600 | -2.32641700 | -1.53973300 |
| H | 6.69633300 | -1.39765900 | 2.64576800 |
| H | 7.73462000 | -1.39923700 | 1.17819900 |
| H | 6.61514600 | -0.02712300 | 1.49465300 |
| H | 6.72517300 | -3.68826200 | 0.36862400 |
| H | 5.96079600 | -3.67085800 | 1.99169800 |
| H | 4.95148100 | -3.94458000 | 0.53900900 |
| H | 7.37051700 | -1.62721000 | -1.46296900 |
| H | 6.36546900 | -0.44528100 | -2.36297800 |
| H | 7.09366100 | 0.02337000 | -0.79714200 |
| H | 5.27405600 | -3.17698000 | -1.83254800 |
| H | 3.72445400 | -2.73141000 | -1.03441100 |
| H | 4.29222000 | -1.81125800 | -2.46357600 |
| H | 2.33200500 | 1.84585300 | 1.21133900 |

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