Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Non-biaryl Atropisomerism at C–B Bond in Sterically Hindered Aminoarylboranes

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Abstract: Sterically hindered aminoarylboranes featuring atropisomerism about the C–B bond were prepared by addition of organomagnesium species onto readily accessible dialkylamine-borane complexes. Some of these aminoarylboranes, isosteres of vinyl styrene derivatives, were resolved by HPLC on chiral stationary phase. They are the first examples of non-biaryl type system which display slow rotation about a C–B bond.

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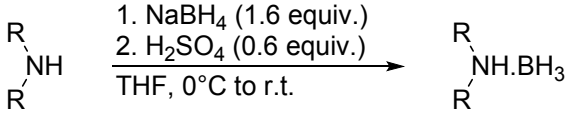
1. General Considerations

All chemicals were used without further purification. Solvents were dried and purified according to the standard procedures before their use. Silica gel chromatography was performed using 230–400 mesh silica gel purchased from Merck Analyses. Analytical thin layer chromatography (TLC) was carried out using 0.25 mm silica plates purchased from Merck. Eluted plates were visualized using ultraviolet light or stained in aqueous $KMnO_4$ ($KMnO_4$ 3g, K_2CO_3 20g, aqueous 5% NaOH 5 mL, H_2O 300 mL). ^1H, ^{13}C and ^{11}B NMR spectra were recorded at room temperature (25°C) in chloroform-d_3 or acetone-d_6, DMSO-d_8 or C_6D_6 using Bruker Avance 300 (300 MHz) unless otherwise stated. ^1H and ^{13}C NMR chemical shifts (δ) are given in ppm relative to tetramethylsilane (internal standard). *J* values are quoted in Hertz. The following abbreviations were used to describe the multiplicities: s = singlet, bs = broad singlet, d = doublet, m = multiplet, t = triplet, dd = doublet of doublet, td = triplet of doublet, q = quadruplet, quint = quintuplet. The carbon signal bound to the boron was not observed in most cases due to quadrupolar relaxation. ^{11}B NMR spectra were recorded at 25°C and chemical shifts (δ) are given in ppm relative to $BF_3.OEt_2$ (internal standard). GC-MS analyses were performed on HP 6890 series GC-system equipped with a J&W Scientific DB-1701 capillary column, a HP 5973 mass selective detector (EI) using the following method: 70°C for 1 min then 20°C/min until 230°C then 6 min at 230°C. Infrared spectra (IR) were recorded on a Perkin-Elmer Paragon 1000 PC FT-IR spectrometer as neat films on NaCl windows or as solids with KBr pellets. The melting points (m.p.) were recorded on a Mettler Toledo DSC1-star system using the following method: 30°C to 300°C at 10°C/min. Separation of enantiomers was performed by high performance liquid chromatography HPLC on a 1260 Infinity II Agilent HPLC bearing a Quaternary Pump with an operating pressure of up to 600 bar. The chiral column used was purchased from Phenomenex and is a Lux® 3 µm Cellulose-1, LC Column 100 x 4.6 mm. The stationary phase is a Cellulose tris(3,5 dimethylphenylcarbamate) and the flow used was a 1 mL/min with a 20µL injection volume. Circular dichroism (CD) spectra were measured on a Jasco J-815 (190-800nm) equipped with a xenon-mercury lamp and running under nitrogen atmosphere. The sample temperature is maintained between 4 and 20°C using a Peltier device (PFD-425S/15). All samples were stirred at 1000rpm during measurements, and every spectrum was taken as the average of 4 -10 scans with wavelengths between 200 to 400 nm.

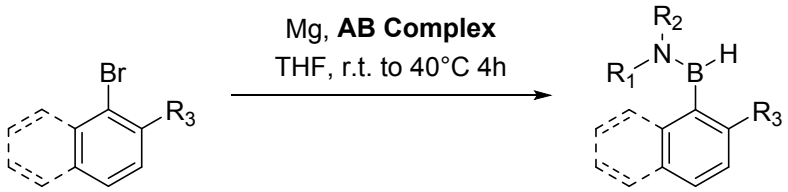
2. General Procedures

General Procedure A for the synthesis of amine-borane complexes



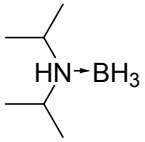
To a stirred solution of the amine (70.6 mL, 0.5 mol) and $NaBH_4$ (30 g, 0.79 mol) in THF (500 mL) was added, at 0°C over a period of 45 minutes, sulfuric acid (16 mL, 0.3 mol). The mixture was allowed to warm to room temperature and stirred for 3 hours. The crude was concentrated under vacuum and the residue was solubilized with CH_2Cl_2, and then filtrated to eliminate all solid residues. The filtrate was washed with water (4x100 mL). The organic phase was dried over Na_2SO_4 and concentrated under reduced pressure to give the amine-borane complex.

General Procedure B for the synthesis of arylaminoboranes

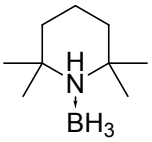


To a solution of magnesium (1.3 equiv.; 1.3 mmol) in dry THF (1 mL/mmol) was added the amine-borane complex (1.1 equiv.; 1.1 mmol). The requisite bromo substituted naphthalene or benzene (1.0 equiv; 1 mmol) was then added and the resulting mixture was heated to 40°C for 4 to 8h (according to the substrate). After cooling the mixture back to room temperature, all volatiles were concentrated. Then, the grey foam was diluted in dry hexane and the magnesium salts filtered. The resulting crude product was obtained with high purity after concentrating all volatiles. Several washes using DABCO and dry Hexane/Pentane or Methylcyclohexane followed by filtration / concentration of all volatiles allowed to isolate pure products.

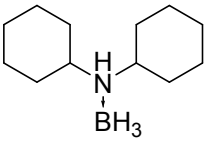
3. Characterization of amine-boranes and compounds 10a-10n



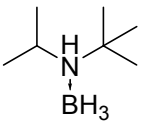
***N*-diisopropylamine-borane complex [105416-38-4]:** Diisopropylamine-borane ($C_6H_{18}BN$) was synthesized according to **General Procedure A** from diisopropylamine [108-18-9] on a 0.5 mol scale and obtained as a colorless oil which solidified upon cooling (50.8 g, 90%). **m.p.** 20-25 °C (hexane). **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 0.96 (d, J = 6.6Hz, 6H, CH_3), 1.05 (d, J = 6.6Hz, 6H, CH_3), 1.91 (q, $J_{H\text{-}B}$ = 91Hz, 3H, CH_3), 2.72 – 2.90 (m, 2H, CH). **^{13}C NMR (75 MHz, C_6D_6)** δ (ppm) 19.0, 21.1, 52.1. **^{11}B NMR (96 MHz, C_6D_6)** δ (ppm) -21.3 (q, $J_{H\text{-}B}$ = 91,4 Hz). Data were in good agreement with those from literature.



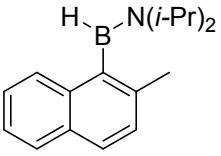
(2,2,6,6-tetramethyl-1-piperidine)-borane complex [99432-15-2]: TMP•BH_3 ($C_9H_{22}BN$) was synthesized according to **General Procedure A** from 2,2,6,6-tetramethyl-1-pyperidine [768-66-1] on a 5 mmol scale and obtained as a yellow oil (504 mg, 65%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.18 (s, 6H, CH_3), 1.22 (s, 6H, CH_3), 1.32 – 1.48 (m, 4H, CH_2), 1.58 (m, 2H, CH_2). **^{13}C NMR (75 MHz, C_6D_6)** δ (ppm) 16.6, 20.6, 34.0, 41.1, 58.5. **^{11}B NMR (96 MHz, C_6D_6)** δ (ppm) -21.1 (q, $J_{H\text{-}B}$ = 98,0 Hz). Data were in good agreement with those from literature.



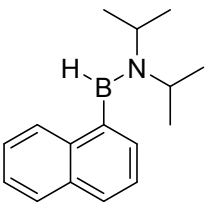
(*N,N*-dicyclohexylamine)-borane complex [131765-96-3]: Dicyclohexylamine-borane ($C_{12}H_{26}BN$) was synthesized according to **General Procedure A** from *N,N*-dicyclohexylamine [101-83-7] on a 0.5 mol scale and obtained as white shining solid (88,5 g, 91%). **m.p.** 121-122°C (hexane) **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.01 – 1.36 (m, 7H, CH_2), 1.48 – 1.95 (m, 13H, CH_2), 2.75 – 2.89 (m, 2H, CH), 2.96 (s, 1H, NH). **^{13}C NMR (75 MHz, C_6D_6)** δ (ppm) 25.4, 25.5, 25.6, 25.7, 29.7, 29.9, 30.8, 31.2, 51.9, 53.0, 60.5, 60.7. **^{11}B NMR (96 MHz, C_6D_6)** δ (ppm) -21.1 (q, $J_{H\text{-}B}$ = 98,0 Hz). Data were in good agreement with those from literature.



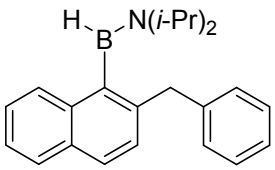
(*N-tert*-butyl-*N*-isopropylamine)-borane complex: *N-tert*-butyl-*N*-isopropylamine)-borane ($C_7H_{20}BN$) was synthesized on a 5 mmol scale according to **General Procedure A** from [7515-80-2] *N*-tert-butyl-*N*-isopropylamine and obtained as a colorless oil (212.9 mg, 33%). **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.30 (d, *J* = 6.9 Hz, 6H, CH_3), 1.33 (s, 9H, CH_3), 3.44 (dq, *J* = 13.1, 6.6 Hz, 1H, CH).**^{13}C NMR (75 MHz, C_6D_6)** δ (ppm) 18.4, 23.7, 27.2, 28.1, 49.0. **^{11}B NMR (96 MHz, C_6D_6)** δ (ppm) --23.72 (q, *J* = 106.4 Hz).



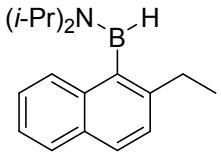
2-*B*-((*N,N*-diisopropylamino)-2-methylnaphth-1-yl)-borane (10a): 10a ($C_{17}H_{24}BN$) was obtained from 1-bromo-2-methylnaphthalene [2586-62-1] (1mmol; 1.0 equiv.) and diisopropylamine-borane complex [55124-35-1] (1.1 mmol; 1.1 equiv.) as a racemic mixture with 62% yield (157.0 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.41 (d, *J* = 6.6 Hz, 6H, CH_3), 1.45 (d, 6.6 Hz, 6H, CH_3), 2.50 (s, 3H, CH_3), 3.21 (hept, *J* = 6.7 Hz, 1H, CH), 3.67 (hept, *J* = 6.7 Hz, 1H, CH), 7.31 – 7.50 (m, 3H, $C_{Ar}H$), 7.75 (d, *J* = 8.4 Hz, 1H, $C_{Ar}H$), 7.80 – 7.87 (m, 1H, $C_{Ar}H$), 7.99 (d, *J* = 8.2 Hz, 1H, $C_{Ar}H$).**^{13}C NMR (75 MHz, C_6D_6)** δ (ppm) 21.6, 21.8, 21.9, 27.1, 27.2, 44.7, 50.9, 124.4, 125.0, 126.6, 127.6, 128.1, 128.2, 131.3, 134.7, 135.8. Carbon adjacent to boron not observed.**^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 39.4. **HPLC:** The separation of the racemate was performed on a Phenomenex Cellulose-1 column at 0 °C. (99:1 hexane:isopropanol; 1mL/min). tr_1 = 3.66 min; tr_2 = 3.78 min.



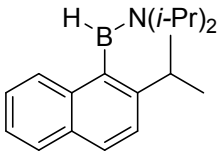
2-*B*-((*N,N*-diisopropylamino)-1-naphth-1-yl)-borane (10b): 10b ($C_{16}H_{22}BN$) was obtained from 1-bromonaphthalene [90-11-9] (1mmol; 1.0 equiv.) and diisopropylamine-borane complex [55124-35-1] (1.1 mmol; 1.1 equiv.) as a racemic mixture with 59% yield (139.9 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.02 (d, *J* = 6.7 Hz, 6H, CH_3), 1.38 (d, *J* = 6.7 Hz, 6H, CH_3), 3.28 – 3.37 (m, 2H CH), 7.20 – 7.32 (m, 2H, $C_{Ar}H$), 7.37 (dq, *J* = 6.8, 1.9 Hz, 2H, $C_{Ar}H$), 7.67 – 7.81 (m, 3H, $C_{Ar}H$).**^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 27.2, 45.8, 53.2, 122.6, 125.8, 127.6. Carbon adjacent to boron was not observed.**^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 38.3.



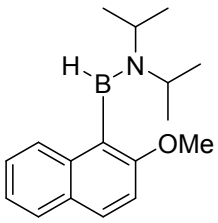
2-*B*-((*N*,*N*-diisopropylamino)-2-benzylnaphth-1-yl)-borane (10c): 10c ($C_{23}H_{28}BN$) was obtained from 1-bromo-2-benzylnaphthalene [108978-33-2] (1mmol; 1.0 equiv.) and diisopropylamine-borane complex [55124-35-1] (1.1 mmol; 1.1 equiv.) as a racemic mixture with 79% yield (260.1 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 0.91 (d, *J* = 6.7 Hz, 3H, CH_3), 1.02 (d, *J* = 6.7 Hz, 3H, CH_3), 1.39 (d, *J* = 6.6 Hz, 3H, CH_3), 1.50 (d, *J* = 6.6 Hz, 3H, CH_3), 3.46 (hept, *J* = 6.7 Hz, 1H, CH), 3.61 (hept, *J* = 6.7 Hz, 1H, CH), 3.95 – 4.19 (m, 2H, CH_2), 7.11 – 7.24 (m, 5H, $C_{Ar}H$), 7.35 – 7.43 (m, 2H, $C_{Ar}H$), 7.62 – 7.74 (m, 2H, $C_{Ar}H$), 7.77 – 7.78 (m, 2H, $C_{Ar}H$).**^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 21.5, 21.6, 27.0, 27.2, 41.9, 44.7, 51.0, 124.8, 125.1, 125.8, 127.0, 127.9, 128.0, 128.2, 128.3, 128.5, 128.9, 129.1, 131.6, 134.8, 139.0, 141.6. Carbon adjacent to boron not observed. **^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 40.4. **HPLC:** The separation of the racemate was performed on a Phenomenex Cellulose-1 column at 25 °C. (99:1 hexane:isopropanol; 1mL/min). tr_1 = 5.19 min; tr_2 = 5.49 min.



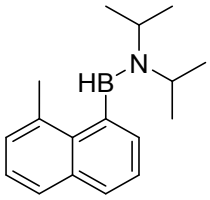
2-*B*-((*N*,*N*-diisopropylamino)-2-ethylnaphth-1-yl)-borane (10d): 10d ($C_{18}H_{26}BN$) was obtained from 1-bromo-2-ethylnaphthalene [39071-00-6] (1mmol; 1.0 equiv.) and diisopropylamine-borane complex [55124-35-1] (1.1 mmol; 1.1 equiv.) as a racemic mixture with 79% yield (211.1 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable.* **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.02 (d, *J* = 6.7 Hz, 3H, CH_3), 1.05 (d, *J* = 6.7 Hz, 3H, CH_3), 1.22 – 1.29 (m, 3H, CH_3), 1.43 (d, *J* = 6.7 Hz, 3H, CH_3), 1.51 (d, *J* = 6.7 Hz, 3H, CH_3), 2.57 – 2.74 (m, 2H, CH_2), 3.48 (hept, *J* = 6.6 Hz, 1H, CH), 3.60 (hept, *J* = 6.6 Hz, 1H, CH), 7.30 – 7.39 (m, 3H, $C_{Ar}H$), 7.61 – 7.67 (m, 1H, $C_{Ar}H$), 7.71 – 7.73 (m, 1H, $C_{Ar}H$), 7.74 – 7.82 (m, 1H, $C_{Ar}H$).**^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 15.5, 15.6, 21.7, 27.2, 29.2, 44.6, 50.8, 68.0, 124.5, 124.9, 126.6, 126.9, 127.8, 128.1, 131.5, 134.7, 142.4. Carbon adjacent to boron was not observed. **^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 40.0. **HPLC:** The separation of the racemate was performed on a Phenomenex Cellulose-1 column at 25 °C. (Heptane; 1mL/min). tr_1 = 9.21 min; tr_2 = 13.06 min.



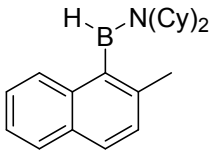
2-*B*-((*N*,*N*-diisopropylamino)-2-isopropylnaphth-1-yl)-borane (10e): 10e ($C_{19}H_{28}BN$) was obtained from 1-bromo-2-isopropylnaphthalene [39071-01-7] (1mmol; 1.0 equiv.) and diisopropylamine-borane complex [55124-35-1] (1.1 mmol; 1.1 equiv.) as a racemic mixture with 82% yield (230.6 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.00 – 1.07 (m, 6H, CH_3), 1.24 – 1.38 (m, 6H, CH_3), 1.40 – 1.47 (m, 3H, CH_3), 1.52 (m, 3H, CH_3), 2.89 – 3.03 (m, 1H, CH), 3.49 (hept, *J* = 6.7 Hz, 1H, CH), 3.62 (hept, *J* = 6.7 Hz, 1H, CH), 7.33 – 7.47 (m, 1H, $C_{Ar}H$), 7.61 – 7.72 (m, 3H, $C_{Ar}H$), 7.73 – 7.87 (m, 2H, $C_{Ar}H$).**^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 21.5, 21.8, 23.5, 24.2, 27.0, 27.2, 34.2, 44.6, 50.7, 123.1, 124.5, 125.7, 127.2, 127.5, 128.1, 131.7, 134.7, 146.9. Carbon adjacent to boron not observed.**^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 40.4. **HPLC:** The separation of the racemate was performed on a Phenomenex Cellulose-1 column at 25 °C. (Heptane; 1mL/min). tr_1 = 5.96 min; tr_2 = 7.26 min.



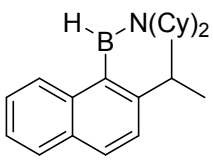
2-*B*-((*N*,*N*-diisopropylamino)-2-methoxynaphth-1-yl)-borane (10f): 10f ($C_{17}H_{24}BNO$) was obtained from 1-bromo-2-methoxynaphthalene [3401-47-6] (1mmol; 1.0 equiv.) and diisopropylamine-borane complex [55124-35-1] (1.1 mmol; 1.1 equiv.) as a racemic mixture with 71% yield (191.1 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.07 (dd, *J* = 13.6, 11.1 Hz, 6H, CH_3), 1.45 (d, *J* = 6.6 Hz, 6H, CH_3), 3.47 (hept, *J* = 6.7 Hz, 1H, CH), 3.67 (hept, *J* = 6.7 Hz, 1H, CH), 3.85 (s, 3H, CH_3), 7.26 (s, 2H, $C_{Ar}H$), 7.60 (d, *J* = 8.2 Hz, 2H, $C_{Ar}H$), 7.76 (dd, *J* = 8.9, 7.6 Hz, 2H, $C_{Ar}H$).**^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 21.8, 21.9, 22.0, 27.3, 27.7, 44.8, 50.9, 124.2, 125.1, 126.3, 127.5, 128.2, 128.3, 131.3, 134.9, 135.7. Carbon adjacent to boron was not observed. **^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 38.2.



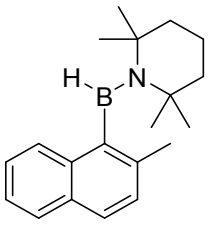
2-*B*-((*N*,*N*-diisopropylamino)-8-methylnaphth-1-yl)-borane (10g): 10g ($C_{17}H_{24}BN$) was obtained from 1-bromo-8-methylnaphthalene [33295-37-3] (1mmol; 1.0 equiv.) and diisopropylamine-borane complex [55124-35-1] (1.1 mmol; 1.1 equiv.) as a racemic mixture with 67% yield (169.6 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.03 (s, 3H, CH_3), 1.08 (d, *J* = 6.7 Hz, 6H, CH_3), 1.37 (d, *J* = 6.7 Hz, 6H, CH_3), 3.45 (hept, *J* = 6.7 Hz, 1H, CH), 3.86 (hept, *J* = 6.8 Hz, 1H, CH), 7.36 – 7.47 (m, 3H, $C_{Ar}H$), 7.78 (dt, *J* = 6.7, 3.5 Hz, 3H, $C_{Ar}H$).**^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 22.1, 27.0, 45.5, 50.3, 124.6, 128.5, 128.7. Carbon adjacent to boron was not observed. **^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 38.9.



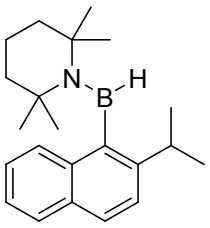
2-*B*-((*N*,*N*-cyclohexylamino)-2-methylnaphth-1-yl)-borane (10h): 10h ($C_{23}H_{32}BN$) was obtained from 1-bromo-2-methylnaphthalene [2586-62-1] (1mmol; 1.0 equiv.) and dicyclohexylamine-borane complex (1.1 mmol; 1.1 equiv.) as a racemic mixture with 86% yield (286.6 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 0.70 – 2.06 (m, 20H, CH_2), 2.40 (s, 3H, CH_3), 2.92 – 3.00 (m, 1H, CH), 3.01 – 3.16 (m, 1H, CH), 7.28 – 7.42 (m, 3H, $C_{Ar}H$), 7.58 – 7.68 (m, 2H, $C_{Ar}H$), 7.71 – 7.77 (m, 1H, $C_{Ar}H$). **^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 22.1, 25.4, 25.6, 25.7, 26.7, 26.8, 32.1, 37.6, 37.8, 55.1, 59.9, 124.3, 124.9, 126.5, 127.6, 128.1, 128.2, 131.3, 134.8, 135.7. Carbon adjacent to boron not observed. **^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 40.6. **HPLC:** The separation of the racemate was performed on a Phenomenex Cellulose-1 column at 0 °C. (99:1 hexane:isopropanol; 1mL/min). tr_1 = 3.60 min; tr_2 = 3.89 min.



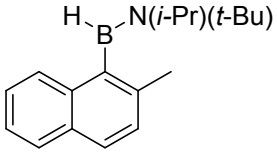
2-*B*-((*N*,*N*-dicyclohexylamino)-2-isopropylnaphth-1-yl)-borane (10i): 10i ($C_{25}H_{36}BN$) was obtained from 1-bromo-2-isopropylnaphthalene [39071-01-7] (1mmol; 1.0 equiv.) and dicyclohexylamine-borane complex (1.1 mmol; 1.1 equiv.) as a racemic mixture with 76% yield (274.6 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 0.95 (m, 4H, CH_2), 1.24 (d, *J* = 6.9 Hz, 3H, CH_3), 1.28 (d, *J* = 6.9 Hz, 3H, CH_3), 1.37 – 2.05 (m, 16H, CH_2), 2.28 – 3.03 (m, 1H, CH), 3.04 – 3.20 (m, 1H, CH), 7.31 – 7.47 (m, 1H, CH), 7.63 – 7.73 (m, 2H, $C_{Ar}H$), 7.71 – 7.84 (m, 2H, $C_{Ar}H$).**^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 23.6, 23.9, 24.2, 25.2, 25.4, 25.5, 25.6, 25.7, 26.7, 32.0, 32.3, 34.3, 37.6, 37.8, 59.7, 123.1, 124.4, 124.8, 125.0, 127.1, 127.9, 128.0, 131.7, 134.7, 146.6. Carbon adjacent to boron not observed. **^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 40.9. **HPLC:** The separation of the racemate was performed on a Phenomenex Cellulose-1 column at 25 °C. (Heptane; 1mL/min). tr_1 = 8.21 min; tr_2 = 11.51 min.



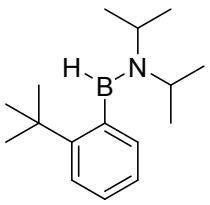
2-*B*-((2,2,6,6-tetramethylpiperidino)-2-methylnaphth-1-yl)-borane (10j): 10j ($C_{20}H_{28}BN$) was obtained from 1-bromo-2-methylnaphthalene [2586-62-1] (1mmol; 1.0 equiv.) and TMP•BH_3 (1.1 mmol; 1.1 equiv.) as a racemic mixture with 49% yield (143.7 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.08 (s, 3H, CH_3), 1.11 (s, 3H, CH_3), 1.59 (s, 3H, CH_3), 1.66 (s, 3H, CH_3), 1.75 – 1.93 (m, 6H, CH_2), 2.43 (s, 3H, CH_3), 7.15 – 7.21 (m, 1H, $C_{Ar}H$), 7.29 – 7.50 (m, 3H, $C_{Ar}H$), 7.55 – 7.71 (m, 1H, $C_{Ar}H$), 7.72 – 7.85 (m, 1H, $C_{Ar}H$). **^{13}C NMR (75 MHz, C_6D_6)** δ (ppm) 20.7, 27.3, 37.1, 37.2, 40.0, 40.3, 41.81, 43.2, 61.9, 62.1, 129.5, 129.8, 131.2, 133.2, 133.5, 133.7, 136.9, 138.2, 138.8. Carbon adjacent to boron not observed. **^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 42.5. **HPLC:** The separation of the racemate was performed on a Phenomenex Cellulose-1 column at 0 °C. (99:1 hexane:isopropanol; 1mL/min). tr_1 = 3.61 min; tr_2 = 3.89 min.



2-*B*-((2,2,6,6-tetramethylpiperidino)-2-isopropylnaphth-1-yl)-borane (10k): (10k) ($C_{22}H_{32}BN$) was obtained from 1-bromo-2-isopropylnaphthalene [39071-01-7] (1mmol; 1.0 equiv.) and TMP•BH_3 (1.1 mmol; 1.1 equiv.) as a racemic mixture with 43% yield (138.1 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.08 (s, 3H, CH_3), 1.13 (s, 3H, CH_3), 1.20 (d, *J* = 6.8 Hz, 3H, CH_3), 1.33 (s, 3H, CH_3), 1.36 (s, 3H, CH_3), 1.38 (d, *J* = 6.8 Hz, 3H, CH_3), 1.81 (m, 6H, CH_2), 3.07 – 3.11 (m, 1H, CH), 7.34 – 7.46 (m, 2H, $C_{Ar}H$), 7.61 – 7.67 (m, 2H, $C_{Ar}H$), 7.72 – 7.84 (m, 2H, $C_{Ar}H$). **^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 15.8, 21.8, 23.9, 24.6, 32.7, 32.8, 34.2, 34.6, 35.3, 35.5, 36.9, 38.3, 123.2, 124.3, 124.5, 125.0, 125.8, 126.5, 127.5, 128.0, 129.0. Carbon adjacent to boron was not observed. **^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 42.0. **HPLC:** The separation of the racemate was performed on a Phenomenex Cellulose-1 column at 25 °C. (Heptane; 1mL/min). tr_1 = 8.64 min; tr_2 = 9.90 min.



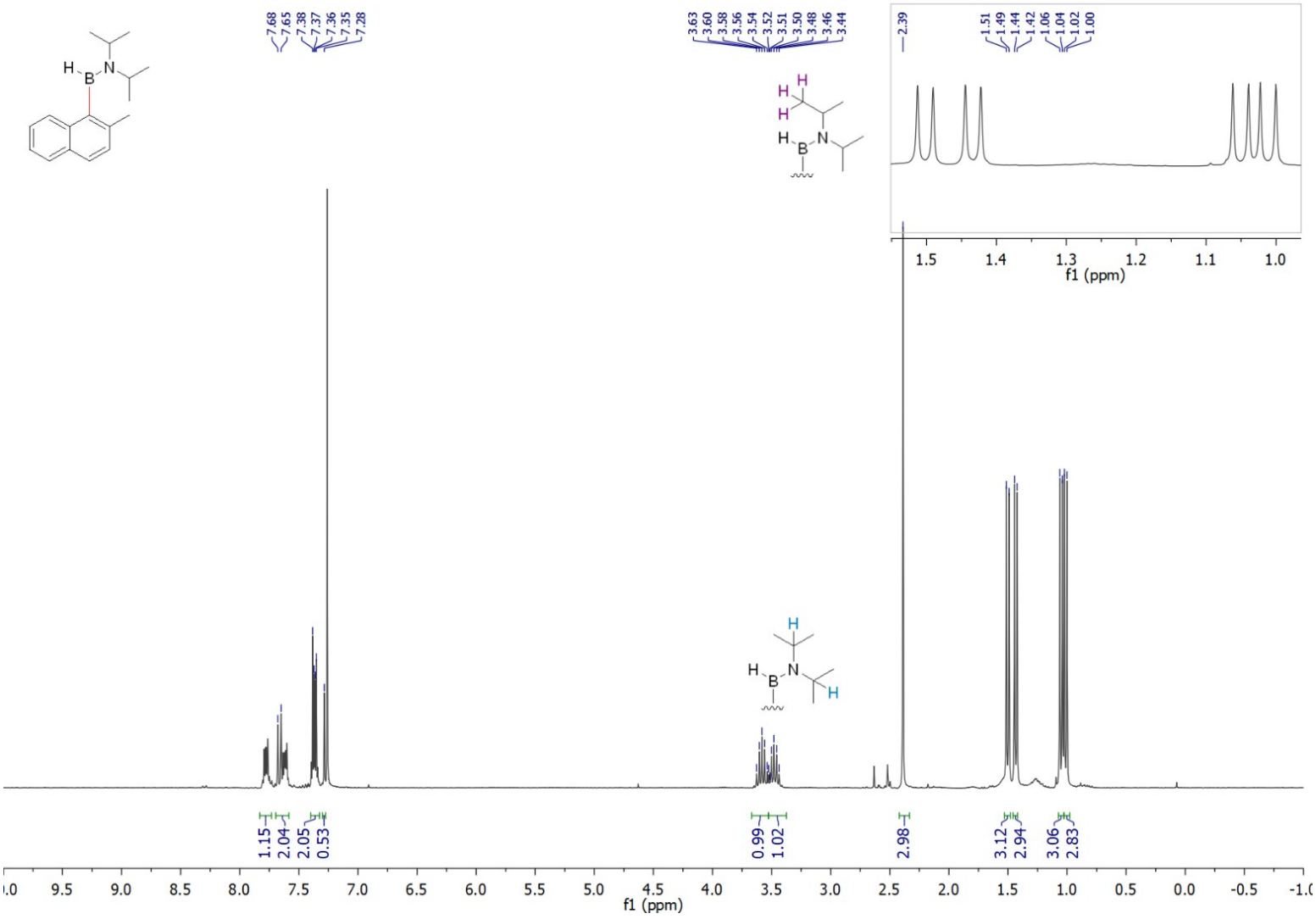
2-*B*-((*N*-*tert*-butyl-*N*-isopropylamino)-2-methylnaphth-1-yl)-borane (10l): (10l) ($C_{18}H_{26}BN$) was obtained from 1-bromo-2-methylnaphthalene [2586-62-1] (1mmol; 1.0 equiv.) and BH_3•NH(*i*-Pr)-(*t*-Bu) (1.1 mmol; 1.1 equiv.) as a racemic mixture with 61% yield (163.0 mg) following the **general procedure B**. **Rf** *unstable on silica.* **MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 0.71 (s, 3H, CH_3), 1.24 (dd, *J* = 9.3, 5.8 Hz, 6H, CH_3), 1.31 (s, 9H, CH_3), 2.50 – 2.81 (m, 6H, CH_3), 2.86 – 3.01 (m, 1H, CH), 3.01 – 3.21 (m, 1H, CH), 7.28 – 7.42 (m, 2H, $C_{Ar}H$), 7.53 – 7.90 (m, 4H, $C_{Ar}H$).**^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 22.4, 27.0, 27.2, 30.2, 48.9, 59.0, 70.7, 124.2, 125.0, 125.3, 125.4, 125.8, 128.1, 128.2, 128.8, 133.6. Carbon adjacent to boron was not observed. **^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 41.0. **HPLC:** The separation of the racemate was performed on a Phenomenex Cellulose-1 column at 25 °C. (99:1 Hexane:isopropanol; 1mL/min). tr_1 = 3.53 min; tr_2 = 3.67 min.



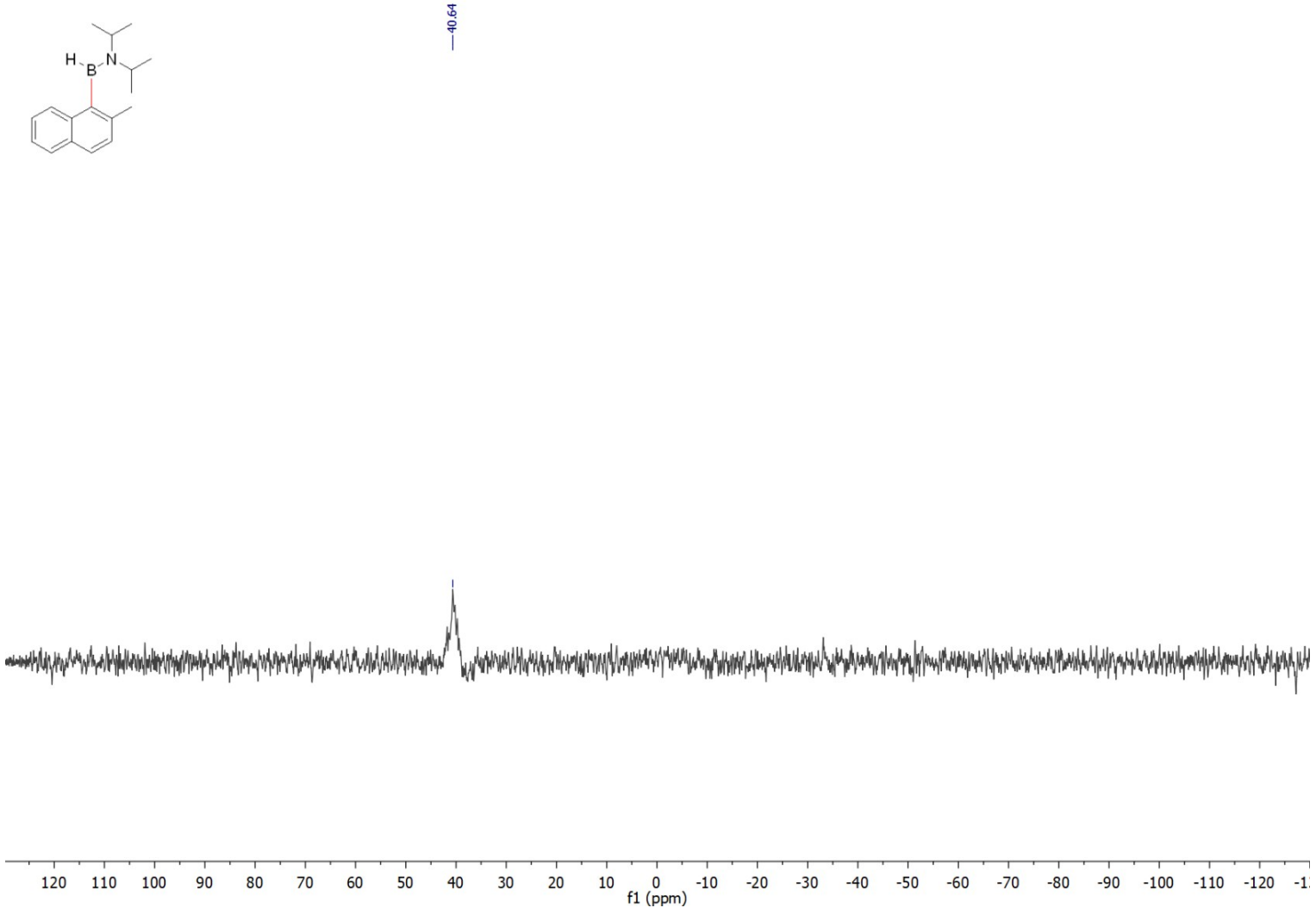
2-*B*-((*N*,*N*-diisopropylamino)-2-*tert*-butyl-phen-1-yl)-borane (10m): (10m) ($C_{16}H_{28}BN$) was obtained from 1-bromo-2-*tert*-butylbenzene [7073-99-6] (1mmol; 1.0 equiv.) and diisopropylamine-borane complex [55124-35-1] (1.1 mmol; 1.1 equiv.) as a racemic mixture with 92% yield (225.6 mg) following the **general procedure B**.**MS (ESI+)** m/z: *unstable*. **^{1}H NMR (300 MHz, $CDCl_3$)** δ (ppm) 1.06 (d, *J* = 6.7 Hz, 6H, CH_3), 1.32 (t, *J* = 3.3 Hz, 6H, CH_3), 3.35 (s, 9H, CH_3), 7.11 (ddd, *J* = 8.4, 6.3, 1.7 Hz, 1H, $C_{Ar}H$), 7.20 (ddd, *J* = 13.4, 8.6, 2.6 Hz, 1H, $C_{Ar}H$), 7.38 (d, *J* = 7.8 Hz, 2H, $C_{Ar}H$).**^{13}C NMR (75 MHz, $CDCl_3$)** δ (ppm) 14.2, 22.5, 26.2, 45.4, 47.5, 51.7, 77.8, 128.0, 132.0, 132.1, 132.4. Carbon adjacent to boron not observed. **^{11}B NMR (96 MHz, $CDCl_3$)** δ (ppm) 38.9.

4. NMR spectra

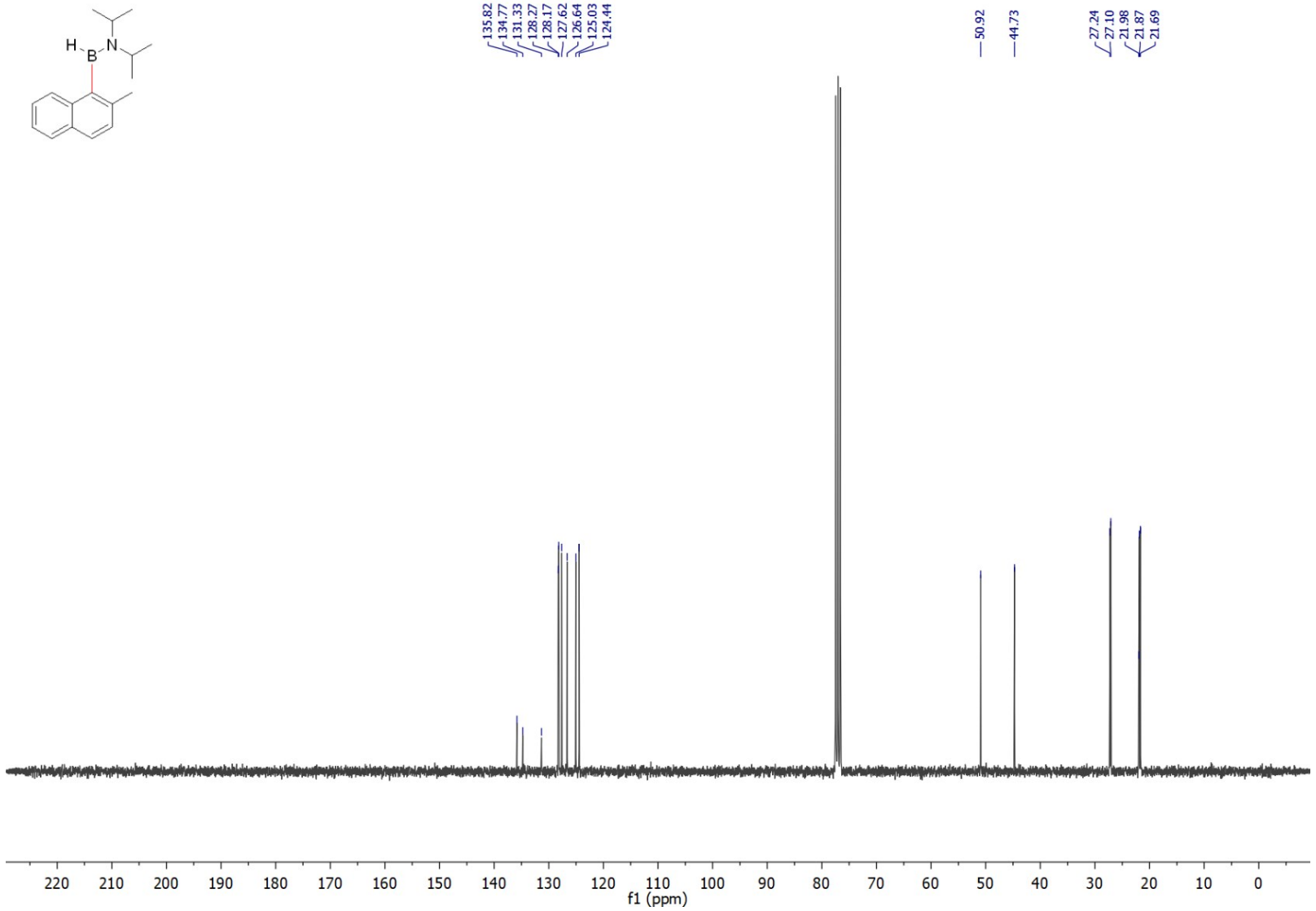
Compound (10a) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



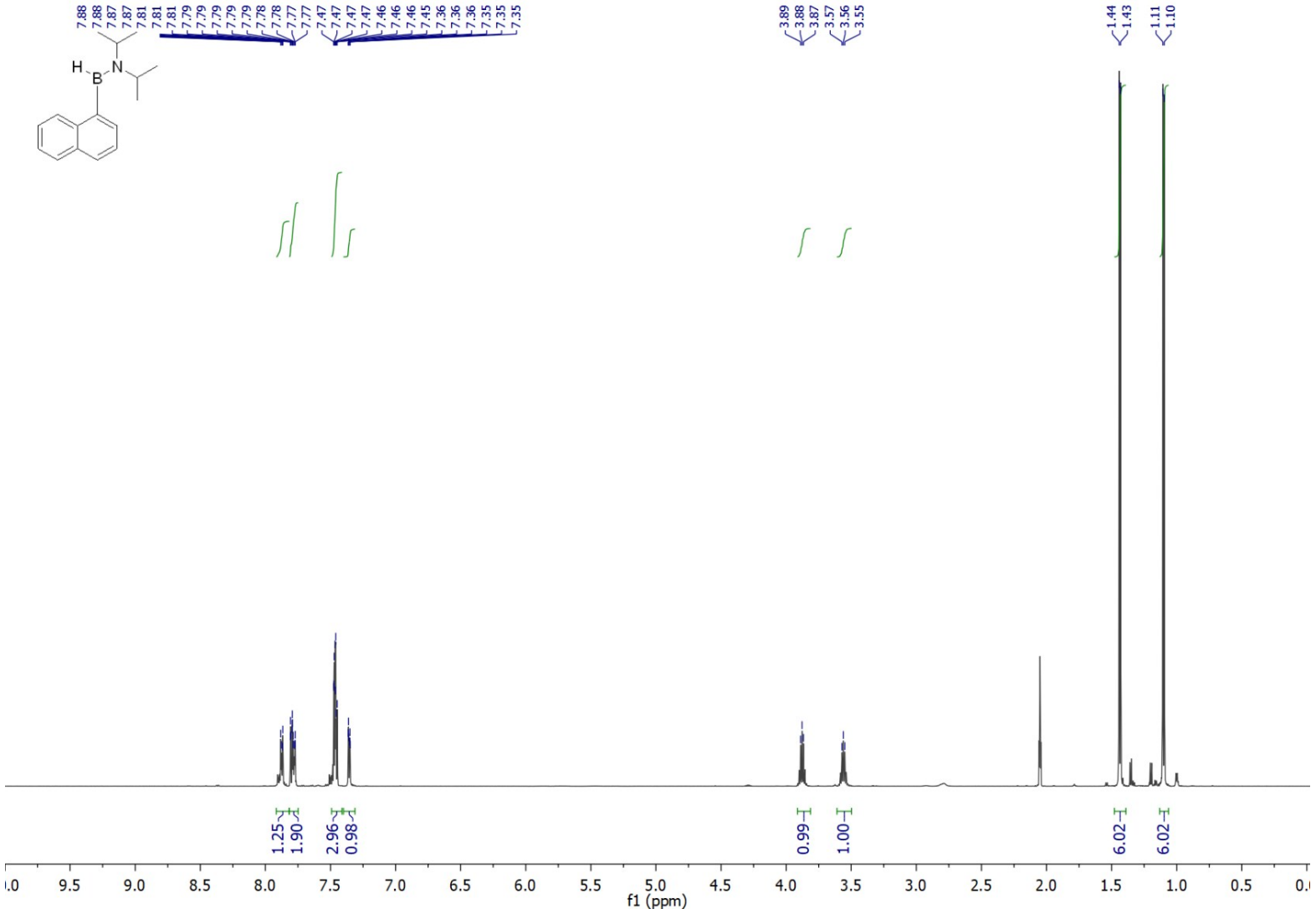
Compound (10a) ^{11}B NMR in $CDCl_3$ at 25°C (96 MHz)



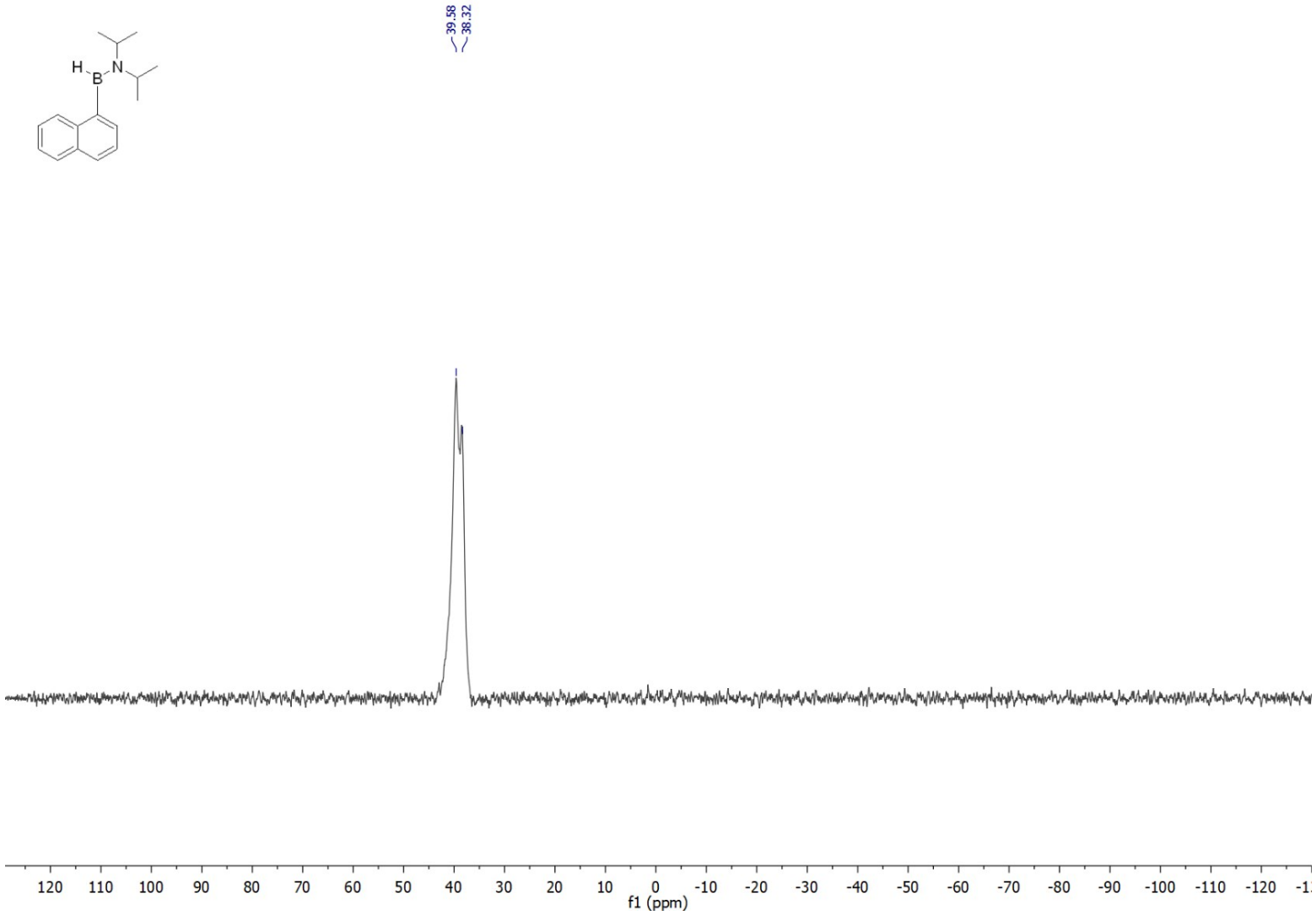
Compound (10a) ^{13}C NMR in $CDCl_3$ at 25°C (75 MHz)



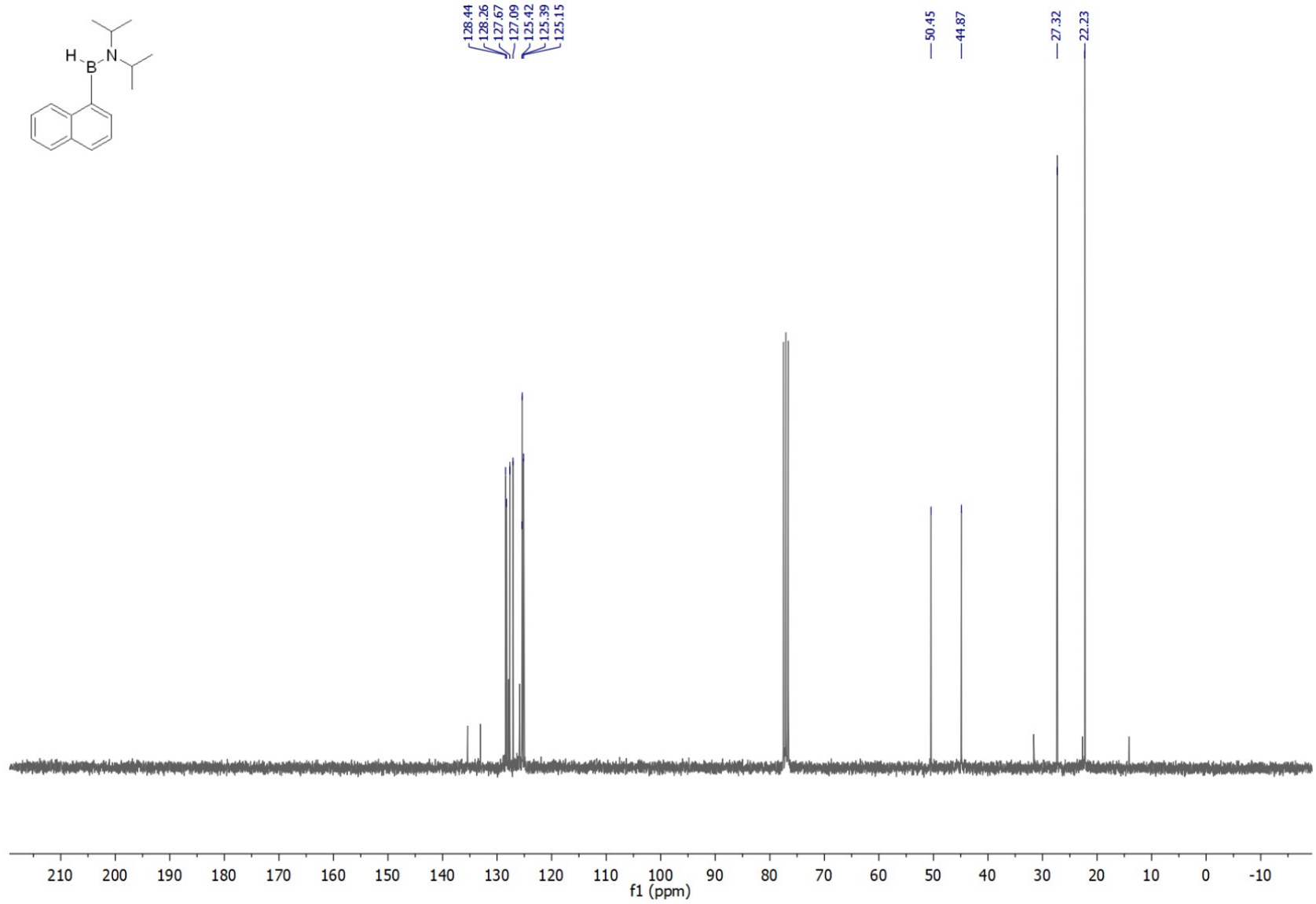
Compound (10b) ^{1}H NMR in Acetone-d_6 at 25°C (300 MHz)



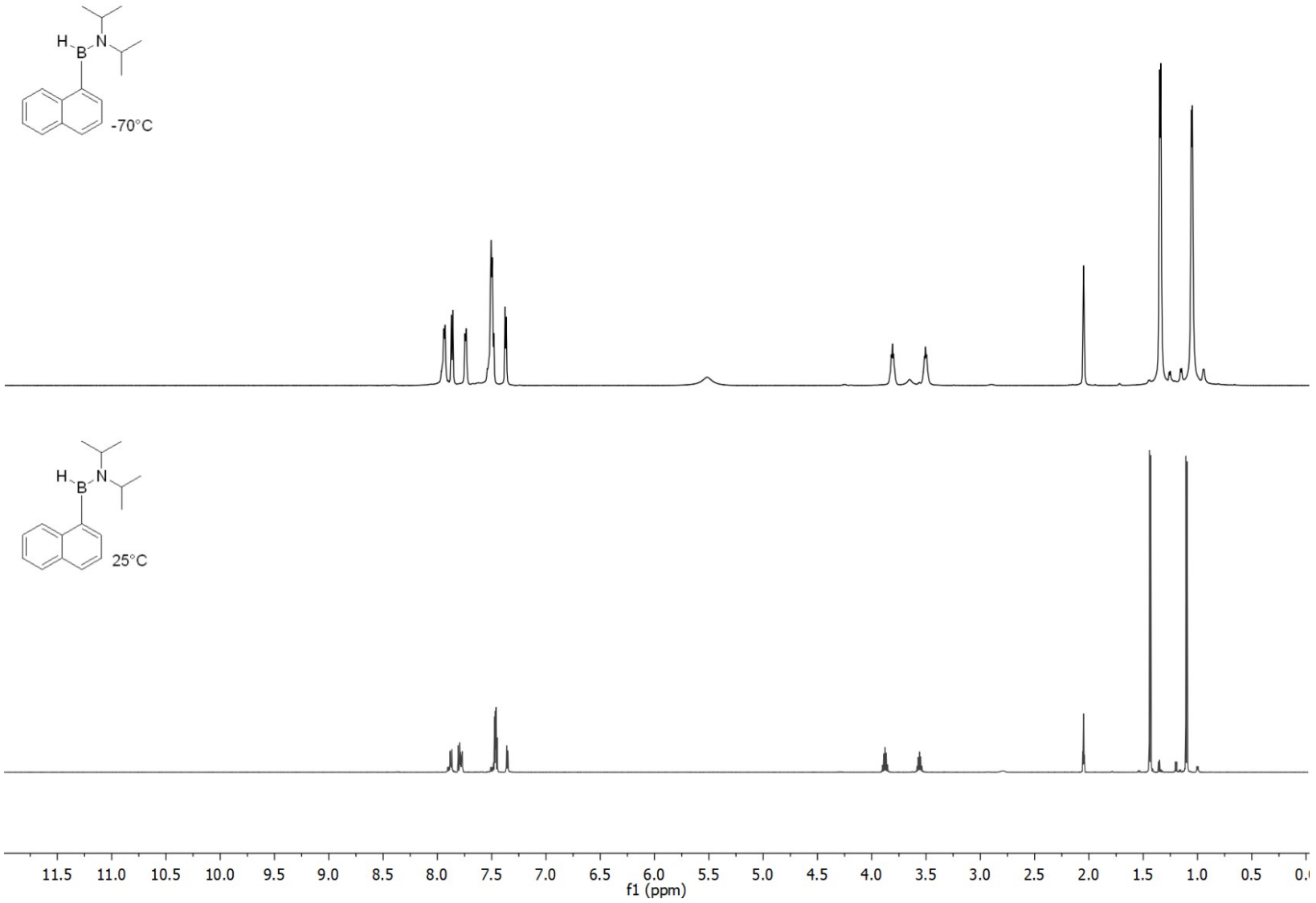
Compound (10b) ^{11}B NMR in Acetone-d_6 at 25°C (196 MHz)



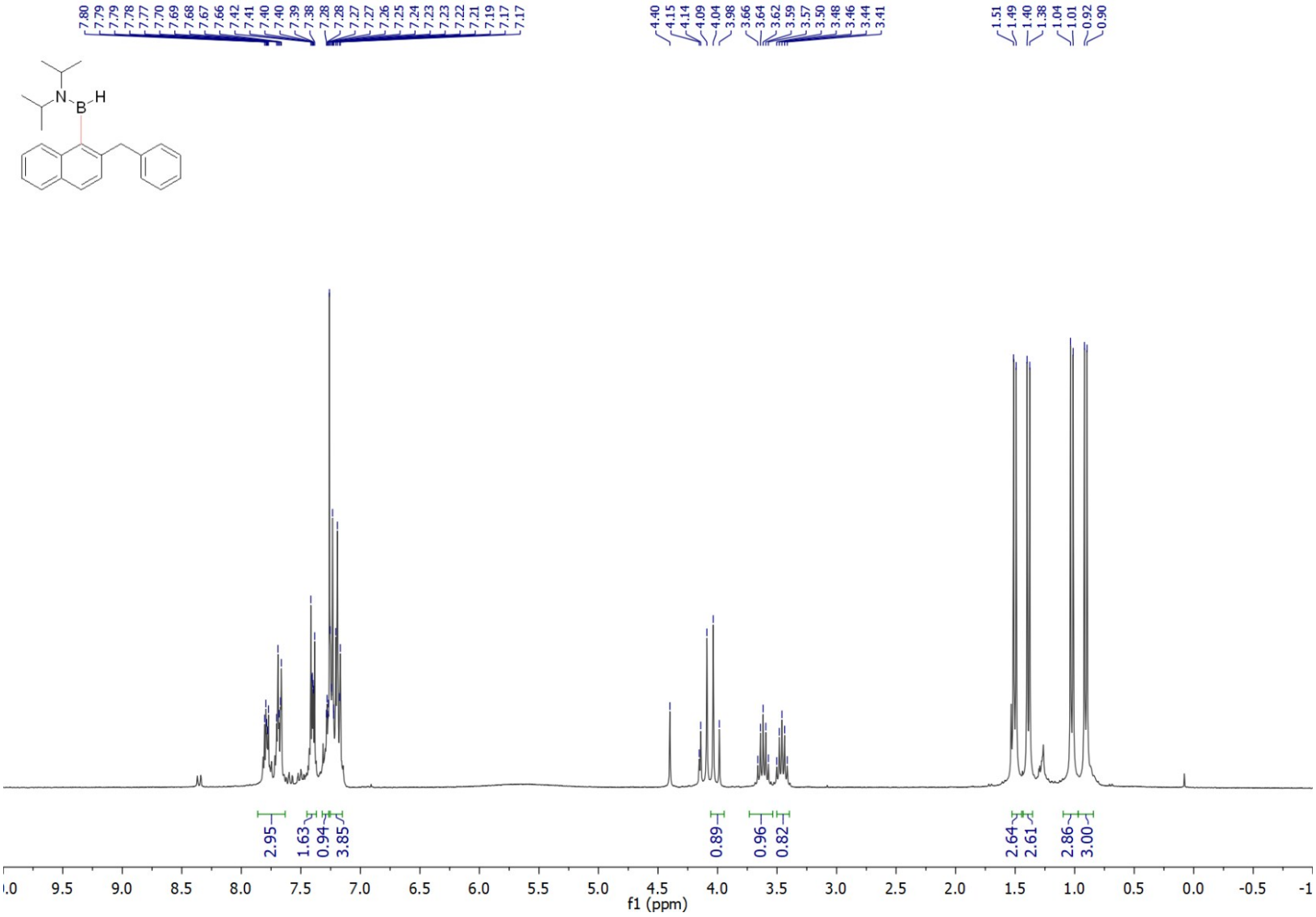
Compound (10b) ^{13}C NMR in Acétone-d_6 at 25°C (75 MHz)



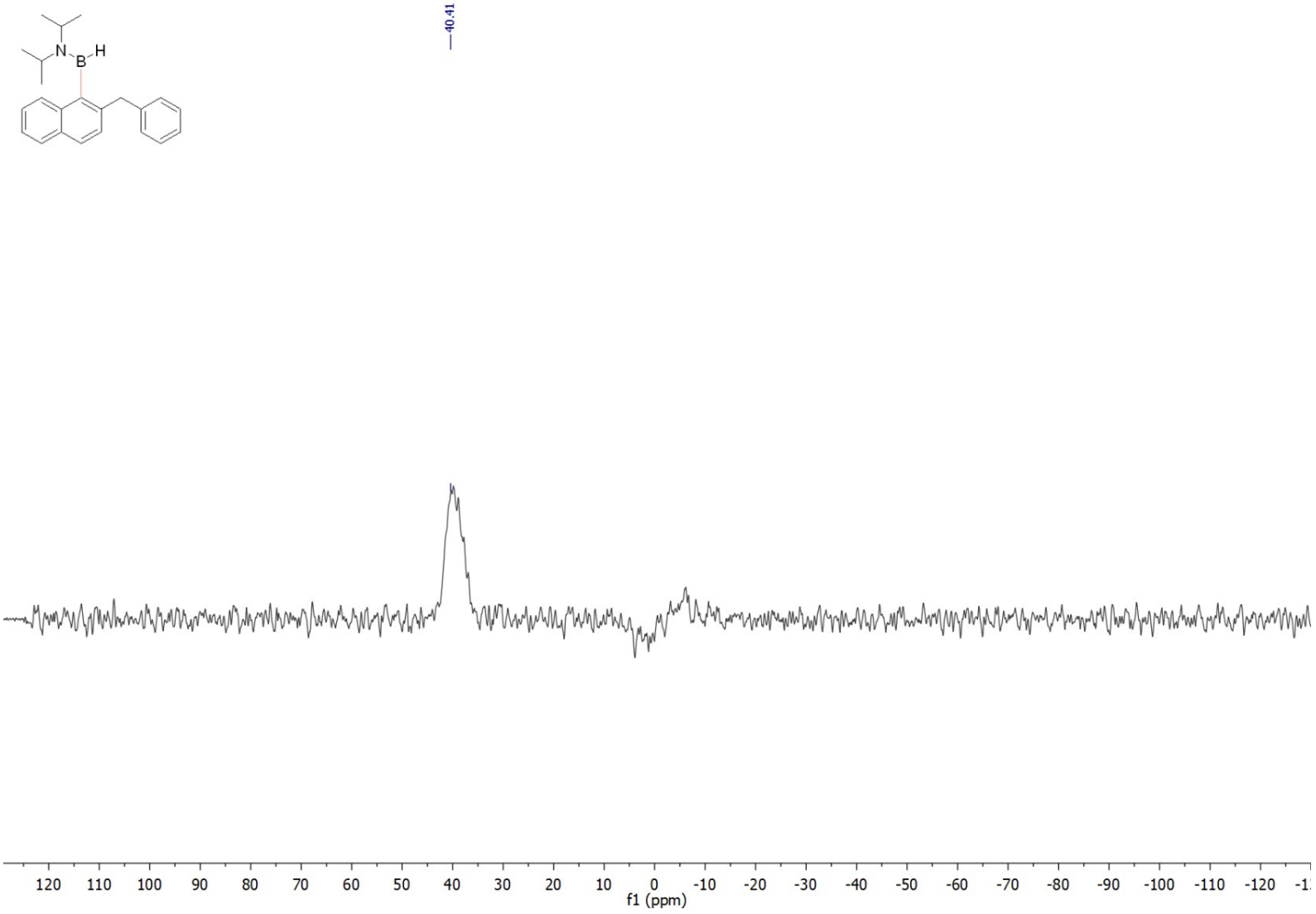
Compound (10b) VTNMR in Acetone-d_6 based on ^{1}H NMR at 25°C and -70°C (600 MHz) – *No apparent coalescence*



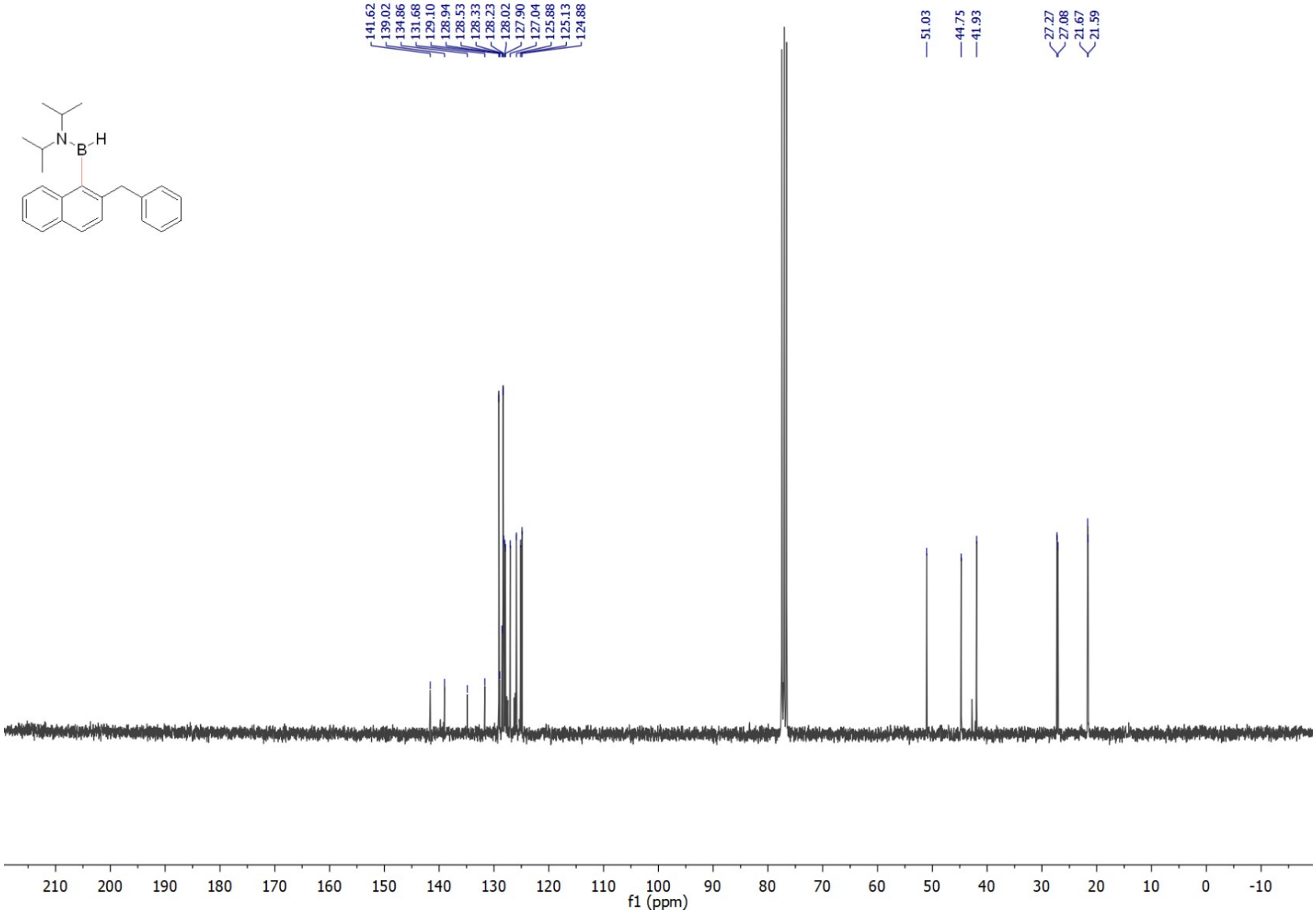
Compound (10c) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



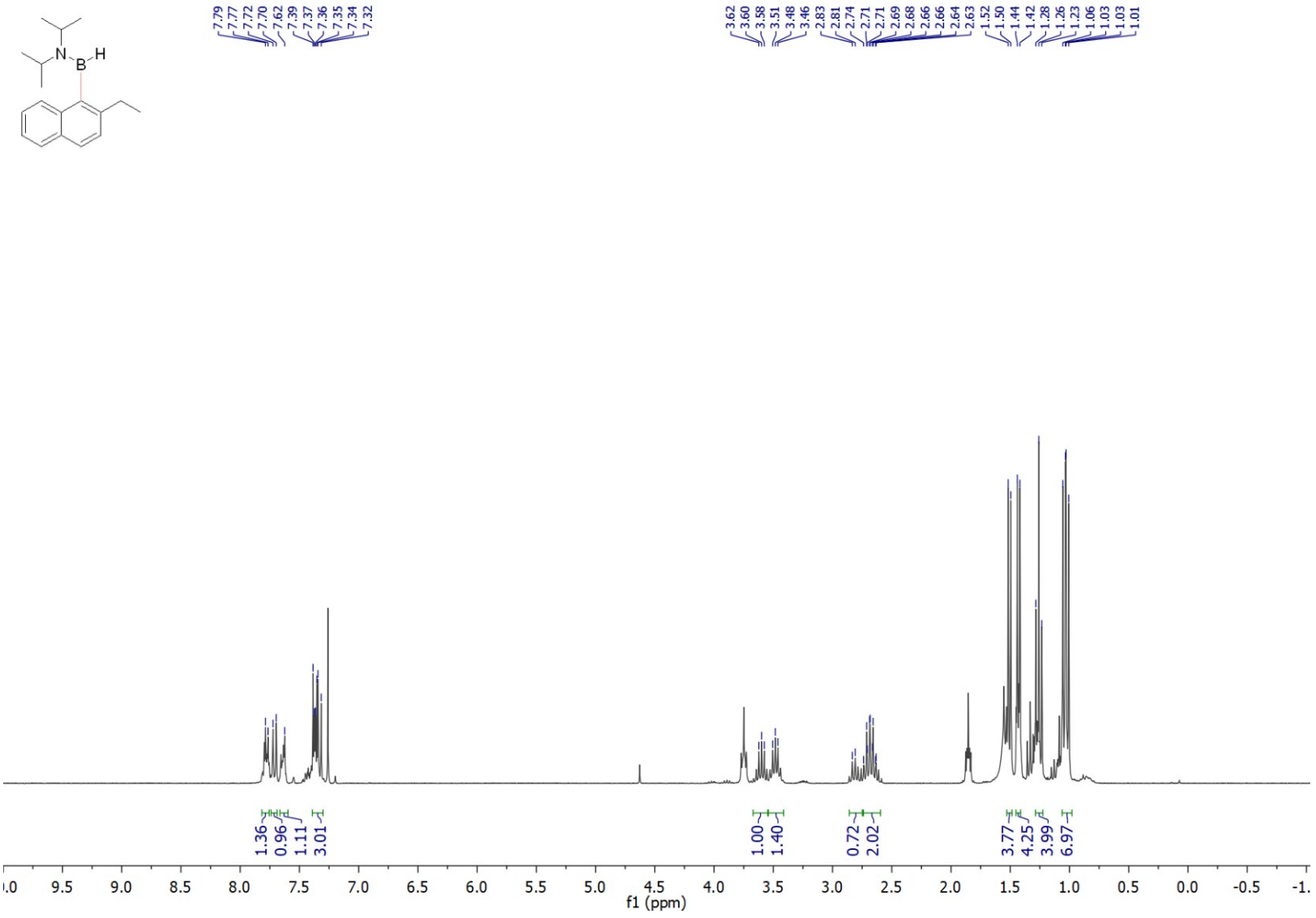
Compound (10c) ^{11}B NMR in $CDCl_3$ at 25°C (196 MHz)



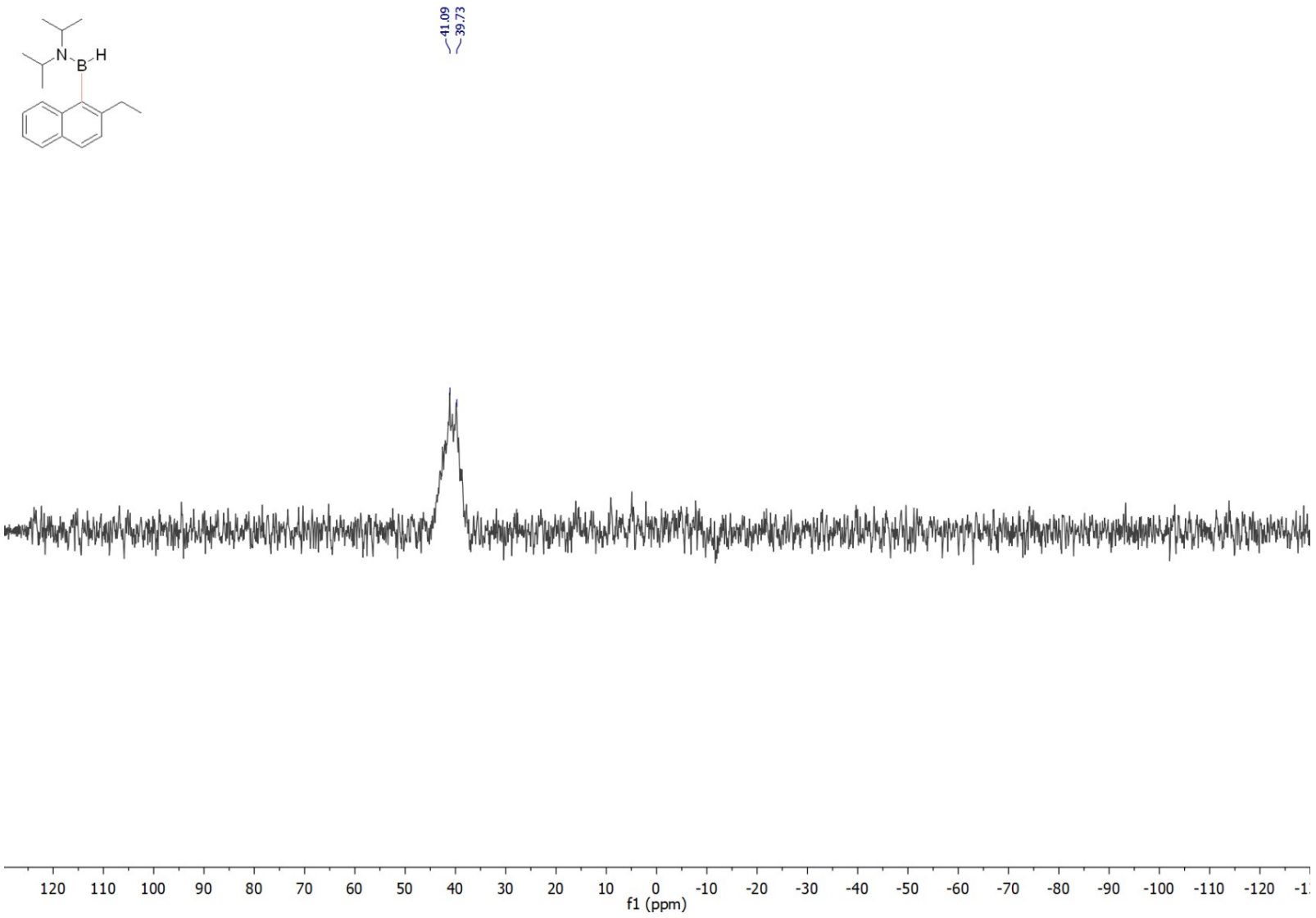
Compound (10c) ^{13}C NMR in $CDCl_3$ at 25°C (75 MHz)



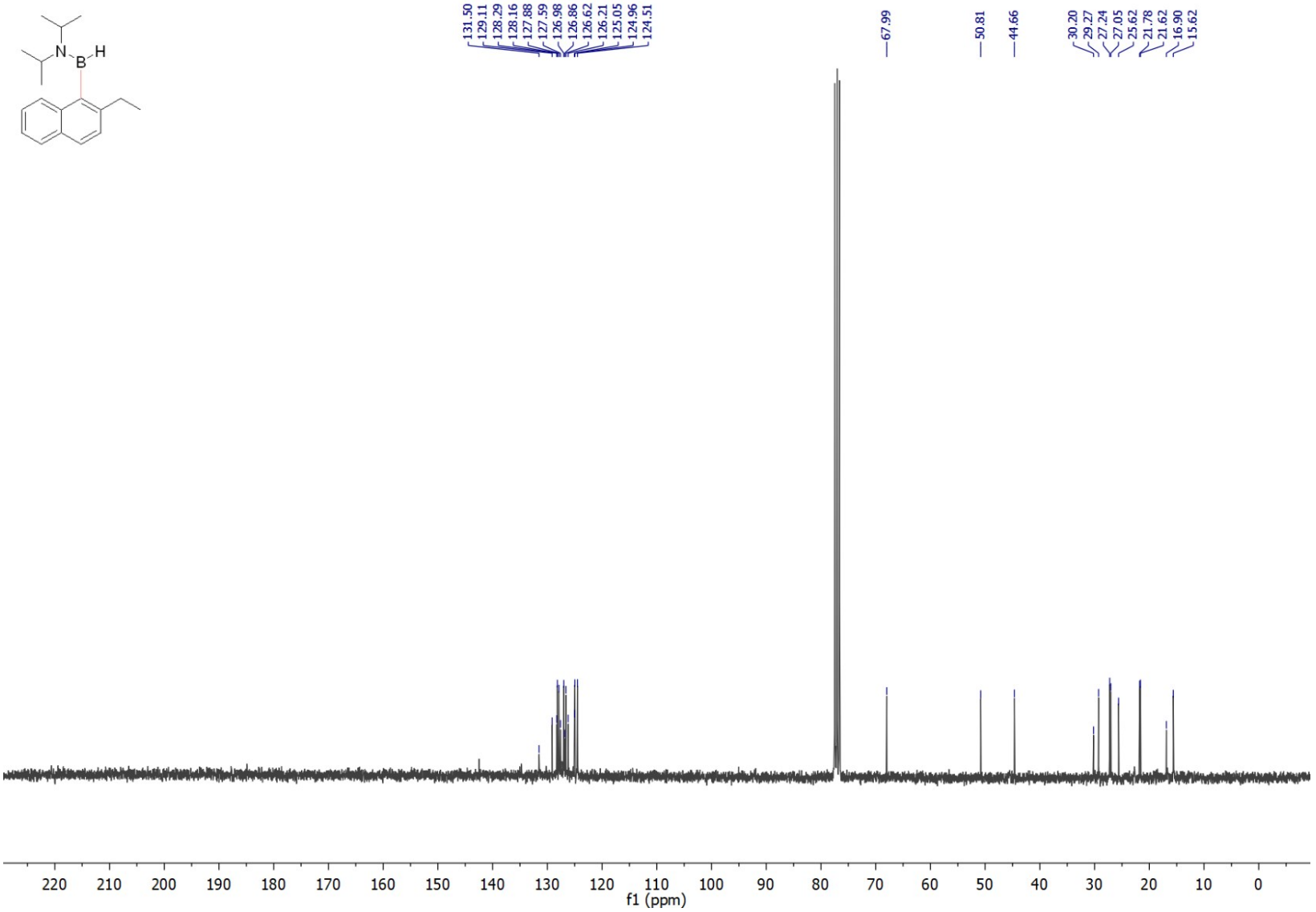
Compound (10d) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



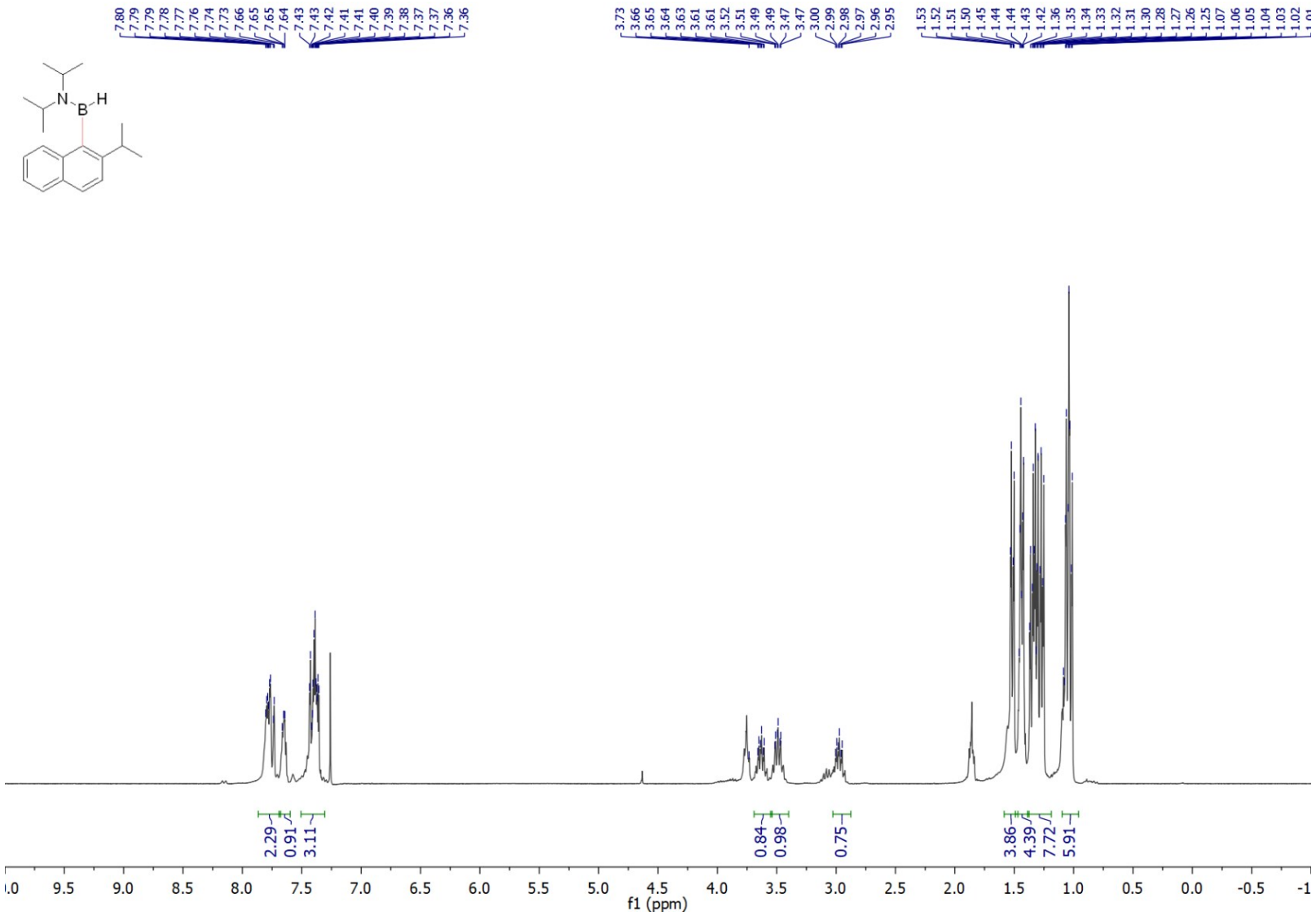
Compound (10d) ^{11}B NMR in $CDCl_3$ at 25°C (196 MHz)



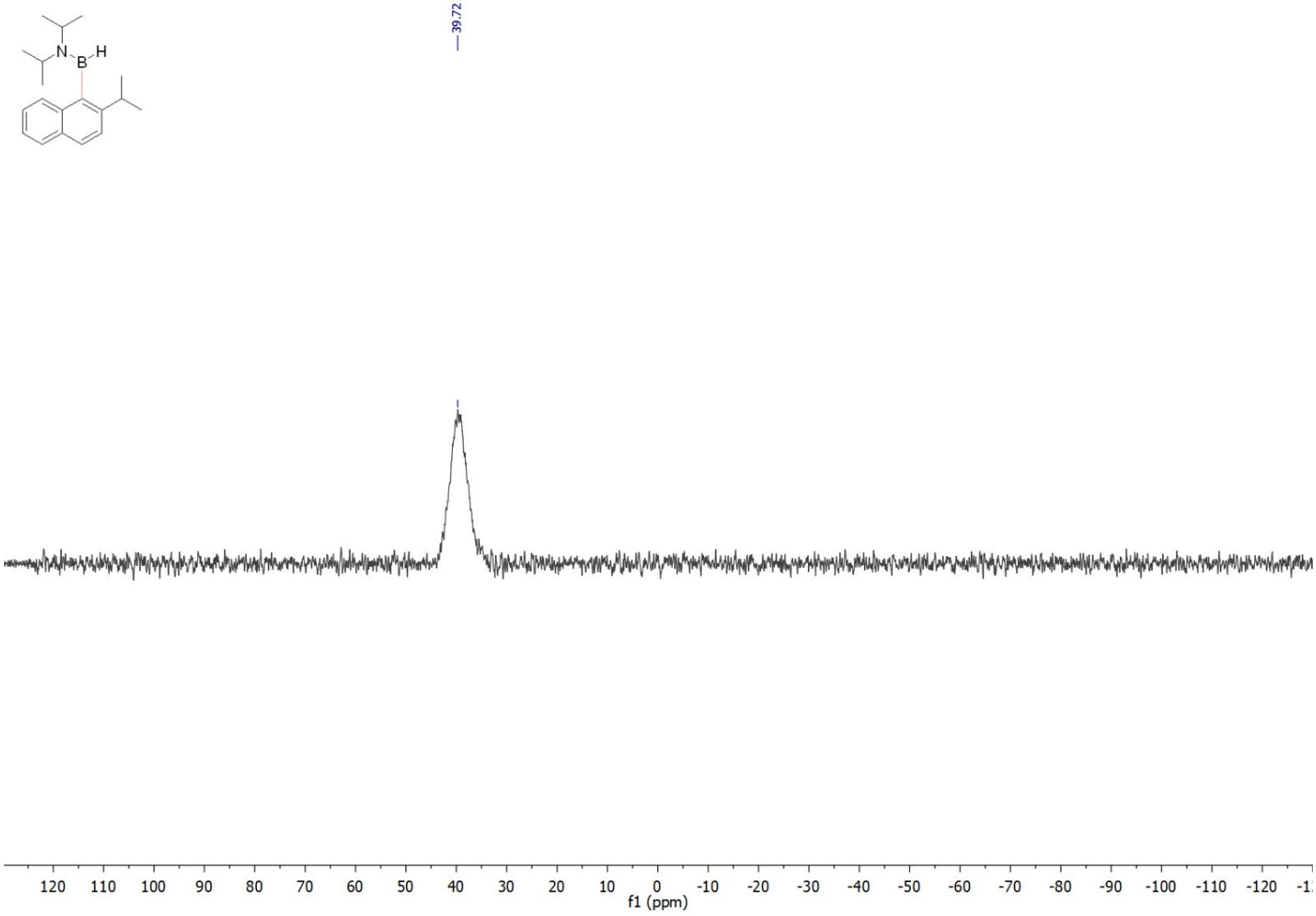
Compound (10d) ^{13}C NMR in $CDCl_3$ at 25°C (75 MHz)



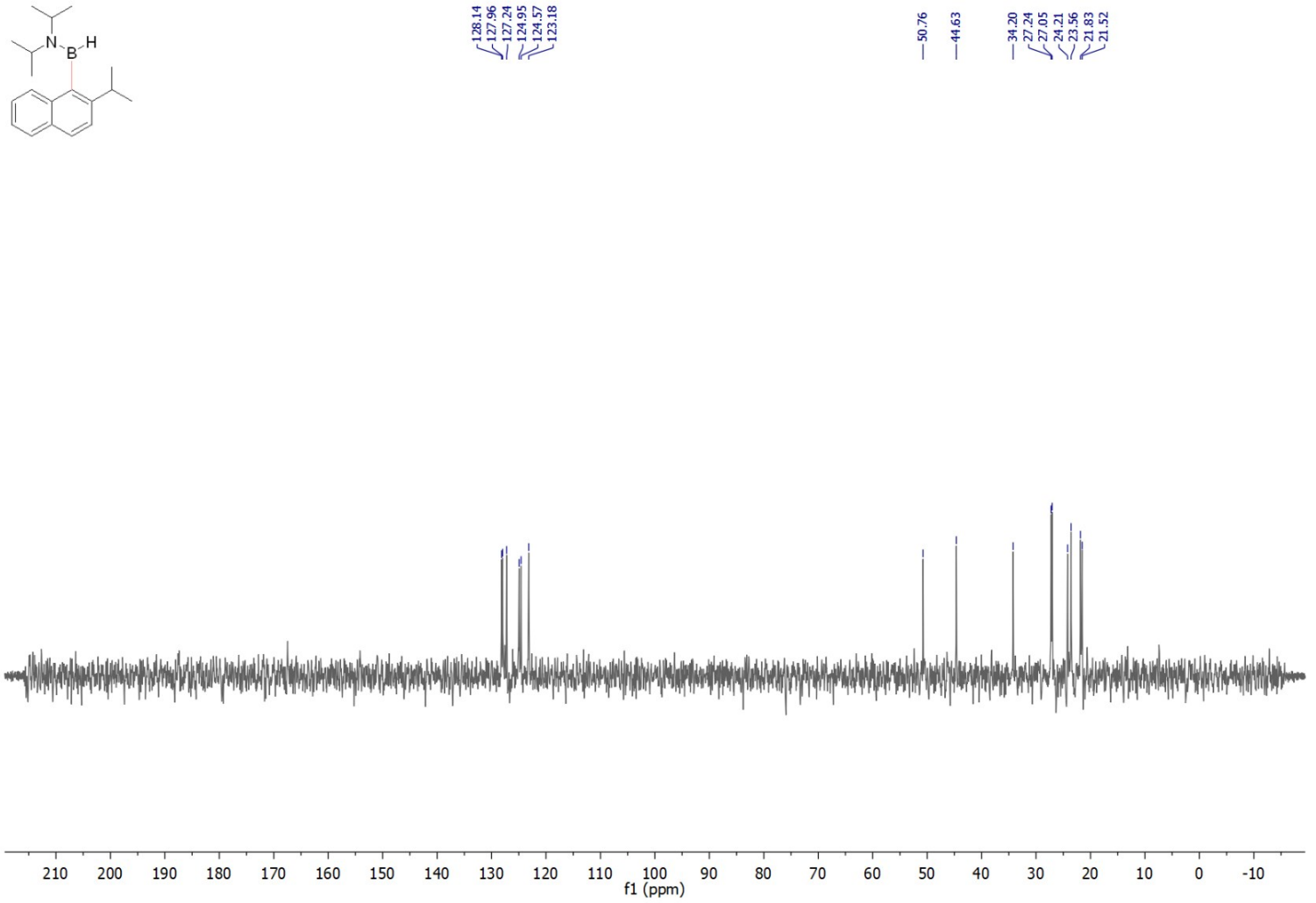
Compound (10e) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



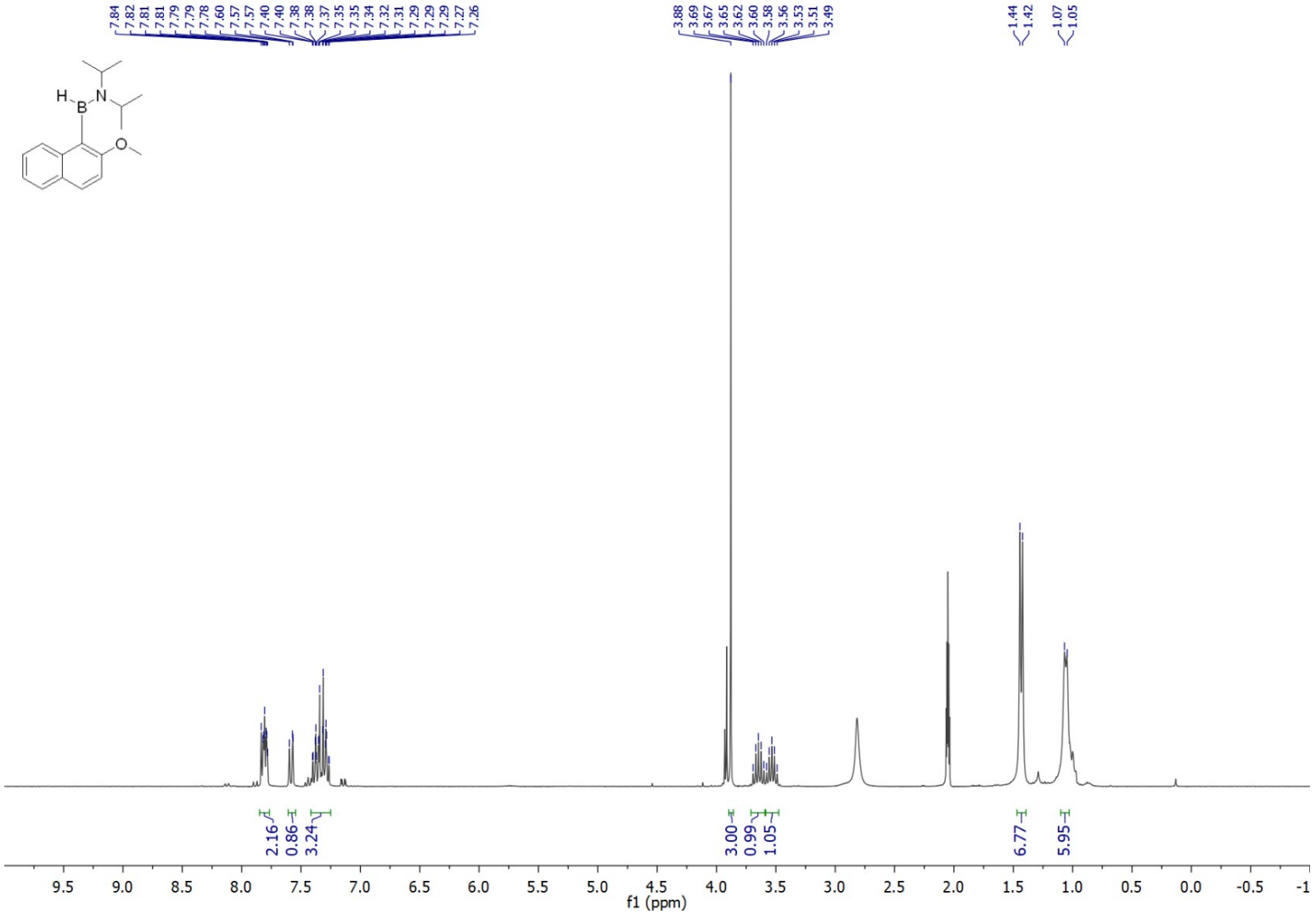
Compound (10e) ^{11}B NMR in $CDCl_3$ at 25°C (196 MHz)



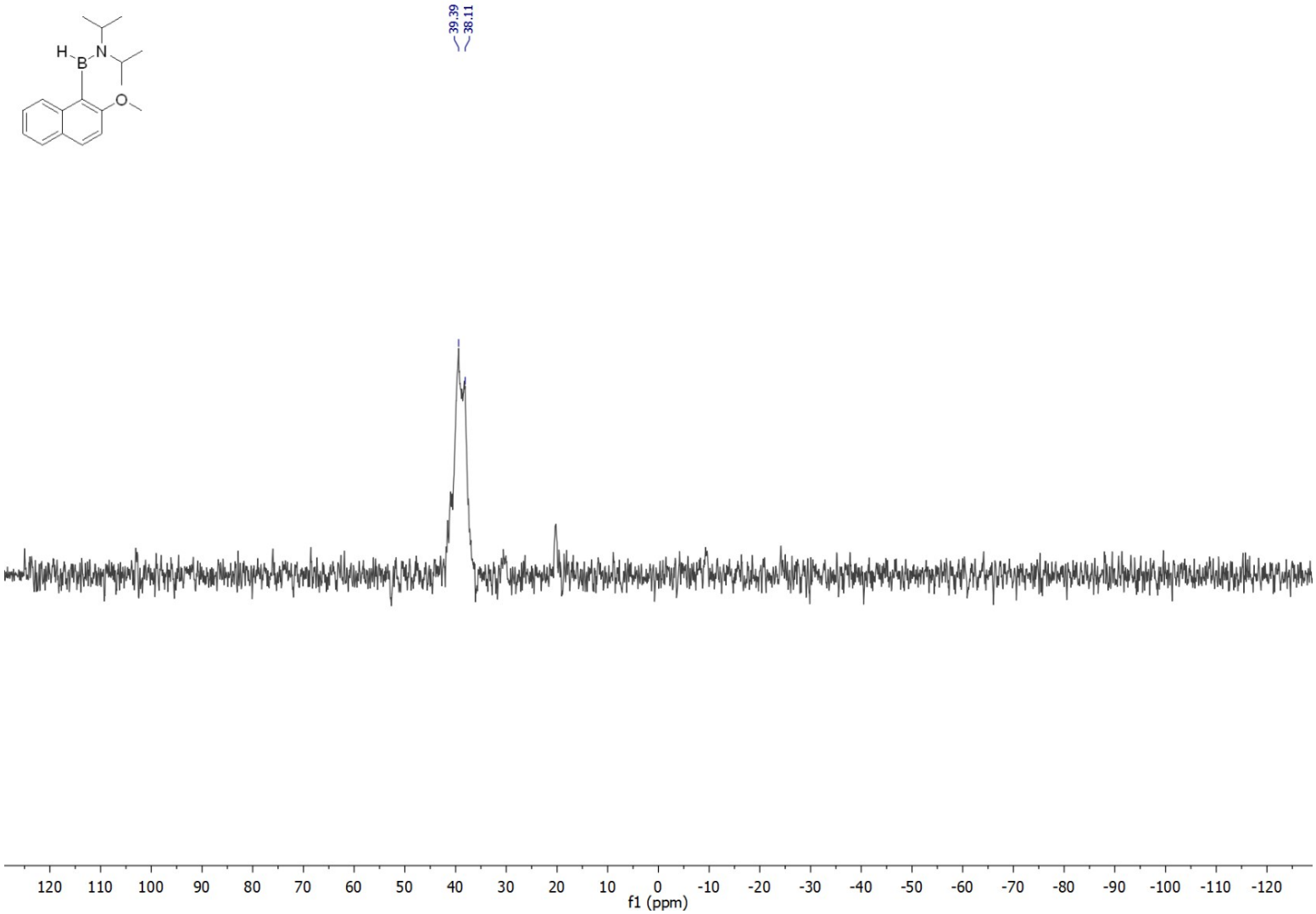
Compound (10e) ^{13}C NMR in $CDCl_3$ at 25°C (75 MHz)



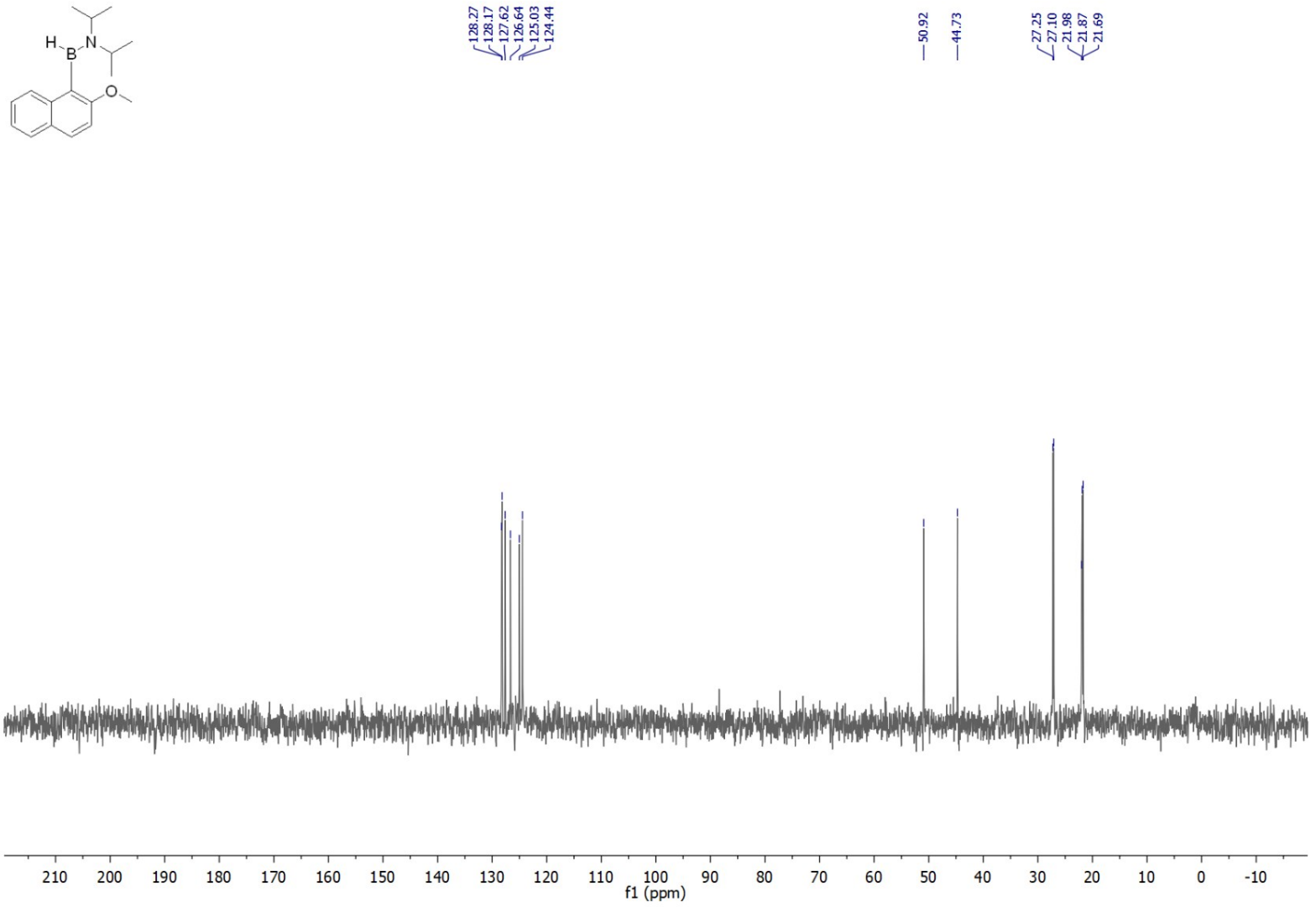
Compound (10f) ^{1}H NMR in Acetone-d_6 at 25°C (300 MHz)



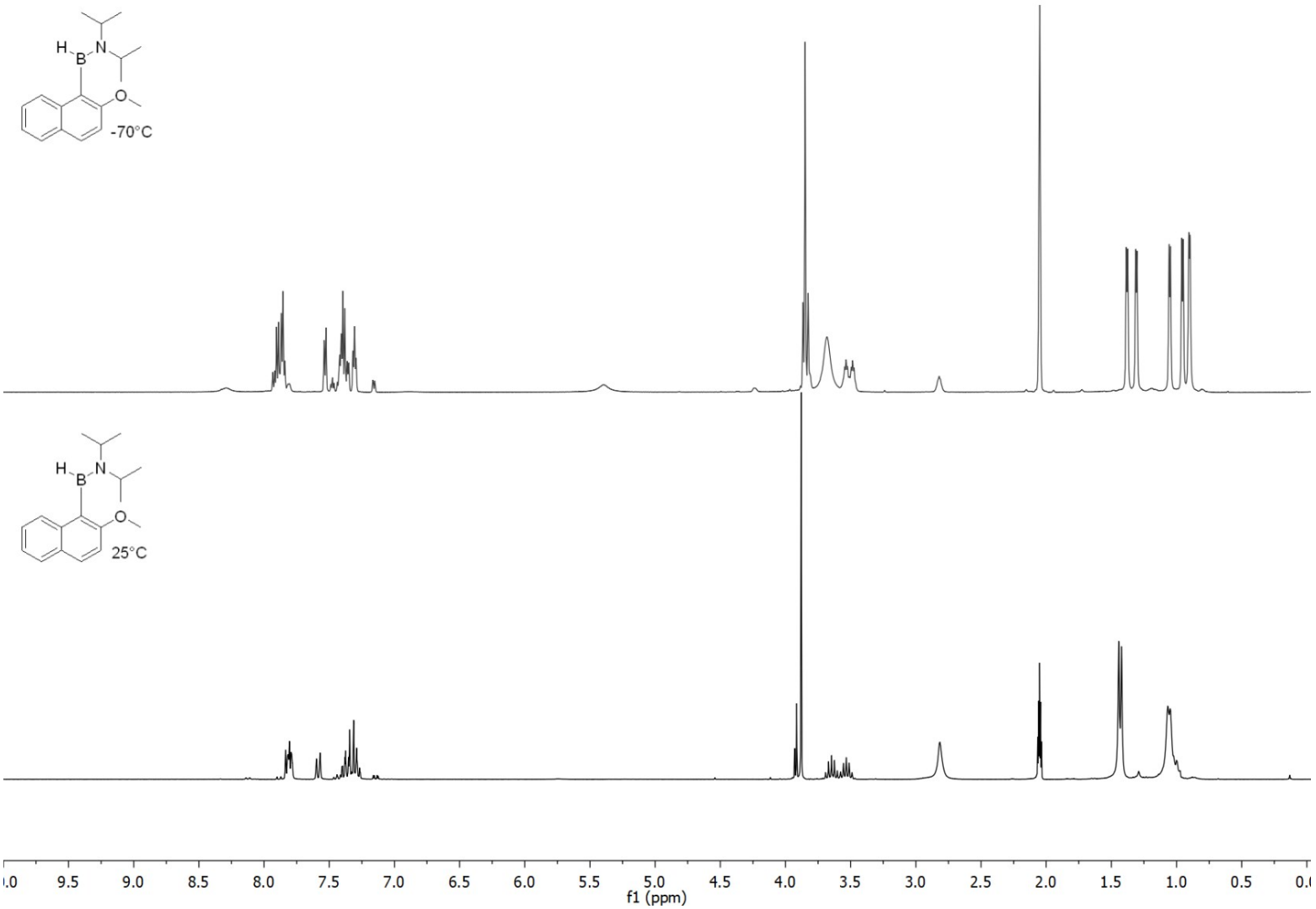
Compound (10f) ^{11}B NMR in Acetone-d_6 at 25°C (196 MHz)



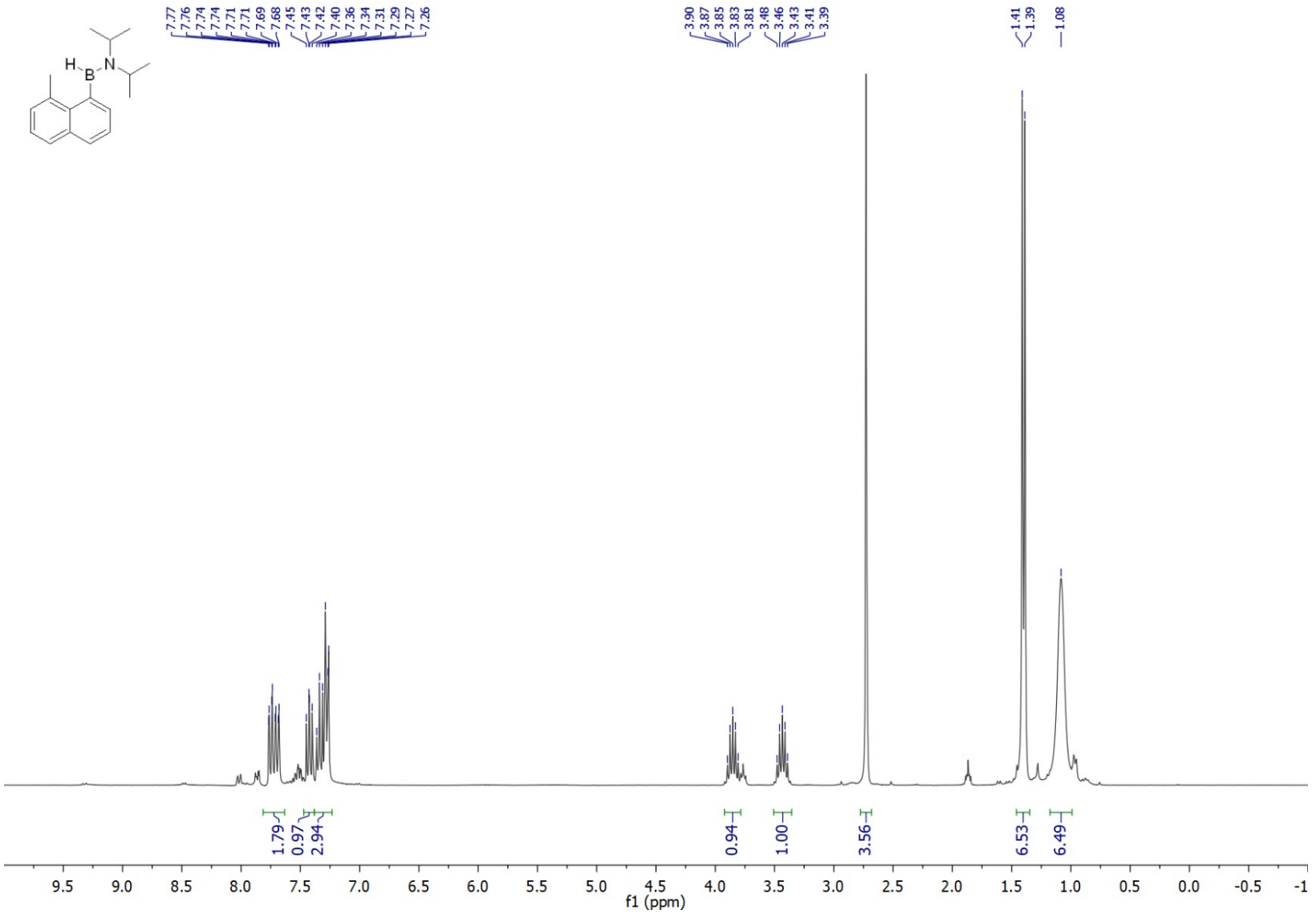
Compound (10f) ^{13}C NMR in C_6D_6 at 25°C (75 MHz)



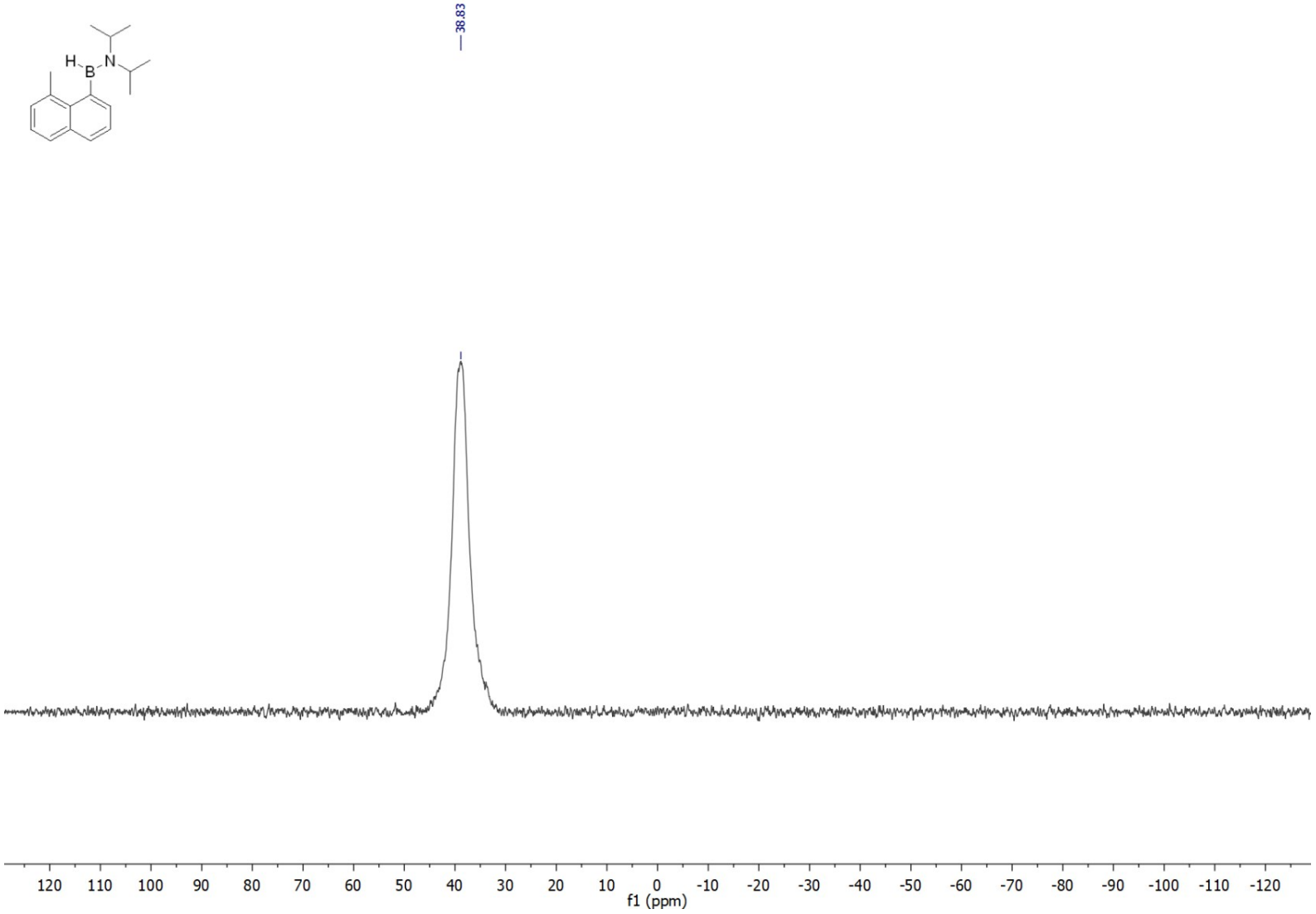
Compound (10f) VTNMR in Acetone-d_6 based on ^{1}H NMR at 25°C and -70°C (600 MHz) – *Coalescence observed*



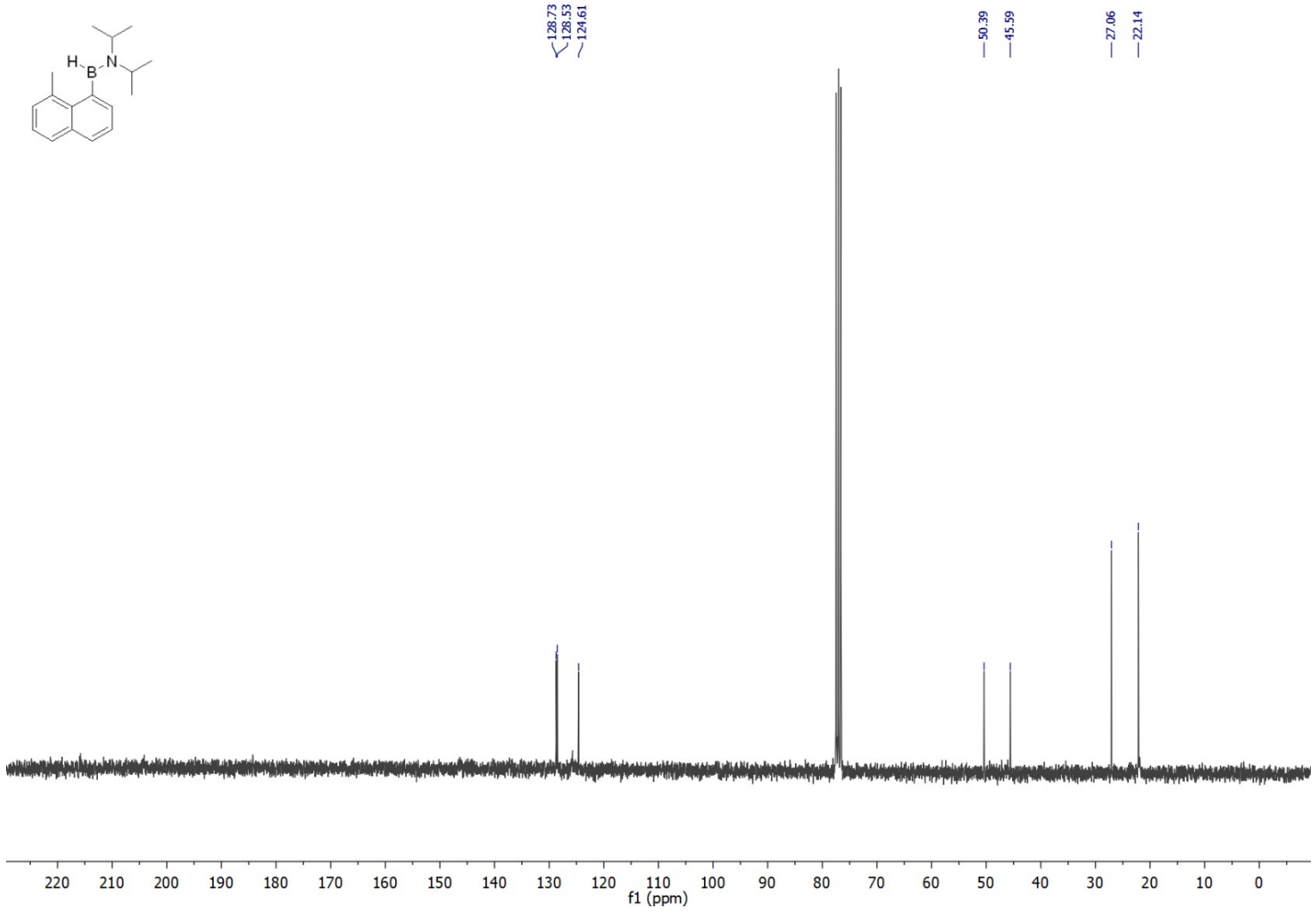
Compound (10g) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



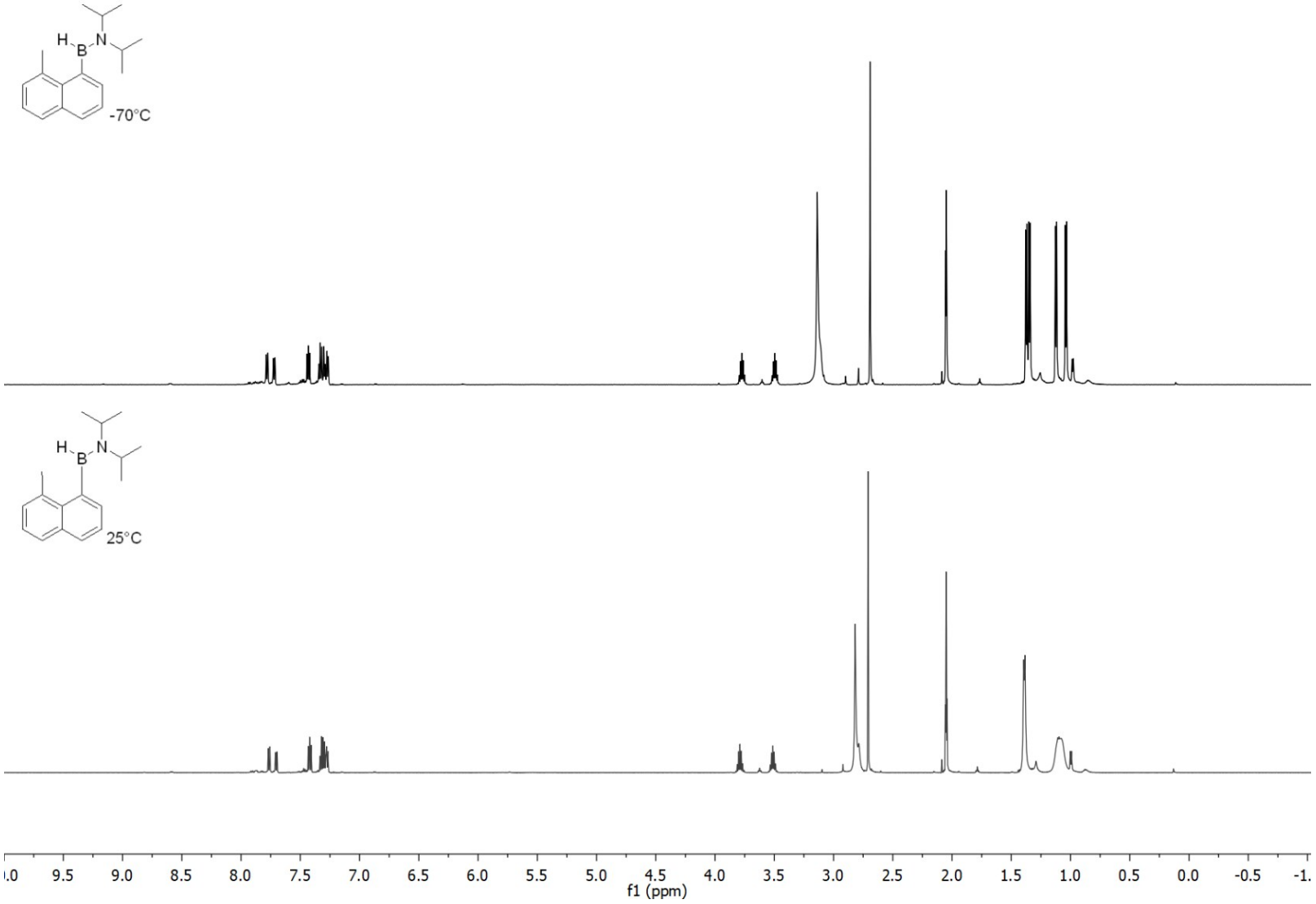
Compound (10g) ^{11}B NMR in $CDCl_3$ at 25°C (196 MHz)



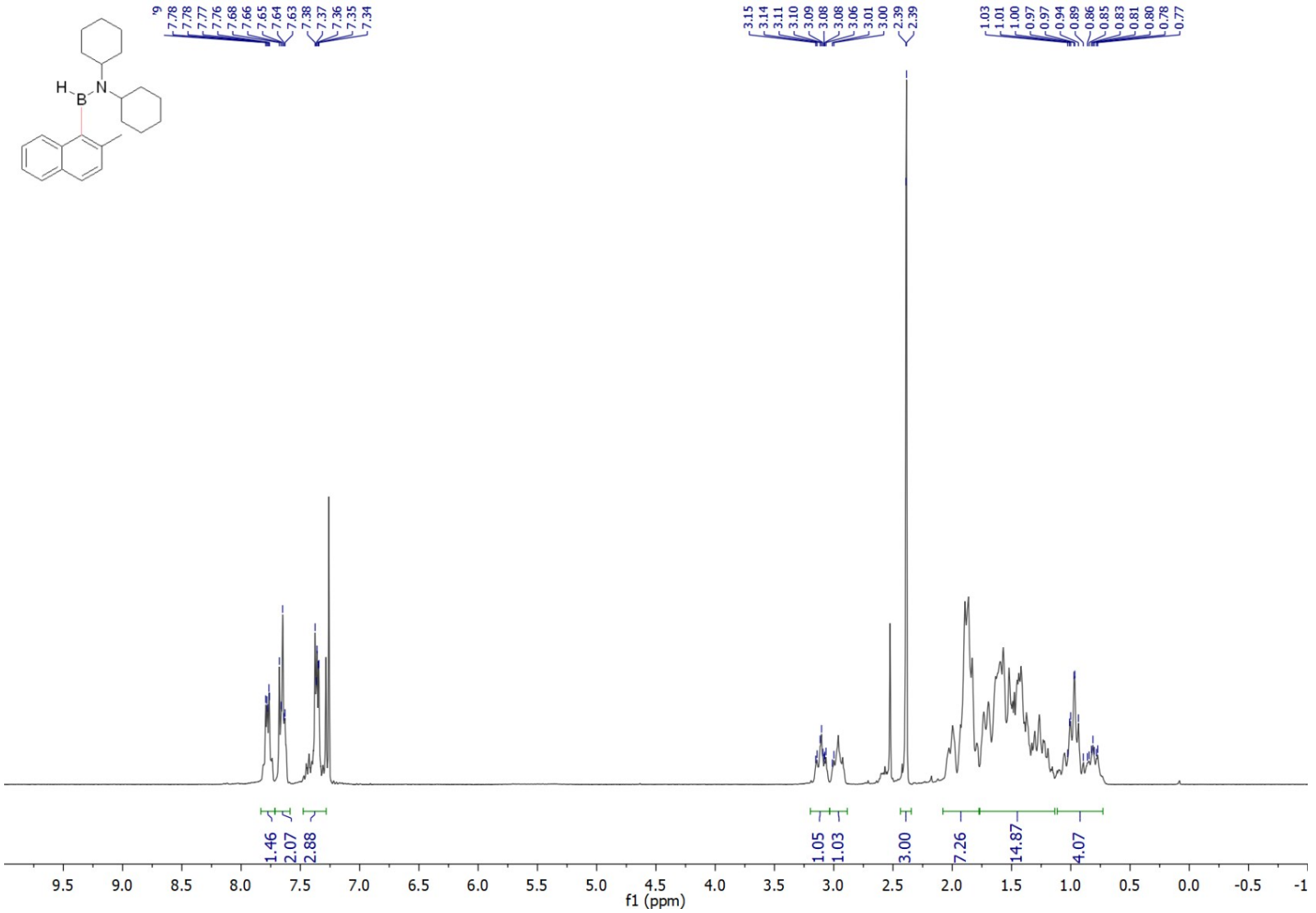
Compound (10g) ^{13}C NMR in $CDCl_3$ at 25°C (75 MHz)



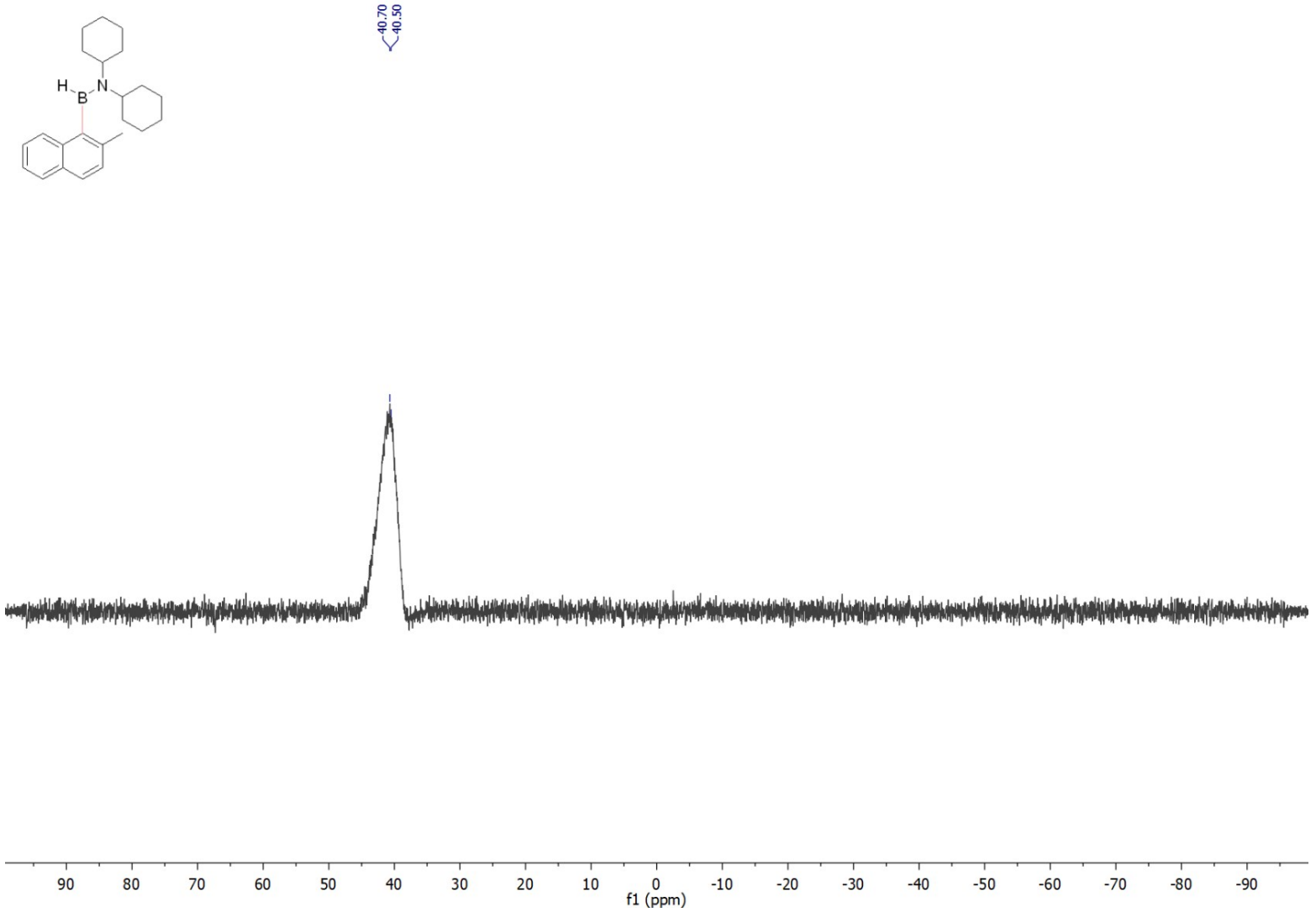
Compound (10g) VTNMR in Acetone-d_6 based on ^{1}H NMR at 25°C and -70°C (600 MHz) – *Coalescence observed*



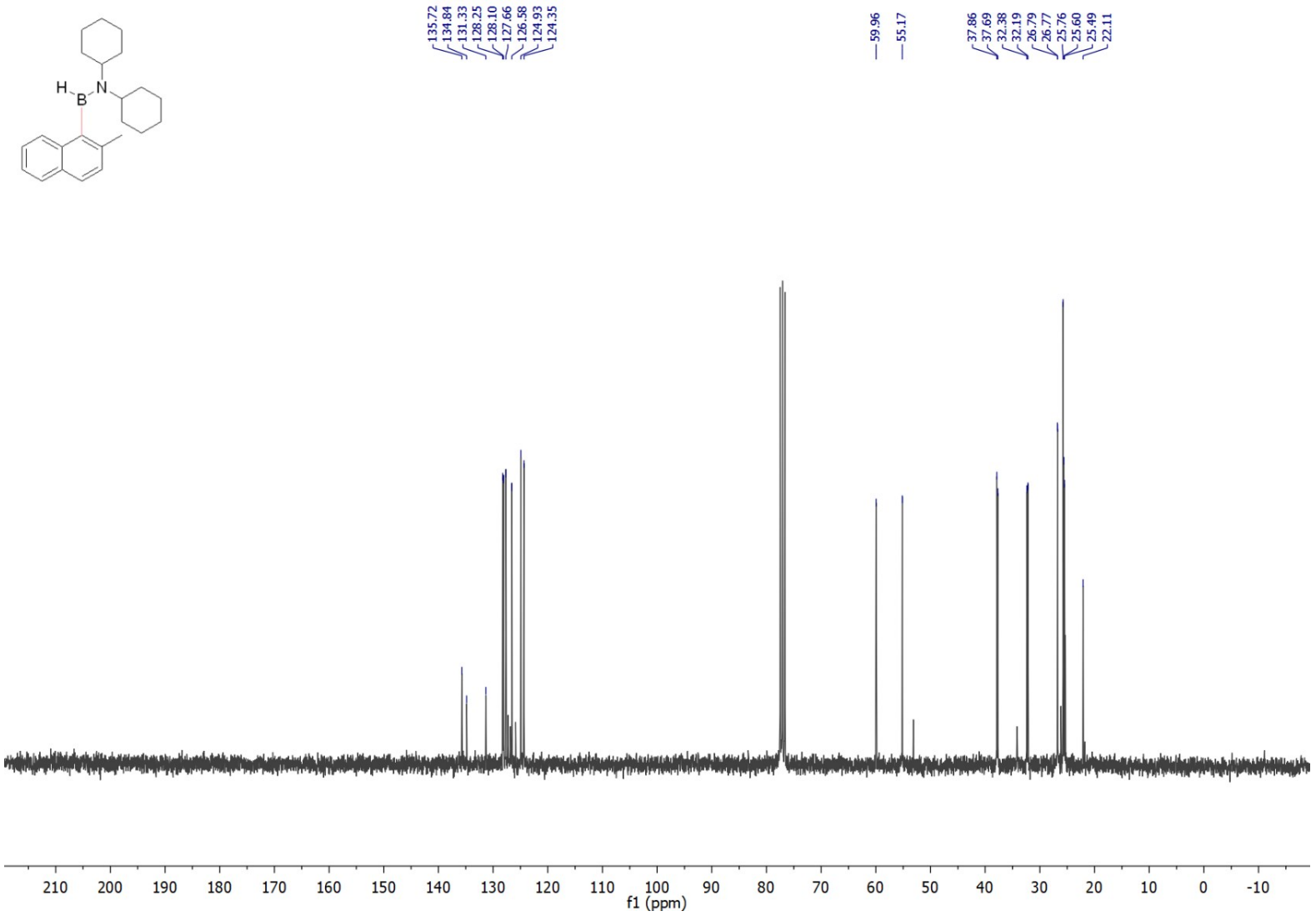
Compound (10h) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



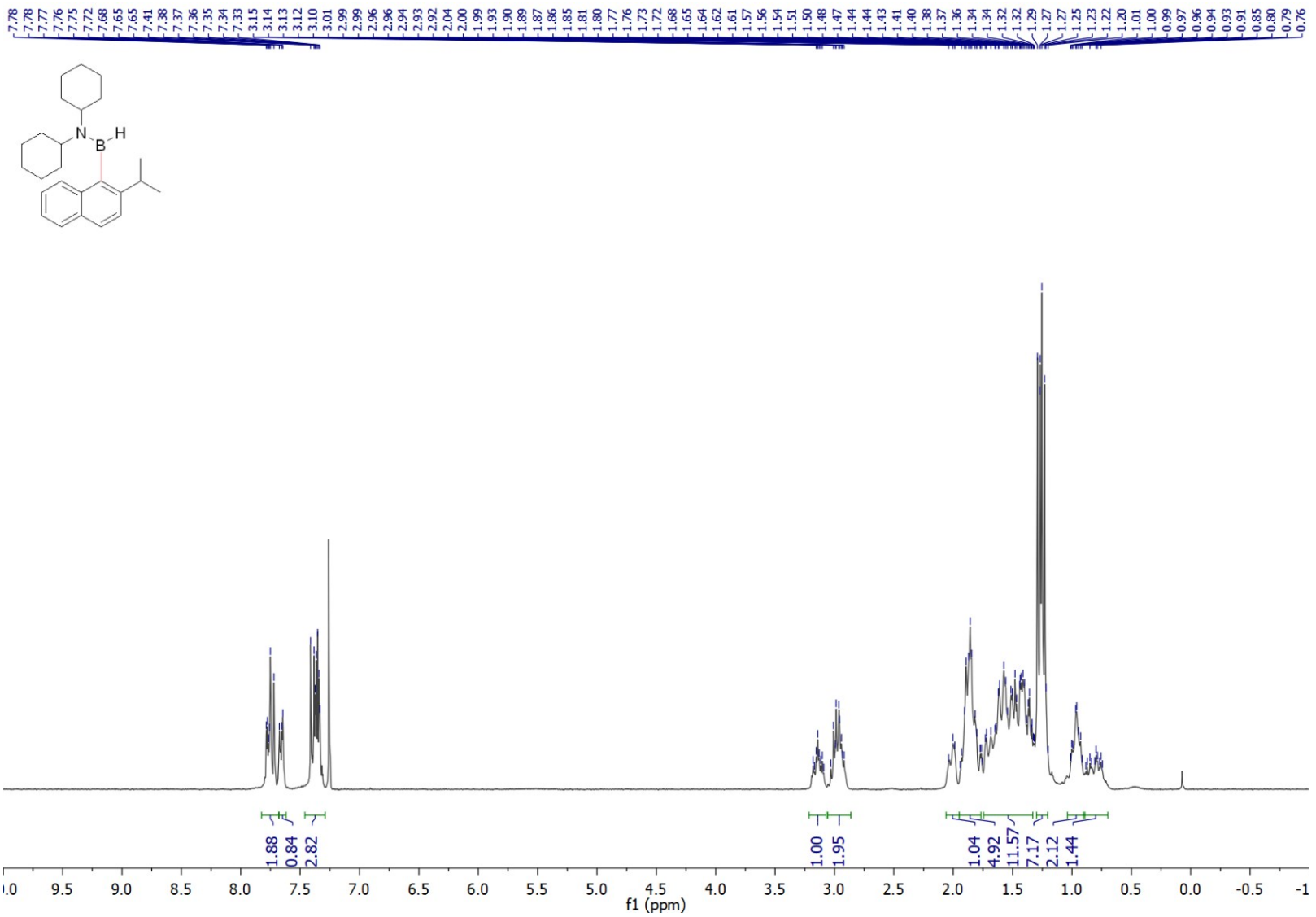
Compound (10h) ^{11}B NMR in $CDCl_3$ at 25°C (196 MHz)



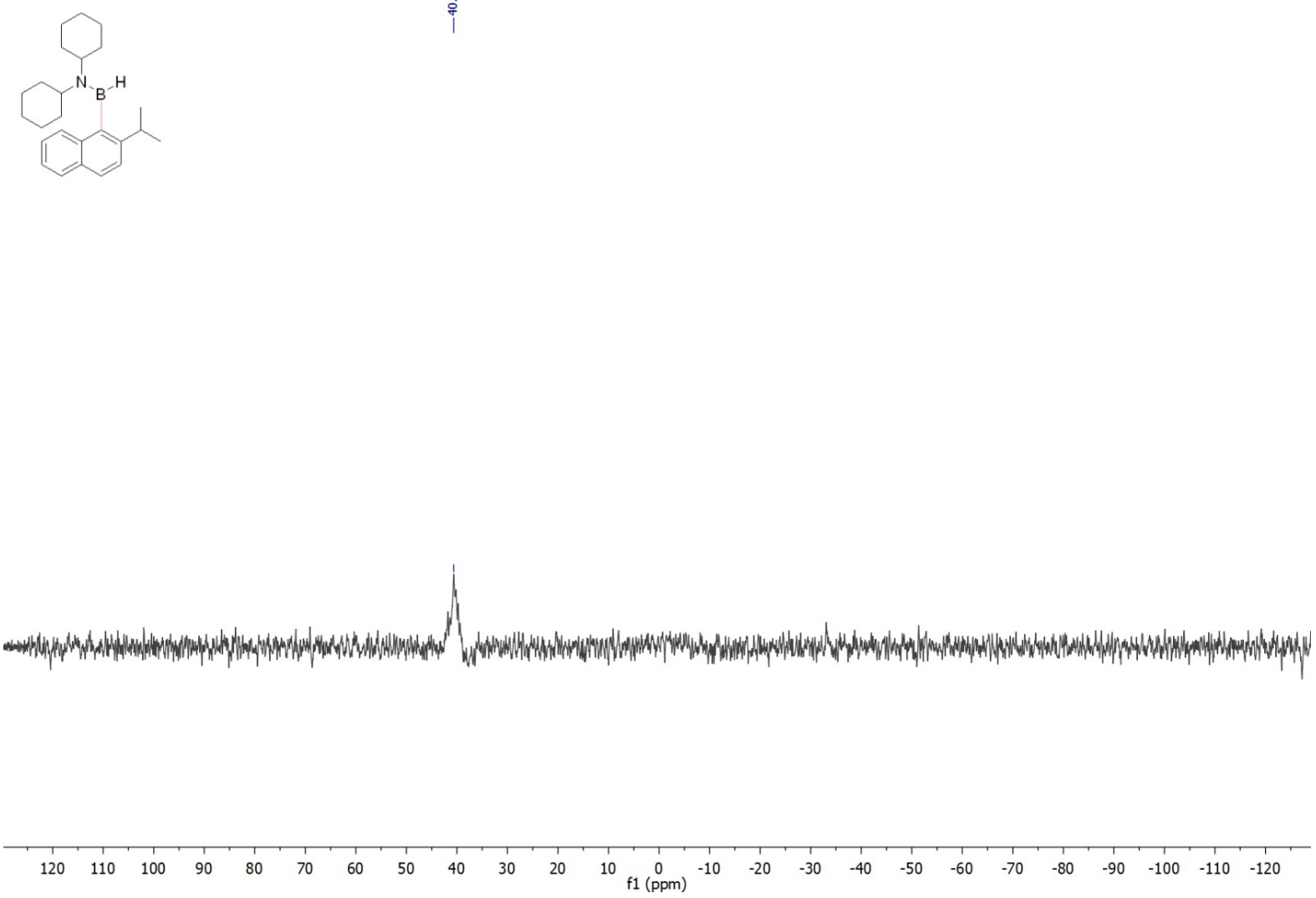
Compound (10h) ^{13}C NMR in $CDCl_3$ at 25°C (75 MHz)



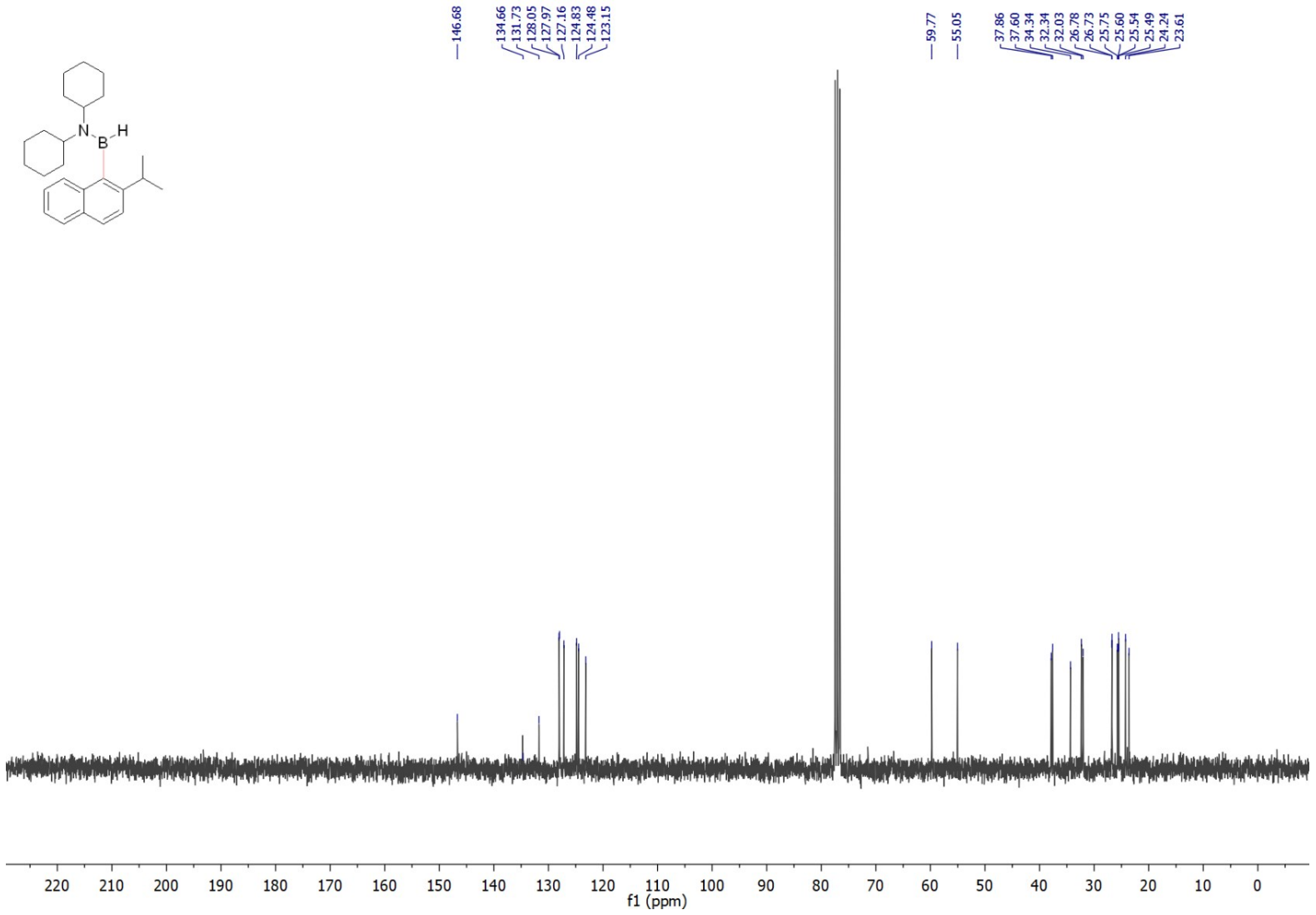
Compound (10i) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



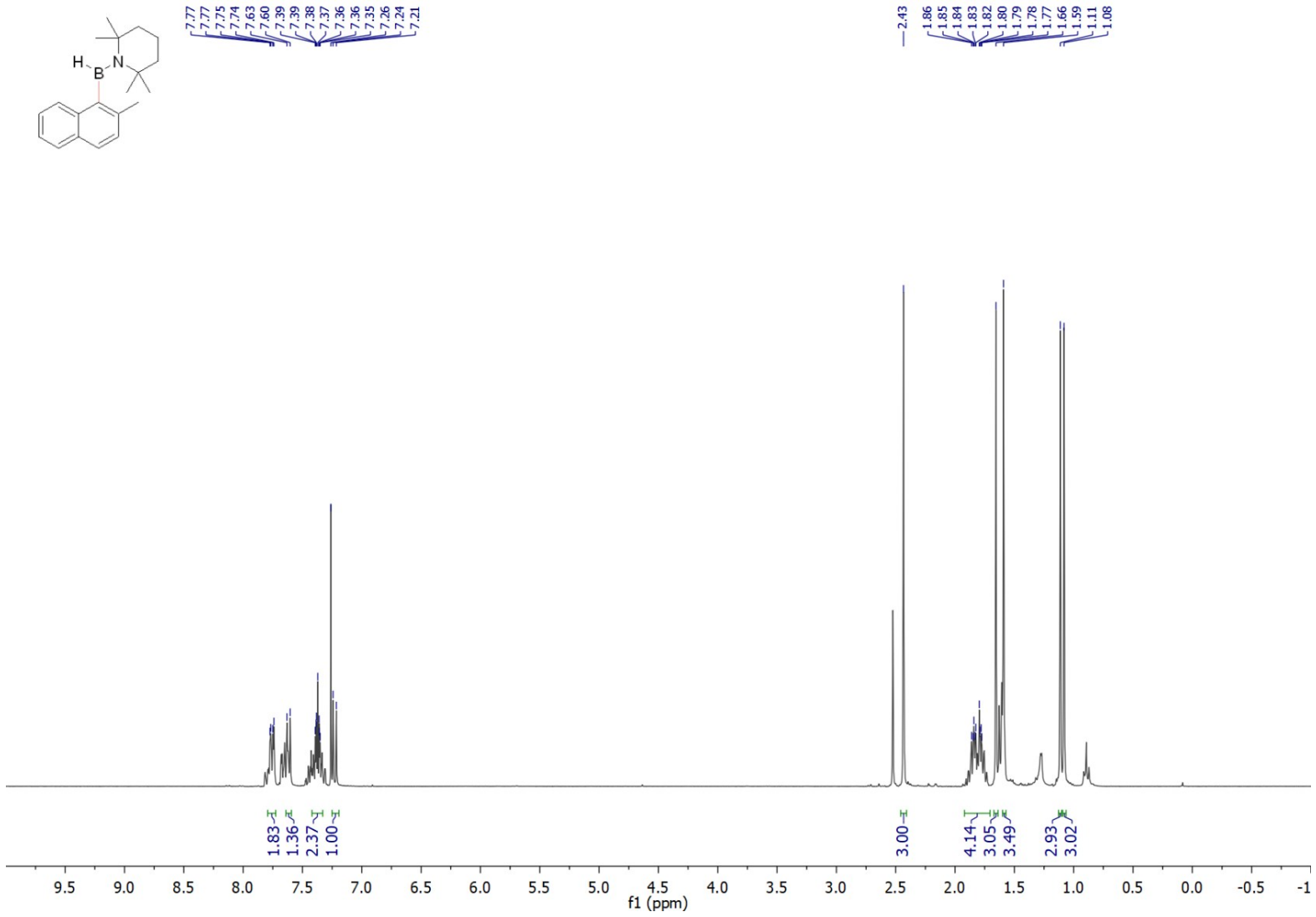
Compound (10i) ^{11}B NMR in C_6D_6 at 25°C (196 MHz)



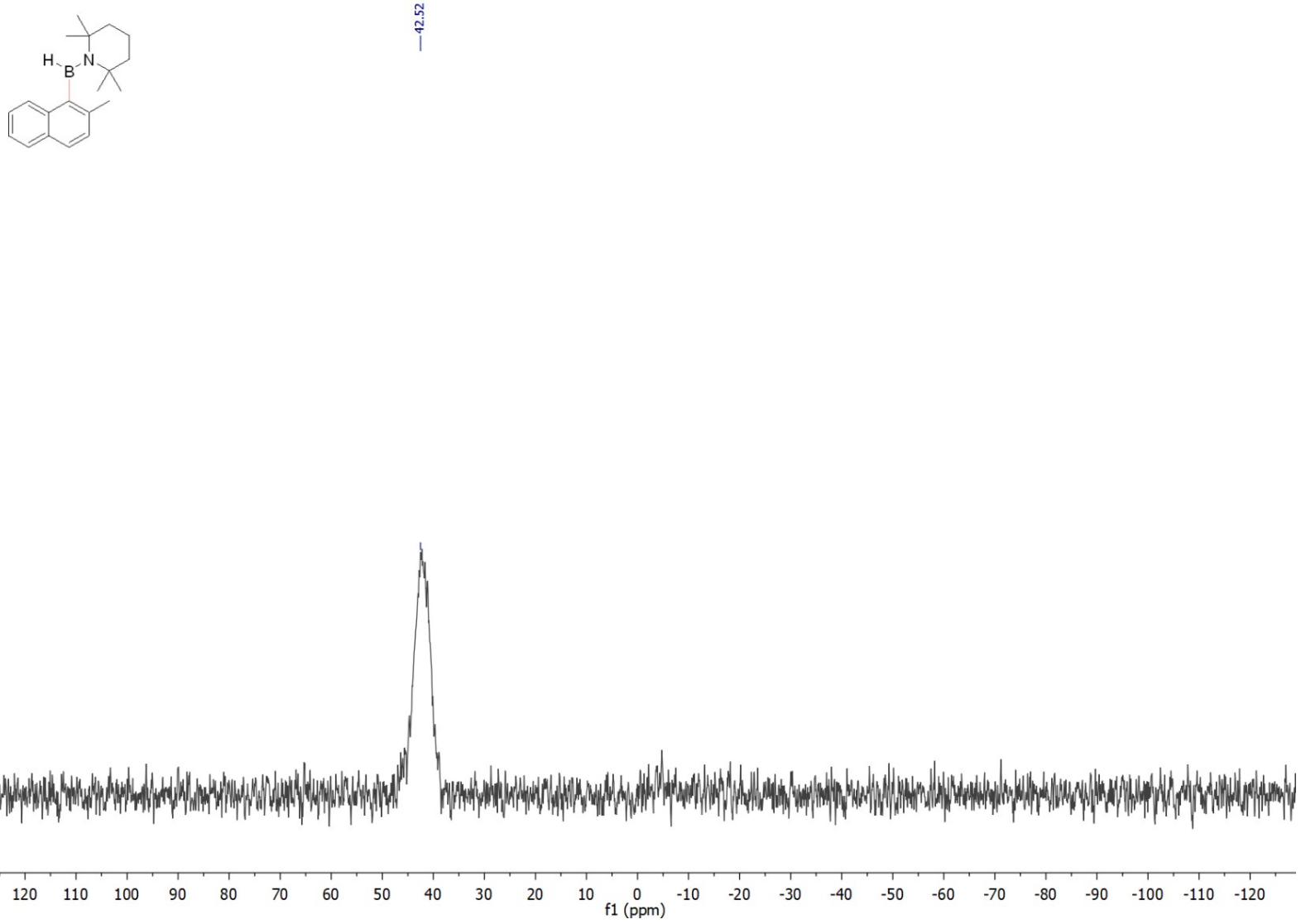
Compound (10i) ^{13}C NMR in $CDCl_3$ at 25°C (75 MHz)



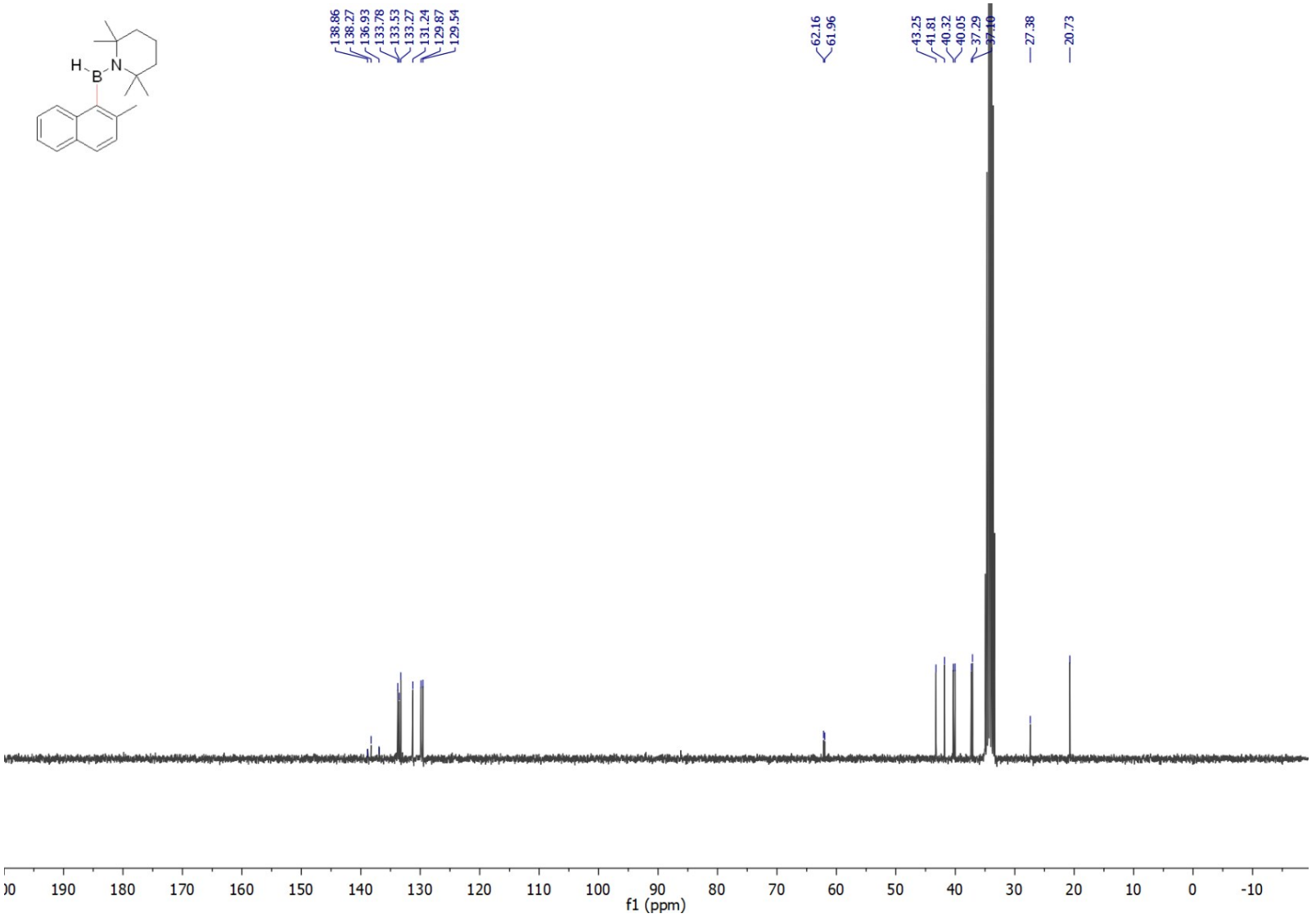
Compound (10j) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



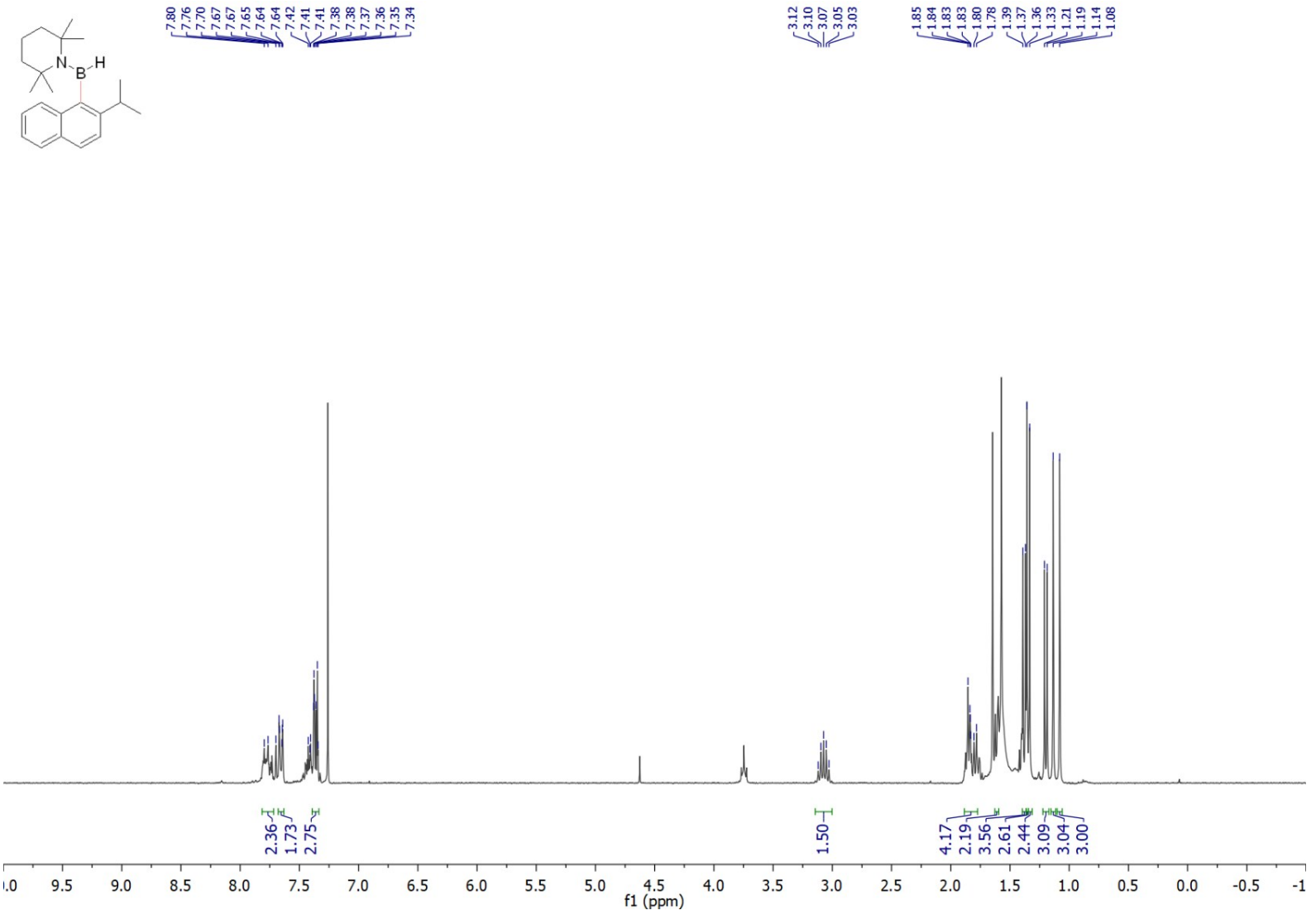
Compound (10j) ^{11}B NMR in $CDCl_3$ at 25°C (196 MHz)



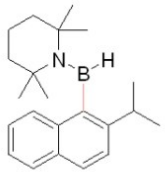
Compound (10j) ^{13}C NMR in C_6D_6 at 25°C (75 MHz)



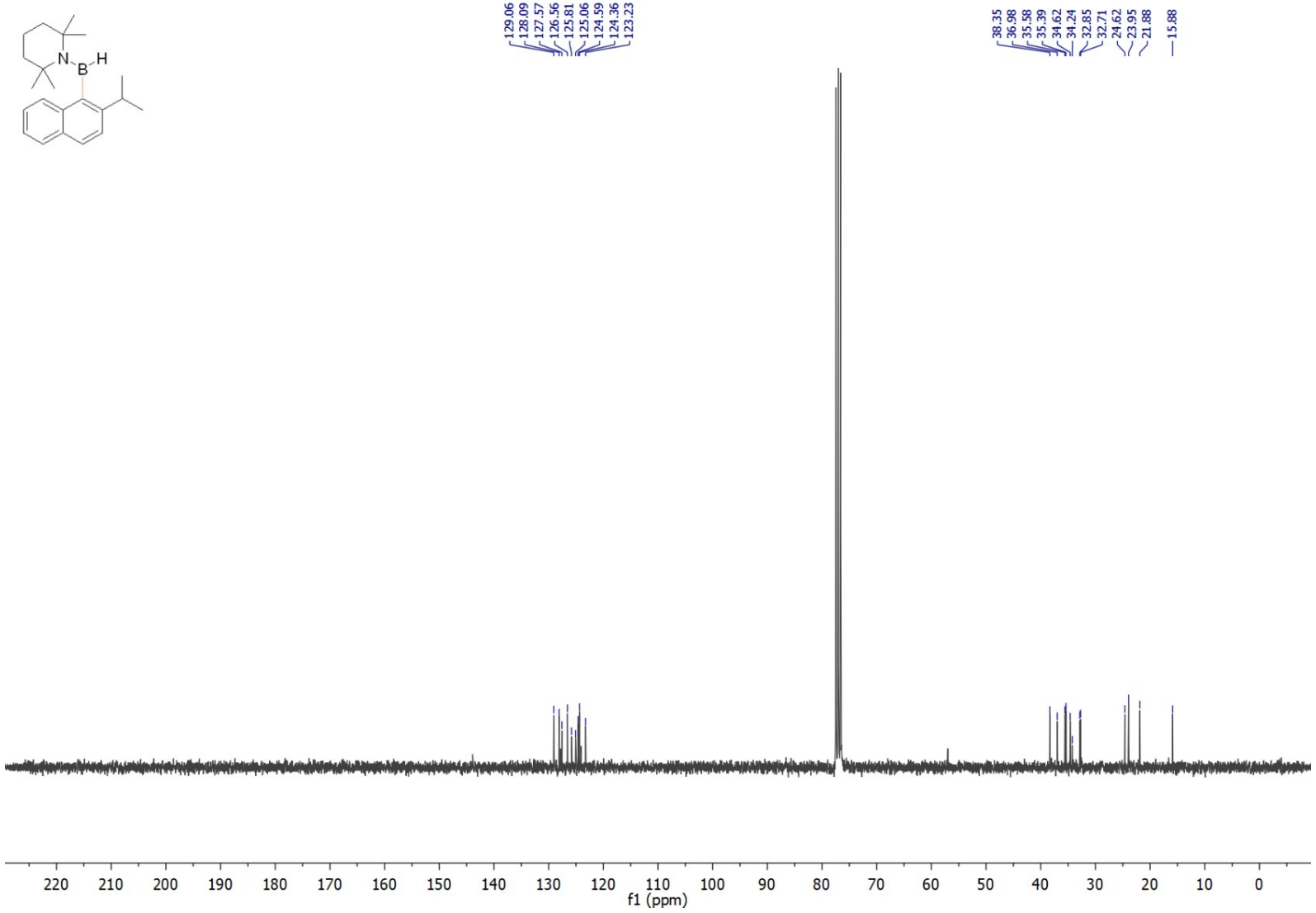
Compound (10k) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



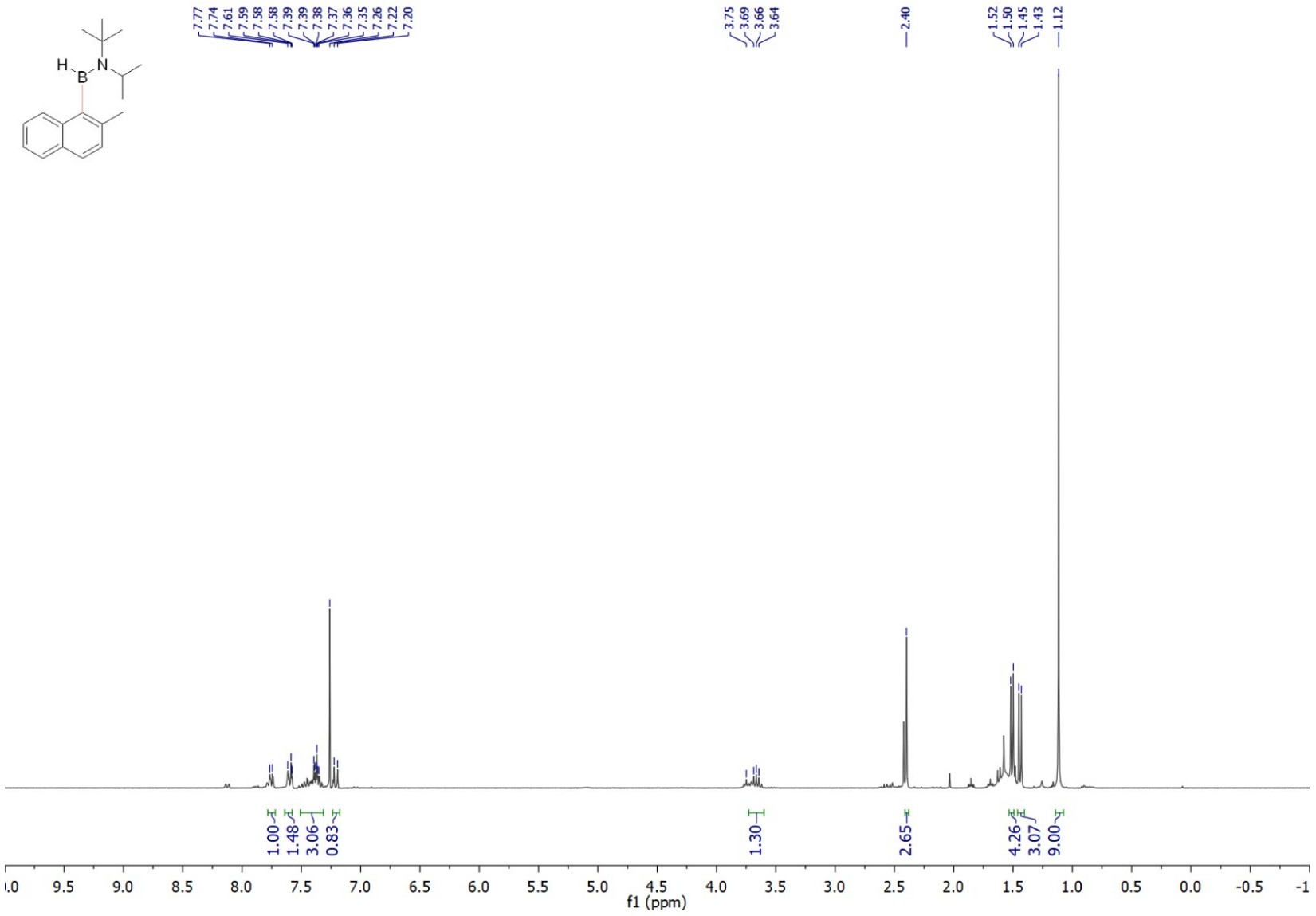
Compound (10k) ^{11}B NMR in $CDCl_3$ at 25°C (196 MHz)



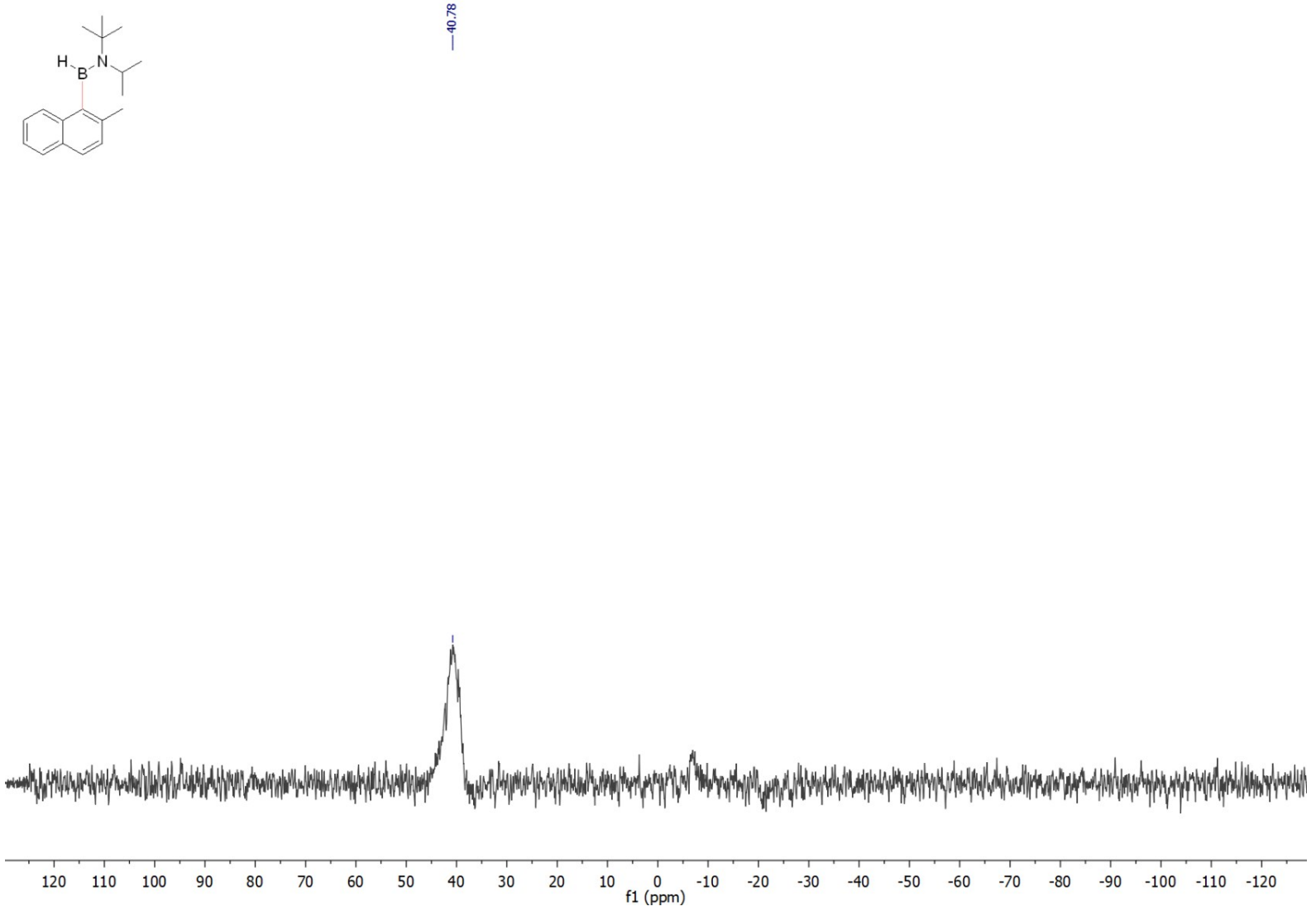
Compound (10k) ^{13}C NMR in $CDCl_3$ at 25°C (75 MHz)



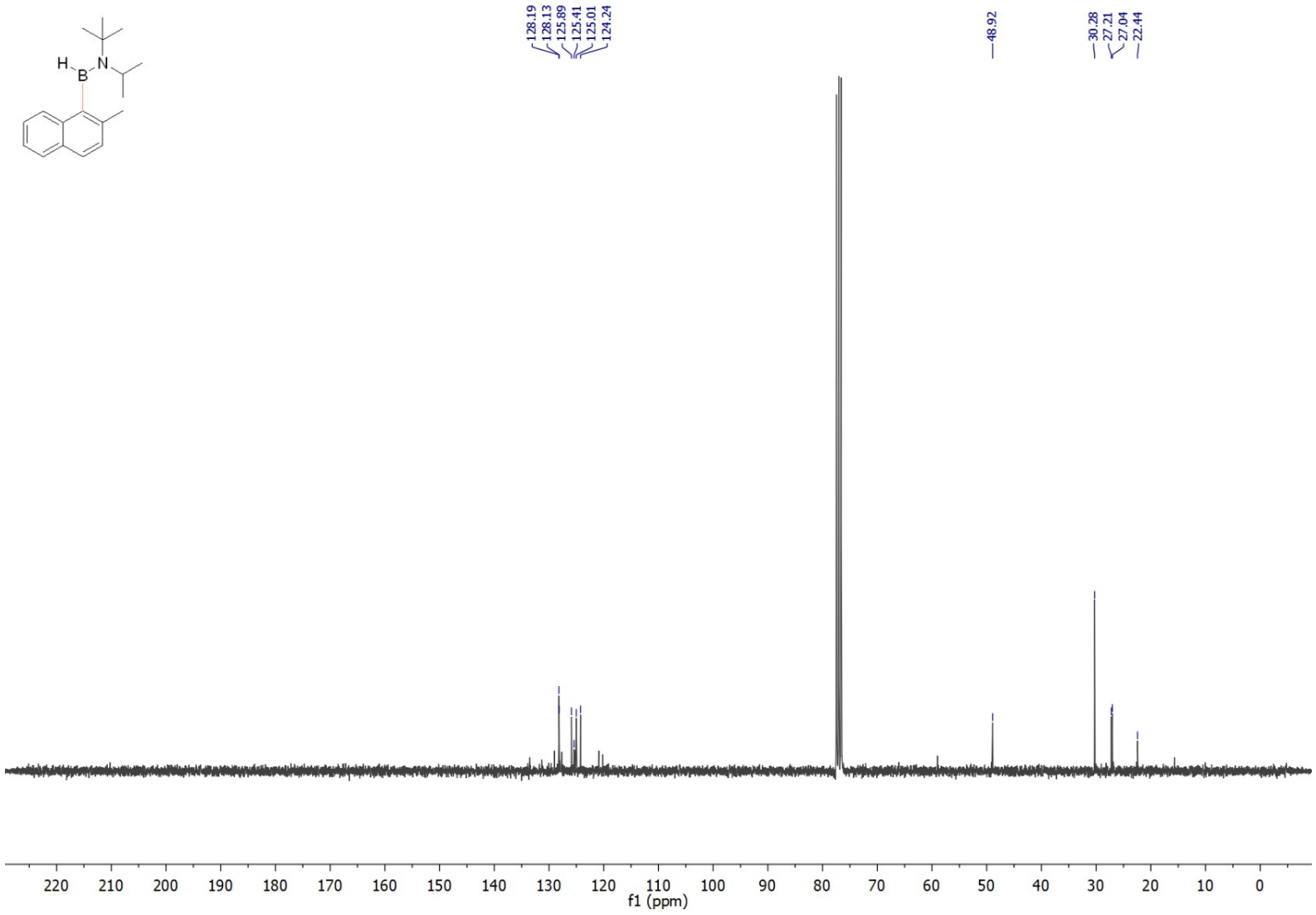
Compound (10l) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



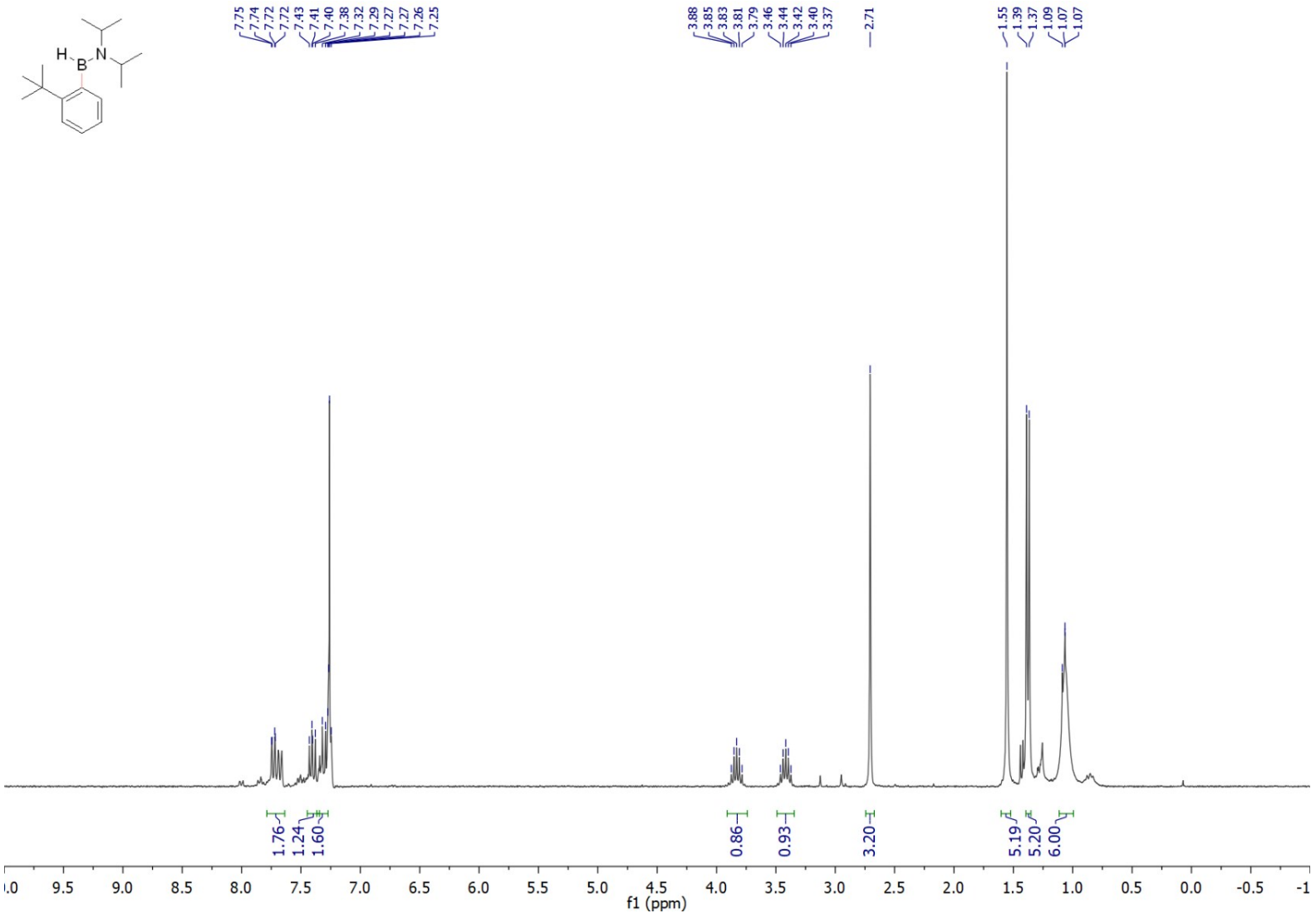
Compound (10l) ^{11}B NMR in $CDCl_3$ at 25°C (196 MHz)



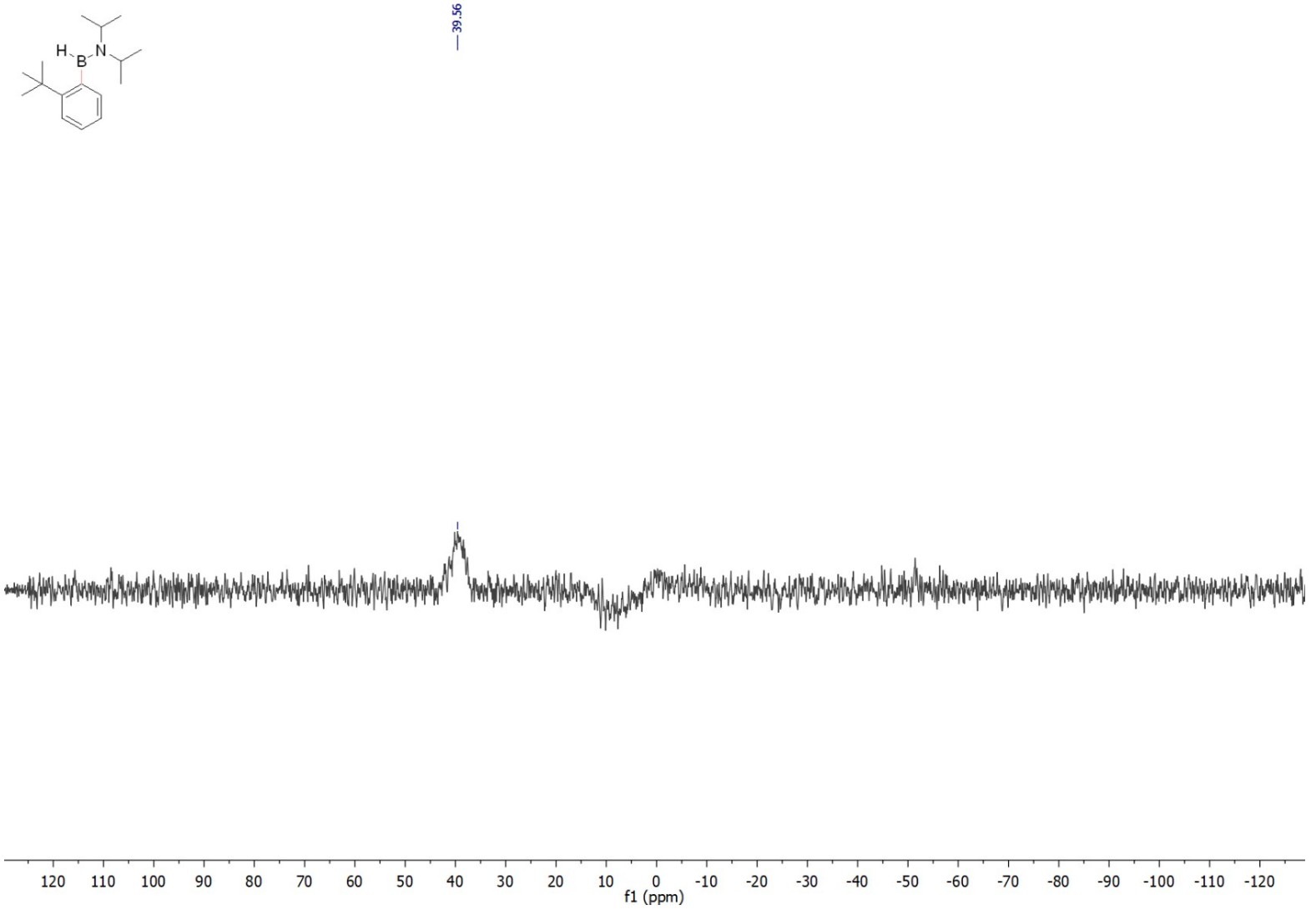
Compound (10l) ^{13}C NMR in $CDCl_3$ at 25°C (75 MHz)



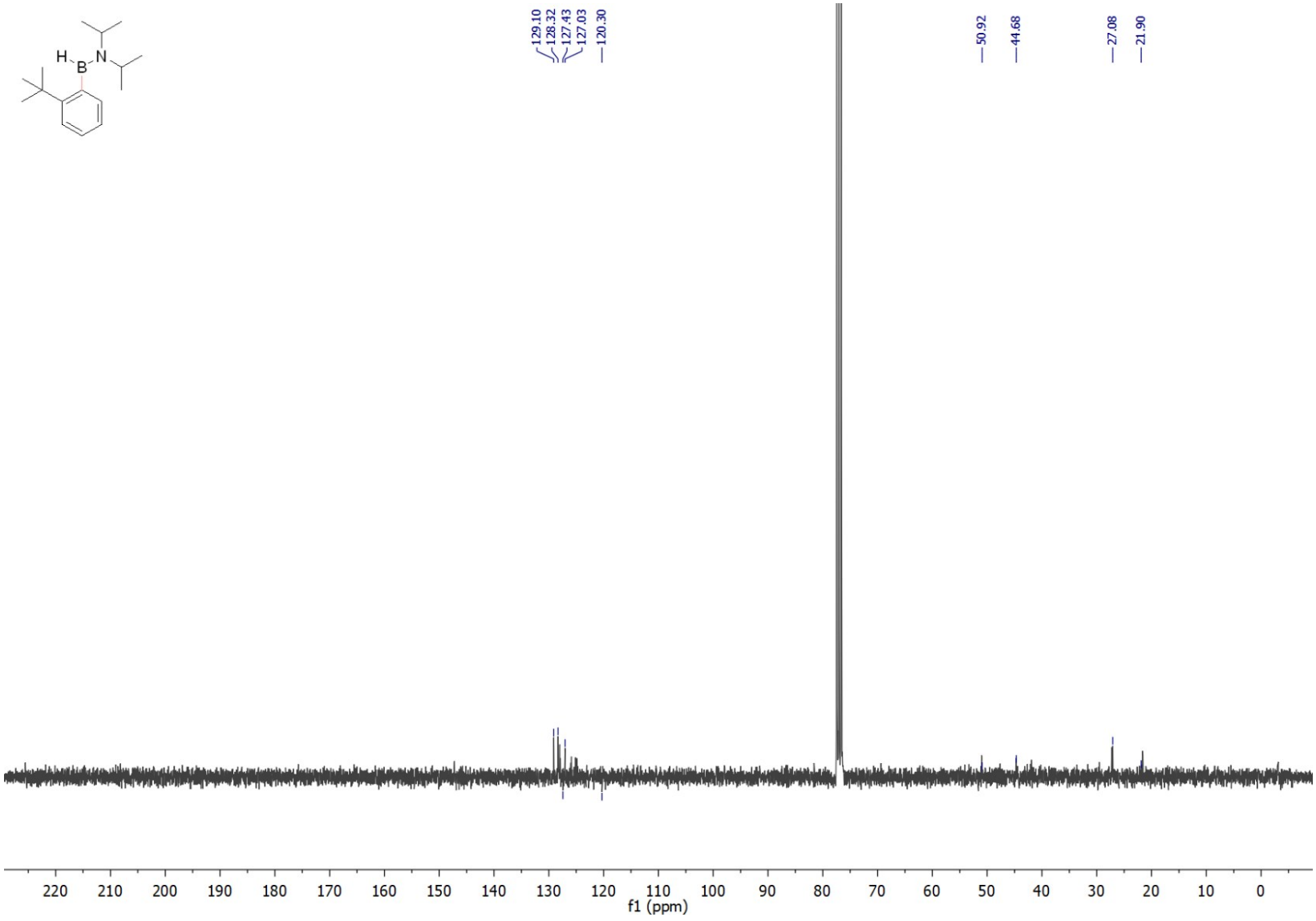
Compound (10m) ^{1}H NMR in $CDCl_3$ at 25°C (300 MHz)



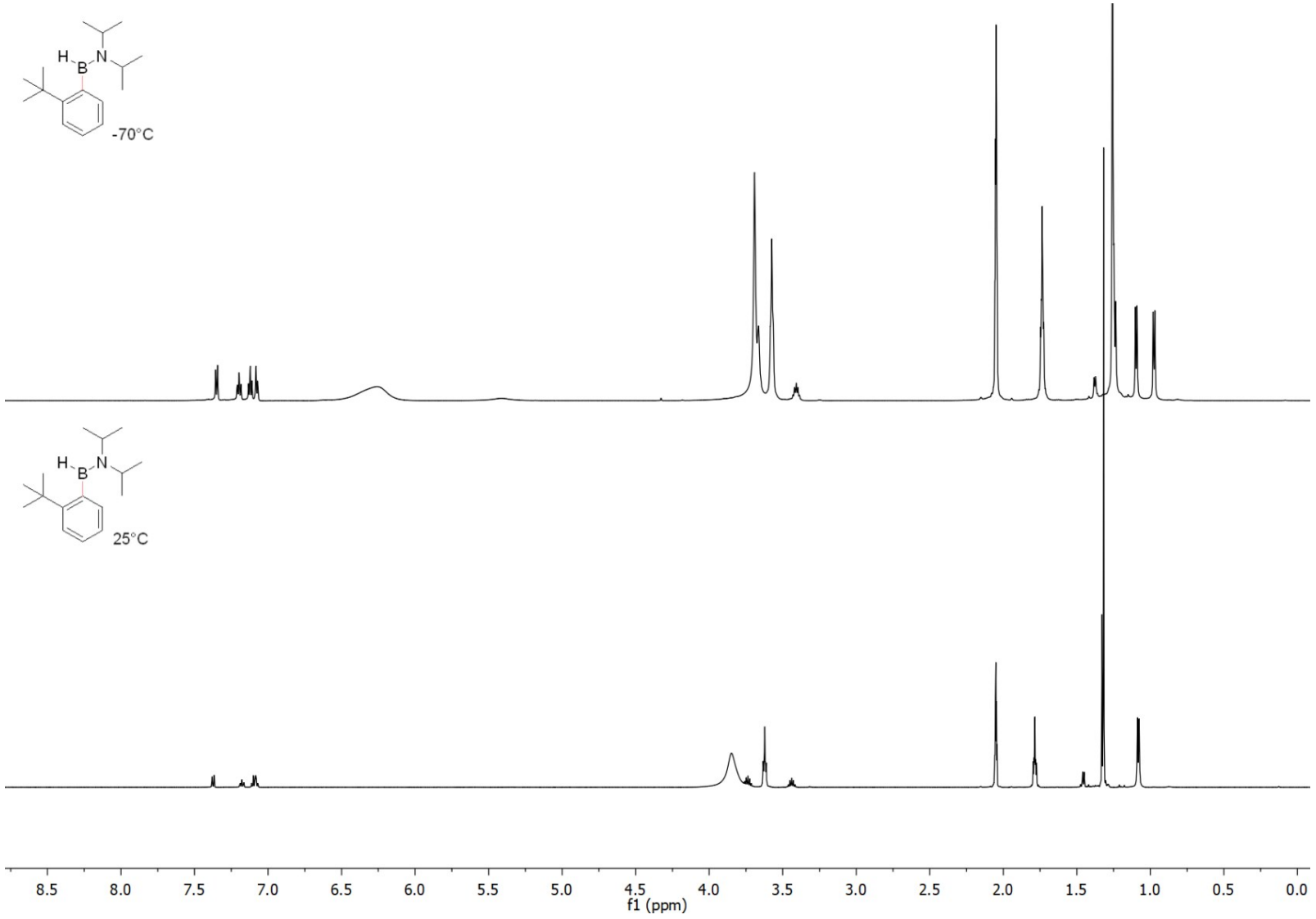
Compound (10m) ^{11}B NMR in $CDCl_3$ at 25°C (196 MHz)



Compound (10m) ^{13}C NMR in $CDCl_3$ at 25°C (75 MHz)



Compound (10m) VTNMR in Acetone-d_6 based on ^{1}H NMR at 25°C and -70°C (600 MHz) – *Coalescence observed*



5. Atropisomers characterization *via* Circular Dichroism

a) Principle and process

This spectroscopic technique is mainly used to determine the thermodynamic parameters of compounds exhibiting an axial chirality. It is based on the degeneration of the chiroptical signal of a sample at a given temperature. Indeed, when the sample goes from one enantiopure compound to a racemic mixture, the chiroptical signal decays exponentially into the chiroptically mute racemate (meaning that the racemization is complete).

The process goes as follow:

1. Separation of the enantiomers by running an HPLC on a chiral stationary phase
2. Put the enantiopure sample from HPLC into a CD-spectrometer at a given and fixed temperature
3. Study the degeneration of the chiroptical signal of one enantiomer over time
4. Get the data and use Eyring Plot for thermodynamic parameters determination

b) Eyring Plot and ∆G‡ determination

The Eyring equation in chemical kinetics relates the reaction rate to temperature. In its linear form it conforms to the standard slope-intercept form of the straight-line equation where:

$$\ln\left(\frac{krac}{T}\right) = \left(-\frac{\Delta H^{\ddagger}}{R}\right)\left(\frac{1}{T}\right) + \ln\left(\frac{k_b}{h}\right) + \left(\frac{\Delta S^{\ddagger}}{R}\right)$$

Y = ln(k_{rac}/T)

m = the slope of the line

X = 1/T and

B = the Y-intercept of the line when X = 0

To determine the activation parameters of a system, ΔH‡ and ΔS‡, a plot of ln(k*rac*/T) vs. (1/T) will produce a straight line where the slope = -ΔH‡/R and the y-intercept = ln(kb/h) + (ΔS‡/R) where:

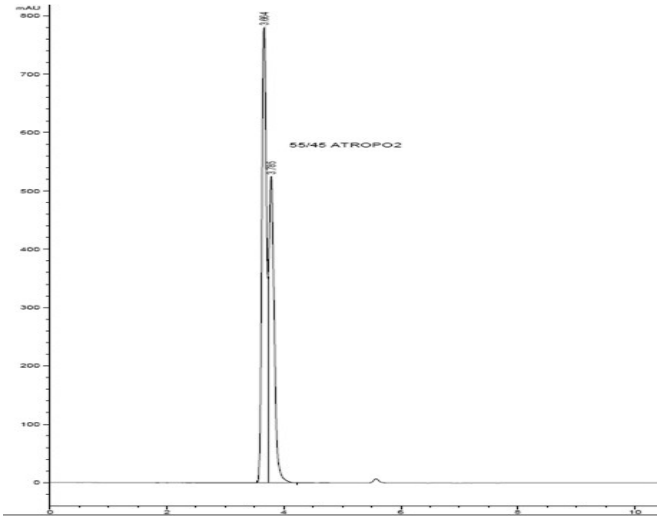
R = gas constant (8.3144621 J/mol.K)
k_B = Boltzmann constant (1.3806488^{-23} J/K)
h = Planck's constant (6.626069^{-34} J.s)
T = temperature in Kelvin, K
k = reaction rate constant, in this case **k*rac* = T.e$^{(m(1/T)+B)}$**
∆H‡ = enthalpy of activation, **= -mR**
∆S‡ = entropy of activation, **= R(B - ln(k_B/h))**
∆G‡ = Gibbs free energy, = **∆H‡ - ∆S‡T**

c) Data

Separation of enantiomers was obtained from a high performance liquid chromatography HPLC on a 1260 Infinity II Agilent HPLC bearing a Quaternary Pump with an operating pressure of up to 600 bar. The chiral column used was purchased from Phenomenex and is a Lux® 3 µm Cellulose-1, LC Column 100 x 4.6 mm. The stationary phase is a Cellulose tris(3,5 dimethylphenylcarbamate) and the flow used was a 1 mL/min with a 20µL injection volume. The mobile phase as well as the temperature of separation were adapted to each sample.

Circular dichroism (CD) spectra were measured on a Jasco J-815 (190-800nm) equipped with a xenon-mercury lamp and running under nitrogen atmosphere. The sample temperature was maintained between 4 and 20°C using a Peltier device (PFD-425S/15). All samples were stirred at 1000rpm during measurements, and every spectrum was taken as the average of 4 -10 scans with wavelengths between 200 to 400 nm.

Compound 10a



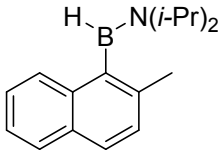


*Figure 1 : Sample **10a** chromatogram at 0°C using Hexane:Isopropanol 99:1 as the mobile phase*

The elution time at 0°C using Cellulose-1 for peak 1 was 3.6 minutes and peak 2 was 3.8 minutes. A sample containing a large excess of peak1 was then studied in CD. The chiroptical decay of **10a** at 10°C is presented here after as an illustration.

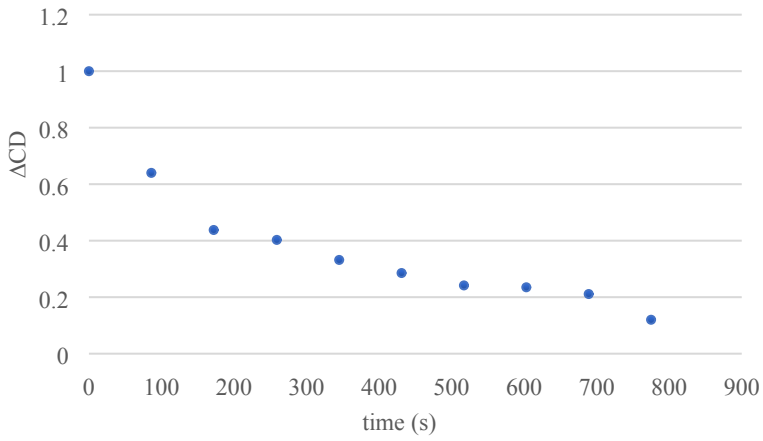
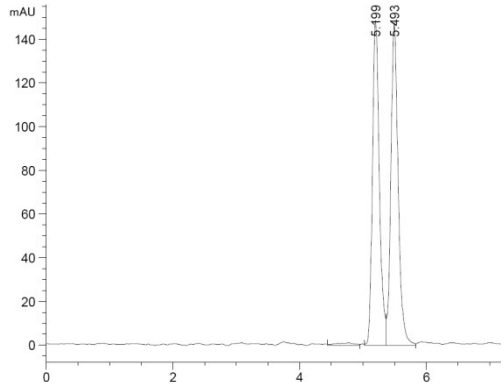


*Figure 2 : Chiroptical degeneration of **10a** at 10°C*

Table 1 : Thermodynamic parameters from CD studies

Temp (K)	k_{rac} (s^{-1})	$t_{1/2}$ (min)	$\Delta G^{\ddagger}_{rac}$ ($kJ.mol^{-1}$)
288	$3.5.10^{-4}$	1.5	82.5±0.1
283	$4.7.10^{-5}$	5	83.4±0.1
277	$1.6.10^{-5}$	18	84.6±0.1

Compound 10c



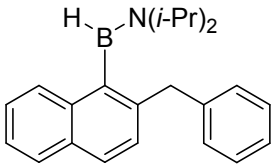


*Figure 3 : Sample **10c** chromatogram at 0°C using Hexane:Isopropanol 99:1 as the mobile phase*

The elution time at 0°C using Cellulose-1 for peak 1 was 5.2 minutes and peak 2 was 5.5 minutes. A sample containing a large excess of peak1 was then studied in CD. The chiroptical decay of **10c** at 10°C is presented here after as an illustration.

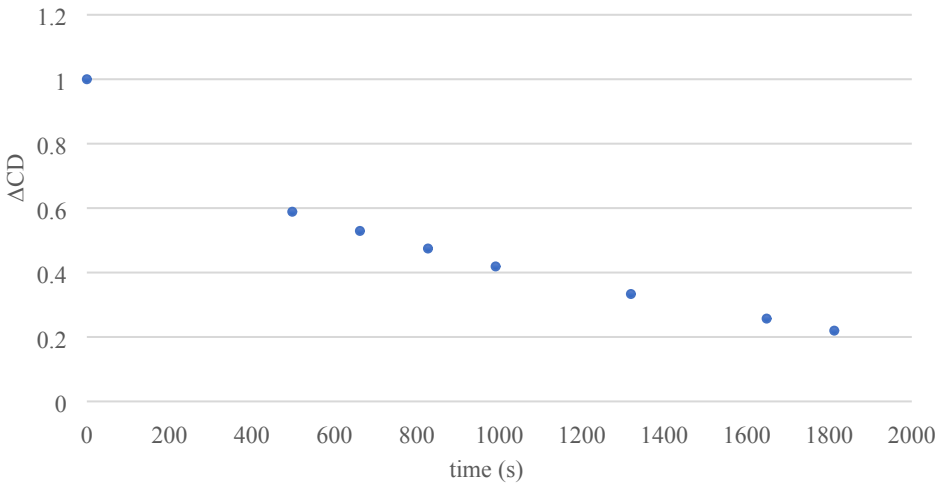
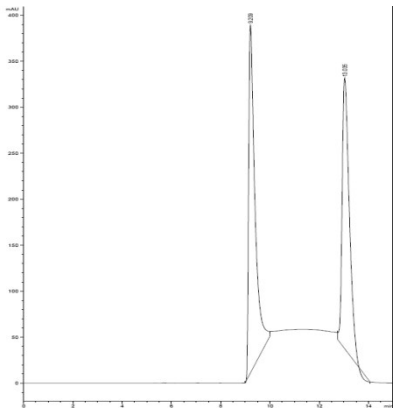


*Figure 4 : Chiroptical degeneration of **10c** at 10°C*

Table 2 : Thermodynamic parameters from CD studies

Temp (K)	k_{rac} (s^{-1})	$t_{1/2}$ (min)	$\Delta G^{\ddagger}_{rac}$ ($kJ.mol^{-1}$)
288	$9.5.10^{-4}$	12	87.1±0.7
283	$8.2.10^{-4}$	14	85.9±0.5
277	$6.4.10^{-4}$	18	84.6±0.4

Compound 10d



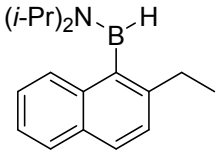


*Figure 5 : Sample **10d** chromatogram at 25°C using Heptane as the mobile phase*

The elution time at 25°C using Cellulose-1 for peak 1 was 9.2 minutes and peak 2 was 13.0 minutes. A sample containing a large excess of peak1 was then studied in CD. The chiroptical decay of **10d** at 10°C is presented here after as an illustration.

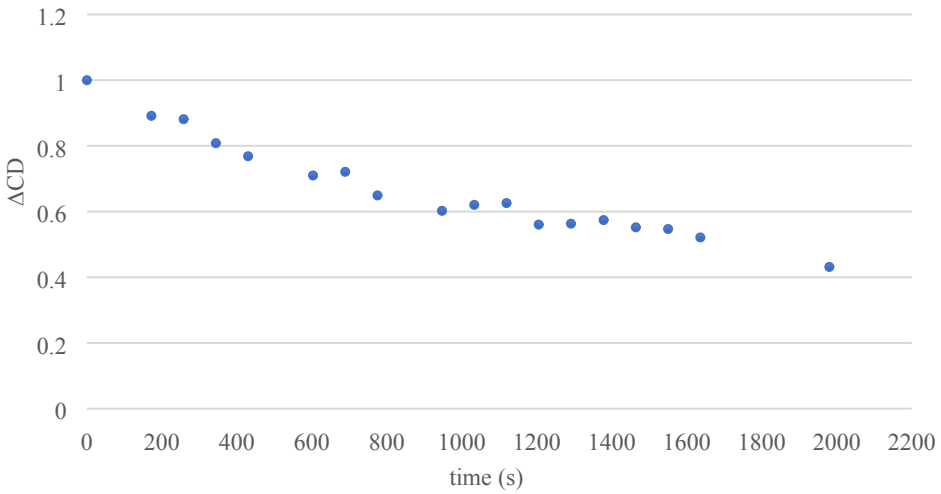
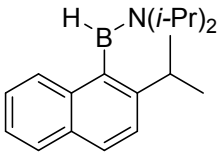


*Figure 6 : Chiroptical degeneration of **10d** at 10°C*

Table 3 : Thermodynamic parameters from CD studies

Temp (K)	k_{rac} (s^{-1})	$t_{1/2}$ (min)	$\Delta G^{\ddagger}_{rac}$ ($kJ.mol^{-1}$)
293	$8.5.10^{-4}$	14	88.4±0.1
283	$3.8.10^{-4}$	31	87.7±0.1
277	$1.7.10^{-4}$	68	87.9±0.1

Compound 10e



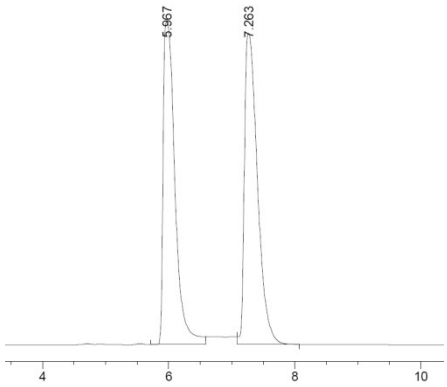


*Figure 7 : Sample **10e** chromatogram at 25°C using Heptane as the mobile phase*

The elution time at 25°C using Cellulose-1 for peak 1 was 5.9 minutes and peak 2 was 7.2 minutes. A sample containing a large excess of peak1 was then studied in CD. The chiroptical decay of **10e** at 10°C is presented here after as an illustration.

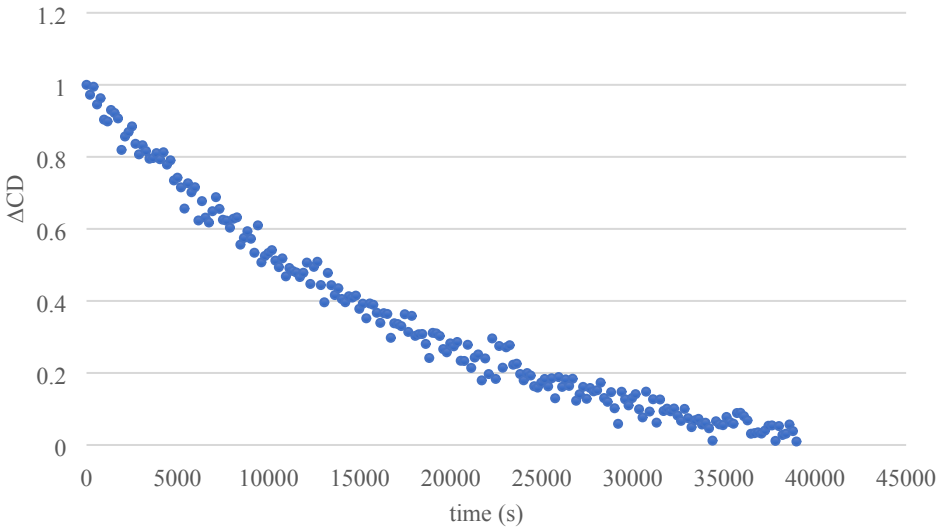
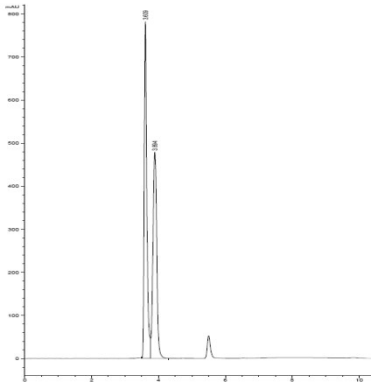


*Figure 8 : Chiroptical degeneration of **10e** at 10°C*

Table 4 : Thermodynamic parameters from CD studies

Temp (K)	k_{rac} (s^{-1})	$t_{1/2}$ (min)	$\Delta G^{\ddagger}_{rac}$ ($kJ.mol^{-1}$)
293	$9.5.10^{-4}$	54	92.2±0.1
288	$8.2.10^{-4}$	68	92.0±0.1
283	$6.4.10^{-4}$	187	92.0±0.1

Compound 10h



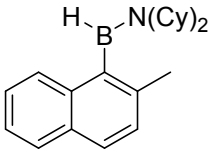


*Figure 9 : Sample **10h** chromatogram at 0°C using Hexane:isopropanol 99:1 as the mobile phase*

The elution time at 0°C using Cellulose-1 for peak 1 was 3.6 minutes and peak 2 was 3.9 minutes. A sample containing a large excess of peak1 was then studied in CD. The chiroptical decay of **10h** at 10°C is presented here after as an illustration.

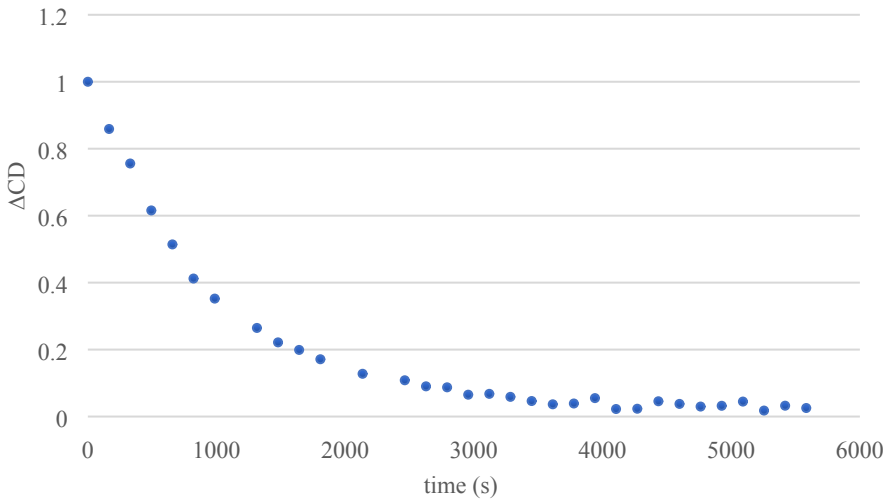


*Figure 10 : Chiroptical degeneration of **10h** at 10°C*

Table 5 : Thermodynamic parameters from CD studies

Temp (K)	k_{rac} (s^{-1})	$t_{1/2}$ (min)	$\Delta G^{\ddagger}_{rac}$ ($kJ.mol^{-1}$)
293	$2.9.10^{-3}$	4	85.8±0.1
283	$8.7.10^{-4}$	13	85.8±0.1
277	$5.0.10^{-4}$	23	85.4±0.1

Compound 10i

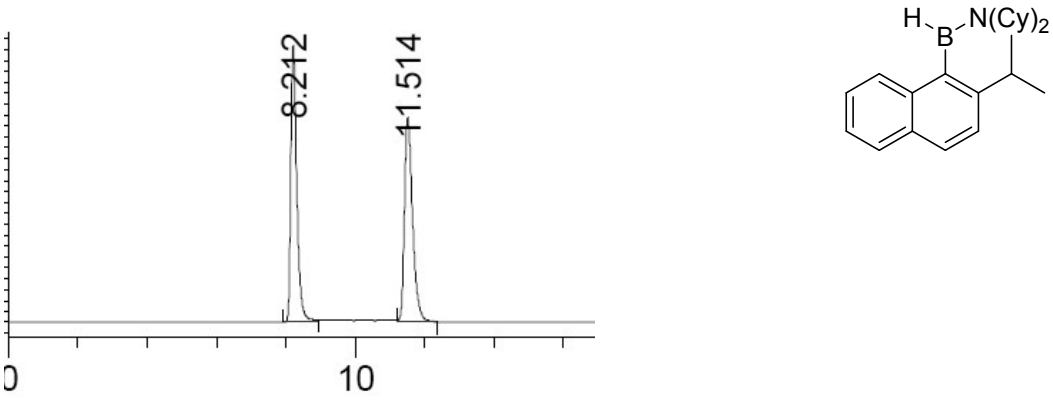


*Figure 11 : Sample **10i** chromatogram at 25°C using Heptane as the mobile phase*

The elution time at 25°C using Cellulose-1 for peak 1 was 8.2 minutes and peak 2 was 11.5 minutes. A sample containing a large excess of peak1 was then studied in CD. The chiroptical decay of **10i** at 10°C is presented here after as an illustration.

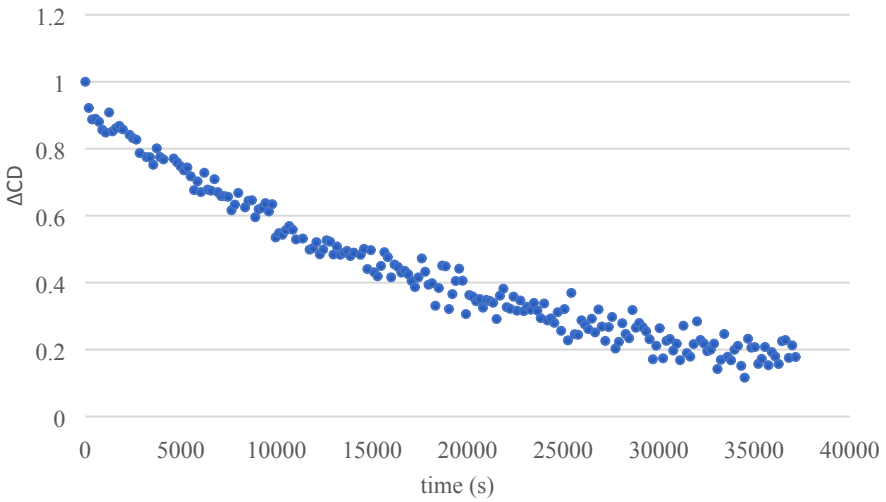
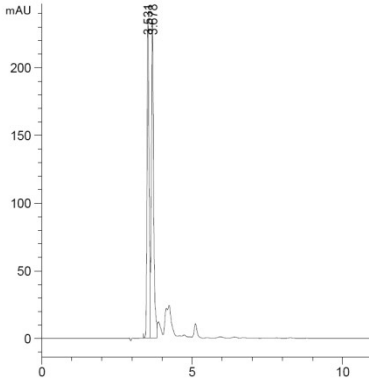


*Figure 12 : Chiroptical degeneration of **10i** at 10°C*

Table 6 : Thermodynamic parameters from CD studies

Temp (K)	k_{rac} (s^{-1})	$t_{1/2}$ (min)	$\Delta G^{\ddagger}_{rac}$ ($kJ.mol^{-1}$)
293	$1.5.10^{-4}$	76	93.4±0.1
288	$8.9.10^{-5}$	130	93.0±0.1
283	$4.7.10^{-5}$	244	92.6±0.1

Compound 10l



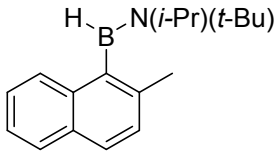


*Figure 13 : Sample **10l** chromatogram at 25°C using Hexane:isopropanol 99:1 as the mobile phase*

The elution time at 25°C using Cellulose-1 for peak 1 was 3.5 minutes and peak 2 was 3.6 minutes. A sample containing a large excess of peak1 was then studied in CD. The chiroptical decay of **10l** at 10°C is presented here after as an illustration.

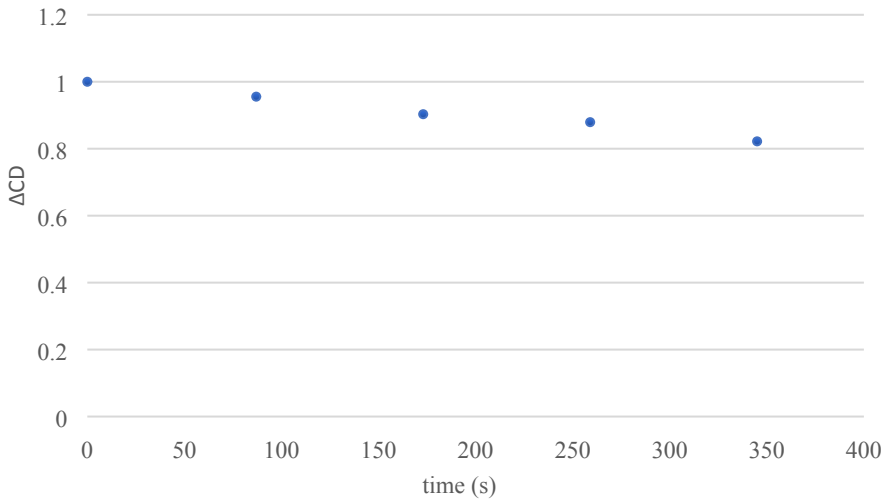


*Figure 14 : Chiroptical degeneration of **10l** at 10°C*

Table 7 : Thermodynamic parameters from CD studies

Temp (K)	k_{rac} (s^{-1})	$t_{1/2}$ (min)	$\Delta G^{\ddagger}_{rac}$ ($kJ.mol^{-1}$)
293	$5.5.10^{-4}$	20	90.0±0.1
283	$1.3.10^{-4}$	89	90.2±0.1
277	$3.2.10^{-5}$	357	91.3±0.1

6. Line Shape Analysis (LSA)

The relatively low-lying barriers of inversion of compounds 10f, 10g, and 10m allows the kinetics to be studied by DNMR. Thus, we evaluated the barrier of inversion of these three products which could not be separated into isomers by DHPLC, by correlating VTNMR results and DNMR line-shape analyses. The diastereotopic protons from the isopropyl groups can be used to determine the rate of inversion by measuring the peaks broadening at half-height.

For the determination of the thermodynamic parameters, a range of rates at different temperatures is required. For the evaluation of the coalescence temperature Tc, a set of spectra at various temperatures for each product were already recorded, which can now be simulated by line-shape analysis. The line-shape analysis gives access to the rates at these temperatures (*i.e. k(T)*). Once the rates are determined by LSA, an Eyring plot and a subsequent linear regression of the data can then be used to determine the thermodynamic parameters.

The LSA were performed using Topspin 4.0.5 (dNMR) and the equations used to determine the thermodynamic parameters are:

$$k_{rac} = \pi\left(\frac{\Delta v}{\sqrt{2}}\right); \quad \Delta G_{rac} = RT_c\left[ln\left(\frac{k_B T_c}{h}\right) - ln\left(\pi\frac{\Delta v}{\sqrt{2}}\right)\right]; \quad t_{1/2rac} = \left(\frac{ln2}{k_{rac}}\right)$$

With k_{rac} being the rate of inversion, Δv being the difference in chemical shift for one peak at 25°C and at the coalescence temperature and T_c being the coalescence temperature.

Thermodynamic parameters determination for compound 10f

Data from VTNMR

*Table 8 :Data from VTNMR results for compound **10f***

T_c (°C)	k_{rac} (s^{-1})	$t_{1/2rac}$ (s)	$\Delta G^{\ddagger}_{Tc}$ ($kJ.mol^{-1}$)
+ 10	$1.33.10^2$	0.005	~59.5

LSA Analysis

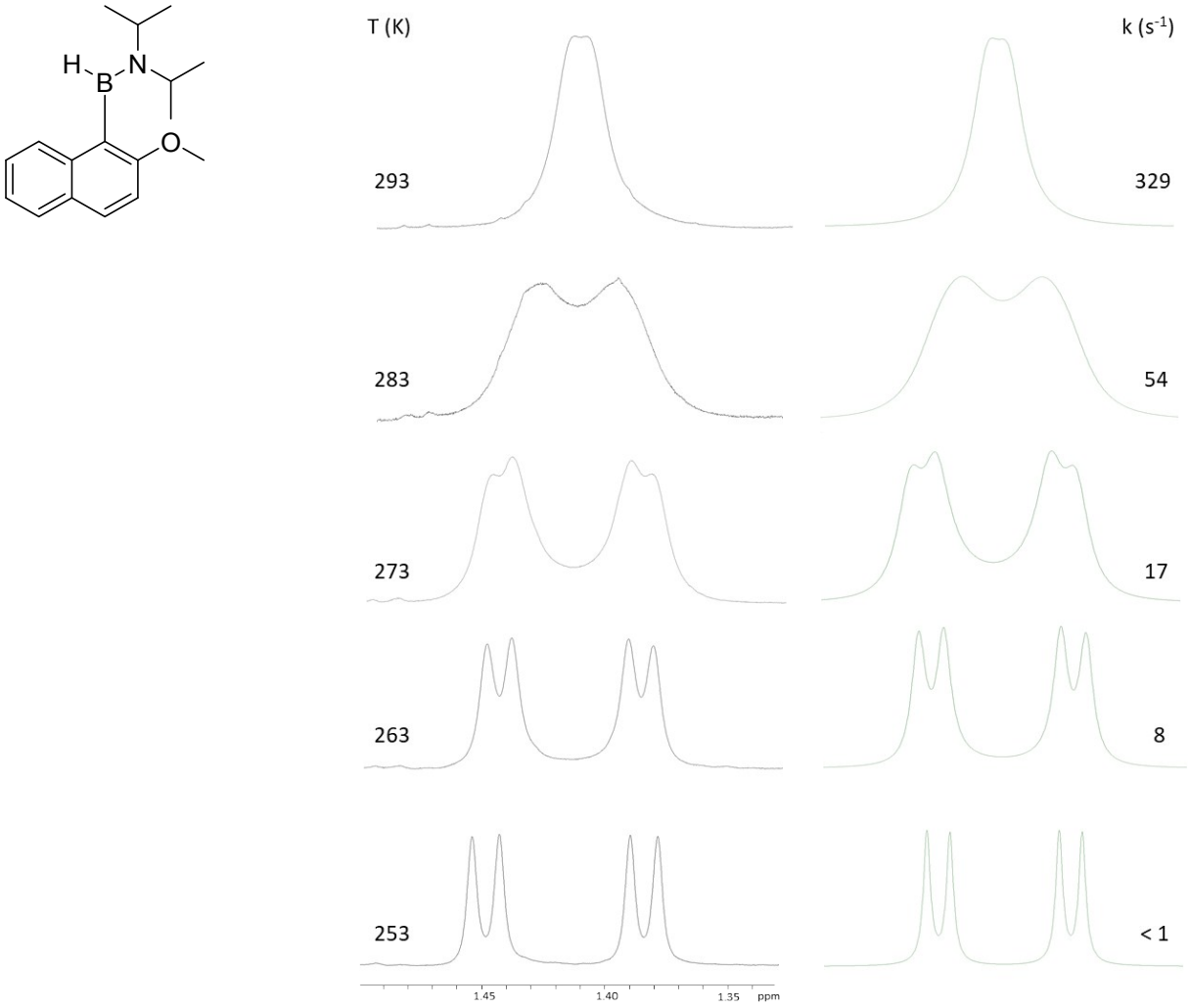


*Figure 15 : LSA analysis for compound **10f**. Left: Experimental spectra in Acetone-d_6 of the two diastereotopic hydrogens from isopropyl groups clearly displaying the temperature dependence of racemization with the resulting coalescence phenomena. Right: Line-shape analysis of the spectra yielding the corresponding calculated k(T).*

*Table 9 : Data from LSA for compound **10f***

ΔH ($kJ.mol^{-1}$)	ΔS ($J.mol^{-1}$)	$\Delta G^{\ddagger}_{Tc}$ ($kJ.mol^{-1}$)
75.5	56.6	~59.5

Thermodynamic parameters determination for compound 10g

Data from VTNMR

*Table 10 :Data from VTNMR results for compound **10g***

T_c (°C)	k_{rac} (s^{-1})	$t_{1/2rac}$ (s)	$\Delta G^{\ddagger}_{Tc}$ ($kJ.mol^{-1}$)
+ 10	$1.33.10^2$	0.005	~59.5

LSA Analysis

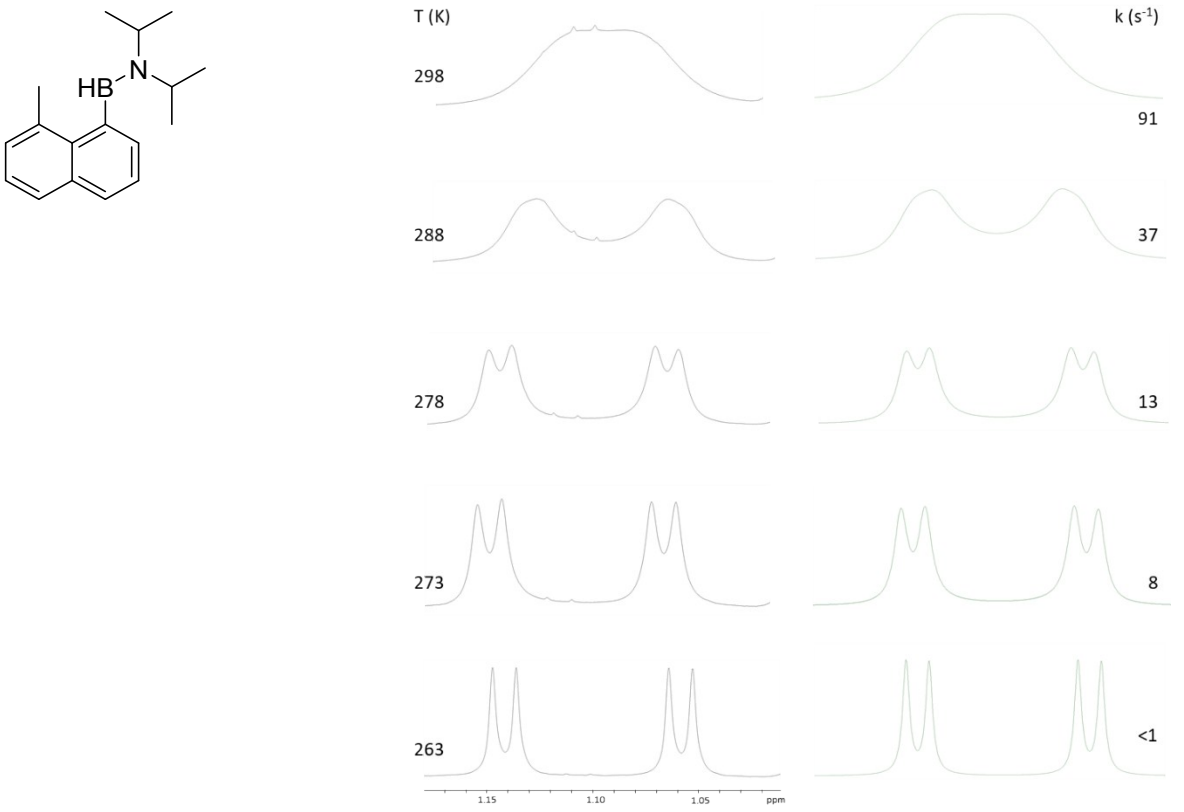


*Figure 16 : LSA analysis for compound **10g**. Left: Experimental spectra in Acetone-d_6 of the two diastereotopic hydrogens from isopropyl groups clearly displaying the temperature dependence of racemization with the resulting coalescence phenomena. Right: Line-shape analysis of the spectra yielding the corresponding calculated k(T).*

*Table 11 : Data from LSA for compound **10g***

ΔH ($kJ.mol^{-1}$)	ΔS ($J.mol^{-1}$)	$\Delta G^{\ddagger}_{Tc}$ ($kJ.mol^{-1}$)
64.2	8.2	61.9

Thermodynamic parameters determination for compound 10m

Data from VTNMR

*Table 12 :Data from VTNMR results for compound **10m***

T_c (°C)	k_{rac} (s^{-1})	$t_{1/2rac}$ (s)	$\Delta G^{‡}_{Tc}$ ($kJ.mol^{-1}$)
- 5	$1.33.10^2$	0.005	~54.3

LSA Analysis

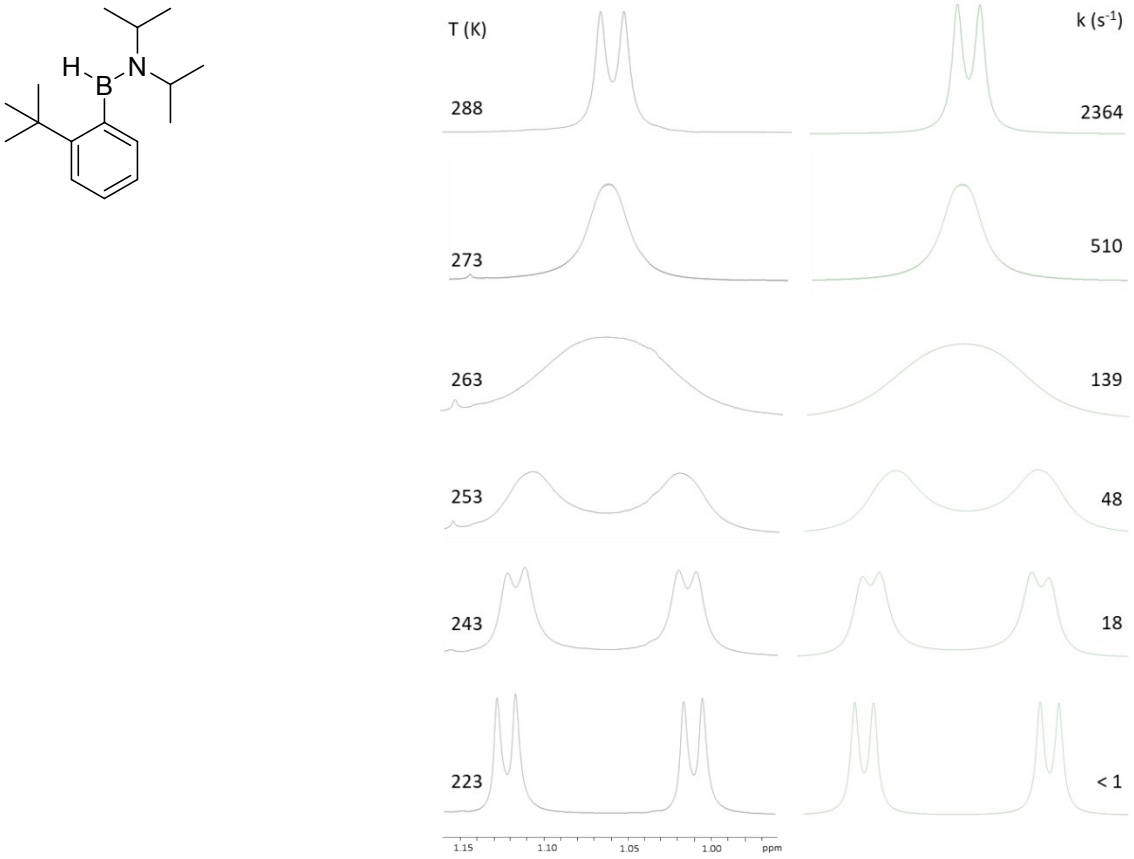


*Figure 17 : LSA analysis for compound **10m**. Left: Experimental spectra in Acetone-d_6 of the two diastereotopic hydrogens from isopropyl groups clearly displaying the temperature dependence of racemization with the resulting coalescence phenomena. Right: Line-shape analysis of the spectra yielding the corresponding calculated k(T).*

*Table 13 : Data from LSA for compound **10m***

ΔH ($kJ.mol^{-1}$)	ΔS ($J.mol^{-1}$)	$\Delta G^{‡}_{Tc}$ ($kJ.mol^{-1}$)
61.8	33.9	52.2

7. DFT Calculation results

All DFT calculations were performed with the Gaussian 16 software package.[1] M06–2X exchange-correlation functional[2] was used with a high-quality triple-ζ def2-TZVPP basis set for molecular structure optimization with the use of SMD solvatation model and Hexane as a solvent. All structures were optimized at 298°K. Frequency calculations were performed to insure that there is no imaginary frequency for local minima. The connectivity between stationary points was established by intrinsic reaction coordinate computations (IRC).

All these computed structures are available on request. This Supporting information contains free Gibbs energies and cartesian coordinates of all structures discussed in the text.

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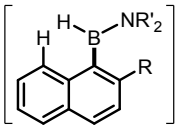
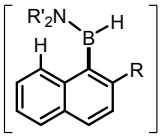
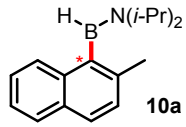
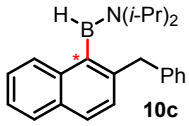
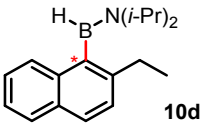
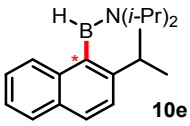
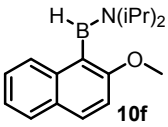
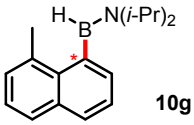
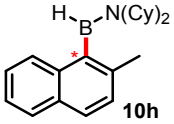
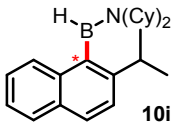
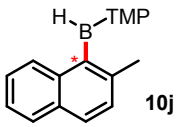
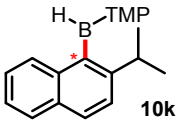
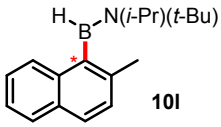
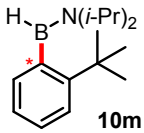
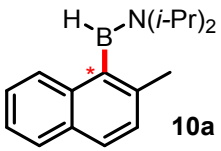
[1] **Gaussian 16**, Revision **A.03**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[2] a) Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *125*, 194101: 1. b) Y. Zhao, D. G. Truhlar *Theor. Chem. Acc.* **2008**, *120*, 215.

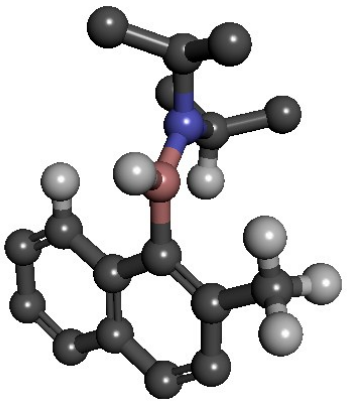
Compound	Experimental ΔG‡ (kJ.mol^{-1}) (at 10°C)	Calc. ΔG‡ H-side 	Calc. ΔG‡ Substituent-side 	difference exp./calc.
 **10a**	83.4±0.1	**97.1**	100.4	13.7
 **10c**	85.9±0.1	106.3	**102.2**	16.3
 **10d**	87.7±0.1	108.1	**101.7**	14.0
 **10e**	92.0±0.1	NA	**104.7**	12.7
 **10f**	59.5	**64.0**	95.5	4.5
 **10g**	61.9	**71.6**	NA	9.6
 **10h**	85.8±0.1	**98.8**	101.3	13.0
 **10i**	92.6±0.1	NA	**105.1**	12.5
 **10j**	ND	132.3	**118.9**	-
 **10k**	ND	NA	**134.8**	-
 **10l**	90.2±0.1	NA	NA	-
 **10m**	52.2	NA	56.0	3.8

NA: not available (impossible to calculate). ND: not determined.

Compound **10a**



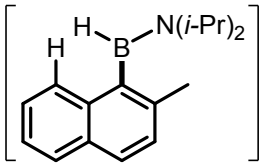
10a

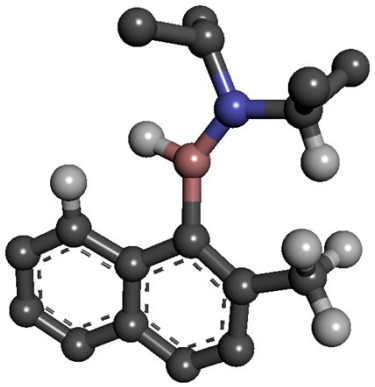


Sum of electronic and thermal Free Energies (Hartrees): -741.553794

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.588731	0.785746	-0.475387
2	6	0	-1.607694	-0.211925	-0.354578
3	6	0	-1.337534	-1.583358	-0.598275
4	1	0	-0.335589	-1.875632	-0.890985
5	6	0	-2.314896	-2.532905	-0.476300
6	1	0	-2.086832	-3.572907	-0.669839
7	6	0	-3.623982	-2.163609	-0.102397
8	1	0	-4.389996	-2.921812	-0.007734
9	6	0	-3.920366	-0.850451	0.135279
10	1	0	-4.923321	-0.555513	0.419844
11	6	0	-2.928260	0.151716	0.015599
12	6	0	-3.215737	1.517795	0.256819
13	1	0	-4.222667	1.799778	0.539843
14	6	0	-2.238255	2.457718	0.130164
15	1	0	-2.464787	3.501948	0.313738
16	6	0	-0.914171	2.103485	-0.239820
17	6	0	0.105701	3.207042	-0.343478
18	1	0	1.046809	2.861205	-0.771085
19	1	0	0.323619	3.627613	0.641093
20	1	0	-0.266549	4.022985	-0.965476
21	5	0	0.877266	0.390128	-0.914337
22	7	0	1.819737	-0.140365	-0.040840
23	6	0	3.188156	-0.465776	-0.492477
24	1	0	3.735860	-0.816762	0.381870
25	6	0	3.180043	-1.594809	-1.515669
26	1	0	4.199275	-1.867611	-1.793571
27	1	0	2.685864	-2.479040	-1.111122
28	1	0	2.650965	-1.288760	-2.419010
29	6	0	3.914305	0.766693	-1.018448
30	1	0	4.951080	0.524203	-1.256555
31	1	0	3.436951	1.140498	-1.924612
32	1	0	3.909265	1.563533	-0.273557
33	6	0	1.540828	-0.382682	1.383042
34	1	0	0.492256	-0.126474	1.529091
35	6	0	1.712888	-1.851022	1.759375
36	1	0	1.413078	-2.003640	2.796725
37	1	0	1.089008	-2.486715	1.130756
38	1	0	2.749145	-2.180427	1.665606
39	6	0	2.371617	0.532119	2.277524
40	1	0	2.094176	0.388594	3.322439
41	1	0	3.439884	0.325564	2.188790
42	1	0	2.200682	1.577392	2.017383
43	1	0	1.203863	0.559234	-2.051910

TS H-side **10a**





Sum of electronic and thermal Free Energies (Hartrees): -741.516869

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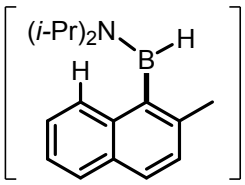
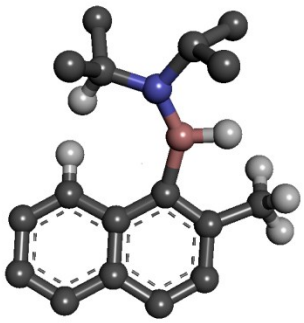
4	1	0	-1.098360	-2.158200	-0.651939
5	6	0	-3.167309	-2.328337	-0.345683
6	1	0	-3.162024	-3.380716	-0.598410
7	6	0	-4.381865	-1.697279	-0.015818
8	1	0	-5.302740	-2.264147	0.012422
9	6	0	-4.377837	-0.357285	0.234341
10	1	0	-5.298949	0.169131	0.453429
11	6	0	-3.176233	0.391468	0.187017
12	6	0	-3.220147	1.792624	0.341458
13	1	0	-4.168831	2.273315	0.547365
14	6	0	-2.089207	2.523041	0.168491
15	1	0	-2.137300	3.603690	0.218799
16	6	0	-0.825832	1.918662	-0.062194
17	6	0	0.280890	2.914057	-0.302714
18	1	0	0.938046	2.598879	-1.109887
19	1	0	0.875433	3.097257	0.594016
20	1	0	-0.151292	3.870160	-0.594580
21	5	0	0.633672	-0.371327	0.055167
22	7	0	2.031500	-0.237430	0.040034
23	6	0	2.830781	-1.490783	0.113752
24	1	0	3.870730	-1.197933	-0.018727
25	6	0	2.723938	-2.166133	1.475480
26	1	0	3.398827	-3.022452	1.524984
27	1	0	2.989041	-1.473687	2.274506
28	1	0	1.709647	-2.522252	1.654509
29	6	0	2.512121	-2.455637	-1.023145
30	1	0	3.232311	-3.275649	-1.028584
31	1	0	1.516281	-2.884483	-0.916053
32	1	0	2.564669	-1.945723	-1.985907
33	6	0	2.866074	0.964707	-0.047675
34	1	0	2.197034	1.801851	0.039729
35	6	0	3.842401	1.090113	1.122084
36	1	0	4.335674	2.062046	1.075542
37	1	0	3.311744	1.024388	2.072286
38	1	0	4.623538	0.329460	1.110359
39	6	0	3.574639	1.070533	-1.394982
40	1	0	4.124017	2.010975	-1.461045
41	1	0	4.290900	0.260348	-1.543439
42	1	0	2.850638	1.036194	-2.210171
43	1	0	0.351570	-1.497032	0.285566

TS Substituent-side **10a**





Sum of electronic and thermal Free Energies (Hartrees): -741.515509

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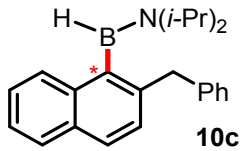
4	1	0	0.536681	-1.827542	-1.024145
5	6	0	2.382336	-2.558192	-0.337376
6	1	0	2.148829	-3.574921	-0.625509
7	6	0	3.647221	-2.255965	0.199412
8	1	0	4.372526	-3.040952	0.365687
9	6	0	3.958489	-0.951458	0.453845
10	1	0	4.944231	-0.677974	0.810432
11	6	0	3.018972	0.083289	0.229764
12	6	0	3.409301	1.433134	0.371331
13	1	0	4.417409	1.659907	0.696557
14	6	0	2.540126	2.422236	0.040046
15	1	0	2.860015	3.456191	0.078189
16	6	0	1.194415	2.144898	-0.315347
17	6	0	0.373060	3.373463	-0.639842
18	1	0	-0.163259	3.745535	0.235421
19	1	0	-0.357815	3.192638	-1.422795
20	1	0	1.038297	4.167964	-0.977535
21	5	0	-0.889331	0.773137	-0.203132
22	7	0	-1.934101	-0.155977	-0.061255
23	6	0	-3.243919	0.379511	0.404072
24	1	0	-3.895399	-0.481356	0.540534
25	6	0	-3.148456	1.060318	1.765173
26	1	0	-4.148781	1.285728	2.139208
27	1	0	-2.650784	0.409795	2.485387
28	1	0	-2.590915	1.994333	1.706305
29	6	0	-3.903510	1.277679	-0.635164
30	1	0	-4.902907	1.565368	-0.304101
31	1	0	-3.323203	2.187249	-0.789742
32	1	0	-3.994105	0.762132	-1.591569
33	6	0	-1.959022	-1.609212	-0.254044
34	1	0	-1.015176	-1.877163	-0.696443
35	6	0	-2.069416	-2.357767	1.070762
36	1	0	-2.019108	-3.434329	0.900930
37	1	0	-1.251241	-2.075461	1.733988
38	1	0	-3.012398	-2.147495	1.578608
39	6	0	-3.025690	-2.053354	-1.255424
40	1	0	-2.900200	-3.116184	-1.466248
41	1	0	-4.041887	-1.914763	-0.885769
42	1	0	-2.922223	-1.506994	-2.193216
43	1	0	-1.309768	1.865814	-0.022455

Compound **10c**



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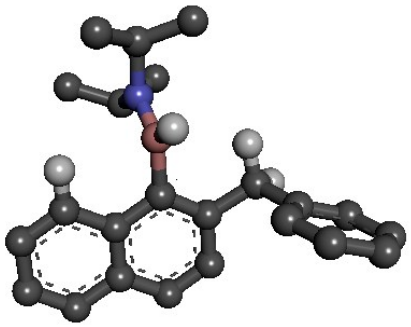
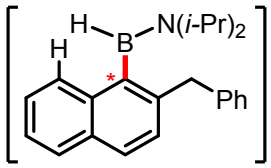


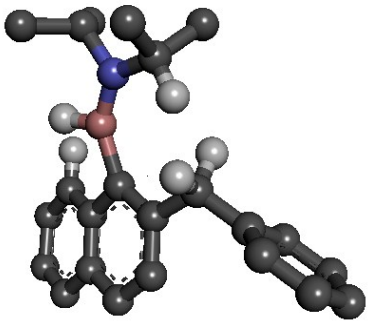
Sum of electronic and thermal Free Energies (Hartrees): -972.524391

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.281872	0.531832	0.006078
2	6	0	-1.058704	1.706709	-0.253745
3	6	0	-2.259604	1.651907	-1.006511
4	1	0	-2.587103	0.696372	-1.399302
5	6	0	-2.999581	2.777435	-1.246986
6	1	0	-3.911372	2.712760	-1.826192
7	6	0	-2.578109	4.026712	-0.746283
8	1	0	-3.170128	4.911104	-0.941031
9	6	0	-1.422406	4.116411	-0.021386
10	1	0	-1.087339	5.071814	0.364164
11	6	0	-0.637793	2.968334	0.240393
12	6	0	0.564930	3.043023	0.986604
13	1	0	0.888050	4.005071	1.365230
14	6	0	1.300155	1.920794	1.217358
15	1	0	2.224601	1.982813	1.780450
16	6	0	0.883185	0.654557	0.729802
17	6	0	1.772106	-0.534826	1.021979
18	1	0	1.269837	-1.458099	0.720740
19	1	0	1.934956	-0.610836	2.099562
20	5	0	-0.718529	-0.874615	-0.571041
21	7	0	-1.730438	-1.652383	-0.020585
22	6	0	-2.066750	-2.978677	-0.578758
23	1	0	-2.852330	-3.397615	0.049611
24	6	0	-2.621812	-2.860053	-1.992702
25	1	0	-2.925761	-3.838429	-2.367874
26	1	0	-3.489758	-2.199690	-2.012676
27	1	0	-1.867041	-2.455825	-2.668236
28	6	0	-0.878885	-3.931612	-0.516425
29	1	0	-1.173420	-4.927864	-0.849708
30	1	0	-0.068640	-3.585063	-1.158536
31	1	0	-0.499912	-4.008380	0.503535
32	6	0	-2.498663	-1.241961	1.165269
33	1	0	-2.152679	-0.239100	1.412357
34	6	0	-3.994958	-1.155683	0.879963
35	1	0	-4.513470	-0.757765	1.752891
36	1	0	-4.191954	-0.490690	0.039009
37	1	0	-4.428286	-2.132471	0.658559
38	6	0	-2.203342	-2.143511	2.360019
39	1	0	-2.731798	-1.781798	3.242801
40	1	0	-2.524587	-3.171446	2.181339
41	1	0	-1.135017	-2.150428	2.579366
42	1	0	-0.141754	-1.305848	-1.525928
43	6	0	3.115464	-0.456968	0.329552
44	6	0	4.300022	-0.636278	1.035958
45	6	0	3.185743	-0.214311	-1.041619
46	6	0	5.529700	-0.580675	0.390573
47	1	0	4.259993	-0.821152	2.102903
48	6	0	4.409916	-0.161519	-1.689387
49	1	0	2.269356	-0.059780	-1.599307
50	6	0	5.587834	-0.344390	-0.974372
51	1	0	6.441345	-0.719558	0.957003
52	1	0	4.446881	0.026844	-2.754410
53	1	0	6.543585	-0.298675	-1.479259

TS H-side **10c**



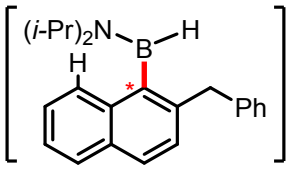
TS H 10c



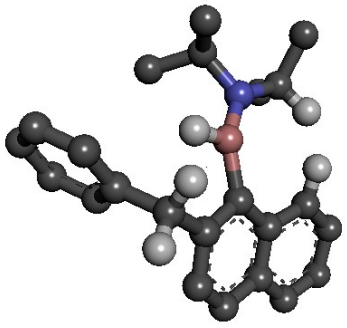
Sum of electronic and thermal Free Energies (Hartrees): -972.483999

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.549719	0.743479	-0.096028
2	6	0	-0.970978	2.136477	-0.004691
3	6	0	-2.211150	2.544137	0.566382
4	1	0	-2.874330	1.806041	0.985669
5	6	0	-2.578794	3.858874	0.650028
6	1	0	-3.524249	4.117010	1.109199
7	6	0	-1.741458	4.879326	0.158312
8	1	0	-2.052194	5.914052	0.212789
9	6	0	-0.524850	4.541779	-0.355606
10	1	0	0.159887	5.303893	-0.707507
11	6	0	-0.108245	3.188927	-0.417520
12	6	0	1.194816	2.873171	-0.853424
13	1	0	1.844860	3.668222	-1.198140
14	6	0	1.642659	1.592505	-0.776871
15	1	0	2.667900	1.372874	-1.041345
16	6	0	0.798782	0.528351	-0.370455
17	6	0	1.461200	-0.835271	-0.250744
18	1	0	0.997168	-1.354750	0.585813
19	5	0	-1.777339	-0.292416	-0.058806
20	7	0	-2.038082	-1.673475	-0.032658
21	6	0	-3.467972	-2.077419	0.081355
22	1	0	-3.470309	-3.159373	0.198147
23	6	0	-4.139306	-1.515650	1.329911
24	1	0	-5.118575	-1.978250	1.464674
25	1	0	-3.537451	-1.721874	2.215899
26	1	0	-4.285128	-0.438498	1.256512
27	6	0	-4.262155	-1.759638	-1.179477
28	1	0	-5.274600	-2.158762	-1.096529
29	1	0	-4.333085	-0.683223	-1.333832
30	1	0	-3.790609	-2.200673	-2.057724
31	6	0	-1.134476	-2.828860	-0.089088
32	1	0	-0.152842	-2.443159	-0.299591
33	6	0	-1.067412	-3.565094	1.245968
34	1	0	-0.333604	-4.370865	1.196578
35	1	0	-0.774818	-2.881554	2.044130
36	1	0	-2.027242	-4.009608	1.514736
37	6	0	-1.460266	-3.773157	-1.246731
38	1	0	-0.682081	-4.534340	-1.318020
39	1	0	-2.410994	-4.291971	-1.121821
40	1	0	-1.487829	-3.226764	-2.189911
41	1	0	-2.802167	0.294599	-0.137369
42	1	0	1.275329	-1.417964	-1.155785
43	6	0	2.947928	-0.806332	0.005867
44	6	0	3.856769	-1.213243	-0.964446
45	6	0	3.436716	-0.365175	1.234823
46	6	0	5.224456	-1.181447	-0.717589
47	1	0	3.490686	-1.556583	-1.924788
48	6	0	4.799252	-0.331068	1.485590
49	1	0	2.737833	-0.040503	1.997052
50	6	0	5.699205	-0.739394	0.507780
51	1	0	5.917117	-1.502737	-1.484416
52	1	0	5.161593	0.013499	2.445269
53	1	0	6.762985	-0.713996	0.702887

TS Substituent-side **10c**



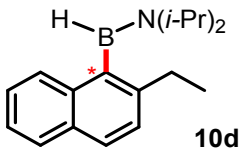
TS Sub 10c



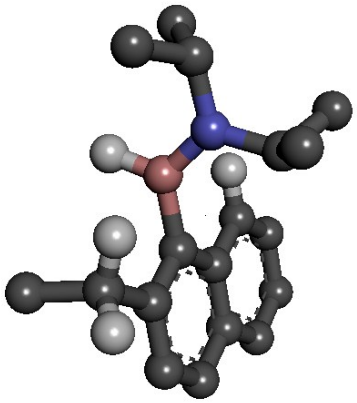
Sum of electronic and thermal Free Energies (Hartrees): -972.48542

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.871247	-0.570046	-0.699503
2	6	0	-2.243780	-0.758482	-0.275010
3	6	0	-3.188517	0.293005	-0.199580
4	1	0	-2.907745	1.265082	-0.550698
5	6	0	-4.472098	0.109053	0.238112
6	1	0	-5.153027	0.949889	0.262940
7	6	0	-4.917727	-1.164694	0.635738
8	1	0	-5.929095	-1.303396	0.993347
9	6	0	-4.063522	-2.223341	0.527495
10	1	0	-4.387368	-3.224195	0.786135
11	6	0	-2.740087	-2.052105	0.054963
12	6	0	-1.910662	-3.178617	-0.130270
13	1	0	-2.289202	-4.161530	0.122590
14	6	0	-0.670832	-3.019691	-0.660051
15	1	0	-0.049629	-3.887450	-0.845755
16	6	0	-0.138767	-1.736062	-0.949226
17	6	0	1.272853	-1.779682	-1.506045
18	1	0	1.412967	-1.029182	-2.280357
19	1	0	1.396238	-2.747245	-1.999773
20	5	0	0.049350	0.746556	-0.670222
21	7	0	0.001373	2.090459	-0.255374
22	6	0	1.314574	2.719818	0.064498
23	1	0	1.085570	3.664546	0.553455
24	6	0	2.132307	1.912197	1.069377
25	1	0	2.966297	2.515261	1.433617
26	1	0	1.517451	1.625391	1.923890
27	1	0	2.543390	1.005686	0.625008
28	6	0	2.125279	3.030925	-1.187464
29	1	0	3.042735	3.558673	-0.921168
30	1	0	2.403250	2.109490	-1.700512
31	1	0	1.559282	3.653592	-1.879950
32	6	0	-1.140219	2.974397	0.008000
33	1	0	-1.984057	2.547083	-0.510531
34	6	0	-1.461349	3.047372	1.495525
35	1	0	-2.337666	3.672989	1.673278
36	1	0	-1.660439	2.050446	1.890329
37	1	0	-0.625642	3.475656	2.053399
38	6	0	-0.988562	4.365279	-0.611976
39	1	0	-1.942954	4.887402	-0.533336
40	1	0	-0.242074	4.984359	-0.115465
41	1	0	-0.732206	4.291584	-1.668785
42	1	0	1.165622	0.468313	-0.935309
43	6	0	2.381824	-1.635289	-0.482110
44	6	0	2.179767	-1.869807	0.874195
45	6	0	3.652392	-1.248410	-0.906372
46	6	0	3.221195	-1.722688	1.782996
47	1	0	1.197701	-2.153729	1.230570
48	6	0	4.692736	-1.097227	-0.002230
49	1	0	3.821090	-1.049690	-1.958577
50	6	0	4.480160	-1.334494	1.350338
51	1	0	3.042055	-1.904423	2.834780
52	1	0	5.668781	-0.786961	-0.352156
53	1	0	5.288027	-1.212103	2.059365

Compound **10d**



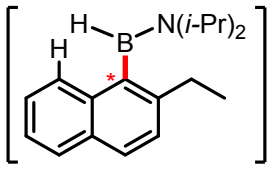
10d



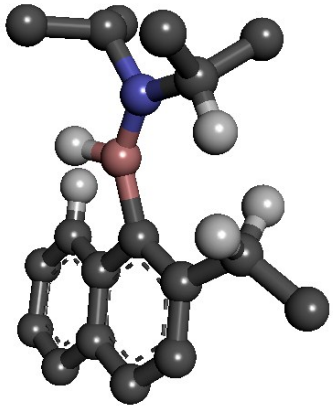
Sum of electronic and thermal Free Energies (Hartrees): -780.835263

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.588242	0.637973	-0.239312
2	6	0	-1.594112	-0.375352	-0.315240
3	6	0	-1.307315	-1.672856	-0.814053
4	1	0	-0.301710	-1.890493	-1.154751
5	6	0	-2.273124	-2.639029	-0.878414
6	1	0	-2.032809	-3.620479	-1.265849
7	6	0	-3.587454	-2.362595	-0.445241
8	1	0	-4.344297	-3.133875	-0.499253
9	6	0	-3.900212	-1.122233	0.035662
10	1	0	-4.907165	-0.898417	0.366982
11	6	0	-2.920531	-0.102834	0.110698
12	6	0	-3.226371	1.188755	0.603558
13	1	0	-4.236248	1.398252	0.934800
14	6	0	-2.260524	2.148967	0.658775
15	1	0	-2.500327	3.136493	1.037181
16	6	0	-0.932172	1.885617	0.236770
17	6	0	0.065719	3.017834	0.272855
18	1	0	1.081844	2.623960	0.347549
19	1	0	-0.101317	3.622417	1.167146
20	5	0	0.889850	0.366118	-0.730226
21	7	0	1.820933	-0.360199	0.004232
22	6	0	3.204313	-0.543555	-0.481114
23	1	0	3.738546	-1.104327	0.285519
24	6	0	3.237393	-1.367968	-1.762044
25	1	0	4.266969	-1.551717	-2.072885
26	1	0	2.746069	-2.330503	-1.614129
27	1	0	2.726365	-0.842287	-2.569462
28	6	0	3.921901	0.790587	-0.649415
29	1	0	4.964576	0.629061	-0.927176
30	1	0	3.450929	1.388058	-1.430549
31	1	0	3.898110	1.360336	0.280426
32	6	0	1.519717	-0.948192	1.318931
33	1	0	0.462996	-0.754087	1.497391
34	6	0	1.718724	-2.460840	1.333496
35	1	0	1.391406	-2.865370	2.291865
36	1	0	1.130964	-2.937051	0.548680
37	1	0	2.765361	-2.739853	1.200583
38	6	0	2.311810	-0.264724	2.429370
39	1	0	2.024468	-0.670712	3.399950
40	1	0	3.386566	-0.417329	2.313070
41	1	0	2.114763	0.807903	2.435262
42	1	0	1.241303	0.820840	-1.778868
43	6	0	-0.045113	3.904193	-0.968300
44	1	0	0.669516	4.726999	-0.930062
45	1	0	0.147953	3.323146	-1.870944
46	1	0	-1.047046	4.327359	-1.052860

TS H-side **10d**



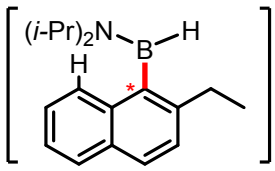
TS H 10d



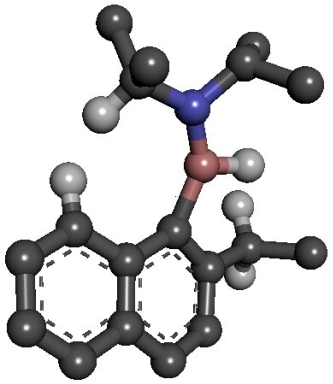
Sum of electronic and thermal Free Energies (Hartrees): -780.794170

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.691804	0.310102	-0.022885
2	6	0	1.916129	-0.482409	-0.049197
3	6	0	1.964241	-1.850733	-0.447902
4	1	0	1.067242	-2.341807	-0.784647
5	6	0	3.129493	-2.566356	-0.467762
6	1	0	3.111729	-3.597704	-0.795465
7	6	0	4.350150	-1.979543	-0.080404
8	1	0	5.261579	-2.562176	-0.082145
9	6	0	4.364021	-0.660856	0.262834
10	1	0	5.290273	-0.165530	0.528100
11	6	0	3.174204	0.108988	0.254303
12	6	0	3.234979	1.494007	0.503889
13	1	0	4.187274	1.944202	0.757222
14	6	0	2.119267	2.257536	0.363534
15	1	0	2.201882	3.326874	0.490028
16	6	0	0.851767	1.692049	0.076829
17	6	0	-0.284777	2.673034	-0.129041
18	1	0	-0.924586	2.274146	-0.914253
19	5	0	-0.641466	-0.582601	0.054943
20	7	0	-2.042228	-0.454978	0.057716
21	6	0	-2.824046	-1.723560	0.066020
22	1	0	-3.869168	-1.438855	-0.038444
23	6	0	-2.507031	-2.616001	-1.128976
24	1	0	-3.219662	-3.441310	-1.176017
25	1	0	-2.574407	-2.050705	-2.059351
26	1	0	-1.506373	-3.040874	-1.057415
27	6	0	-2.695190	-2.475983	1.384690
28	1	0	-3.361199	-3.340685	1.390531
29	1	0	-1.675868	-2.831639	1.532901
30	1	0	-2.958966	-1.834314	2.225484
31	6	0	-2.904624	0.732423	0.046608
32	1	0	-2.257868	1.582521	0.169636
33	6	0	-3.635747	0.893908	-1.283352
34	1	0	-4.206114	1.824055	-1.290156
35	1	0	-2.923558	0.920511	-2.109175
36	1	0	-4.336679	0.077573	-1.466350
37	6	0	-3.866196	0.771938	1.234818
38	1	0	-4.380926	1.733744	1.247464
39	1	0	-4.630830	-0.004197	1.193567
40	1	0	-3.319728	0.667634	2.172530
41	1	0	-0.361177	-1.720150	0.216901
42	6	0	0.114968	4.089962	-0.532371
43	1	0	0.802713	4.083874	-1.379009
44	1	0	-0.774123	4.648028	-0.826237
45	1	0	0.584501	4.639501	0.282573
46	1	0	-0.883514	2.734094	0.783195

TS Substituent-side **10d**



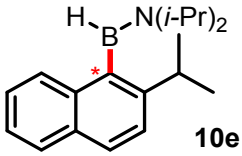
TS Sub 10d



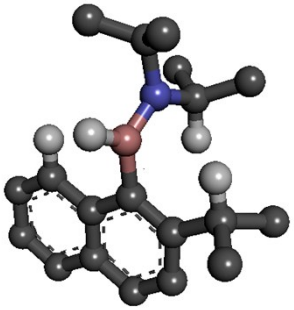
Sum of electronic and thermal Free Energies (Hartrees): -780.796616

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.709298	0.585914	-0.406340
2	6	0	1.696208	-0.459326	-0.213599
3	6	0	1.454112	-1.827185	-0.485559
4	1	0	0.540680	-2.102566	-0.975653
5	6	0	2.382717	-2.805818	-0.250728
6	1	0	2.149122	-3.833622	-0.496387
7	6	0	3.645281	-2.481996	0.277083
8	1	0	4.369333	-3.259504	0.479920
9	6	0	3.957138	-1.167385	0.475251
10	1	0	4.942392	-0.879485	0.821779
11	6	0	3.020115	-0.142862	0.202962
12	6	0	3.414976	1.212376	0.280377
13	1	0	4.424481	1.450836	0.592642
14	6	0	2.548859	2.184518	-0.100066
15	1	0	2.870888	3.219223	-0.118249
16	6	0	1.201284	1.893507	-0.442947
17	6	0	0.402184	3.122433	-0.829443
18	1	0	-0.465719	2.861367	-1.427646
19	1	0	1.046871	3.726860	-1.472888
20	5	0	-0.887310	0.528752	-0.256188
21	7	0	-1.931727	-0.395897	-0.082613
22	6	0	-3.244037	0.154457	0.357773
23	1	0	-3.899331	-0.701001	0.508879
24	6	0	-3.157651	0.867632	1.702521
25	1	0	-4.159844	1.107154	2.062506
26	1	0	-2.668571	0.233618	2.442966
27	1	0	-2.595866	1.797803	1.624724
28	6	0	-3.893513	1.028911	-0.707777
29	1	0	-4.898299	1.318429	-0.395140
30	1	0	-3.315966	1.938417	-0.873247
31	1	0	-3.969557	0.493803	-1.654689
32	6	0	-1.956772	-1.855167	-0.222532
33	1	0	-1.007284	-2.140981	-0.640439
34	6	0	-2.086828	-2.555569	1.126765
35	1	0	-2.034362	-3.637460	0.996044
36	1	0	-1.278056	-2.249822	1.791137
37	1	0	-3.036947	-2.327849	1.613355
38	6	0	-3.010667	-2.333134	-1.221898
39	1	0	-2.884468	-3.402865	-1.393931
40	1	0	-4.031444	-2.180285	-0.870877
41	1	0	-2.893807	-1.819808	-2.176634
42	1	0	-1.310196	1.624915	-0.108973
43	6	0	-0.013553	3.968739	0.372815
44	1	0	-0.541692	4.867702	0.053086
45	1	0	-0.667026	3.404267	1.038160
46	1	0	0.858398	4.278097	0.950830

Compound **10e**



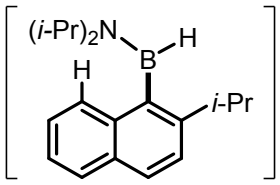
10e



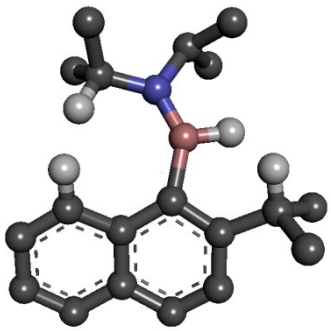
Sum of electronic and thermal Free Energies (Hartrees): -820.116571

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.630401	0.252494	-0.406540
2	6	0	-1.792116	-0.569585	-0.241363
3	6	0	-1.733691	-1.978320	-0.404124
4	1	0	-0.787820	-2.441226	-0.662007
5	6	0	-2.844522	-2.759528	-0.239850
6	1	0	-2.776723	-3.831427	-0.371565
7	6	0	-4.082216	-2.175406	0.101948
8	1	0	-4.954679	-2.801989	0.231505
9	6	0	-4.174117	-0.821873	0.268682
10	1	0	-5.119181	-0.362500	0.532588
11	6	0	-3.040717	0.009031	0.101727
12	6	0	-3.114331	1.413153	0.269498
13	1	0	-4.066452	1.861438	0.526678
14	6	0	-2.002859	2.184044	0.109145
15	1	0	-2.077443	3.257132	0.238913
16	6	0	-0.745327	1.614933	-0.227169
17	6	0	0.440997	2.545337	-0.393492
18	1	0	1.318816	1.929625	-0.603500
19	5	0	0.709726	-0.448394	-0.869216
20	7	0	1.794865	-0.695696	-0.035625
21	6	0	2.990306	-1.412006	-0.525958
22	1	0	3.669343	-1.511348	0.320522
23	6	0	2.647404	-2.819545	-0.999491
24	1	0	3.555402	-3.362223	-1.266882
25	1	0	2.132999	-3.375039	-0.214203
26	1	0	2.001793	-2.786616	-1.877545
27	6	0	3.711576	-0.614320	-1.605395
28	1	0	4.626986	-1.123578	-1.910557
29	1	0	3.076565	-0.499007	-2.484496
30	1	0	3.975758	0.379020	-1.240598
31	6	0	1.824797	-0.293147	1.377977
32	1	0	0.899884	0.257850	1.547477
33	6	0	1.821550	-1.504206	2.305487
34	1	0	1.779543	-1.180864	3.346297
35	1	0	0.953988	-2.134315	2.107112
36	1	0	2.722924	-2.108123	2.183849
37	6	0	2.988856	0.645887	1.683362
38	1	0	2.904030	1.019153	2.704873
39	1	0	3.953579	0.142597	1.599510
40	1	0	2.988664	1.502427	1.008464
41	1	0	0.784497	-0.824197	-2.001899
42	6	0	0.242544	3.491485	-1.579009
43	1	0	1.118304	4.128775	-1.713008
44	1	0	0.078211	2.935258	-2.502406
45	1	0	-0.620875	4.140390	-1.419841
46	6	0	0.720846	3.336622	0.885462
47	1	0	0.843776	2.675878	1.744832
48	1	0	1.630813	3.929828	0.778081
49	1	0	-0.096865	4.024607	1.107878

TS Substituent-side **10e**



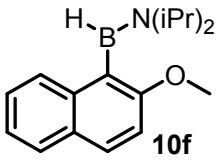
TS Sub 10e



Sum of electronic and thermal Free Energies (Hartrees): -820.076792

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.703375	0.308798	-0.252156
2	6	0	-1.490374	-0.903955	-0.147212
3	6	0	-1.061037	-2.163498	-0.631838
4	1	0	-0.168215	-2.212189	-1.226889
5	6	0	-1.802723	-3.304676	-0.479784
6	1	0	-1.438545	-4.237254	-0.890832
7	6	0	-3.047328	-3.267432	0.174550
8	1	0	-3.619699	-4.174861	0.312169
9	6	0	-3.544432	-2.060380	0.575775
10	1	0	-4.529581	-1.988999	1.020798
11	6	0	-2.808323	-0.866809	0.387633
12	6	0	-3.402054	0.385123	0.667686
13	1	0	-4.400231	0.413048	1.087749
14	6	0	-2.746278	1.528286	0.341529
15	1	0	-3.238772	2.481595	0.482936
16	6	0	-1.406974	1.510650	-0.130738
17	6	0	-0.831209	2.872853	-0.495643
18	1	0	0.124083	2.721741	-0.990935
19	5	0	0.882067	0.496860	-0.088027
20	7	0	2.060764	-0.265054	-0.047112
21	6	0	3.284465	0.414469	0.460077
22	1	0	4.073857	-0.334703	0.458153
23	6	0	3.743454	1.541938	-0.456727
24	1	0	4.704426	1.933306	-0.118364
25	1	0	3.859487	1.184307	-1.480313
26	1	0	3.026423	2.362885	-0.459151
27	6	0	3.136241	0.879974	1.904100
28	1	0	4.096436	1.234931	2.282746
29	1	0	2.417832	1.694976	1.986434
30	1	0	2.797656	0.060522	2.539056
31	6	0	2.300810	-1.667338	-0.399049
32	1	0	1.377986	-2.042280	-0.806381
33	6	0	3.350433	-1.822193	-1.499128
34	1	0	3.396590	-2.865691	-1.813582
35	1	0	3.087539	-1.216460	-2.366774
36	1	0	4.350947	-1.537744	-1.171767
37	6	0	2.623834	-2.517743	0.826453
38	1	0	2.720990	-3.565800	0.539348
39	1	0	3.560750	-2.217227	1.298560
40	1	0	1.824602	-2.437075	1.563835
41	1	0	1.117677	1.608313	0.251407
42	6	0	-1.730882	3.589062	-1.508812
43	1	0	-1.240043	4.500250	-1.854449
44	1	0	-1.928535	2.958798	-2.376517
45	1	0	-2.689539	3.878015	-1.076798
46	6	0	-0.607295	3.749800	0.735680
47	1	0	0.072148	3.272626	1.442588
48	1	0	-0.184414	4.714211	0.448579
49	1	0	-1.549263	3.940273	1.253935

Compound **10f**



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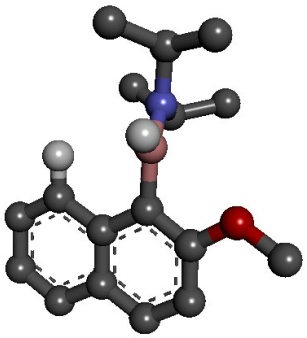
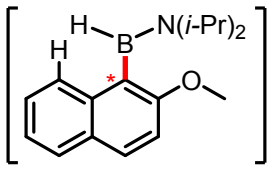


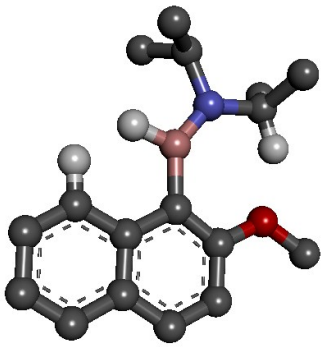
Sum of electronic and thermal Free Energies (Hartrees): -816.76382

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.584534	0.532278	-0.427624
2	6	0	1.579128	-0.478003	-0.343506
3	6	0	1.278933	-1.842019	-0.610865
4	1	0	0.266536	-2.105392	-0.893717
5	6	0	2.239651	-2.808655	-0.521880
6	1	0	1.988857	-3.840447	-0.731311
7	6	0	3.565189	-2.473342	-0.162122
8	1	0	4.316328	-3.248959	-0.095389
9	6	0	3.890817	-1.172971	0.095350
10	1	0	4.903875	-0.902529	0.368449
11	6	0	2.915597	-0.147796	0.012088
12	6	0	3.231148	1.202222	0.274432
13	1	0	4.247400	1.460351	0.545985
14	6	0	2.277708	2.178949	0.191799
15	1	0	2.544098	3.204812	0.399375
16	6	0	0.953079	1.833388	-0.160871
17	5	0	-0.905572	0.253648	-0.871451
18	7	0	-1.852110	-0.343855	-0.046679
19	6	0	-3.242314	-0.545828	-0.502578
20	1	0	-3.791378	-0.976348	0.334593
21	6	0	-3.915125	0.775327	-0.856686
22	1	0	-4.968159	0.614110	-1.093063
23	1	0	-3.849633	1.475196	-0.022937
24	1	0	-3.436762	1.232930	-1.722736
25	6	0	-3.308114	-1.538915	-1.656206
26	1	0	-4.344443	-1.727502	-1.940894
27	1	0	-2.780962	-1.148472	-2.527436
28	1	0	-2.850218	-2.488270	-1.375254
29	6	0	-1.570174	-0.738990	1.341243
30	1	0	-0.506459	-0.559467	1.492001
31	6	0	-2.334503	0.132821	2.333246
32	1	0	-2.058963	-0.129894	3.355394
33	1	0	-2.100647	1.185602	2.172143
34	1	0	-3.414189	0.000848	2.238201
35	6	0	-1.825335	-2.223858	1.583188
36	1	0	-1.509739	-2.492025	2.592084
37	1	0	-2.882285	-2.479932	1.492151
38	1	0	-1.259901	-2.835120	0.879665
39	1	0	-1.238533	0.566878	-1.974601
40	6	0	0.274537	4.118756	-0.055365
41	1	0	-0.648814	4.672047	-0.206415
42	1	0	0.639607	4.305205	0.957706
43	1	0	1.018628	4.461678	-0.778440
44	8	0	-0.045020	2.759157	-0.247925

TS H-side **10f**



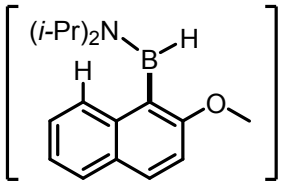
TS H 10f



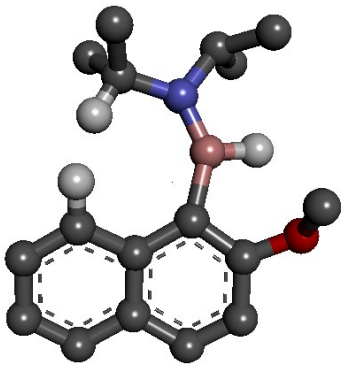
Sum of electronic and thermal Free Energies (Hartrees): -816.741008

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.702628	0.243280	0.000160
2	6	0	1.977945	-0.454417	0.000086
3	6	0	2.118290	-1.874766	0.000183
4	1	0	1.246387	-2.502616	0.000370
5	6	0	3.338904	-2.491416	0.000075
6	1	0	3.380351	-3.573101	0.000161
7	6	0	4.536211	-1.750401	-0.000128
8	1	0	5.493473	-2.253741	-0.000208
9	6	0	4.458397	-0.390578	-0.000187
10	1	0	5.355583	0.216698	-0.000313
11	6	0	3.206238	0.272581	-0.000078
12	6	0	3.176436	1.680177	-0.000122
13	1	0	4.112291	2.225539	-0.000261
14	6	0	1.993955	2.349786	-0.000001
15	1	0	1.993340	3.428474	-0.000045
16	6	0	0.775734	1.632219	0.000134
17	5	0	-0.620283	-0.649838	0.000196
18	7	0	-2.015847	-0.483236	0.000054
19	6	0	-2.833586	-1.728063	0.000026
20	1	0	-3.874251	-1.410706	-0.000301
21	6	0	-2.633068	-2.557358	-1.263141
22	1	0	-3.346631	-3.383046	-1.286612
23	1	0	-2.786222	-1.945565	-2.152802
24	1	0	-1.628541	-2.977155	-1.306881
25	6	0	-2.633685	-2.556946	1.263559
26	1	0	-3.347080	-3.382784	1.286847
27	1	0	-1.629086	-2.976504	1.308015
28	1	0	-2.787500	-1.944926	2.152949
29	6	0	-2.845905	0.730482	-0.000243
30	1	0	-2.161195	1.561368	-0.000072
31	6	0	-3.693937	0.842582	-1.266179
32	1	0	-4.217768	1.799922	-1.273839
33	1	0	-3.060996	0.794289	-2.152940
34	1	0	-4.449574	0.058731	-1.340730
35	6	0	-3.694716	0.842731	1.265158
36	1	0	-4.218435	1.800135	1.272431
37	1	0	-4.450497	0.058981	1.339288
38	1	0	-3.062340	0.794420	2.152319
39	1	0	-0.369132	-1.803937	0.000377
40	6	0	-0.387514	3.734534	0.000392
41	1	0	-1.434017	4.032242	0.000350
42	1	0	0.095300	4.136871	0.893365
43	1	0	0.095439	4.137158	-0.892373
44	8	0	-0.388815	2.324317	0.000173

TS Substituent-side **10f**



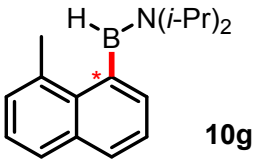
TS Sub 10f



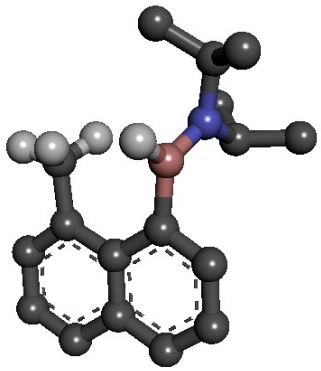
Sum of electronic and thermal Free Energies (Hartrees): -816.728963

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.702765	0.651342	-0.094850
2	6	0	-1.739980	-0.360670	-0.085612
3	6	0	-1.542621	-1.689847	-0.532148
4	1	0	-0.619915	-1.942296	-1.019509
5	6	0	-2.523463	-2.643636	-0.470976
6	1	0	-2.323481	-3.638558	-0.847027
7	6	0	-3.794057	-2.333680	0.044950
8	1	0	-4.559734	-3.094895	0.108480
9	6	0	-4.057241	-1.045014	0.412625
10	1	0	-5.043469	-0.760451	0.759044
11	6	0	-3.066467	-0.039415	0.324025
12	6	0	-3.408688	1.307620	0.592318
13	1	0	-4.417692	1.541812	0.908535
14	6	0	-2.494053	2.288875	0.391812
15	1	0	-2.734791	3.334786	0.524038
16	6	0	-1.164809	1.958913	0.035704
17	5	0	0.883123	0.563012	0.118291
18	7	0	1.932113	-0.365824	0.071151
19	6	0	3.278229	0.118025	0.484171
20	1	0	3.961356	-0.717133	0.341155
21	6	0	3.788014	1.250748	-0.399609
22	1	0	4.832842	1.463501	-0.166909
23	1	0	3.720762	0.977184	-1.453648
24	1	0	3.215717	2.164751	-0.242611
25	6	0	3.329113	0.486123	1.961841
26	1	0	4.352622	0.727385	2.254231
27	1	0	2.702436	1.353032	2.169398
28	1	0	2.981671	-0.342928	2.578924
29	6	0	1.932636	-1.778156	-0.319217
30	1	0	0.911458	-2.029982	-0.549516
31	6	0	2.757699	-2.026250	-1.579985
32	1	0	2.657940	-3.066979	-1.891367
33	1	0	2.410268	-1.389970	-2.394589
34	1	0	3.819795	-1.832518	-1.423229
35	6	0	2.348157	-2.697853	0.827717
36	1	0	2.229661	-3.738736	0.523622
37	1	0	3.390118	-2.559214	1.119063
38	1	0	1.719162	-2.523917	1.701027
39	1	0	1.269487	1.611259	0.517911
40	6	0	0.261639	3.209602	-1.369965
41	1	0	0.832248	4.134950	-1.325300
42	1	0	0.938128	2.384563	-1.599007
43	1	0	-0.491110	3.283133	-2.159747
44	8	0	-0.362992	3.058322	-0.107413

Compound **10g**



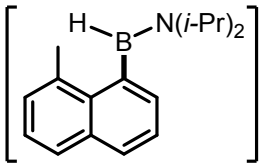
10g



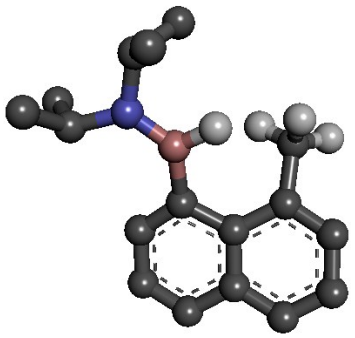
Sum of electronic and thermal Free Energies (Hartrees): -741.549737

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.529179	0.592234	-0.610946
2	6	0	-1.745685	-0.083262	-0.269154
3	6	0	-1.829270	-1.503190	-0.085445
4	6	0	-3.030328	-2.069405	0.257373
5	1	0	-3.082803	-3.142276	0.395689
6	6	0	-4.198143	-1.300072	0.433506
7	1	0	-5.125587	-1.788250	0.702538
8	6	0	-4.148594	0.050199	0.263678
9	1	0	-5.033423	0.661031	0.393635
10	6	0	-2.931842	0.686277	-0.087109
11	6	0	-2.897180	2.090608	-0.257364
12	1	0	-3.813336	2.651345	-0.118057
13	6	0	-1.734049	2.719968	-0.589025
14	1	0	-1.707047	3.793874	-0.720460
15	6	0	-0.558559	1.963301	-0.758678
16	5	0	0.877498	-0.061410	-0.917625
17	7	0	1.965777	0.046495	-0.055843
18	6	0	3.299064	-0.452302	-0.451285
19	1	0	3.977857	-0.231808	0.372356
20	6	0	3.292882	-1.963475	-0.649462
21	1	0	4.298032	-2.323893	-0.873777
22	1	0	2.938928	-2.471154	0.248758
23	1	0	2.640242	-2.239515	-1.478779
24	6	0	3.827745	0.275637	-1.681059
25	1	0	4.848115	-0.041574	-1.901739
26	1	0	3.209688	0.062591	-2.553504
27	1	0	3.829285	1.354099	-1.517886
28	6	0	1.872255	0.614864	1.297367
29	1	0	0.827932	0.891993	1.433359
30	6	0	2.220311	-0.410810	2.372865
31	1	0	2.061992	0.021419	3.361533
32	1	0	1.588024	-1.294897	2.285476
33	1	0	3.263254	-0.727135	2.316117
34	6	0	2.710597	1.881524	1.437734
35	1	0	2.566878	2.318546	2.426653
36	1	0	3.776672	1.678821	1.319461
37	1	0	2.417739	2.620517	0.691496
38	1	0	1.059605	-0.570992	-1.981607
39	6	0	-0.633298	-2.395987	-0.266464
40	1	0	0.193354	-2.105097	0.384234
41	1	0	-0.893963	-3.426848	-0.032100
42	1	0	-0.265782	-2.370966	-1.293060
43	1	0	0.356048	2.485092	-1.020499

TS H-side **10g**



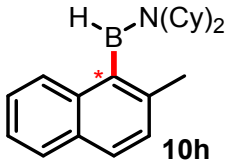
TS H 10g



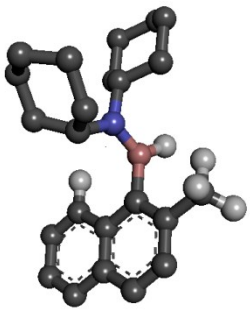
Sum of electronic and thermal Free Energies (Hartrees): -741.522529

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.540912	0.559441	-0.213653
2	6	0	-1.868405	-0.007890	-0.065522
3	6	0	-2.195589	-1.394059	-0.257617
4	6	0	-3.461294	-1.832488	0.054252
5	1	0	-3.698678	-2.877190	-0.109154
6	6	0	-4.474536	-0.973738	0.513282
7	1	0	-5.449220	-1.371801	0.762117
8	6	0	-4.234319	0.366636	0.552513
9	1	0	-5.017752	1.068786	0.809391
10	6	0	-2.953925	0.872310	0.225078
11	6	0	-2.772666	2.274019	0.134366
12	1	0	-3.619680	2.918357	0.336600
13	6	0	-1.572741	2.789203	-0.248664
14	1	0	-1.444519	3.854670	-0.386257
15	6	0	-0.467253	1.927621	-0.389817
16	5	0	0.728411	-0.350031	0.060606
17	7	0	2.097376	-0.047324	0.101988
18	6	0	3.057631	-1.174157	0.185018
19	1	0	4.046149	-0.753425	0.006141
20	6	0	3.065357	-1.819226	1.565611
21	1	0	3.818272	-2.607736	1.613987
22	1	0	3.285809	-1.085771	2.340615
23	1	0	2.092967	-2.262869	1.782065
24	6	0	2.829319	-2.210049	-0.911685
25	1	0	3.648360	-2.931139	-0.920474
26	1	0	1.900519	-2.758315	-0.754712
27	1	0	2.783282	-1.729524	-1.890017
28	6	0	2.719335	1.280940	0.027590
29	1	0	1.937013	1.995999	0.250732
30	6	0	3.777754	1.509757	1.107120
31	1	0	4.082060	2.556852	1.085537
32	1	0	3.372126	1.297826	2.096237
33	1	0	4.676070	0.909677	0.963415
34	6	0	3.265873	1.563462	-1.367398
35	1	0	3.681179	2.570761	-1.425989
36	1	0	4.061281	0.860075	-1.623740
37	1	0	2.476536	1.468190	-2.114195
38	1	0	0.498740	-1.471980	0.356874
39	6	0	-1.292842	-2.394874	-0.942046
40	1	0	-0.744997	-3.017860	-0.235674
41	1	0	-1.905656	-3.054112	-1.557042
42	1	0	-0.565539	-1.911930	-1.591772
43	1	0	0.477276	2.392435	-0.622192

Compound **10h**



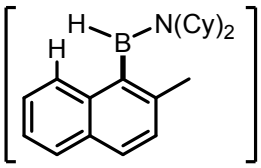
10h



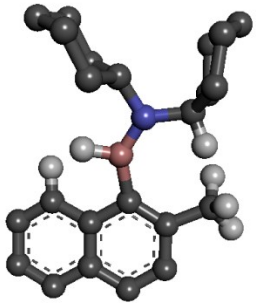
Sum of electronic and thermal Free Energies (Hartrees): -974.87997

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.730141	1.040089	0.074202
2	6	0	2.645344	0.137887	-0.556397
3	6	0	2.227612	-0.746900	-1.583970
4	1	0	1.190637	-0.730000	-1.898730
5	6	0	3.106177	-1.610268	-2.179235
6	1	0	2.765425	-2.274995	-2.962228
7	6	0	4.458896	-1.637994	-1.780101
8	1	0	5.146283	-2.324127	-2.256876
9	6	0	4.896061	-0.797345	-0.794825
10	1	0	5.933119	-0.809001	-0.481455
11	6	0	4.007898	0.104661	-0.161839
12	6	0	4.441656	0.980750	0.863417
13	1	0	5.481127	0.958621	1.167497
14	6	0	3.561122	1.836619	1.452485
15	1	0	3.898687	2.505472	2.236122
16	6	0	2.196590	1.878701	1.063170
17	6	0	1.290588	2.844634	1.780544
18	1	0	0.318262	2.935423	1.296502
19	5	0	0.219138	1.117028	-0.385369
20	7	0	-0.753611	0.190460	-0.018221
21	6	0	-2.151346	0.362156	-0.451733
22	1	0	-2.718267	-0.470228	-0.044713
23	6	0	-2.780535	1.638266	0.108343
24	1	0	-2.677324	1.641436	1.196499
25	1	0	-2.227760	2.502083	-0.271165
26	6	0	-2.305362	0.295835	-1.971237
27	1	0	-1.731217	1.108392	-2.424187
28	1	0	-1.878856	-0.642723	-2.333909
29	6	0	-0.446463	-0.946811	0.864447
30	1	0	0.634279	-0.907667	0.981062
31	6	0	-1.034497	-0.804063	2.279961
32	1	0	-0.391477	-1.384593	2.949004
33	1	0	-0.948962	0.238985	2.591453
34	6	0	-0.756569	-2.332008	0.262792
35	1	0	-0.049808	-3.027142	0.725690
36	1	0	-0.518051	-2.319751	-0.802513
37	1	0	-0.115707	2.030232	-1.079978
38	6	0	-2.462089	-1.321589	2.459822
39	1	0	-2.726960	-1.271452	3.517681
40	1	0	-3.181176	-0.686208	1.936934
41	6	0	-2.162473	-2.893277	0.500403
42	1	0	-2.170090	-3.945338	0.208710
43	1	0	-2.899694	-2.402980	-0.138518
44	6	0	-2.579573	-2.761831	1.964213
45	1	0	-1.928049	-3.395168	2.575719
46	1	0	-3.597049	-3.131608	2.100886
47	6	0	-4.247924	1.748919	-0.299188
48	1	0	-4.811616	0.925285	0.152778
49	1	0	-4.676338	2.673650	0.090549
50	6	0	-3.773166	0.413140	-2.377740
51	1	0	-4.323246	-0.454737	-1.997998
52	1	0	-3.862602	0.390147	-3.464939
53	6	0	-4.402691	1.685860	-1.816751
54	1	0	-3.910505	2.555855	-2.263030
55	1	0	-5.457011	1.740375	-2.093121
56	1	0	1.118645	2.522079	2.810255
57	1	0	1.738502	3.838733	1.825712

TS H-side **10h**



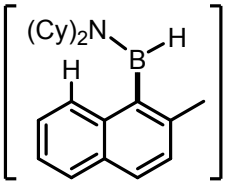
TS H 10h



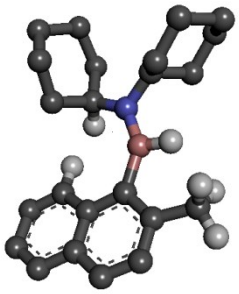
Sum of electronic and thermal Free Energies (Hartrees): -974.842464

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.852608	-0.676011	-0.045657
2	6	0	2.980538	0.243336	0.083589
3	6	0	2.846589	1.590104	0.529101
4	1	0	1.879421	1.962488	0.821580
5	6	0	3.918775	2.431555	0.648828
6	1	0	3.762992	3.440495	1.008236
7	6	0	5.219020	2.001180	0.322842
8	1	0	6.056306	2.681369	0.403349
9	6	0	5.404646	0.706863	-0.063299
10	1	0	6.396273	0.330406	-0.283655
11	6	0	4.313171	-0.190892	-0.158008
12	6	0	4.547937	-1.551188	-0.448645
13	1	0	5.558819	-1.883174	-0.652081
14	6	0	3.517564	-2.433307	-0.404865
15	1	0	3.710099	-3.488071	-0.557218
16	6	0	2.175856	-2.024430	-0.181084
17	6	0	1.210928	-3.180924	-0.086328
18	1	0	0.460705	-3.022927	0.683296
19	5	0	0.439120	0.074866	-0.175256
20	7	0	-0.931951	-0.231119	-0.210955
21	6	0	-1.874697	0.910216	-0.192760
22	1	0	-2.870973	0.483253	-0.132560
23	6	0	-1.726594	1.796210	1.046271
24	1	0	-1.762959	1.171560	1.942189
25	1	0	-0.747341	2.280864	1.031786
26	6	0	-1.841031	1.753585	-1.468459
27	1	0	-0.860702	2.226251	-1.563178
28	1	0	-1.969494	1.104120	-2.336573
29	6	0	-1.553218	-1.561668	-0.212496
30	1	0	-0.773173	-2.211981	-0.568199
31	6	0	-1.956088	-2.048472	1.189100
32	1	0	-1.934804	-3.144268	1.178923
33	1	0	-1.196423	-1.723003	1.902885
34	6	0	-2.701692	-1.760920	-1.230963
35	1	0	-2.642643	-2.811951	-1.529062
36	1	0	-2.488665	-1.179443	-2.129455
37	1	0	0.593771	1.237951	-0.330124
38	6	0	-3.353473	-1.620090	1.632452
39	1	0	-3.561949	-2.033080	2.620879
40	1	0	-3.411087	-0.532358	1.733096
41	6	0	-4.142090	-1.520043	-0.758128
42	1	0	-4.821529	-1.974420	-1.481981
43	1	0	-4.389203	-0.456922	-0.749614
44	6	0	-4.396287	-2.104756	0.628859
45	1	0	-4.348706	-3.197598	0.575967
46	1	0	-5.402717	-1.848408	0.963353
47	6	0	-2.819924	2.862251	1.079795
48	1	0	-3.797189	2.375254	1.172681
49	1	0	-2.699415	3.495294	1.960404
50	6	0	-2.927605	2.827721	-1.434293
51	1	0	-3.911827	2.346694	-1.432116
52	1	0	-2.878493	3.436791	-2.338360
53	6	0	-2.800891	3.706567	-0.192246
54	1	0	-1.857029	4.259070	-0.239715
55	1	0	-3.602096	4.447226	-0.168666
56	1	0	0.712397	-3.387057	-1.035227
57	1	0	1.761444	-4.082253	0.180490

TS Substituent-side **10h**



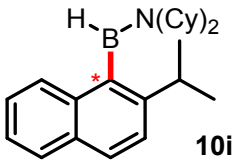
TS Sub 10h



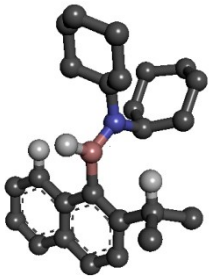
Sum of electronic and thermal Free Energies (Hartrees): -974.841442

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.720800	-1.068808	-0.254201
2	6	0	-2.748263	-0.046663	-0.215854
3	6	0	-2.542839	1.285784	-0.649641
4	1	0	-1.596772	1.550884	-1.075665
5	6	0	-3.517486	2.244664	-0.592651
6	1	0	-3.303026	3.243858	-0.949496
7	6	0	-4.795197	1.941263	-0.087711
8	1	0	-5.558205	2.706042	-0.032814
9	6	0	-5.059563	0.660638	0.301416
10	1	0	-6.042860	0.383431	0.661809
11	6	0	-4.069357	-0.348330	0.223370
12	6	0	-4.402759	-1.681195	0.541917
13	1	0	-5.406229	-1.908554	0.880968
14	6	0	-3.481506	-2.663780	0.373178
15	1	0	-3.756149	-3.693164	0.565790
16	6	0	-2.149158	-2.384246	-0.027878
17	6	0	-1.287831	-3.622252	-0.177537
18	1	0	-0.622828	-3.764179	0.675668
19	5	0	-0.120834	-0.945231	-0.306552
20	7	0	0.903894	0.020543	-0.375276
21	6	0	2.281011	-0.478787	-0.147857
22	1	0	2.930384	0.389195	-0.135917
23	6	0	2.485650	-1.160338	1.207737
24	1	0	2.120026	-0.506895	2.002598
25	1	0	1.897551	-2.079007	1.252984
26	6	0	2.784986	-1.377482	-1.279436
27	1	0	2.186001	-2.291828	-1.303641
28	1	0	2.637748	-0.872334	-2.236461
29	6	0	0.760592	1.463402	-0.665976
30	1	0	0.020139	1.512265	-1.457038
31	6	0	0.242460	2.239050	0.554158
32	1	0	-0.263529	3.145357	0.203000
33	1	0	-0.509713	1.634791	1.061500
34	6	0	1.981628	2.179030	-1.290961
35	1	0	1.553621	2.993702	-1.881783
36	1	0	2.472371	1.516955	-2.007035
37	1	0	0.361423	-2.008973	-0.135675
38	6	0	1.352982	2.649331	1.514817
39	1	0	0.921317	3.149777	2.382712
40	1	0	1.870990	1.759430	1.887892
41	6	0	3.011682	2.816977	-0.347951
42	1	0	3.633709	3.498807	-0.931185
43	1	0	3.693276	2.072843	0.068688
44	6	0	2.350788	3.559661	0.808174
45	1	0	1.821435	4.440134	0.429560
46	1	0	3.111249	3.920066	1.502605
47	6	0	3.961695	-1.497197	1.415035
48	1	0	4.545615	-0.570626	1.445289
49	1	0	4.100952	-1.987817	2.379766
50	6	0	4.257366	-1.730432	-1.074627
51	1	0	4.858182	-0.816457	-1.138542
52	1	0	4.600520	-2.388144	-1.874962
53	6	0	4.485827	-2.382825	0.286827
54	1	0	3.961379	-3.343382	0.315411
55	1	0	5.546408	-2.595516	0.432058
56	1	0	-1.929142	-4.500151	-0.243013
57	1	0	-0.670381	-3.592942	-1.071467

Compound **10i**



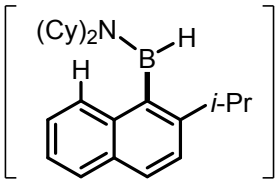
10i



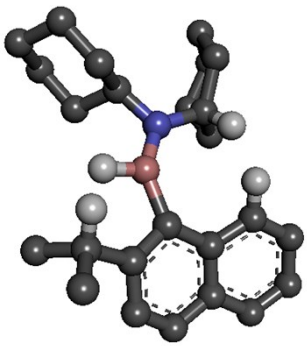
Sum of electronic and thermal Free Energies (Hartrees): -1053.443118

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.693748	0.089758	-0.524131
2	6	0	-2.573223	-0.977783	-0.152175
3	6	0	-2.111668	-2.315516	-0.044827
4	1	0	-1.069895	-2.531823	-0.253111
5	6	0	-2.953722	-3.331178	0.316521
6	1	0	-2.580179	-4.344104	0.389740
7	6	0	-4.310622	-3.065812	0.596427
8	1	0	-4.968372	-3.875503	0.883463
9	6	0	-4.788776	-1.788571	0.504097
10	1	0	-5.828965	-1.573260	0.717512
11	6	0	-3.939346	-0.720506	0.128956
12	6	0	-4.414561	0.609339	0.024712
13	1	0	-5.458326	0.811263	0.233132
14	6	0	-3.568815	1.615594	-0.332993
15	1	0	-3.949274	2.627088	-0.411421
16	6	0	-2.196931	1.370871	-0.608444
17	6	0	-1.322851	2.545560	-1.003761
18	1	0	-0.300783	2.176066	-1.117064
19	5	0	-0.202204	-0.272110	-0.906886
20	7	0	0.902224	-0.062571	-0.084440
21	6	0	2.247374	-0.473603	-0.525132
22	1	0	2.937647	-0.226462	0.275731
23	6	0	2.354977	-1.983134	-0.742327
24	1	0	2.045161	-2.498514	0.170564
25	1	0	1.661347	-2.280111	-1.533502
26	6	0	2.715950	0.295835	-1.760179
27	1	0	2.032914	0.089705	-2.588664
28	1	0	2.661473	1.368204	-1.555836
29	6	0	0.777726	0.550833	1.247157
30	1	0	-0.278235	0.805697	1.322142
31	6	0	1.068729	-0.414844	2.411049
32	1	0	0.509443	-0.040121	3.273998
33	1	0	0.648741	-1.393476	2.171300
34	6	0	1.550544	1.874085	1.415182
35	1	0	1.017717	2.442937	2.183799
36	1	0	1.471418	2.455130	0.493706
37	1	0	-0.012185	-0.788739	-1.968154
38	6	0	-1.757190	3.133772	-2.347311
39	1	0	-1.099714	3.954885	-2.638239
40	1	0	-1.731841	2.378512	-3.133476
41	1	0	-2.774864	3.525181	-2.290600
42	6	0	-1.307414	3.626274	0.078461
43	1	0	-1.030327	3.212458	1.048846
44	1	0	-0.593121	4.411931	-0.174340
45	1	0	-2.288727	4.093026	0.182221
46	6	0	2.534178	-0.529970	2.835257
47	1	0	2.590653	-1.129332	3.745956
48	1	0	3.121350	-1.066068	2.086166
49	6	0	3.008116	1.764162	1.871751
50	1	0	3.370845	2.763000	2.122318
51	1	0	3.651516	1.407785	1.064934
52	6	0	3.139800	0.849549	3.088491
53	1	0	2.615185	1.310754	3.932085
54	1	0	4.186984	0.758087	3.381306
55	6	0	3.777542	-2.379405	-1.131933
56	1	0	4.454813	-2.158954	-0.299447
57	1	0	3.832100	-3.455375	-1.304657
58	6	0	4.136575	-0.107552	-2.150060
59	1	0	4.827148	0.186790	-1.352181
60	1	0	4.445373	0.431401	-3.047141
61	6	0	4.242773	-1.614727	-2.368678
62	1	0	3.617574	-1.898234	-3.221337
63	1	0	5.268370	-1.889450	-2.620890

TS Substituent-side **10i**



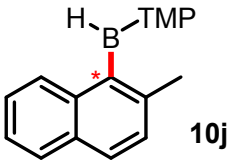
TS Sub 10i



Sum of electronic and thermal Free Energies (Hartrees): -1053.403063

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.692527	0.468380	-0.339226
2	6	0	2.493517	-0.736956	-0.228956
3	6	0	2.124086	-1.974008	-0.808920
4	1	0	1.243445	-2.016489	-1.421024
5	6	0	2.885397	-3.105381	-0.684325
6	1	0	2.563606	-4.020337	-1.164867
7	6	0	4.087875	-3.083738	0.044752
8	1	0	4.676482	-3.984511	0.155396
9	6	0	4.517582	-1.899253	0.570910
10	1	0	5.463722	-1.837583	1.094956
11	6	0	3.761432	-0.713660	0.416019
12	6	0	4.288582	0.523003	0.850781
13	1	0	5.241919	0.539278	1.365139
14	6	0	3.631802	1.673547	0.557032
15	1	0	4.079529	2.620780	0.826748
16	6	0	2.353471	1.672016	-0.063289
17	6	0	1.809263	3.057730	-0.395097
18	1	0	0.956500	2.944610	-1.056875
19	5	0	0.097776	0.628328	-0.397361
20	7	0	-1.058881	-0.175396	-0.435332
21	6	0	-2.339810	0.505342	-0.134629
22	1	0	-3.103718	-0.264065	-0.111952
23	6	0	-2.386199	1.170726	1.243277
24	1	0	-2.078759	0.452052	2.005745
25	1	0	-1.673915	1.997437	1.277167
26	6	0	-2.759993	1.498572	-1.220361
27	1	0	-2.039847	2.320677	-1.251711
28	1	0	-2.727785	1.006528	-2.194733
29	6	0	-1.131725	-1.620556	-0.733214
30	1	0	-0.400438	-1.773831	-1.516018
31	6	0	-0.738905	-2.479112	0.477014
32	1	0	-0.364680	-3.441983	0.112065
33	1	0	0.090001	-1.996479	0.994970
34	6	0	-2.444191	-2.133210	-1.373590
35	1	0	-2.141400	-2.985288	-1.988523
36	1	0	-2.831687	-1.385303	-2.068183
37	1	0	-0.209525	1.752092	-0.195847
38	6	0	1.356927	3.803068	0.859995
39	1	0	0.964275	4.788585	0.602764
40	1	0	0.581304	3.249648	1.390151
41	1	0	2.193552	3.945988	1.547240
42	6	0	2.838191	3.889754	-1.168882
43	1	0	3.223627	3.342809	-2.030023
44	1	0	2.365837	4.804098	-1.531547
45	1	0	3.685437	4.186638	-0.550164
46	6	0	-1.902657	-2.743794	1.426245
47	1	0	-1.552717	-3.318160	2.285189
48	1	0	-2.291279	-1.797139	1.816261
49	6	0	-3.558673	-2.638105	-0.445583
50	1	0	-4.267195	-3.214851	-1.043401
51	1	0	-4.131720	-1.813205	-0.017722
52	6	0	-3.015846	-3.488540	0.698035
53	1	0	-2.614572	-4.427856	0.303640
54	1	0	-3.823968	-3.750801	1.382633
55	6	0	-3.789076	1.704244	1.529397
56	1	0	-4.495621	0.867690	1.567790
57	1	0	-3.814426	2.182052	2.510151
58	6	0	-4.157409	2.048355	-0.938002
59	1	0	-4.883688	1.230074	-0.994958
60	1	0	-4.438388	2.771140	-1.705831
61	6	0	-4.232485	2.686269	0.447261
62	1	0	-3.577429	3.563137	0.472697
63	1	0	-5.245279	3.040559	0.646949

Compound **10j**



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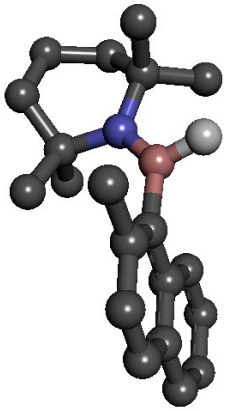
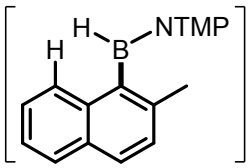


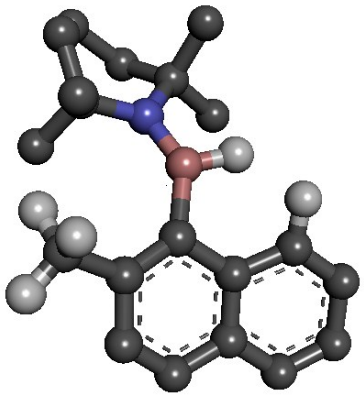
Sum of electronic and thermal Free Energies (Hartrees): -858.205180

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.680136	3.251665	-0.431597
2	1	0	-0.312051	2.965370	-0.781758
3	6	0	1.595122	2.065932	-0.277561
4	6	0	2.942179	2.313516	0.089336
5	1	0	3.260410	3.339453	0.237125
6	6	0	3.831476	1.295118	0.259986
7	1	0	4.857442	1.495808	0.543571
8	6	0	3.426021	-0.045529	0.052539
9	6	0	4.330108	-1.125854	0.193020
10	1	0	5.353105	-0.910901	0.477823
11	6	0	3.927507	-2.412622	-0.030192
12	1	0	4.627858	-3.230228	0.077771
13	6	0	2.594420	-2.676694	-0.409338
14	1	0	2.282285	-3.696078	-0.594902
15	6	0	1.699315	-1.651368	-0.545198
16	1	0	0.678080	-1.864826	-0.837952
17	6	0	2.078900	-0.303163	-0.314235
18	6	0	1.148483	0.774990	-0.453442
19	5	0	-0.325602	0.489264	-0.950524
20	7	0	-1.446704	0.043805	-0.242758
21	6	0	-2.695596	-0.234015	-1.046549
22	6	0	-3.721658	-1.045985	-0.245550
23	1	0	-4.615262	-1.128422	-0.865458
24	1	0	-3.344050	-2.062282	-0.136407
25	6	0	-4.081564	-0.459094	1.117702
26	1	0	-4.963942	0.176868	1.036536
27	1	0	-4.351957	-1.271687	1.793335
28	6	0	-2.928552	0.351531	1.705493
29	1	0	-2.955878	0.305334	2.794730
30	1	0	-3.028275	1.406120	1.439419
31	6	0	-1.536939	-0.102644	1.244787
32	6	0	-2.372980	-1.080377	-2.284163
33	1	0	-1.821289	-0.529094	-3.040330
34	1	0	-3.304812	-1.424034	-2.736649
35	1	0	-1.790301	-1.958662	-2.001118
36	6	0	-3.322169	1.089746	-1.493149
37	1	0	-3.633419	1.695922	-0.642466
38	1	0	-4.199027	0.900795	-2.115704
39	1	0	-2.607133	1.667042	-2.079782
40	6	0	-1.249397	-1.543728	1.681199
41	1	0	-1.343343	-1.625178	2.766193
42	1	0	-0.228122	-1.815805	1.413157
43	1	0	-1.922782	-2.269044	1.231395
44	6	0	-0.538092	0.801293	1.970436
45	1	0	-0.597833	1.827053	1.605427
46	1	0	0.487242	0.455267	1.876541
47	1	0	-0.788488	0.803596	3.032268
48	1	0	-0.473610	0.672061	-2.120212
49	1	0	1.092629	3.971177	-1.141611
50	1	0	0.557137	3.775109	0.519835

TS H-side **10j**



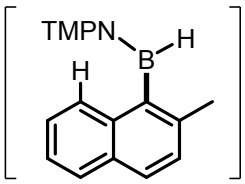
TS H-side 10j



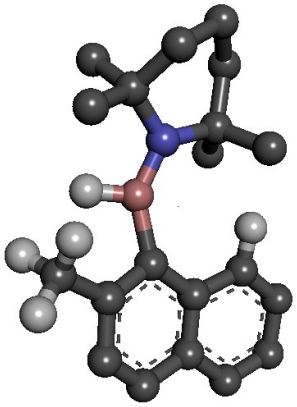
Sum of electronic and thermal Free Energies (Hartrees): -858.154786

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.452883	3.112590	0.506755
2	1	0	-0.440242	3.230106	1.591933
3	6	0	-1.362367	1.966431	0.124669
4	6	0	-2.562328	2.412762	-0.491216
5	1	0	-2.648492	3.463493	-0.735642
6	6	0	-3.579267	1.572897	-0.810532
7	1	0	-4.459792	1.933254	-1.328385
8	6	0	-3.523237	0.228875	-0.395615
9	6	0	-4.651991	-0.606138	-0.589598
10	1	0	-5.497482	-0.199806	-1.131406
11	6	0	-4.689175	-1.868935	-0.080668
12	1	0	-5.556500	-2.500060	-0.220136
13	6	0	-3.588782	-2.322531	0.671404
14	1	0	-3.627447	-3.295070	1.144749
15	6	0	-2.471128	-1.549991	0.828709
16	1	0	-1.682342	-1.941842	1.445831
17	6	0	-2.352515	-0.243909	0.263527
18	6	0	-1.162738	0.606639	0.395319
19	5	0	0.165384	-0.300922	0.548649
20	7	0	1.540953	-0.251083	0.214231
21	6	0	2.193837	-1.552670	-0.170617
22	6	0	3.249606	-1.274094	-1.252888
23	1	0	3.672809	-2.230383	-1.561949
24	1	0	2.715661	-0.879127	-2.120214
25	6	0	4.366678	-0.319347	-0.838368
26	1	0	5.223214	-0.881088	-0.463296
27	1	0	4.720660	0.225536	-1.714142
28	6	0	3.893942	0.639639	0.249334
29	1	0	4.426828	1.590902	0.185001
30	1	0	4.133240	0.230009	1.228662
31	6	0	2.391180	0.967080	0.211623
32	6	0	1.201827	-2.526572	-0.828916
33	1	0	0.551028	-3.021197	-0.112850
34	1	0	1.766839	-3.302835	-1.347492
35	1	0	0.577215	-2.011922	-1.560638
36	6	0	2.795305	-2.254497	1.049673
37	1	0	3.596376	-1.684977	1.515672
38	1	0	3.196737	-3.229001	0.763228
39	1	0	2.015183	-2.414742	1.795659
40	6	0	2.124546	1.784323	-1.063347
41	1	0	2.490412	2.808278	-0.961737
42	1	0	1.066304	1.805998	-1.314589
43	1	0	2.643001	1.333195	-1.909606
44	6	0	2.125936	1.713640	1.529417
45	1	0	2.618139	1.173166	2.338920
46	1	0	1.073615	1.760528	1.780557
47	1	0	2.525762	2.729301	1.503710
48	1	0	-0.122119	-1.404542	0.821970
49	1	0	-0.841452	4.040291	0.091064
50	1	0	0.570571	3.017573	0.180260

TS Substituent-side **10j**



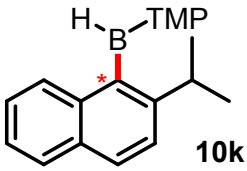
TS Sub-side 10j

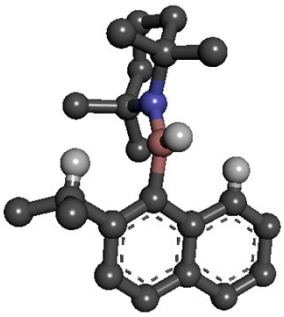


Sum of electronic and thermal Free Energies (Hartrees): -858.159910

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.864938	3.406155	-0.205076
2	1	0	0.487929	3.755495	0.757822
3	6	0	1.708017	2.154128	-0.061758
4	6	0	3.101676	2.414385	-0.072090
5	1	0	3.432210	3.443047	-0.141546
6	6	0	4.016521	1.418555	0.031236
7	1	0	5.077740	1.633402	0.064149
8	6	0	3.585524	0.076742	0.046293
9	6	0	4.554208	-0.956631	0.055051
10	1	0	5.598349	-0.672884	0.107963
11	6	0	4.191985	-2.268594	-0.023696
12	1	0	4.937292	-3.052509	-0.023733
13	6	0	2.825498	-2.580931	-0.136215
14	1	0	2.515586	-3.612145	-0.247860
15	6	0	1.875910	-1.595727	-0.117899
16	1	0	0.857286	-1.893093	-0.236040
17	6	0	2.189387	-0.217127	0.008963
18	6	0	1.202685	0.850140	0.055895
19	5	0	-0.396177	0.889962	0.328203
20	7	0	-1.583336	0.135181	0.166326
21	6	0	-2.881127	0.891193	0.082986
22	6	0	-3.786038	0.182258	-0.938703
23	1	0	-4.692164	0.777061	-1.058706
24	1	0	-3.261833	0.218610	-1.896833
25	6	0	-4.149903	-1.259254	-0.593282
26	1	0	-5.107261	-1.292205	-0.071562
27	1	0	-4.285785	-1.828975	-1.513035
28	6	0	-3.087310	-1.896022	0.296231
29	1	0	-3.034069	-2.973034	0.123085
30	1	0	-3.368783	-1.779504	1.340114
31	6	0	-1.659543	-1.350159	0.102480
32	6	0	-2.695853	2.308872	-0.479134
33	1	0	-2.256513	2.998668	0.236263
34	1	0	-3.675555	2.701739	-0.755145
35	1	0	-2.073730	2.292097	-1.375483
36	6	0	-3.541942	1.024837	1.457462
37	1	0	-3.808577	0.067795	1.898878
38	1	0	-4.451053	1.625193	1.381296
39	1	0	-2.856099	1.531573	2.138406
40	6	0	-1.182000	-1.827932	-1.280992
41	1	0	-0.912552	-2.886208	-1.266620
42	1	0	-0.334516	-1.251902	-1.645303
43	1	0	-1.986101	-1.702803	-2.007220
44	6	0	-0.878080	-1.906018	1.308473
45	1	0	-1.476758	-1.753416	2.207220
46	1	0	0.068047	-1.404691	1.480230
47	1	0	-0.690348	-2.976746	1.202824
48	1	0	-0.651547	1.956616	0.763242
49	1	0	0.008548	3.266672	-0.858964
50	1	0	1.477182	4.202855	-0.626094

Compound **10k**

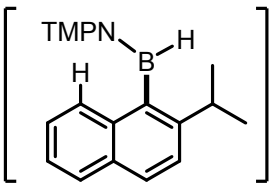




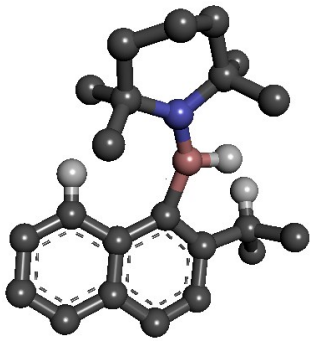
Sum of electronic and thermal Free Energies (Hartrees): -936.768014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.526453	3.749304	-0.974770
2	1	0	-0.435765	3.270811	-1.950680
3	1	0	0.290481	4.464720	-0.869227
4	1	0	-1.457167	4.318572	-0.966502
5	6	0	-0.740951	3.423197	1.506950
6	1	0	-0.029914	4.236402	1.665068
7	1	0	-0.649914	2.718769	2.334668
8	1	0	-1.748186	3.844468	1.533280
9	6	0	-0.484585	2.731853	0.164785
10	1	0	0.526717	2.317817	0.198013
11	6	0	-1.454415	1.576011	-0.011391
12	6	0	-2.789754	1.853544	-0.406614
13	1	0	-3.066686	2.869627	-0.658284
14	6	0	-3.732805	0.871594	-0.469215
15	1	0	-4.746849	1.097044	-0.776422
16	6	0	-3.404165	-0.457806	-0.110136
17	6	0	-4.368991	-1.493989	-0.123455
18	1	0	-5.379681	-1.256888	-0.433487
19	6	0	-4.038218	-2.765357	0.252758
20	1	0	-4.783921	-3.549240	0.242778
21	6	0	-2.719615	-3.057752	0.661903
22	1	0	-2.464854	-4.063750	0.968505
23	6	0	-1.767011	-2.076683	0.671490
24	1	0	-0.755474	-2.311356	0.983396
25	6	0	-2.072953	-0.746928	0.283169
26	6	0	-1.079540	0.282631	0.292638
27	5	0	0.367953	-0.007951	0.865474
28	7	0	1.543511	-0.427393	0.224913
29	6	0	2.803661	-0.376018	1.061117
30	6	0	3.961626	-1.178971	0.450747
31	1	0	4.861146	-0.923043	1.012981
32	1	0	3.775303	-2.244395	0.618350
33	6	0	4.148866	-0.957306	-1.032912
34	1	0	4.370478	0.089772	-1.253048
35	1	0	4.992067	-1.543389	-1.401166
36	6	0	2.865649	-1.395663	-1.701105
37	1	0	2.691683	-2.449222	-1.460470
38	1	0	2.932677	-1.325474	-2.787728
39	6	0	1.636694	-0.583206	-1.270366
40	6	0	2.573737	-0.992484	2.448868
41	1	0	2.020677	-0.343025	3.120880
42	1	0	3.544518	-1.189249	2.906953
43	1	0	2.040133	-1.939947	2.362562
44	6	0	3.236104	1.083067	1.246002
45	1	0	3.518310	1.551966	0.303918
46	1	0	4.093995	1.137600	1.919106
47	1	0	2.422887	1.661995	1.686846
48	6	0	0.430330	-1.347528	-1.822281
49	1	0	0.638754	-1.618049	-2.858949
50	1	0	-0.482890	-0.760854	-1.815310
51	1	0	0.262948	-2.266892	-1.261642
52	6	0	1.674398	0.793826	-1.941575
53	1	0	2.512282	1.401289	-1.601560
54	1	0	0.751867	1.333068	-1.734174
55	1	0	1.756896	0.677871	-3.023954
56	1	0	0.443485	0.212472	2.033911

TS Substituent-side **10k**



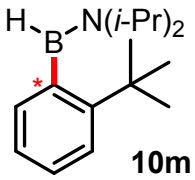
TS Sub-side 10k



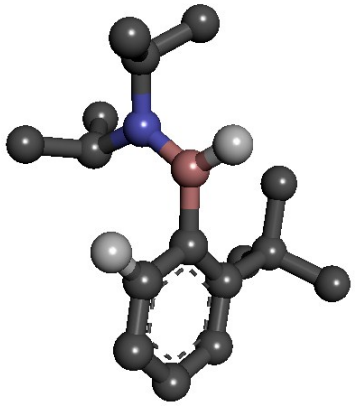
Sum of electronic and thermal Free Energies (Hartrees): -936.716798

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.125029	0.326232	0.199439
2	6	0	-1.917172	-0.897083	0.126748
3	6	0	-1.459471	-2.157144	0.585058
4	1	0	-0.479655	-2.231486	1.007554
5	6	0	-2.219270	-3.294452	0.529051
6	1	0	-1.813207	-4.222716	0.910131
7	6	0	-3.515360	-3.267503	-0.014563
8	1	0	-4.106713	-4.171485	-0.070704
9	6	0	-4.015873	-2.074386	-0.447541
10	1	0	-5.020750	-2.007106	-0.846583
11	6	0	-3.254426	-0.884691	-0.360149
12	6	0	-3.843988	0.344178	-0.724853
13	1	0	-4.843740	0.350525	-1.142012
14	6	0	-3.177350	1.498323	-0.484241
15	1	0	-3.663395	2.439375	-0.701230
16	6	0	-1.851429	1.520064	0.030043
17	6	0	-1.369990	2.934605	0.360519
18	1	0	-0.500090	2.870970	1.003270
19	5	0	0.474159	0.589191	0.240338
20	7	0	1.746820	-0.031997	0.105860
21	6	0	2.911381	0.940582	0.056202
22	6	0	2.764747	1.862152	-1.162015
23	1	0	3.609880	2.551135	-1.207007
24	1	0	2.743652	1.282667	-2.085887
25	1	0	1.855053	2.453582	-1.114760
26	6	0	2.981311	1.778609	1.337260
27	1	0	3.903021	2.364552	1.341590
28	1	0	2.145290	2.468719	1.429245
29	1	0	2.989174	1.126727	2.212317
30	6	0	1.973804	-1.511604	0.108460
31	6	0	1.709198	-2.013944	1.539304
32	1	0	1.634364	-3.103599	1.576305
33	1	0	2.550119	-1.716928	2.168243
34	1	0	0.825286	-1.573373	1.991299
35	6	0	1.100794	-2.103568	-1.009671
36	1	0	0.972033	-3.179623	-0.879982
37	1	0	0.125242	-1.643963	-1.090924
38	1	0	1.611394	-1.935339	-1.960593
39	1	0	0.637385	1.747720	0.286055
40	6	0	-0.988908	3.701080	-0.905513
41	1	0	-0.618752	4.698018	-0.659136
42	1	0	-0.220080	3.175013	-1.471360
43	1	0	-1.856825	3.818235	-1.558319
44	6	0	-2.412810	3.722303	1.163576
45	1	0	-2.778856	3.145807	2.013853
46	1	0	-1.952781	4.634514	1.547008
47	1	0	-3.271478	4.024159	0.563898
48	6	0	3.409333	-1.994682	-0.241019
49	1	0	3.318340	-2.931237	-0.792173
50	1	0	3.960419	-2.226529	0.672057
51	6	0	4.271377	0.239588	-0.083693
52	1	0	4.985506	0.987402	-0.429188
53	1	0	4.619624	-0.094282	0.898740
54	6	0	4.211060	-0.963556	-0.999317
55	1	0	5.209511	-1.342503	-1.219819
56	1	0	3.740933	-0.711540	-1.953108

Compound **10k**



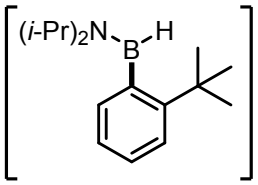
10m



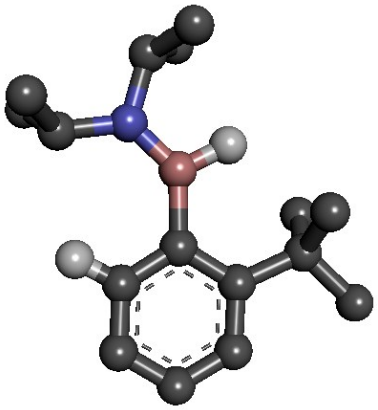
Sum of electronic and thermal Free Energies (Hartrees): -705.797852

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.749172	0.691058	-0.586571
2	6	0	0.728438	2.087335	-0.748090
3	6	0	1.835110	2.882562	-0.513017
4	6	0	3.014598	2.282689	-0.094935
5	1	0	3.895606	2.879244	0.103147
6	6	0	3.058335	0.910143	0.067021
7	1	0	3.986786	0.461681	0.396721
8	6	0	1.950220	0.088855	-0.177558
9	6	0	2.142511	-1.418006	0.048155
10	5	0	-0.637891	0.023175	-0.951480
11	7	0	-1.740649	0.067729	-0.100909
12	6	0	-3.062130	-0.421997	-0.541916
13	1	0	-3.755210	-0.254050	0.282407
14	6	0	-3.583137	0.366046	-1.737666
15	1	0	-4.598181	0.052913	-1.987118
16	1	0	-3.595693	1.434273	-1.517304
17	1	0	-2.953429	0.204863	-2.612850
18	6	0	-3.035515	-1.919974	-0.822524
19	1	0	-4.032322	-2.278594	-1.084149
20	1	0	-2.364868	-2.142559	-1.653635
21	1	0	-2.690387	-2.472537	0.052311
22	6	0	-1.669299	0.560197	1.282324
23	1	0	-0.627473	0.832170	1.448920
24	6	0	-2.512697	1.816081	1.479053
25	1	0	-2.392642	2.194709	2.494909
26	1	0	-2.204047	2.597456	0.784178
27	1	0	-3.575268	1.619129	1.324338
28	6	0	-2.031212	-0.522217	2.296400
29	1	0	-1.872286	-0.149134	3.308874
30	1	0	-3.077355	-0.823237	2.218859
31	1	0	-1.409750	-1.407938	2.159803
32	1	0	-0.803054	-0.413237	-2.050356
33	6	0	3.299756	-1.926356	-0.824427
34	1	0	3.435926	-2.999483	-0.675063
35	1	0	3.091038	-1.753044	-1.881440
36	1	0	4.242049	-1.435579	-0.583098
37	6	0	2.476981	-1.667715	1.525788
38	1	0	1.668560	-1.315772	2.170038
39	1	0	2.615300	-2.736176	1.705335
40	1	0	3.391376	-1.155936	1.826316
41	1	0	-0.193690	2.559678	-1.071825
42	1	0	1.778915	3.954489	-0.650709
43	6	0	0.907825	-2.246067	-0.300228
44	1	0	0.051065	-1.982510	0.321580
45	1	0	0.627735	-2.133833	-1.348326
46	1	0	1.121557	-3.302766	-0.128974

TS Substituent-side **10m**



TS Sub-side 10m



Sum of electronic and thermal Free Energies (Hartrees): -705.776501

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.764090	0.754957	-0.000034
2	6	0	-0.605021	2.148624	0.000005
3	6	0	-1.654918	3.052689	0.000001
4	6	0	-2.945774	2.568322	-0.000041
5	1	0	-3.793854	3.241052	-0.000046
6	6	0	-3.152910	1.197375	-0.000075
7	1	0	-4.175677	0.857841	-0.000104
8	6	0	-2.109967	0.267805	-0.000072
9	6	0	-2.497259	-1.228355	-0.000105
10	5	0	0.492862	-0.226528	-0.000033
11	7	0	1.881855	-0.020084	0.000041
12	6	0	2.750621	-1.226904	0.000068
13	1	0	3.778464	-0.869483	0.000174
14	6	0	2.576428	-2.063425	1.262165
15	1	0	3.318718	-2.863041	1.288990
16	1	0	2.701758	-1.447621	2.153376
17	1	0	1.587590	-2.520592	1.297657
18	6	0	2.576640	-2.063319	-1.262128
19	1	0	3.318903	-2.862962	-1.288875
20	1	0	1.587789	-2.520440	-1.297842
21	1	0	2.702164	-1.447450	-2.153267
22	6	0	2.647009	1.233422	0.000112
23	1	0	1.934805	2.044303	0.000037
24	6	0	3.486678	1.393219	1.266389
25	1	0	3.961287	2.375337	1.273417
26	1	0	2.857983	1.310630	2.153302
27	1	0	4.279271	0.647087	1.335878
28	6	0	3.486923	1.393224	-1.266004
29	1	0	3.961506	2.375354	-1.272946
30	1	0	4.279550	0.647114	-1.335336
31	1	0	2.858403	1.310615	-2.153039
32	1	0	0.245045	-1.378755	-0.000099
33	6	0	-2.001663	-1.920295	1.283243
34	1	0	-2.246674	-2.984285	1.246636
35	1	0	-0.934676	-1.825259	1.450190
36	1	0	-2.511307	-1.490655	2.148137
37	6	0	-4.019678	-1.444960	-0.000118
38	1	0	-4.497328	-1.026126	-0.886589
39	1	0	-4.214231	-2.518409	-0.000133
40	1	0	-4.497339	-1.026148	0.886357
41	1	0	0.381236	2.575982	0.000041
42	1	0	-1.456314	4.116335	0.000032
43	6	0	-2.001647	-1.920244	-1.283474
44	1	0	-2.511276	-1.490566	-2.148357
45	1	0	-0.934656	-1.825207	-1.450400
46	1	0	-2.246664	-2.984235	-1.246914