Hydroboration of vinyl halides with mesitylborane : a direct access to (mesityl)(alkyl)haloboranes

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Supporting information

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II. General considerations

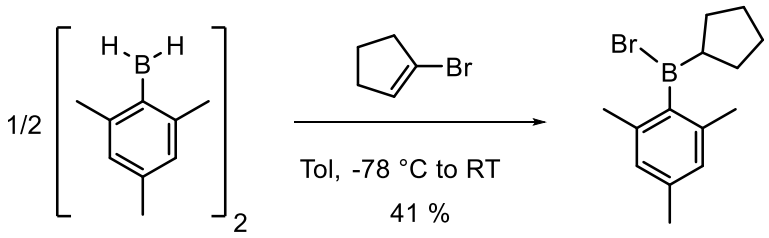
All reactions and manipulations were carried out under an atmosphere of dry argon using standard Schlenk techniques or in a glove-box. All solvents were purged with argon and dried using an MBRAUN Solvent Purification System (SPS). ^{1}H, ^{13}C, ^{31}P, ^{11}B NMR spectra were recorded on Bruker AV 400. Chemical shifts were expressed in positive sign, in parts per million, calibrated to residual ^{1}H (5.32 ppm for CD_2Cl_2, 7.16 ppm for C_6D_6) and ^{13}C (53.84 ppm for CD_2Cl_2, 128.06 ppm for C_6D_6) solvent signals and external $BF_3{\cdot}Et_2O$, 85% H_3PO_4 respectively. Mass spectra were recorded on an Q-Exactive or an MAXIS 4G Mass spectrometer. 1-bromo-cyclopentene[1] and mesitylborane[2] were prepared according to literature procedures. 1-bromo-cyclohexene and 1-bromo-cycloheptene were purchased from Fluorochem, 1-chloro-cyclopentene and 2-bromobutene were purchased from Merck. Elemental analyses were performed at the ScanMat-CRMPO on a ThermoFisher Flash 1112 Series.

Rem: Under the experimental conditions used to record the HRMS spectra, the ionisation of the halogen-boron bond occurs preventing any observation of the molecular peak of the synthesised halogenoboranes **2a-e**.

1. F. Zhan and G. Liang, *Angew. Chem. Int. Ed.*, 2013, **52**, 1266.
2. N. Matsumi and Y. Chujo, *Polym. Bull.*, 1997, **38**, 531.

III. Synthetic procedures

1. Bromo(*c*-pentyl)mesitylborane 2a

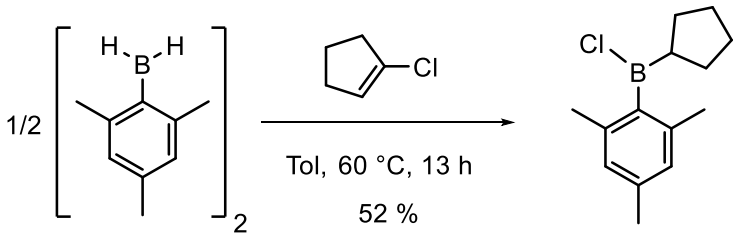


1-bromocyclopentene (1.01 g, 6.87 mmol, 1.0 eq.) in toluene (5 mL) was added dropwise over one minute to a -78 °C cooled solution of mesitylborane (0.91 g, 6.87 mmol) in toluene (5 mL). The cold bath was then removed and the solution allowed to warm up slowly to room temperature. After one hour at room temperature, volatiles were removed under reduced pressure and the residue was distilled (100 °C, $2.7.10^{-2}$ mmbar) giving the expected compound as an orange oil in 41 % yield.

HRMS (ESI), solvent CH_2Cl_2: exact mass (monoisotopic) calcd for $[M\text{-}Br]^+$ $[C_{14}H_{20}{}^{11}B]^+$, 199.16526; found 199.1653 (0 ppm).

^1H NMR (C_6D_6, 400 MHz): δ = 1.37-1.49 (m, 2H, CH_2), 1.51-1.74 (m, 4H, CH_2), 1.75-1.85 (m, 2H, CH_2), 1.95 (m, 1H, CH *c*pent), 2.13 (s, 9H, CH_3 *o*Mes and CH_3 *p*Mes), 6.66 (s, 2H, CH Mes); $^{11}B\{^1H\}$ (C_6D_6, 128 MHz): δ = 80.8 (s); $^{13}C\{^1H\}$ NMR (C_6D_6, 100 MHz) δ = 21.2 (s, CH_3 *p*Mes), 22.0 (s, CH_3 *o*Mes), 27.4 (s, CH_2), 30.7 (s, CH_2), 43.4 (br., CH *c*pent), 128.0 (s, CH Mes), 135.5 (s, C *o*Mes), 138.4 (s, C *p*Mes), 141.6 (br., C *ipso*Mes).

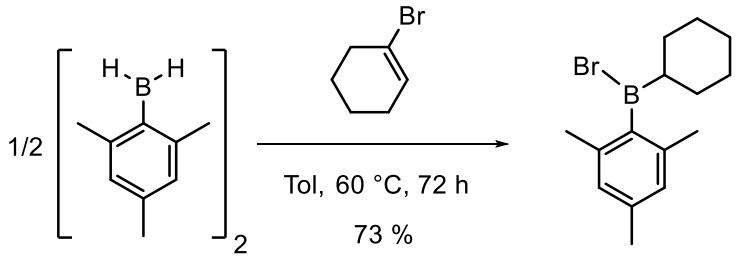
2. Chloro(*c*-pentyl)mesitylborane 2b



1-chlorocyclopentene (336 mg, 3.28 mmol, 1.02 eq.) was added dropwise to a solution of mesitylborane (424 mg, 3.21 mmol) in toluene (3 mL) and the resulting solution was heated at 60 °C for 13 hours under stirring. The volatiles were then removed under reduced pressure and the residue was extracted with pentane. Pentane was evaporated under reduced pressure and the remaining yellowish oil was distilled under reduced pressure (85 °C, $2.0.10^{-2}$ mmbar) giving the expected compound as a colorless oil in 52 % yield.

^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 1.61-1.80 (m, 6H, CH_2), 1.91-2.02 (m, 2H, CH_2), 2.06-2.16 (m, 1H, CH *c*pent), 2.25 (s, 6H, CH_3 *o*Mes), 2.32 (s, 3H, CH_3 *p*Mes), 6.85 (s, 2H, CH Mes); ^{11}B{^{1}H} (CD_2Cl_2, 128 MHz): δ = 77.5 (s); ^{13}C{^{1}H} NMR (CD_2Cl_2, 100 MHz) δ = 21.4 (s, CH_3 *p*Mes), 22.1 (s, CH_3 *o*Mes), 27.7 (s, CH_2), 30.3 (s, CH_2), 41.0 (br., CH *c*pent), 127.9 (s, CH Mes), 136.6 (s, C *o*Mes), 138.8 (s, C *p*Mes), 140.1 (br., C *ipso*Mes).

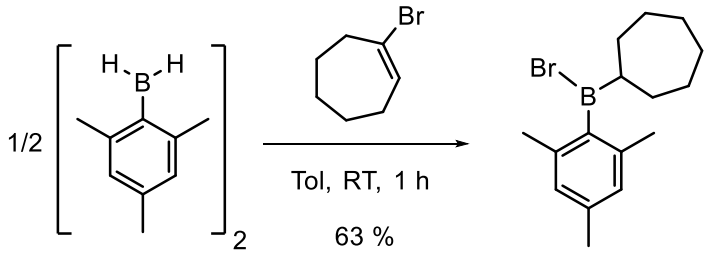
3. Bromo(*c*-hexyl)mesitylborane 2c



1-bromocyclohexene (524.6 mg, 380 μL, 3.26 mmol) was added dropwise over one minute to a solution of mesitylborane (430 mg, 3.26 mmol, 1 eq.) under stirring in toluene (3 mL) and the resulting clear yellow solution was heated to 60 °C for 72 hours. The volatiles were then removed under reduced pressure, the compound extracted with pentane, the pentane solution was filtered and concentrated to dryness under vacuum. The residue was distilled (110 °C, 2.10^{-2} mmbar) giving the expected compound as a colorless oil in 73 % yield.

^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 1.18-1.43 (m, 4H, CH_2), 1.59 (m, 1H, CH *c*hex), 1.64-1.82 (m, 4H, CH_2), 1.93-2.02 (m, 2H, CH_2), 2.17 (s, 6H, CH_3 *o*Mes), 2.28 (s, 6H, CH_3 *p*Mes), 6.80 (s, 2H, CH Mes); ^{11}B{^{1}H} (CD_2Cl_2, 128 MHz): δ = 80.5 (s); ^{13}C{^{1}H} NMR (CD_2Cl_2, 100 MHz) δ = 21.2 (s, CH_3 *p*Mes), 22.0 (s, CH_3 *o*Mes), 26.9 (s, CH_2), 27.8 (s, CH_2), 29.3 (s, CH_2), 42.3 (br., CH *c*hex), 127.9 (s, CH Mes), 135.7 (s, C *o*Mes), 138.8 (s, C *p*Mes), 141.2 (br., C *ipso*Mes).

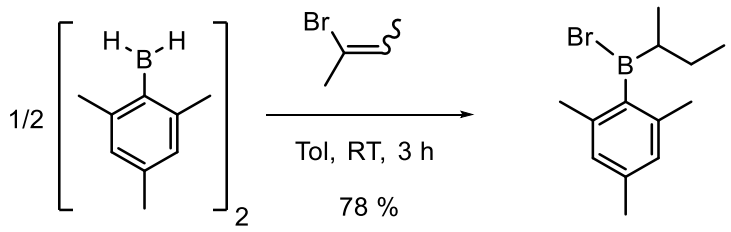
4. Bromo(*c*-heptyl)mesitylborane 2d



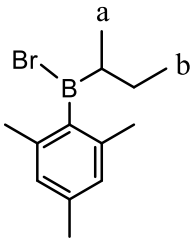
1-bromocycloheptene (626.0 mg, 477.8 μL, 3.58 mmol) was added dropwise over one minute to a solution of mesitylborane (472 mg, 3.58 mmol, 1 eq.) under stirring in toluene (3.3 mL) and the resulting clear yellow solution stirred for 1 hour at room temperature. The volatiles were then removed under reduced pressure, the compound extracted with pentane, the pentane solution was filtered and concentrated to dryness under vacuum. The residue was distilled (125 °C, 3.10^{-2} mmbar) giving the expected compound as a colorless oil in 63 % yield.

^{1}H NMR (C_6D_6, 400 MHz): δ = 1.45-1.72 (m, 8H, CH_2), 1.73-1.87 (m, 3H, CH_2 and CH *c*hept), 2.03-2.12 (m, 2H, CH_2), 1.95 (m, 1H, CH *c*pent), 2.22 (s, 6H, CH_3 *o*Mes), 2.32 (s, 3H, CH_3 *p*Mes), 6.84 (s, 2H, CH Mes); ^{11}B{^{1}H} (C_6D_6, 128 MHz): δ = 80.2 (s); ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz) δ = 21.3 (s, CH_3 *p*Mes), 22.1 (s, CH_3 *o*Mes), 28.9 (s, CH_2), 29.6 (s, CH_2), 30.6 (s, CH_2), 43.4 (br., CH *c*hept), 128.1 (s, CH Mes), 135.8 (s, C *o*Mes), 138.9 (s, C *p*Mes), 141.5 (br., C *ipso*Mes).

5. Bromo(*sec*-butyl)mesitylborane 2e



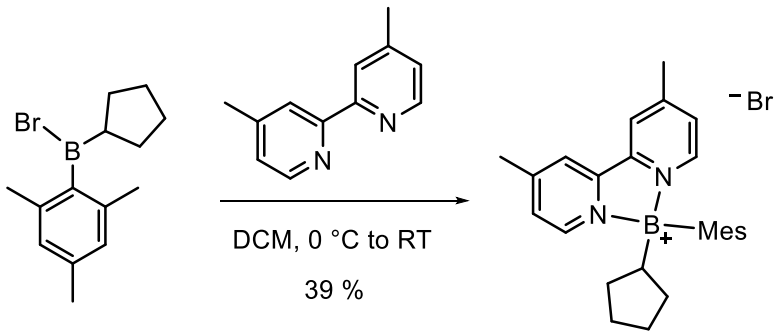
2-bromo-but-2-ene (as a mixture of *cis* / *trans* isomers, 420.3 mg, 316.5 μL, 3.11 mmol) was added dropwise to a solution of mesitylborane (411 mg, 3.11 mmol, 1 eq.) under stirring in toluene (2.9 mL) and the resulting clear yellow solution stirred for 3 hours at room temperature. The volatiles were then removed under reduced pressure, the compound extracted with pentane, the pentane solution was filtered and concentrated to dryness under vacuum. The residue was distilled (72 °C, 3.10^{-2} mmbar) giving the expected compound as a colorless liquid in 78 % yield.



^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 0.99 (pseudo-t, 3H, $^{3}J_{HH}$ = 7.3 Hz, CH_{3a}), 1.14 (d, 3H, CH_{3b}), 1.44 (m, 1H, CH_2), 1.62 (m, 1H, B-CH), 1.83 (m, 1H, CH_2), 2.17 (s, 6H, CH_3 *o*Mes), 2.27 (s, 3H, CH_3 *p*Mes), 6.79 (s, 2H, CH Mes); ^{11}B{^{1}H} (CD_2Cl_2, 128 MHz): δ = 81.2 (s); ^{13}C{^{1}H} NMR (CD_2Cl_2, 100 MHz) δ = 13.4 (s, CH_{3A}), 15.3 (s, CH_{3B}), 21.2 (s, CH_3 *p*Mes), 22.0 (s, CH_3 *o*Mes), 26.3 (s, CH_2), 38.4 (br., B-CH), 128.0 (s, CH Mes), 135.8 (s, C *o*Mes), 138.9 (s, C *p*Mes), 141.3 (br., C *ipso*Mes).

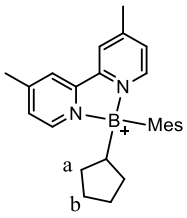
C *ipso*Mes was tentatively attributed based on ^{1}H,^{13}C HMBC NMR experiments.

6. Bipyridine(*c*-pentyl)mesitylborane 3a



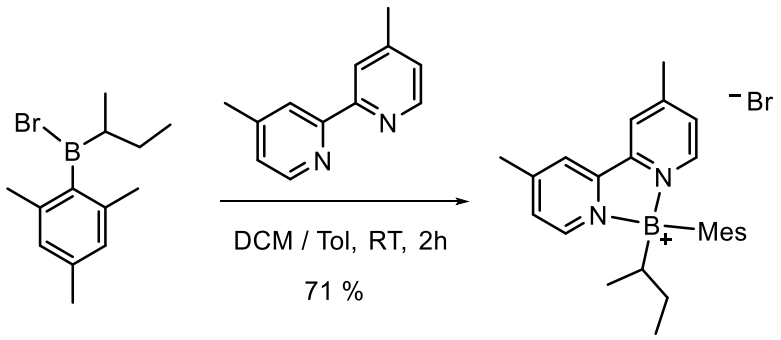
4,4'-dimethyl-bipyridine (64 mg, 0.35 mmol, 0.95 eq.) in solution in dichloromethane (2 mL) was added to an ice-cold solution of bromoborane (102 mg, 0.37 mmol) in dichloromethane (2 mL) and the ice bath was removed allowing the reaction mixture to warm up slowly to room temperature. After 30 minutes at room temperature, pentane (10 mL) was added under strong stirring leading to the precipitation of a redish powder. The mother liquor was eliminated by filtration and the powder was washed with pentane (2 times 5 mL). The powder was then solubilized in DCM (2.2 mL) and the resulting solution was saturated by the addition of pentane (3 mL). The cloudy mixture was then filtered in a new schlenk affording colorless crystals of the expected compound at -20 °C with a yield of 39 %. Single crystals suitable for X-ray diffraction were obtained in the same way.

HRMS (ESI), solvent CH_3OH / CH_2Cl_2 90/10: exact mass (monoisotopic) calcd for $[C_{26}H_{32}N_2{}^{11}B]^+$, 383.2653; found 383.2658 (1 ppm).



^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 0.25-0.41 (m, 2H, CH_2a), 0.91 (br. s, 3H, CH_3 *o*Mes), 1.16 (m, 2H, CH_2b), 1.17-1.29 (m, 2H, CH_2a), 1.29-1.44 (m, 2H, CH_2b), 2.15 (m, 1H, CH-B), 2.20 (s, 3H, CH_3 *p*Mes), 2.71-2.89 (br. s, 3H, CH_3 *o*Mes), 2.84 (s, 6H, CH_3 *p*Py), 6.61 (br. s, 1H, CH Mes), 6.94 (br. s, 1H, CH Mes), 6.67 (d, 2H, $^3J_{HH}$ = 5.9 Hz, CH Py), 8.25 (d, 2H, $^3J_{HH}$ = 5.9 Hz, CH Py), 10.07 (s, 2H, CH Py); ^{11}B{^{1}H} (CD_2Cl_2, 128 MHz): δ = 8.5 (br. s); ^{13}C{^{1}H} NMR (CD_2Cl_2, 100 MHz): δ = 20.7 (s, CH_3 *p*Mes), 22.4 (s, CH_3 *p*Py), 23.0 (br., CH_3 *o*Mes), 25.5 (br., CH_3 *o*Mes), 26.0 (s, CH_2b), 28.6 (s, CH_2a), 36.1 (s, CH-B), 126.2 (s, CH Py), 129.0 (s, CH Py), 131.6 (br., CH *m*Mes), 138.3 (s, C *p*Mes), 141.2 (s, CH Py), 146.4 (s, C *o*Py), 158.6 (s, C *p*Py). The resonance signal corresponding to the B-**C**(Mes) carbon was not observed.

7. Bipyridine(*sec*-butyl)mesitylborane 3e



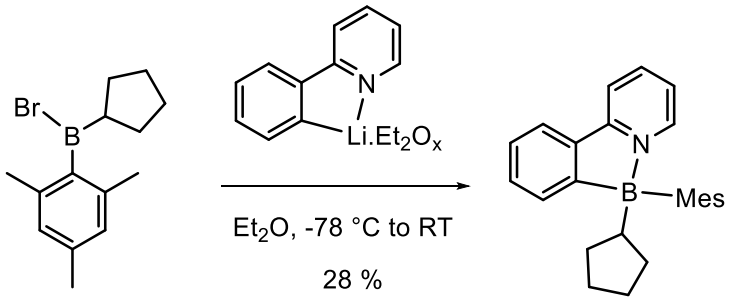
4,4'-dimethyl-bipyridine (448.5 mg, 2.43 mmol, 1 eq.) in solution in dichloromethane (8 mL) was added dropwise at room temperature to a solution of bromoborane (650 mg, 2.43 mmol) in toluene (2 mL) and the reaction mixture was allowed to stir for 2 hours. The reaction mixture was then filtered in a new schlenk and the reaction schlenk was washed with DCM (2 mL). Pentane (30 mL) was then added under strong stirring leading to the precipitation of a orange oil. The mother liquor was eliminated by canula. The oil was then suspended in pentane (40 mL) turning into a yellow / green powder under strong stirring. The mother liquor was then eliminated by filtration and the powder was dried under vacuum (yield 71 %).

HRMS (ESI), solvent CH_2Cl_2: exact mass (monoisotopic) calcd for $[C_{25}H_{32}N_2{}^{11}B]^+$, 371.2653; found 371.2651 (1 ppm).

Due to low symmetry in solution, different sets of ^{13}C resonance signals are observed for the two pyridyl heterocycles.

^1H NMR (CD_2Cl_2, 400 MHz): δ = 0.20 (m, 1H, CH_2), 0.23 (d, 3H, $^3J_{HH}$ = 6.7 Hz, CH_3), 0.82 (t, 3H, $^3J_{HH}$ = 7.3 Hz, CH_3), 0.94 (br., 3H, CH_3 *o*Mes), 0.98 (m, 1H, CH_2), 1.77 (m, 1H, CH-B), 2.20 (s, 3H, CH_3 *p*Mes), 2.76 (br., 3H, CH_3 *o*Mes), 2.82 (s, 3H, CH_3 Py), 2.82 (s, 3H, CH_3 Py), 6.62 (br., 1H, CH Mes), 6.94 (br., 1H, CH Mes), 7.74 (m, 2H, CH Py), 8.28 (m, 2H, CH Py), 10.05 (s, 2H, CH Py); $^{11}B\{^1H\}$ (CD_2Cl_2, 128 MHz): δ = 9.0 (br. s); $^{13}C\{^1H\}$ NMR (CD_2Cl_2, 100 MHz): δ = 13.4 (s, CH_3), 13.7 (s, CH_3), 20.6 (s, CH_3 *p*Mes), 22.3 (s, CH_3 *p*Py), 23.0 (br., CH_3 *o*Mes), 25.0 (s, CH_2), 26.0 (br., CH_3 *o*Mes), 29.3 (s, CH-B), 125.9 (s, CH Py), 125.9 (s, CH Py), 129.0 (s, CH Py), 129.2 (s, CH Py), 131.7 (br., CH *m*Mes), 138.1 (s, C *p*Mes), 141.2 (s, CH Py), 141.3 (s, CH Py), 143.9 (br., C *o*Mes), 144.6 (br., C *o*Mes), 146.2 (s, C *o*Py), 146.4 (s, C *o*Py), 158.5 (s, C *p*Py), 158.5 (s, C *p*Py). The resonance signal corresponding to the B-**C**(Mes) carbon was not observed.

8. Phenylpyridine(*c*-pentyl)mesitylborane 4a



n-butyl lithium (2.46 mmol, 0.98 mL, 2.5 M in hexanes, 1 eq.) was added dropwise to a solution of 2-(2-bromophenyl)pyridine (575 mg, 2.46 mmol) in diethylether (5 mL) at -78 °C leading to the formation of a yellow precipitate and the reaction mixture was allowed to warm up to -65 °C over 25 min. Then, the reaction mixture was cooled down to -78 °C and bromoborane (754 mg, 2.70 mmol, 1.1 eq.) in solution in diethylether (4 mL) cooled down to -78 °C was added dropwise. After the completion of the addition, the cold bath was removed allowing the reaction mixture to warm up to room temperature giving a green mixture.

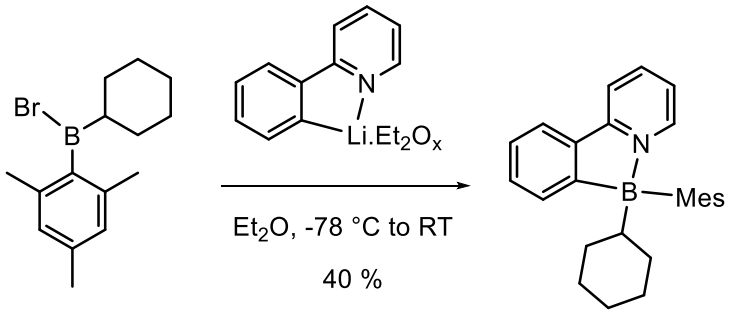
Volatiles were eliminated under reduced pressure and the residue was extracted with pentane (2 times 20 mL) and the organic fractions were combined and filtered by canula. The expected compound starts then to crash out of pentane and the fast crystallization was completed by placing the schlenk at 0 °C (the compound is not pure). The mother liquor was then eliminated by canula and the crystals were solubilized in a mixture dichloromethane / pentane (5 / 40 mL). This cloudy mixture was filtered again by canula in a new schlenk and placed at -20 °C affording 200 mg colorless crystals of the expected compound. The mother liquor was then filtered by canula, concentrated under vacuum and placed at 0 °C affording 45 mg additional crystals of the same compound. Single crystals suitable for X-ray diffraction were obtained in the same way.

HRMS (ESI), solvent CH_3OH / CH_2Cl_2 90/10: exact mass (monoisotopic) calcd for $[C_{25}H_{28}N^{11}B+Na]^+$, 376.2207; found 376.2213 (2 ppm); exact mass (monoisotopic) calcd for $[C_{25}H_{28}N^{11}B+K]^+$, 392.19464; found 392.1948 (0 ppm).

Anal. Calcd. For $[C_{25}H_{28}NB]$; C, 84.99; H, 7.99; N, 3.96. Found: C, 85.07; H, 7.88; N, 3.81.

^{1}H NMR (CD_2Cl_2, 400 MHz): δ = -0.04 (m, 1H, CH_2), 0.75 (m, 1H, CH_2), 0.89-1.51 (m, 6H, CH_2), 1.91 (br. s, 6H, CH_3 Mes), 2.04 (m, 1H, CH *c*pent), 2.18 (s, 3H, CH_3 *p*Mes), 6.67 (br. s, 2H, CH Mes), 7.27-7.41 (m, 2H, H arom.), 7.56 (d, 1H, $^3J_{HH}$ = 7.0 Hz, H arom.), 7.92 (d, 1H, $^3J_{HH}$ = 7.5 Hz, H arom.), 7.99-8.09 (m, 2H, H arom.), 8.28 (d, 1H, $^3J_{HH}$ = 5.7 Hz, H arom.); $^{13}C\{^1H\}$ NMR (CD_2Cl_2, 100 MHz): δ = 20.7 (s, CH_3 *p*Mes), 24.8 (br., CH_3 *o*Mes), 26.1 (s, CH_2), 26.8 (s, CH_2), 29.5 (s, CH_2), 29.8 (s, CH_2), 36.4 (br., CH *c*pent), 118.3, 121.8, 121.8, 125.5 and 129.6 (s, CH arom.), 130.2 (s, CH Mes), 130.8 (s, CH arom.), 134.6 (s, C quat.), 136.9 (s, C quat.), 140.1 (s, CH arom.), 143.5 (s, CH arom.), 158.1 (s, C quat.), 165.6 (s, B-CAr); $^{11}B\{^1H\}$ (CD_2Cl_2, 128 MHz): δ = 3.5 (s). The resonance signal corresponding to three quaternary carbons were not observed.

9. Phenylpyridine(*c*-hexyl)mesitylborane 4c



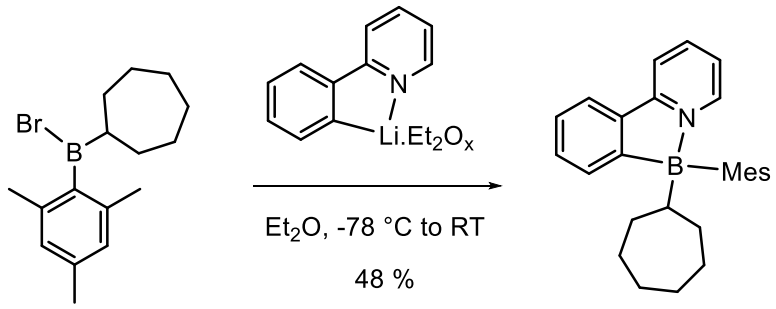
n-butyl lithium (1.04 mmol, 0.42 mL, 2.5 M in hexanes, 1 eq.) was added dropwise to a solution of 2-(2-bromophenyl)pyridine (243.6 mg, 1.04 mmol) in diethylether (2 mL) at -78 °C leading to the formation of a yellow precipitate and the reaction mixture was allowed to warm up to -65 °C over 25 min. Then, the reaction mixture was cooled down to -78 °C and bromoborane (305 mg, 1.04 mmol, 1.0 eq.) in solution in diethylether (2 mL) cooled down to -78 °C was added dropwise. The reaction mixture was then allowed to warm up slowly in the bath until it reached -10 °C. At that stage, the cold bath was removed and the reaction mixture was further stirred at room temperature for 20 minutes giving a green mixture.

The reaction mixture was then filtered over a frit and the reaction schlenk and frit were washed with diethylether (2 mL) giving phase A. The frit was then further washed with diethylether (2 X 3 mL) giving 32 mg of pure compound X as a white solid. The phase A diethylether solution was concentrated to dryness giving a greenish powder that was washed to times with pentane (2 X 10 mL) giving 120 mg of the expected compound as a beige powder (global yield, 40 %).

HRMS (ASAP), 200 °C: exact mass (monoisotopic) calcd for $[C_{26}H_{30}N^{11}B]^{\cdot\cdot}$, 367.24768; found 367.2475 (0 ppm).

^{1}H NMR (CD_2Cl_2, 400 MHz): δ = -0.26 (m, 1H, CH_2), 0.57-0.78 (m, 2H, CH_2), 0.80-0.96 (m, 1H, CH_2), 0.97-1.13 (m, 1H, CH_2), 1.16-1.49 (m, 3H, CH_2), 1.49-1.69 (m, 3H, $2CH_2$ & CH *c*hex), 2.17 (s, 3H, CH_3 *p*Mes), 6.49-6.85 (br. s, 2H, CH Mes), 7.26-7.43 (m, 3H, H arom.), 7.58 (d br., 1H, $^{3}J_{HH}$ = 7.3 Hz, H arom.), 7.89 (d br., 1H, $^{3}J_{HH}$ = 7.6 Hz, H arom.), 8.04 (m, 2H, H arom.), 8.31 (d, 1H, $^{3}J_{HH}$ = 5.7 Hz, H arom.), the CH_3 *o*Mes groups give an extremely broad signal under the aliphatic region of the spectrum; $^{13}C\{^{1}H\}$ NMR (CD_2Cl_2, 100 MHz): δ = 20.6 (s, CH_3 *p*Mes), 25.0 (br., CH_3 *o*Mes), 28.1 (s, CH_2), 29.3 (s, CH_2), 29.4 (s, CH_2), 29.8 (s, CH_2), 30.2 (s, CH_2), 34.8 (br., CH *c*pent), 118.3, 121.6, 121.6, 125.5 and 129.7 (s, CH arom.), 130.2 (s, CH Mes), 130.8 (s, CH arom.), 134.4 (s, C *p*Mes), 137.2 (s, C quat.), 140.1 (s, CH arom.), 143.2 (s, C quat.), 143.7 (s, CH arom.), 157.8 (s, C quat.), 164.8 (s, B-CAr); $^{11}B\{^{1}H\}$ (CD_2Cl_2, 128 MHz): δ = 4.2 (s). The resonance signal corresponding to the two C *o*Mes was not observed.

10. Phenylpyridine(*c*-hexyl)mesitylborane 4d



n-butyl lithium (0.98 mmol, 0.39 mL, 2.5 M in hexanes, 1 eq.) was added dropwise to a solution of 2-(2-bromophenyl)pyridine (228.7 mg, 0.98 mmol) in diethylether (2 mL) at -78 °C leading to the formation of a yellow precipitate and the reaction mixture was allowed to warm up to -65 °C over 25 min. Then, the reaction mixture was cooled down to -78 °C and bromoborane (300.0 mg, 0.98 mmol, 1.0 eq.) in solution in diethylether (2 mL) at room temperature was added dropwise. The reaction mixture was then allowed to warm up slowly in the bath until it reached -10 °C. At that stage, the cold bath was removed and the reaction mixture was further stirred at room temperature for 20 minutes giving a green mixture.

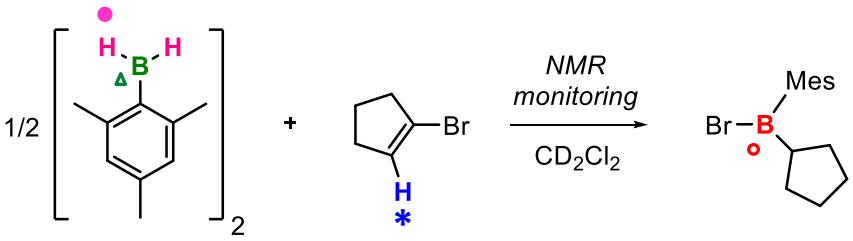
The reaction mixture was then filtered over a frit and the reaction shlenk and frit were washed with diethylether (2 mL). The resulting diethylether solution was then concentrated to dryness giving a greenish powder that was whashed to times with pentane (2 X 6 mL) giving the expected compound as a white powder in 48 % yield.

HRMS (ASAP), 190 °C: exact mass (monoisotopic) calcd for $[C_{27}H_{32}N^{11}B+H]^+$, 382.27006; found 382.2704 (1 ppm).

^{1}H NMR (CD_2Cl_2, 400 MHz): δ = -0.17-0.02 (m, 1H, CH_2), 0.53-1.81 (m, 14H, CH_2 & CH_3 *o*Mes), 2.17 (s, 3H, CH_3 *p*Mes), 2.38-3.23 (br., 3H, CH_3 *o*Mes), 6.15-7.01 (s br., 2H, CH Mes), 7.25-7.43 (m, 3H, H arom.), 7.61 (d br., 1H, $^3J_{HH}$ = 7.2 Hz, H arom.), 7.90 (d br., 1H, $^3J_{HH}$ = 7.6 Hz, H arom.), 8.00-8.09 (m, 2H, H arom.), 8.38 (d, 1H, $^3J_{HH}$ = 5.8 Hz, H arom.); $^{13}C\{^1H\}$ NMR (CD_2Cl_2, 100 MHz): δ = 20.6 (s, CH_3 *p*Mes), 24.4 (br., CH_3 *o*Mes), 25.9 (br., CH_3 *o*Mes), 28.1 (s, CH_2), 28.3 (s, CH_2), 30.2 (s, CH_2), 30.4 (s, CH_2), 31.7 (s, CH_2), 32.2 (s, CH_2), 33.8 (br., CH *c*hept), 118.4, 121.6, 121.6, 125.6 and 129.7 (s, CHarom.), 130.3 (br., CH Mes), 130.8 (s, CH arom.), 134.3 (s, C *p*Mes), 137.4 (s, C quat.), 140.2 (s, CH arom.), 143.0 (br., B-C Mes), 143.8 (s, CH arom.), 158.3 (s, C quat.), 164.6 (br., B-CAr); $^{11}B\{^1H\}$ (CD_2Cl_2, 128 MHz): δ = 4.6 (s). The resonance signals corresponding to two C *o*Mes quaternary carbons were not observed.

IV. NMR monitoring of the reaction between $MesBH_2$ and 1-bromocyclopentene

1-bromocyclopentene (7.5 mg, $5.08.10^{-2}$ mmol, 1.0 eq.) in CD_2Cl_2 (0.2 mL) was added to a -78 °C cooled solution of mesitylborane (6.7 mg, $5.08.10^{-2}$ mmol) in CD_2Cl_2 (0.4 mL) under stirring. The solution was transferred to a pressure NMR tube via canula and the reaction was monitored by ^{1}H, $^{1}H\{^{11}B\}$ and $^{11}B\{^{1}H\}$ NMR experiments starting at -80 °C. No change was observed until 0 °C at what temperature the reaction started. The NMR monitoring does not show the formation of any intermediate, only the starting material disappearance and product formation could be observed.



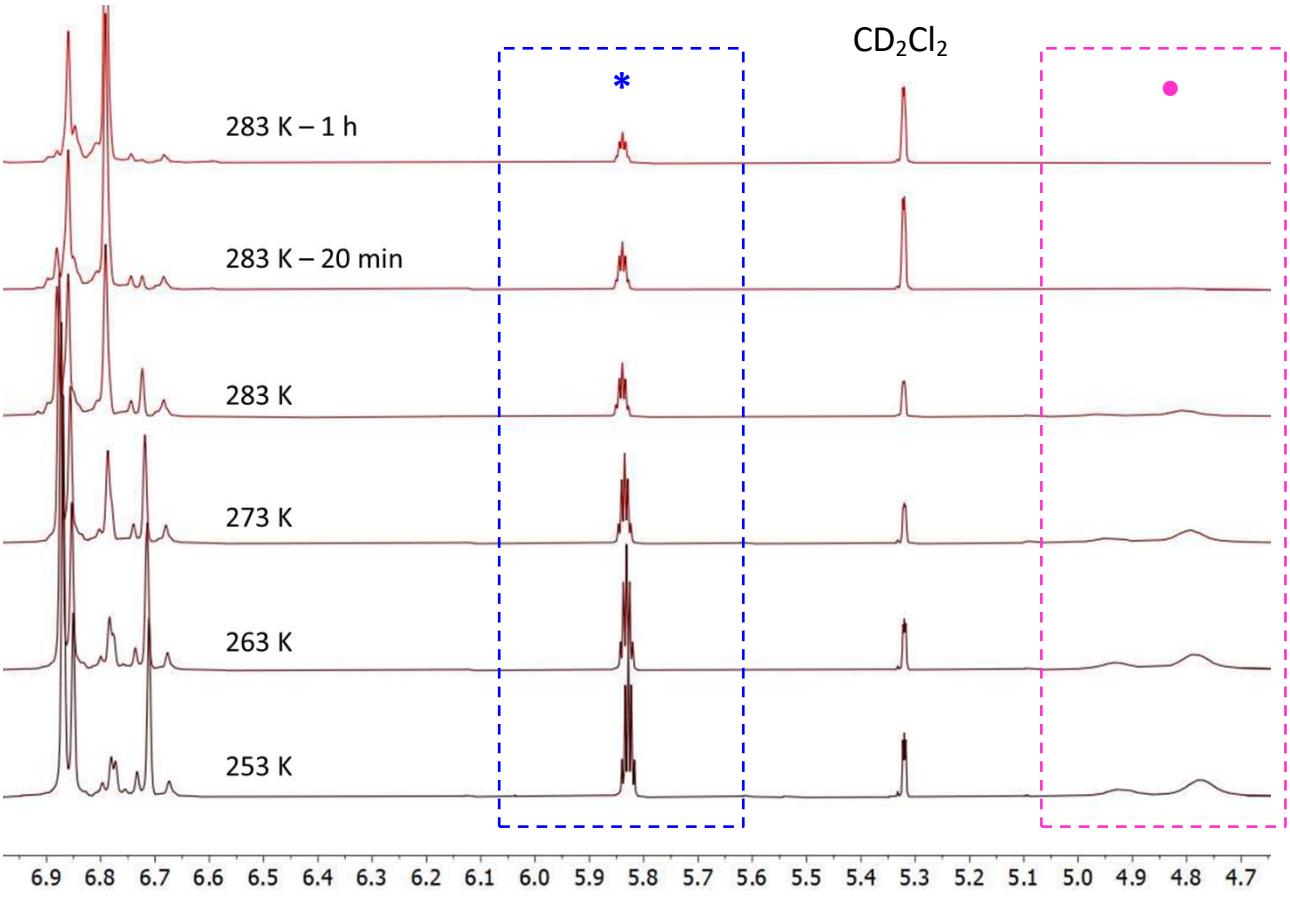


*Figure 1. $^{1}H\{^{11}B\}$ NMR monitoring of the reaction between **1** and 1-bromocyclopentene (400 MHz) in CD_2Cl_2*

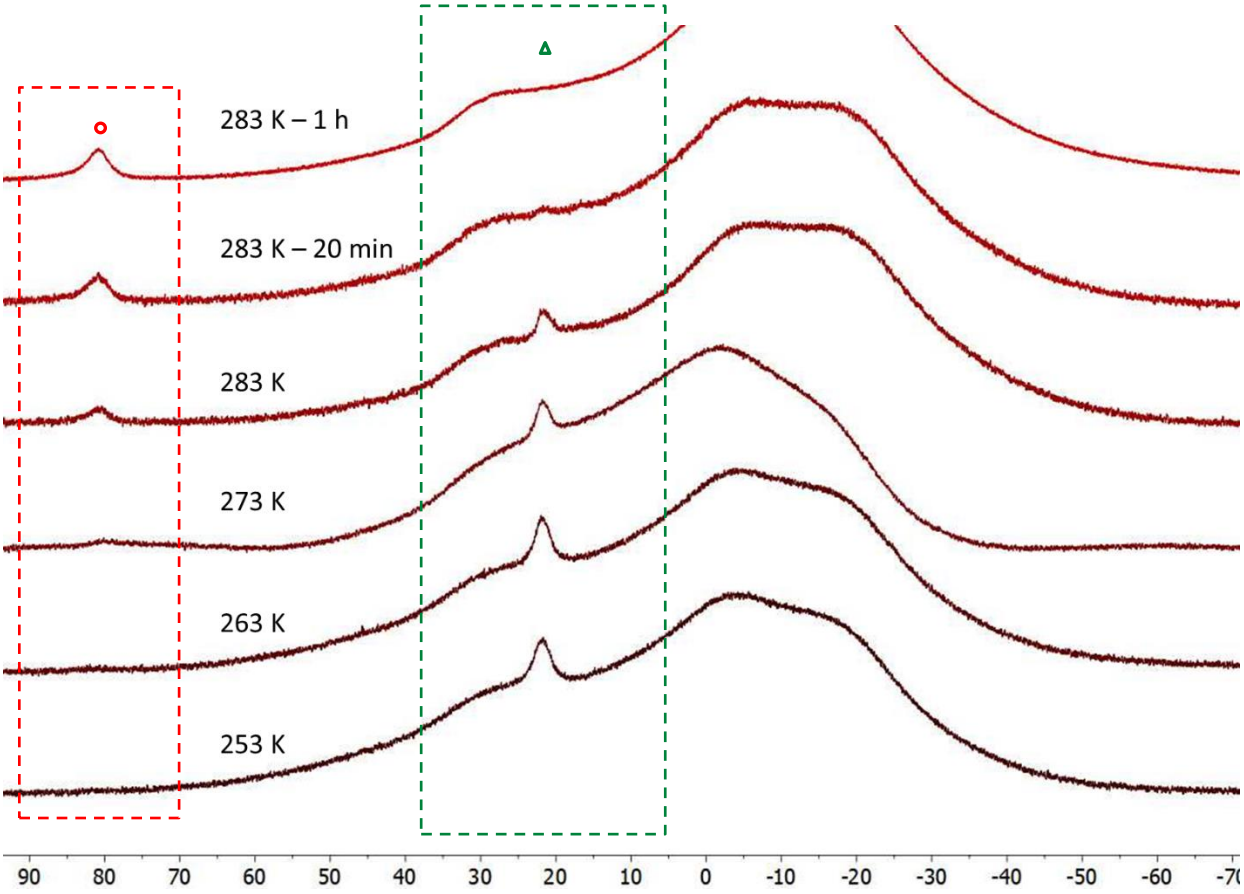
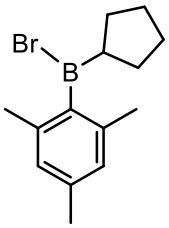


Figure 2. $^{11}B\{^{1}H\}$ *NMR monitoring of the reaction between* ***1*** *and 1-bromocyclopentene (400 MHz) in* CD_2Cl_2

V. NMR spectra

1. NMR spectra of 2a



2a

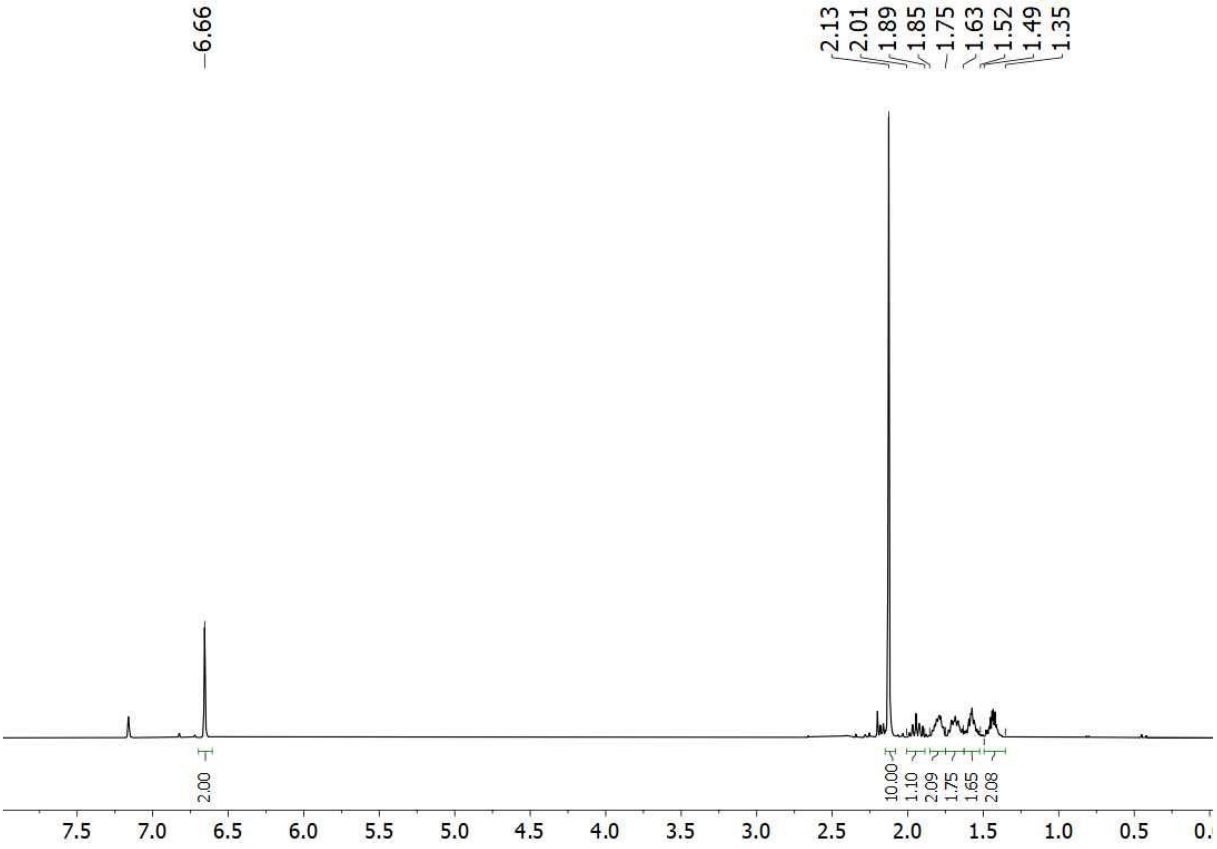


*Figure 3. ^{1}H NMR spectrum of **2a** (400 MHz) in C_6D_6*

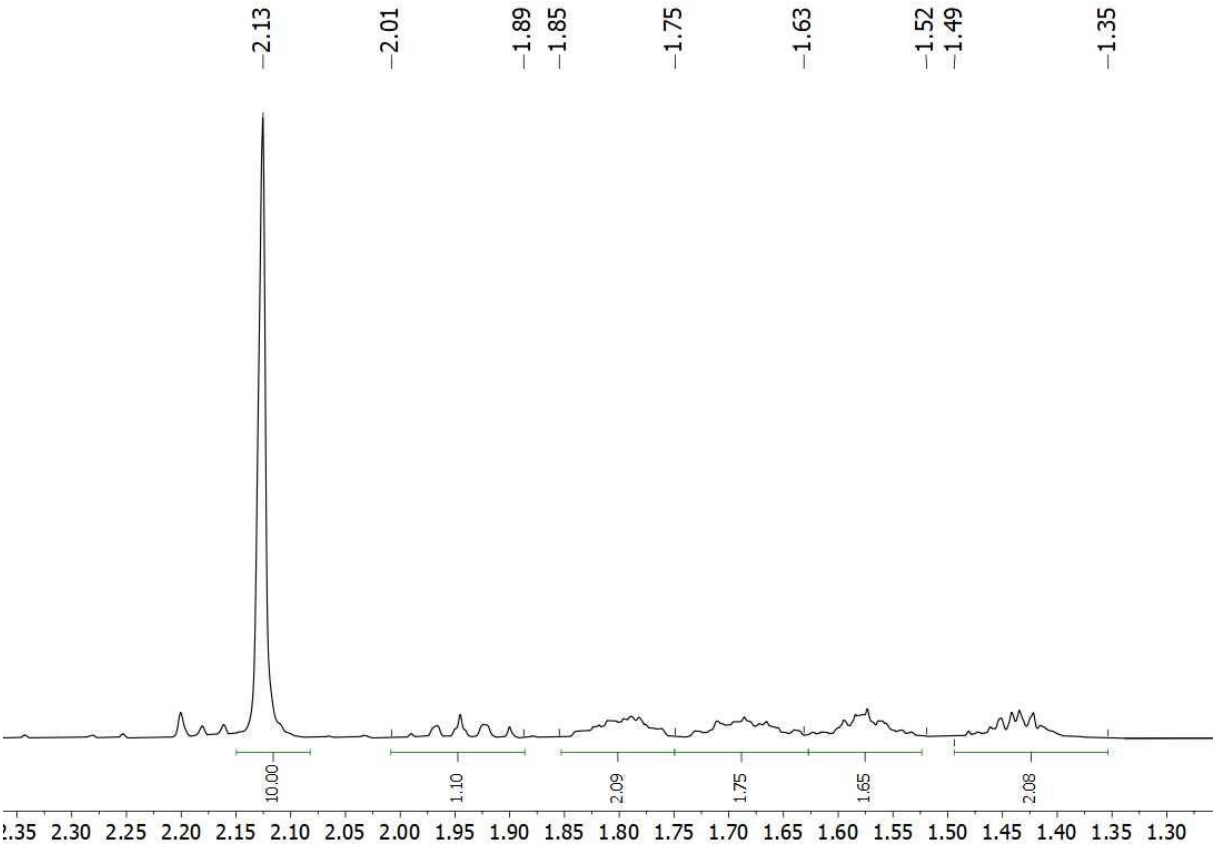


*Figure 4. ^{1}H NMR spectrum of **2a** (400 MHz) in C_6D_6, aliphatic region*

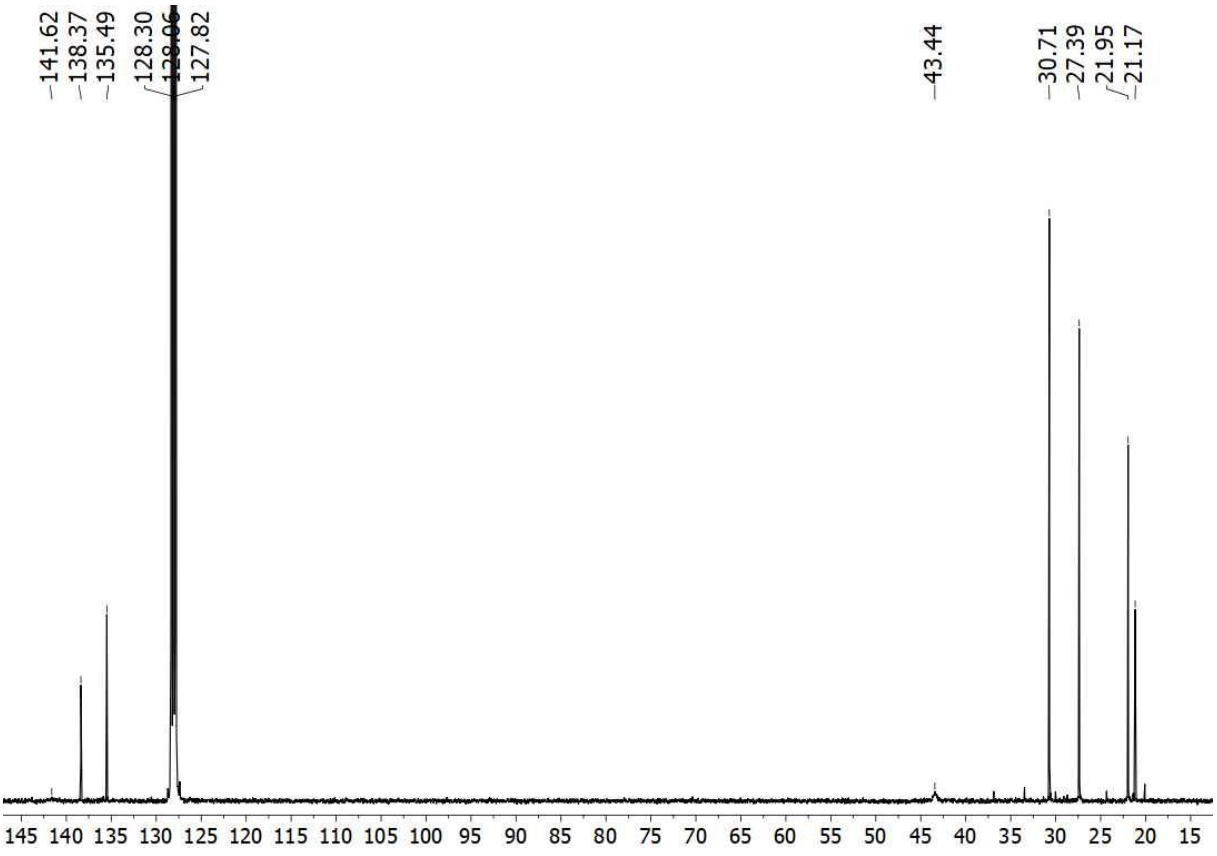


*Figure 5. $^{13}C\{^{1}H\}$ NMR spectrum of **2a** (100 MHz) in C_6D_6*

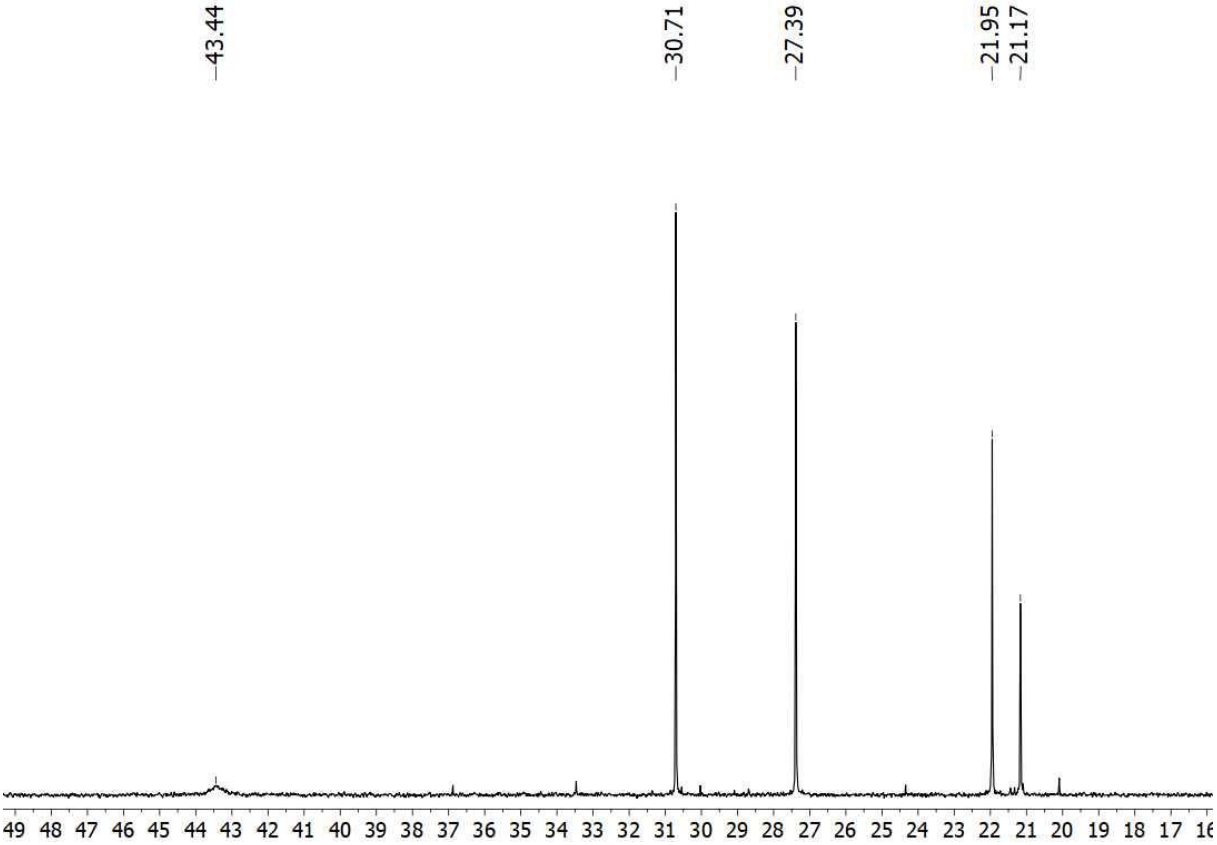


*Figure 6. $^{13}C\{^{1}H\}$ NMR spectrum of **2a** (100 MHz) in C_6D_6, aliphatic region*

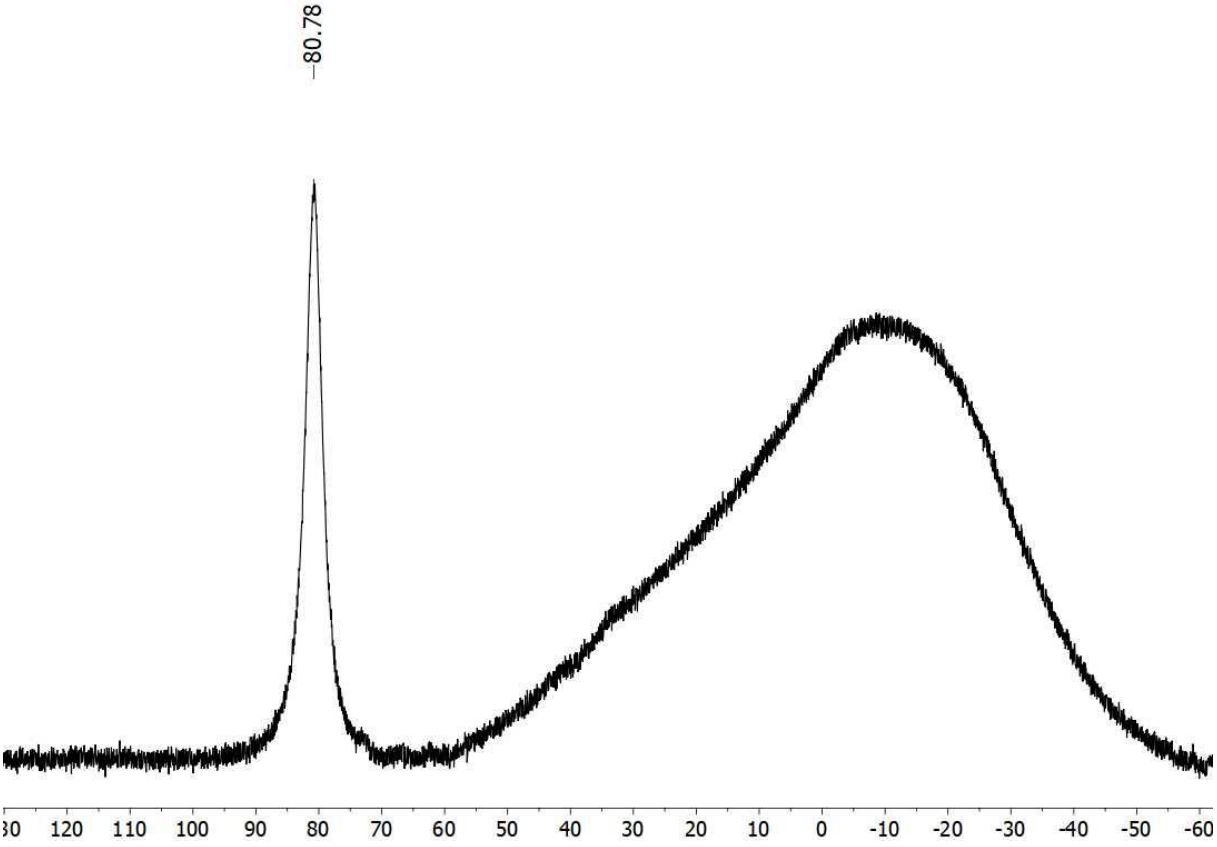
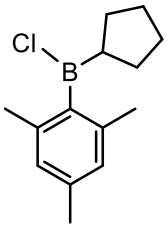


*Figure 7. $^{11}B\{^{1}H\}$ NMR spectrum of **2a** (128 MHz) in C_6D_6*

11.NMR spectra of 2b



2b

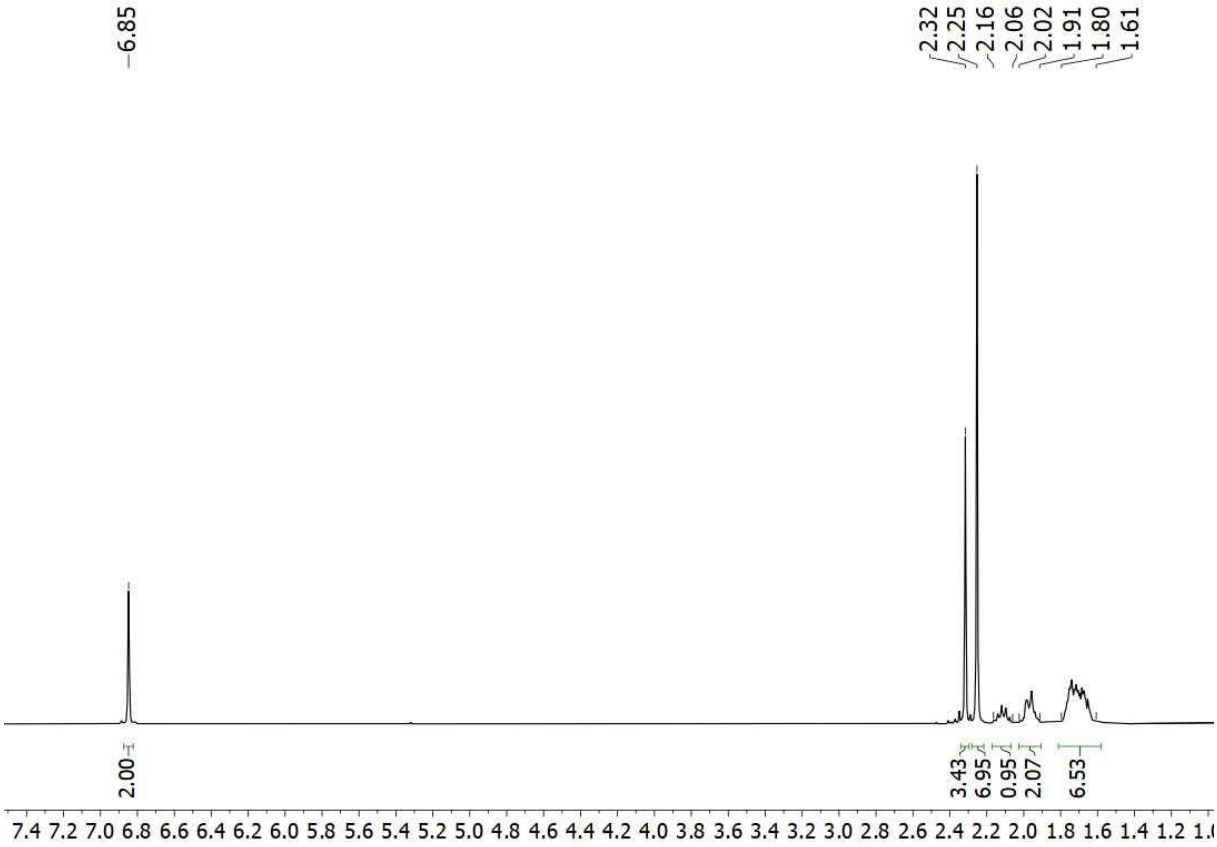


*Figure 8. ^{1}H NMR spectrum of **2b** (400 MHz) in CD_2Cl_2*

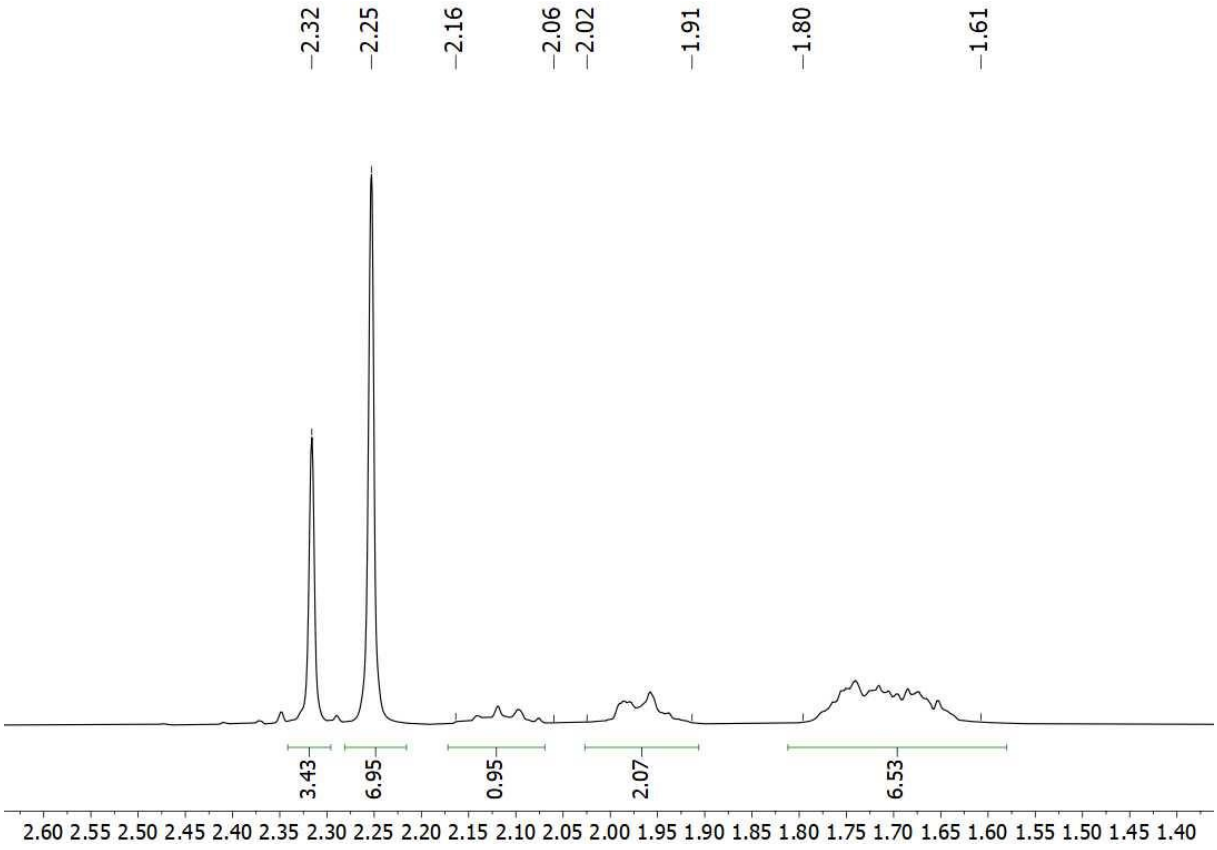


*Figure 9. ^{1}H NMR spectrum of **2b** (400 MHz) in CD_2Cl_2, aliphatic region*

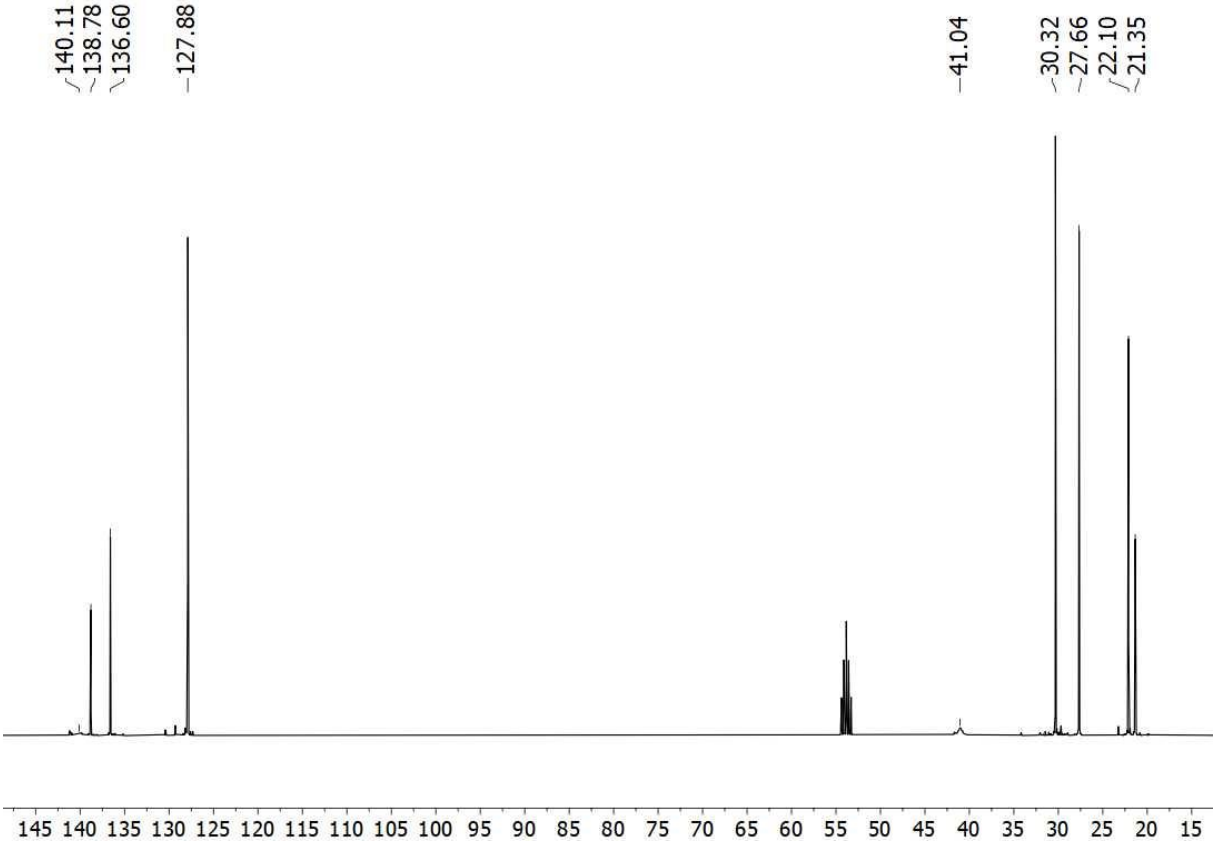


*Figure 10. $^{13}C\{^{1}H\}$ NMR spectrum of **2b** (100 MHz) in CD_2Cl_2*

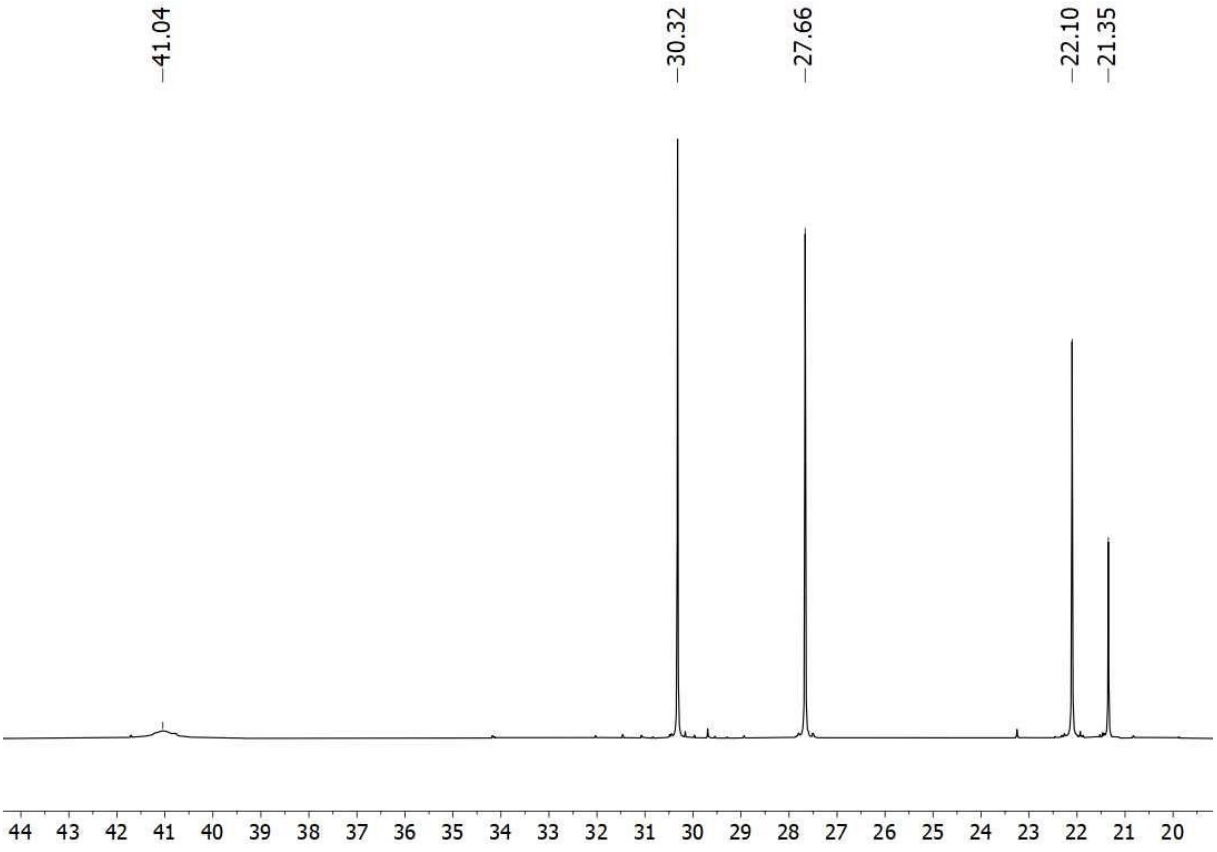


*Figure 11. $^{13}C\{^{1}H\}$ NMR spectrum of **2b** (100 MHz) in CD_2Cl_2, aliphatic region*

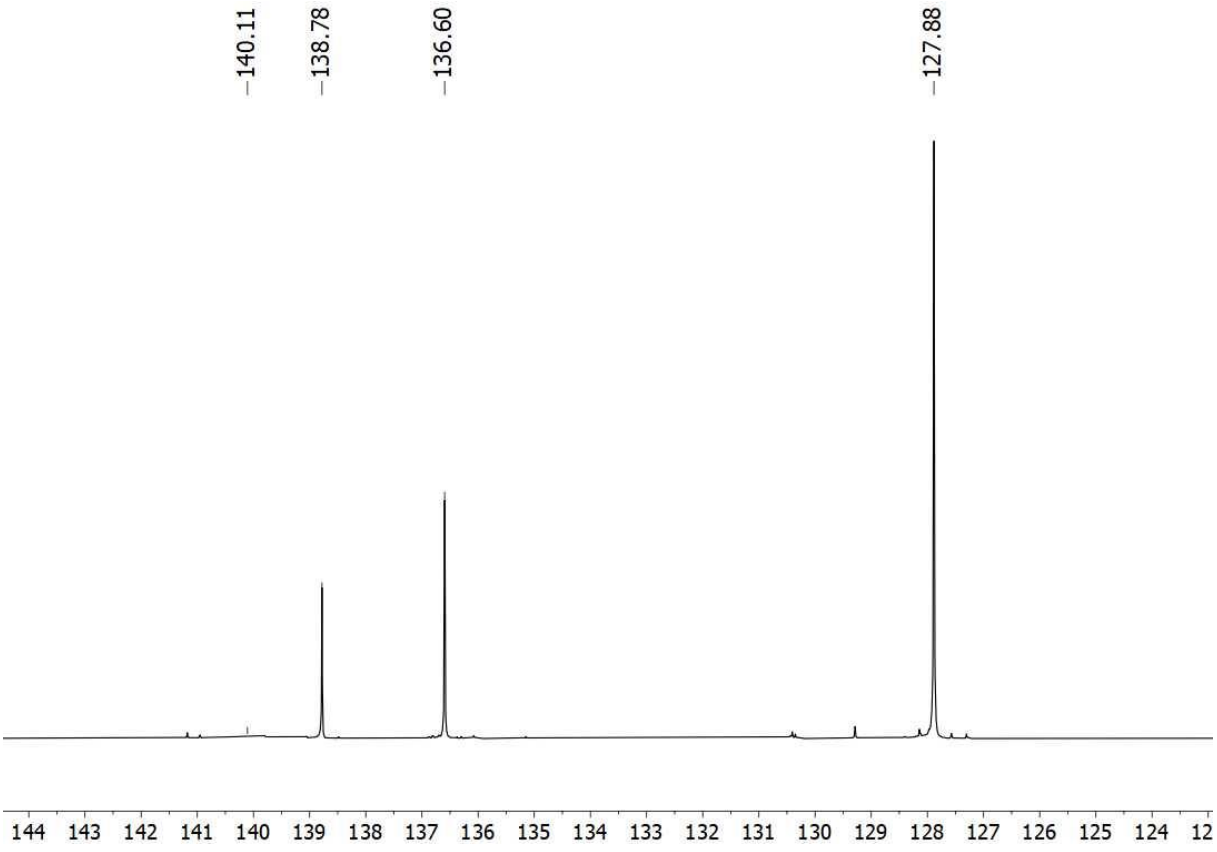


*Figure 12. $^{13}C\{^{1}H\}$ NMR spectrum of **2b** (100 MHz) in CD_2Cl_2, aromatic region*

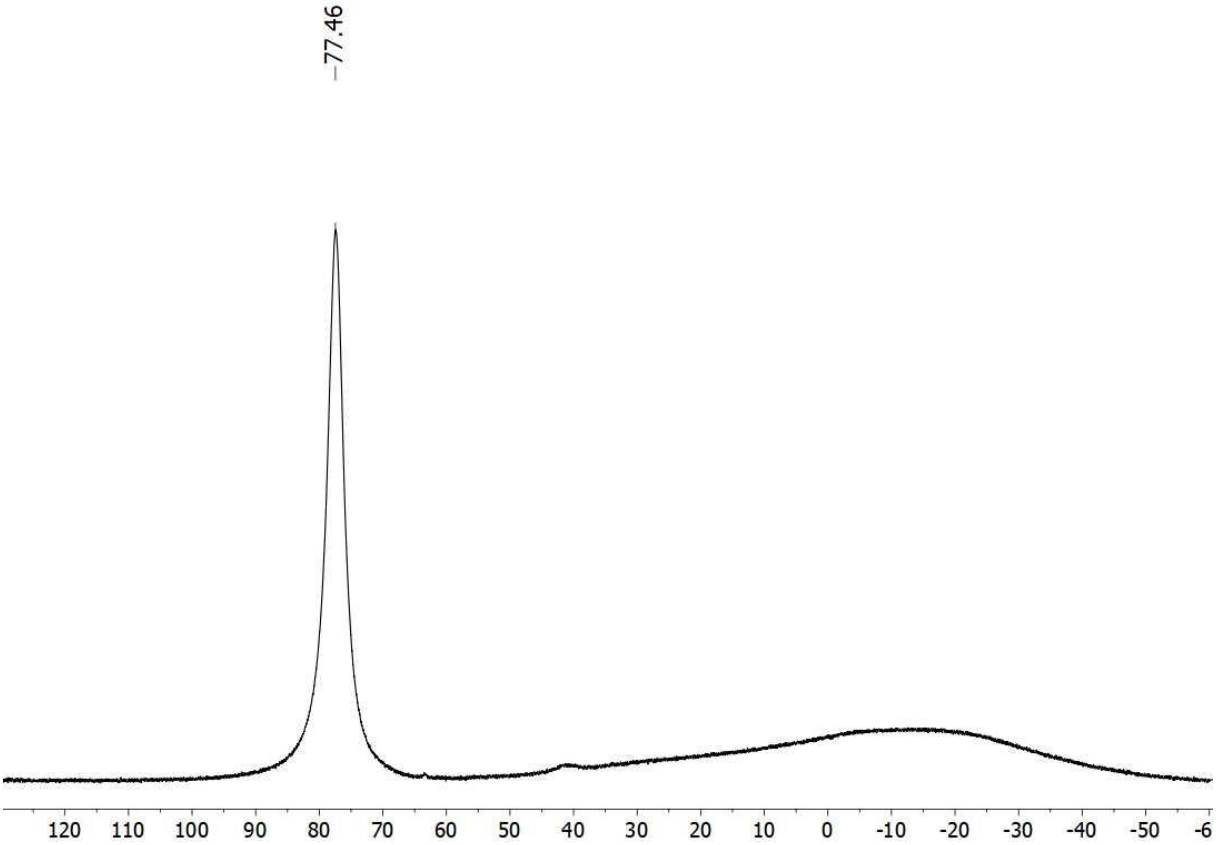
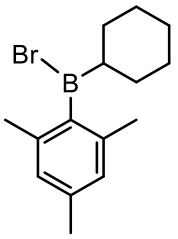


*Figure 13. $^{11}B\{^{1}H\}$ NMR spectrum of **2b** (128 MHz) in CD_2Cl_2*

12.NMR spectra of 2c



2c

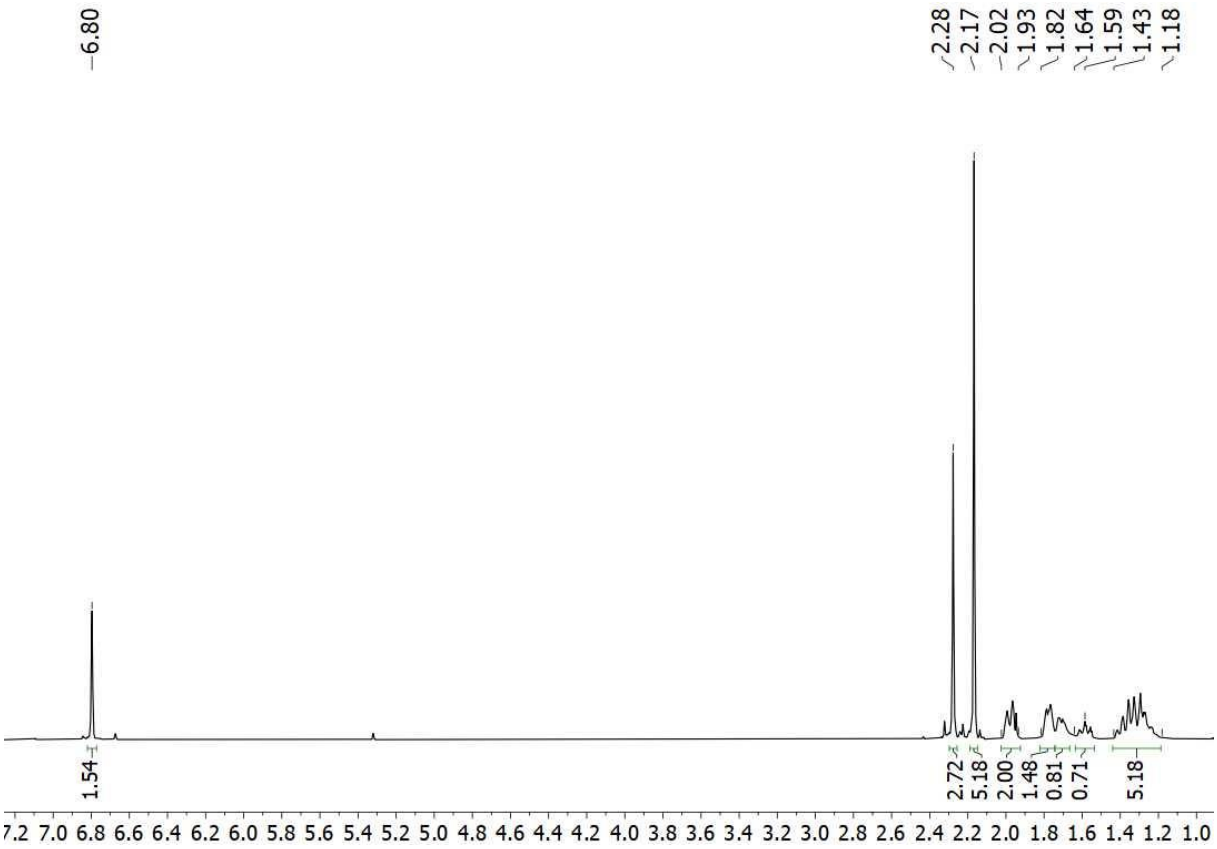


*Figure 14. ^{1}H NMR spectrum of **2c** (400 MHz) in CD_2Cl_2*

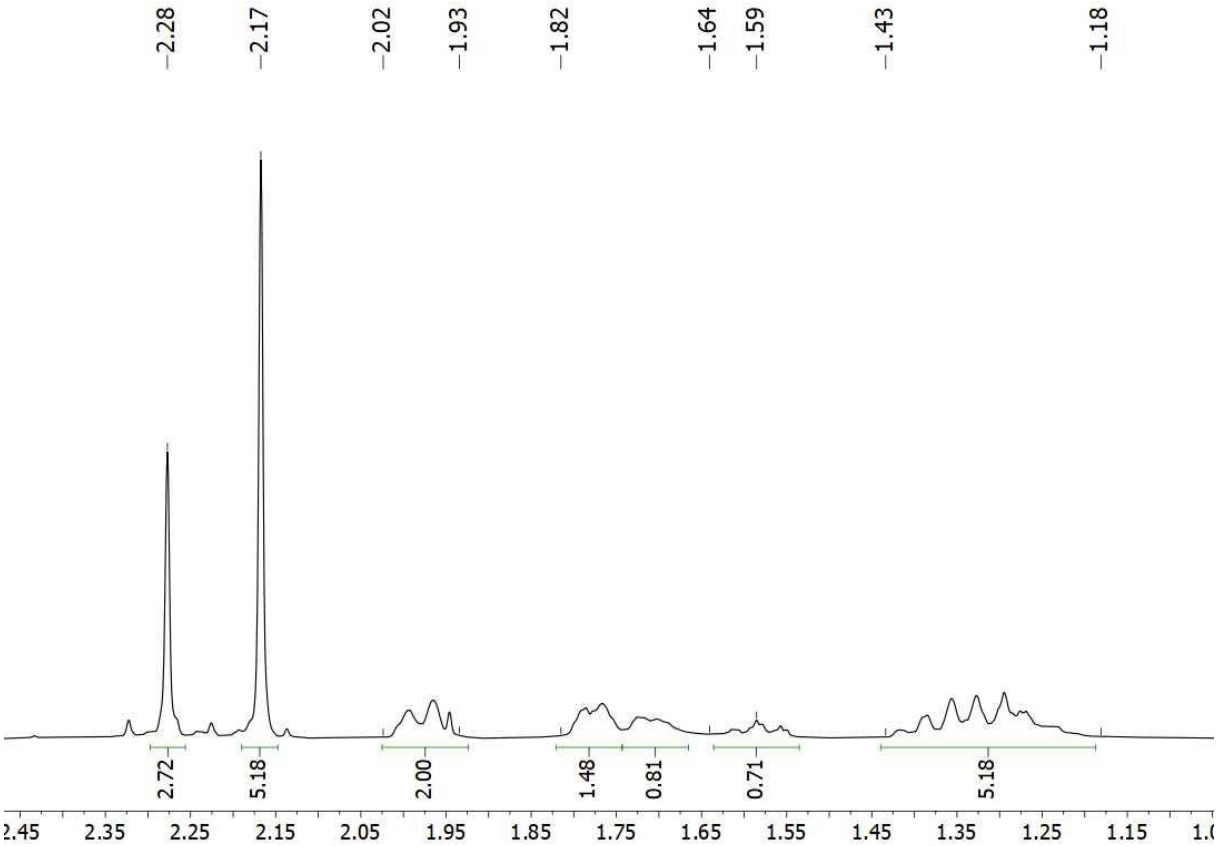


*Figure 15. ^{1}H NMR spectrum of **2c** (400 MHz) in CD_2Cl_2, aliphatic region*

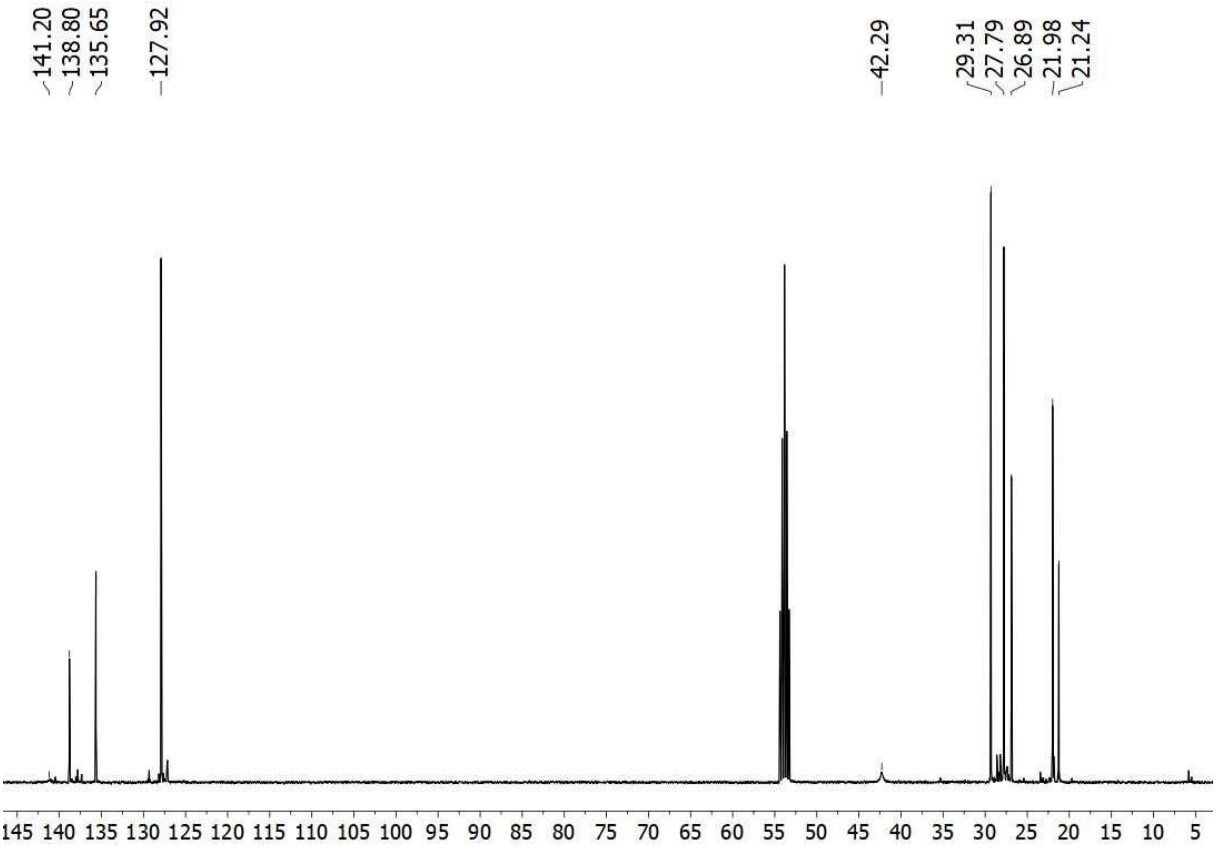


*Figure 16. $^{13}C\{^{1}H\}$ NMR spectrum of **2c** (100 MHz) in CD_2Cl_2*

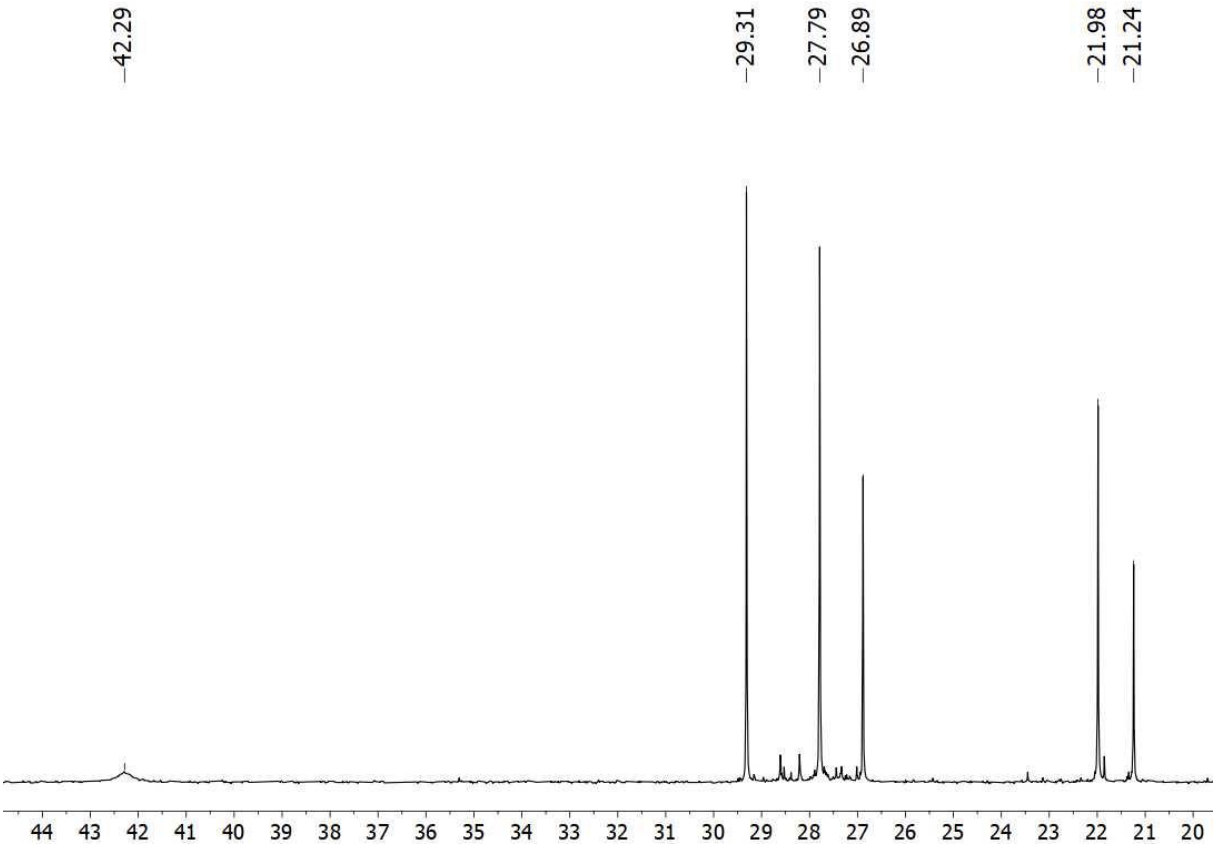


*Figure 17. $^{13}C\{^{1}H\}$ NMR spectrum of **2c** (100 MHz) in CD_2Cl_2, aliphatic region*

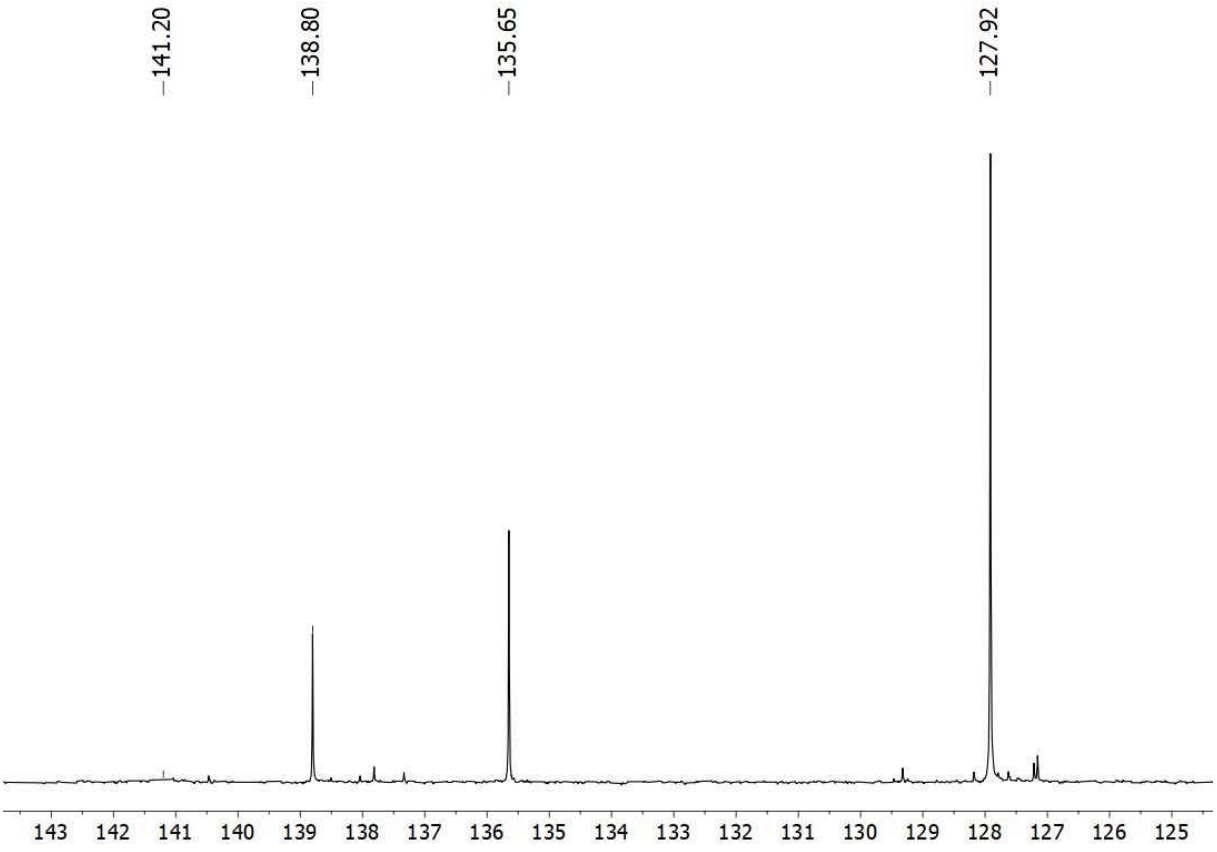


*Figure 18. $^{13}C\{^{1}H\}$ NMR spectrum of **2c** (100 MHz) in CD_2Cl_2, aromatic region*

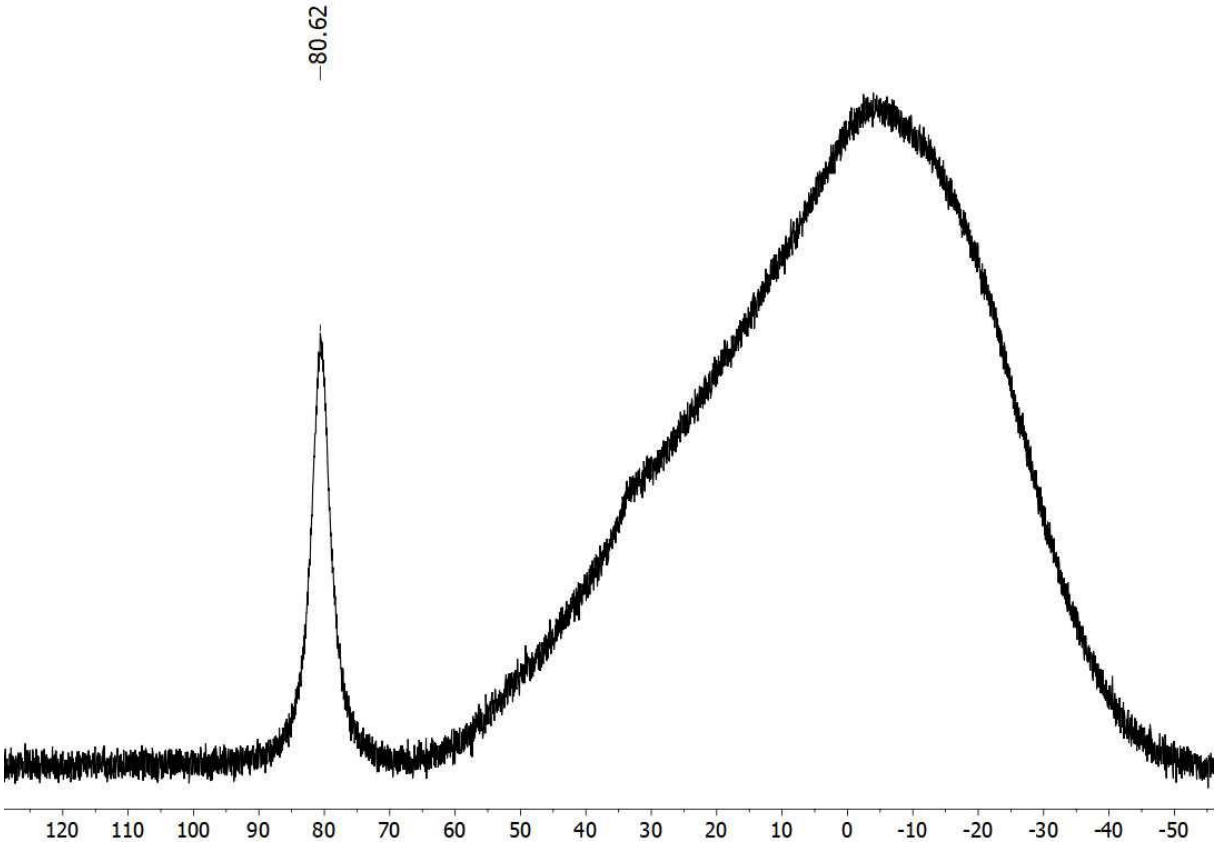
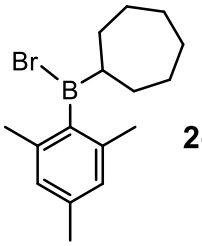


*Figure 19. $^{11}B\{^{1}H\}$ NMR spectrum of **2c** (128 MHz) in CD_2Cl_2*

13.NMR spectra of 2d



2d

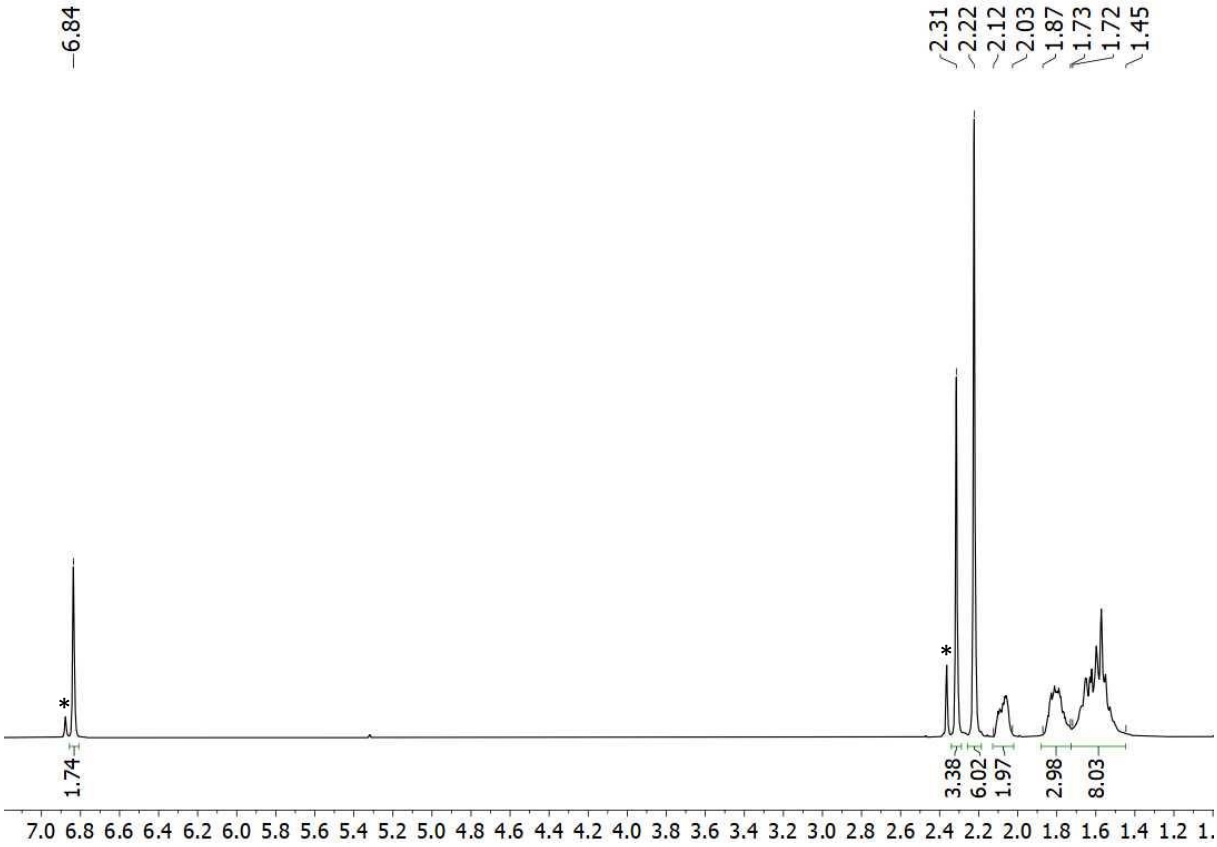


*Figure 20. ^{1}H NMR spectrum of **2d** (400 MHz) in C_6D_6*

* Impurity that couldn't be attributed

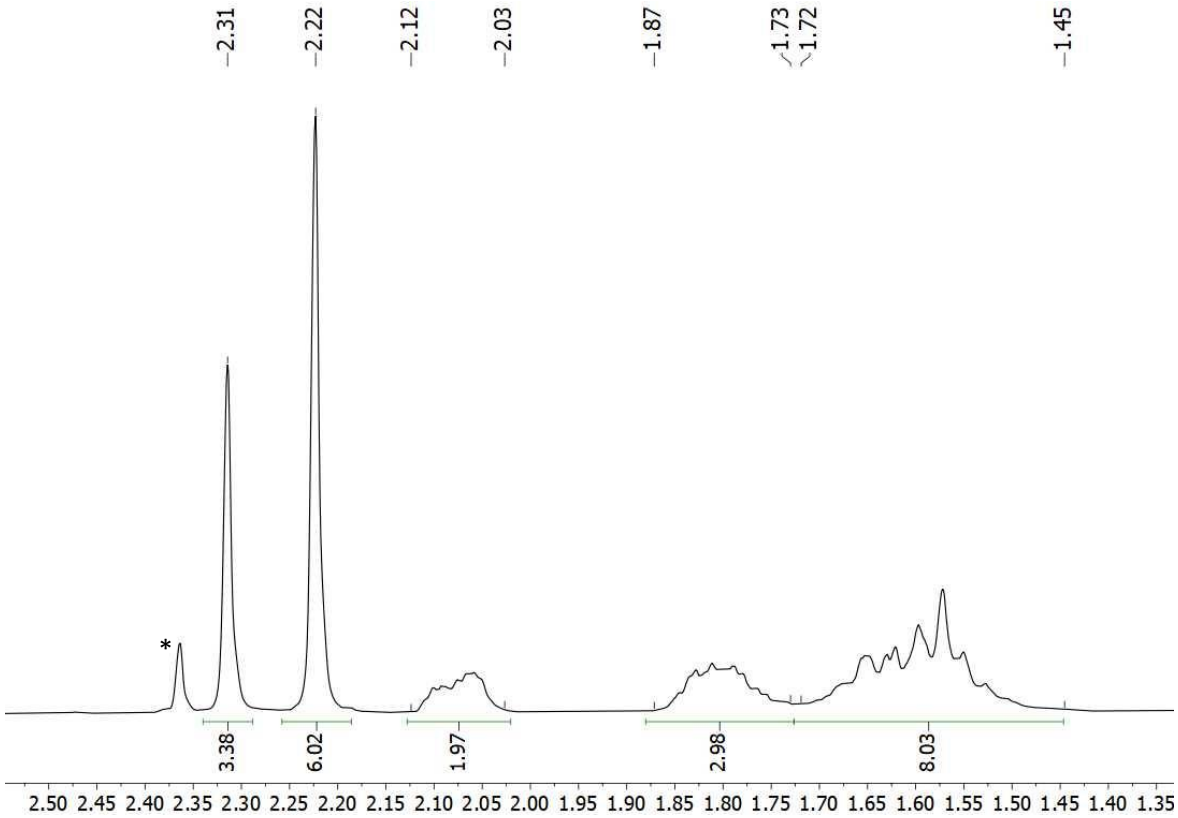


*Figure 21. ^{1}H NMR spectrum of **2d** (400 MHz) in C_6D_6, aliphatic region*

* Impurity that couldn't be attributed

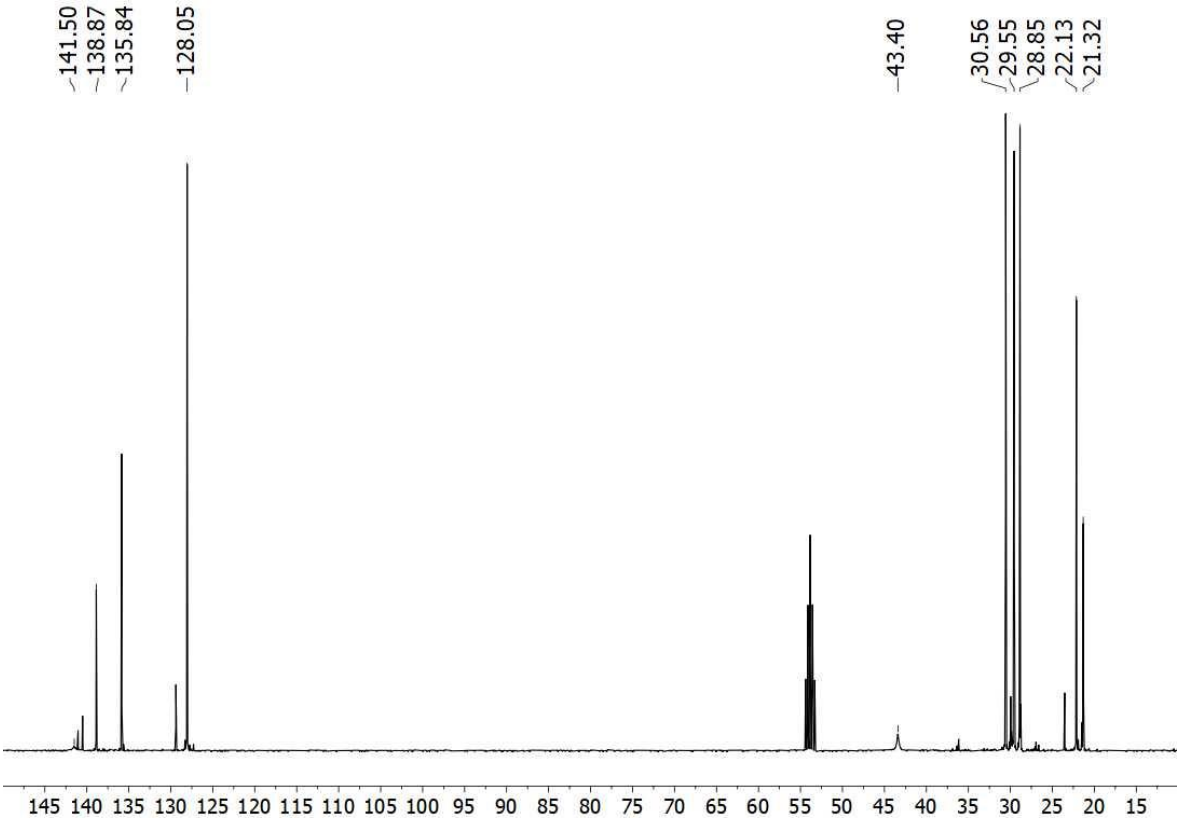
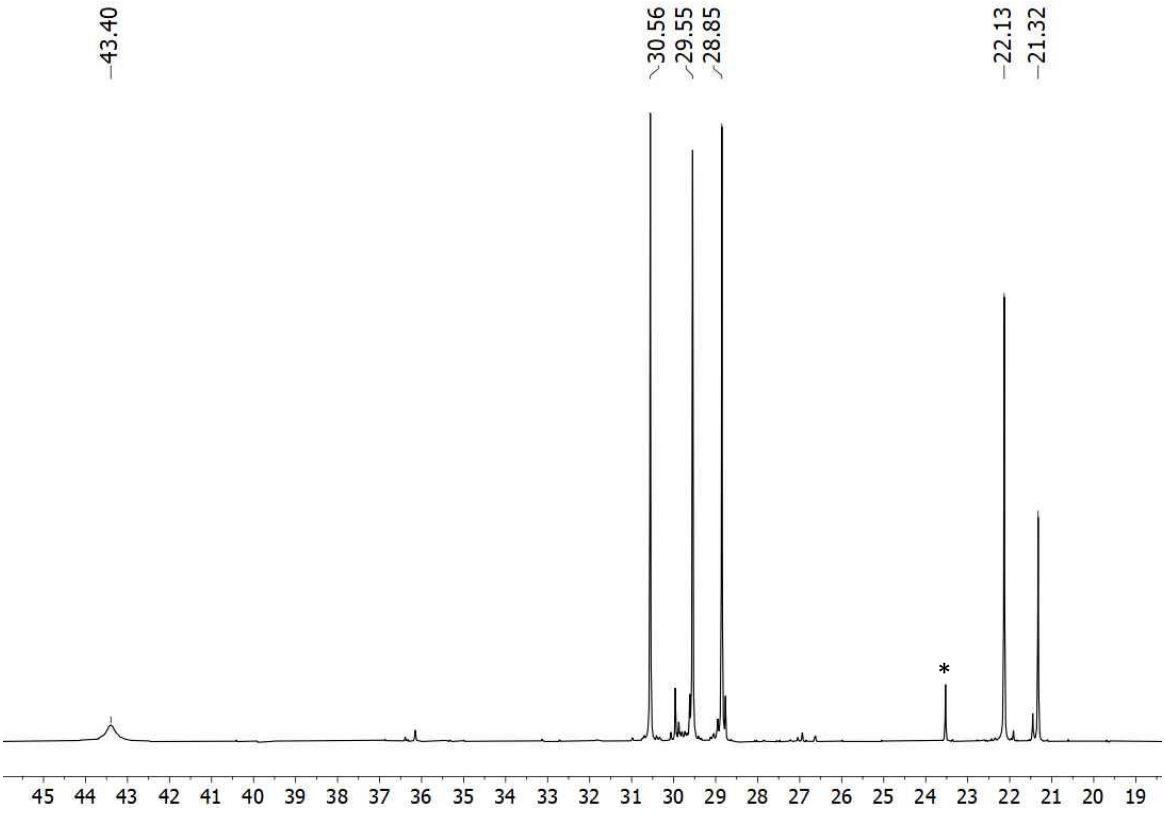


*Figure 22. $^{13}C\{^{1}H\}$ NMR spectrum of **2d** (100 MHz) in C_6D_6*



* Impurity that couldn't be attributed

*Figure 23. $^{13}C\{^{1}H\}$ NMR spectrum of **2d** (100 MHz) in C_6D_6, aliphatic region*

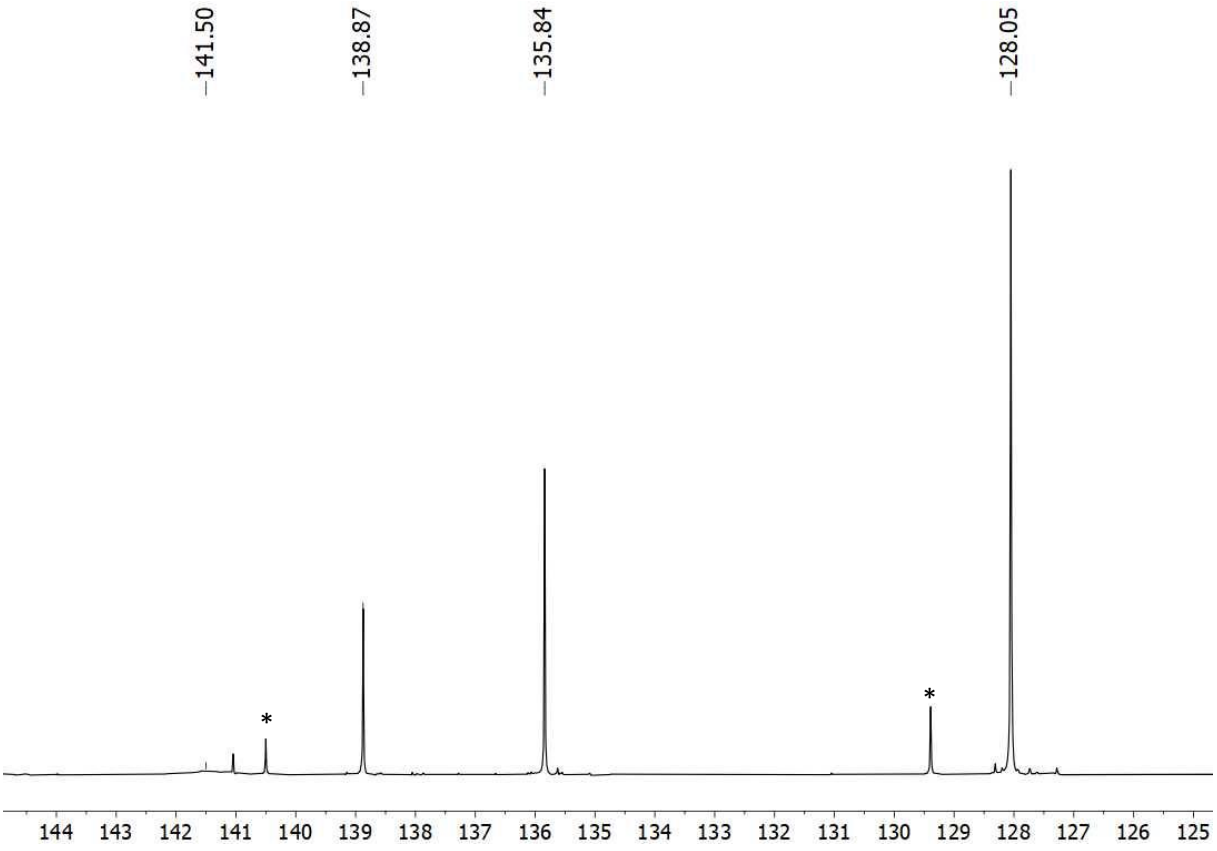


*Figure 24. $^{13}C\{^{1}H\}$ NMR spectrum of **2d** (100 MHz) in C_6D_6, aromatic region*

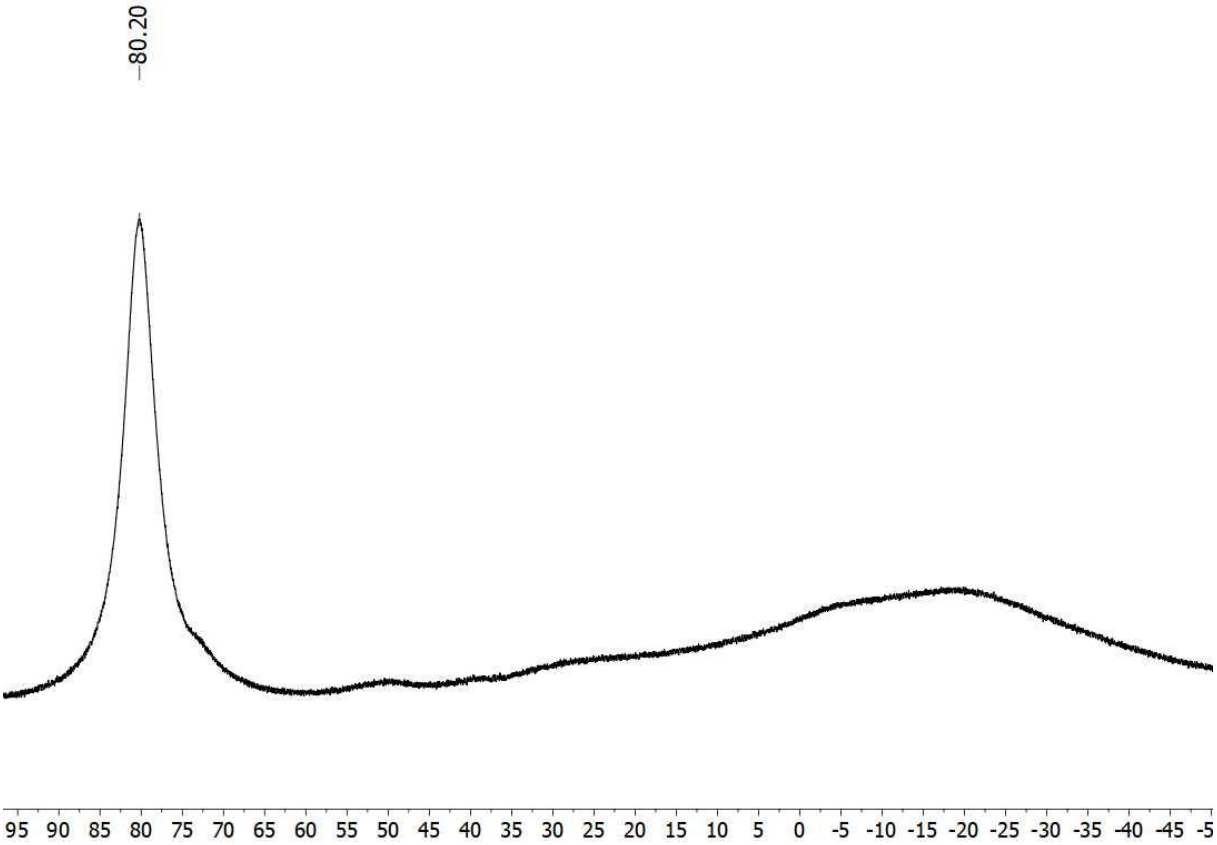
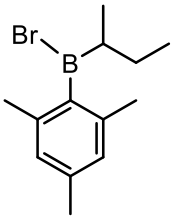


*Figure 25. $^{11}B\{^{1}H\}$ NMR spectrum of **2d** (128 MHz) in C_6D_6*

14.NMR spectra of 2e



2e

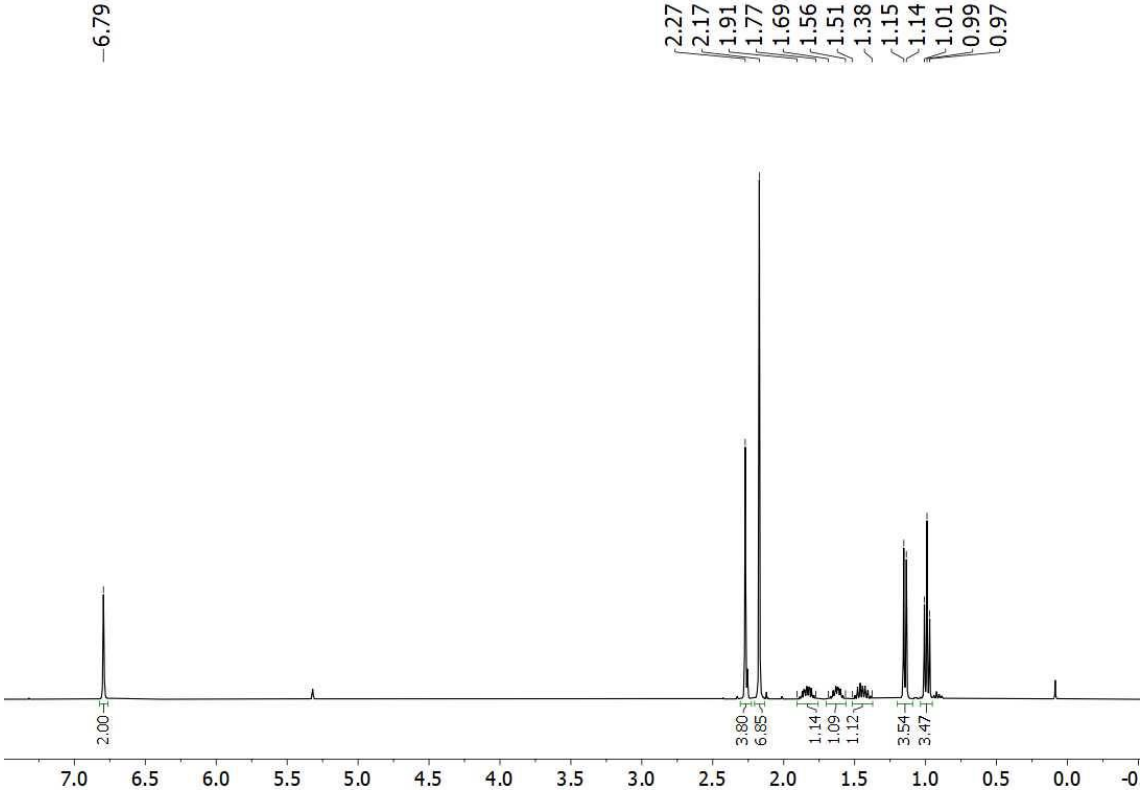


*Figure 26. ^{1}H NMR spectrum of **2e** (400 MHz) in CD_2Cl_2*

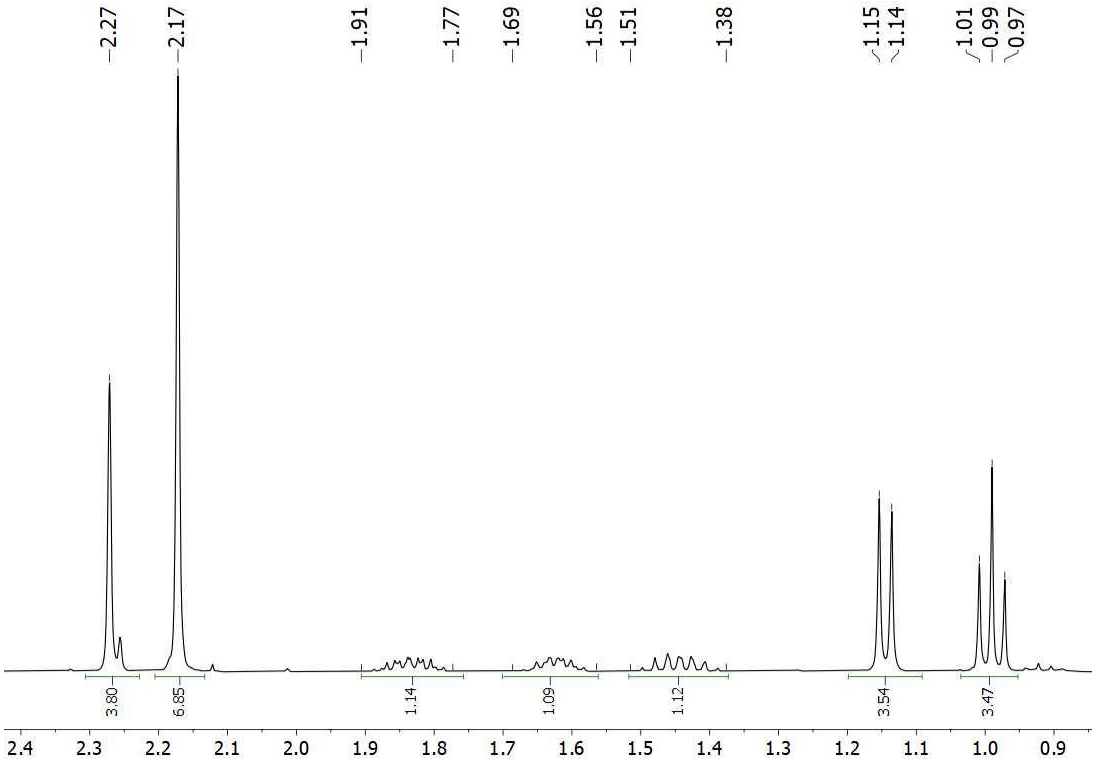


*Figure 27. ^{1}H NMR spectrum of **2e** (400 MHz) in CD_2Cl_2, aliphatic region*

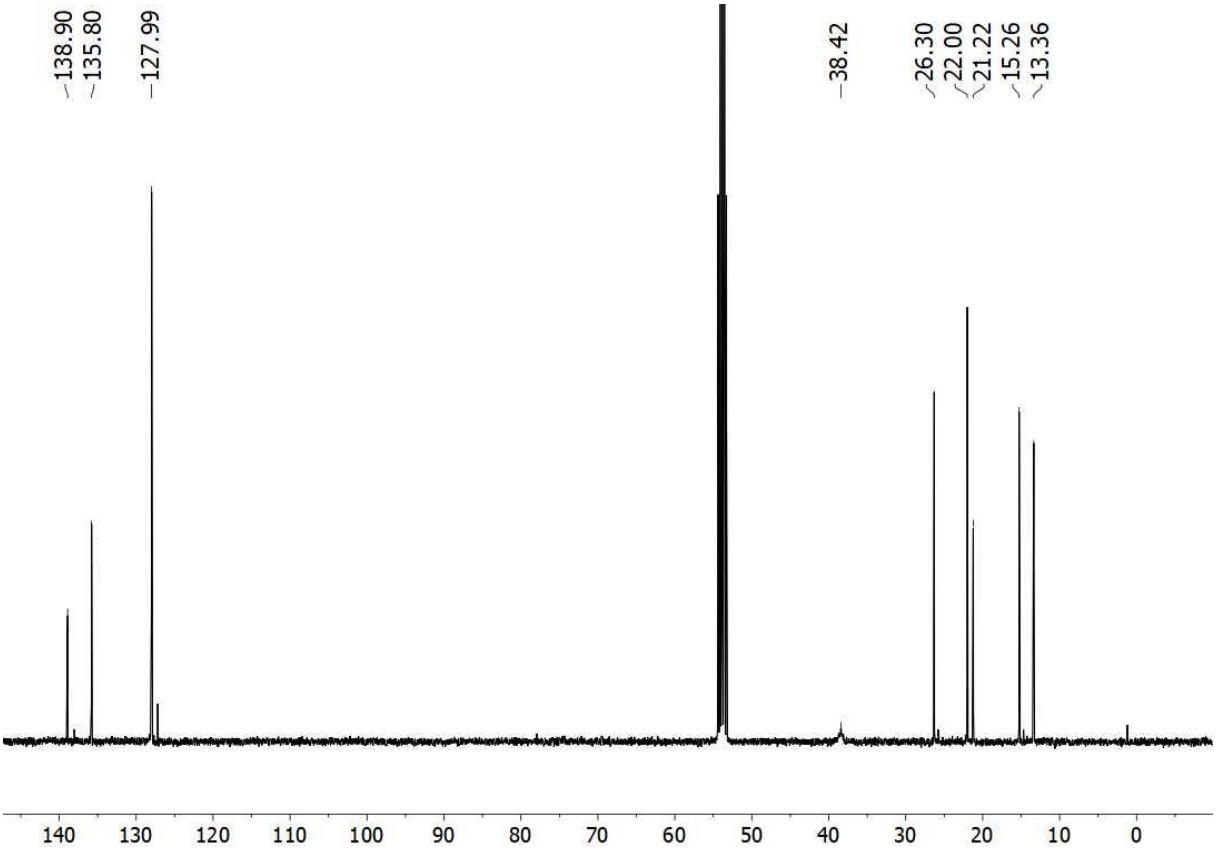


*Figure 28. $^{13}C\{^{1}H\}$ NMR spectrum of **2e** (100 MHz) in CD_2Cl_2*

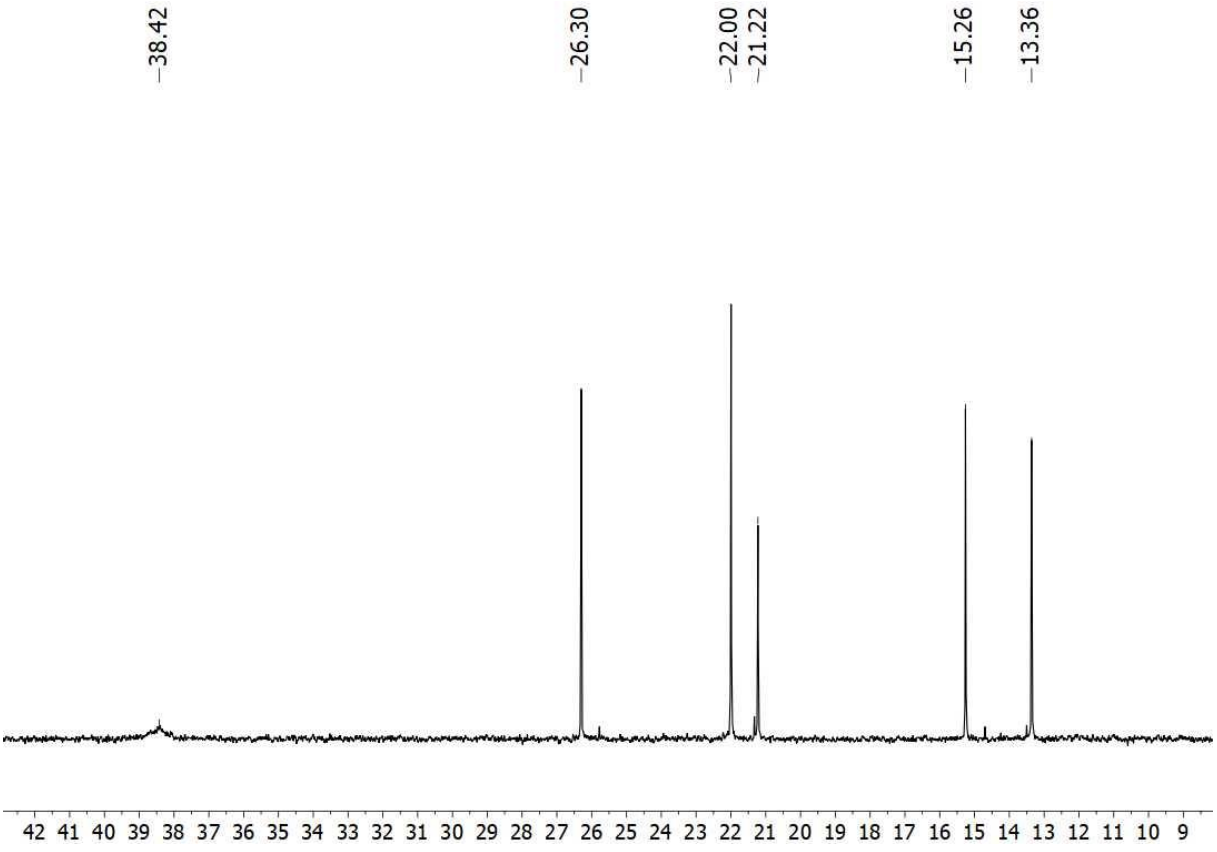


*Figure 29. $^{13}C\{^{1}H\}$ NMR spectrum of **2e** (100 MHz) in CD_2Cl_2, aliphatic region*

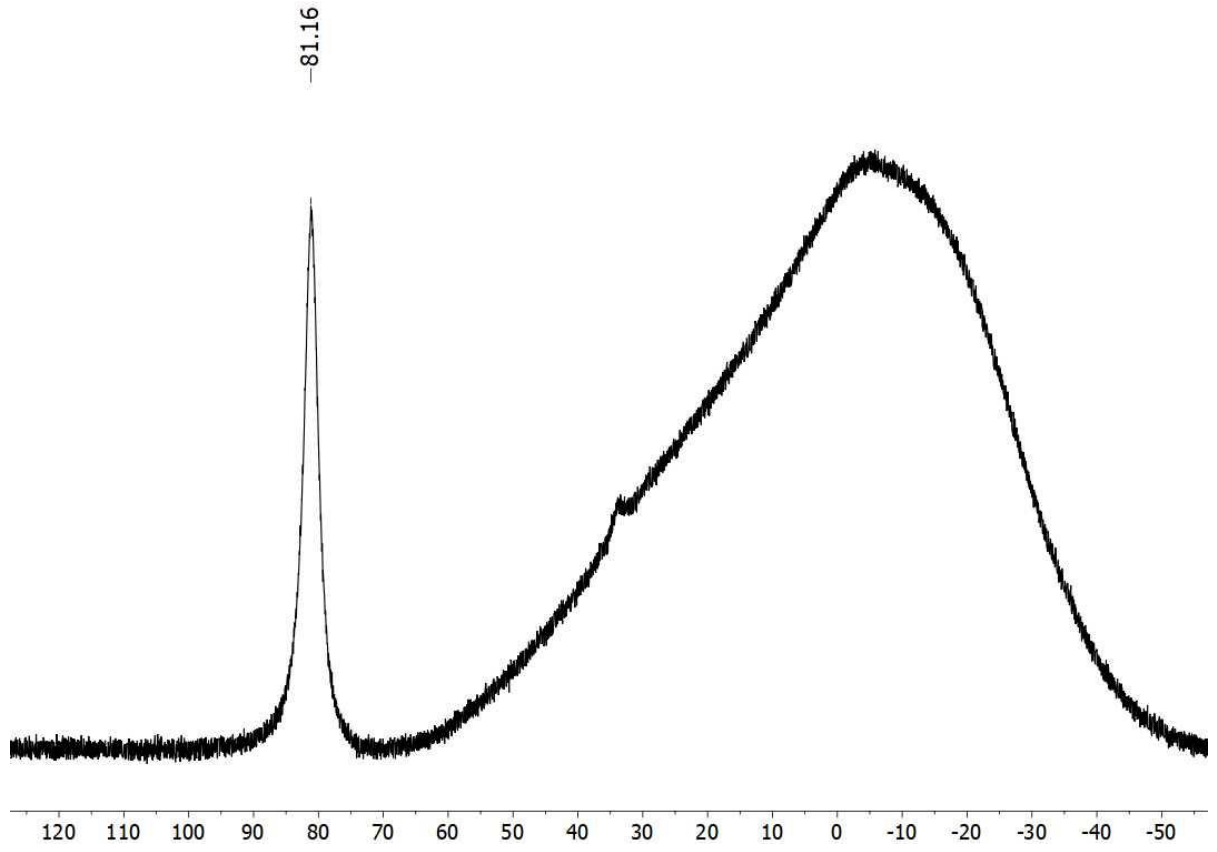
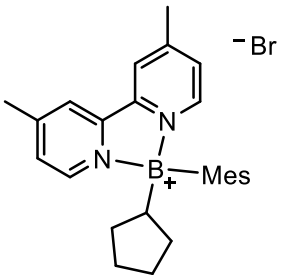


*Figure 30. $^{11}B\{^{1}H\}$ NMR spectrum of **2e** (128 MHz) in CD_2Cl_2*

15.NMR spectra of 3a



3a

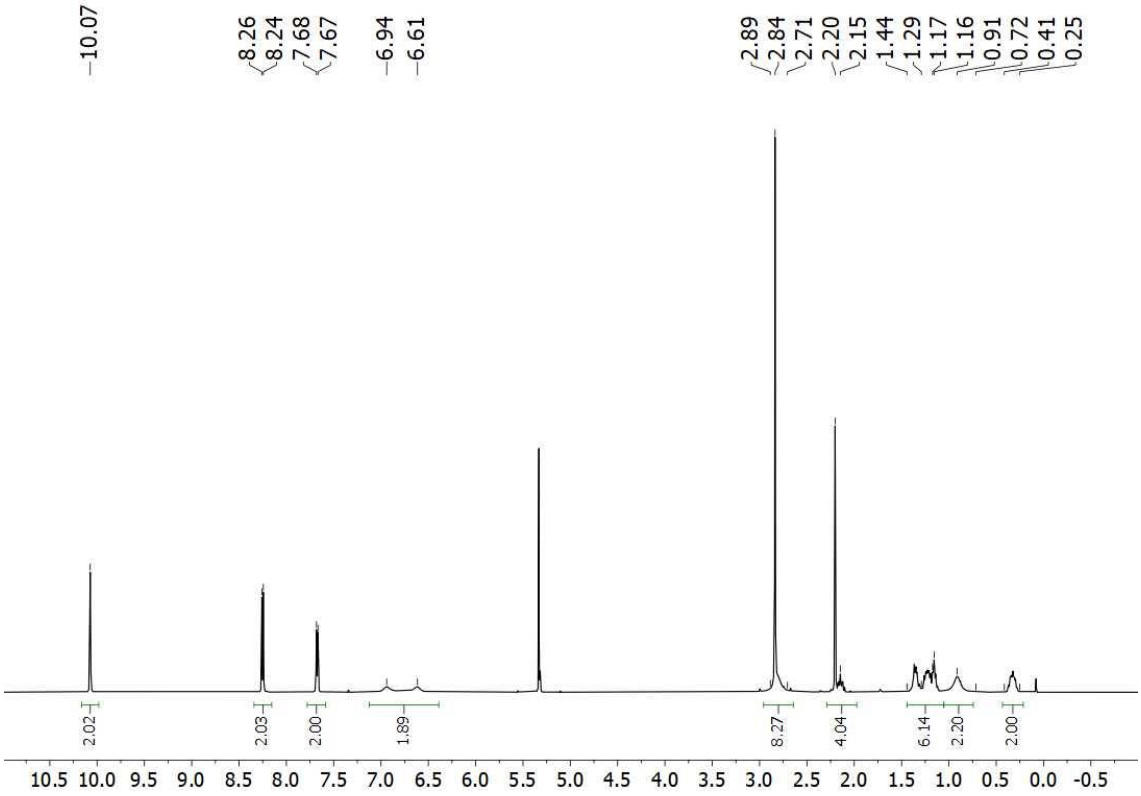


*Figure 31. ^{1}H NMR spectrum of **3a** (400 MHz) in CD_2Cl_2*

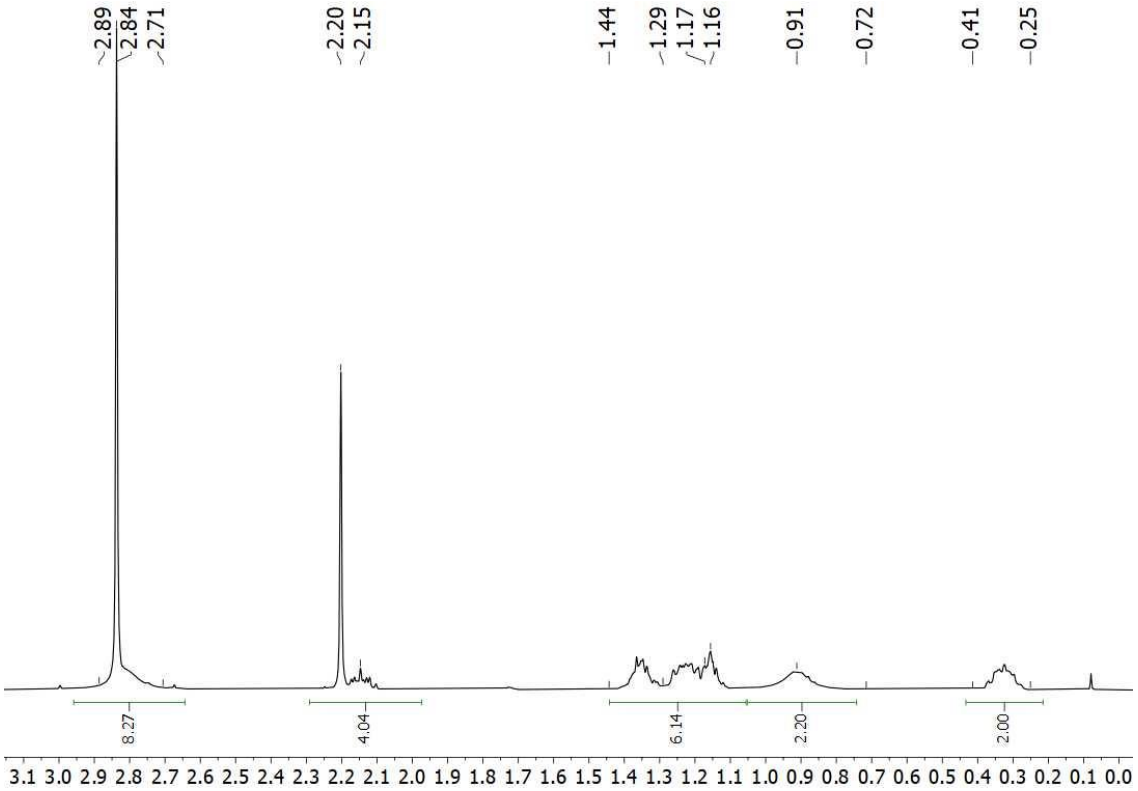


*Figure 32. ^{1}H NMR spectrum of **3a** (400 MHz) in CD_2Cl_2, aliphatic region*

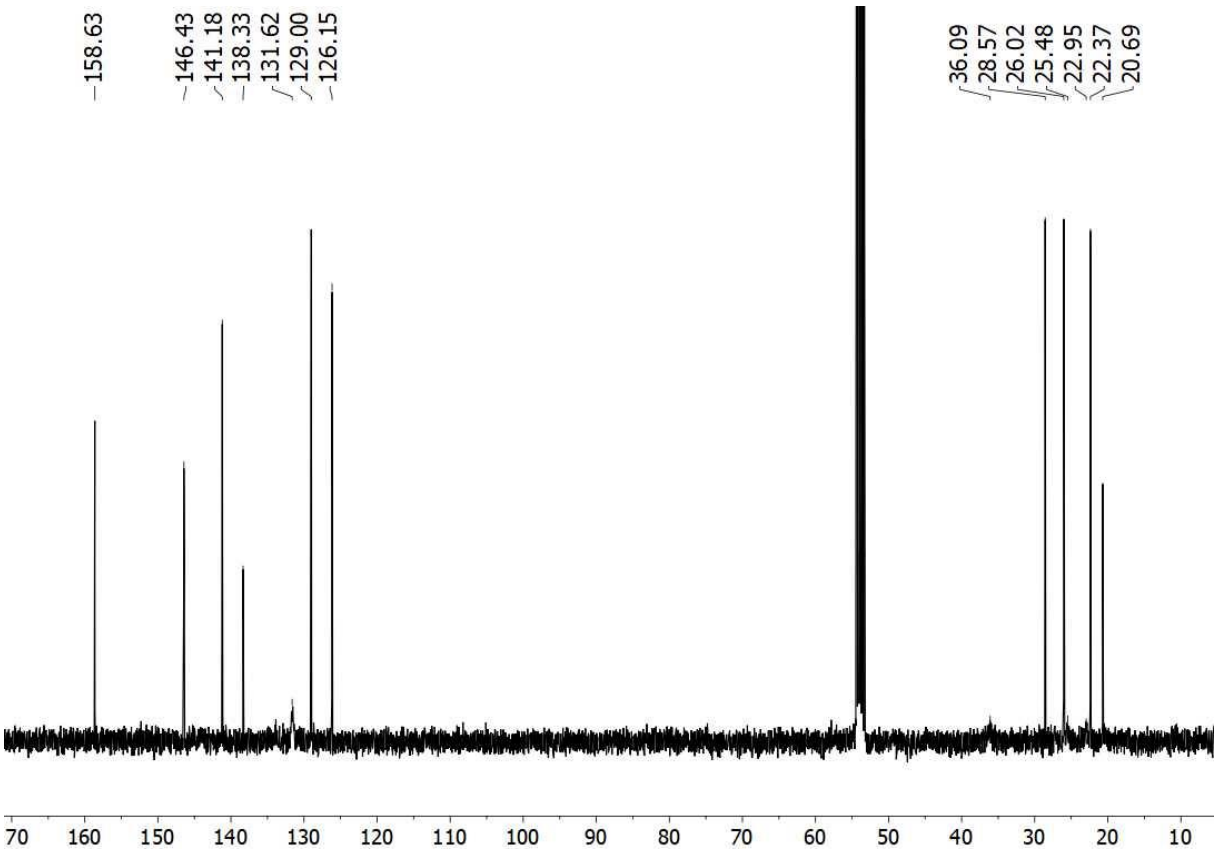


*Figure 33. $^{13}C\{^{1}H\}$ NMR spectrum of **3a** (100 MHz) in CD_2Cl_2*

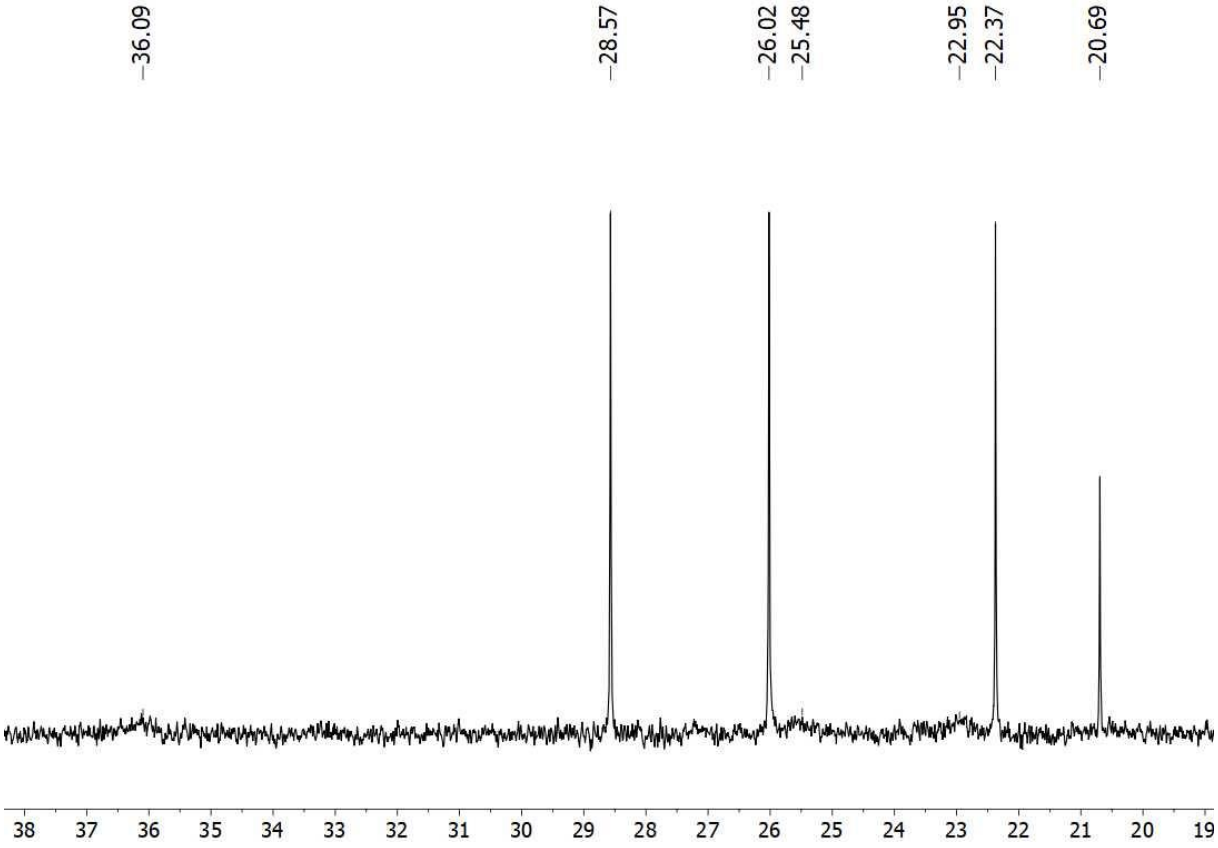


*Figure 34. $^{13}C\{^{1}H\}$ NMR spectrum of **3a** (100 MHz) in CD_2Cl_2, aliphatic region*

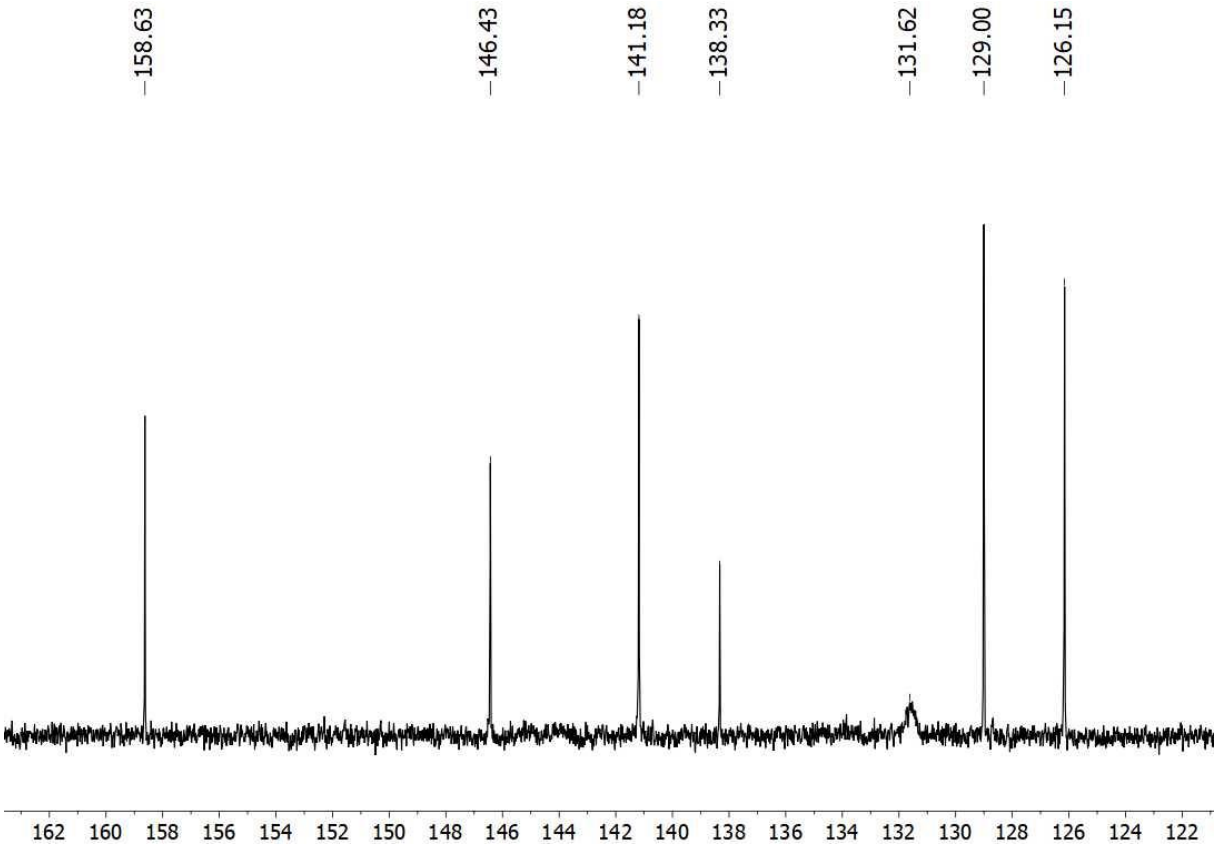


*Figure 35. $^{13}C\{^{1}H\}$ NMR spectrum of **3a** (100 MHz) in CD_2Cl_2, aromatic region*

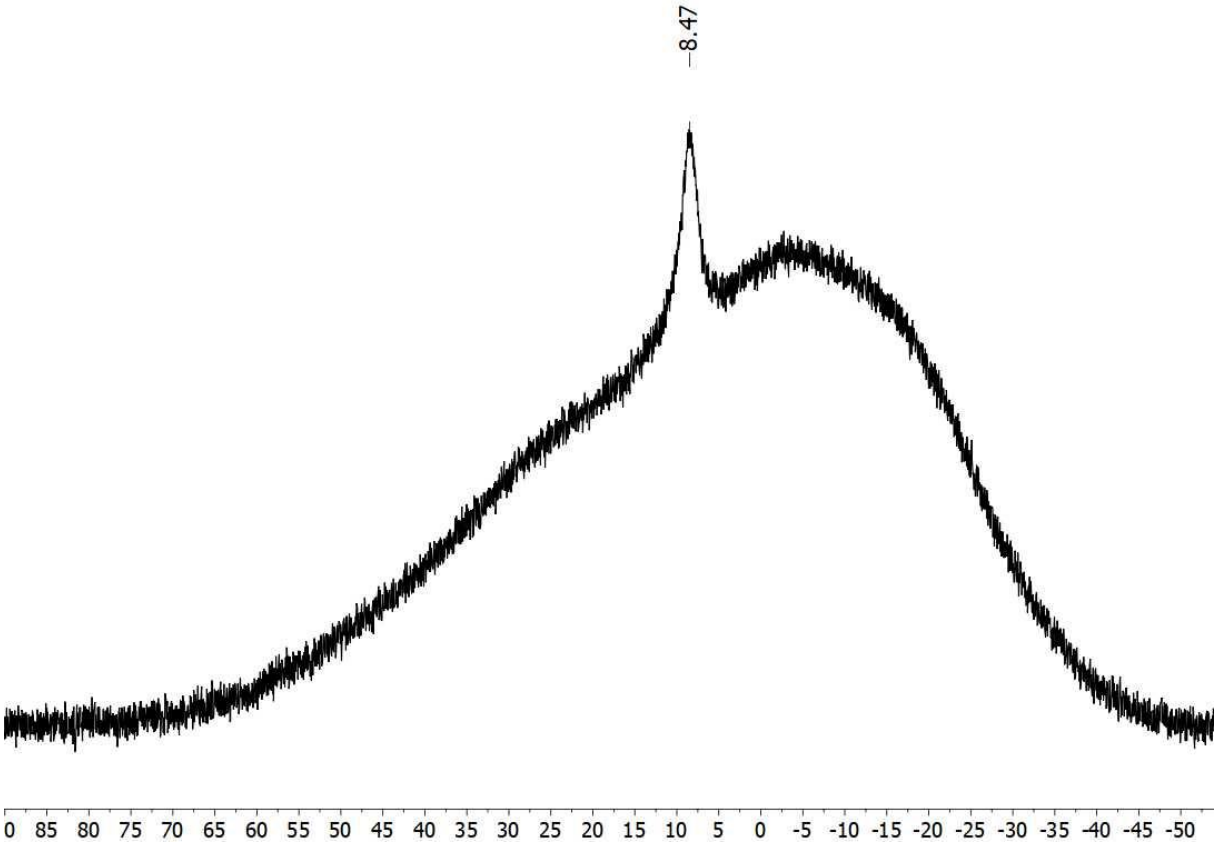
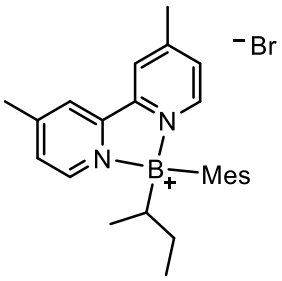


*Figure 36. $^{11}B\{^{1}H\}$ NMR spectrum of **3a** (128 MHz) in CD_2Cl_2*

16.NMR spectra of 3e



3e

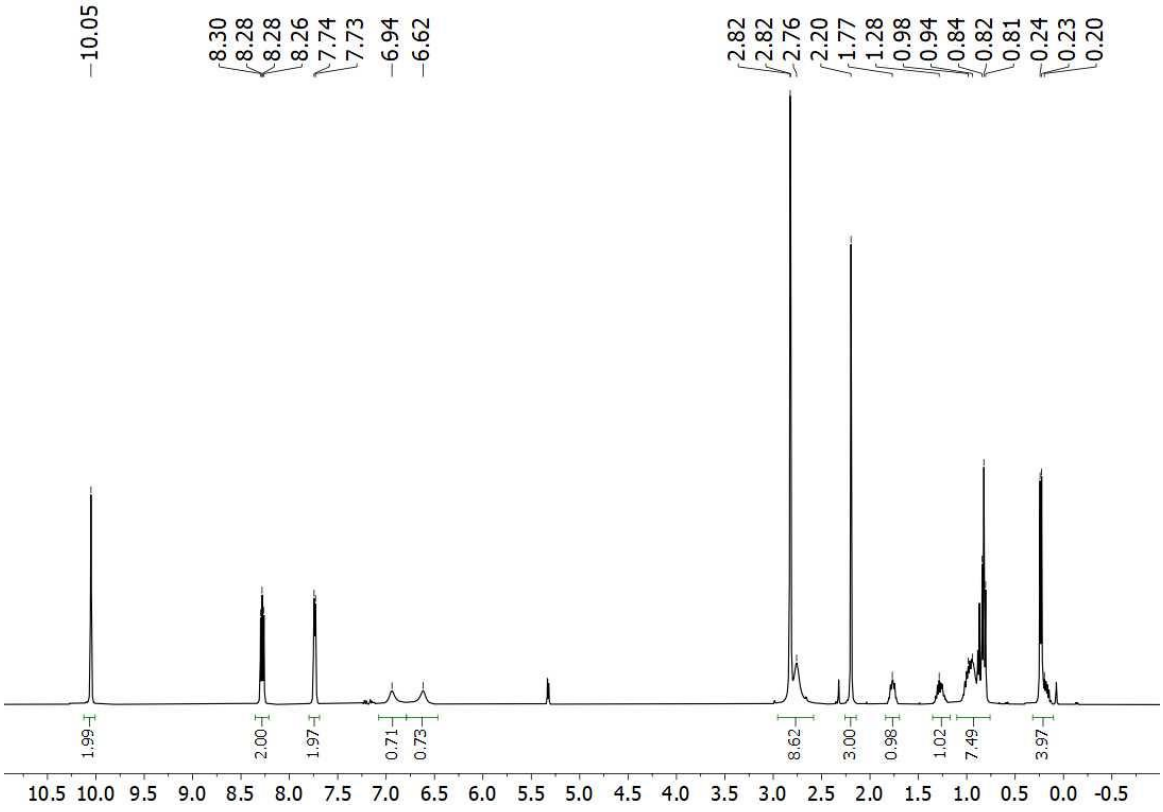


*Figure 37. ^{1}H NMR spectrum of **3e** (400 MHz) in CD_2Cl_2*

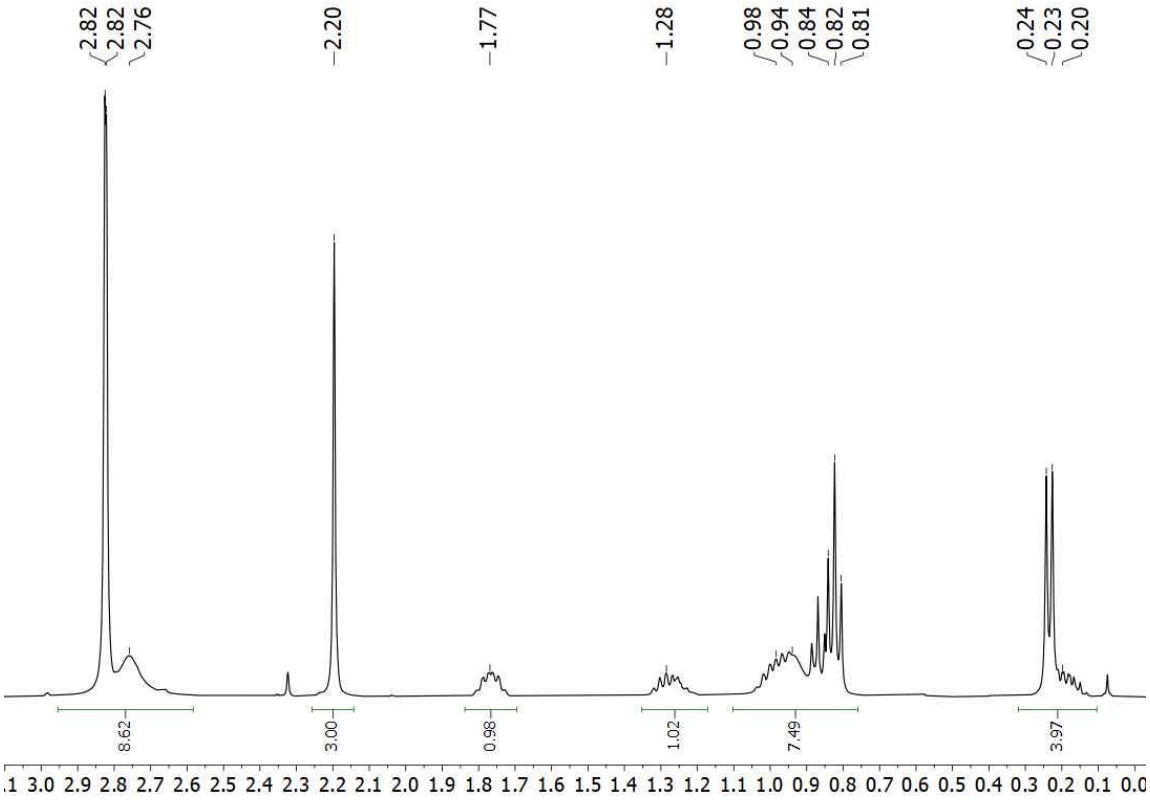


*Figure 38. ^{1}H NMR spectrum of **3e** (400 MHz) in C_2Cl_2, aliphatic region*

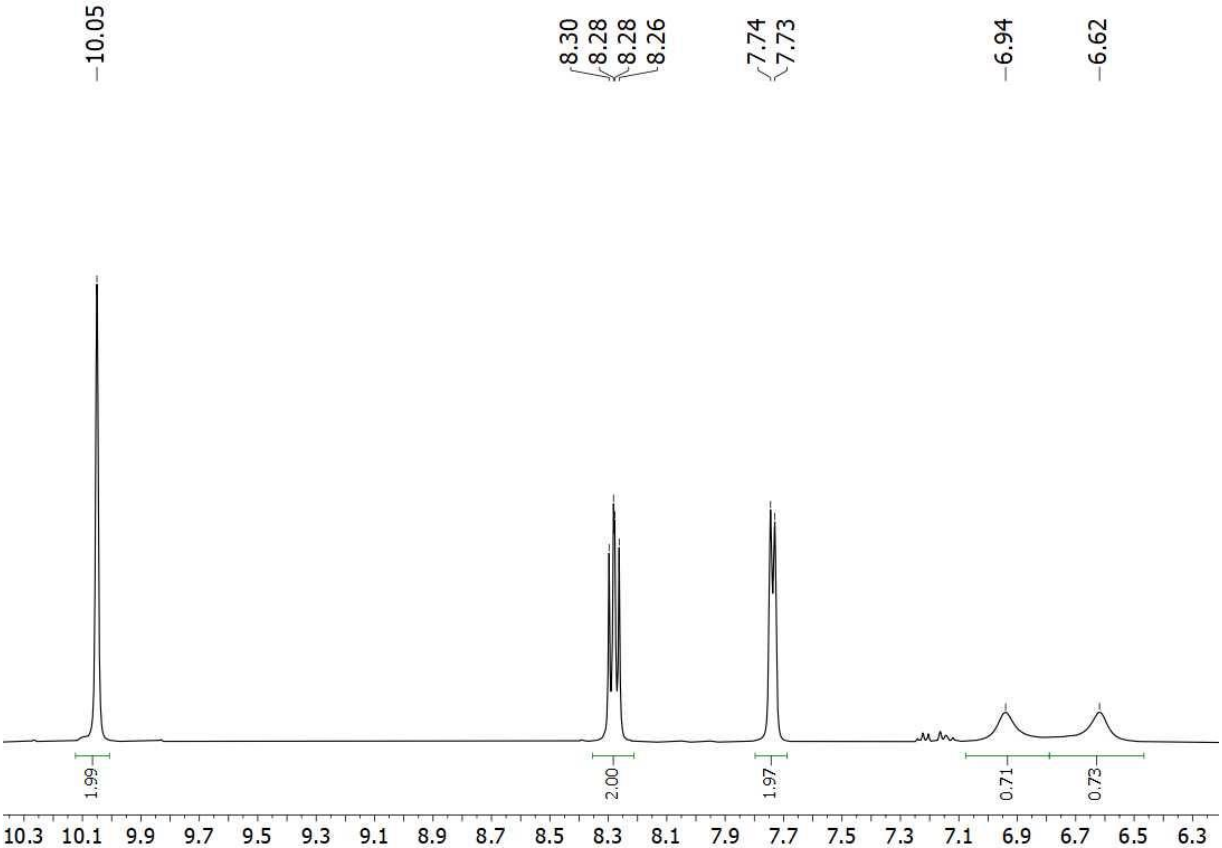


*Figure 39. ^{1}H NMR spectrum of **3e** (400 MHz) in CD_2Cl_2, aromatic region*

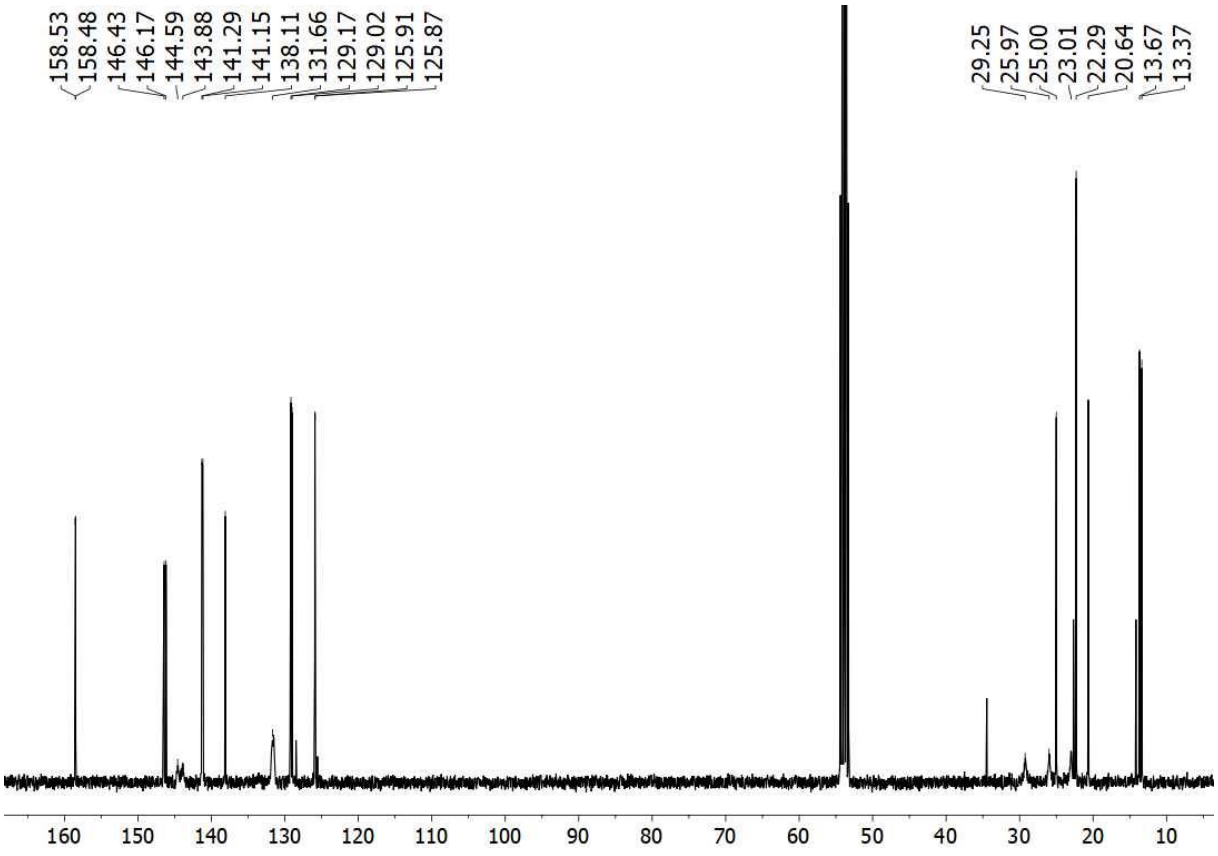


*Figure 40. $^{13}C\{^{1}H\}$ NMR spectrum of **3e** (100 MHz) in CD_2Cl_2*

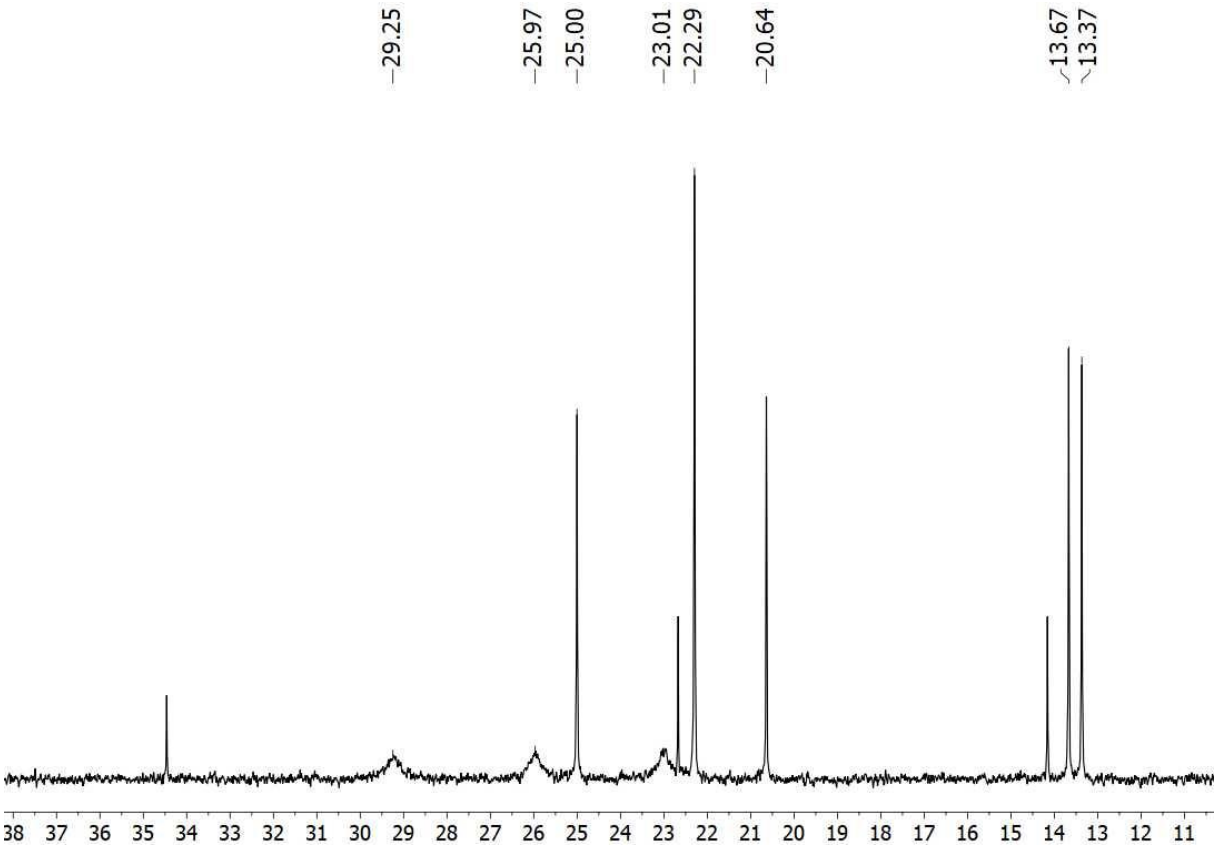


*Figure 41. $^{13}C\{^{1}H\}$ NMR spectrum of **3e** (100 MHz) in CD_2Cl_2, aliphatic region*

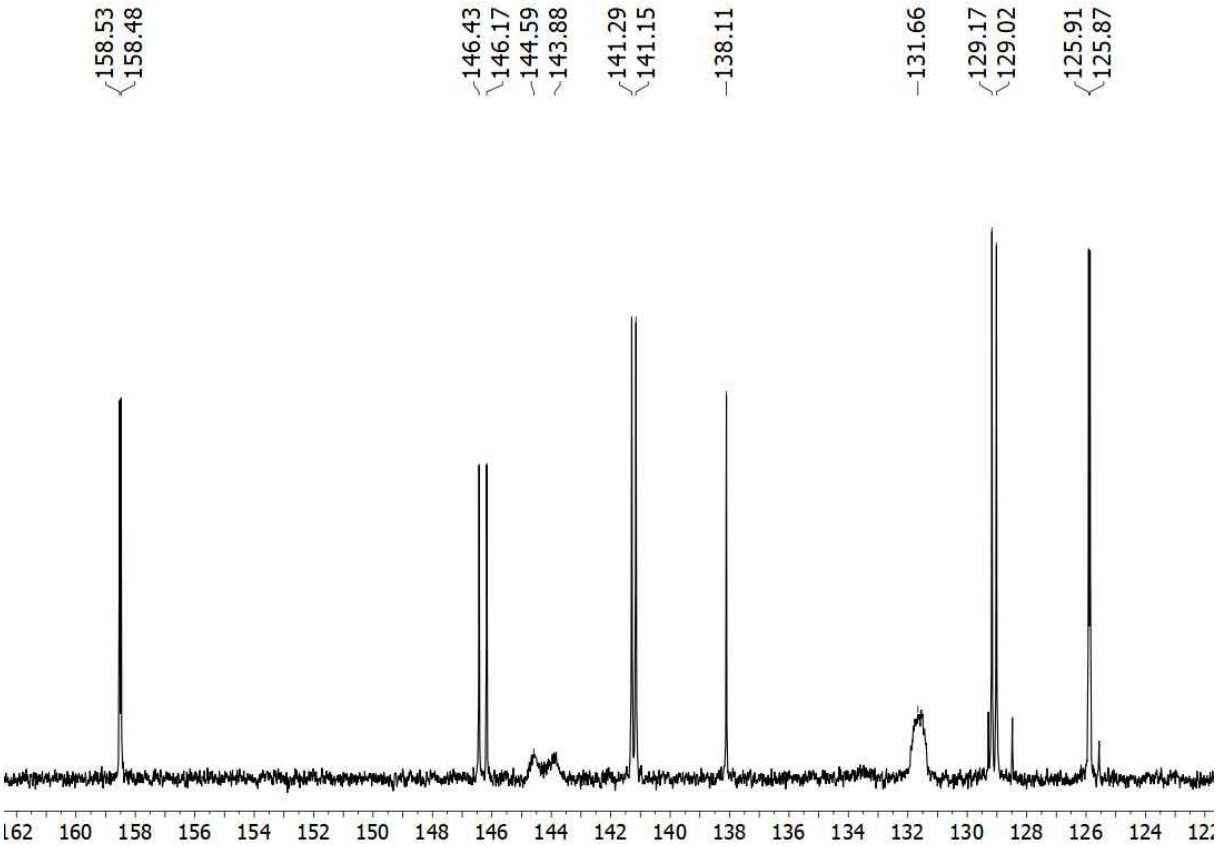


*Figure 42. $^{13}C\{^{1}H\}$ NMR spectrum of **3e** (100 MHz) in CD_2Cl_2, aromatic region*

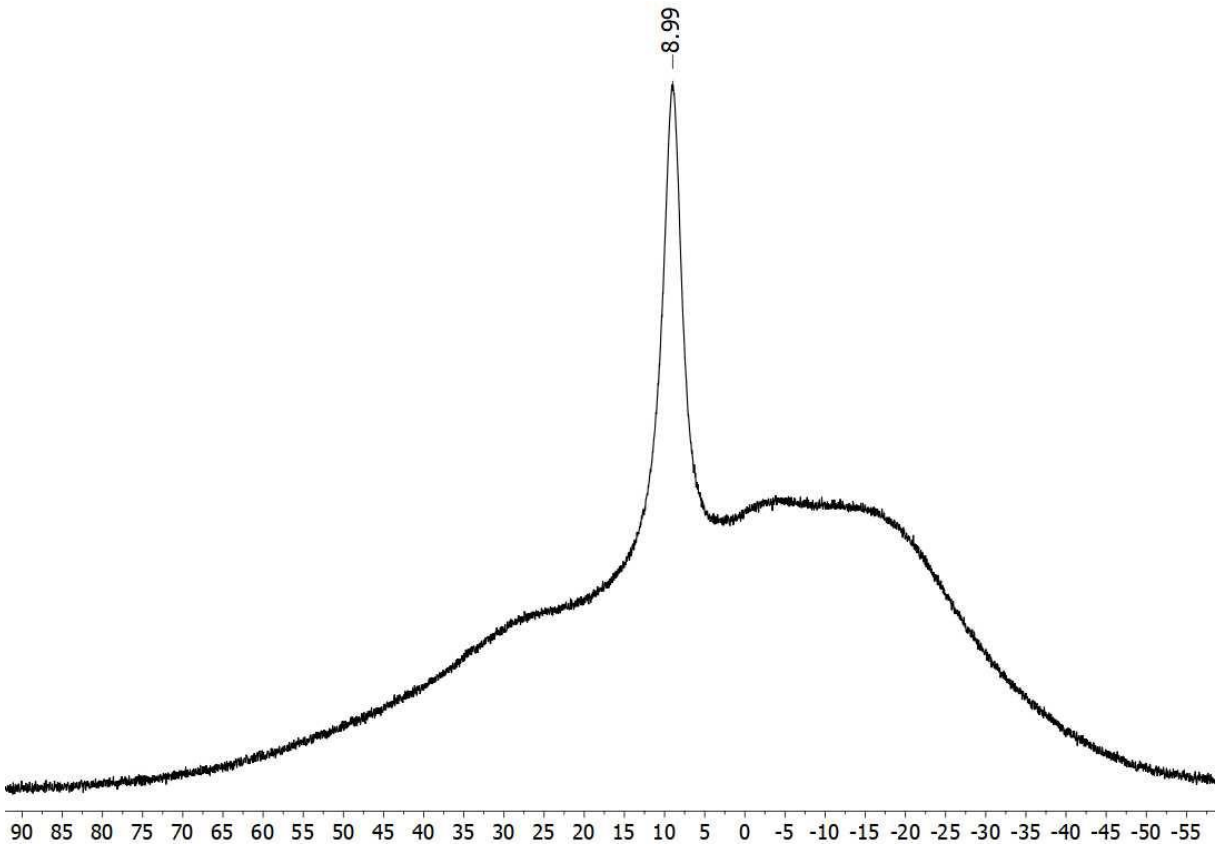
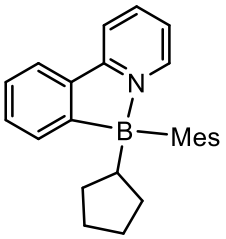


*Figure 43. $^{11}B\{^{1}H\}$ NMR spectrum of **3e** (128 MHz) in CD_2Cl_2*

17.NMR spectra of 4a



4a

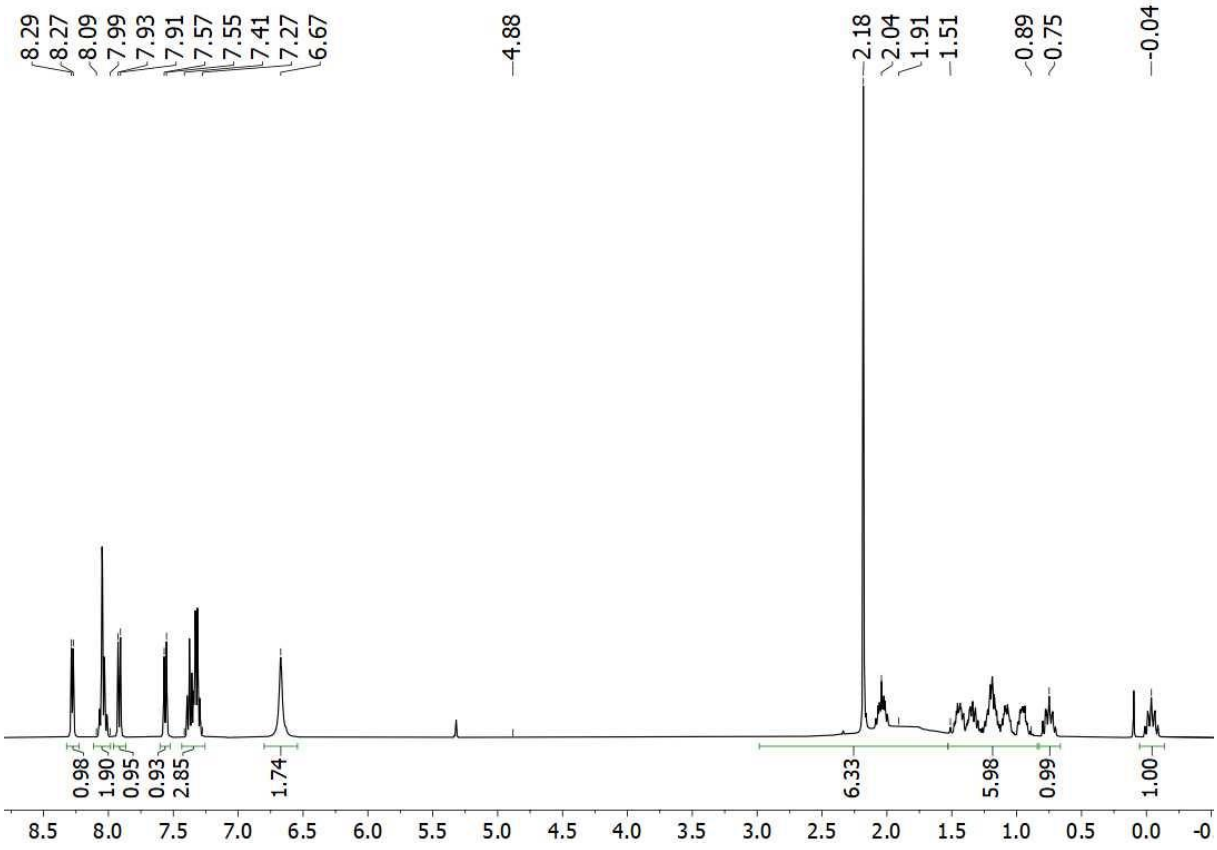


*Figure 44. ^{1}H NMR spectrum of **4a** (400 MHz) in CD_2Cl_2*

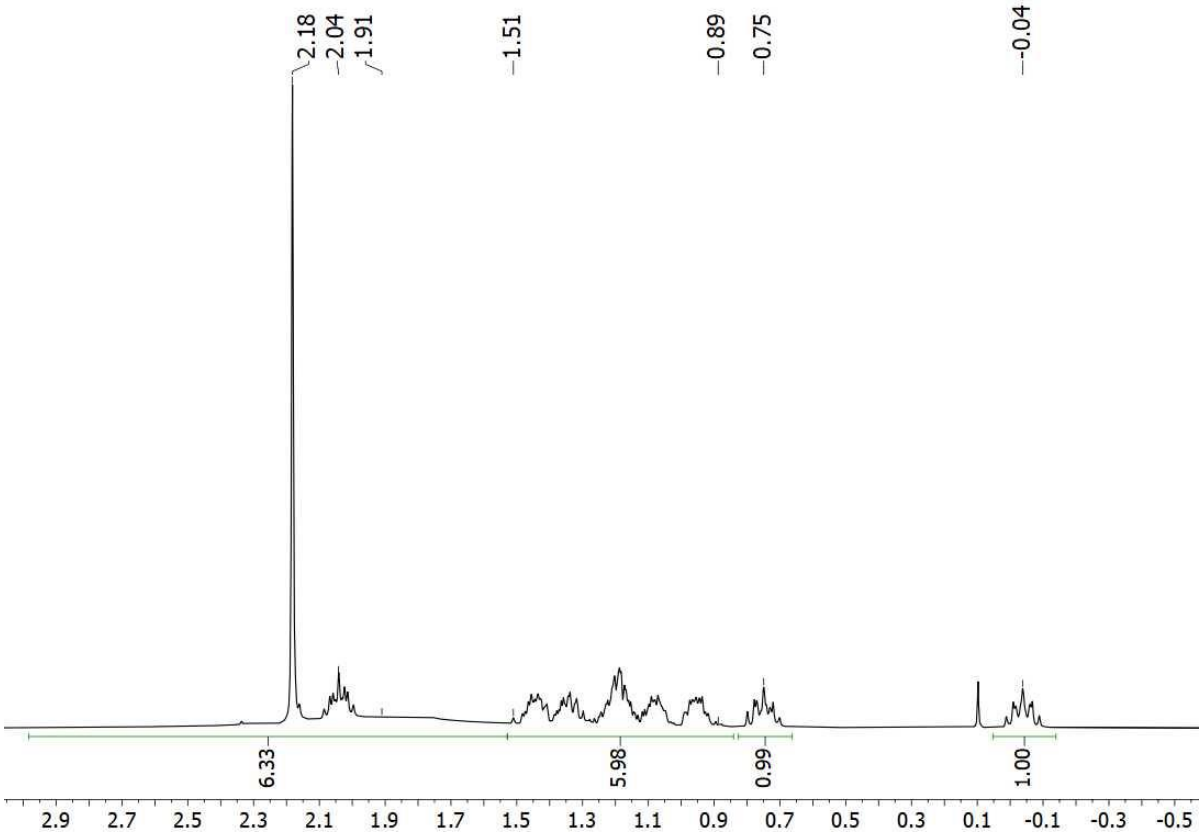


*Figure 45. ^{1}H NMR spectrum of **4a** (400 MHz) in C_2Cl_2, aliphatic region*

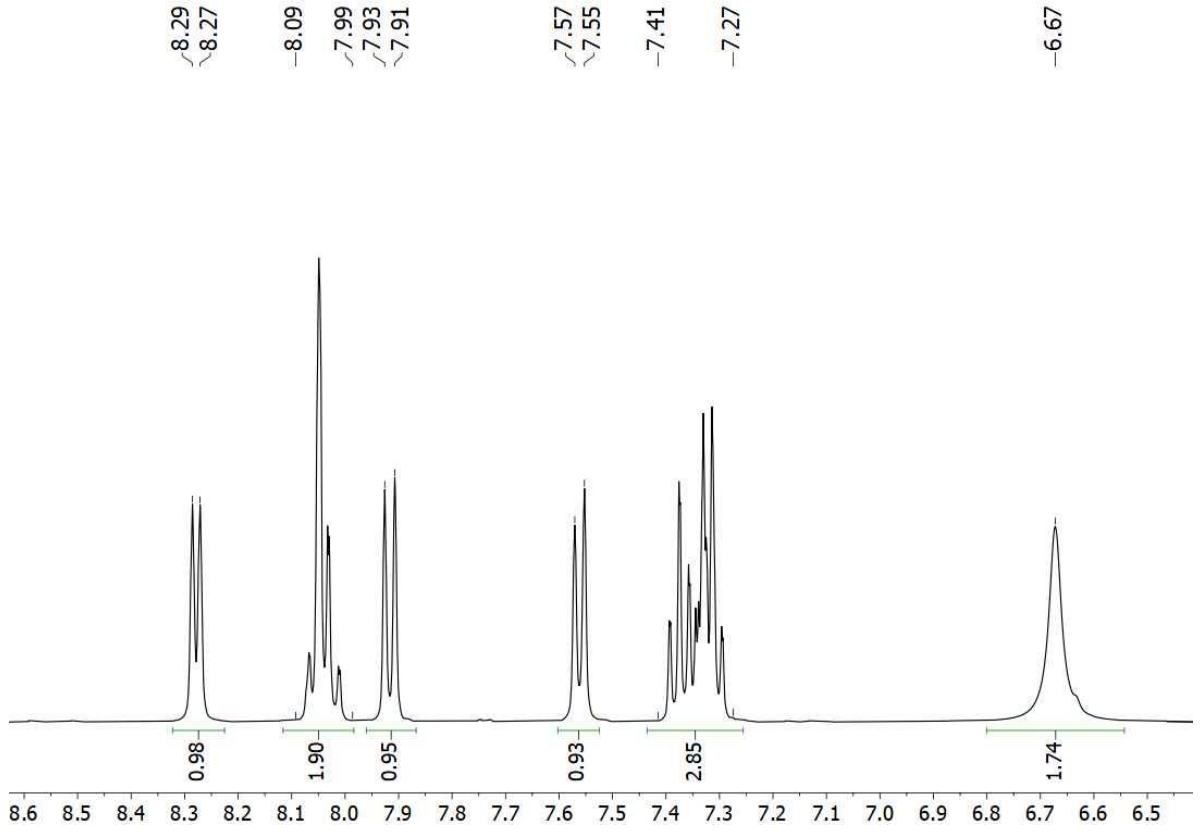


*Figure 46. ^{1}H NMR spectrum of **4a** (400 MHz) in CD_2Cl_2, aromatic region*

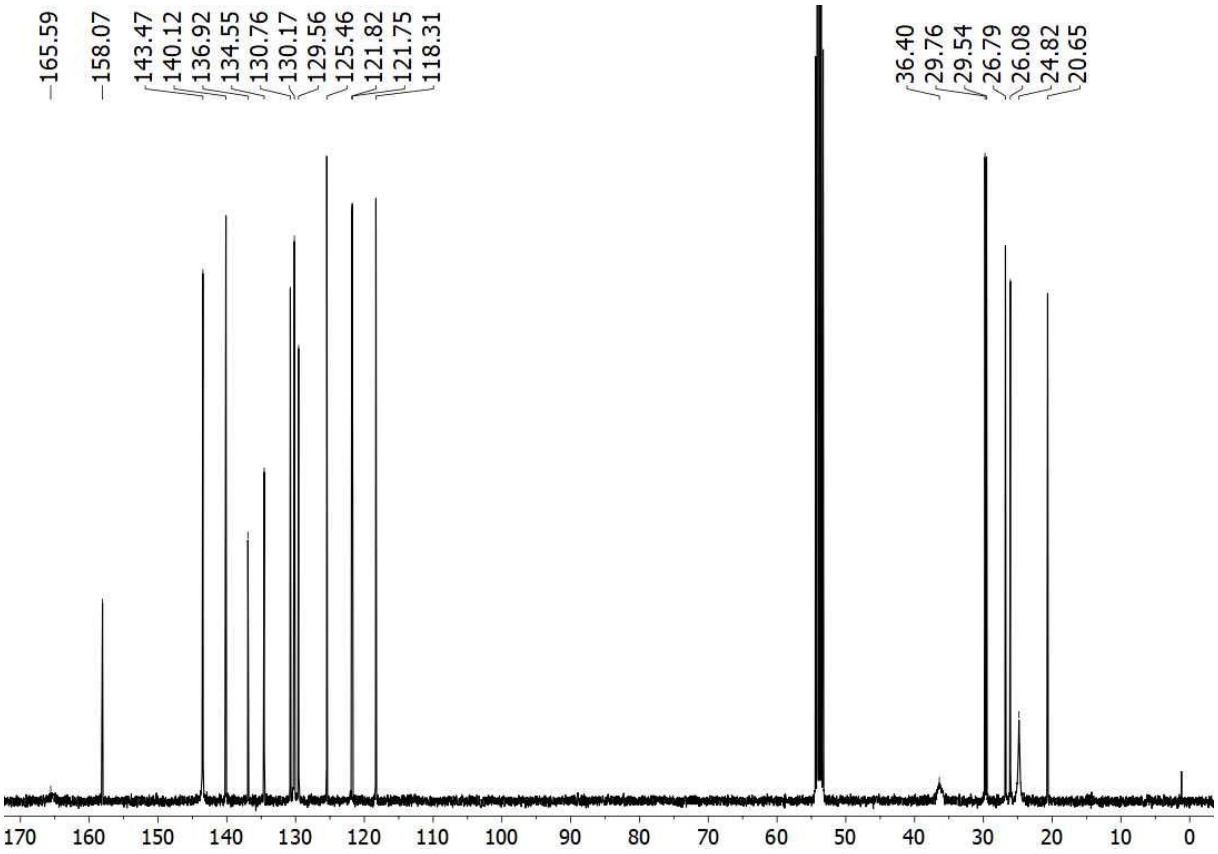


*Figure 47. $^{13}C\{^{1}H\}$ NMR spectrum of **4a** (100 MHz) in CD_2Cl_2*

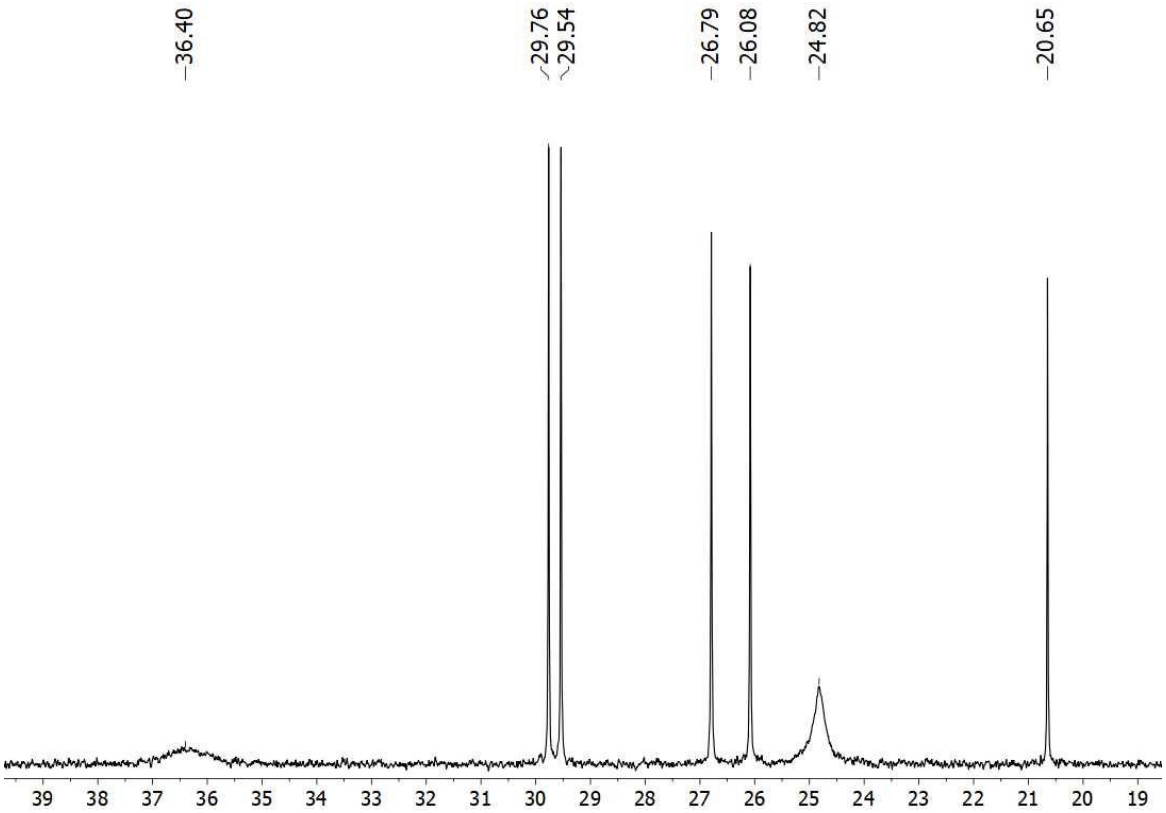


*Figure 48. $^{13}C\{^{1}H\}$ NMR spectrum of **4a** (100 MHz) in CD_2Cl_2, aliphatic region*

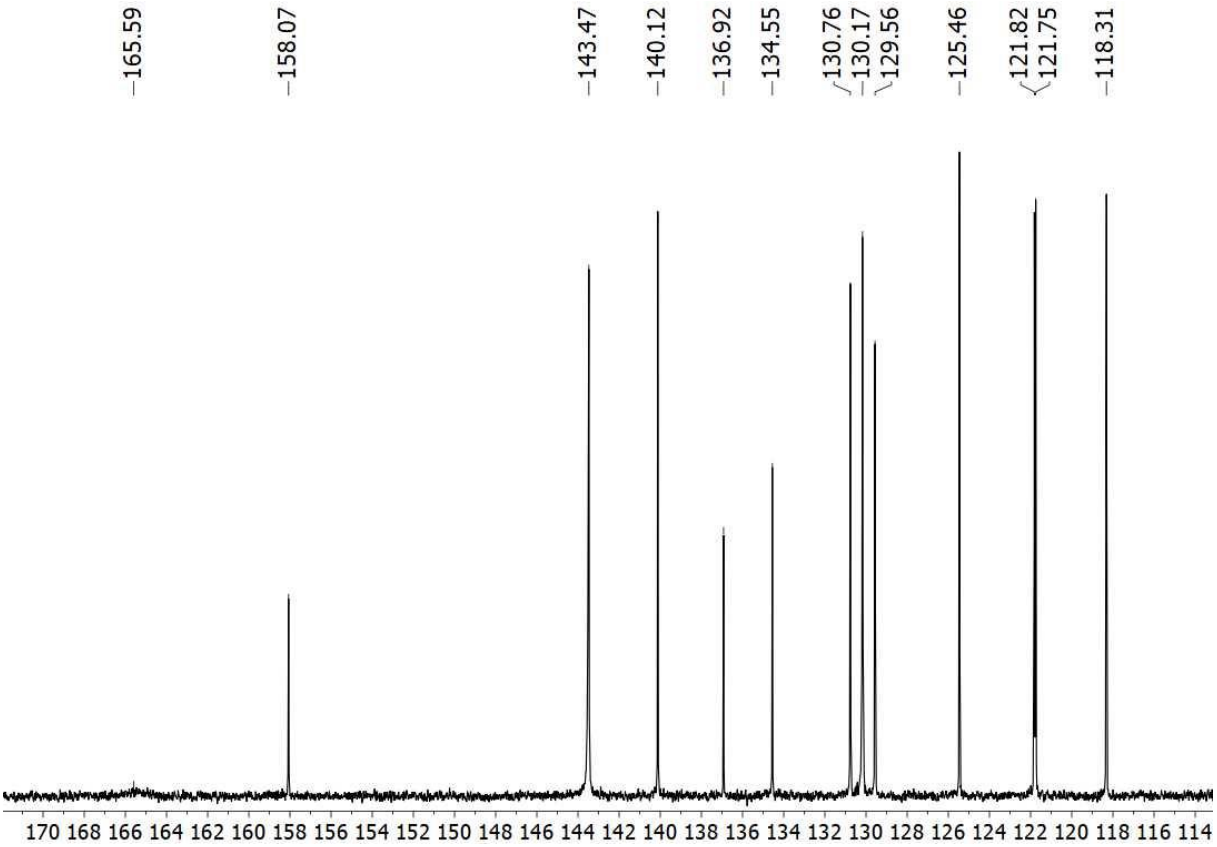


*Figure 49. $^{13}C\{^{1}H\}$ NMR spectrum of **4a** (100 MHz) in CD_2Cl_2, aromatic region*

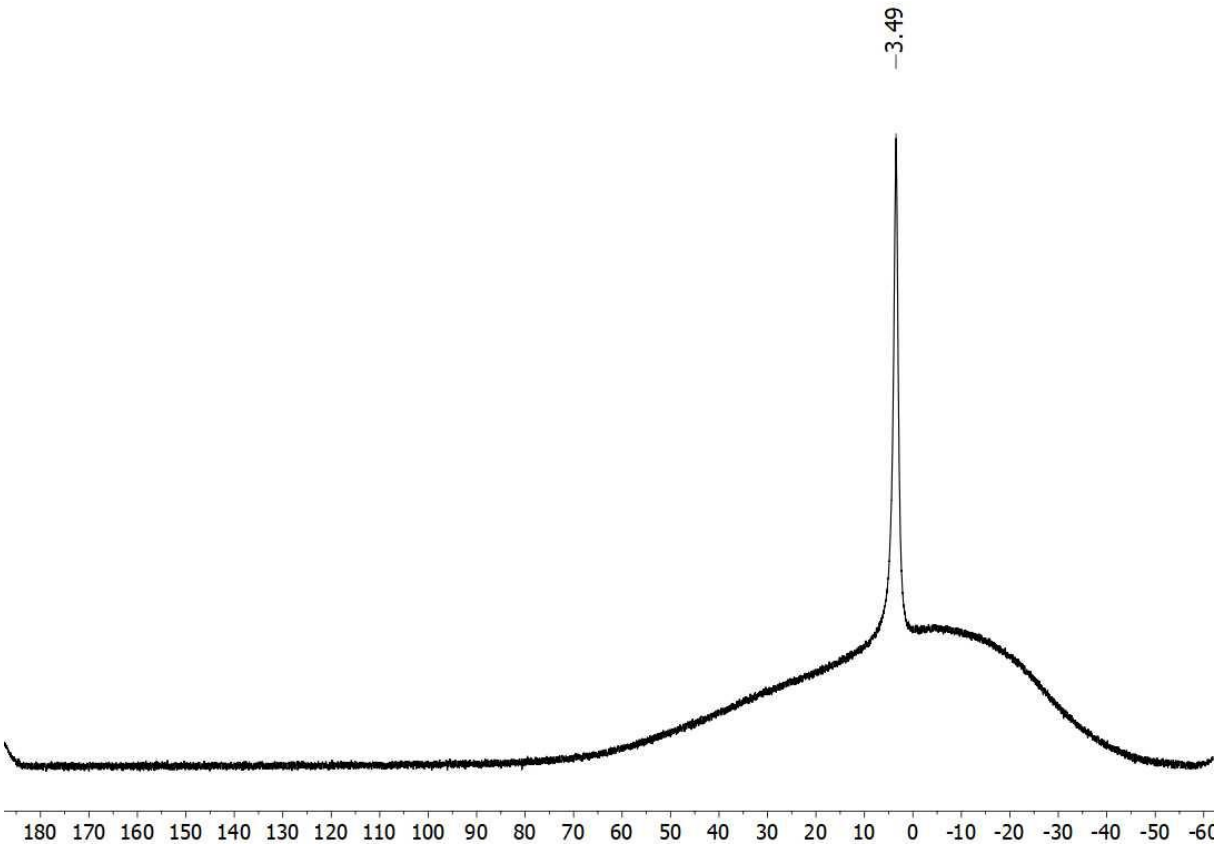
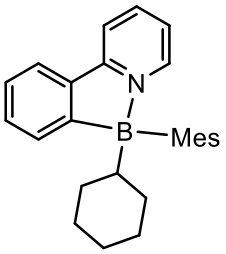


*Figure 50. $^{11}B\{^{1}H\}$ NMR spectrum of **4a** (128 MHz) in CD_2Cl_2*

18.NMR spectra of 4c



4c

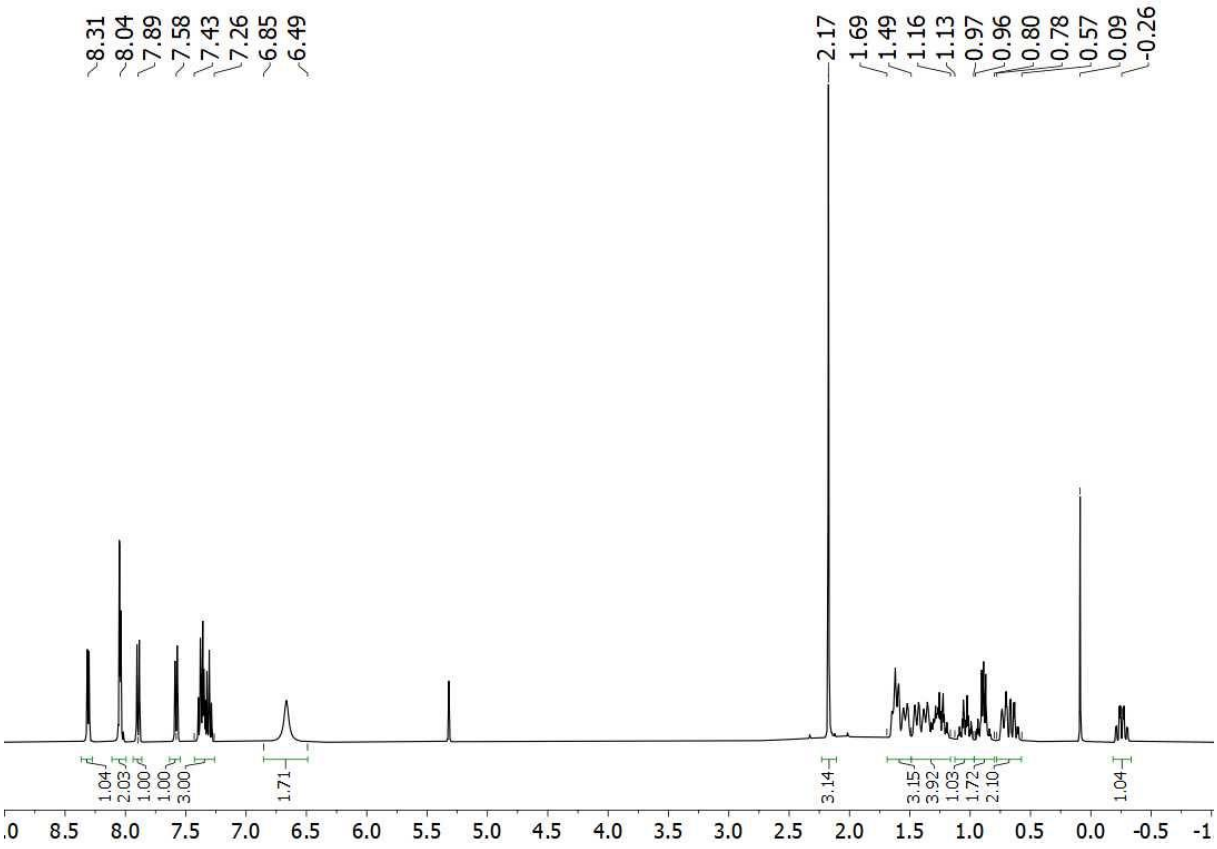


*Figure 51. ^{1}H NMR spectrum of **4c** (400 MHz) in CD_2Cl_2*

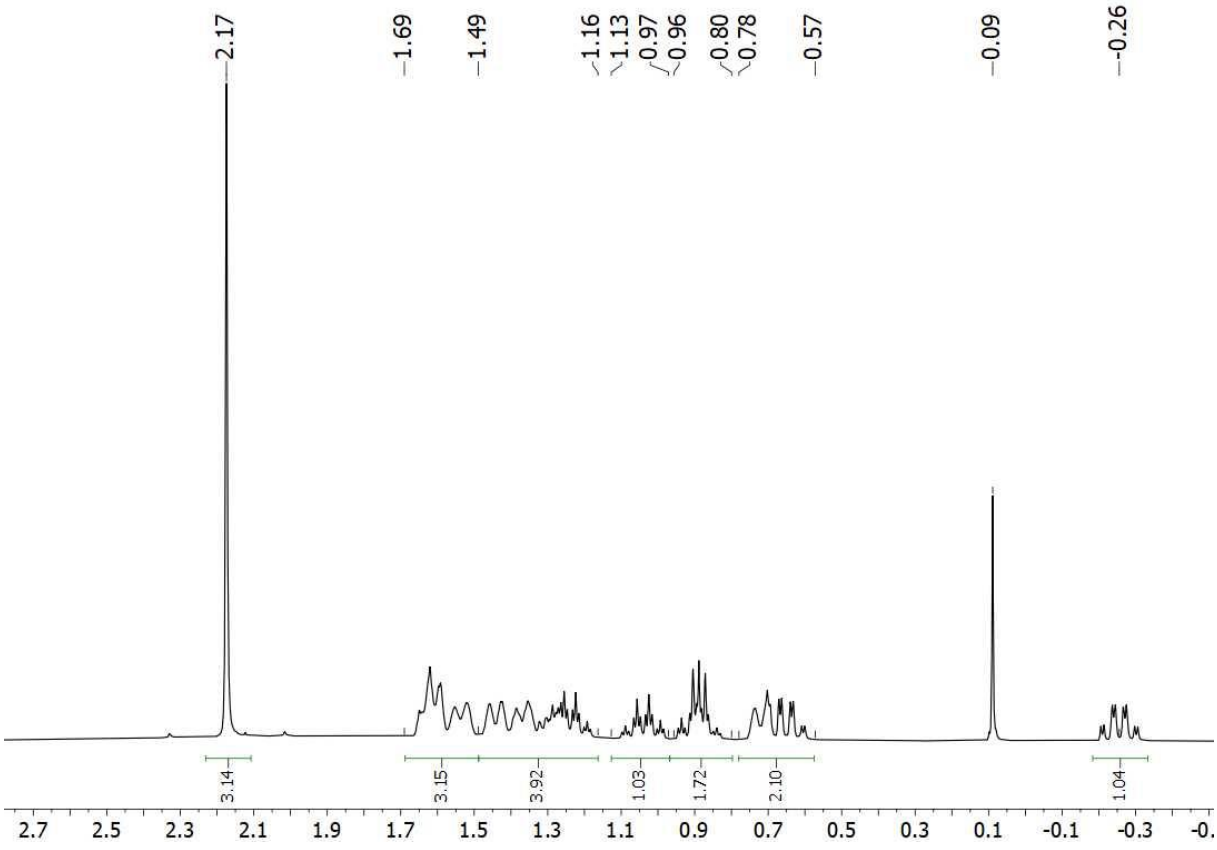


*Figure 52. ^{1}H NMR spectrum of **4c** (400 MHz) in C_2Cl_2, aliphatic region*

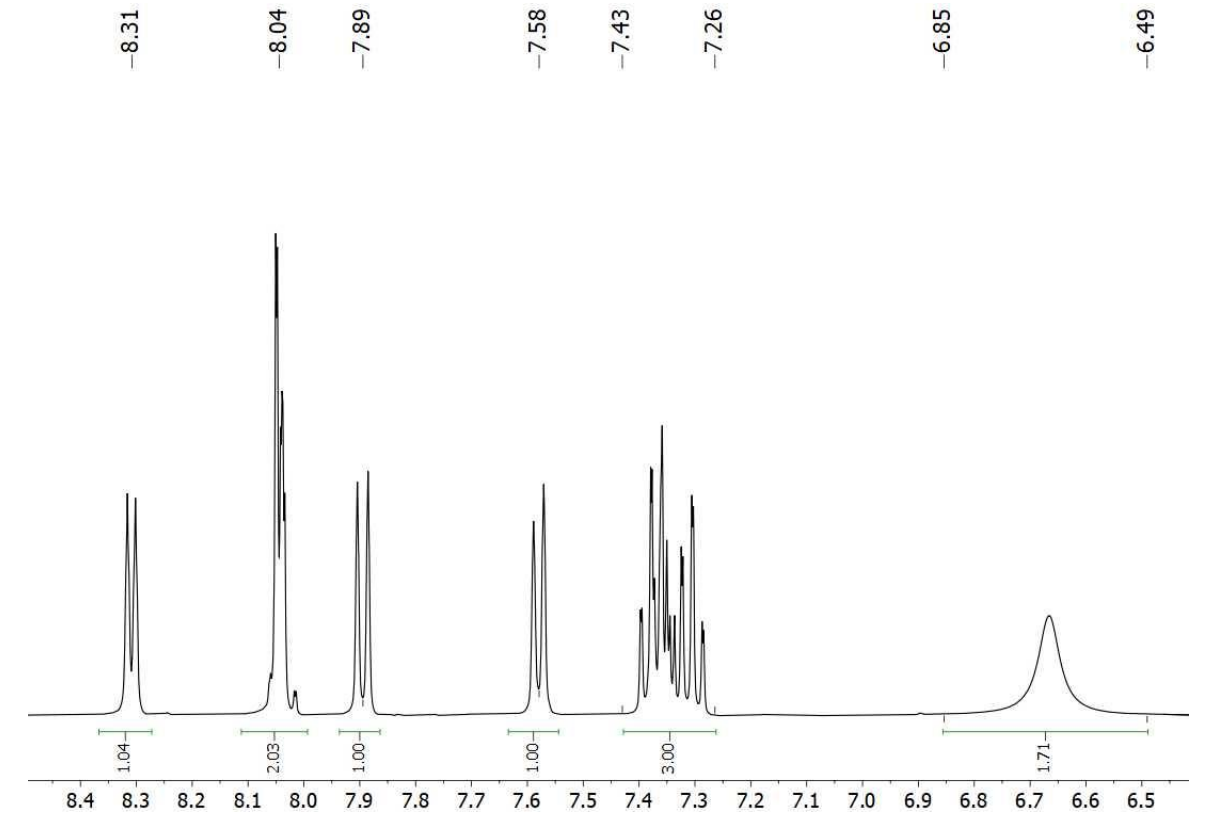


*Figure 53. ^{1}H NMR spectrum of **4c** (400 MHz) in CD_2Cl_2, aromatic region*

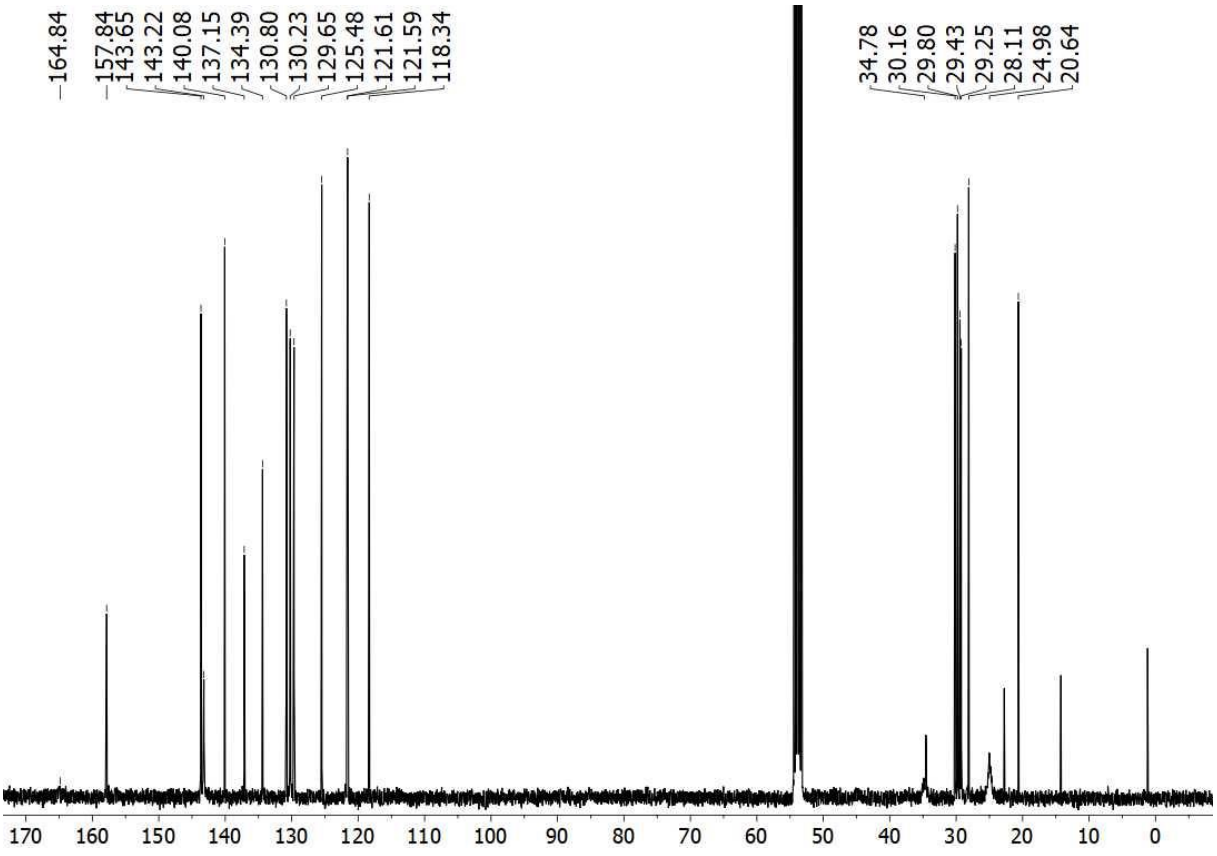


*Figure 54. $^{13}C\{^{1}H\}$ NMR spectrum of **4c** (100 MHz) in CD_2Cl_2*

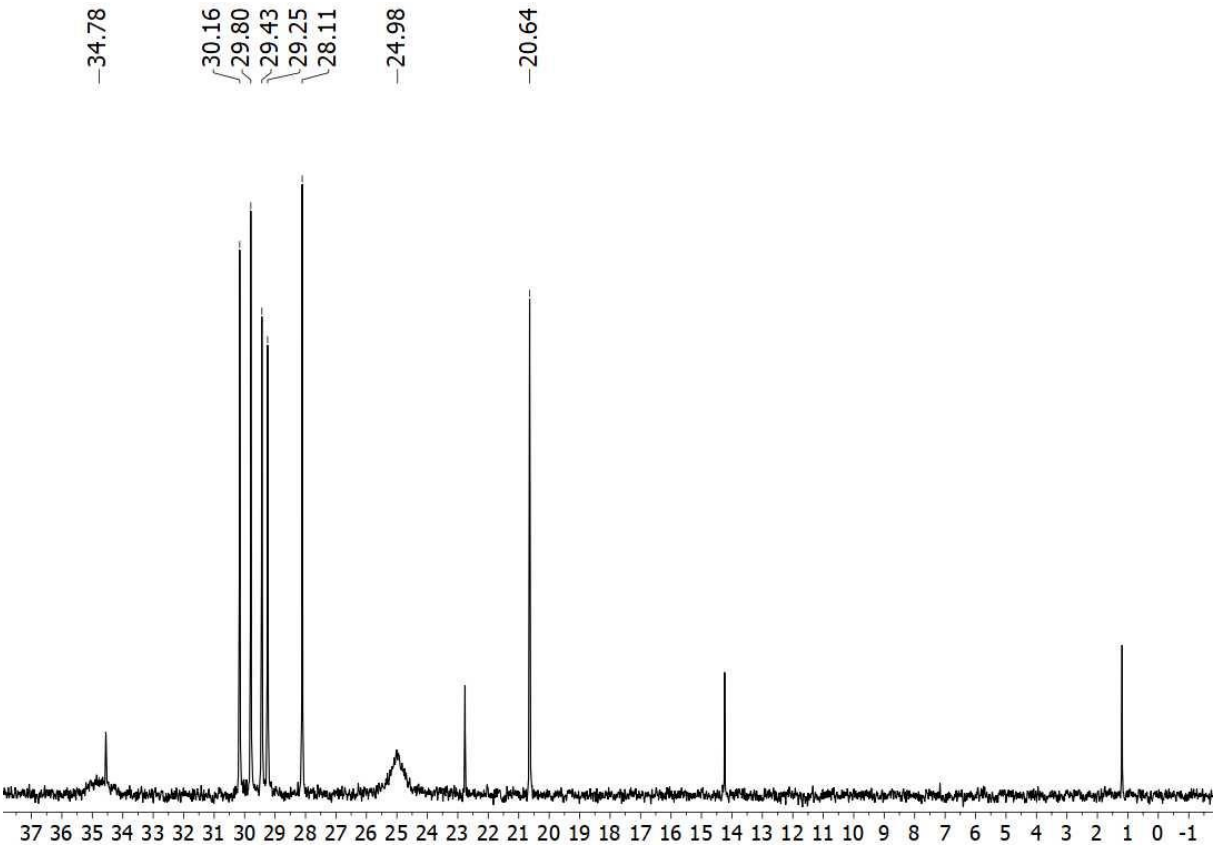


*Figure 55. $^{13}C\{^{1}H\}$ NMR spectrum of **4c** (100 MHz) in CD_2Cl_2, aliphatic region*

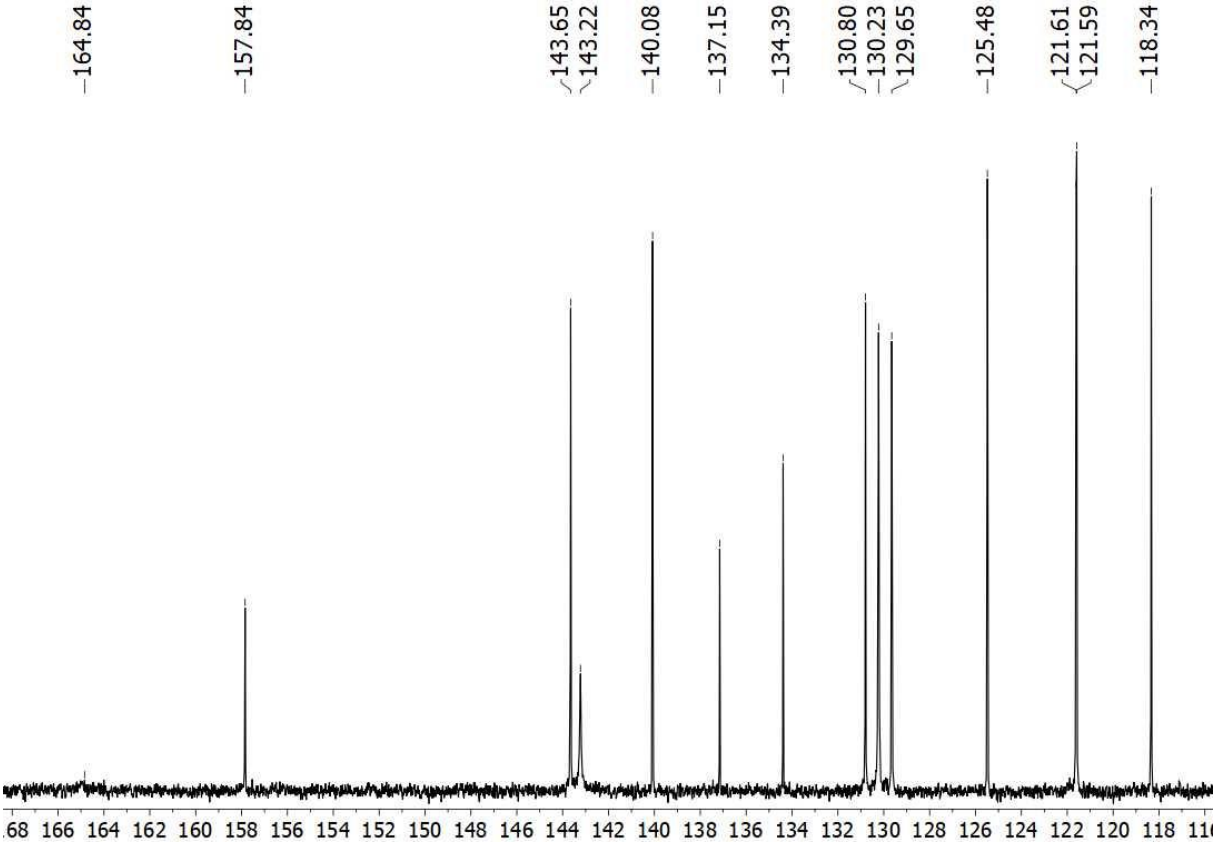


*Figure 56. $^{13}C\{^{1}H\}$ NMR spectrum of **4c** (100 MHz) in CD_2Cl_2, aromatic region*

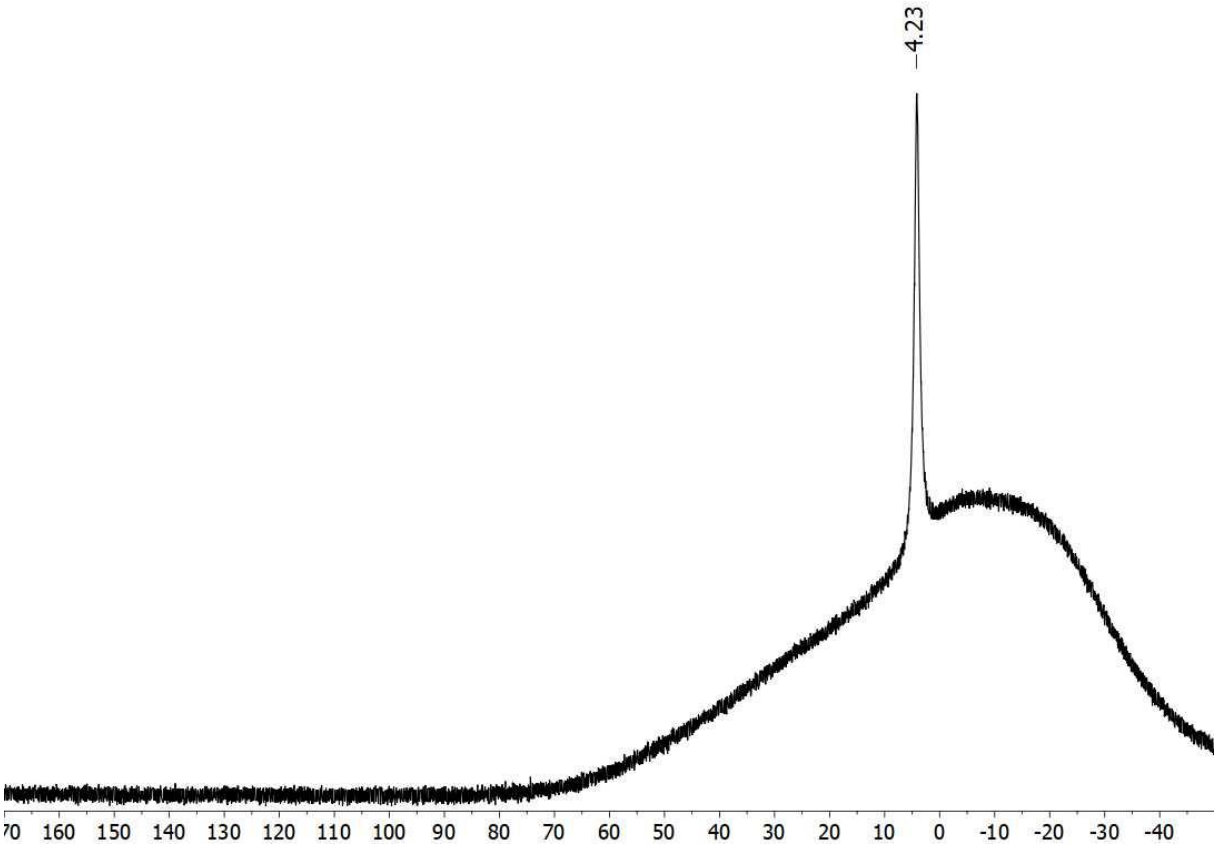
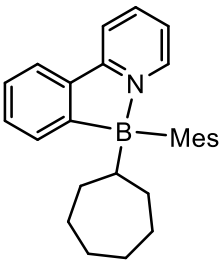


*Figure 57. $^{11}B\{^{1}H\}$ NMR spectrum of **4c** (128 MHz) in CD_2Cl_2*

19. NMR spectra of 4d



4d

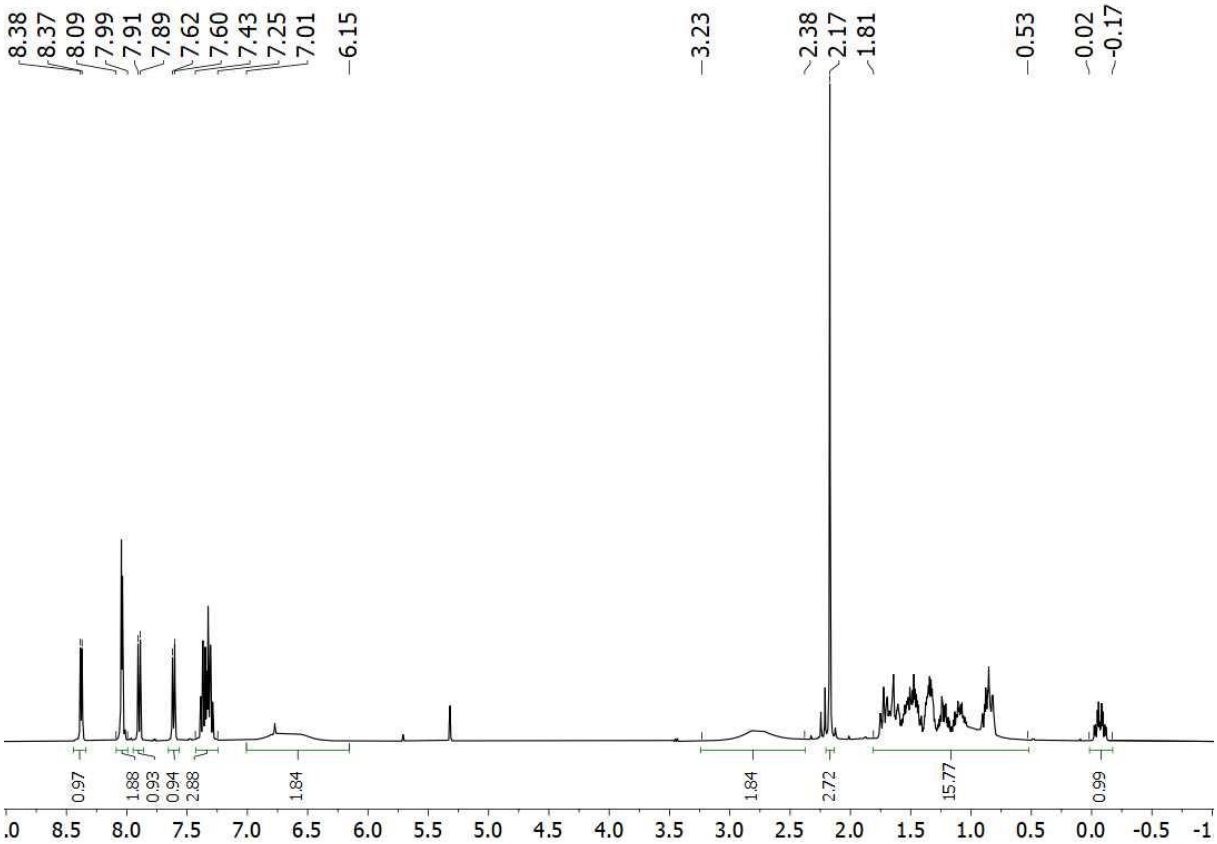


*Figure 58. ^{1}H NMR spectrum of **4d** (400 MHz) in CD_2Cl_2*

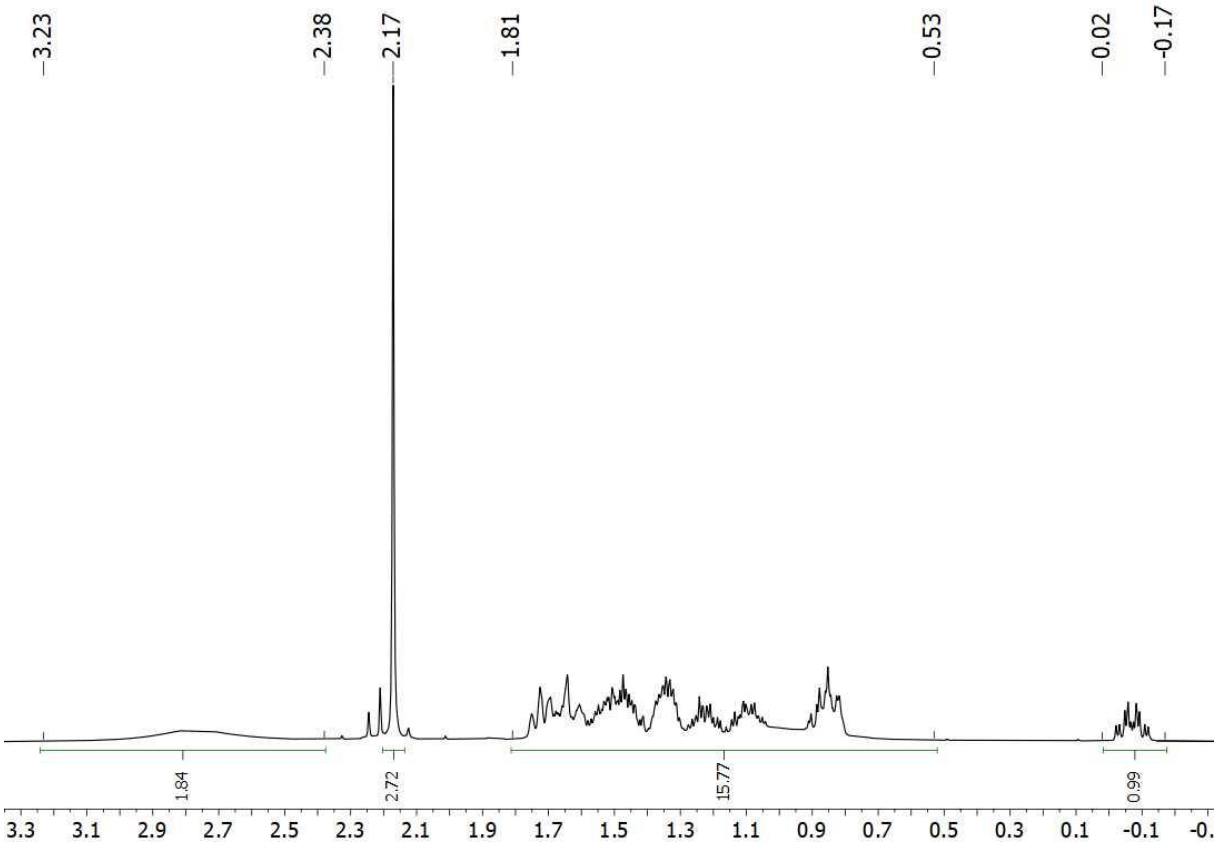


*Figure 59. ^{1}H NMR spectrum of **4d** (400 MHz) in C_2Cl_2, aliphatic region*

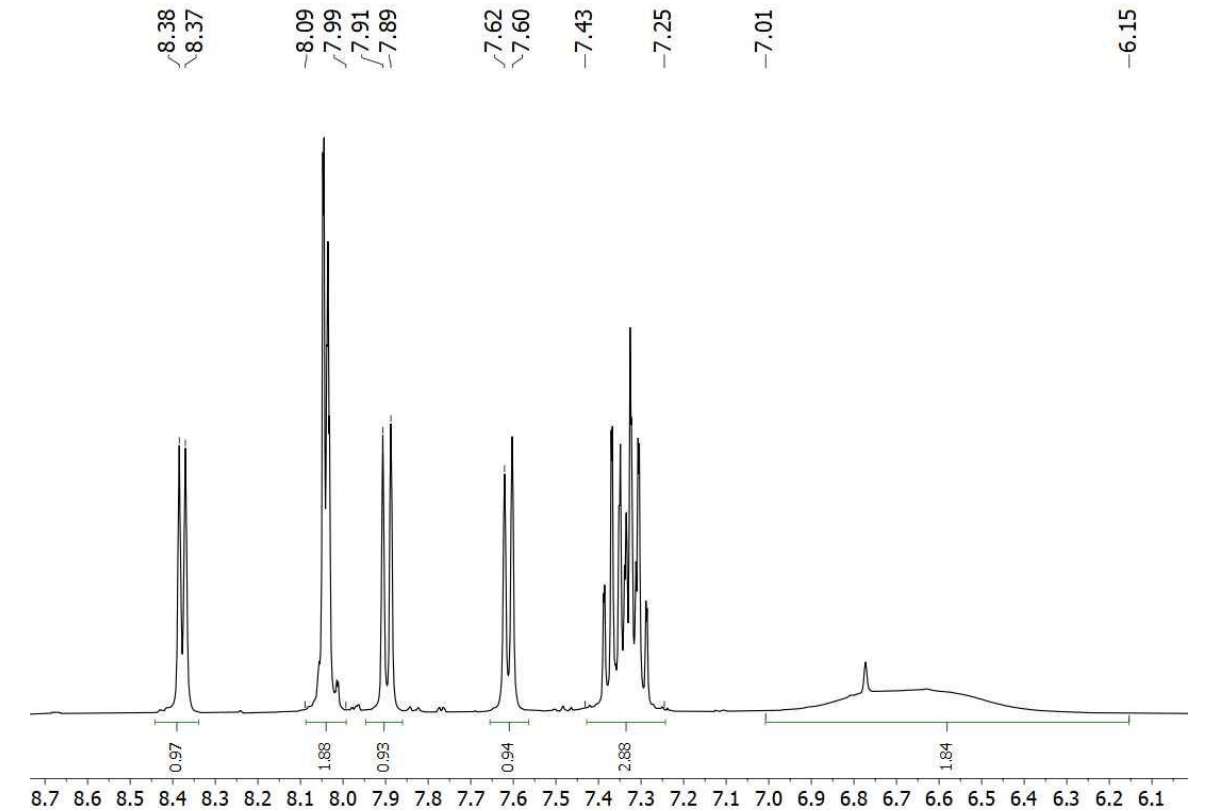


*Figure 60. ^{1}H NMR spectrum of **4d** (400 MHz) in CD_2Cl_2, aromatic region*

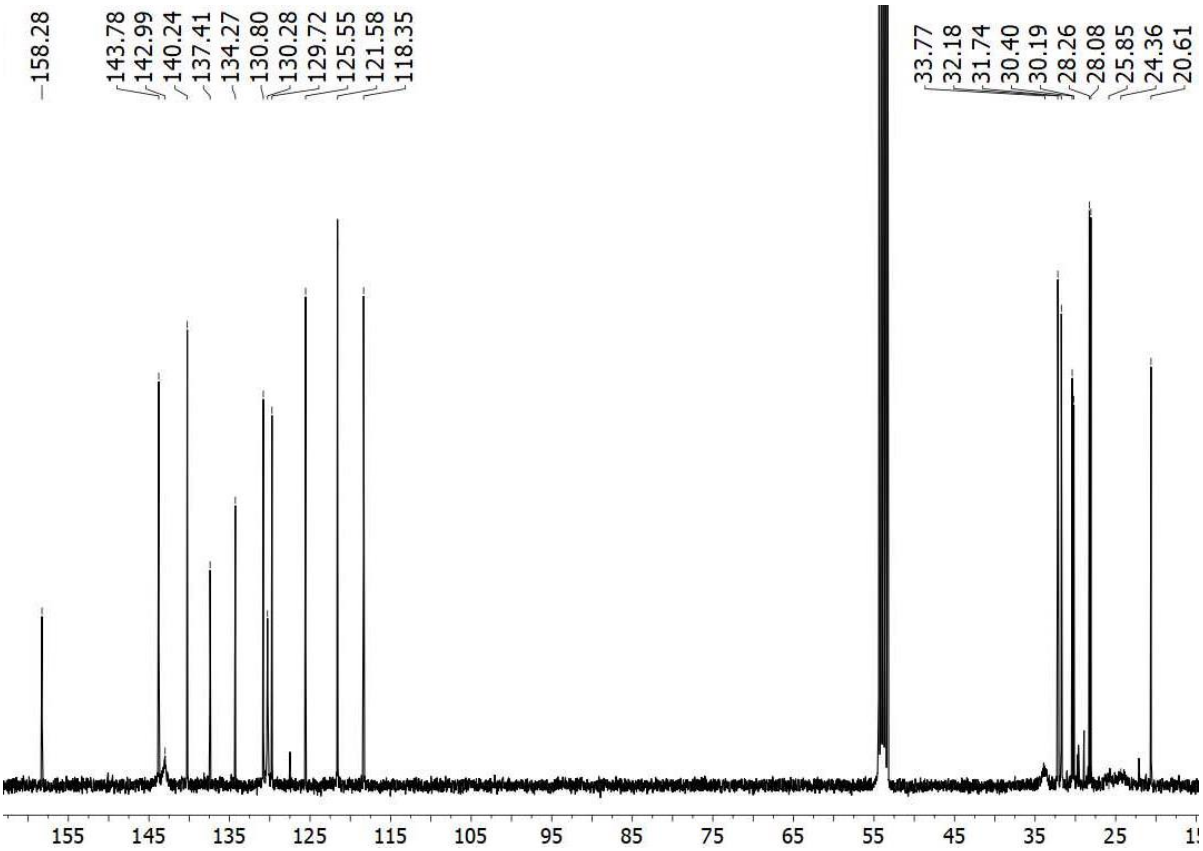


*Figure 61. $^{13}C\{^{1}H\}$ NMR spectrum of **4d** (100 MHz) in CD_2Cl_2*

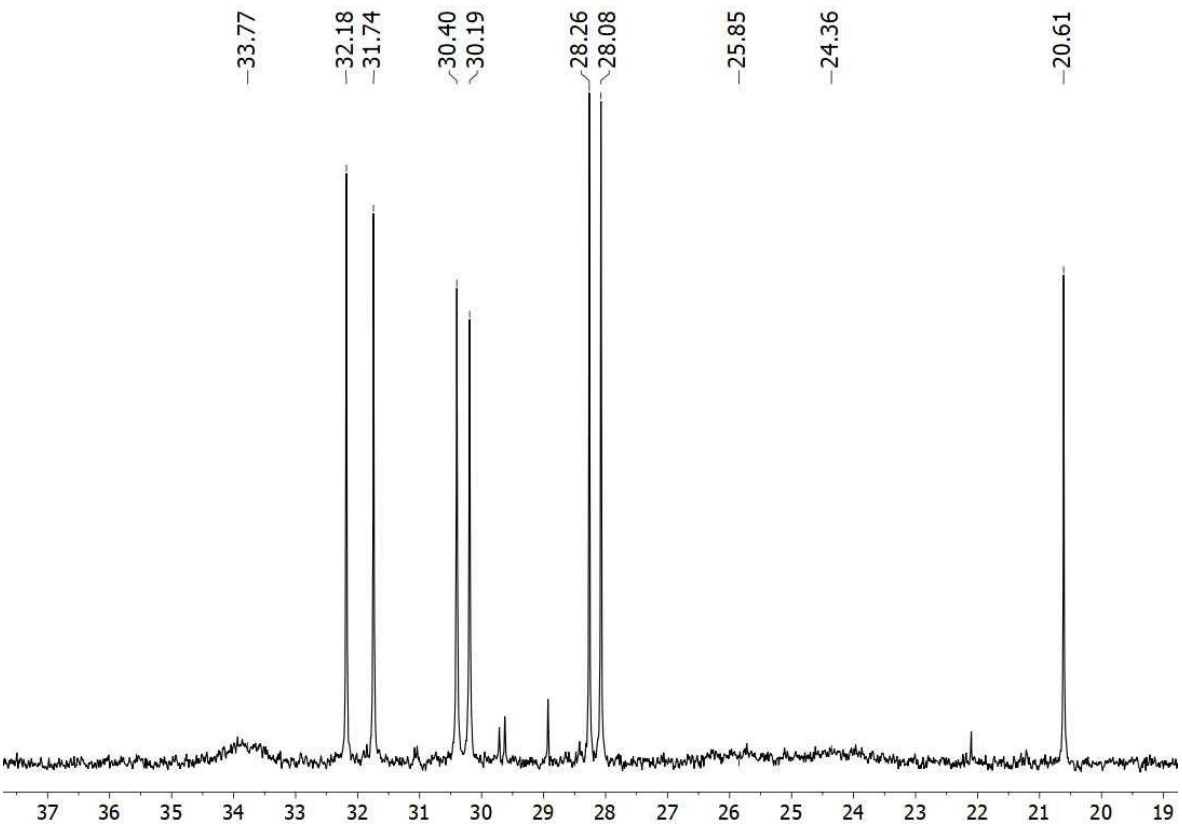


*Figure 62. $^{13}C\{^{1}H\}$ NMR spectrum of **4d** (100 MHz) in CD_2Cl_2, aliphatic region*

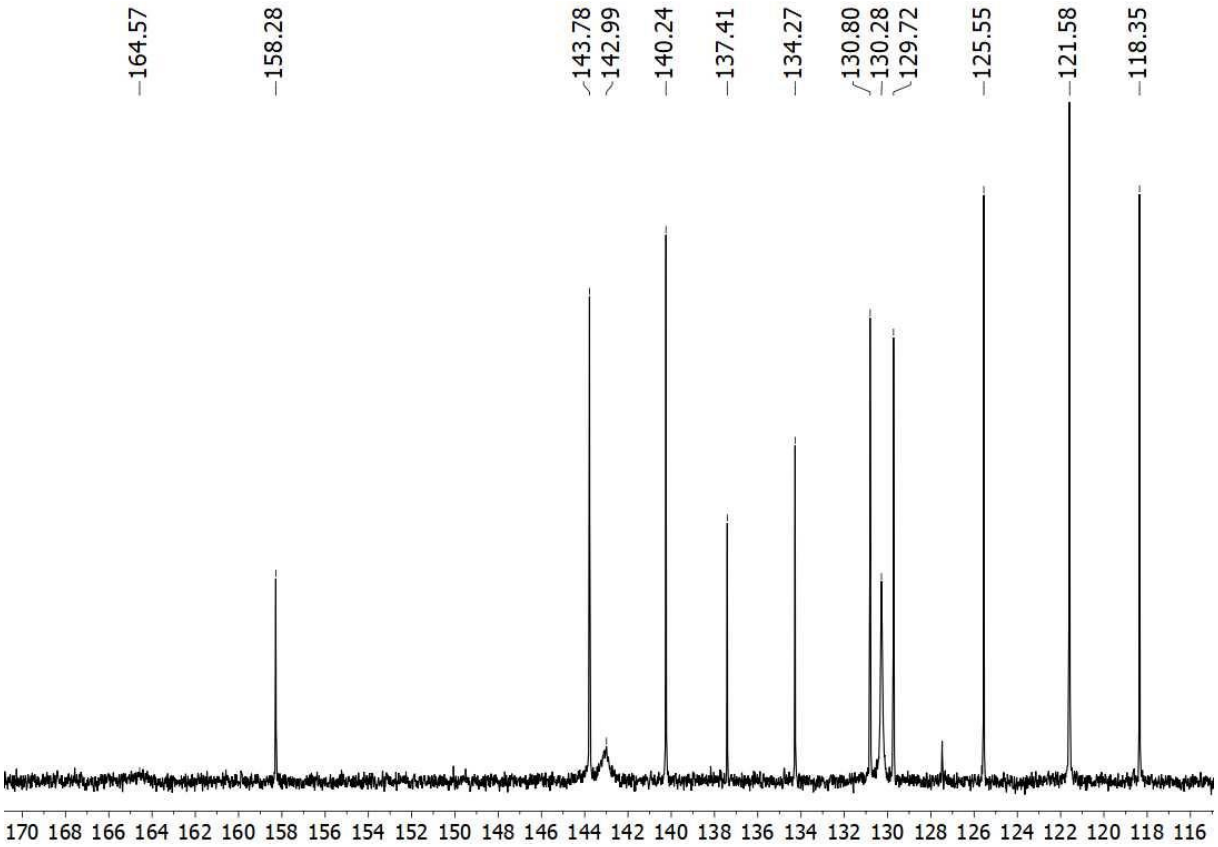


*Figure 63. $^{13}C\{^{1}H\}$ NMR spectrum of **4d** (100 MHz) in CD_2Cl_2, aromatic region*

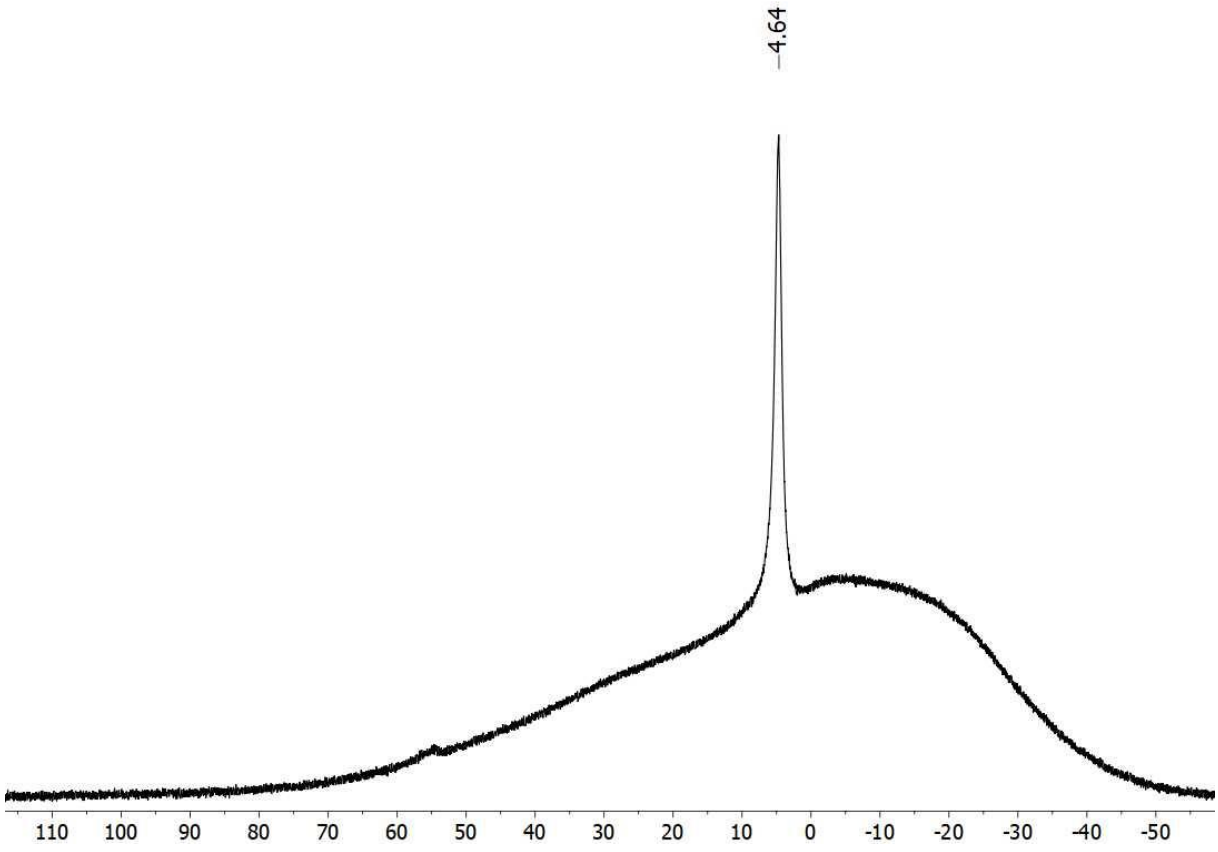


*Figure 64. $^{11}B\{^{1}H\}$ NMR spectrum of **4d** (128 MHz) in CD_2Cl_2*

VI. Crystallographic data

The structures were solved by dual-space algorithm using the *SHELXT* program,[3] and then refined with full-matrix least-squares methods based on F^2 (*SHELXL*).[4]

3a : ($2(C_{26}H_{32}BN_2)$,$3(CH_2Cl_2)$,2(Br)); *M* = 1181.29. D8 VENTURE Bruker AXS diffractometer equipped with a (CMOS) PHOTON 100 detector, [*], Mo-Kα radiation (λ = 0.71073 Å, multilayer monochromator), *T* = 150 K; monoclinic $P2_1/c$ (I.T.#14), a = 18.7324(16), b = 13.6027(16), c = 46.542(4) Å, β = 96.679(3) °, *V* = 11779(2) $Å^3$. *Z* = 8, *d* = 1.332 $g.cm^{-3}$, μ = 1.687 mm^{-1}. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters. A final refinement on F^2 with 26999 unique intensities and 1263 parameters converged at ωR_F^2 = 0.1497 (R_F = 0.0673) for 16616 observed reflections with $I > 2\sigma(I)$.

4a : ($C_{25}H_{28}BN$); *M* = 353.29. D8 VENTURE Bruker AXS diffractometer equipped with a (CMOS) PHOTON 100 detector, [*], Mo-*Kα* radiation (*λ* = 0.71073 Å, multilayer monochromator), *T* = 150 K; monoclinic $P\,2_1/n$ (I.T.#14), *a* = 8.4771(14), *b* = 20.873(3), *c* = 11.7953(16) Å, *β* = 94.067(5) °, *V* = 2081.8(5) $Å^3$. *Z* = 4, *d* = 1.127 $g.cm^{-3}$, *μ* = 0.064 mm^{-1}. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters. A final refinement on F^2 with 4774 unique intensities and 244 parameters converged at ωR_F^2 = 0.1620 (R_F = 0.0590) for 3587 observed reflections with $I > 2\sigma(I)$.

4c : ($C_{26}H_{30}BN$); *M* = 367.32 . D8 VENTURE Bruker AXS diffractometer equipped with a (CMOS) PHOTON 100 detector [*], Mo-*Kα* radiation (*λ* = 0.71073 Å, multilayer monochromator) , *T* = 150 K; monoclinic $P2_1/n$ (I.T.#14), *a* = 8.3499(7), *b* = 20.1352(16), *c* = 12.4684(9) Å, *β* = 92.264(3), *V* = 2094.6(3) $Å^3$. *Z* = 4, *d* = 1.165 $g.cm^{-3}$, *μ* = 0.066 mm^{-1}. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters. A final refinement on F^2 with 4794 unique intensities and 253 parameters converged at ωR_F^2 = 0.1367 (R_F = 0.0617) for 3852 observed reflections with $I > 2\sigma(I)$.

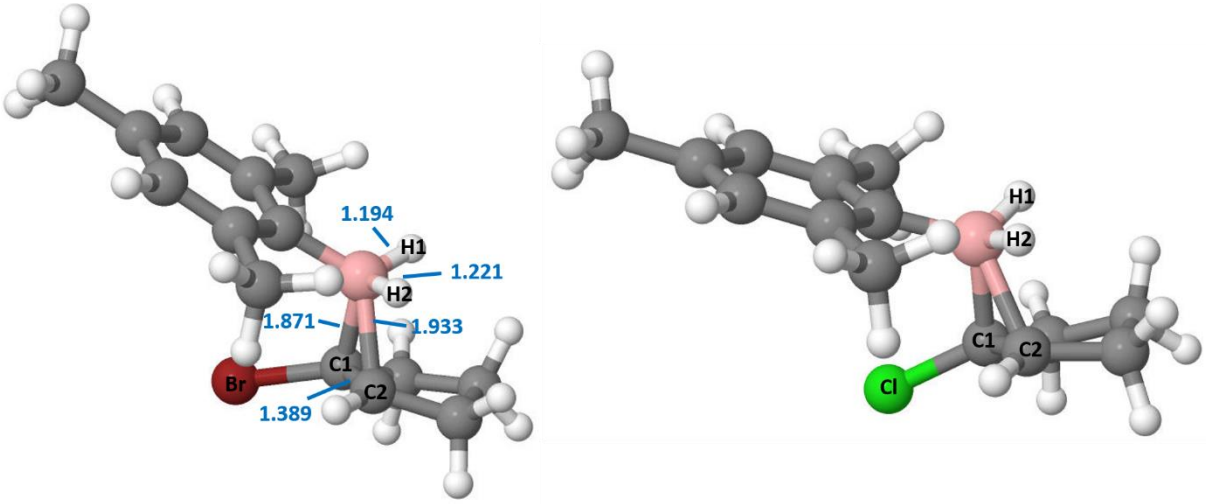
4d : ($C_{27}H_{32}BN$); *M* = 381.34. APEXII, Bruker-AXS diffractometer equipped with a CCD plate detector, Mo-Kα radiation (λ = 0.71073 Å, graphite monochromator), *T* = 150 K; monoclinic $P2_1/n$ (I.T.#14), a = 11.5003(11), b = 10.5542(10), c = 18.008(2) Å, β = 90.335(4) °, *V* = 2185.7(4) $Å^3$. *Z* = 4, *d* = 1.159 $g.cm^{-3}$, μ = 0.065 mm^{-1}. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters. A final refinement on F^2 with 4940 unique intensities and 274 parameters converged at $\omega R(F^2)$ = 0.1395 ($R(F)$ = 0.0650) for 2888 observed reflections with $I > 2\sigma(I)$.

3. G. M. Sheldrick, *Acta Cryst. A*, 2015, **71**, 3.
4. G. Sheldrick, *Acta Cryst. C*, 2015, **71**, 3.

VII. Computational details

Calculations were carried out using the Gaussian09 package[S1-DFT] at the DFT level by means of the hybrid density functional B3LYP.[S2-DFT] Polarized all electron double-zeta 6-31G(d,p) basis set were used for the H, C, B, Cl and Br atoms. To check the validity of the employed basis set we repeated all the calculation by using a polarized all electron triple-zeta 6-311G(d,p) basis set for the H, C, B, Cl and Br atoms and by adding diffuse functions at the B, Cl and Br centres. The results obtained are very similar to those computed with the double-zeta 6-31G(d,p) basis set (less than 2 kcal.mol^{-1}) and they are shown in Figure S11-DFT and S12-DFT The nature of the optimized stationary points has been verified by means of analytical frequency calculations at 298.15 K and 1 atm. The geometry optimizations have been achieved without any geometrical constraints. The calculated profiles were simulated with a dispersion corrected functional and a solvation model. More precisely, dispersion corrections were treated with the D3 version of Grimme's dispersion with the Becke-Johnson damping [S3-DFT] and the solvent effect included by means of continuum model SMD.[S4-DFT] As experimentally, benzene was used as solvent. Energy data are reported in the gas phase. The electron density and partial charge distribution were examined in terms of localized electron-pair bonding units using the NBO program. [S5-DFT, S6-DFT]

1. **Figure S1-DFT**. DFT-optimised structures of **TS-B1C1**, for the Br and Cl derivative.



2. **Table S1-DFT.** Relevant bond length distances and Wiberg bond indexes for **TS-B1C1**, in the Br and Cl derivative.

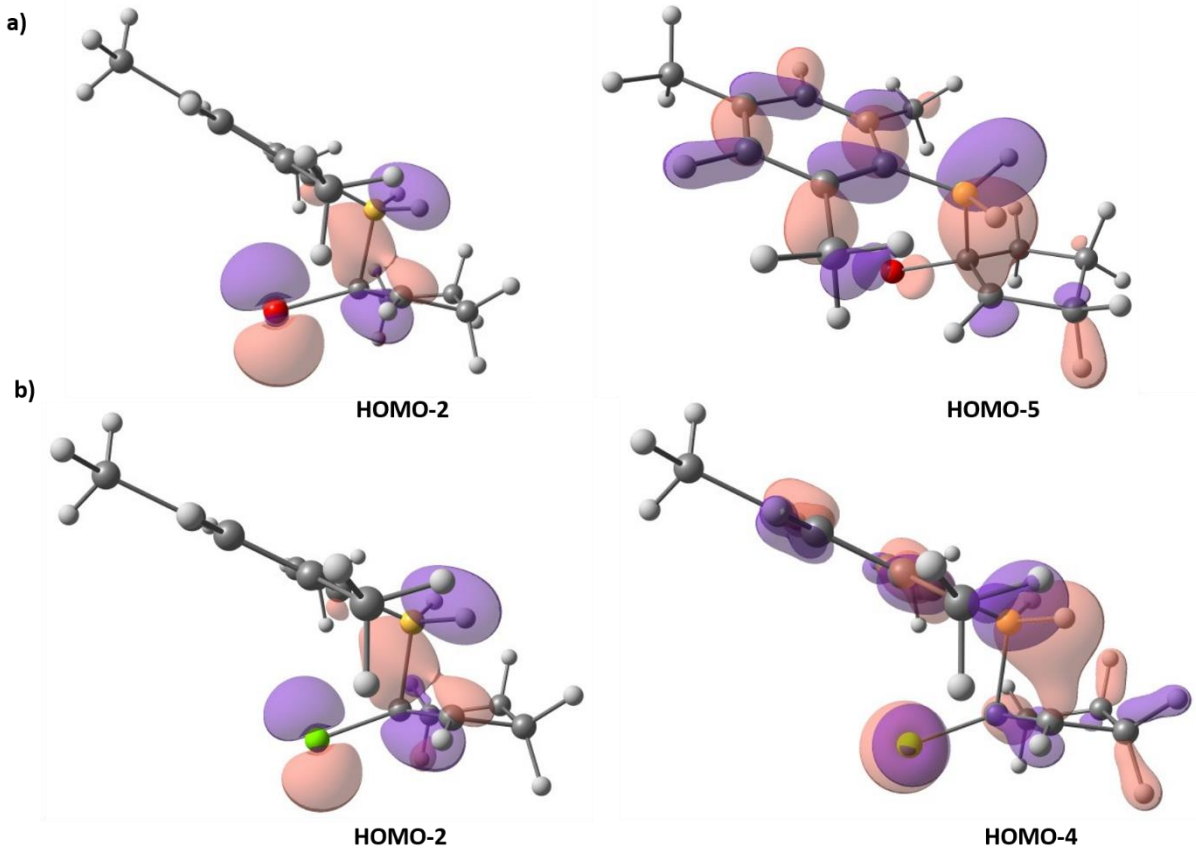
	C1-X	C1-B	C1-C2	C2-B	C2-H2	B-H2	B-H1
			Bond Lengths (Å)				
TS-B1C1$_{,Br}$	1.920	1.871	1.389	1.933	1.857	1.221	1.194
TS-B1C1$_{,Cl}$	1.767	1.860	1.392	1.924	1.833	1.223	1.194

Wiberg bond indexes							
TS-B1C1$_{,Br}$	1.01	0.49	1.35	0.38	0.11	0.77	0.94
TS-B1C1$_{,Cl}$	1.03	0.5	1.33	0.38	0.12	0.76	0.94

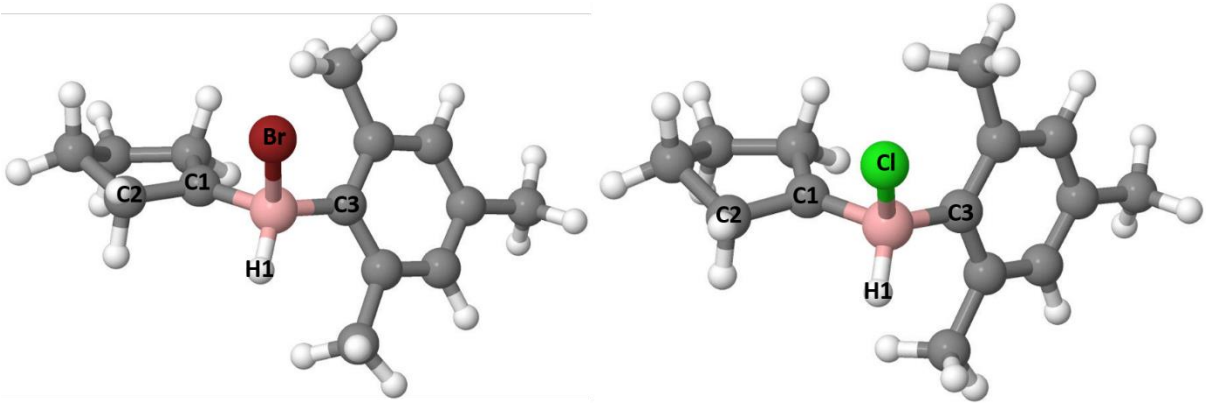
3. **Table S2-DFT.** Natural charges for **TS-B1C1**, in the Br and Cl derivative.

	X	C1	B	C2	H2	H1
TS-B1C1$_{Br}$	0.084	-0.197	-0.021	-0.149	0.102	0.012
TS-B1C1$_{Cl}$	0.010	-0.128	-0.025	-0.151	0.109	0.012

4. **Figure S2-DFT**. Relevant DFT computed frontier molecular orbitals for **TS-B1C1$_{Br}$** (a) and **TS-B1C1$_{Cl}$** (b).



5. **Figure S3-DFT.** DFT optimised structure of **TS-C1P**, for the Br and Cl derivative.



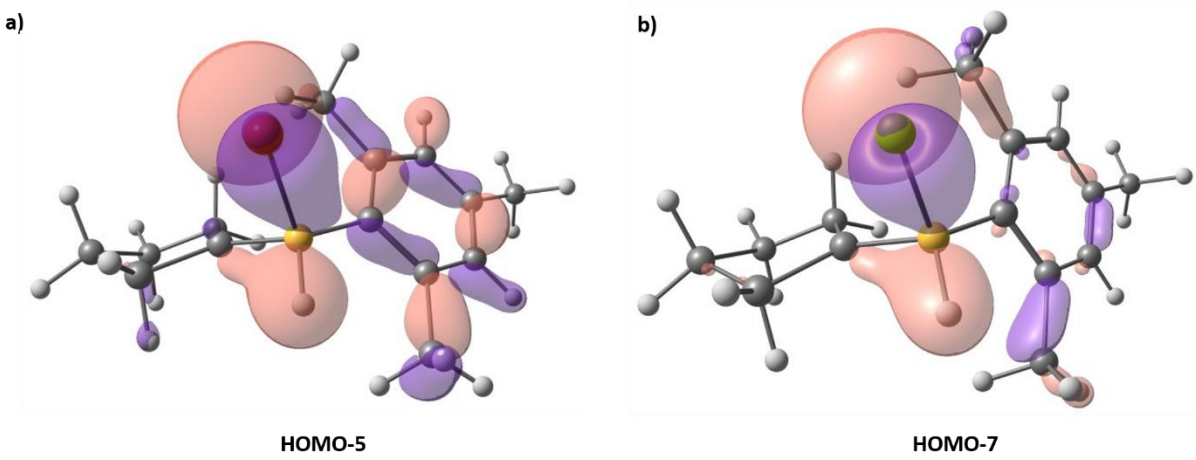
6. **Table S3-DFT.** Relevant bond length distances, angles and Wiberg bond indexes for **TS-C1P**, in the Br (left) and Cl (right) derivative.

	C1-X	C1-B	C1-H1	B-Br	B-H1	B-C3	C1-B-C3
			Bond lengths (Å) and angles (°)				
TS-C1P$_{Br}$	2.850	1.574	2.199	2.137	1.206	1.600	119.65
TS-C1P$_{Cl}$	2.685	1.588	2.245	1.962	1.206	1.605	116.13
			Wiberg bond indexes				
TS-C1P$_{Br}$	0.16	0.92	0.05	0.81	0.90	0.90	-
TS-C1P$_{Cl}$	0.15	0.88	0.04	0.81	0.92	0.89	-

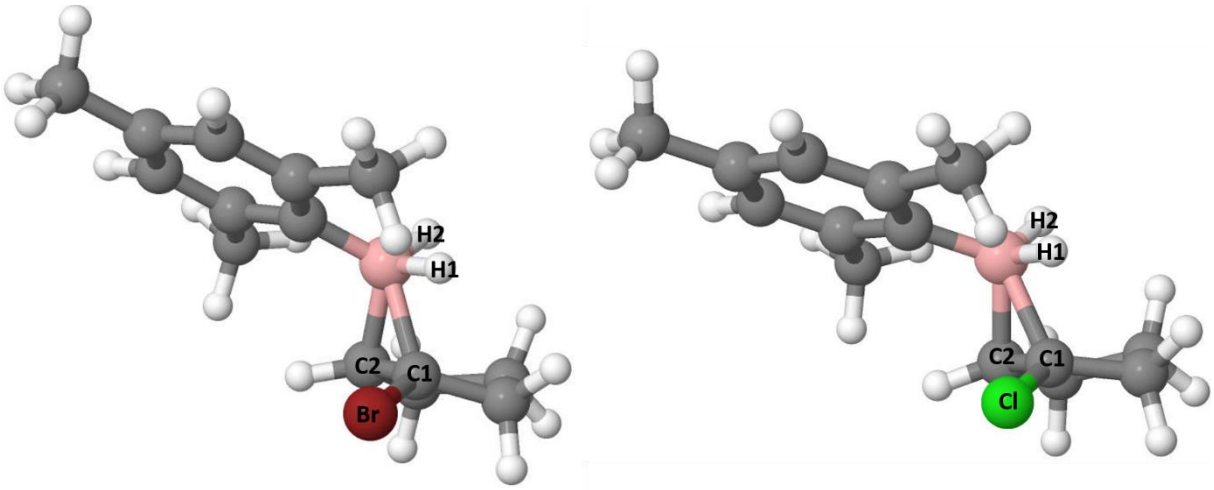
7. **Table S4-DFT.** Natural charges for **TS-C1P**, in the Br and Cl derivative.

	X	C1	B	C3	H1
TS-C1P$_{Br}$	-0.218	0.186	0.096	-0.319	0.029
TS-C1P$_{Cl}$	-0.280	0.210	0.146	-0.314	0.010

8. **Figure S4-DFT**. Relevant DFT computed frontier molecular orbitals for **TS-C1P$_{Br}$** (a) and **TS-C1P$_{Cl}$** (b).



9. **Figure S5-DFT.** DFT optimised structure of **TS-B2C2**, for the Bromo and Chloro derivative



10. **Table S5-DFT.** Relevant bond length distances and Wiberg bond indexes for **TS-B2C2**, in the Br and Cl derivative.

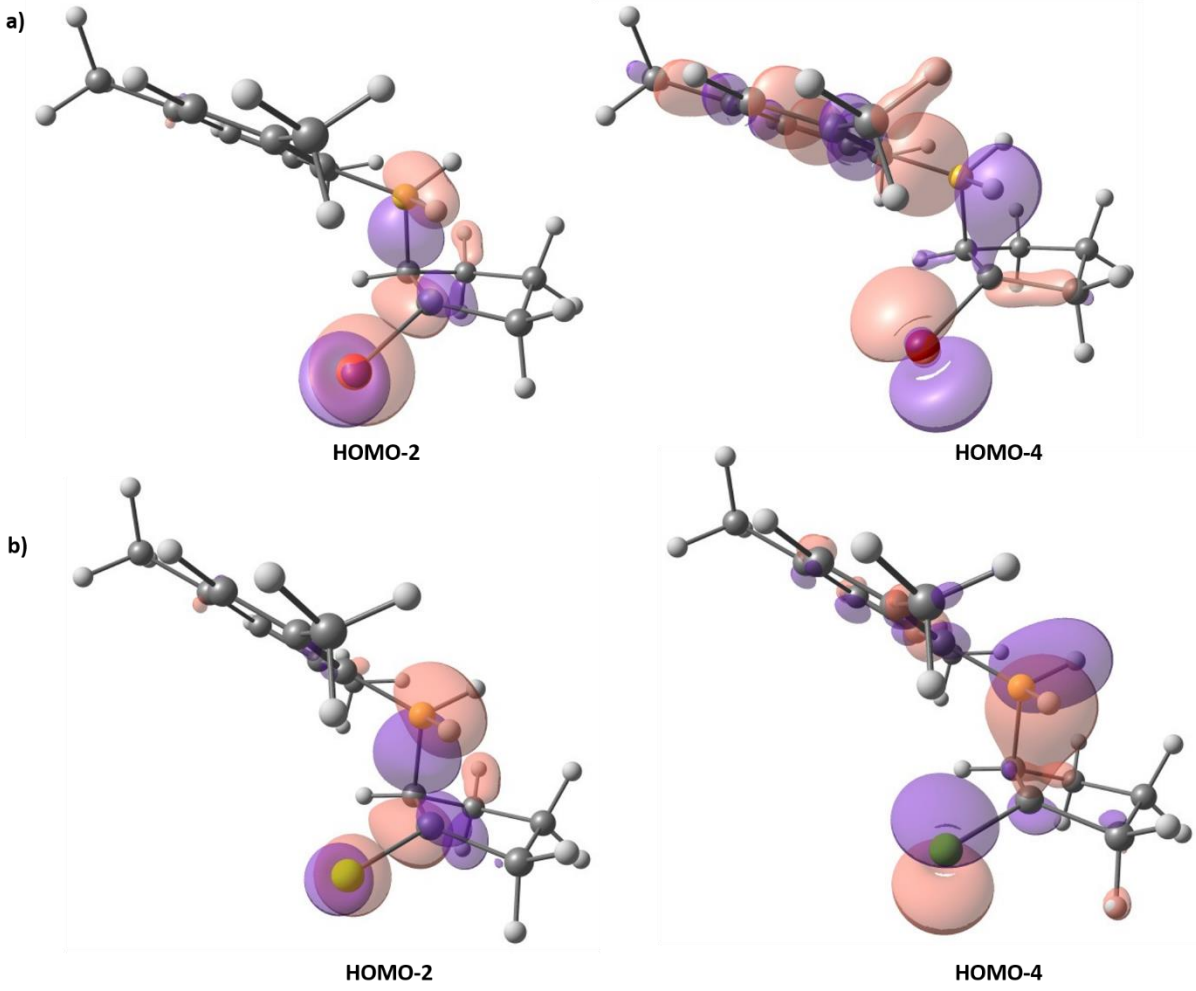
	C2-B	C1-C2	C1-B	C1-X	C1-H1	B-H1	B-H2
			Bond lengths (Å)				
TS-B2C2$_{Br}$	1.779	1.398	1.911	1.914	1.775	1.231	1.201
TS-B2C2$_{Cl}$	1.774	1.401	1.914	1.756	1.767	1.233	1.200

	Wiberg bond indexes						
TS-B2C2$_{Br}$	0.57	1.29	0.39	1.04	0.15	0.72	0.92
TS-B2C2$_{Cl}$	0.58	1.28	0.39	1.06	0.15	0.71	0.92

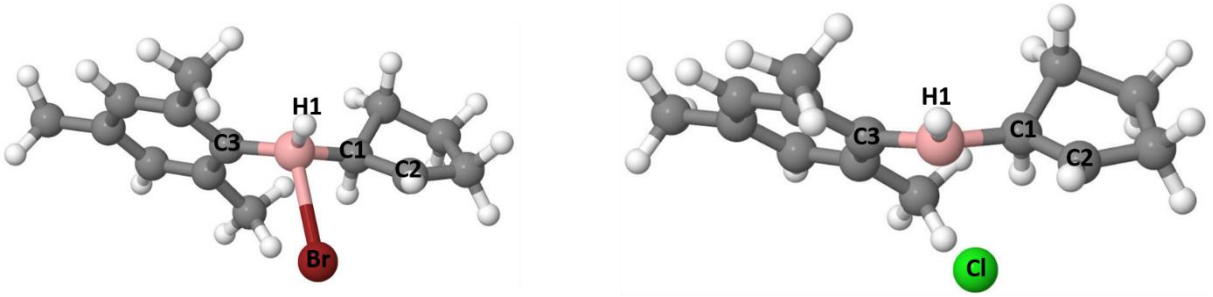
11. **Table S6-DFT.** Natural charges for **TS-B2C2**, in the Br and Cl derivative.

	X	C2	B	C1	H1	H2
TS-B2C2$_{Br}$	0.111	-0.359	-0.029	-0.053	0.134	0.029
TS-B2C2$_{Cl}$	0.041	-0.365	-0.029	0.024	0.133	0.027

12. **Figure S6-DFT**. Relevant DFT computed frontier molecular orbitals for **TS-B2C2$_{Br}$** (a) and **TS-B2C2$_{Cl}$** (b).



13. **Figure S7-DFT.** DFT optimised structure of **TS-C2D2**, for the Br and Cl derivative.



The geometry displays the halogen atom simultaneously interacting with both the B centre and the C2 carbon of the forming cyclopentene, as shown, respectively, in the Homo -4 and Homo – 3 orbitals (see **Figure S8-DFT**).

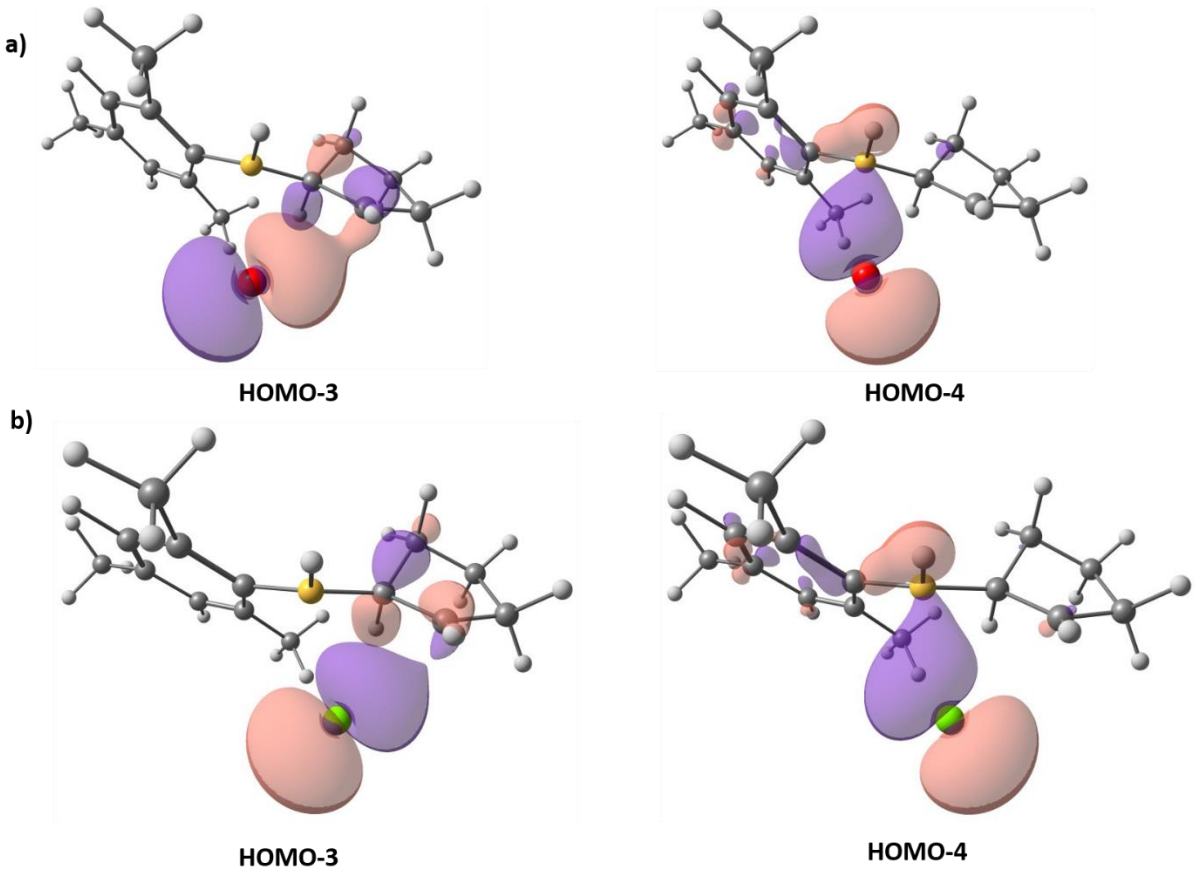
14. **Table S7-DFT.** Relevant bond length distances, angles and Wiberg bond indexes for **TS-C2D2**, in the Br and Cl derivative.

	B-C1	B-X	B-H1	C1-C2	C2-X	B-C3	C1-B-C3
			Bond lengths (Å) and angles (°)				
TS-C2D2$_{Br}$	1.621	2.472	1.196	1.457	2.803	1.574	124.3
TS-C2D2$_{Cl}$	1.614	2.379	1.195	1.457	2.635	1.571	125.0
			Wiberg bond indexes				
TS-C2D2$_{Br}$	0.805	0.527	0.971	1.154	0.364	0.925	-
TS-C2D2$_{Cl}$	0.808	0.454	0.970	0.147	0.347	0.926	-

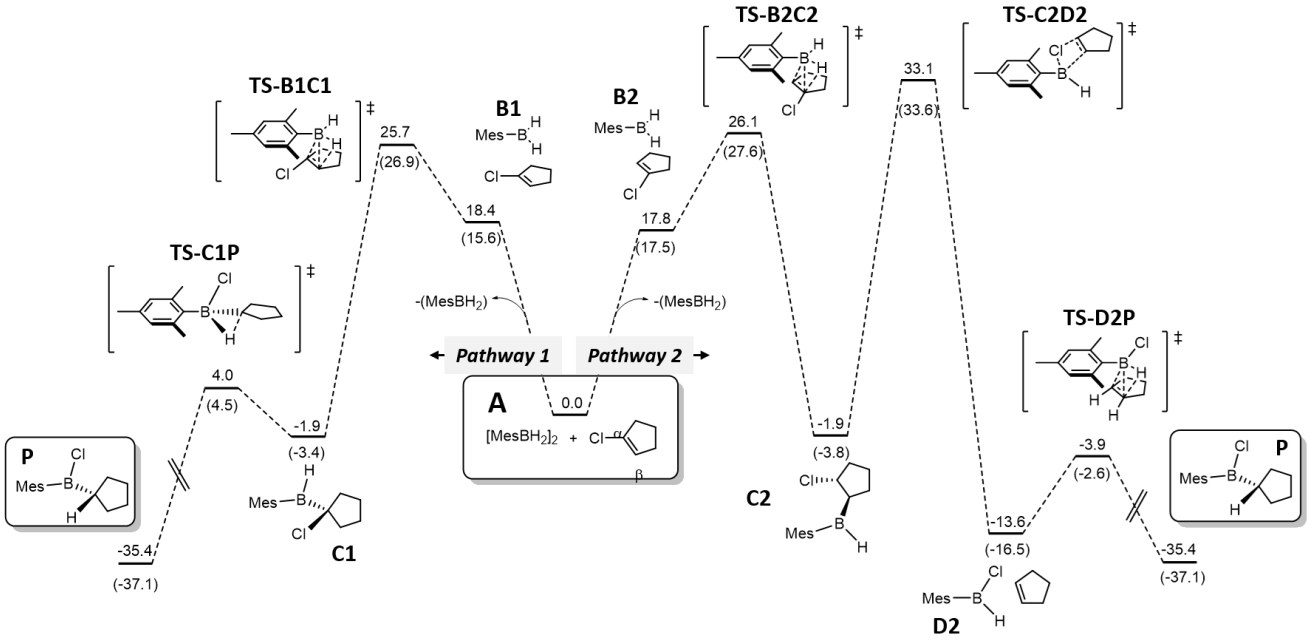
15. **Table S8-DFT.** Natural charges for **TS-C2D2**, in the Br and Cl derivative.

	X	C1	B	C2	H1
TS-C2D2$_{Br}$	-0.362	-0.650	0.407	0.220	-0.059
TS-C2D2$_{Cl}$	-0.442	-0.656	0.467	0.237	-0.063

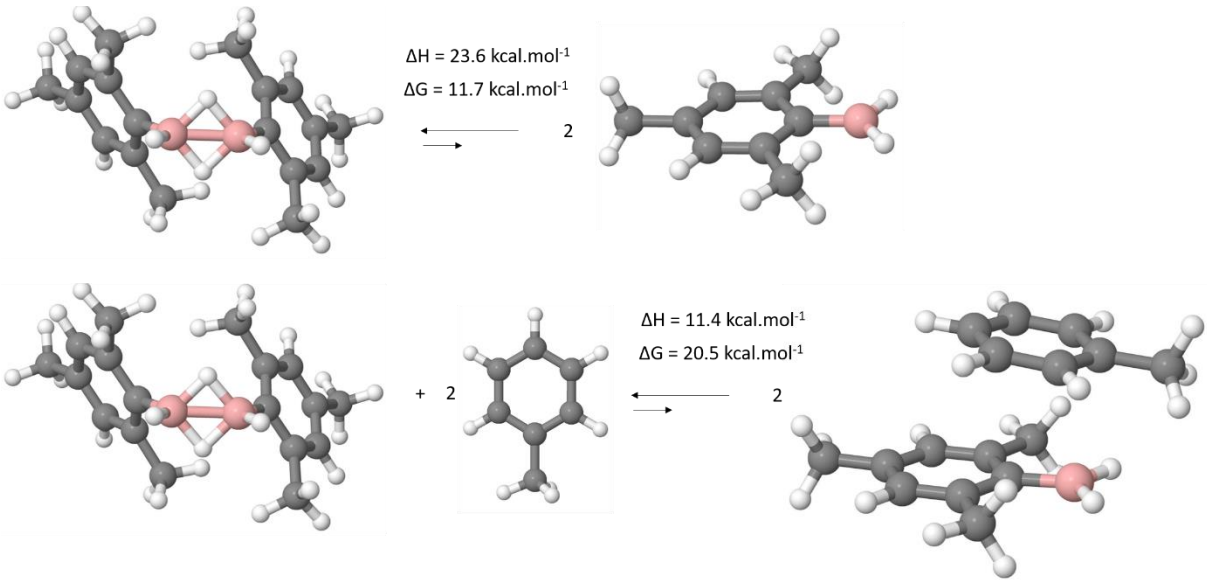
16. **Figure S8-DFT**. Relevant DFT computed frontier molecular orbitals for **TS-C2D2$_{,Br}$** (a) and **TS-C2D2$_{,Cl}$** (b).



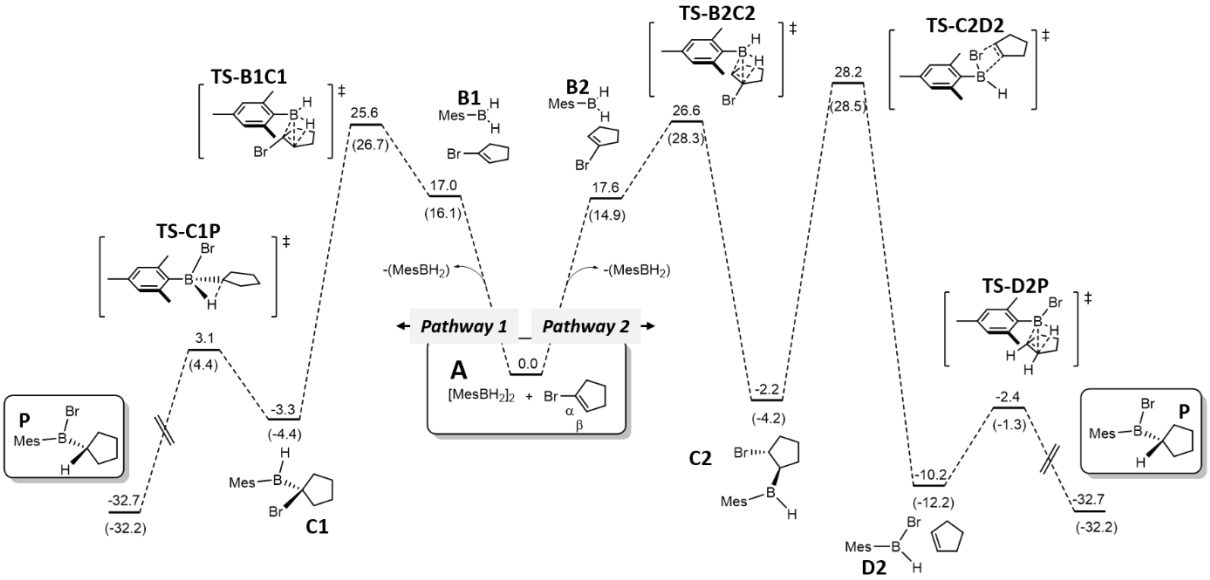
17. **Figure S9-DFT**. DFT computed enthalpy (free enthalpy) profile of the reaction between mesityl borane and chlorocyclopentene at the B3LYP-D3/6-31G(d,p) level of theory. The two pathways 1 and 2 from either α- or β-hydroboration are given.



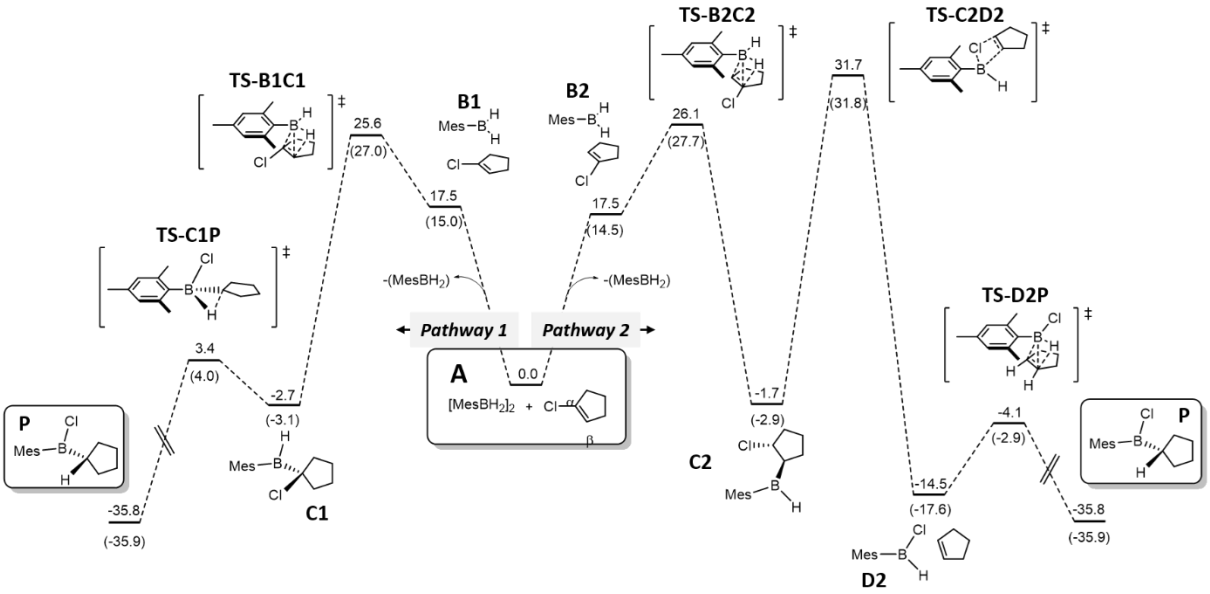
18. **Figure S10-DFT.** DFT computed enthalpy and free enthalpy values for the dissociation of the mesitylborane dimer to give the monomeric species MesBH2 without (a) and with (b) an explicit toluene molecule.



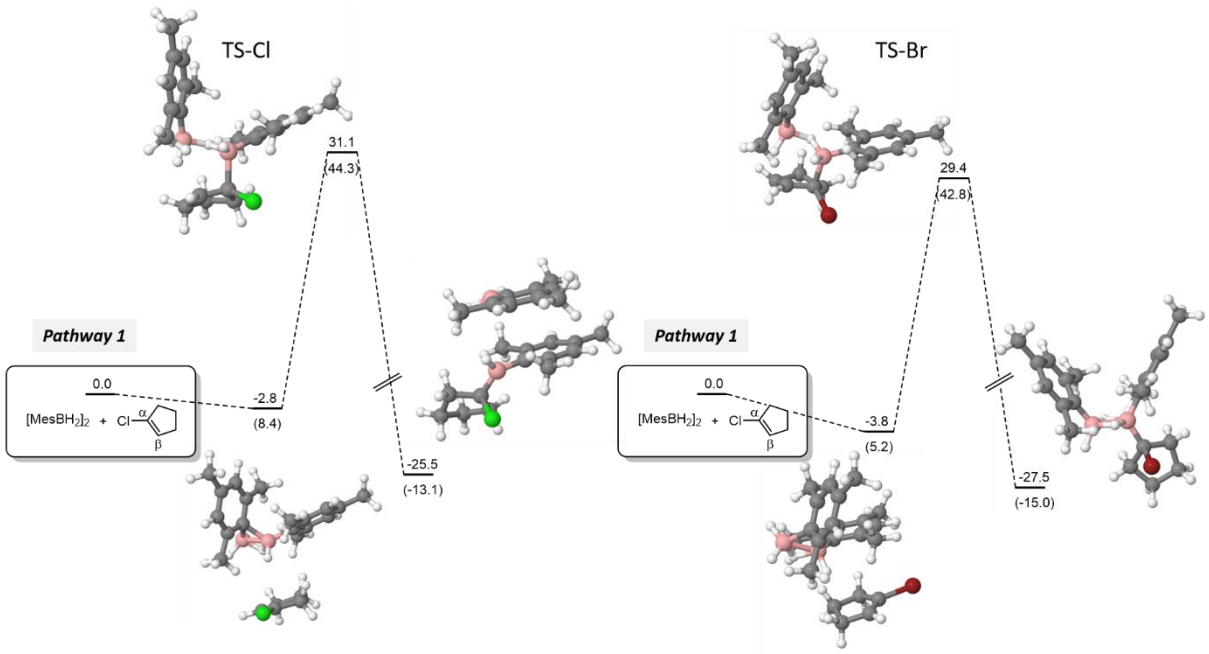
19. **Figure S11-DFT:** DFT computed enthalpy (free enthalpy) profile of the reaction between $MesBH_2$ and *c*-pent-Br at the B3LYP-D3/6-311G(d,p) level of theory. Pathways 1 and 2 from α– and β–hydroboration, respectively, are shown.



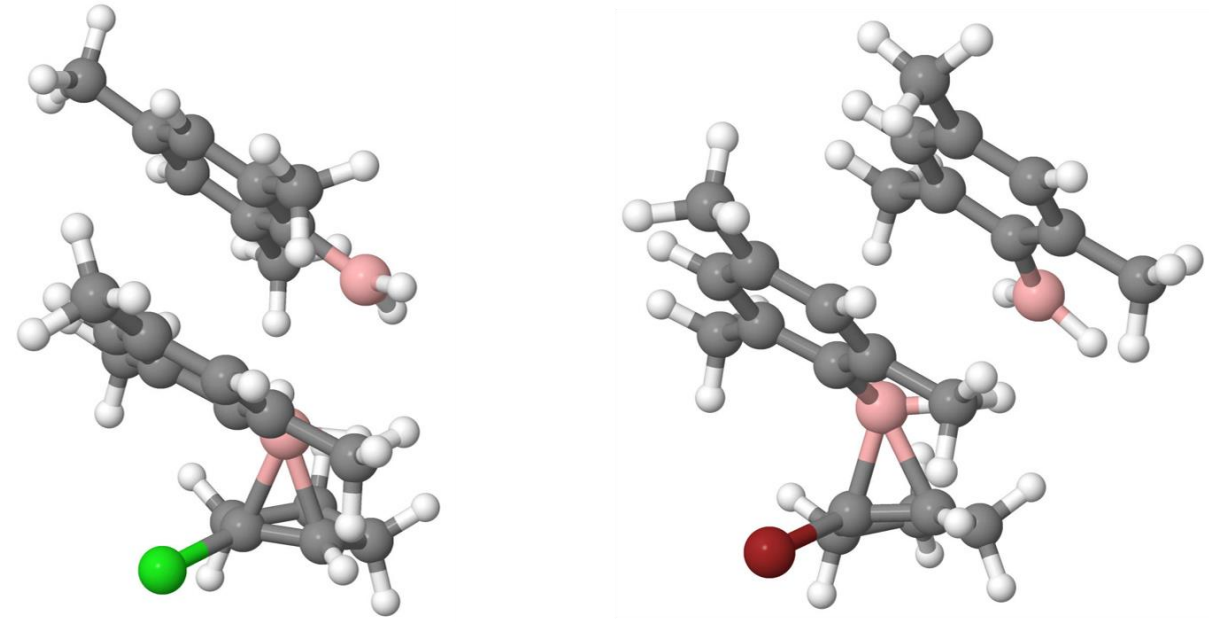
20. **Figure S12-DFT:** DFT computed enthalpy(free enthalpy) profile of the reaction between $MesBH_2$ and *c*-pent-Cl at the B3LYP-D3/6-311G(d,p) level of theory. Pathways 1 and 2 from α– and β–hydroboration, respectively, are shown.



21. **Figure S13-DFT:** DFT computed enthalpy(free enthalpy) profile of the reaction between $MesBH_2$ and *c*-pent-Cl and *c*-pent-Br at the B3LYP-D3/6-31G(d,p) level of theory involving a dinuclear transition state. Only pathways 1 from α– hydroboration is shown.



22. **Figure S14_DFT:** Geometry of the α-hydroboration transition state reaction (B3LYP-D3/6-31G(d,p)) displaying the second mesityl-borane molecule close to the reactive monomer without any type of assistance.



TS for the α-hydroboration-Cl

TS for the α-hydroboration-Br

VIII. Geometries of all computed complexes (B3LYP-D3/6-31G(d,p))

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[dimer_cis_mesityle_borane]

Enthalpies= -751.025171 / Free Energies= -751.097299

B	-0.877352	2.233881	0.162290
H	-0.154998	2.251791	-0.957295
H	-1.372471	3.320015	0.212574
H	0.154993	2.251913	0.956985
B	0.877350	2.233850	-0.162599
H	1.372477	3.319973	-0.213024
C	-1.756342	0.935258	0.265197
C	-2.781427	0.756866	-0.695320
C	-1.587783	-0.050518	1.263481
C	-3.582570	-0.387100	-0.664673
C	-2.415578	-1.178078	1.271946
C	-3.413361	-1.370755	0.313504
H	-4.356104	-0.512638	-1.419197
H	-2.274269	-1.928278	2.046786
C	1.756331	0.935211	-0.265346
C	1.587710	-0.050734	-1.263451
C	2.781486	0.756989	0.695133
C	2.415520	-1.178288	-1.271786
C	3.582634	-0.386972	0.664621
C	3.413367	-1.370795	-0.313380
H	2.274166	-1.928619	-2.046490
H	4.356224	-0.512379	1.419112
C	-2.999326	1.783550	-1.781994
H	-3.149194	2.786026	-1.365815
H	-2.138250	1.846381	-2.459648
H	-3.873930	1.537568	-2.390550
C	-0.532377	0.079941	2.337372
H	0.475041	-0.021237	1.921061
H	-0.587285	1.048156	2.847708
H	-0.651610	-0.696104	3.098482
C	-4.306114	-2.585374	0.353220
H	-5.226579	-2.383659	0.916092
H	-4.605040	-2.895537	-0.652997
H	-3.809327	-3.432058	0.836564
C	2.999462	1.783862	1.781614
H	3.149329	2.786261	1.365248
H	2.138423	1.846831	2.459304
H	3.874093	1.537968	2.390165
C	0.532242	0.079541	-2.337304
H	-0.475155	-0.021533	-1.920918
H	0.587149	1.047656	-2.847831
H	0.651413	-0.696654	-3.098271
C	4.306108	-2.585429	-0.352894
H	5.226917	-2.383594	-0.915157
H	4.604427	-2.895860	0.653422
H	3.809578	-3.431974	-0.836743

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mesityle_borane /

Enthalpies= -375.493779 / Free Energies= -375.539316

C	0.443820	-1.223594	-0.001351
C	1.179670	-0.000003	0.003455
C	0.443877	1.223601	-0.001501
C	-0.950181	1.202451	-0.010856
C	-1.665337	0.000051	-0.012720
C	-0.950218	-1.202395	-0.010714
H	-1.497911	2.141741	-0.017861
H	-1.497985	-2.141667	-0.017600

C	-3.170505	0.000020	0.012383
H	-3.580055	-0.886589	-0.480548
H	-3.540095	-0.002249	1.045747
H	-3.580059	0.888703	-0.476764
C	1.131632	2.570128	-0.000882
H	1.772947	2.698735	-0.878169
H	0.394372	3.377437	-0.003322
H	1.768502	2.699983	0.879385
C	1.131543	-2.570136	-0.000557
H	1.772870	-2.698863	-0.877818
H	1.768400	-2.699898	0.879735
H	0.394267	-3.377430	-0.002908
B	2.711359	-0.000029	0.011279
H	3.335122	-1.018192	0.014874
H	3.335153	1.018116	0.014753

13

Bromopentene

Enthalpies= -2766.056140 / Free Energies= -2766.093860

C	3.909072	1.926340	0.049359
C	3.593330	1.624515	1.540218
C	2.183761	1.081543	1.499926
C	1.834788	0.794207	0.246209
C	2.907876	1.076164	-0.773238
H	3.725072	2.986605	-0.149235
H	4.949271	1.716933	-0.212121
H	3.684890	2.514246	2.173059
H	4.276592	0.871881	1.958885
H	3.347512	0.134179	-1.127492
H	2.525094	1.599696	-1.654828
Br	0.178443	0.017904	-0.283385
H	1.574111	0.912648	2.379892

36

[B1-Br]

Enthalpies= -3141.558975 / Free Energies= -3141.627048

C	-1.227177	1.391155	-1.621856
C	-0.472350	0.185340	-1.635374
C	-1.171554	-1.042113	-1.445828
C	-2.552307	-1.041813	-1.255900
C	-3.289783	0.147231	-1.238309
C	-2.609428	1.353044	-1.423610
B	1.051693	0.202134	-1.845991
C	2.123219	1.009196	0.577466
C	1.728491	-0.172482	1.068940
C	2.806906	-1.223979	1.072930
C	3.916192	-0.559884	0.217772
C	3.582087	0.956683	0.190181
Br	0.038496	-0.519764	1.855259
C	-0.451103	-2.370641	-1.431948
C	-4.782102	0.116830	-1.034920
C	-0.576161	2.742108	-1.811667
H	-3.171856	2.283649	-1.409357
H	-3.070321	-1.987172	-1.109994
H	-5.285750	-0.363820	-1.882532
H	-5.049322	-0.456128	-0.139848
H	-5.195037	1.123675	-0.928849
H	0.160382	2.953987	-1.029533
H	-0.047427	2.808705	-2.767353
H	-1.324849	3.538688	-1.785963
H	0.070910	-2.562776	-2.374345
H	0.298207	-2.406645	-0.636266
H	-1.155269	-3.190175	-1.263951
H	1.682646	-0.808588	-1.896893
H	1.629674	1.211840	-2.111244
H	1.523829	1.910775	0.562599
H	4.176374	1.518459	0.924341
H	3.774011	1.407439	-0.788112

H 4.916083 -0.760530 0.609608

H 3.871524 -0.956160 -0.799055

H 3.129262 -1.418034 2.104437

H 2.463969 -2.178293 0.661849

36

[TS-B1C1-Br]

Enthalpies= -3141.548063 / Free Energies= -3141.610903

C 0.268586 1.302935 0.035784

C 1.000388 0.098780 0.134412

C 0.270935 -1.118740 0.124521

C -1.121322 -1.110290 0.020057

C -1.845809 0.082187 -0.068920

C -1.129553 1.277615 -0.060420

B 2.586989 0.039159 0.189784

C 3.653526 1.024030 1.466193

C 3.189181 -0.193995 1.945612

C 4.318381 -1.208209 2.056067

C 5.431148 -0.590164 1.179242

C 5.132255 0.929192 1.164613

Br 1.769467 -0.310303 3.233564

C 0.971338 -2.453193 0.236661

C -3.350438 0.067009 -0.173243

C 0.940774 2.656787 0.047946

H -1.670296 2.218937 -0.134714

H -1.657281 -2.057681 0.012238

H -3.687732 -0.546055 -1.017206

H -3.811390 -0.352794 0.729270

H -3.751886 1.075259 -0.311531

H 1.283393 2.930999 1.054300

H 1.811576 2.693515 -0.613789

H 0.246384 3.439446 -0.271114

H 1.675066 -2.617471 -0.586218

H 1.544210 -2.526359 1.167022

H 0.248486 -3.274110 0.229617

H 3.166810 -0.878047 -0.308966

H 3.092361 1.035165 -0.304340

H 3.161331 1.970394 1.647049

H 5.645974 1.439883 1.990120

H 5.422427 1.425217 0.235287

H 6.428854 -0.808965 1.566497

H 5.372207 -0.988403 0.165052

H 4.625750 -1.269021 3.106569

H 4.021289 -2.208738 1.735251

36

[C1-Br]

Enthalpies= -3141.594844 / Free Energies= -3141.660310

C 1.179151 3.098390 -1.725420

C 1.949731 2.926604 -0.421313

C 1.409733 4.056360 0.457263

C 1.186965 5.247836 -0.493658

C 0.959294 4.619900 -1.898399

B 2.196029 1.539506 0.283221

Br 3.955493 3.313314 -0.772584

C 1.715951 0.141949 -0.203440

C 0.911067 -0.583162 0.725714

C 0.362824 -1.812314 0.367954

C 0.607078 -2.391387 -0.883812

C 1.419969 -1.696748 -1.776002

C 1.966474 -0.444347 -1.465185

C 0.599868 -0.028128 2.098790

C 0.010423 -3.729221 -1.238497

C 2.851668 0.194959 -2.510015

H 2.661290 1.633670 1.379884

H 0.445558 3.702627 0.850922

H 1.642672 -2.138811 -2.744820

H -0.264935 -2.339625 1.082983

H	1.511951	0.146804	2.679528
H	0.067257	0.928773	2.049364
H	-0.029866	-0.721380	2.663201
H	3.568061	-0.535657	-2.901674
H	2.263315	0.546260	-3.366261
H	3.423457	1.038917	-2.125566
H	0.316640	-4.503019	-0.524968
H	-1.085311	-3.693283	-1.218178
H	0.316183	-4.053641	-2.237053
H	2.046680	4.276081	1.315888
H	2.076408	5.883654	-0.502298
H	0.347583	5.869937	-0.170891
H	1.672733	5.028336	-2.619040
H	-0.041474	4.830000	-2.285963
H	1.660313	2.629549	-2.582465
H	0.220036	2.583437	-1.578571

36

[TS-C1P-Br]

Enthalpies= -3141.583166 / Free Energies= -3141.645241

C	0.783053	3.049819	-1.614095
C	1.626147	2.993393	-0.401871
C	1.815132	4.387782	0.069482
C	1.403150	5.309260	-1.092608
C	0.286913	4.498864	-1.774192
B	2.151053	1.701515	0.328000
Br	4.253810	2.050848	0.174662
C	1.668596	0.259807	-0.170331
C	0.907147	-0.544929	0.725880
C	0.425660	-1.794944	0.330782
C	0.671892	-2.314246	-0.943732
C	1.422334	-1.535376	-1.818941
C	1.916552	-0.272958	-1.457981
C	0.583006	-0.098549	2.137126
C	0.155702	-3.674904	-1.339038
C	2.704637	0.453201	-2.529581
H	1.941567	1.924380	1.494281
H	1.042740	4.452027	0.862575
H	1.637587	-1.915957	-2.815941
H	-0.153872	-2.385317	1.037775
H	1.488278	0.095561	2.721538
H	-0.009082	0.822843	2.158380
H	0.009218	-0.869595	2.660018
H	3.421830	-0.226817	-3.002191
H	2.045357	0.810408	-3.331704
H	3.275575	1.295316	-2.142928
H	0.660022	-4.471382	-0.777953
H	-0.916727	-3.772167	-1.134586
H	0.314484	-3.869722	-2.403790
H	2.772422	4.573191	0.556549
H	2.251695	5.443202	-1.773386
H	1.083135	6.297557	-0.755464
H	0.118251	4.775187	-2.817214
H	-0.659284	4.626926	-1.235975
H	1.513179	2.812449	-2.410959
H	0.049110	2.239467	-1.663949

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[P-Br]

Enthalpies= -3141.640377 / Free Energies= -3141.706775

C	0.086467	2.998466	-0.839956
C	1.376044	3.083590	0.009439
C	2.264761	4.175283	-0.698971
C	1.368205	4.785613	-1.804399
C	-0.069668	4.413609	-1.410257
B	2.106242	1.735981	0.306541
Br	3.733914	1.842130	1.395670
C	1.663254	0.324504	-0.172960

C	0.899570	-0.518588	0.662837
C	0.486429	-1.764865	0.189539
C	0.816325	-2.208586	-1.096312
C	1.573619	-1.364982	-1.912389
C	1.999678	-0.108179	-1.471274
C	0.532866	-0.075592	2.059609
C	0.372146	-3.567716	-1.575416
C	2.828954	0.775539	-2.373266
H	1.106552	3.491945	0.995957
H	2.576447	4.929839	0.027560
H	1.838114	-1.690614	-2.915930
H	-0.107236	-2.406044	0.837858
H	1.422843	0.029854	2.690597
H	0.025918	0.897162	2.056277
H	-0.136165	-0.792334	2.543397
H	2.954035	0.331596	-3.364614
H	2.365059	1.759700	-2.509773
H	3.830132	0.944087	-1.958453
H	0.888177	-4.368445	-1.031502
H	-0.701951	-3.716615	-1.418535
H	0.579561	-3.704751	-2.640417
H	3.182680	3.755691	-1.119670
H	1.606695	4.328124	-2.772115
H	1.519291	5.864001	-1.913889
H	-0.772913	4.470336	-2.247310
H	-0.432859	5.092116	-0.627291
H	0.213044	2.279172	-1.657732
H	-0.775960	2.665114	-0.254211

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[B2-Br]

Enthalpies= -3141.558995 / Free Energies= -3141.627502

C	-1.283447	0.336493	-1.594171
C	-0.797894	-0.981556	-1.350815
C	-1.725566	-1.959746	-0.896445
C	-3.065772	-1.619379	-0.698330
C	-3.536797	-0.327136	-0.941775
C	-2.629048	0.637575	-1.393021
B	0.683335	-1.331633	-1.574151
C	1.616339	-0.089537	1.033621
C	1.849672	-1.405058	0.943350
C	3.273440	-1.658060	0.507247
C	3.764846	-0.264697	0.027814
C	2.798393	0.767257	0.662913
H	1.160692	-2.183971	1.244721
C	-1.304535	-3.381831	-0.603145
C	-4.984145	0.029980	-0.723472
C	-0.367495	1.445977	-2.056113
H	-2.983425	1.648644	-1.580947
H	-3.762021	-2.376380	-0.345259
H	-5.083863	0.855457	-0.009152
H	-5.456801	0.358627	-1.656616
H	-5.554962	-0.819438	-0.338965
H	0.423598	1.635089	-1.324732
H	0.121770	1.206456	-3.005017
H	-0.925214	2.377024	-2.190348
H	-0.543169	-3.425755	0.182401
H	-2.158723	-3.978187	-0.270781
H	-0.876890	-3.870090	-1.484149
H	1.077672	-2.453375	-1.472931
H	1.456190	-0.526135	-1.993194
Br	0.028324	0.696091	1.706963
H	3.213758	1.232092	1.566949
H	2.531844	1.580611	-0.018647
H	4.807017	-0.074077	0.294699
H	3.683473	-0.209761	-1.060230
H	3.859410	-2.026019	1.361048

H 3.342694 -2.416718 -0.278283

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[TS-B2C2-Br]

Enthalpies= -3141.546535 / Free Energies= -3141.608312

C 0.267175 1.251273 -0.266185

C 0.981286 0.099414 0.157812

C 0.227772 -1.056603 0.469867

C -1.173051 -1.027924 0.429198

C -1.873845 0.122429 0.074009

C -1.129322 1.249600 -0.287954

B 2.574919 0.068401 0.187976

C 3.576236 0.852617 1.613735

C 3.202328 -0.487209 1.757143

C 4.451213 -1.354884 1.664219

C 5.492114 -0.437949 0.977667

C 5.059573 0.999889 1.344720

H 2.366576 -0.765866 2.383339

C 0.884906 -2.372930 0.825355

C -3.381313 0.154694 0.052000

C 0.976320 2.492951 -0.761800

H -1.653870 2.147144 -0.609880

H -1.726484 -1.932854 0.673165

H -3.775896 0.874181 0.779897

H -3.761372 0.456480 -0.930980

H -3.806433 -0.824755 0.289617

H 1.587049 2.964481 0.013265

H 1.641783 2.262861 -1.601677

H 0.254405 3.238100 -1.109133

H 1.092022 -2.461631 1.899498

H 0.230803 -3.210200 0.563485

H 1.832890 -2.510913 0.299610

H 3.205474 -0.603929 -0.581936

H 3.033218 1.187385 -0.043115

Br 2.659480 2.272196 2.511805

H 5.518606 1.324366 2.286024

H 5.290568 1.748869 0.584065

H 6.514712 -0.649236 1.298700

H 5.448199 -0.570966 -0.105162

H 4.772490 -1.619159 2.679866

H 4.284503 -2.284803 1.114587

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[C2-Br]

Enthalpies= -3141.591646 / Free Energies= -3141.657243

C -1.762107 0.459489 -1.736460

C -0.950126 -0.509904 -1.075409

C -1.601752 -1.601935 -0.442084

C -2.994874 -1.706190 -0.480762

C -3.788558 -0.744988 -1.108867

C -3.150541 0.335627 -1.727903

B 0.582659 -0.315283 -1.076475

C 2.512261 0.494339 0.404772

C 1.620586 -0.699946 0.043602

C 2.706037 -1.723275 -0.398084

C 3.973930 -1.406900 0.459191

C 3.657634 -0.097040 1.221232

H 1.162023 -1.053101 0.972218

C -0.841486 -2.701713 0.265157

C -5.290107 -0.865426 -1.133381

C -1.159862 1.664210 -2.424419

H -3.753439 1.094848 -2.221243

H -3.474517 -2.560595 -0.009009

H -5.764760 0.002526 -0.661163

H -5.666668 -0.914070 -2.161819

H -5.630045 -1.761998 -0.607892

H -0.608328 2.300108 -1.724151

H -0.455854 1.371736 -3.210166

H -1.941121 2.276606 -2.882875

H -0.542754 -2.397514 1.274939

H -1.465958 -3.593491 0.370529

H 0.063574 -2.994846 -0.271076

H 1.080968 0.244581 -2.015247

H 2.876803 0.999372 -0.491635

Br 1.509316 1.918726 1.369219

H 3.303510 -0.313192 2.233675

H 4.511692 0.580080 1.302317

H 4.201229 -2.218375 1.155872

H 4.848938 -1.283577 -0.185414

H 2.360813 -2.751608 -0.264462

H 2.931376 -1.596811 -1.462691

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[TS-C2D2-Br]

Enthalpies= -3141.541123 / Free Energies= -3141.604404

C -1.456745 0.625434 -1.723381

C -0.741191 0.189144 -0.572840

C -1.422952 -0.678782 0.322619

C -2.730440 -1.095666 0.055649

C -3.418779 -0.683211 -1.086141

C -2.761012 0.181394 -1.962150

B 0.750644 0.656866 -0.393574

C 3.077191 0.571733 0.601799

C 1.916394 -0.247230 0.277741

C 2.600803 -1.537927 -0.265435

C 3.792062 -1.707827 0.710696

C 4.242196 -0.253461 0.998034

H 1.547056 -0.571560 1.262677

C -0.800002 -1.167641 1.610985

C -4.839057 -1.118869 -1.341534

C -0.861198 1.581777 -2.735727

H -3.280695 0.525959 -2.853596

H -3.228106 -1.755651 0.763359

H -5.053464 -1.180768 -2.413167

H -5.046071 -2.096691 -0.895462

H -5.554096 -0.406789 -0.909491

H -0.535290 2.515393 -2.267335

H 0.013373 1.160397 -3.242129

H -1.599723 1.831262 -3.503319

H -0.348023 -0.344647 2.172533

H -1.555370 -1.632668 2.251184

H -0.027192 -1.926375 1.434977

H 1.183321 1.411626 -1.213757

H 3.185349 1.610546 0.317704

Br 0.979864 2.174845 1.543643

H 4.556903 -0.047886 2.030613

H 5.093275 0.062489 0.374894

H 3.448943 -2.186168 1.633569

H 4.605669 -2.312988 0.304724

H 1.912654 -2.386011 -0.260414

H 2.950067 -1.391156 -1.293537

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[D2-Br]

Enthalpies= -3141.604995 / Free Energies= -3141.673965

C -0.872878 0.344223 -1.593408

C -0.722469 0.352575 -0.171309

C -1.570582 -0.498785 0.591134

C -2.500941 -1.317848 -0.056854

C -2.650227 -1.320594 -1.443288

C -1.827544 -0.474382 -2.194065

B 0.370221 1.280158 0.395179

C 2.826172 -0.370480 0.525377

C 2.009050 -1.161179 1.233426

C 1.518118 -2.339313 0.429824

C 1.961022 -1.995749 -1.017469

C	3.036947	-0.886368	-0.877220
H	1.763326	-1.014868	2.280094
C	-1.510414	-0.594156	2.096314
C	-3.671089	-2.198158	-2.118219
C	-0.028634	1.208877	-2.505977
H	-1.930873	-0.459262	-3.276434
H	-3.128014	-1.973445	0.541884
H	-3.218224	-2.787486	-2.923189
H	-4.136836	-2.889559	-1.410820
H	-4.467612	-1.596528	-2.572405
H	-0.110331	2.272094	-2.261686
H	1.032529	0.948664	-2.445897
H	-0.343068	1.081628	-3.545273
H	-1.891976	0.313421	2.572649
H	-2.113406	-1.436569	2.446004
H	-0.490874	-0.732676	2.462057
H	1.210378	1.743228	-0.295954
H	3.332738	0.507103	0.913846
Br	0.382957	2.091600	2.167377
H	4.056279	-1.285182	-0.982172
H	2.935378	-0.101708	-1.635818
H	2.330479	-2.869601	-1.560402
H	1.103280	-1.605577	-1.570374
H	1.981498	-3.267027	0.795563
H	0.434426	-2.479020	0.507071

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[TS-D2P-Br]

Enthalpies= -3141.592990 / Free Energies= -3141.655430

C	0.813165	1.256914	-0.274497
C	1.316064	-0.039561	0.007469
C	0.380045	-1.093517	0.148426
C	-0.992625	-0.841770	0.030498
C	-1.488150	0.433760	-0.238261
C	-0.563417	1.468520	-0.395176
B	2.879511	-0.332333	0.137876
C	3.520496	0.665256	1.504394
C	3.667584	-0.673035	1.874172
C	5.115107	-1.090613	1.891654
C	5.887250	0.120843	1.309260
C	4.889024	1.307333	1.326782
H	2.906257	-1.245168	2.393559
C	0.805632	-2.521998	0.411214
C	-2.969418	0.693401	-0.351114
C	1.722366	2.451107	-0.460969
H	-0.922727	2.470237	-0.622890
H	-1.691662	-1.667945	0.140099
H	-3.350837	1.221516	0.531975
H	-3.201523	1.317552	-1.220984
H	-3.533234	-0.239323	-0.445279
H	2.070655	2.857039	0.496829
H	2.608893	2.200824	-1.047173
H	1.193090	3.259658	-0.973451
H	1.497021	-2.888265	-0.355269
H	1.307998	-2.638785	1.378952
H	-0.062167	-3.187775	0.418168
Br	4.016502	-0.067760	-1.538899
H	3.061137	-1.509571	0.364034
H	2.676580	1.251195	1.843463
H	5.067372	1.969677	2.182387
H	4.955541	1.912658	0.419501
H	6.789420	0.337303	1.886743
H	6.189972	-0.092287	0.284139
H	5.366376	-1.266660	2.946115
H	5.299702	-2.028351	1.360086

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[cloropentene]

Enthalpies= -654.843358 / Free Energies= -654.879774

C	3.900268	1.919509	0.046704
C	3.581195	1.621333	1.538260
C	2.173595	1.077011	1.497291
C	1.825794	0.789559	0.242926
C	2.896928	1.073807	-0.777418
H	3.723356	2.980588	-0.153569
H	4.939911	1.704071	-0.211887
H	3.671745	2.513403	2.167994
H	4.265314	0.871247	1.960041
H	3.333459	0.132219	-1.136638
H	2.510584	1.602510	-1.654601
Cl	0.305633	0.067602	-0.247275
H	1.562026	0.903999	2.375419

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[B1-Cl]

Enthalpies= -1030.345367 / Free Energies= -1030.412851

C	-1.191745	1.384177	-1.163057
C	-0.435980	0.180668	-1.227014
C	-1.136719	-1.054575	-1.104304
C	-2.519048	-1.062995	-0.924928
C	-3.257550	0.123868	-0.858124
C	-2.575779	1.336870	-0.978107
B	1.089705	0.207177	-1.433271
C	2.138517	0.920585	1.005055
C	1.776448	-0.301954	1.417418
C	2.880514	-1.323670	1.350752
C	3.973523	-0.573424	0.548375
C	3.598043	0.932547	0.619441
Cl	0.231536	-0.715412	2.111408
C	-0.418379	-2.383392	-1.162207
C	-4.751063	0.083031	-0.665699
C	-0.539999	2.742512	-1.285220
H	-3.138655	2.265850	-0.926267
H	-3.038575	-2.014089	-0.830672
H	-5.019258	-0.487878	0.230610
H	-5.172204	1.087078	-0.565535
H	-5.245590	-0.405672	-1.513786
H	0.179994	2.923393	-0.480213
H	0.007689	2.848035	-2.226474
H	-1.290650	3.536487	-1.242505
H	0.084589	-2.532179	-2.122994
H	0.347134	-2.459814	-0.385493
H	-1.121410	-3.208824	-1.020405
H	1.719263	-0.800984	-1.530809
H	1.666070	1.226444	-1.662141
H	1.514333	1.804058	1.054443
H	4.177076	1.461263	1.389388
H	3.779030	1.450594	-0.327237
H	4.977064	-0.771308	0.931970
H	3.944802	-0.902046	-0.492739
H	3.204777	-1.582133	2.367438
H	2.558584	-2.252952	0.870833

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[TS-B1C1-Cl]

Enthalpies= -1030.333860 / Free Energies= -1030.394883

C	0.256404	1.323331	0.095917
C	1.001087	0.123762	0.139555
C	0.285452	-1.099851	0.075451
C	-1.107134	-1.102523	-0.026012
C	-1.844654	0.084962	-0.062690
C	-1.141478	1.286668	-0.002464
B	2.588266	0.077998	0.195046
C	3.638829	0.996319	1.519784
C	3.174960	-0.250093	1.929861
C	4.306815	-1.265398	1.994365

C	5.423298	-0.597799	1.160517
C	5.119376	0.919854	1.224627
Cl	1.857755	-0.425699	3.094000
C	1.002740	-2.429695	0.118314
C	-3.348984	0.057810	-0.170742
C	0.914801	2.682173	0.167525
H	-1.692465	2.224407	-0.034684
H	-1.632241	-2.054667	-0.076013
H	-3.805567	-0.431765	0.698041
H	-3.763244	1.067994	-0.238799
H	-3.676795	-0.498016	-1.057217
H	1.275266	2.906907	1.179814
H	1.772916	2.762102	-0.507226
H	0.207081	3.473014	-0.097341
H	1.695844	-2.546860	-0.721792
H	1.591098	-2.539893	1.034982
H	0.289465	-3.258169	0.082502
H	3.183390	-0.788255	-0.372028
H	3.079951	1.117010	-0.221950
H	3.144610	1.927906	1.763574
H	5.624969	1.386314	2.080630
H	5.416598	1.465493	0.325718
H	6.418981	-0.832819	1.543408
H	5.374638	-0.941282	0.126085
H	4.606198	-1.379080	3.043032
H	4.015163	-2.248221	1.618490

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[C1-Cl]

Enthalpies= -1030.377789 / Free Energies= -1030.443106

C	-1.475942	1.289315	-1.101353
C	-0.686065	0.136417	-0.899179
C	-1.328974	-1.110475	-0.713169
C	-2.721510	-1.177121	-0.729872
C	-3.513217	-0.035666	-0.908245
C	-2.871036	1.189297	-1.093444
B	0.856113	0.278371	-0.933449
C	2.811043	1.285263	0.436639
C	1.893083	0.059303	0.228207
C	2.921314	-1.059740	-0.041024
C	4.128623	-0.752303	0.878534
C	4.023540	0.754733	1.232372
Cl	1.069511	-0.288639	1.870059
C	-0.522446	-2.376081	-0.540750
C	-5.017413	-0.136861	-0.897248
C	-0.822697	2.641276	-1.264709
H	-3.466967	2.087599	-1.238196
H	-3.204837	-2.143550	-0.602848
H	-5.387354	-0.434998	0.091263
H	-5.484746	0.818444	-1.152435
H	-5.373916	-0.888127	-1.611125
H	-0.467168	3.031393	-0.302888
H	0.045802	2.593011	-1.933024
H	-1.520687	3.376745	-1.674875
H	0.203345	-2.508344	-1.352157
H	0.032095	-2.362952	0.403008
H	-1.168118	-3.258849	-0.534504
H	1.385175	0.641747	-1.949186
H	3.130010	1.625806	-0.555562
H	2.298146	2.118073	0.923174
H	3.851717	0.882934	2.303875
H	4.931675	1.309688	0.979986
H	4.079272	-1.362922	1.783298
H	5.068523	-0.995641	0.375087
H	2.502183	-2.056232	0.107977
H	3.218364	-0.983346	-1.094334

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[TS-C1P-Cl]

Enthalpies= -1030.368397 / Free Energies= -1030.430553

C	0.773429	2.984712	-1.539872
C	1.664274	2.954737	-0.363762
C	1.785262	4.337414	0.142386
C	1.268699	5.268693	-0.969661
C	0.190106	4.406141	-1.649535
B	2.352421	1.674135	0.275760
Cl	4.210365	2.123344	-0.168349
C	1.797365	0.251580	-0.219610
C	0.861978	-0.413702	0.620494
C	0.290426	-1.630987	0.235383
C	0.608071	-2.243668	-0.977682
C	1.511287	-1.586665	-1.811309
C	2.101701	-0.364965	-1.459650
C	0.426497	0.156593	1.955823
C	0.012049	-3.575649	-1.358122
C	3.076590	0.217077	-2.461597
H	2.298637	1.827179	1.470655
H	1.042366	4.314203	0.967583
H	1.767229	-2.034938	-2.769258
H	-0.423158	-2.113604	0.900270
H	1.267594	0.262642	2.648615
H	-0.026955	1.149728	1.860057
H	-0.315065	-0.495649	2.426625
H	4.113340	0.023204	-2.168434
H	2.920786	-0.231705	-3.447771
H	2.993518	1.299820	-2.568627
H	0.039921	-3.734988	-2.440557
H	0.562557	-4.403568	-0.893017
H	-1.029286	-3.659312	-1.029542
H	2.744378	4.567365	0.608483
H	2.083552	5.487681	-1.668896
H	0.890543	6.218658	-0.585874
H	-0.019128	4.700061	-2.680215
H	-0.750269	4.460229	-1.089067
H	1.484969	2.794630	-2.367448
H	0.084223	2.135715	-1.575638

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[P-Cl]

Enthalpies= -1030.431166 / Free Energies= -1030.496871

C	0.135024	2.997255	-0.784312
C	1.418832	3.051011	0.074999
C	2.335717	4.127179	-0.622386
C	1.457391	4.766534	-1.726581
C	0.010126	4.419577	-1.344272
B	2.127918	1.688967	0.365300
Cl	3.597113	1.747394	1.407749
C	1.672093	0.294089	-0.159845
C	0.877817	-0.550983	0.643974
C	0.449607	-1.779670	0.138227
C	0.794428	-2.202929	-1.150335
C	1.584325	-1.358385	-1.934073
C	2.023953	-0.118192	-1.460445
C	0.497133	-0.132556	2.045115
C	0.307259	-3.528479	-1.679421
C	2.882550	0.768427	-2.331953
H	1.151405	3.459619	1.061793
H	2.662573	4.869109	0.110575
H	1.864368	-1.670465	-2.937639
H	-0.168141	-2.422002	0.762529
H	1.367622	-0.125771	2.711558
H	0.070605	0.877632	2.065412
H	-0.244222	-0.810651	2.476561
H	3.875946	0.922361	-1.893748
H	3.025416	0.335120	-3.325653

H	2.430225	1.758005	-2.467452
H	0.801792	-3.790008	-2.619198
H	0.492306	-4.337564	-0.964335
H	-0.773267	-3.509164	-1.868045
H	3.244575	3.689703	-1.044984
H	1.692096	4.314542	-2.697777
H	1.630786	5.842740	-1.823875
H	-0.686296	4.496829	-2.185358
H	-0.344962	5.098813	-0.558232
H	0.254591	2.282294	-1.606989
H	-0.738430	2.675760	-0.208241

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[B2-Cl]

Enthalpies= -1030.346319 / Free Energies= -1030.409817

C	-1.112818	0.655080	-1.297097
C	-0.627490	-0.666062	-1.070955
C	-1.555457	-1.650465	-0.630994
C	-2.895838	-1.312687	-0.428584
C	-3.366635	-0.017136	-0.653728
C	-2.458659	0.953528	-1.091948
B	0.854721	-1.012827	-1.298164
C	1.747456	0.200170	1.313777
C	1.995995	-1.111959	1.205968
C	3.425838	-1.341432	0.779319
C	3.907096	0.064981	0.326857
C	2.920273	1.076801	0.961693
H	1.313225	-1.900984	1.495420
C	-1.135253	-3.077388	-0.360563
C	-4.813811	0.337356	-0.430143
C	-0.198017	1.769483	-1.750386
H	-2.813170	1.966919	-1.266592
H	-3.592326	-2.074525	-0.086597
H	-4.912987	1.151138	0.297500
H	-5.286016	0.681216	-1.357999
H	-5.385168	-0.517875	-0.059561
H	0.611659	1.937472	-1.034509
H	0.268882	1.548119	-2.715203
H	-0.752190	2.706673	-1.852748
H	-0.373678	-3.135195	0.423807
H	-1.989802	-3.678552	-0.037947
H	-0.708387	-3.551443	-1.249701
H	1.247796	-2.136619	-1.217494
H	1.626729	-0.201562	-1.707557
Cl	0.274845	0.901483	1.927929
H	3.318986	1.539646	1.874200
H	2.644950	1.890873	0.284199
H	4.942843	0.263118	0.612423
H	3.842633	0.134586	-0.761390
H	4.008836	-1.717177	1.631686
H	3.511643	-2.085793	-0.018192

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[TS-B2C2-Cl]

Enthalpies= -1030.333221 / Free Energies= -1030.393831

C	0.262488	1.257159	-0.251209
C	0.978618	0.102499	0.160123
C	0.227786	-1.057917	0.463401
C	-1.172785	-1.033735	0.418081
C	-1.876063	0.117386	0.069625
C	-1.134235	1.250940	-0.277302
B	2.572406	0.064320	0.188483
C	3.582217	0.870677	1.600778
C	3.194406	-0.465367	1.762787
C	4.436787	-1.343656	1.686369
C	5.485479	-0.447061	0.984311
C	5.066440	0.999756	1.327785
H	2.359655	-0.720599	2.401178

C	0.890488	-2.371729	0.816806
C	-3.383549	0.144042	0.040214
C	0.969031	2.507999	-0.727761
H	-1.660914	2.150347	-0.590444
H	-1.724129	-1.942142	0.653581
H	-3.784615	0.860498	0.767490
H	-3.759781	0.446304	-0.944113
H	-3.806053	-0.837577	0.273466
H	1.572418	2.975050	0.055644
H	1.641129	2.290523	-1.565721
H	0.245734	3.253166	-1.072137
H	1.118789	-2.450121	1.887365
H	0.231764	-3.211198	0.574605
H	1.828800	-2.513672	0.274700
H	3.198066	-0.616469	-0.577809
H	3.037140	1.180499	-0.051313
Cl	2.752902	2.200754	2.392637
H	5.525983	1.335416	2.265246
H	5.302525	1.734981	0.555386
H	6.506274	-0.662926	1.307987
H	5.439781	-0.597629	-0.096200
H	4.756295	-1.593395	2.706233
H	4.263792	-2.281610	1.152548

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[C2-Cl]

Enthalpies= -1030.377720 / Free Energies= -1030.443805

C	-1.496133	0.457754	-1.715504
C	-0.762806	-0.348296	-0.797063
C	-1.496918	-1.192868	0.080459
C	-2.891340	-1.220470	0.024059
C	-3.609374	-0.409095	-0.858666
C	-2.891428	0.425400	-1.719551
B	0.779855	-0.249225	-0.797661
C	2.742736	0.818902	0.478361
C	1.769760	-0.368426	0.421220
C	2.782024	-1.543126	0.303630
C	4.051335	-1.102369	1.100032
C	3.835283	0.387370	1.455588
H	1.275318	-0.425159	1.396295
C	-0.819311	-2.108665	1.075038
C	-5.115479	-0.418324	-0.865978
C	-0.803845	1.393940	-2.681014
H	-3.434455	1.060119	-2.415847
H	-3.434494	-1.890900	0.686278
H	-5.513984	-0.153050	-1.849766
H	-5.512176	-1.399055	-0.586532
H	-5.513627	0.309265	-0.146987
H	-0.200736	2.144798	-2.160334
H	-0.128702	0.854308	-3.353398
H	-1.536597	1.924859	-3.295147
H	-0.485682	-1.559576	1.962751
H	-1.510686	-2.883535	1.418331
H	0.054793	-2.609247	0.652307
H	1.329608	0.001254	-1.835909
H	3.156134	1.028684	-0.510986
Cl	1.919936	2.380734	0.968677
H	3.458375	0.492694	2.477543
H	4.739743	0.994633	1.367346
H	4.185653	-1.702510	2.004132
H	4.950221	-1.236393	0.491413
H	2.356480	-2.475854	0.682065
H	3.039378	-1.712954	-0.747833

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[TS-C2D2-Cl]

Enthalpies= -1030.322049 / Free Energies= -1030.384263

C	-1.464793	0.620475	-1.730352

C	-0.743286	0.173844	-0.587448
C	-1.426119	-0.686021	0.315186
C	-2.743275	-1.081261	0.064544
C	-3.438732	-0.657593	-1.068964
C	-2.778173	0.195418	-1.953849
B	0.754076	0.621728	-0.426764
C	3.050881	0.577737	0.592312
C	1.922897	-0.272842	0.236033
C	2.661764	-1.539059	-0.289774
C	3.819785	-1.681286	0.733068
C	4.211597	-0.216342	1.060801
H	1.548023	-0.611822	1.214111
C	-0.792769	-1.195581	1.590714
C	-4.867824	-1.073239	-1.307684
C	-0.865942	1.561809	-2.755025
H	-3.302517	0.545540	-2.840268
H	-3.242153	-1.734757	0.777300
H	-5.100243	-1.115970	-2.376394
H	-5.078742	-2.055366	-0.873006
H	-5.567327	-0.360080	-0.852719
H	-0.525273	2.495453	-2.297521
H	-0.001324	1.125155	-3.265581
H	-1.607900	1.813166	-3.518615
H	-0.323635	-0.386257	2.157193
H	-1.546019	-1.658653	2.234706
H	-0.032461	-1.962058	1.394952
H	1.175922	1.403629	-1.225902
H	3.159795	1.605662	0.270184
Cl	1.033221	2.026102	1.472792
H	4.440214	-0.013989	2.116362
H	5.096263	0.128831	0.505659
H	3.457480	-2.186855	1.633397
H	4.669432	-2.251140	0.350695
H	1.997973	-2.406116	-0.312449
H	3.045544	-1.379370	-1.303285

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[D2-Cl]

Enthalpies= -1030.396400 / Free Energies= -1030.464094

C	-0.715952	0.662743	-1.345534
C	-0.590369	0.725585	0.076790
C	-1.450181	-0.097068	0.857379
C	-2.371278	-0.939457	0.226574
C	-2.496797	-0.995280	-1.161298
C	-1.659511	-0.180246	-1.930188
B	0.487002	1.677154	0.635624
C	2.957173	0.016017	0.811668
C	2.124247	-0.765524	1.510812
C	1.650545	-1.954137	0.712585
C	2.136418	-1.637685	-0.727471
C	3.201450	-0.518393	-0.578674
H	1.852914	-0.605971	2.549389
C	-1.410125	-0.136744	2.366108
C	-3.509015	-1.895375	-1.819399
C	0.141808	1.494324	-2.276015
H	-1.743583	-0.208429	-3.013961
H	-3.008749	-1.571494	0.839527
H	-3.051356	-2.493035	-2.615253
H	-3.966691	-2.579333	-1.099564
H	-4.312882	-1.309728	-2.281693
H	0.023147	2.567299	-2.096946
H	1.205902	1.267965	-2.162358
H	-0.129872	1.298845	-3.316718
H	-1.792573	0.789603	2.804827
H	-2.022897	-0.962049	2.738783
H	-0.395640	-0.268579	2.748411
H	1.323037	2.146688	-0.058903

H	3.453860	0.899675	1.199616
Cl	0.482545	2.402932	2.274359
H	4.225539	-0.910919	-0.656986
H	3.110870	0.254968	-1.350248
H	2.528820	-2.520509	-1.238885
H	1.294077	-1.267251	-1.316259
H	2.097014	-2.878517	1.106609
H	0.564055	-2.085677	0.761158

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[TS-D2P-Cl]

Enthalpies= -1030.381045 / Free Energies= -1030.441928

C	0.824205	1.249407	-0.285955
C	1.317668	-0.047610	0.007349
C	0.376046	-1.094761	0.154400
C	-0.994950	-0.835191	0.030825
C	-1.481883	0.441154	-0.249244
C	-0.550506	1.469225	-0.412218
B	2.884028	-0.337403	0.144057
C	3.501012	0.640993	1.526902
C	3.683946	-0.704260	1.861519
C	5.141945	-1.087789	1.849440
C	5.878800	0.154582	1.286387
C	4.852342	1.316576	1.337732
H	2.949148	-1.298708	2.394014
C	0.792070	-2.523565	0.430185
C	-2.961441	0.709135	-0.365763
C	1.744103	2.435093	-0.473506
H	-0.902931	2.471521	-0.647931
H	-1.699367	-1.656156	0.145170
H	-3.343697	1.230822	0.520837
H	-3.187065	1.342490	-1.230588
H	-3.529586	-0.219834	-0.470447
H	2.110375	2.824992	0.484073
H	2.619932	2.181891	-1.074171
H	1.217608	3.255150	-0.970256
H	1.491564	-2.896769	-0.325459
H	1.281243	-2.637486	1.405140
H	-0.078628	-3.185627	0.430024
Cl	3.954331	-0.080260	-1.378615
H	3.048382	-1.518406	0.393267
H	2.652000	1.200449	1.897250
H	5.030706	1.970689	2.199604
H	4.890724	1.938242	0.439888
H	6.778641	0.380952	1.863757
H	6.183955	-0.029452	0.256520
H	5.411411	-1.281833	2.896075
H	5.340868	-2.008175	1.293570

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[mesitylene-toluene]

Enthalpies= -646.974728 / Free Energies= -647.038682

B	0.637232	1.751775	-1.806202
H	-1.568931	2.062697	0.997381
C	-1.624071	1.131268	0.440195
C	1.382500	0.474741	-1.395655
C	2.037748	0.378890	-0.132464
C	2.644478	-0.814544	0.254409
C	2.637829	-1.943386	-0.573632
C	2.012886	-1.849561	-1.818737
C	1.395386	-0.669778	-2.241497
C	-1.157935	-0.051354	1.014169
C	-1.216920	-1.247990	0.299921
C	-1.757433	-1.255401	-0.986602
C	-2.232291	-0.073468	-1.553526
C	-2.168702	1.140233	-0.853084
C	0.749857	-0.658355	-3.607520
C	3.281932	-3.226439	-0.117753

C	2.092517	1.546947	0.823834
C	-2.720435	2.410121	-1.451033
H	-1.798937	-2.180779	-1.553379
H	-0.731056	-0.035160	2.012536
H	0.096054	1.845882	-2.865255
H	0.621801	2.718529	-1.106867
H	-2.655684	-0.085459	-2.554449
H	-0.832089	-2.164406	0.736199
H	2.008120	-2.717743	-2.473371
H	3.134105	-0.874142	1.223957
H	2.599576	2.410130	0.381450
H	1.090346	1.878709	1.108434
H	2.630831	1.275004	1.736175
H	0.851156	-1.633781	-4.091886
H	-0.315098	-0.420501	-3.545486
H	1.206483	0.089173	-4.263927
H	4.330524	-3.068261	0.158926
H	2.775616	-3.625907	0.769300
H	3.249188	-3.992809	-0.896904
H	-2.163083	3.287423	-1.110882
H	-3.769202	2.556240	-1.162573
H	-2.681070	2.387751	-2.543629

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[toluene]

Enthalpies= -271.471223 / Free Energies= -271.506403

H	-1.390326	1.613400	-0.105208
C	-1.820499	0.722722	-0.554692
C	-1.454715	-0.536750	-0.082496
C	-1.995749	-1.702801	-0.643391
C	-2.914674	-1.570294	-1.690985
C	-3.284289	-0.310764	-2.167732
C	-2.737992	0.840842	-1.601546
H	-3.024954	1.821595	-1.969327
H	-3.345491	-2.463192	-2.136949
H	-0.739838	-0.620689	0.732626
H	-4.000594	-0.231288	-2.980667
C	-1.577605	-3.061151	-0.137594
H	-0.537819	-3.282345	-0.408132
H	-2.203549	-3.854621	-0.555472
H	-1.643406	-3.119755	0.954414

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[B1-concerted-Cl] scf done: -1406.407478 / Sum of electronic and thermal Energies= -1405.874018 / Sum of electronic and thermal Enthalpies= -1405.873074 / Sum of electronic and thermal Free Energies= -1405.963709

B	0.546544	0.201861	-0.545685
H	1.494652	0.352885	-3.025058
H	4.013502	2.013819	1.493352
H	1.195859	1.113298	-1.228548
B	1.797372	0.153562	-1.889568
H	2.941589	0.315047	-1.593745
C	1.164044	-1.265113	-1.265250
C	0.227997	-1.996915	-2.073850
C	2.024689	-2.023647	-0.390610
C	0.153739	-3.384563	-1.969374
C	1.891271	-3.403646	-0.307853
C	0.959904	-4.103931	-1.084663
H	-0.560650	-3.920273	-2.589097
H	2.538457	-3.956970	0.367376
C	-1.006684	0.502690	-0.618834
C	-1.863797	-0.280468	0.197343
C	-1.586466	1.551324	-1.370707
C	-3.238410	-0.034699	0.222634
C	-2.968494	1.775084	-1.315475
C	-3.815041	0.991358	-0.531417
H	-3.875013	-0.654474	0.851092
H	-3.393179	2.585845	-1.903295
C	-1.317053	-1.409150	1.039881

H	-0.465302	-1.085927	1.646921
H	-2.084028	-1.801379	1.713821
H	-0.963005	-2.240875	0.421269
C	-0.763019	2.465881	-2.250836
H	0.035569	2.967756	-1.693505
H	-0.282168	1.927437	-3.073502
H	-1.391777	3.245465	-2.689824
C	-5.299157	1.252727	-0.471982
H	-5.589652	1.683974	0.494198
H	-5.615357	1.950760	-1.252612
H	-5.874081	0.327862	-0.593631
C	3.120269	-1.383360	0.417421
H	4.023159	-1.281614	-0.196707
H	2.858090	-0.387041	0.770646
H	3.375286	-2.004375	1.280187
C	-0.733415	-1.341754	-3.027173
H	-0.422294	-0.344831	-3.329288
H	-0.845567	-1.957911	-3.924783
H	-1.720849	-1.254030	-2.561858
C	0.821410	-5.594957	-0.948691
H	0.246340	-5.843507	-0.047893
H	0.301358	-6.032305	-1.804847
H	1.798119	-6.078790	-0.849198
C	2.198777	1.835208	2.633577
C	2.984102	2.306147	1.665659
C	2.250837	3.331956	0.839335
C	0.789361	3.288381	1.379074
C	0.818053	2.428686	2.671371
H	1.014147	0.279385	0.545461
Cl	2.670413	0.634638	3.821969
H	0.681041	3.022741	3.583958
H	0.044114	1.654237	2.674508
H	0.397043	4.290375	1.567732
H	0.132061	2.814710	0.648298
H	2.706542	4.324039	0.960077
H	2.301805	3.097411	-0.230613

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[TS-B1C1-concerted-Cl] scf done: -1406.351070 / Sum of electronic and thermal Energies= -1405.819973 / Sum of electronic and thermal Enthalpies= -1405.819029 / Sum of electronic and thermal Free Energies= -1405.906467

B	-0.080582	0.280732	0.459850
H	1.817514	0.551642	-1.922011
H	2.633128	0.736722	1.798690
H	0.442727	0.479788	-0.692459
B	1.575505	-0.196131	-1.002796
H	2.318611	0.067254	-0.063274
C	1.333880	-1.726578	-1.318154
C	0.492960	-2.112711	-2.391811
C	1.937373	-2.749632	-0.550891
C	0.287736	-3.464048	-2.680771
C	1.716553	-4.095391	-0.868869
C	0.895865	-4.475426	-1.931715
H	-0.363667	-3.734834	-3.509581
H	2.195953	-4.866228	-0.269058
C	-1.646135	0.396692	0.238498
C	-2.495866	-0.430034	1.034968
C	-2.267085	1.230028	-0.725933
C	-3.882060	-0.345553	0.906693
C	-3.664411	1.280495	-0.828242
C	-4.492198	0.520279	-0.007556
H	-4.508664	-0.984946	1.524741
H	-4.111775	1.928860	-1.578742
C	-1.948490	-1.471753	1.985884
H	-1.306062	-1.039941	2.755532
H	-2.766368	-1.998790	2.485747
H	-1.349120	-2.214836	1.449287
C	-1.503325	2.083330	-1.718153

H	-1.447149	3.130625	-1.399027
H	-0.487384	1.732364	-1.890352
H	-2.014968	2.080554	-2.685714
C	-5.993674	0.605665	-0.105695
H	-6.424364	1.055250	0.797531
H	-6.306732	1.212525	-0.960151
H	-6.444879	-0.387251	-0.212567
C	2.822944	-2.434658	0.634407
H	3.679606	-1.811439	0.355959
H	2.269687	-1.896027	1.412897
H	3.213615	-3.352415	1.083959
C	-0.235288	-1.076744	-3.214088
H	0.437878	-0.289479	-3.568970
H	-0.717357	-1.529676	-4.085579
H	-1.018540	-0.589744	-2.622442
C	0.656834	-5.928313	-2.259976
H	-0.392242	-6.206612	-2.100412
H	0.887800	-6.145713	-3.309321
H	1.272103	-6.585669	-1.638652
C	0.629158	1.607043	1.477327
C	2.018918	1.440615	1.248492
C	2.572621	2.570766	0.459924
C	1.329811	3.320814	-0.059916
C	0.265454	3.030603	1.014785
H	0.316044	-0.686489	1.014958
Cl	0.091974	1.233607	3.164893
H	0.383002	3.718297	1.859927
H	-0.763950	3.096545	0.667233
H	1.513634	4.389015	-0.191652
H	1.034073	2.908561	-1.025361
H	3.091557	3.182434	1.221025
H	3.316017	2.290253	-0.287969

[C1-concerted-Cl] scf done: -1406.447675 / Sum of electronic and thermal Energies= -1405.910139 / Sum of electronic and thermal Enthalpies= -1405.909195 / Sum of electronic and thermal Free Energies= -1405.997968

B	0.605467	0.658673	-0.168819
H	2.852288	-0.187781	-0.921070
H	3.290019	2.134402	-0.308031
H	1.057214	0.567783	-1.433570
B	1.698854	-0.479282	-1.008805
H	1.968241	2.947293	-1.139974
C	1.265633	-1.841743	-1.662976
C	0.422791	-1.965046	-2.787266
C	1.796955	-3.021126	-1.082721
C	0.116584	-3.234529	-3.291204
C	1.465062	-4.272160	-1.605831
C	0.619935	-4.400457	-2.712300
H	-0.530389	-3.312849	-4.162174
H	1.878682	-5.166210	-1.144175
C	-0.961902	0.459899	-0.174099
C	-1.579027	-0.513356	0.651310
C	-1.782659	1.269619	-0.986408
C	-2.967730	-0.641744	0.656100
C	-3.174888	1.109894	-0.960615
C	-3.788061	0.163621	-0.143554
H	-3.424969	-1.390993	1.298770
H	-3.789794	1.742694	-1.597457
C	-0.760590	-1.438168	1.522473
H	-0.061462	-0.891352	2.163478
H	-1.406209	-2.035417	2.171769
H	-0.176659	-2.137052	0.912435
C	-1.223995	2.308123	-1.937286
H	-1.635940	3.301417	-1.726815
H	-0.136140	2.391726	-1.895719
H	-1.488104	2.069777	-2.973859
C	-5.287063	0.002161	-0.114395

H	-5.778227	0.703891	-0.794358
H	-5.584785	-1.011731	-0.406403
H	-5.686889	0.174414	0.891731
C	2.719549	-2.942442	0.111830
H	3.614778	-2.349396	-0.107712
H	2.236442	-2.468818	0.975080
H	3.044724	-3.938234	0.425080
C	-0.170955	-0.756926	-3.472448
H	0.564794	0.041838	-3.613790
H	-0.560743	-1.020108	-4.459835
H	-1.000160	-0.345509	-2.889055
C	0.250736	-5.760712	-3.247764
H	1.108228	-6.441759	-3.241821
H	-0.532970	-6.226158	-2.636513
H	-0.126911	-5.699855	-4.272695
C	1.293786	1.912242	0.592282
C	2.375305	2.707637	-0.148321
C	2.580341	4.001852	0.668489
C	1.276124	4.191906	1.495126
C	0.359286	3.012918	1.105966
H	1.225268	-0.423862	0.214428
Cl	2.110435	1.161388	2.130652
H	-0.292925	2.669317	1.911043
H	-0.289667	3.301272	0.273404
H	1.497062	4.163801	2.565072
H	0.792364	5.151862	1.292741
H	3.441835	3.896986	1.332868
H	2.784299	4.852999	0.012487

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[B1-concerted-Br] scf done: -3517.622466 / Sum of electronic and thermal Energies= -3517.088302 / Sum of electronic and thermal Enthalpies= -3517.087357 / Sum of electronic and thermal Free Energies= -3517.182818

B	0.902692	0.033486	-1.296823
H	1.304115	0.019854	-3.929339
H	1.646984	0.750510	3.240498
H	1.428751	0.871806	-2.156900
B	1.829246	-0.153119	-2.873178
H	3.017309	-0.053473	-2.835505
C	1.266328	-1.500415	-2.054904
C	0.136490	-2.194476	-2.611362
C	2.248197	-2.286705	-1.348146
C	0.004396	-3.569788	-2.427453
C	2.054273	-3.650644	-1.174161
C	0.938725	-4.312086	-1.703705
H	-0.856213	-4.076919	-2.855414
H	2.796624	-4.225464	-0.626638
C	-0.614262	0.412385	-1.049374
C	-1.307332	-0.293888	-0.032624
C	-1.297447	1.456238	-1.714783
C	-2.634831	0.018213	0.266621
C	-2.626186	1.751048	-1.380381
C	-3.318241	1.038915	-0.400015
H	-3.142426	-0.536476	1.051799
H	-3.131800	2.561047	-1.901516
C	-0.631891	-1.397346	0.745166
H	0.314566	-1.055178	1.173847
H	-1.265866	-1.739553	1.566576
H	-0.404762	-2.261511	0.112015
C	-0.638772	2.298592	-2.784915
H	0.280408	2.776245	-2.427593
H	-0.366069	1.710402	-3.666960
H	-1.310252	3.095676	-3.116154
C	-4.747688	1.366331	-0.049284
H	-5.117890	2.216754	-0.629152
H	-5.412760	0.515919	-0.242149
H	-4.848517	1.614749	1.013681
C	3.531055	-1.699632	-0.823892

H	4.272745	-1.641567	-1.629124
H	3.403202	-0.689930	-0.433585
H	3.947152	-2.330970	-0.034208
C	-0.966523	-1.510661	-3.372226
H	-0.663283	-0.557335	-3.798113
H	-1.316511	-2.157822	-4.182431
H	-1.817172	-1.321043	-2.709393
C	0.756696	-5.788026	-1.483078
H	1.675611	-6.338264	-1.711578
H	0.515649	-5.991883	-0.432647
H	-0.051014	-6.192672	-2.097809
C	-0.121954	1.769673	2.561370
C	1.181668	1.496704	2.607038
C	1.947538	2.425455	1.695518
C	0.836521	3.132687	0.870531
C	-0.493268	2.892708	1.631627
H	1.604195	0.130854	-0.337140
Br	-1.450397	0.921908	3.631303
H	-0.815254	3.769921	2.208511
H	-1.314772	2.621750	0.963746
H	1.041933	4.195268	0.719000
H	0.767089	2.662654	-0.111532
H	2.536890	3.137606	2.290416
H	2.655929	1.890341	1.053432

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[TS-B1C1-concerted-Br] scf done: -3517.566207 / Sum of electronic and thermal Energies= -3517.035389 / Sum of electronic and thermal Enthalpies= -3517.034445 / Sum of electronic and thermal Free Energies= -3517.122891

B	-0.069334	0.272898	0.477379
H	1.773347	0.578460	-1.955819
H	2.645373	0.725676	1.771756
H	0.439328	0.483377	-0.680261
B	1.568467	-0.178705	-1.035065
H	2.336912	0.077946	-0.116958
C	1.320968	-1.706987	-1.358345
C	0.453941	-2.085091	-2.412822
C	1.940783	-2.737100	-0.611830
C	0.239431	-3.435154	-2.705508
C	1.711745	-4.079591	-0.933704
C	0.866840	-4.451688	-1.981414
H	-0.435294	-3.699845	-3.517361
H	2.201804	-4.855228	-0.348705
C	-1.638468	0.376318	0.268731
C	-2.476010	-0.474840	1.052253
C	-2.273139	1.224470	-0.673359
C	-3.863769	-0.394135	0.940123
C	-3.671785	1.272217	-0.758784
C	-4.487550	0.491690	0.054586
H	-4.481002	-1.051641	1.548551
H	-4.129536	1.933819	-1.491382
C	-1.913578	-1.538277	1.969512
H	-1.269072	-1.121141	2.745498
H	-2.723437	-2.085230	2.460959
H	-1.312007	-2.261221	1.408623
C	-1.525172	2.091533	-1.666302
H	-1.506291	3.144115	-1.360310
H	-0.497264	1.771360	-1.824555
H	-2.025952	2.060614	-2.639160
C	-5.990210	0.577706	-0.021401
H	-6.315234	1.188896	-0.868341
H	-6.443824	-0.414279	-0.125943
H	-6.407053	1.024078	0.889990
C	2.848977	-2.430918	0.558625
H	3.698671	-1.803488	0.268790
H	2.309904	-1.900115	1.352295
H	3.249836	-3.351969	0.992254
C	-0.295598	-1.044089	-3.209646

H	0.368452	-0.256101	-3.579723
H	-0.802416	-1.492708	-4.069265
H	-1.060911	-0.558462	-2.594330
C	0.656328	-5.901927	-2.338239
H	1.305633	-6.205203	-3.169851
H	0.881055	-6.560088	-1.493180
H	-0.375678	-6.092422	-2.650862
C	0.643040	1.608536	1.469999
C	2.032634	1.449141	1.246388
C	2.588821	2.587610	0.472242
C	1.346338	3.338189	-0.049094
C	0.276566	3.034032	1.017343
H	0.342299	-0.697363	1.015713
Br	0.099802	1.220017	3.325082
H	0.386601	3.717675	1.866052
H	-0.751016	3.099840	0.665493
H	1.526696	4.408379	-0.168961
H	1.058152	2.933675	-1.020314
H	3.103029	3.194333	1.240828
H	3.337028	2.312699	-0.272923

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[C1-concerted-Br] scf done: -3517.663509 / Sum of electronic and thermal Energies= -3517.126142 / Sum of electronic and thermal Enthalpies= -3517.125198 / Sum of electronic and thermal Free Energies= -3517.215096

B	0.602218	0.659671	-0.160921
H	2.849704	-0.179389	-0.927903
H	3.308874	2.104834	-0.248362
H	1.050166	0.568620	-1.431234
B	1.696230	-0.473733	-1.008303
H	2.027286	2.911789	-1.144265
C	1.263159	-1.837048	-1.661939
C	0.423052	-1.957991	-2.788615
C	1.793373	-3.017943	-1.083803
C	0.117764	-3.226144	-3.296360
C	1.462983	-4.267715	-1.611061
C	0.619972	-4.393487	-2.719435
H	-0.527322	-3.302197	-4.168940
H	1.876117	-5.162856	-1.151078
C	-0.964036	0.452712	-0.163235
C	-1.579717	-0.524781	0.658156
C	-1.785829	1.262029	-0.975304
C	-2.968500	-0.653135	0.664067
C	-3.177928	1.102227	-0.948231
C	-3.790017	0.154974	-0.131479
H	-3.424766	-1.405184	1.304139
H	-3.793525	1.735102	-1.584329
C	-0.760154	-1.456080	1.520800
H	-0.054247	-0.914161	2.157999
H	-1.404266	-2.053750	2.171248
H	-0.183082	-2.154280	0.903529
C	-1.228842	2.297602	-1.930709
H	-1.638881	3.292009	-1.721864
H	-0.140457	2.379558	-1.894144
H	-1.497403	2.056220	-2.965383
C	-5.289070	-0.005428	-0.099676
H	-5.780817	0.695551	-0.780009
H	-5.588058	-1.019591	-0.389364
H	-5.687066	0.168999	0.906817
C	2.712944	-2.942810	0.113356
H	3.601638	-2.336794	-0.096985
H	2.222625	-2.486007	0.981610
H	3.048896	-3.938493	0.415402
C	-0.168861	-0.748352	-3.472589
H	0.567806	0.049874	-3.612062
H	-0.558179	-1.009614	-4.460673
H	-0.998088	-0.337086	-2.889269
C	0.251822	-5.752322	-3.259202

H	1.109378	-6.433298	-3.253969
H	-0.532759	-6.219539	-2.650435
H	-0.124343	-5.688645	-4.284524
C	1.276001	1.927639	0.580524
C	2.396062	2.690640	-0.132419
C	2.590293	4.002691	0.659798
C	1.277494	4.209282	1.468463
C	0.348785	3.049741	1.055665
H	1.231825	-0.420850	0.217577
Br	2.095448	1.126640	2.297481
H	-0.342406	2.730117	1.837147
H	-0.259900	3.350341	0.196859
H	1.482154	4.161836	2.540814
H	0.813958	5.179901	1.270427
H	3.445784	3.915365	1.334348
H	2.797974	4.839372	-0.013376

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[TS-alpha-Cl-dimer] scf done: -1406.373881 / Sum of electronic and thermal Energies= -1405.843445 / Sum of electronic and thermal Enthalpies= -1405.842501 / Sum of electronic and thermal Free Energies= -1405.928161

B	1.265239	2.000503	-1.239224
B	-0.734382	2.562110	1.333682
C	-0.055019	1.390777	2.051344
C	2.132463	0.751599	-0.785550
C	3.061948	0.787681	0.277941
C	3.684337	-0.388211	0.713724
C	3.416662	-1.624577	0.128672
C	2.522161	-1.655562	-0.944221
C	1.894563	-0.498270	-1.411783
C	0.839246	1.608366	3.141701
C	1.514620	0.535333	3.717589
C	1.347078	-0.773397	3.248217
C	0.453367	-0.995932	2.199500
C	-0.250771	0.051330	1.605038
C	1.967894	3.743835	-1.597627
C	0.873710	4.768929	-1.790704
C	0.023411	4.210965	-2.958957
C	0.974180	3.273859	-3.737588
C	2.003202	2.879024	-2.688868
Cl	3.499557	2.131480	-3.257790
C	0.976185	-0.618477	-2.606711
C	4.046756	-2.891770	0.649795
C	3.443535	2.076478	0.966365
C	-1.203480	-0.279151	0.482190
C	2.141355	-1.903572	3.845125
C	1.081214	2.988041	3.711069
H	0.167078	1.827367	-1.671094
H	-1.581065	2.390993	0.511412
H	-0.459036	3.696015	1.597664
H	1.107147	2.781598	-0.305999
H	0.316627	-2.007608	1.827848
H	2.197650	0.716359	4.544370
H	2.313558	-2.604779	-1.434115
H	4.391742	-0.334472	1.538400
H	-1.153717	-1.342327	0.233103
H	-2.238359	-0.045161	0.755859
H	-0.973673	0.292285	-0.418608
H	1.446140	3.686385	2.952296
H	0.165133	3.422674	4.124342
H	1.823402	2.948828	4.513190
H	2.147727	-1.855727	4.939384
H	1.743695	-2.877397	3.546986
H	3.185305	-1.854658	3.513477
H	4.135179	2.668077	0.351386
H	2.573341	2.700072	1.178688
H	3.948857	1.879968	1.915612
H	0.970564	-1.642773	-2.990635

H	-0.056660	-0.347718	-2.365881
H	1.295396	0.038401	-3.422586
H	3.343069	-3.458383	1.272560
H	4.354870	-3.554223	-0.166371
H	4.928744	-2.680037	1.261987
H	2.811901	3.913366	-0.942484
H	1.375860	5.702020	-2.078380
H	0.295974	4.965488	-0.884300
H	-0.376036	5.007311	-3.590928
H	-0.821260	3.645084	-2.563269
H	1.493140	3.810087	-4.541182
H	0.468489	2.412293	-4.178596

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[TS-alpha-Br-dimer] scf done: -3517.587855 / Sum of electronic and thermal Energies= -3517.057764 / Sum of electronic and thermal Enthalpies= -3517.056820 / Sum of electronic and thermal Free Energies= -3517.143429

B	1.251500	1.978074	-1.250097
B	-0.675314	2.593746	1.314436
C	-0.030496	1.409495	2.044582
C	2.129282	0.738600	-0.791992
C	3.058575	0.785643	0.270686
C	3.685873	-0.384036	0.715437
C	3.423938	-1.625550	0.138997
C	2.532501	-1.667201	-0.936171
C	1.900029	-0.516091	-1.412052
C	0.861181	1.610920	3.139926
C	1.515728	0.526246	3.718153
C	1.330147	-0.778922	3.245562
C	0.436861	-0.985438	2.193312
C	-0.248556	0.073849	1.597851
C	1.928342	3.748829	-1.573580
C	0.817987	4.757279	-1.762543
C	-0.007310	4.201857	-2.949220
C	0.971211	3.295254	-3.730443
C	1.993482	2.902266	-2.674467
Br	3.644872	2.133129	-3.282727
C	0.989388	-0.647318	-2.611562
C	4.058648	-2.886732	0.669001
C	3.438955	2.081975	0.944508
C	-1.205115	-0.240722	0.473500
C	2.103717	-1.922580	3.844100
C	1.121091	2.985697	3.713158
H	0.174112	1.785233	-1.723238
H	-1.531182	2.440916	0.498149
H	-0.368453	3.721594	1.570106
H	1.040722	2.735312	-0.306617
H	0.285110	-1.994309	1.819810
H	2.196978	0.695283	4.548987
H	2.330267	-2.620316	-1.421163
H	4.392583	-0.320867	1.540016
H	-1.175475	-1.305422	0.227514
H	-2.235778	0.013569	0.745242
H	-0.963382	0.323266	-0.428926
H	1.502776	3.679389	2.958360
H	0.208866	3.434169	4.120294
H	1.856453	2.933606	4.520855
H	2.096871	-1.882503	4.938724
H	1.698205	-2.889504	3.534332
H	3.152394	-1.883949	3.526299
H	4.129623	2.664687	0.319877
H	2.568742	2.707277	1.151354
H	3.946452	1.897213	1.894935
H	0.998229	-1.671590	-2.995549
H	-0.047969	-0.388070	-2.377596
H	1.307881	0.013505	-3.424618
H	3.349554	-3.463715	1.275849
H	4.390849	-3.543095	-0.142772

H	4.925915	-2.666312	1.298888
H	2.752766	3.917017	-0.894385
H	1.306663	5.703955	-2.028921
H	0.227403	4.928049	-0.859364
H	-0.415333	4.999385	-3.574179
H	-0.844536	3.612703	-2.572111
H	1.488757	3.853810	-4.519166
H	0.487229	2.432205	-4.192281

IX. Geometries of all computed complexes (B3LYP-D3/6-311G(d,p))

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[mesityl_borane_dimer_TZ] scf done: -751.604816 / Sum of electronic and thermal Energies= -751.189756 / Sum of electronic and thermal Enthalpies= -751.188812 / Sum of electronic and thermal Free Energies= -751.261332

B	-0.876154	2.229730	0.161905
H	-0.155394	2.246089	-0.959181
H	-1.367938	3.314014	0.213119
H	0.155402	2.246234	0.958814
B	0.876161	2.229704	-0.162270
H	1.367947	3.313980	-0.213650
C	-1.759137	0.934484	0.263799
C	-2.786352	0.760937	-0.691788
C	-1.587326	-0.053500	1.256013
C	-3.584621	-0.381952	-0.663406
C	-2.412597	-1.180139	1.261151
C	-3.411189	-1.369032	0.306889
H	-4.359894	-0.503949	-1.414056
H	-2.268959	-1.931944	2.031381
C	1.759140	0.934442	-0.263973
C	1.587330	-0.053689	-1.256042
C	2.786349	0.761032	0.691645
C	2.412597	-1.180332	-1.261010
C	3.584610	-0.381866	0.663439
C	3.411180	-1.369089	-0.306710
H	2.268962	-1.932251	-2.031128
H	4.359878	-0.503754	1.414113
C	-3.008916	1.789727	-1.773912
H	-3.150904	2.789785	-1.353827
H	-2.154022	1.848327	-2.457013
H	-3.888625	1.547447	-2.373227
C	-0.531800	0.073489	2.328737
H	0.473172	-0.026669	1.911066
H	-0.588435	1.038726	2.840539
H	-0.651882	-0.704563	3.085012
C	-4.302816	-2.583457	0.343824
H	-5.221243	-2.380004	0.906011
H	-4.599265	-2.890790	-0.662105
H	-3.805643	-3.428634	0.825395
C	3.008920	1.789983	1.773615
H	3.150895	2.789981	1.353382
H	2.154037	1.848677	2.456723
H	3.888640	1.547795	2.372950
C	0.531811	0.073153	-2.328792
H	-0.473165	-0.026941	-1.911116
H	0.588457	1.038318	-2.840730
H	0.651895	-0.705006	-3.084957
C	4.302799	-2.583527	-0.343443
H	5.221274	-2.380143	-0.905576
H	4.599164	-2.890748	0.662546
H	3.805658	-3.428753	-0.824958

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[mesityl_borane_TZ] scf done: -375.781688 / Sum of electronic and thermal Energies= -375.577898 / Sum of electronic and thermal Enthalpies= -375.576953 / Sum of electronic and thermal Free Energies= -375.622611

C	0.442088	-1.221629	0.006677
C	1.178373	0.000868	0.003379
C	0.444965	1.223329	-0.008183
C	-0.947141	1.202043	-0.015637
C	-1.661451	0.003177	-0.010634
C	-0.948334	-1.198285	-0.001448
H	-1.493291	2.139856	-0.027714
H	-1.496158	-2.135451	-0.001349

C	-3.165338	-0.000631	0.011156
H	-3.570508	-0.796048	-0.619324
H	-3.534134	-0.174669	1.028216
H	-3.573646	0.952801	-0.329510
C	1.131313	2.569332	-0.016273
H	1.769672	2.691838	-0.894366
H	0.392860	3.373096	-0.022671
H	1.767183	2.703320	0.861852
C	1.127839	-2.567900	0.015620
H	1.767188	-2.700978	-0.860206
H	1.762773	-2.691651	0.895983
H	0.389063	-3.371406	0.018125
B	2.708532	-0.000147	0.009592
H	3.329116	-1.016557	0.018424
H	3.330225	1.015613	0.006328

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[Bromopentene_TZ] scf done: -2768.957756 / Sum of electronic and thermal Energies= -2768.844994 / Sum of electronic and thermal Enthalpies= -2768.844050 / Sum of electronic and thermal Free Energies= -2768.881807

C	3.910199	1.926236	0.049343
C	3.592876	1.625354	1.538669
C	2.184075	1.081869	1.497796
C	1.837485	0.796003	0.247506
C	2.908531	1.077717	-0.772774
H	3.728298	2.984822	-0.149626
H	4.948013	1.713003	-0.210219
H	3.681723	2.514041	2.169569
H	4.273363	0.872980	1.957099
H	3.346677	0.136843	-1.125875
H	2.525649	1.603559	-1.650273
Br	0.176243	0.012365	-0.280754
H	1.576678	0.912069	2.376789

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[B1-Br_TZ] scf done: -3144.749421 / Sum of electronic and thermal Energies= -3144.429736 / Sum of electronic and thermal Enthalpies= -3144.428791 / Sum of electronic and thermal Free Energies= -3144.494816

C	-1.236458	1.436841	-1.549284
C	-0.492229	0.228841	-1.631868
C	-1.200842	-1.001205	-1.517711
C	-2.578989	-0.999403	-1.329380
C	-3.305570	0.190589	-1.242686
C	-2.616397	1.397573	-1.352959
B	1.029465	0.246187	-1.840493
C	2.128303	0.997147	0.665766
C	1.778979	-0.219492	1.086966
C	2.882563	-1.239443	1.004467
C	3.958008	-0.491746	0.176518
C	3.577122	1.011818	0.242613
Br	0.104671	-0.665591	1.873800
C	-0.495157	-2.334237	-1.592460
C	-4.796461	0.159238	-1.038975
C	-0.575716	2.790772	-1.656408
H	-3.170619	2.328467	-1.285244
H	-3.104889	-1.945393	-1.241442
H	-5.059458	-0.419719	-0.148447
H	-5.207099	1.164025	-0.923684
H	-5.298010	-0.314558	-1.889176
H	0.134690	2.959113	-0.842559
H	-0.019350	2.897879	-2.590060
H	-1.322316	3.586108	-1.615146
H	-0.004299	-2.478158	-2.558272
H	0.275184	-2.422048	-0.824312
H	-1.204381	-3.151879	-1.450343
H	1.655882	-0.762002	-1.916358
H	1.613668	1.260470	-2.053691
H	1.502440	1.877359	0.709998
H	4.171455	1.549792	0.991397
H	3.728678	1.520637	-0.712197
H	4.966473	-0.681190	0.545567

H	3.913299	-0.828871	-0.859382
H	3.229272	-1.491428	2.013142
H	2.555879	-2.170011	0.535326

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[TS-B1C1-Br_TZ] scf done: -3144.736054 / Sum of electronic and thermal Energies= -3144.416090 / Sum of electronic and thermal Enthalpies= -3144.415146 / Sum of electronic and thermal Free Energies= -3144.477946

C	0.256602	1.320619	0.091627
C	0.998789	0.121894	0.133401
C	0.283056	-1.099413	0.063598
C	-1.107262	-1.099774	-0.031239
C	-1.842680	0.086363	-0.060205
C	-1.139395	1.284885	-0.001140
B	2.585340	0.074829	0.195102
C	3.649479	0.995597	1.524661
C	3.187040	-0.246253	1.935356
C	4.318507	-1.261425	1.995053
C	5.431303	-0.594789	1.156194
C	5.126169	0.920999	1.220133
Br	1.769217	-0.424672	3.227876
C	0.997097	-2.430208	0.094540
C	-3.346625	0.060443	-0.162068
C	0.914362	2.678833	0.162246
H	-1.688462	2.221615	-0.031266
H	-1.632582	-2.049529	-0.083329
H	-3.796151	-0.439652	0.702081
H	-3.759046	1.070325	-0.215204
H	-3.675144	-0.482890	-1.053885
H	1.247913	2.913755	1.179524
H	1.786069	2.748334	-0.492504
H	0.213101	3.463579	-0.129034
H	1.681196	-2.542620	-0.751275
H	1.591531	-2.546301	1.004281
H	0.280813	-3.253722	0.060396
H	3.176800	-0.799882	-0.355869
H	3.080577	1.107136	-0.229130
H	3.158085	1.927691	1.759908
H	5.636022	1.388487	2.071168
H	5.414758	1.465426	0.320026
H	6.425848	-0.827833	1.537491
H	5.379506	-0.939374	0.124378
H	4.625687	-1.376474	3.039207
H	4.025859	-2.242028	1.620170

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[C1-Br_TZ] scf done: -3144.785634 / Sum of electronic and thermal Energies= -3144.462119 / Sum of electronic and thermal Enthalpies= -3144.461175 / Sum of electronic and thermal Free Energies= -3144.527612

C	1.225921	3.068696	-1.737194
C	1.998261	2.918768	-0.432307
C	1.401844	4.014692	0.454356
C	1.088123	5.196268	-0.485000
C	0.959896	4.579830	-1.905820
B	2.240556	1.536568	0.282624
Br	3.986754	3.391664	-0.771950
C	1.731059	0.148370	-0.191698
C	0.915322	-0.563143	0.735198
C	0.337519	-1.772841	0.368564
C	0.563082	-2.345535	-0.887237
C	1.392041	-1.667868	-1.773471
C	1.970064	-0.434900	-1.453953
C	0.628764	-0.013613	2.114298
C	-0.069017	-3.663155	-1.251018
C	2.891110	0.180630	-2.480292
H	2.720841	1.632818	1.369392
H	0.469149	3.602763	0.861963
H	1.604128	-2.109158	-2.742915
H	-0.298910	-2.290571	1.080045
H	1.551238	0.155005	2.676932
H	0.098862	0.943132	2.076344
H	0.008236	-0.707687	2.684256

H	3.651289	-0.544542	-2.786493
H	2.342523	0.466158	-3.383320
H	3.415748	1.058314	-2.109426
H	0.217826	-4.447464	-0.543602
H	-1.161417	-3.595524	-1.229402
H	0.227754	-3.986601	-2.250630
H	2.036017	4.269939	1.302498
H	1.899646	5.925617	-0.455928
H	0.179171	5.715372	-0.175829
H	1.697573	5.019636	-2.579416
H	-0.022624	4.759832	-2.346135
H	1.718667	2.617585	-2.594691
H	0.283250	2.527085	-1.590102

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[TS-C1P-Br_TZ] scf done: -3144.772698 / Sum of electronic and thermal Energies= -3144.451961 / Sum of electronic and thermal Enthalpies= -3144.451016 / Sum of electronic and thermal Free Energies= -3144.513523

C	0.812191	3.071004	-1.648385
C	1.620797	2.997982	-0.417646
C	1.785781	4.379917	0.085859
C	1.403309	5.322475	-1.067052
C	0.314598	4.519713	-1.797435
B	2.130776	1.701500	0.312004
Br	4.254224	2.034319	0.178537
C	1.653201	0.258343	-0.179328
C	0.910675	-0.549394	0.727663
C	0.433432	-1.800267	0.339228
C	0.666632	-2.317981	-0.935800
C	1.402765	-1.538599	-1.818193
C	1.893493	-0.275274	-1.465093
C	0.607701	-0.107881	2.144243
C	0.153640	-3.681285	-1.322559
C	2.679784	0.446022	-2.539504
H	1.930789	1.924566	1.475454
H	0.986084	4.419790	0.852659
H	1.611974	-1.920187	-2.814006
H	-0.130451	-2.393680	1.053331
H	1.521347	0.098770	2.707536
H	0.002175	0.802317	2.175863
H	0.058082	-0.888465	2.674983
H	3.425376	-0.224463	-2.976433
H	2.025842	0.762848	-3.359937
H	3.218317	1.311974	-2.165633
H	0.663536	-4.470089	-0.759180
H	-0.916173	-3.778383	-1.113876
H	0.309314	-3.879127	-2.385364
H	2.720533	4.565950	0.611004
H	2.269699	5.476349	-1.717681
H	1.065765	6.298910	-0.719063
H	0.178447	4.813207	-2.838379
H	-0.647092	4.633459	-1.287769
H	1.561371	2.849701	-2.430741
H	0.082332	2.262099	-1.730668

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[P-Br_TZ] scf done: -3144.833484 / Sum of electronic and thermal Energies= -3144.509050 / Sum of electronic and thermal Enthalpies= -3144.508106 / Sum of electronic and thermal Free Energies= -3144.571829

C	0.112060	2.999526	-0.793829
C	1.422352	3.063771	0.024689
C	2.285262	4.185401	-0.666466
C	1.358248	4.828079	-1.725993
C	-0.066377	4.430171	-1.313289
B	2.152641	1.709303	0.266063
Br	3.829047	1.774744	1.303483
C	1.683084	0.308837	-0.215817
C	0.937175	-0.533422	0.632340
C	0.496031	-1.766764	0.157593
C	0.782520	-2.198914	-1.139766
C	1.523565	-1.355904	-1.966872
C	1.975203	-0.110608	-1.526246

C	0.626466	-0.112514	2.048419
C	0.305240	-3.544857	-1.621109
C	2.790074	0.769361	-2.442899
H	1.173517	3.436345	1.029199
H	2.609280	4.915511	0.076450
H	1.751558	-1.671042	-2.980606
H	-0.087218	-2.406385	0.813814
H	1.510967	-0.196508	2.687961
H	0.290020	0.927897	2.098675
H	-0.157610	-0.734773	2.484048
H	3.837642	0.811173	-2.125964
H	2.771228	0.400113	-3.470009
H	2.413835	1.796922	-2.455044
H	0.809250	-4.355700	-1.084660
H	-0.769074	-3.668483	-1.455691
H	0.500614	-3.679652	-2.686821
H	3.191625	3.786259	-1.125006
H	1.577170	4.410805	-2.714006
H	1.497791	5.909299	-1.794978
H	-0.785487	4.506032	-2.132646
H	-0.418098	5.078499	-0.502547
H	0.221986	2.309640	-1.636402
H	-0.731320	2.643977	-0.197426

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[B2-Br_TZ] scf done: -3144.749566 / Sum of electronic and thermal Energies= -3144.428841 / Sum of electronic and thermal Enthalpies= -3144.427897 / Sum of electronic and thermal Free Energies= -3144.496706

C	-1.283423	0.335842	-1.613398
C	-0.806164	-0.984459	-1.374605
C	-1.735177	-1.955615	-0.912438
C	-3.068700	-1.605846	-0.704585
C	-3.532218	-0.313326	-0.946194
C	-2.623020	0.644051	-1.403038
B	0.668848	-1.343203	-1.607311
C	1.616928	-0.149412	1.070977
C	1.888948	-1.448680	0.938456
C	3.308540	-1.644003	0.464355
C	3.753521	-0.221275	0.030168
C	2.760587	0.758166	0.704781
H	1.230293	-2.258159	1.220008
C	-1.320930	-3.377360	-0.614323
C	-4.974718	0.052675	-0.719276
C	-0.365305	1.439547	-2.081922
H	-2.971869	1.655577	-1.587634
H	-3.766198	-2.356246	-0.346006
H	-5.062304	0.879836	-0.008038
H	-5.448766	0.379300	-1.650407
H	-5.545732	-0.791351	-0.328435
H	0.443134	1.612750	-1.368447
H	0.098810	1.202918	-3.042279
H	-0.916726	2.374986	-2.195194
H	-0.572786	-3.418776	0.181685
H	-2.180201	-3.969407	-0.293566
H	-0.883022	-3.864508	-1.488367
H	1.056595	-2.464087	-1.509665
H	1.447566	-0.538522	-2.007257
Br	0.007001	0.563993	1.791015
H	3.172991	1.214895	1.611760
H	2.453552	1.573605	0.046462
H	4.788277	-0.009122	0.301432
H	3.667107	-0.131410	-1.053176
H	3.921042	-2.028193	1.289290
H	3.380129	-2.367817	-0.350919

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[TS-B2C2-Br_TZ] scf done: -3144.734048 / Sum of electronic and thermal Energies= -3144.414389 / Sum of electronic and thermal Enthalpies= -3144.413445 / Sum of electronic and thermal Free Energies= -3144.475436

C	0.266061	1.249247	-0.267976
C	0.978743	0.099671	0.157502
C	0.227271	-1.055205	0.468452

C	-1.171306	-1.025368	0.430006
C	-1.870913	0.123011	0.076684
C	-1.128032	1.247462	-0.287264
B	2.572019	0.071691	0.192886
C	3.576333	0.850954	1.618336
C	3.202790	-0.487781	1.757994
C	4.450304	-1.355391	1.663406
C	5.491277	-0.438958	0.979059
C	5.057317	0.998068	1.344317
H	2.370416	-0.767598	2.384669
C	0.884495	-2.371881	0.818445
C	-3.377522	0.156077	0.056798
C	0.974516	2.487810	-0.769606
H	-1.651802	2.142755	-0.610258
H	-1.723628	-1.929158	0.672195
H	-3.767107	0.879663	0.780586
H	-3.756216	0.450694	-0.926937
H	-3.800754	-0.820455	0.301449
H	1.572452	2.971467	0.005526
H	1.648806	2.249320	-1.597755
H	0.252533	3.222374	-1.133112
H	1.094226	-2.459676	1.890166
H	0.228343	-3.205135	0.556630
H	1.828229	-2.508748	0.288491
H	3.205374	-0.587554	-0.581753
H	3.026865	1.195851	-0.024372
Br	2.664095	2.270554	2.533595
H	5.521262	1.323426	2.280855
H	5.283506	1.743288	0.581261
H	6.510606	-0.648368	1.304880
H	5.451814	-0.573562	-0.101736
H	4.770439	-1.621150	2.677051
H	4.282225	-2.281876	1.112331

[C2-Br_TZ] scf done: -3144.784665 / Sum of electronic and thermal Energies= -3144.460336 / Sum of electronic and thermal Enthalpies= -3144.459391 / Sum of electronic and thermal Free Energies= -3144.527169

C	-1.680840	0.099690	-1.966232
C	-0.929405	-0.666353	-1.025981
C	-1.646090	-1.520125	-0.145011
C	-3.036391	-1.596550	-0.220178
C	-3.768385	-0.831692	-1.125944
C	-3.069794	0.015058	-1.988236
B	0.607121	-0.513673	-1.016301
C	2.619704	0.450058	0.273856
C	1.624794	-0.709794	0.166423
C	2.612440	-1.890192	-0.065279
C	3.910447	-1.527114	0.720885
C	3.738712	-0.058381	1.177232
H	1.159161	-0.831335	1.146548
C	-0.962145	-2.394410	0.880094
C	-5.270941	-0.903727	-1.170004
C	-1.017504	1.044933	-2.942322
H	-3.625639	0.616493	-2.700933
H	-3.563487	-2.272375	0.445981
H	-5.637214	-0.929636	-2.199671
H	-5.644058	-1.788575	-0.650486
H	-5.716106	-0.024813	-0.690815
H	-0.439445	1.818857	-2.431479
H	-0.328490	0.518535	-3.607780
H	-1.767653	1.542923	-3.559716
H	-0.653546	-1.813180	1.754029
H	-1.643469	-3.171153	1.233233
H	-0.075578	-2.887734	0.481480
H	1.138348	-0.164517	-2.031021
H	2.994393	0.739745	-0.707388
Br	1.767797	2.124946	0.948617
H	3.411228	-0.014270	2.218161
H	4.649903	0.534683	1.086525

H	4.051028	-2.185075	1.580377
H	4.788025	-1.640817	0.081495
H	2.182815	-2.838438	0.259919
H	2.835723	-1.987115	-1.131774

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[TS-C2D2-Br_TZ] scf done: -3144.732482 / Sum of electronic and thermal Energies= -3144.411835 / Sum of electronic and thermal Enthalpies= -3144.410891 / Sum of electronic and thermal Free Energies= -3144.475140

C	-1.459038	0.626178	-1.731900
C	-0.732331	0.160698	-0.600592
C	-1.408749	-0.714079	0.290569
C	-2.720995	-1.111950	0.034626
C	-3.418516	-0.675158	-1.089490
C	-2.767455	0.197774	-1.958442
B	0.756754	0.612736	-0.435099
C	3.079630	0.581564	0.580719
C	1.916972	-0.240270	0.287365
C	2.586700	-1.558639	-0.206172
C	3.783124	-1.695453	0.765079
C	4.243173	-0.234894	0.977858
H	1.550722	-0.522399	1.285518
C	-0.777423	-1.225827	1.564311
C	-4.844011	-1.095460	-1.333466
C	-0.872034	1.598625	-2.732014
H	-3.296280	0.561531	-2.834238
H	-3.215869	-1.775820	0.737456
H	-5.070058	-1.140022	-2.401658
H	-5.051979	-2.075961	-0.898442
H	-5.543173	-0.382287	-0.882208
H	-0.529630	2.515492	-2.247006
H	-0.014016	1.178120	-3.262810
H	-1.622697	1.871592	-3.476639
H	-0.348799	-0.410144	2.150927
H	-1.524212	-1.723669	2.185915
H	0.011751	-1.958106	1.366481
H	1.188941	1.379872	-1.236785
H	3.180005	1.618293	0.293944
Br	0.994434	2.241589	1.557808
H	4.599583	0.019133	1.983787
H	5.070873	0.049740	0.309929
H	3.444581	-2.126688	1.710609
H	4.585982	-2.324019	0.379389
H	1.892041	-2.397253	-0.160587
H	2.928359	-1.455945	-1.240330

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[D2-Br_TZ] scf done: -3144.796347 / Sum of electronic and thermal Energies= -3144.473192 / Sum of electronic and thermal Enthalpies= -3144.472248 / Sum of electronic and thermal Free Energies= -3144.539933

C	-0.845246	0.595046	-1.494965
C	-0.716758	0.509905	-0.076311
C	-1.471378	-0.489844	0.602669
C	-2.278106	-1.361249	-0.124310
C	-2.393049	-1.285094	-1.512785
C	-1.673282	-0.294607	-2.177010
B	0.278448	1.481973	0.569944
C	2.647816	-0.473821	0.095463
C	2.159793	-1.178128	1.118624
C	1.482997	-2.446463	0.663920
C	1.882541	-2.553643	-0.830008
C	2.382875	-1.141848	-1.231067
H	2.211505	-0.877548	2.158349
C	-1.431517	-0.679048	2.097778
C	-3.267481	-2.253342	-2.262229
C	-0.139461	1.651607	-2.316318
H	-1.759915	-0.212207	-3.255427
H	-2.832559	-2.127593	0.408047
H	-2.894729	-3.277360	-2.157276
H	-4.290217	-2.242595	-1.873769
H	-3.305913	-2.016871	-3.327019
H	-0.435237	2.659866	-2.015536

H	0.946654	1.596353	-2.218106
H	-0.386505	1.534226	-3.372775
H	-1.908084	0.154562	2.618416
H	-1.959390	-1.593293	2.375510
H	-0.411528	-0.747276	2.477819
H	1.072462	2.073945	-0.070074
H	3.157930	0.477992	0.184857
Br	0.335193	2.070901	2.432961
H	3.271553	-1.177235	-1.868487
H	1.617906	-0.590727	-1.789052
H	2.696039	-3.274927	-0.941040
H	1.054807	-2.891485	-1.455426
H	1.793811	-3.319574	1.246058
H	0.397077	-2.362023	0.781665

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[Ts-D2P-Br_TZ] scf done: -3144.783139 / Sum of electronic and thermal Energies= -3144.460662 / Sum of electronic and thermal Enthalpies= -3144.459718 / Sum of electronic and thermal Free Energies= -3144.522618

C	0.808459	1.256468	-0.262292
C	1.309399	-0.038650	0.016216
C	0.375927	-1.093171	0.148278
C	-0.993953	-0.841637	0.026104
C	-1.487962	0.432484	-0.239423
C	-0.565300	1.466799	-0.387873
B	2.870772	-0.331720	0.150115
C	3.528060	0.670396	1.496583
C	3.672478	-0.663948	1.877501
C	5.115959	-1.086460	1.890584
C	5.893013	0.119240	1.305247
C	4.897242	1.306731	1.310505
H	2.913477	-1.227013	2.405365
C	0.803083	-2.521406	0.404005
C	-2.967947	0.691436	-0.358610
C	1.716707	2.451597	-0.438264
H	-0.923766	2.467110	-0.614197
H	-1.691541	-1.667536	0.127490
H	-3.349322	1.218996	0.522593
H	-3.194525	1.313454	-1.229236
H	-3.528987	-0.240703	-0.454249
H	2.024770	2.873382	0.524526
H	2.623103	2.199560	-0.988491
H	1.201150	3.245196	-0.983214
H	1.498037	-2.878618	-0.361048
H	1.299111	-2.638913	1.372802
H	-0.062701	-3.186724	0.401334
Br	3.996898	-0.113310	-1.556763
H	3.050901	-1.506335	0.381874
H	2.691774	1.261481	1.838769
H	5.078065	1.975630	2.157967
H	4.964720	1.903403	0.399933
H	6.788043	0.338221	1.889025
H	6.207292	-0.099805	0.286836
H	5.370010	-1.261288	2.942841
H	5.294552	-2.024272	1.361000

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[cloropentene_TZ] scf done: -655.035353 / Sum of electronic and thermal Energies= -654.922234 / Sum of electronic and thermal Enthalpies= -654.921290 / Sum of electronic and thermal Free Energies= -654.957721

C	3.901212	1.919168	0.046532
C	3.580748	1.621938	1.536735
C	2.174304	1.077257	1.494976
C	1.828992	0.790672	0.244581
C	2.896896	1.075167	-0.776242
H	3.725809	2.978560	-0.153718
H	4.938427	1.700657	-0.210699
H	3.668643	2.513016	2.164421
H	4.261888	0.872306	1.958869
H	3.331964	0.134884	-1.134922
H	2.509536	1.605015	-1.649631
Cl	0.308051	0.065408	-0.244414

H 1.563340 0.902812 2.370762

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[B1-Cl_TZ] scf done: -1030.827256 / Sum of electronic and thermal Energies= -1030.506184 / Sum of electronic and thermal Enthalpies= -1030.505239 / Sum of electronic and thermal Free Energies= -1030.572487

C -1.188991 1.383234 -1.188510

C -0.431253 0.183149 -1.260313

C -1.123504 -1.052966 -1.118313

C -2.499082 -1.064526 -0.911373

C -3.239211 0.117917 -0.836577

C -2.566341 1.330844 -0.977115

B 1.090078 0.215526 -1.477621

C 2.139626 0.929812 1.011174

C 1.757062 -0.280773 1.422317

C 2.841219 -1.321231 1.369610

C 3.958172 -0.591806 0.582365

C 3.599621 0.918726 0.632142

Cl 0.194053 -0.667375 2.094640

C -0.402415 -2.378546 -1.183399

C -4.727651 0.072046 -0.618059

C -0.545351 2.742612 -1.326395

H -3.130873 2.256184 -0.919583

H -3.012355 -2.015109 -0.801142

H -4.976781 -0.508898 0.275013

H -5.147203 1.072848 -0.500074

H -5.232260 -0.407057 -1.463587

H 0.179065 2.929457 -0.529070

H -0.008540 2.842650 -2.272317

H -1.299633 3.530545 -1.281674

H 0.072725 -2.531462 -2.155786

H 0.383323 -2.445183 -0.428872

H -1.098547 -3.202597 -1.015916

H 1.724423 -0.786697 -1.565859

H 1.662853 1.235426 -1.695430

H 1.526388 1.819379 1.044091

H 4.181285 1.449720 1.395639

H 3.788887 1.420683 -0.319529

H 4.948853 -0.795904 0.989732

H 3.948805 -0.930212 -0.454016

H 3.147308 -1.585818 2.388246

H 2.508499 -2.241297 0.883927

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[TS-B1C1-Cl_TZ] scf done: -1030.813642 / Sum of electronic and thermal Energies= -1030.493304 / Sum of electronic and thermal Enthalpies= -1030.492360 / Sum of electronic and thermal Free Energies= -1030.553450

C 0.255432 1.323778 0.091737

C 1.000439 0.127254 0.136943

C 0.288262 -1.096204 0.075751

C -1.102107 -1.100728 -0.020996

C -1.840474 0.083334 -0.056743

C -1.140519 1.284026 -0.001323

B 2.587370 0.084746 0.196483

C 3.641508 0.994907 1.523883

C 3.171150 -0.250529 1.922907

C 4.296836 -1.269704 1.989211

C 5.419019 -0.604070 1.163346

C 5.119657 0.913460 1.230326

Cl 1.851448 -0.417887 3.088600

C 1.007540 -2.423780 0.117656

C -3.344145 0.053014 -0.161786

C 0.911727 2.683297 0.151471

H -1.692010 2.219141 -0.035628

H -1.624871 -2.052143 -0.068527

H -3.794230 -0.448348 0.701313

H -3.759390 1.061684 -0.216063

H -3.669082 -0.491273 -1.054356

H 1.281388 2.910351 1.157688

H 1.760343 2.759429 -0.532793

H 0.199492 3.468703 -0.109616

H 1.700102 -2.535677 -0.721350

H	1.593790	-2.533139	1.033627
H	0.295602	-3.250865	0.079674
H	3.185805	-0.767650	-0.381733
H	3.074999	1.132459	-0.202983
H	3.152973	1.924167	1.777376
H	5.625209	1.374860	2.087074
H	5.419181	1.459369	0.334681
H	6.409534	-0.841728	1.552146
H	5.375792	-0.944456	0.129741
H	4.592013	-1.388237	3.036730
H	4.003608	-2.247620	1.607813

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[C1-Cl_TZ] scf done: -1030.860642 / Sum of electronic and thermal Energies= -1030.538378 / Sum of electronic and thermal Enthalpies= -1030.537434 / Sum of electronic and thermal Free Energies= -1030.601345

C	-1.461933	1.278044	-1.097826
C	-0.683766	0.118905	-0.907898
C	-1.334018	-1.120503	-0.718463
C	-2.724691	-1.172742	-0.716459
C	-3.506005	-0.025338	-0.881918
C	-2.855513	1.191218	-1.072138
B	0.859273	0.244246	-0.950832
C	2.789811	1.284882	0.416388
C	1.891182	0.045661	0.214064
C	2.930957	-1.064943	-0.034025
C	4.131316	-0.730712	0.883219
C	4.007594	0.777915	1.217569
Cl	1.056820	-0.294823	1.853530
C	-0.537445	-2.392640	-0.557548
C	-5.010011	-0.113577	-0.858645
C	-0.797166	2.622482	-1.267895
H	-3.443285	2.094102	-1.207587
H	-3.215018	-2.132999	-0.585030
H	-5.367997	-0.486061	0.106510
H	-5.468794	0.862404	-1.029860
H	-5.380323	-0.799919	-1.626686
H	-0.435066	3.009355	-0.309307
H	0.065603	2.562642	-1.940064
H	-1.489846	3.360910	-1.676826
H	0.191614	-2.517381	-1.364852
H	0.008827	-2.396350	0.389204
H	-1.189413	-3.268391	-0.568039
H	1.389064	0.578268	-1.972693
H	3.105170	1.623197	-0.575995
H	2.264115	2.109991	0.897520
H	3.836602	0.917832	2.285775
H	4.907173	1.338438	0.955680
H	4.089108	-1.329018	1.794246
H	5.073177	-0.966681	0.384240
H	2.522214	-2.060869	0.131507
H	3.229764	-1.002435	-1.085799

36

[TS-C1P-Cl_TZ) scf done: -1030.849322 / Sum of electronic and thermal Energies= -1030.528588 / Sum of electronic and thermal Enthalpies= -1030.527644 / Sum of electronic and thermal Free Energies= -1030.590064

C	0.749505	3.006271	-1.533760
C	1.660916	2.959245	-0.378178
C	1.781368	4.327314	0.156356
C	1.238430	5.279842	-0.922681
C	0.156097	4.424997	-1.603030
B	2.364646	1.675289	0.231897
Cl	4.214487	2.127231	-0.270398
C	1.806468	0.250198	-0.248307
C	0.935391	-0.443663	0.635011
C	0.364830	-1.662496	0.265046
C	0.617794	-2.248771	-0.974015
C	1.461208	-1.567937	-1.844269
C	2.052012	-0.343848	-1.508457
C	0.571635	0.096891	2.002840
C	0.008147	-3.576913	-1.343327

C	2.968197	0.258719	-2.551446
H	2.359415	1.823523	1.424142
H	1.053014	4.277843	0.992739
H	1.670665	-1.997915	-2.819497
H	-0.296868	-2.167827	0.962955
H	1.452571	0.222868	2.636920
H	0.080760	1.073247	1.947427
H	-0.113700	-0.585618	2.510150
H	4.013613	0.013153	-2.344815
H	2.724254	-0.135571	-3.541200
H	2.918333	1.344556	-2.598788
H	0.461634	-4.391684	-0.768492
H	-1.066096	-3.596019	-1.136414
H	0.152179	-3.800609	-2.402733
H	2.743632	4.554811	0.612895
H	2.037748	5.522037	-1.629350
H	0.859047	6.214777	-0.509887
H	-0.070152	4.738688	-2.622091
H	-0.774134	4.461062	-1.027852
H	1.439698	2.835751	-2.381726
H	0.063529	2.156699	-1.569026

36

[P-Cl_TZ] scf done: -1030.916203 / Sum of electronic and thermal Energies= -1030.591092 / Sum of electronic and thermal Enthalpies= -1030.590148 / Sum of electronic and thermal Free Energies= -1030.653737

C	-1.375293	1.326243	-0.408817
C	-0.834552	0.021294	-0.382332
C	-1.705956	-1.084102	-0.391282
C	-3.086376	-0.871691	-0.415361
C	-3.631442	0.409841	-0.454319
C	-2.756359	1.499062	-0.456475
B	0.710759	-0.151450	-0.313283
C	1.584237	0.178385	0.934787
C	1.902068	-1.151366	1.703049
C	3.211341	-0.841088	2.439917
C	4.016765	-0.057465	1.398259
C	2.975986	0.852171	0.707356
H	1.084292	-1.442596	2.364978
C	-1.178177	-2.499532	-0.378123
C	-5.122263	0.626178	-0.491787
C	-0.470968	2.537243	-0.404154
H	-3.161360	2.506135	-0.493178
H	-3.750713	-1.730473	-0.406863
H	-5.464966	1.175586	0.390916
H	-5.414414	1.211245	-1.369282
H	-5.661726	-0.322396	-0.526308
H	0.018953	2.668417	0.565863
H	0.318145	2.461420	-1.158754
H	-1.035628	3.448190	-0.611526
H	-0.847320	-2.806562	-1.375038
H	-0.324482	-2.614106	0.294619
H	-1.950424	-3.200931	-0.055617
Cl	1.542394	-0.837299	-1.758699
H	2.072805	-1.975277	1.002742
H	0.995203	0.798704	1.615852
H	2.970074	1.846199	1.161496
H	3.206859	0.985867	-0.350557
H	4.845732	0.507491	1.831209
H	4.441781	-0.755208	0.669491
H	3.004835	-0.211020	3.312526
H	3.721140	-1.741800	2.791421

36

[B2-Cl_TZ] scf done: -1030.827344 / Sum of electronic and thermal Energies= -1030.506238 / Sum of electronic and thermal Enthalpies= -1030.505294 / Sum of electronic and thermal Free Energies= -1030.573278

C	-1.104873	0.650809	-1.307569
C	-0.629043	-0.673483	-1.089506
C	-1.559274	-1.650928	-0.643786
C	-2.892516	-1.302865	-0.429952
C	-3.354340	-0.005804	-0.649160

C	-2.444112	0.957543	-1.091163
B	0.847585	-1.028731	-1.324478
C	1.741362	0.174824	1.325056
C	2.014920	-1.126021	1.208847
C	3.444914	-1.325271	0.771962
C	3.902016	0.094866	0.339355
C	2.891285	1.079485	0.977571
H	1.346698	-1.929221	1.485579
C	-1.147425	-3.079023	-0.373140
C	-4.795990	0.358738	-0.414479
C	-0.185908	1.760178	-1.760760
H	-2.791677	1.972401	-1.259090
H	-3.591035	-2.058347	-0.084248
H	-4.881229	1.171712	0.313186
H	-5.269791	0.704652	-1.338727
H	-5.368604	-0.491688	-0.040166
H	0.629690	1.915204	-1.051473
H	0.268603	1.540855	-2.729954
H	-0.734362	2.699911	-1.850573
H	-0.398203	-3.138150	0.420792
H	-2.007599	-3.675526	-0.063173
H	-0.711819	-3.550041	-1.257157
H	1.235959	-2.150384	-1.239481
H	1.623502	-0.220791	-1.723357
Cl	0.249838	0.839487	1.938773
H	3.278598	1.547017	1.890214
H	2.596398	1.886538	0.303216
H	4.928827	0.308592	0.637861
H	3.847211	0.175975	-0.746724
H	4.037574	-1.704544	1.613427
H	3.536754	-2.053772	-0.037056

36

[TS-B2C2-Cl_TZ] scf done: -1030.812510 / Sum of electronic and thermal Energies= -1030.492480 / Sum of electronic and thermal Enthalpies= -1030.491536 / Sum of electronic and thermal Free Energies= -1030.552364

C	0.264431	1.252824	-0.252954
C	0.976930	0.098684	0.158789
C	0.225907	-1.058795	0.461804
C	-1.172418	-1.030416	0.420090
C	-1.872297	0.120307	0.074209
C	-1.129938	1.249661	-0.274896
B	2.570088	0.059813	0.190922
C	3.576454	0.865666	1.599041
C	3.195561	-0.470673	1.759852
C	4.441063	-1.342585	1.683744
C	5.486499	-0.440160	0.986363
C	5.057716	1.003018	1.329061
H	2.364944	-0.728455	2.399003
C	0.886312	-2.374004	0.810218
C	-3.378918	0.150870	0.047712
C	0.972773	2.499822	-0.734031
H	-1.654126	2.148166	-0.588209
H	-1.724422	-1.936467	0.654307
H	-3.773173	0.873983	0.769369
H	-3.753669	0.444341	-0.937911
H	-3.801482	-0.826398	0.290559
H	1.560130	2.977686	0.052667
H	1.656676	2.273240	-1.557581
H	0.251406	3.234949	-1.097595
H	1.116295	-2.451440	1.878531
H	0.224427	-3.208552	0.567925
H	1.820548	-2.516429	0.264786
H	3.197232	-0.608175	-0.580972
H	3.032307	1.180930	-0.035822
Cl	2.739059	2.187166	2.398744
H	5.514784	1.339962	2.265345
H	5.289971	1.737685	0.557638
H	6.504824	-0.649281	1.315352
H	5.446893	-0.590980	-0.092406

H	4.759334	-1.592874	2.701889
H	4.272950	-2.277574	1.147274

36

[C2-Cl_TZ] scf done: -1030.861560 / Sum of electronic and thermal Energies= -1030.536876 / Sum of electronic and thermal Enthalpies= -1030.535932 / Sum of electronic and thermal Free Energies= -1030.601041

C	-1.600038	0.784710	-1.450543
C	-0.787438	-0.183064	-0.789842
C	-1.436736	-1.281942	-0.169213
C	-2.826705	-1.391646	-0.216924
C	-3.619994	-0.432046	-0.841649
C	-2.985003	0.653076	-1.449927
B	0.742024	0.030365	-0.770066
C	2.672146	0.803878	0.743401
C	1.779328	-0.375753	0.339562
C	2.858131	-1.384087	-0.147383
C	4.131599	-1.104936	0.711426
C	3.830490	0.180114	1.515432
H	1.325411	-0.761975	1.255242
C	-0.678334	-2.384168	0.533793
C	-5.119761	-0.557449	-0.873025
C	-1.003848	1.996034	-2.130610
H	-3.588138	1.410808	-1.941119
H	-3.303895	-2.250291	0.245084
H	-5.595712	0.302122	-0.390812
H	-5.489934	-0.593905	-1.902389
H	-5.456657	-1.460566	-0.360716
H	-0.455601	2.628153	-1.427148
H	-0.302153	1.710627	-2.918481
H	-1.789095	2.605181	-2.582160
H	-0.389411	-2.085529	1.546021
H	-1.302098	-3.275615	0.626339
H	0.228712	-2.670136	0.001226
H	1.237715	0.626635	-1.683330
H	3.024988	1.344417	-0.135200
Cl	1.767283	2.070019	1.714684
H	3.492731	-0.064550	2.525299
H	4.685803	0.852240	1.599912
H	4.352848	-1.939015	1.379588
H	5.002388	-0.969986	0.066819
H	2.510727	-2.413270	-0.049284
H	3.077019	-1.218465	-1.206144

36

[TS-C2D2-Cl_TZ] scf done: -1030.804655 / Sum of electronic and thermal Energies= -1030.483573 / Sum of electronic and thermal Enthalpies= -1030.482629 / Sum of electronic and thermal Free Energies= -1030.545730

C	-1.462532	0.615555	-1.738408
C	-0.736835	0.156544	-0.604125
C	-1.416705	-0.703205	0.299031
C	-2.734650	-1.088572	0.053936
C	-3.432583	-0.657022	-1.072134
C	-2.776211	0.197544	-1.954791
B	0.756428	0.596255	-0.451622
C	3.051403	0.582639	0.589964
C	1.922093	-0.263688	0.242560
C	2.646371	-1.545539	-0.265249
C	3.807587	-1.678518	0.751593
C	4.210823	-0.212420	1.041814
H	1.547437	-0.583412	1.226546
C	-0.782314	-1.214796	1.571699
C	-4.863413	-1.065660	-1.304561
C	-0.868054	1.564233	-2.757183
H	-3.304433	0.554751	-2.833565
H	-3.233057	-1.739849	0.765946
H	-5.101724	-1.097304	-2.370461
H	-5.072774	-2.049431	-0.877526
H	-5.552772	-0.353251	-0.837369
H	-0.523127	2.489889	-2.291047
H	-0.010720	1.128754	-3.276920
H	-1.615359	1.823978	-3.509865

H	-0.327566	-0.404714	2.145483
H	-1.533341	-1.689684	2.206138
H	-0.013746	-1.968431	1.371350
H	1.174322	1.399144	-1.225162
H	3.150441	1.616522	0.292166
Cl	1.042561	2.058753	1.524562
H	4.475854	0.014659	2.081980
H	5.078777	0.117448	0.452670
H	3.446242	-2.160282	1.663272
H	4.647320	-2.263047	0.375391
H	1.975474	-2.404519	-0.270124
H	3.025143	-1.404434	-1.281582

36

[D2-Cl_TZ] scf done: -1030.880280 / Sum of electronic and thermal Energies= -1030.557240 / Sum of electronic and thermal Enthalpies= -1030.556296 / Sum of electronic and thermal Free Energies= -1030.624547

C	-0.715501	0.734764	-1.330043
C	-0.579010	0.737611	0.090824
C	-1.433208	-0.111727	0.843726
C	-2.357276	-0.925776	0.186539
C	-2.494742	-0.922691	-1.198526
C	-1.665684	-0.077614	-1.939164
B	0.508073	1.655570	0.678758
C	2.969111	-0.086974	0.839403
C	2.149803	-0.885077	1.527215
C	1.636697	-2.031900	0.693507
C	2.073637	-1.652778	-0.745538
C	3.162489	-0.560962	-0.579894
H	1.909038	-0.765139	2.576788
C	-1.383719	-0.211406	2.348190
C	-3.511347	-1.794812	-1.884127
C	0.142438	1.596439	-2.230285
H	-1.759567	-0.060021	-3.020449
H	-2.988029	-1.582615	0.776583
H	-3.054436	-2.374642	-2.691304
H	-3.976957	-2.491544	-1.184711
H	-4.305044	-1.188513	-2.332983
H	0.061321	2.657446	-1.984097
H	1.199565	1.330508	-2.156674
H	-0.160785	1.471491	-3.271274
H	-1.793710	0.683841	2.821753
H	-1.970436	-1.067199	2.687226
H	-0.366474	-0.328259	2.722038
H	1.367796	2.111174	0.010091
H	3.485130	0.773560	1.248486
Cl	0.502937	2.341869	2.334265
H	4.174196	-0.967559	-0.705544
H	3.061607	0.246847	-1.310785
H	2.430584	-2.513673	-1.313050
H	1.218727	-1.238130	-1.280792
H	2.090147	-2.974206	1.027149
H	0.553730	-2.159091	0.775236

36

[TS-D2P-Cl_TZ] scf done: -1030.863450 / Sum of electronic and thermal Energies= -1030.540629 / Sum of electronic and thermal Enthalpies= -1030.539685 / Sum of electronic and thermal Free Energies= -1030.600997

C	0.819556	1.250822	-0.278511
C	1.312570	-0.043672	0.015644
C	0.374535	-1.091610	0.157687
C	-0.994148	-0.834176	0.029640
C	-1.480972	0.439275	-0.250602
C	-0.552621	1.467388	-0.409077
B	2.877208	-0.330413	0.156621
C	3.506517	0.644036	1.527638
C	3.685567	-0.700562	1.863301
C	5.139658	-1.089450	1.843983
C	5.880869	0.149371	1.281600
C	4.858597	1.313817	1.331093
H	2.953069	-1.287844	2.401986
C	0.793612	-2.519277	0.429895

C	-2.959539	0.704873	-0.373883
C	1.738301	2.436356	-0.463751
H	-0.905418	2.467176	-0.646226
H	-1.696174	-1.655371	0.138635
H	-3.340434	1.236510	0.505109
H	-3.181448	1.325573	-1.246618
H	-3.524783	-0.224877	-0.468115
H	2.096315	2.825924	0.494982
H	2.615999	2.184007	-1.058712
H	1.213012	3.252012	-0.964956
H	1.499877	-2.882630	-0.321738
H	1.273322	-2.632774	1.407489
H	-0.073819	-3.182381	0.417672
Cl	3.940768	-0.092471	-1.378404
H	3.041815	-1.509907	0.407340
H	2.665078	1.206134	1.905049
H	5.042476	1.969911	2.187758
H	4.895997	1.929655	0.431486
H	6.777180	0.373273	1.861603
H	6.189390	-0.035076	0.254774
H	5.413000	-1.285836	2.887377
H	5.332070	-2.007705	1.286063

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