Experimental Details

$TMSN_3$ was purchased from TCI and used without further purification. Chloroborole (**1**)[1] and $[PPh_4]N_3$[2] and were prepared according to published methods.

All manipulations were performed either under an atmosphere of dry argon or *in vacuo* using standard Schlenk, high vacuum line or glovebox techniques. Deuterated solvents were dried over molecular sieves and degassed by three freeze-pump-thaw cycles prior to use. All other solvents were distilled and degassed from appropriate drying agents. All solvents were stored under argon over activated 3 or 4 Å molecular sieves. Liquid-phase NMR spectra were acquired on a Bruker Avance 400 MHz NMR spectrometer (^{1}H: 400.1 MHz, ^{11}B: 128.4 MHz, ^{13}C: 100.7 MHz, ^{31}P 162.0 MHz). VT-NMR spectra were acquired on a Bruker Neo 400 MHz (^{1}H: 400.1 MHz, ^{11}B: 128.4 MHz, ^{13}C: 100.7 MHz, ^{31}P 162.0 MHz, ^{14}N: 28.9 MHz). Chemical shifts (δ) are reported in ppm and internally referenced to the solvent signal (^{13}C NMR) or the residual protic signal (^{1}H NMR) of the deuterated solvent. ^{11}B chemical shifts were externally referenced to $[BF_3{\cdot}OEt_2]$ and ^{14}N NMR spectra were externally referenced to $MeNO_2$. ^{1}H and ^{13}C signals were assigned based on data from DEPT-135, HSQC, HMBC and COSY experiments. C_B denotes carbon atoms attached to boron within the borole ring; C_q denotes quaternary carbon atoms.

Photolysis reactions were performed under a mercury vapor lamp (current: 19 A, voltage: 26 V). IR spectra were acquired in the argon atmosphere of a glovebox on a Bruker Alpha spectrometer equipped with a diamond-ATR module.

Caution! All manipulations requiring the isolation of bulk (*ca 50-300 mg)* of azide-containing materials were performed using custom-made stainless-steel/FEP reaction vessels, which do not produce shrapnel in the event of a detonation, as a precaution against the potential formation of unforeseen explosive azide-containing side-products. Although the reaction of tetraphenylphosphonium azide with dichloromethane is much slower, if occurring at all, than the borole/azide complexation reactions performed herein, the use of large excesses of azide salts could potentially lead to the formation of dangerous amounts of azidomethanes.[3]

<u>Generation of azidoborole 2</u>

In a typical experiment, a dichloromethane (0.3 mL) solution of $TMSN_3$ (8.6 mg, 0.070 mmol) was added via gas phase diffusion to a solution of **1** (30 mg, 0.070 mmol) in dichloromethane (0.4 mL) at *ca* -78 °C under nitrogen in a J.Y.-type NMR tube. The sample was analyzed by multinuclear NMR spectroscopy at temperatures between -75 °C and 25 °C. At low temperatures, even chloroborole could not be detected by ^{11}B NMR spectroscopy, even though it was still in solution. This is presumably due to efficient quadrupolar relaxation and to the higher viscosity of the solution at those temperatures. Although the bulk of $TMSN_3$ was converted to TMSCl rather quickly at -75 °C (as assessed by ^{1}H NMR spectroscopy), the putative azidoborole **2** could not be directly observed by ^{11}B NMR spectroscopy. The aromatic region of the ^{1}H NMR spectrum was poorly defined, and ^{14}N NMR spectroscopy indicated the evolution of small amounts of dinitrogen (*ca* -70 ppm) even at -75 °C. Warming up the solution accelerated the dinitrogen evolution. At room temperature, two broad main signals could be observed by ^{11}B NMR spectroscopy (10.3 and 36.7 ppm) and the ^{1}H NMR spectrum was rather complex in the aromatic region, featuring a broad "continuum" of peaks between 6.5 and 7.5 ppm. Drying the mixture *in vacuo* yielded an orange-red solid which has never formed crystalline materials despite our best efforts.

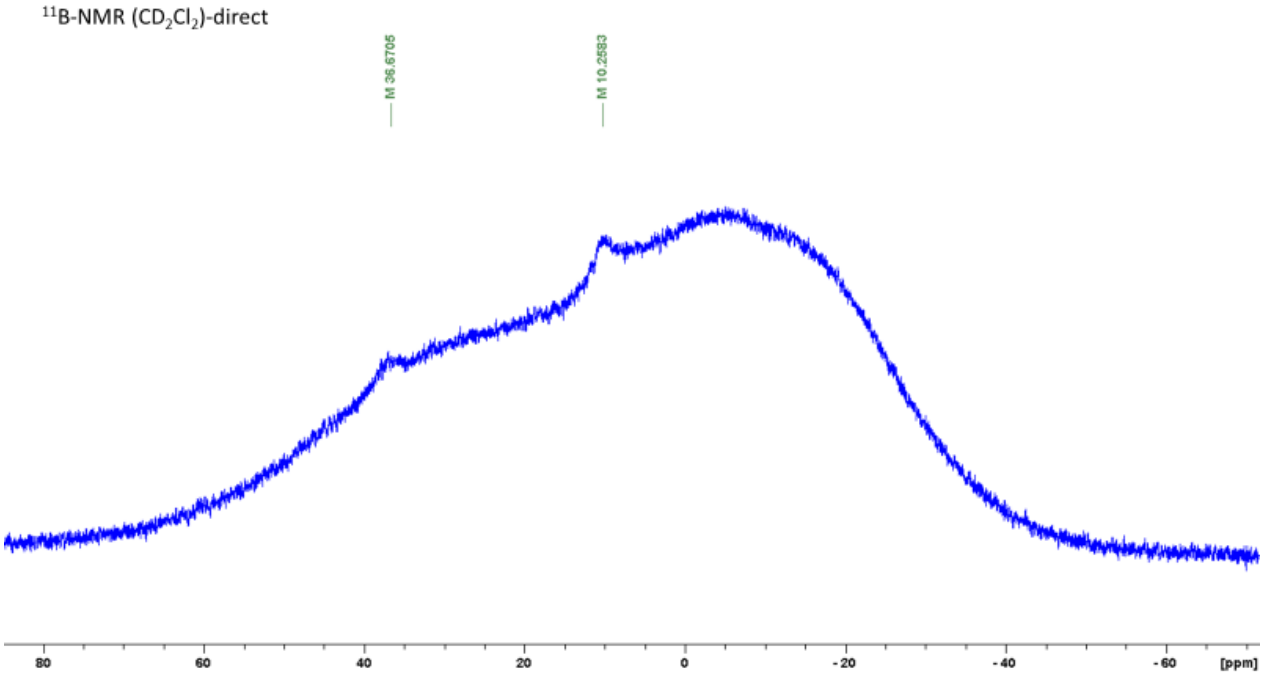


Figure S1 : ^{11}B NMR spectrum in CD_2Cl_2 of the resulting material obtained by treatment of **1** with trimethylsilyl azide at low temperature with subsequent warming to room temperature.

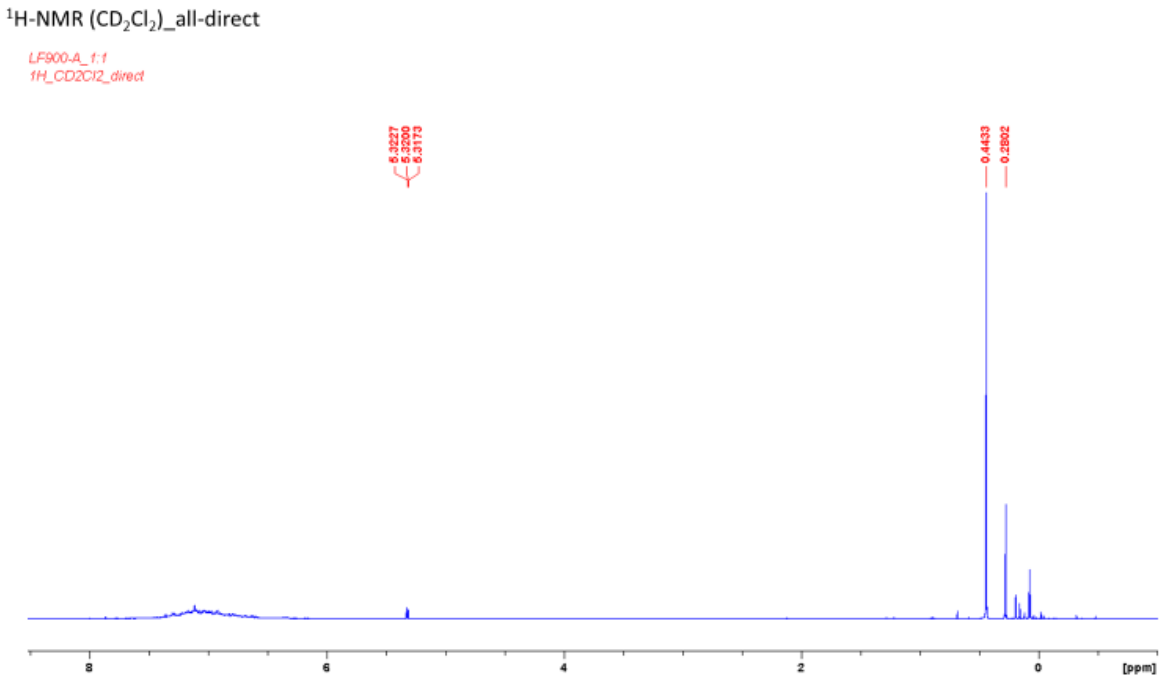


Figure S2 : ^{1}H NMR spectrum in CD_2Cl_2 of the resulting material obtained by treatment of **1** with trimethylsilyl azide at low temperature with subsequent warming to room temperature.

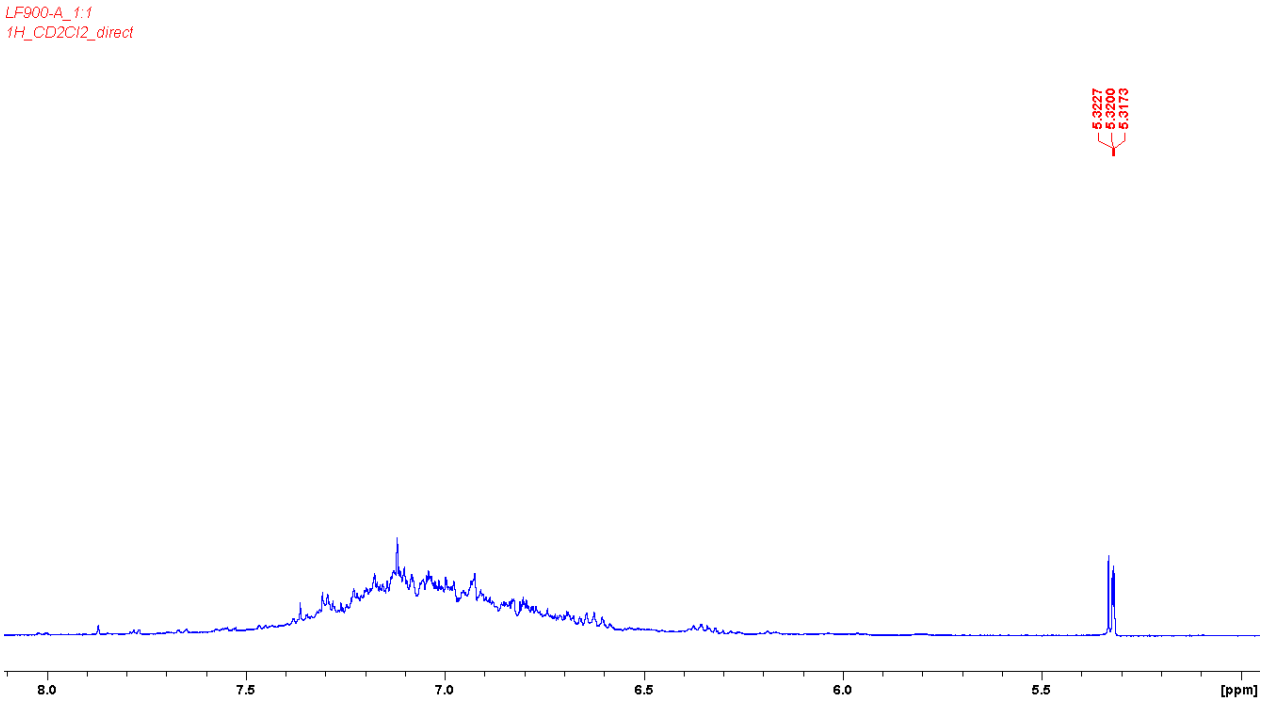


Figure S3 : Aromatic region of the ^{1}H NMR spectrum in CD_2Cl_2 of the material obtained by treatment of **1** with trimethylsilyl azide at low temperature with subsequent warming up to room temperature.

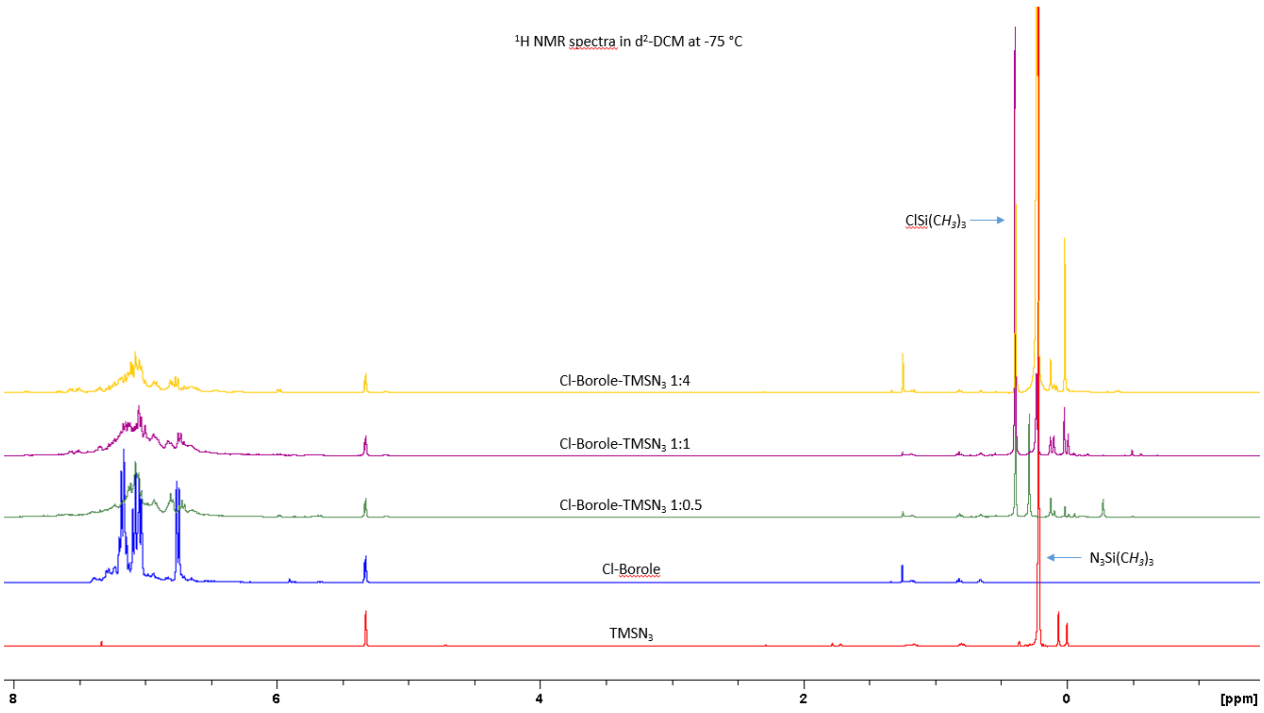


Figure S4 : ^{1}H NMR spectrum at -75 °C in CD_2Cl_2 of the reaction between **1** and trimethylsilyl azide, showing the consumption of $TMSN_3$ and **1** and the formation of TMSCl.

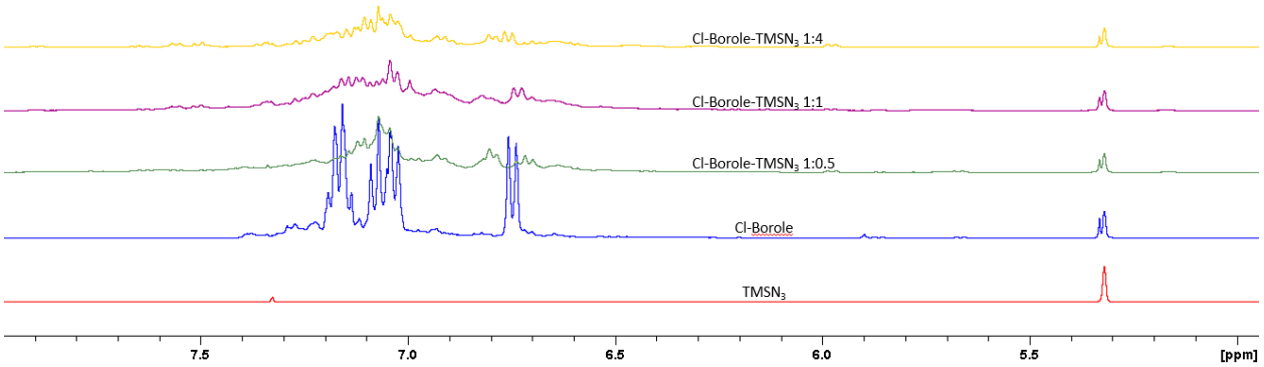


Figure S5 : Aromatic region of ^{1}H NMR spectra of Cl-Borole and $TMSN_3$ in different ratios at -75 °C.

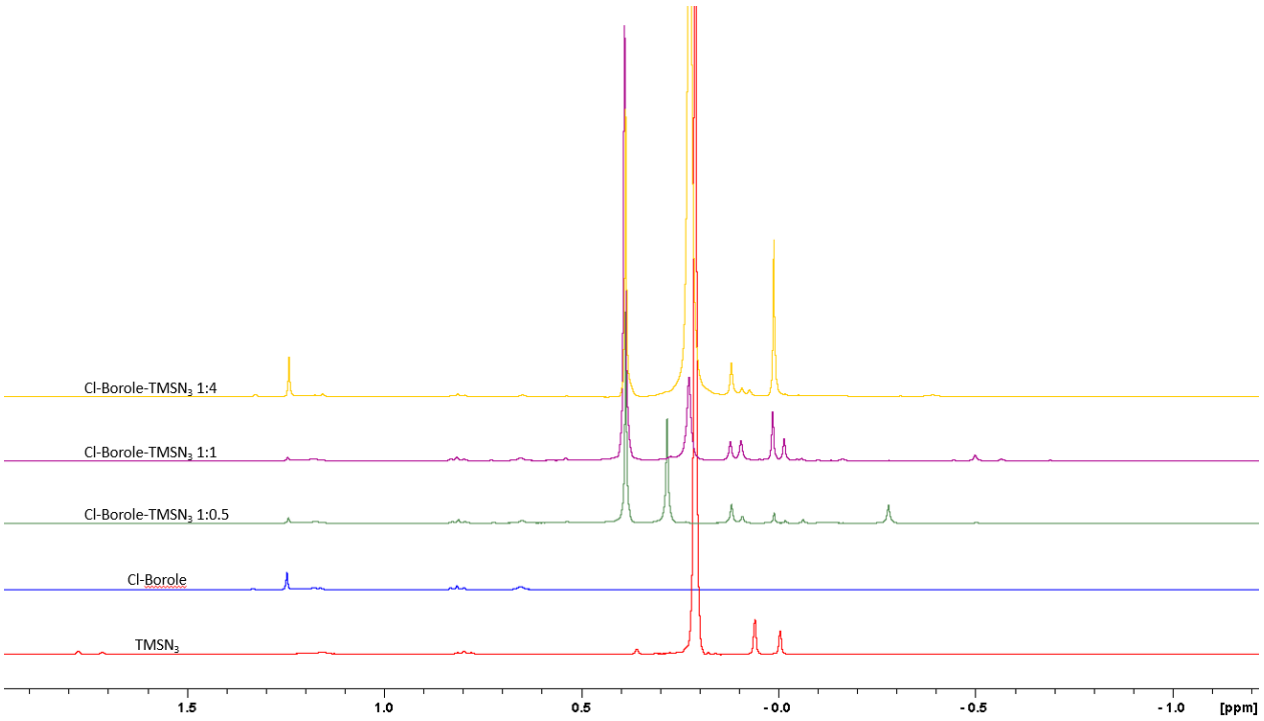


Figure S6 : Aliphatic region of ^{1}H NMR spectra of Cl-Borole and $TMSN_3$ in different ratios at -75 °C.

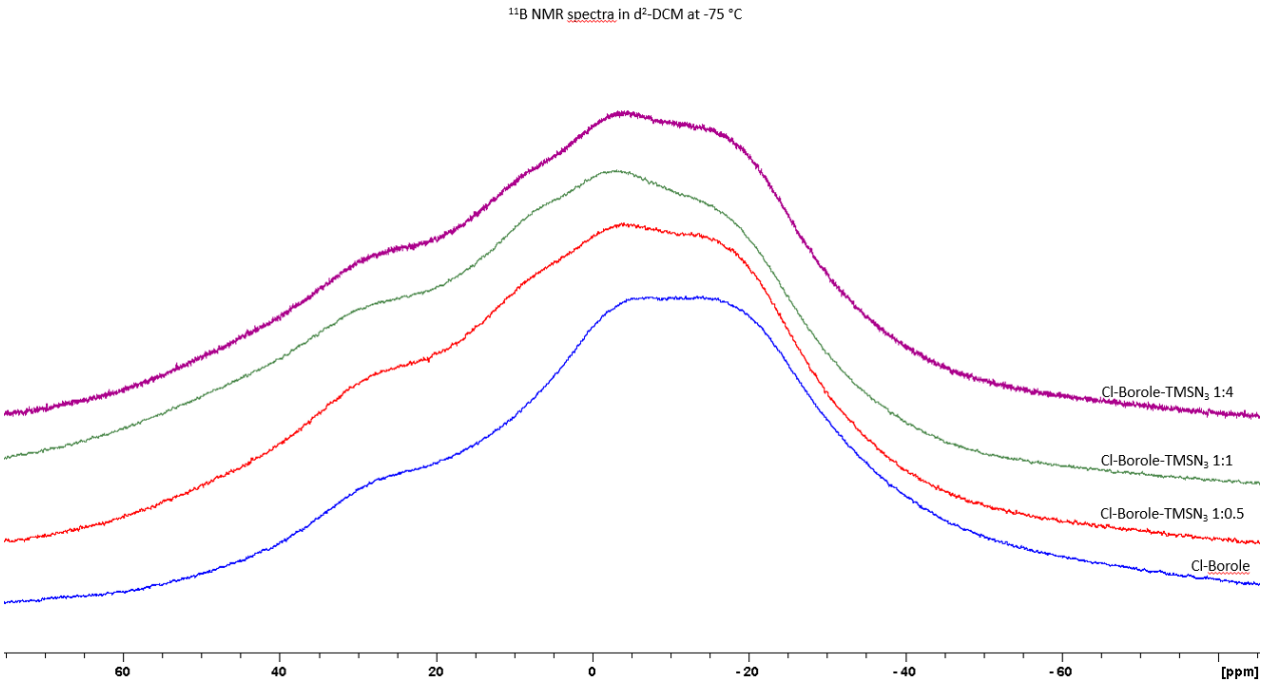


Figure S7 : ^{11}B NMR spectra of the reaction of **1** and $TMSN_3$ in different ratios at -75 °C, hardly showing any unambiguous signal.

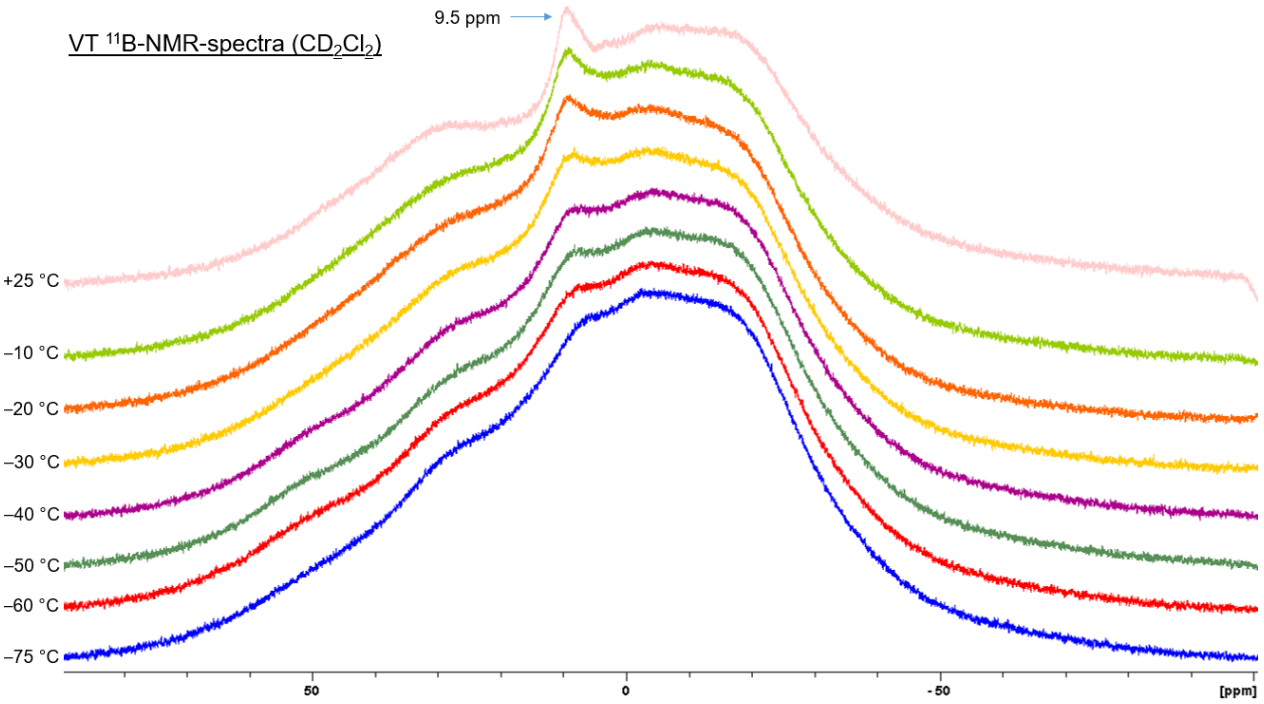


Figure S8 : Variable-temperature ^{11}B NMR spectrum in CD_2Cl_2 of the reaction between **1** and trimethylsilyl azide.

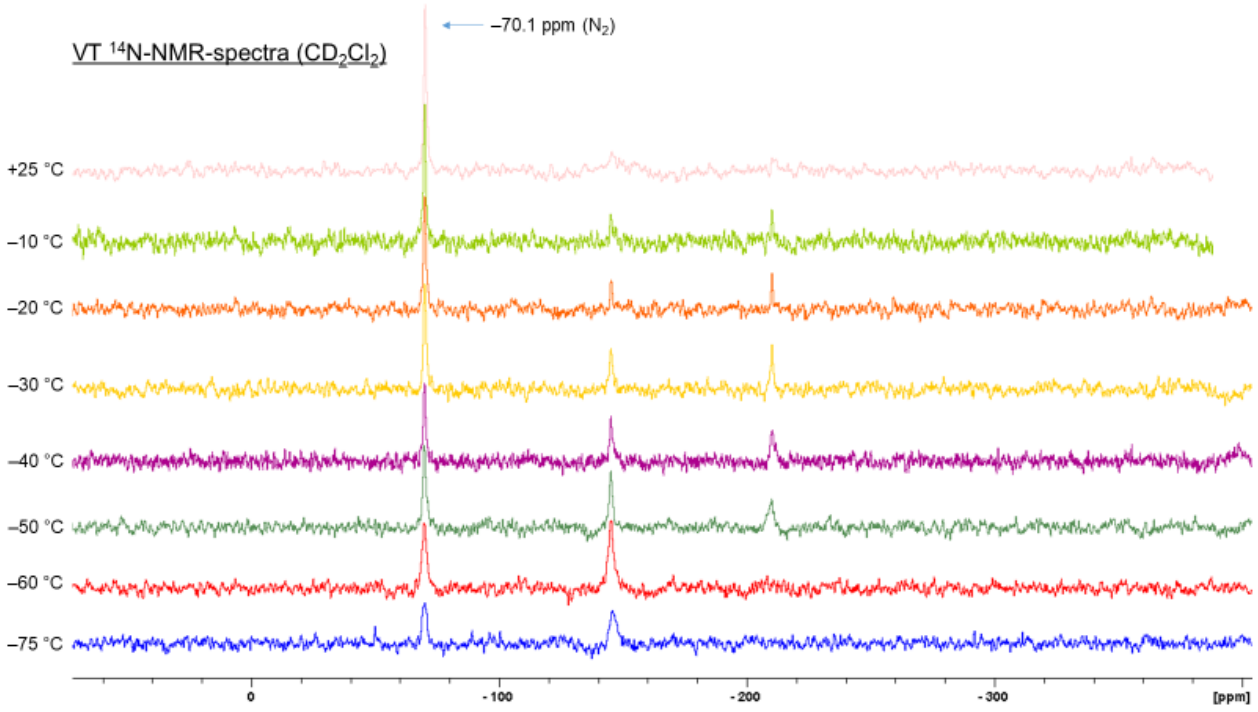
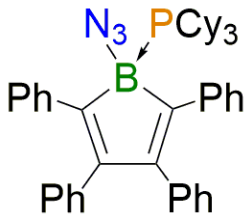


Figure S9 : Variable-temperature ^{14}N NMR spectrum in CD_2Cl_2 of the reaction between **1** and trimethylsilyl azide. Signals at *ca* -145 and -205 ppm belong to residual $TMSN_3$.

Synthesis of Azidoborole·PCy_3 3a



$C_{46}H_{53}BN_3P$ (689.730 $gmol^{-1}$)

1 (95.0 mg; 0.24 mmol) was dissolved in CH_2Cl_2 (1 mL) at –78 °C and trimethylsilyl azide (40.7 mg; 0.35 mmol) in CH_2Cl_2 (1 mL) was added dropwise. A color change from deep purple to

deep red was observed. The reaction mixture was stirred for 1 h at –78 °C and subsequently 72.8 mg (0.26 mmol) tricyclohexylphosphine in CH_2Cl_2 (1 mL) was added dropwise. The color changed to bright yellow and precipitation was monitored. After warming to room temperature, all volatiles were removed *in vacuo*. The remaining yellow solid was washed with pentane (8 x 8 mL) and dried whereupon **3a** was isolated in 72% (119 mg, 0.17 mmol) yield. Single crystals suitable for X-ray diffraction were grown via gas-phase diffusion of pentane into a saturated solution of **3a** in CH_2Cl_2 (see Crystal Structure Determinations).

^{1}H NMR (CD_2Cl_2): δ = 7.31–7.19 (m, 4H, C*H*, C_6H_5), 7.19–7.06 (m, 4H, C*H*, C_6H_5), 7.06–6.83 (m, 12H, C*H*, C_6H_5), 2.00–1.83 (m, 6H, CH_2, C_6H_{11}), 1.78–1.67 (m, 9H (3H, C*H*, 6H CH_2), C_6H_{11}), 1.67–1.60 (m, 4H, CH_2, C_6H_{11}), 1.60–1.47 (m, 6H, CH_2, C_6H_{11}), 1.25–1.19 (m, 2H, CH_2, C_6H_{11}), 0.98–0.71 (m, 6H, CH_2, C_6H_{11}) ppm.

^{11}B NMR (CD_2Cl_2): δ = –1.8 (broad) ppm.

^{13}C{^{1}H} NMR (CD_2Cl_2): δ = 153.7 (d, $^2J_{P–C}$ = 9.4 Hz, C_q, $2C_B$), 143.3 (C_q, 4C), 140.3 (C_q, $2C_q$), 130.4 (*C*H, 4C), 129.3 (*C*H, 4C), 127.9 (*C*H, 4C), 127.5 (*C*H, 4C), 125.9 (*C*H, 2C), 125.1 (*C*H, 2C), 32.4 (d, $^1J_{P–C}$ = 25.9 Hz, *C*H, 3C, P(C_6H_{11})$_3$), 29.1 (d, $^2J_{P–C}$ = 3.1 Hz, *C*H$_2$, 6C, P(C_6H_{11})$_3$), 27.8 (d, $^3J_{P–C}$ = 10.3 Hz, *C*H, 6C, P(C_6H_{11})$_3$), 26.7 (*C*H, 3C, P(C_6H_{11})$_3$) ppm.

Comment: The number of C_q, CH and CH_2 atoms were deduced from a combination of ^{13}C, ^{1}H HSQC and ^{13}C, ^{1}H HMBC NMR spectroscopy.

^{31}P{^{1}H} NMR (CD_2Cl_2): δ = 0.5 (bm) ppm.

HRMS-ASAP: $[M–N_2]+H^+$ 661.410, 662.407, 663.410, 664.414, 665.417 (calculated: 661.412, 662.408, 663.412, 664.415, 665.418).

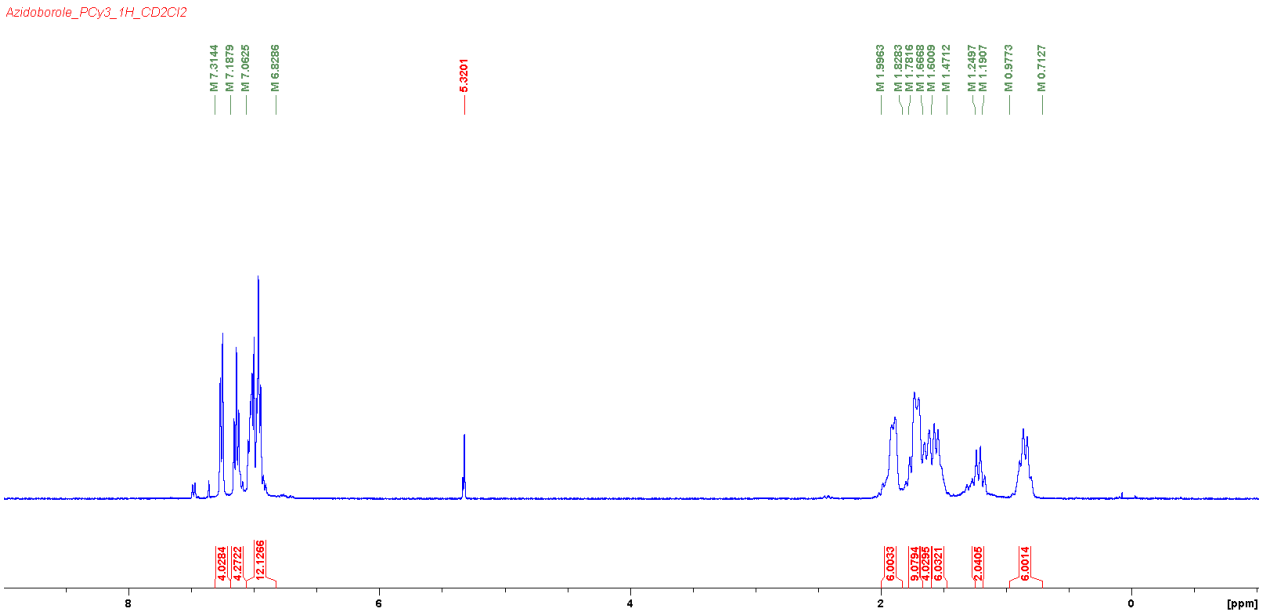


Figure S10 : ^{1}H NMR spectrum in CD_2Cl_2 of compound azidoborole·PCy_3 (**3a**).

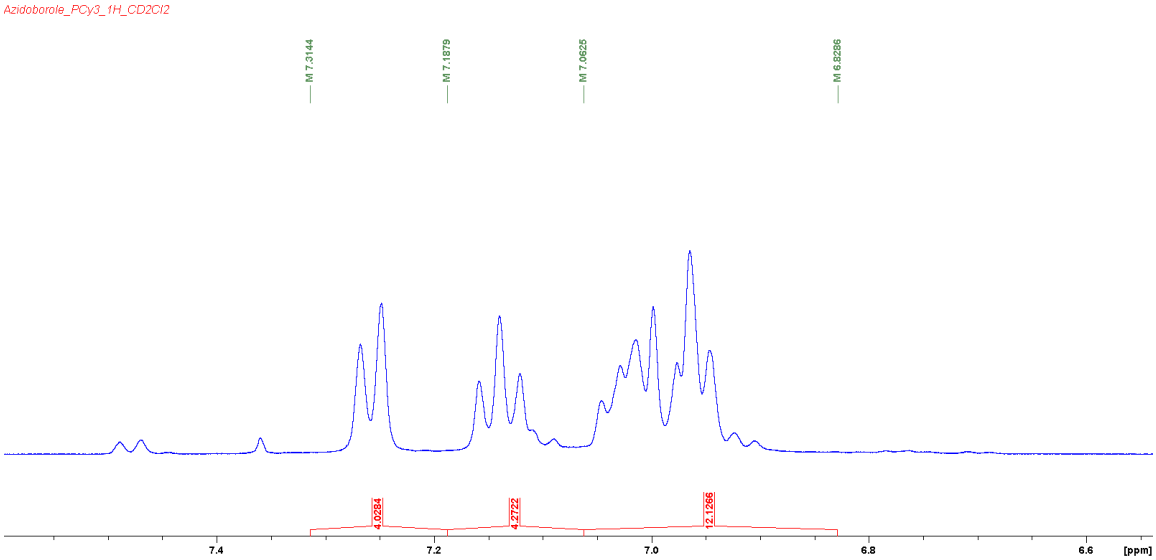


Figure S11 : Extended aromatic region of ^{1}H NMR spectrum of compound **3a**.

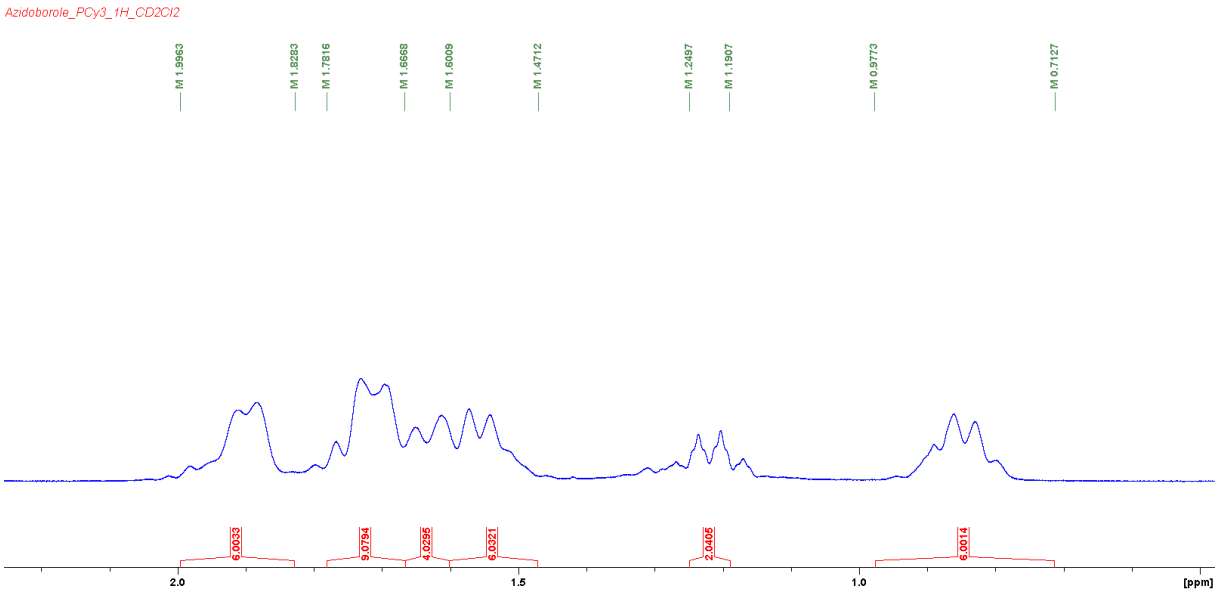


Figure S12 : Extended aliphatic region of ^{1}H NMR spectrum of compound **3a**.

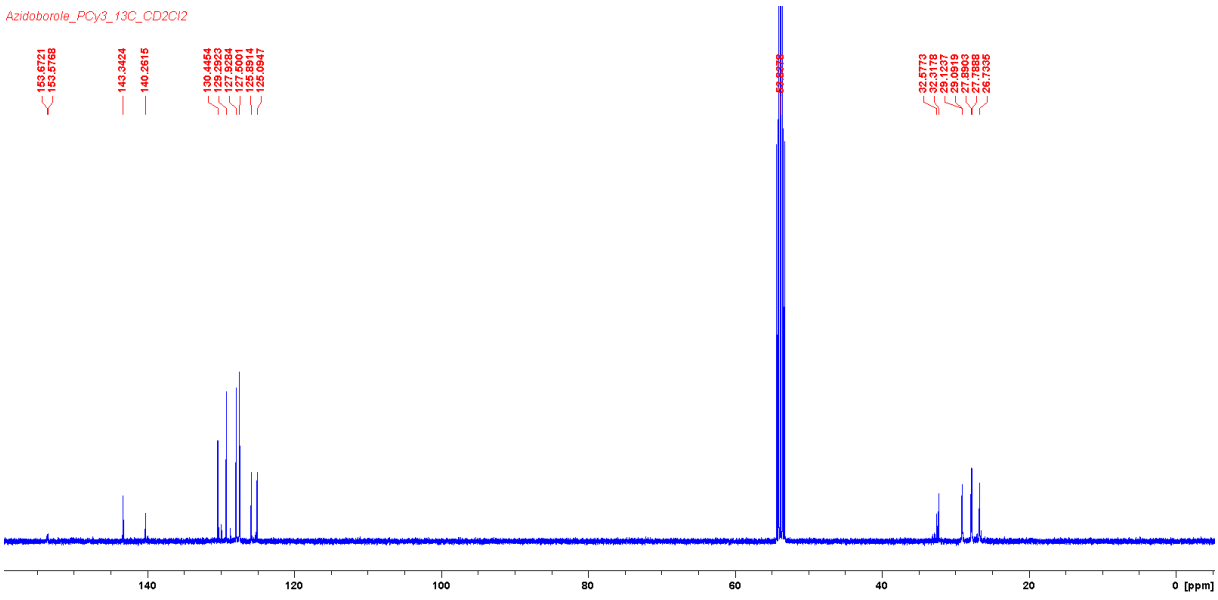


Figure S13 : ^{13}C NMR spectrum of compound **3a** in CD_2Cl_2.

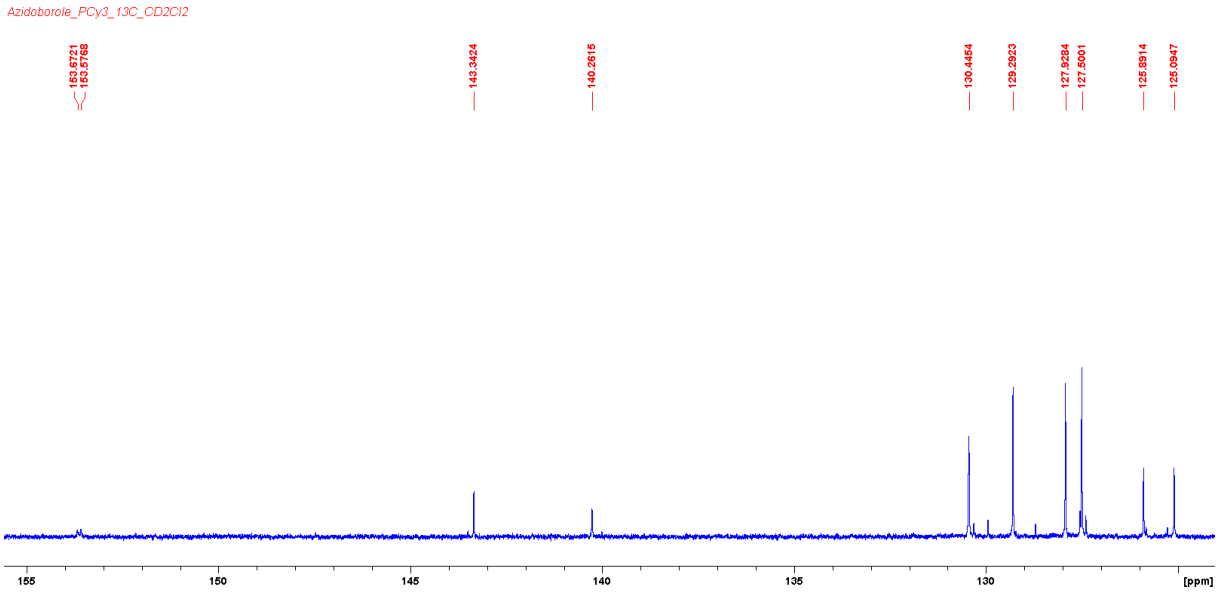


Figure S14 : Extended aromatic region of ^{13}C NMR spectrum of compound **3a**.

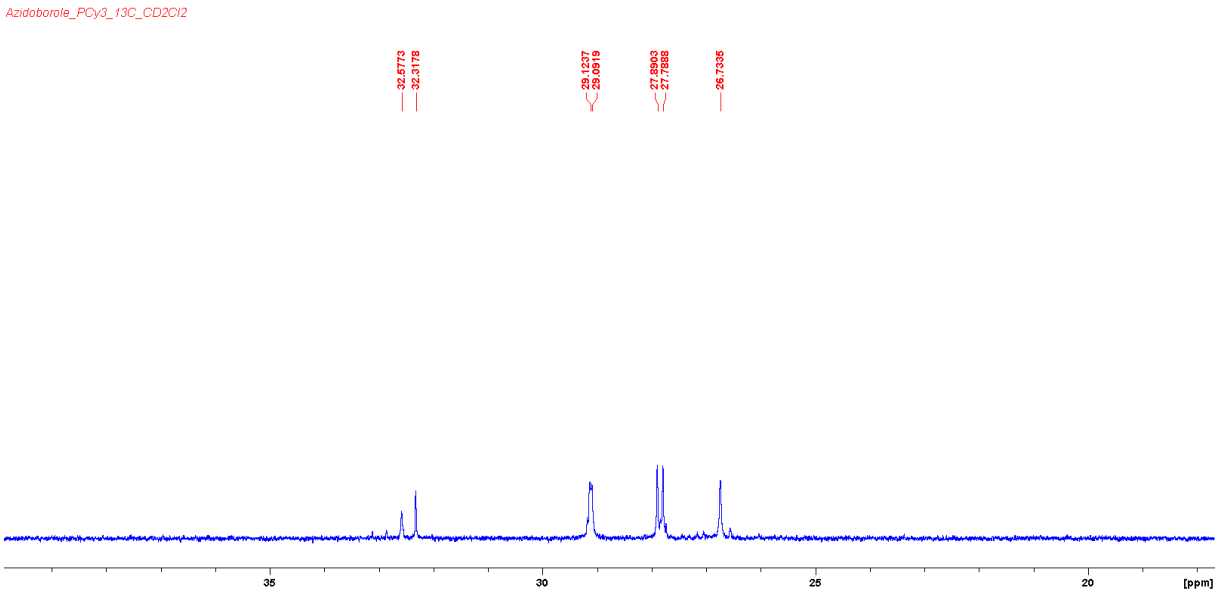


Figure S15 : Extended aliphatic region of ^{13}C NMR spectrum of compound **3a**.

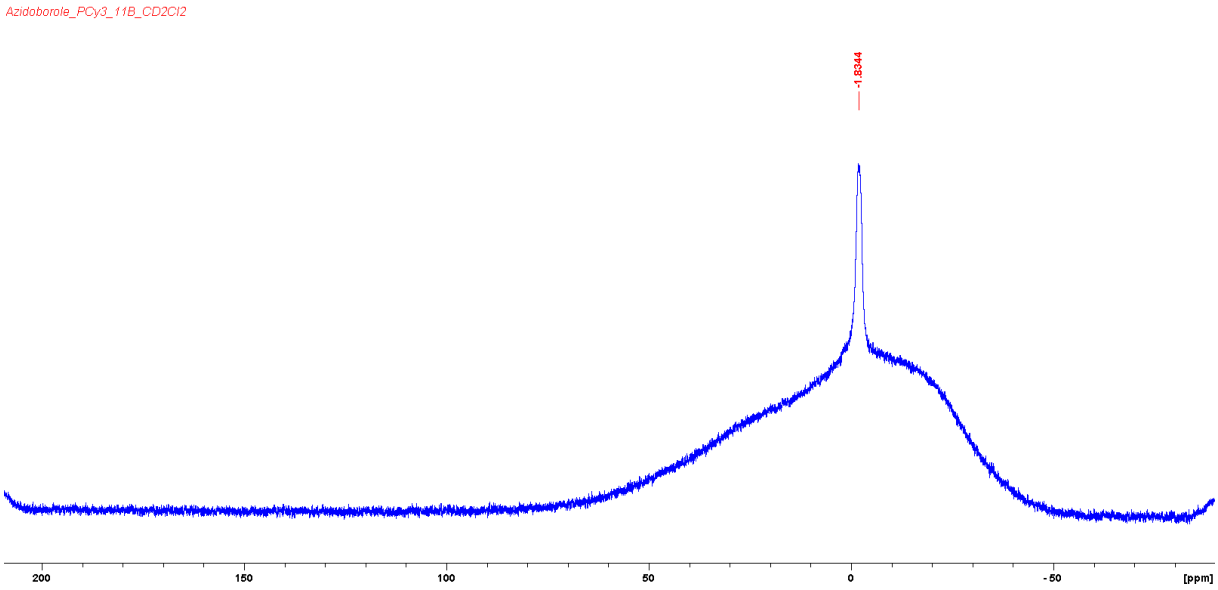


Figure S16 : ^{11}B NMR spectrum of compound **3a** in CD_2Cl_2.

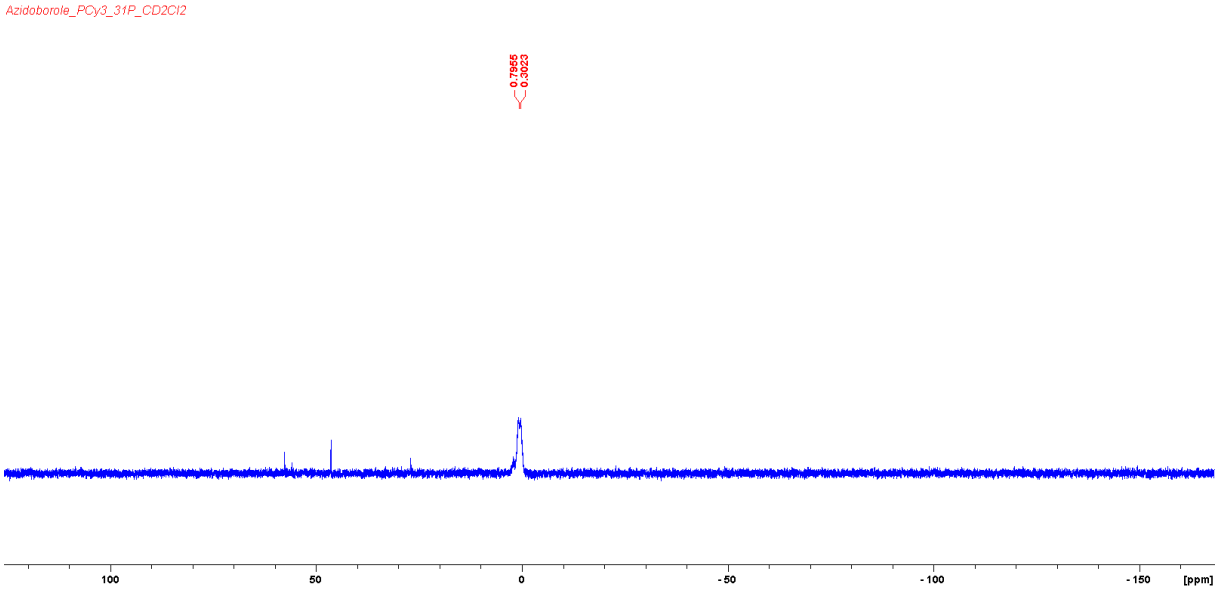


Figure S17 : $^{31}P\{^{1}H\}$ NMR spectrum of compound **3a** in CD_2Cl_2.

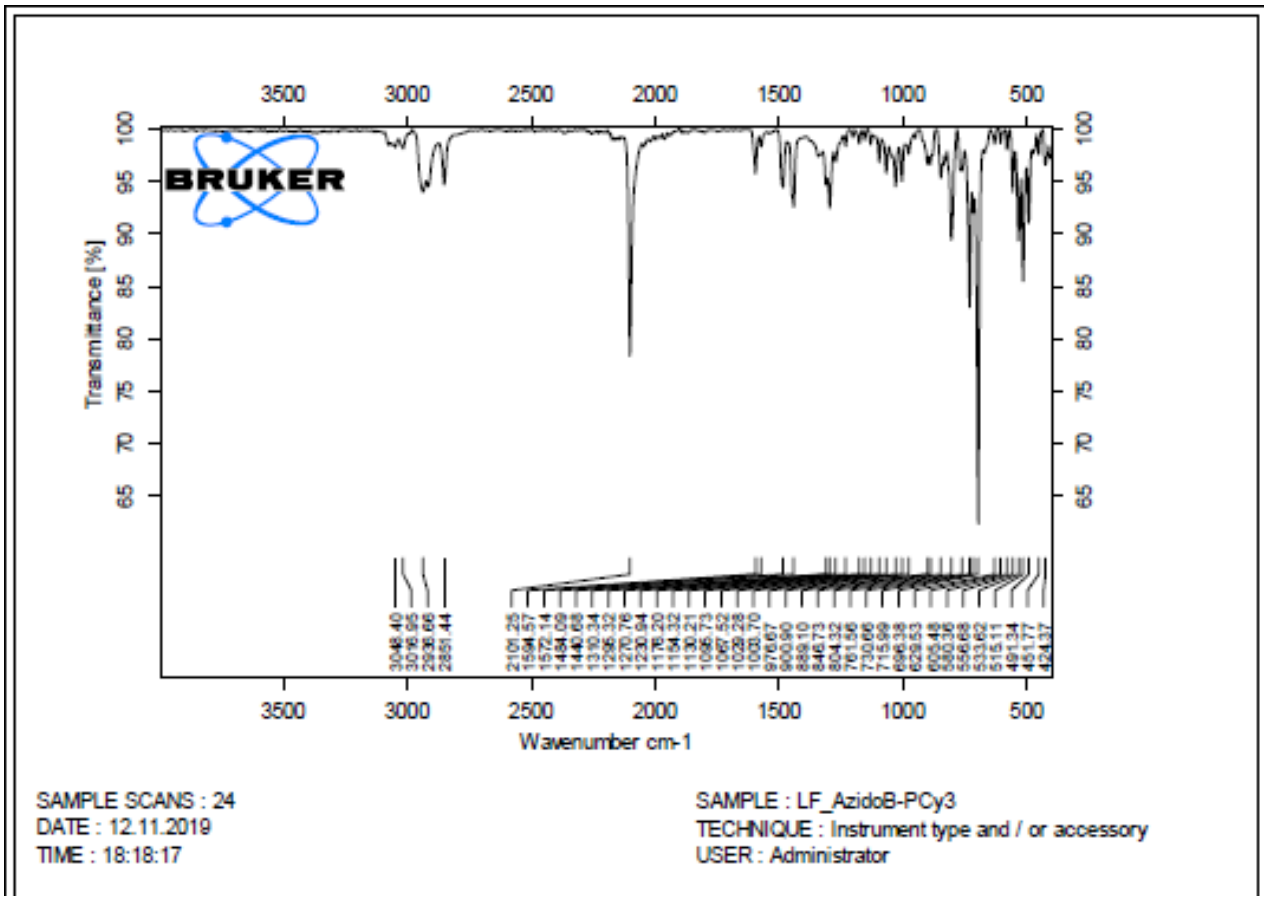
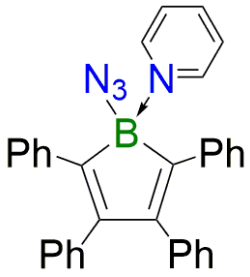


Figure S18 : ATR-IR spectrum of isolated **3a**.

Synthesis of Azidoborole*pyridine 3b



$C_{33}H_{25}BN_4$ (488.398 gmol^{-1})

1 (97.0 mg; 0.24 mmol) was dissolved in CH_2Cl_2 (1 mL) at –78 °C and trimethylsilyl azide (37.2 mg; 0.32 mmol) in CH_2Cl_2 (1 mL) was added dropwise. A color change from deep purple to deep red was observed. The reaction mixture was stirred for 1 h at –78 °C and subsequently pyridine (0.10 mL, 98.2 mg, 1.24 mmol) was added dropwise. The color changed to bright yellow and precipitation was monitored. After warming to room temperature, all volatiles were removed

in vacuo. The remaining yellow solid was washed with pentane (5 x 8 mL) and dried whereupon **3b** was isolated in 77% (93.0 mg, 0.19 mmol) yield. Single crystals suitable for X-ray diffraction were grown via gas-phase diffusion of pentane into a saturated solution of **3b** in benzene (see Crystal Structure Determinations).

^{1}H NMR (C_6D_6): δ = 8.54–8.28 (m, 2H, C*H*, C_6H_5/ NC_5H_5), 7.30–7.23 (m, 4H, C*H*, C_6H_5/ NC_5H_5), 7.23–7.18 (m, 4H, C*H*, C_6H_5/ NC_5H_5), 7.07–6.94 (m, 8H, C*H*, C_6H_5/ NC_5H_5), 6.94–6.88 (m, 2H, C*H*, C_6H_5/ NC_5H_5), 6.88–6.81 (m, 2H, C*H*, C_6H_5/ NC_5H_5), 6.49–6.37 (m, 1H, C*H*, C_6H_5/ NC_5H_5), 6.18–6.08 (m, 2H, C_6H_5/ NC_5H_5) ppm.

^{11}B NMR (C_6D_6): δ = 4.9 ppm.

^{13}C{^{1}H} NMR (C_6D_6): δ = 152.5 (C_q, 2C$_B$), 144.1 (*C*H, 2C), 141.5 (C_q, 4C$_q$), 140.4 (*C*H, 1C), 139.3 (C_q, 2C), 130.7 (*C*H, 4C), 128.8 (*C*H, 4C), 128.3 (*C*H, 4C), 128.1 (*C*H, 4C), 126.5 (*C*H, 2C), 125.5 (*C*H, 2C), 125.3 (*C*H, 2C) ppm.

Comment: The number of C_q and CH atoms were deduced from a combination of ^{13}C, ^{1}H HSQC and ^{13}C, ^{1}H HMBC NMR spectroscopy.

HRMS-ASAP: [M]+H$^+$ 488.220, 489.224, 490.227, 491.212 (calculated: 488.228, 489.224, 490.228, 491.231).

HRMS-ASAP: [M–N$_2$]+H$^+$: 460.221, 461.218, 462.221, 463.225. (calculated: 460.222, 461.218, 462.222, 463.225).

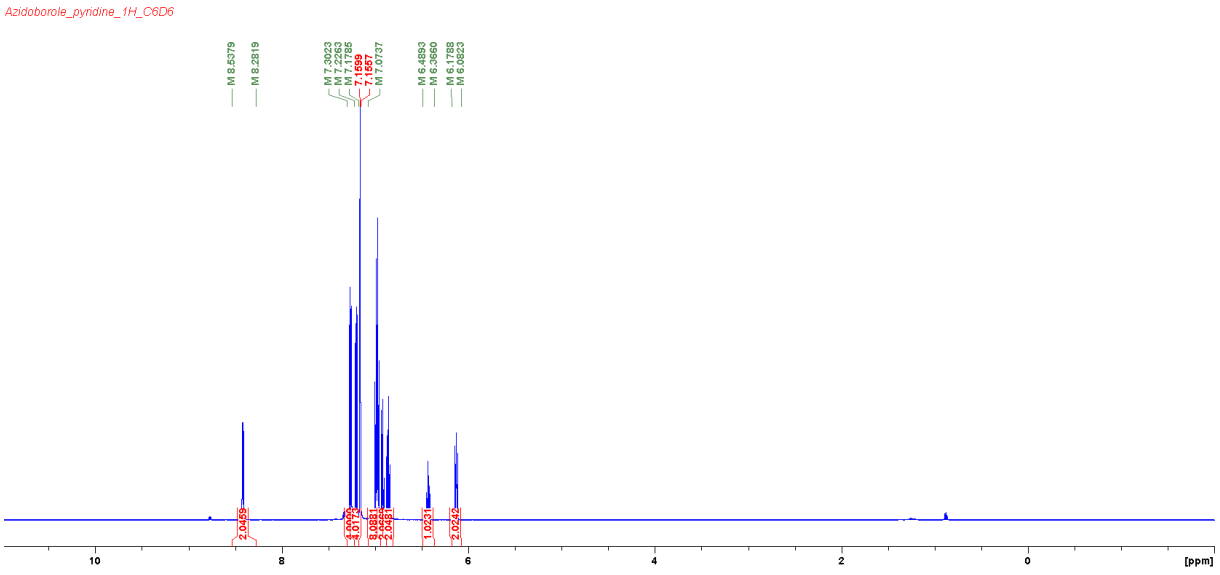


Figure S19 : ^{1}H NMR spectrum of compound **3b** in C_6D_6.

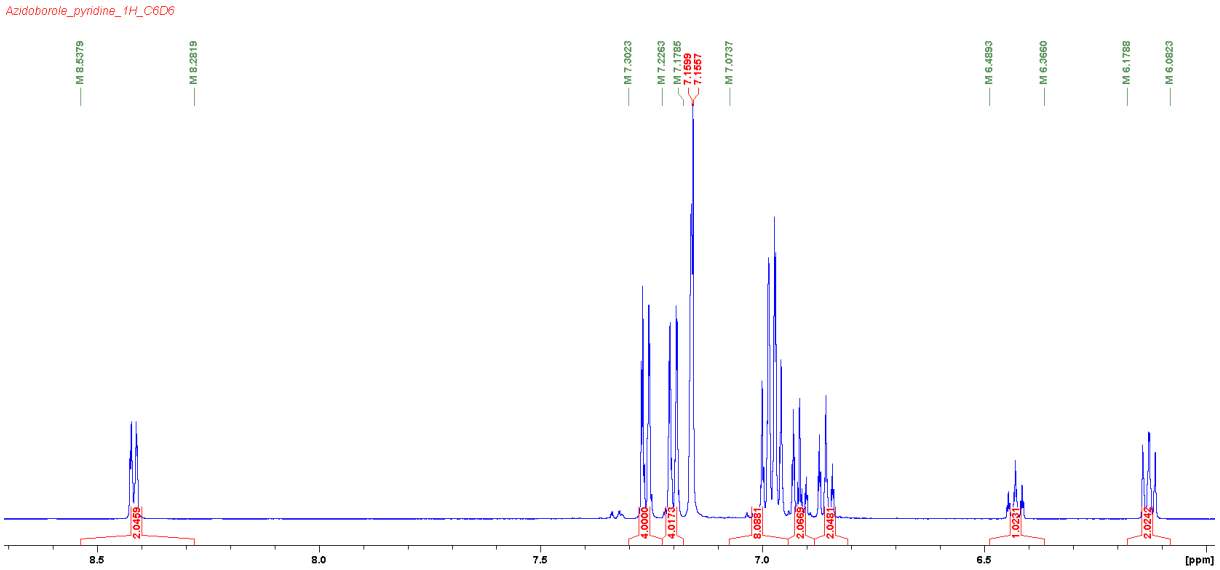


Figure S20 : Extended aromatic region of ^{1}H NMR spectrum of compound **3b**.

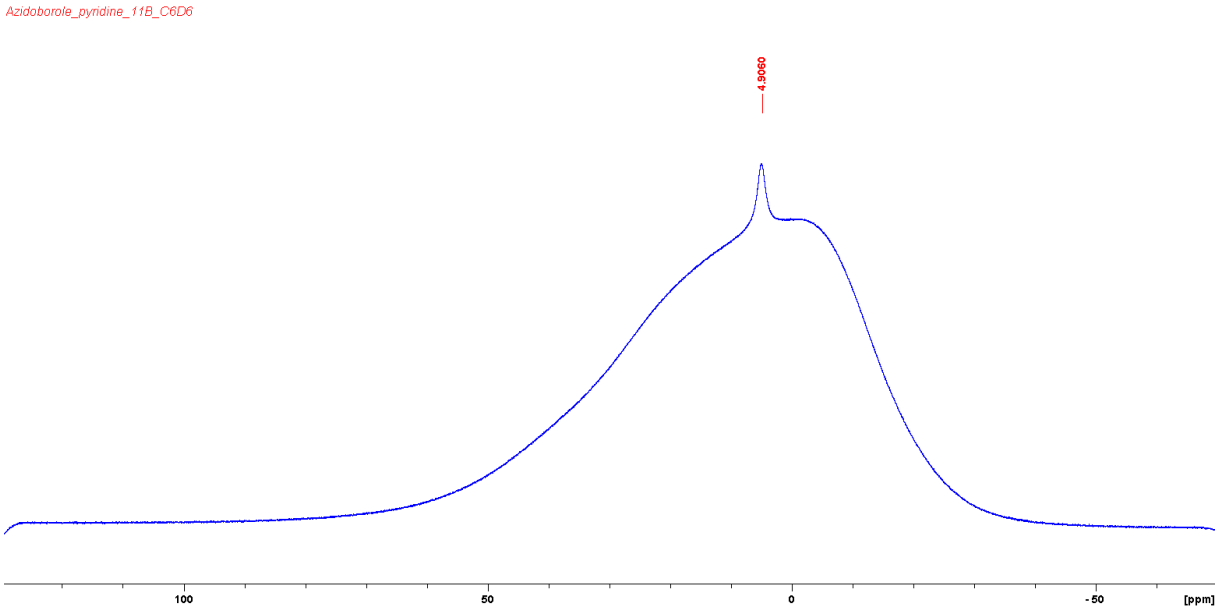


Figure S21 : ^{11}B NMR spectrum of compound **3b** in C_6D_6.

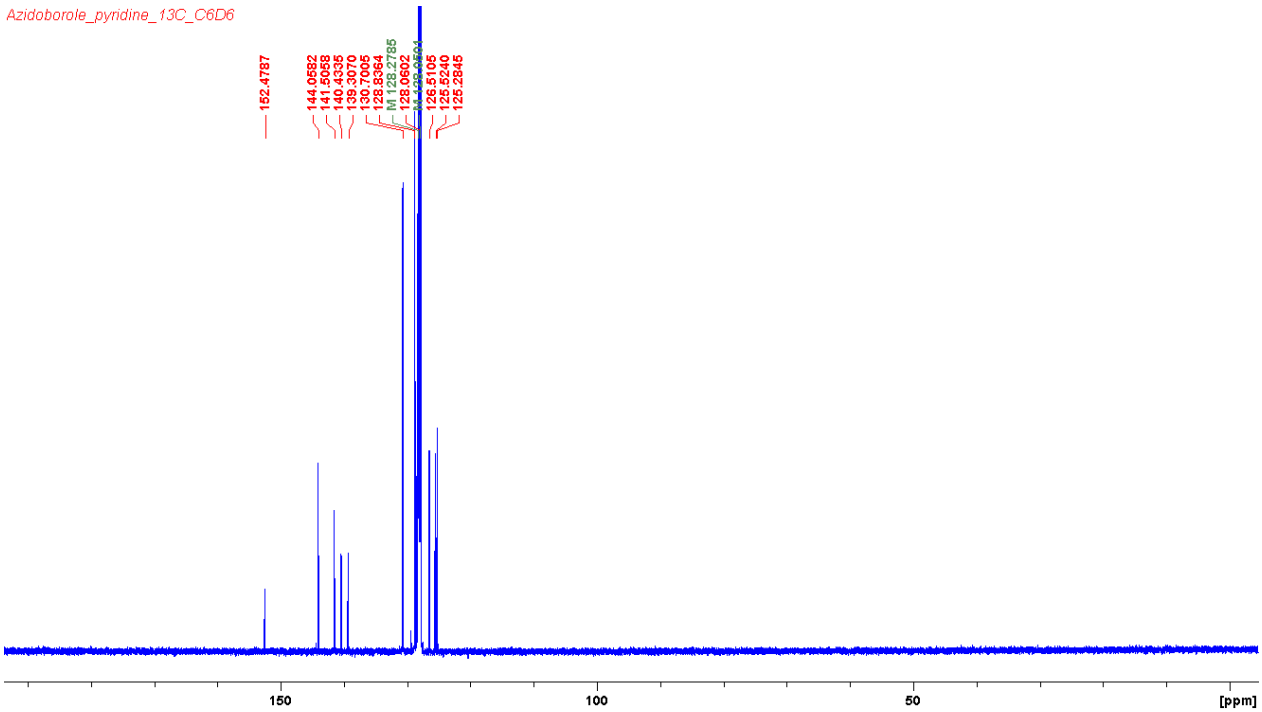


Figure S22 : ^{13}C NMR spectrum of compound **3b** in C_6D_6.

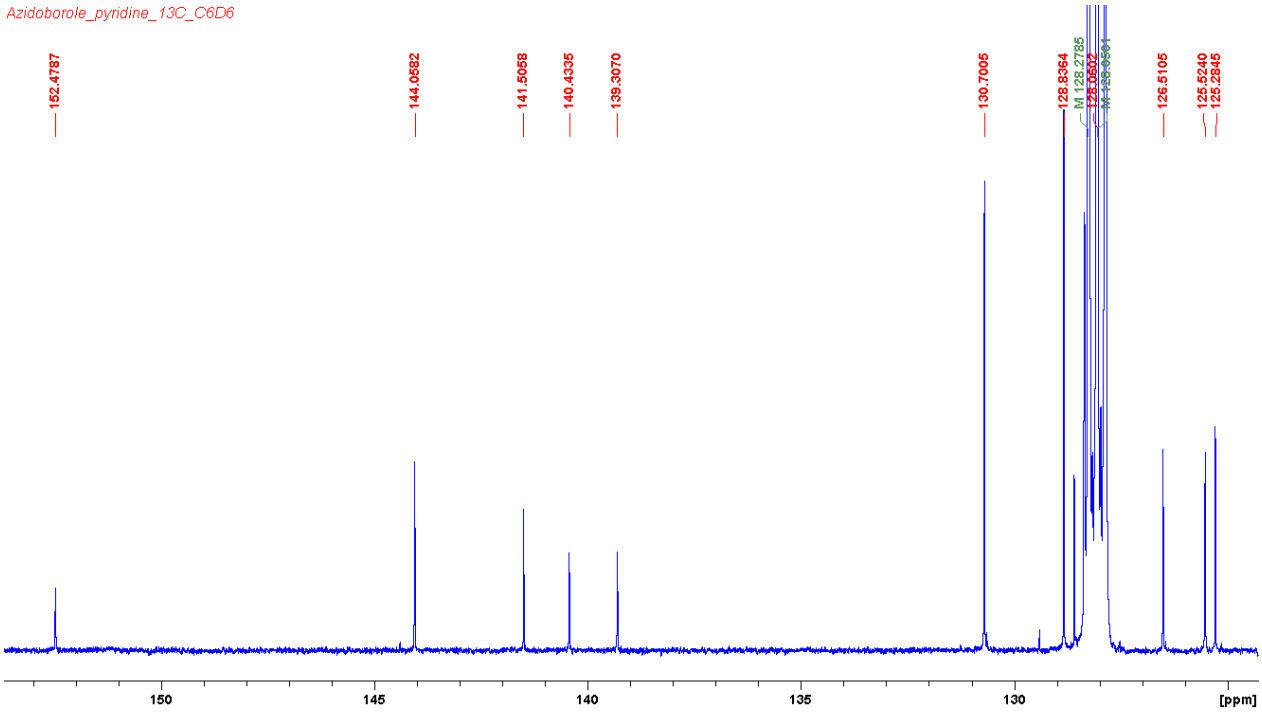


Figure S23 : Extended aromatic region of ^{13}C NMR spectrum of compound **3b**.

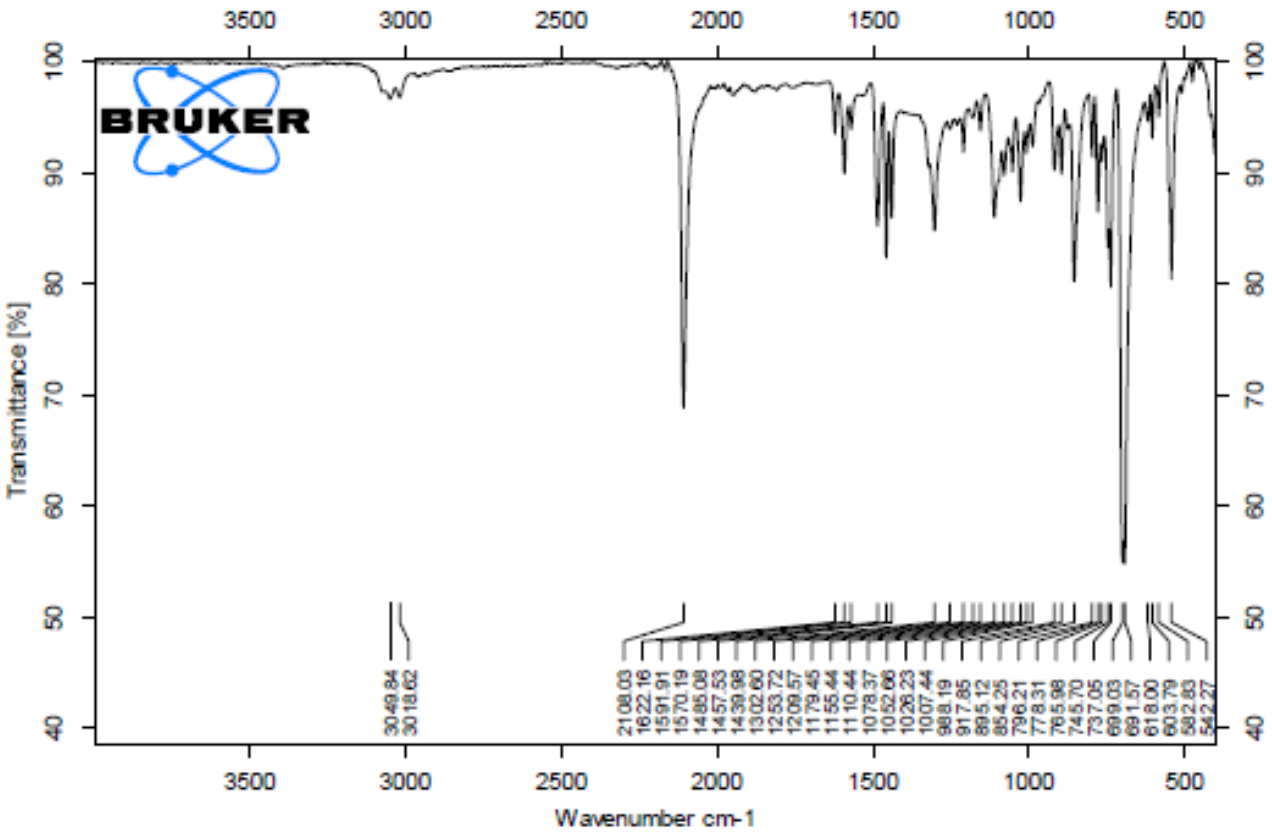
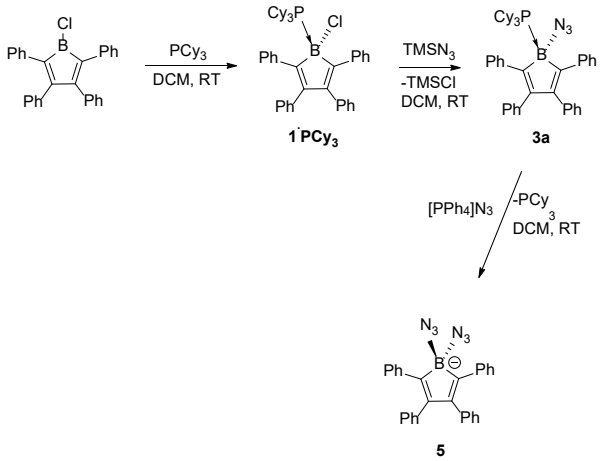


Figure S24 : ATR-IR spectrum of isolated **3b**.

Reaction of 1·PCy$_3$ adduct with azide sources



Chloroborole-PCy$_3$ adduct (**1·PCy$_3$**) was generated *in situ* by treating a CD_2Cl_2 solution of **1** (28 mg; 70 µmol) with a PCy$_3$ solution (20 mg; 70 µmol) in the same solvent, leading to a color change

from a deep purple solution to an orange one. The resulting species was attributed to the **1**·PCy_3 [4] adduct.

$^{31}P\{^1H\}$ NMR (CD_2Cl_2): δ = 2.1ppm

^{11}B NMR (CD_2Cl_2): δ = -1.5 ppm.

$TMSN_3$ (11 mg; 96 μmol) was added to the previous mixture, which resulted in a color change from orange to yellow and in the formation of a precipitate. The formation of trimethylsilyl chloride was observed by ^1H NMR spectroscopy. The mixture was left to react overnight in a J. Young-type NMR tube. The end species was attributed to the azidoborole·PCy_3 adduct (**3a**).

$^{31}P\{^1H\}$ NMR (CD_2Cl_2): δ = 0.52 (bm) ppm.

^{11}B NMR (CD_2Cl_2): δ = -1.8 ppm.

$[PPh_4]N_3$ (26 mg; 68 μmol) was then added to the mixture, resulting in a color change to bright yellow. The appearance of free PCy_3 was observed by ^{31}P NMR spectroscopy (signal at δ = 10.5 ppm). The resulting final borole-derived species in solution was identified as **5**.

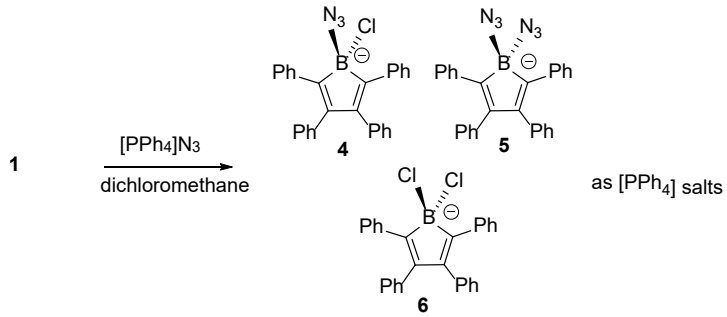
^{11}B NMR (CD_2Cl_2): δ = 2.4 ppm

At no point could the formation of N_2, an expected azide decomposition product, be observed by ^{14}N NMR spectroscopy.

Bright yellow crystals were formed from the slow evaporation of a benzene extract, which were analyzed by single-crystal X-ray diffraction and shown to be of $[PPh_4]$**5** (see Crystal Structure Determinations).

Our computations indicate that, while proper intermediates for the associative mechanism were not found, dissociation of the PR_3 group (R = Me for decreasing computational costs) is +19.9 kcal mol^{-1}, while the further addition of N_3^- leading to **5** is exergonic by –34.6 kcal mol^{-1} (see Figure S58). These results support the feasibility of the formation of **5** from **3a** through the dissociative pathway.

Synthesis of $[PPh_4]$[borolate-$(Cl,N_3)_2$]mixture ($[PPh_4]$[4-mix])



Dichloromethane was condensed over a mixture of $[PPh_4]N_3$ (154 mg; 0.404 mmol) and **1** (162 mg; 0.403 mmol) at -196 °C. Upon thawing, the mixture turned to deep purple, then dark orange, then light orange. After stirring, the volatiles were removed *in vacuo*. Dichloromethane and pentane were added to the solid product, which yielded a two-phase system from which the cloudy pale orange light phase was removed (crystals suitable for X-ray diffraction were obtained from this extract, see Crystal Structure Determinations) and the heavy, darker orange phase was evaporated to dryness *in vacuo* again, yielding the desired mixture of compounds as a yellow foam-like solid (213 mg; 0.271 mmol; 67 % recovered yield based on **1**)

^{11}B NMR (CD_2Cl_2): δ = 2.4, 4.3 and 6.8 ppm (overlapping signals)

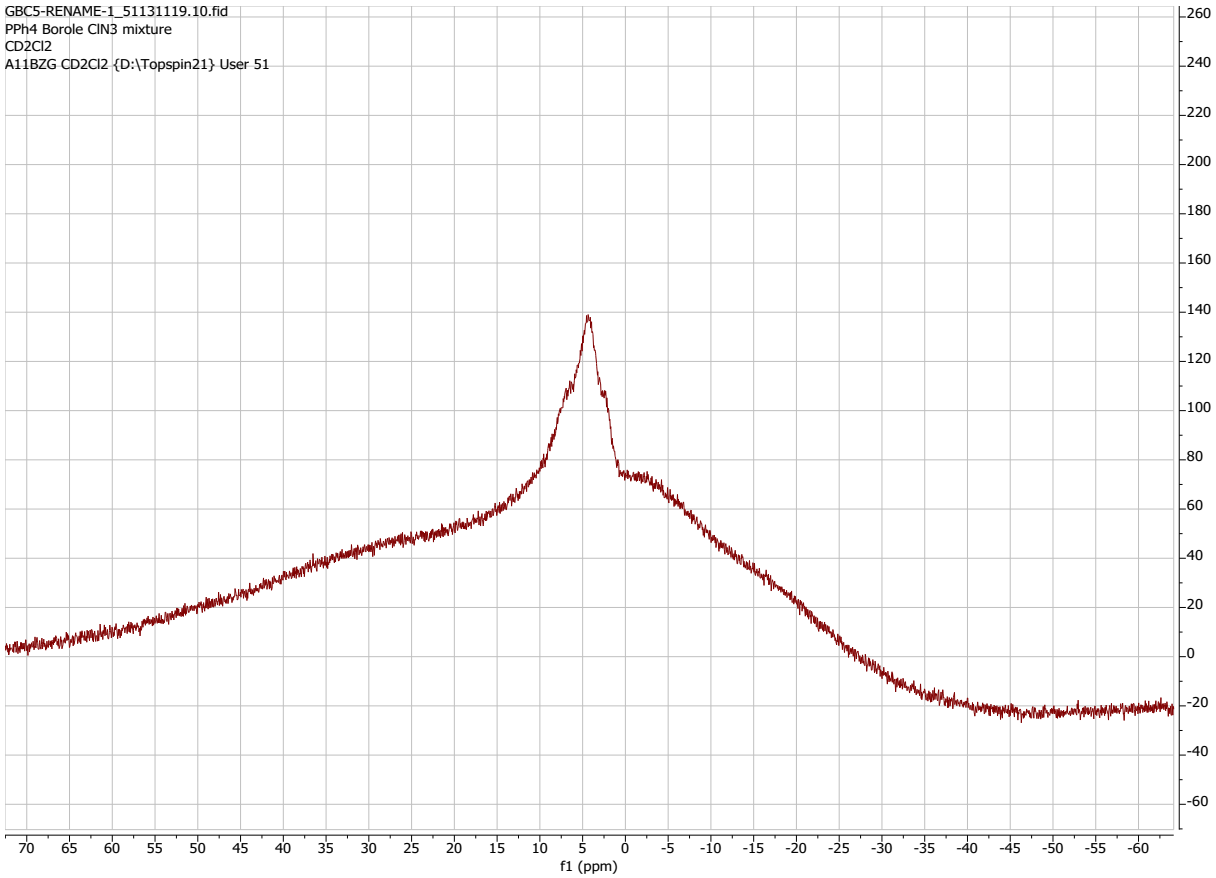


Figure S25 : ^{11}B NMR of [PPh_4][**4-mix**] in CD_2Cl_2.

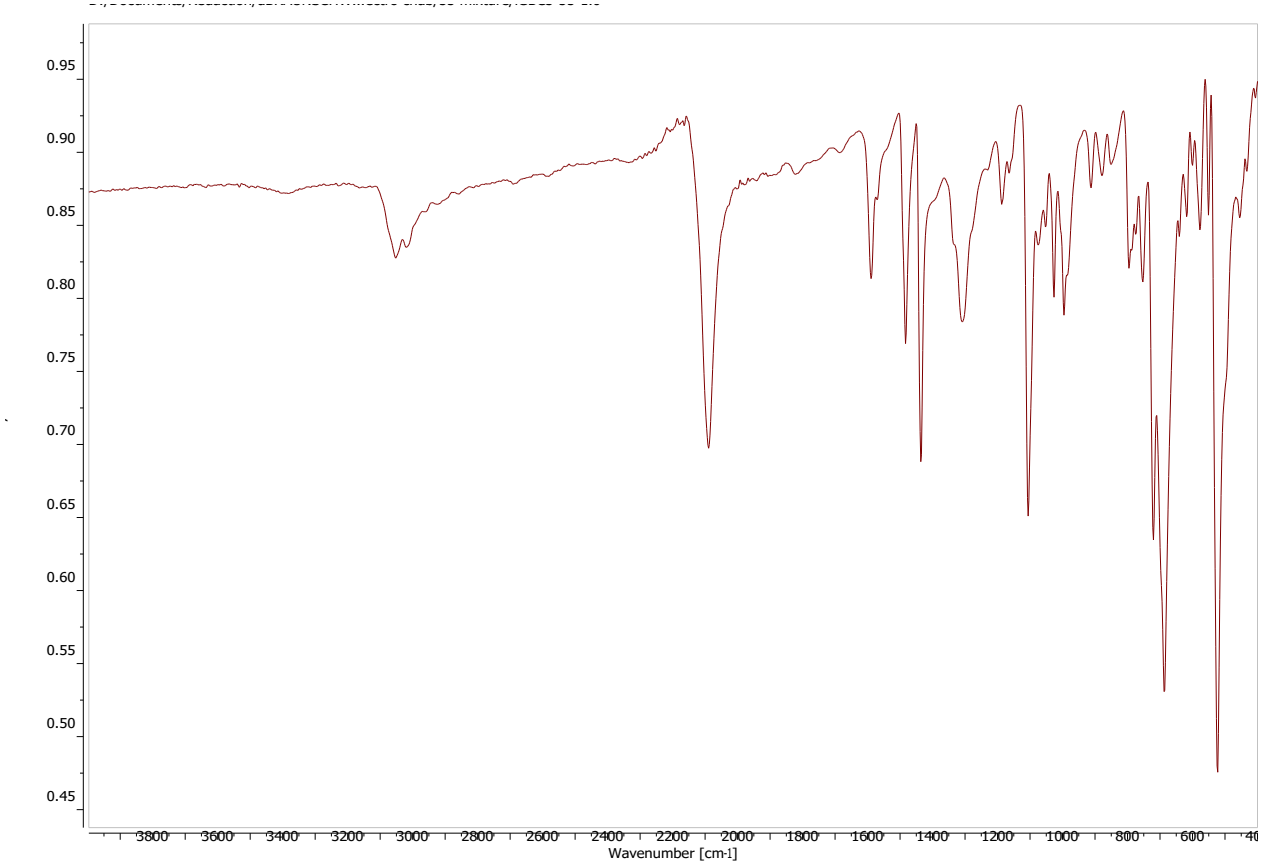
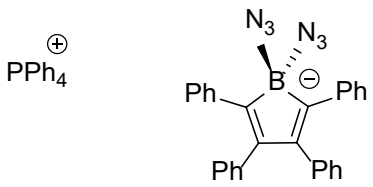


Figure S26 : ATR IR spectrum of isolated [PPh_4][**4-mix**].

Crystals were obtained by slow evaporation of DCM/pentane extracts and always display severe substitutional disorder, as expected from the mixture of complex salts by ^{11}B NMR (See Crystal Structure Determination).

<u>Synthesis of [PPh_4][diazidoborolate] ([PPh_4][5])</u>



A sample of the **[PPh_4][4-mix]** mixture of salts (119 mg; 0.152 mmol) was dissolved in dichloromethane. To the resulting solution, a $TMSN_3$ (43 mg; 0.37 mmol) solution in

dichloromethane was added. The mixture was left to react for several days, yielding a yellow-orange solution, which was evaporated to dryness *in vacuo*, yielding a yellow foam-like solid (50 mg, 63 μmol, 42% recovered yield based on **[PPh_4][4-mix]**. The crude isolated product contains leftover excess $TMSN_3$, which can be removed by washing with non-polar solvents.

^{1}H NMR (CD_2Cl_2): δ = 7.91 (m, 4H, PPh_4^+), 7.74 (m, 8H, PPh_4^+), 7.60 (m, 8H, PPh_4^+), 7.25 (m, 4H, C*H*, C_6H_5), 7.03 (2x m, 10H, C*H*, C_6H_5), 6.94 (m, 6H, C*H*, C_6H_5).

^{11}B NMR (CD_2Cl_2): δ = 2.4 ppm.

^{13}C{^{1}H} NMR (CD_2Cl_2): δ = 148.9 (C_q, 2C), 143.4 (C_q, 2C), 141.0 (C_q, 2C), 136.1 (d, J = 3.6 Hz, *C*H, 4C, PPh_4^+), 134.8 (d, J = 10 Hz, *C*H, 8C, PPh_4^+), 131.0 (d, J = 13 Hz, *C*H, 8C, PPh_4^+), 130.8 (*C*H, 4C), 129.4 (*C*H, 4C), 127.5 (*C*H, 4C), 127.4 (*C*H, 4C), 125.3 (*C*H, 2C), 124.2 (*C*H, 2C), 117.9 (d, J = 90 Hz, P-*C*, 4C, PPh_4^+).

The C_q carbons belonging to C_B could not be detected.

^{31}P{^{1}H} NMR (CD_2Cl_2): δ = 23.3 ppm.

HRMS-ESI: $[M]^-$ 451.1850 (calculated: 451.1848); [PPh_4^+] 339.1289 (calculated 339.1297)

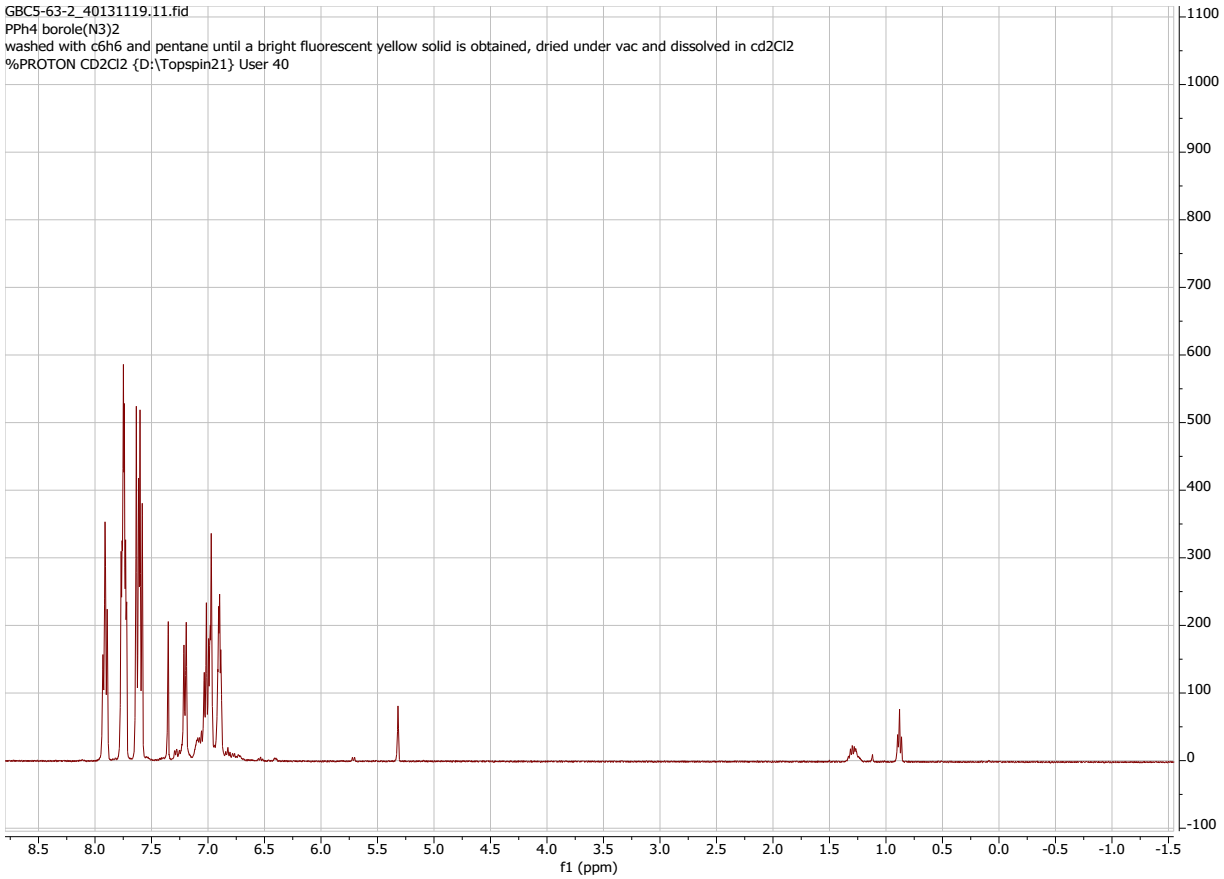


Figure S27 : ^{1}H NMR spectrum of **[PPh$_4$][5]** in CD_2Cl_2. Signals at *ca* 1 ppm belong to residual pentane, used to remove excess $TMSN_3$.

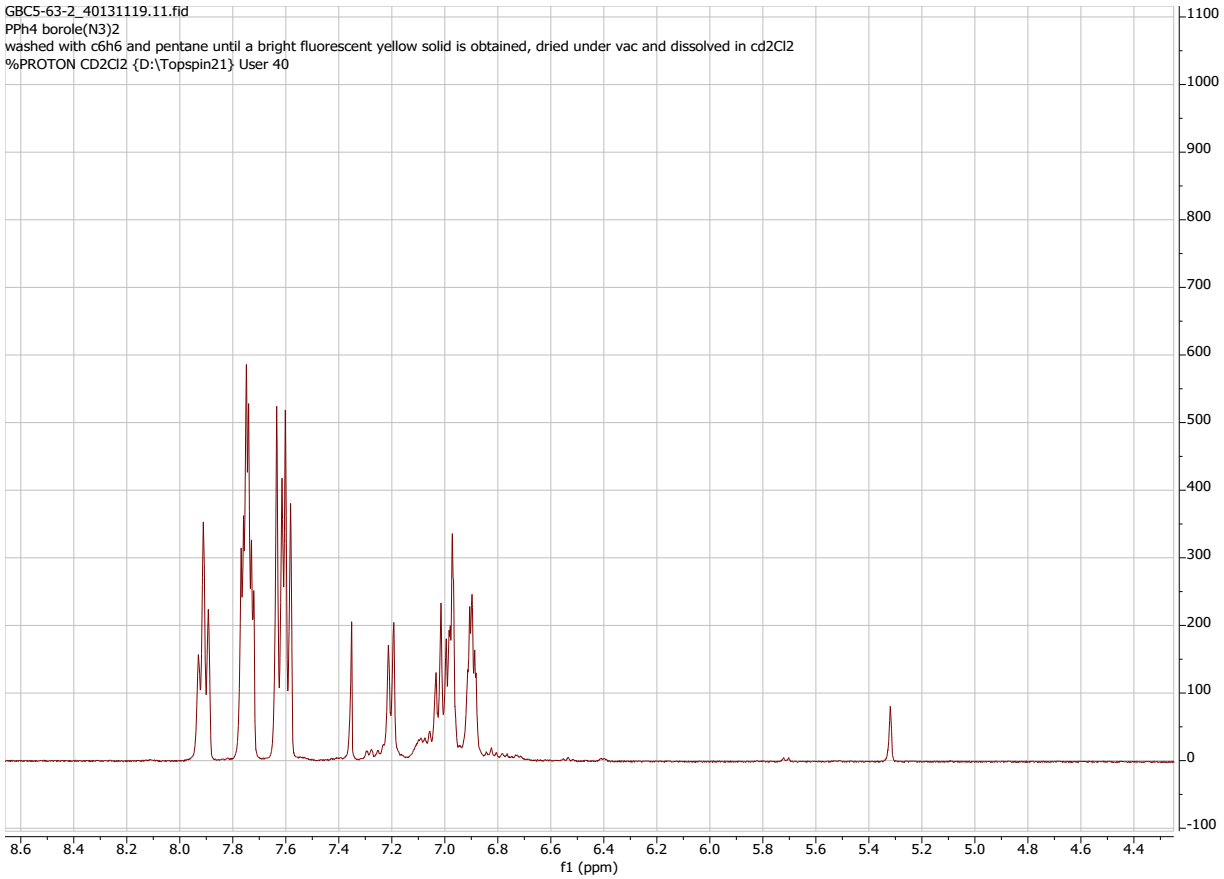


Figure S28 : Extended aromatic region of the ^{1}H NMR spectrum of **[PPh$_4$][5]**.

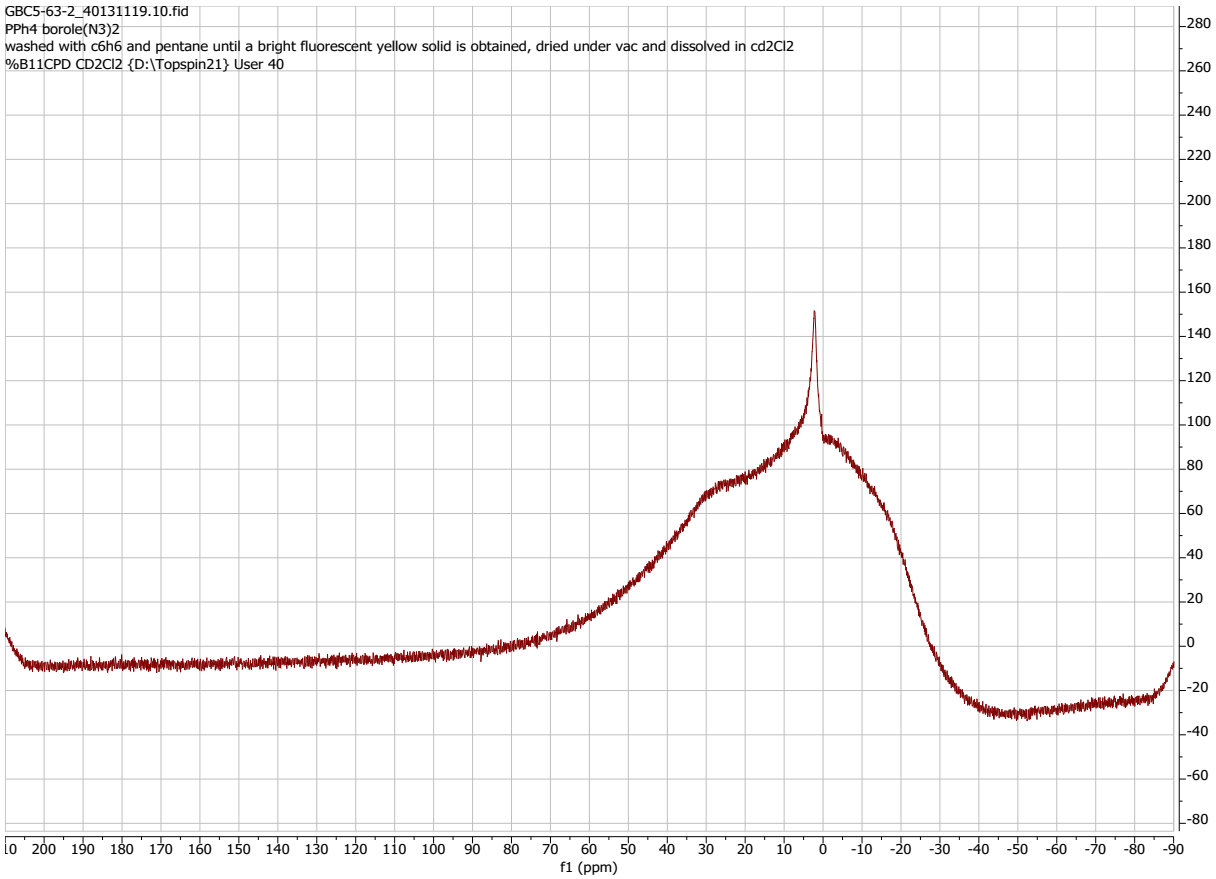


Figure S29 : ^{11}B NMR spectrum of **[PPh$_4$][5]** in CD_2Cl_2.

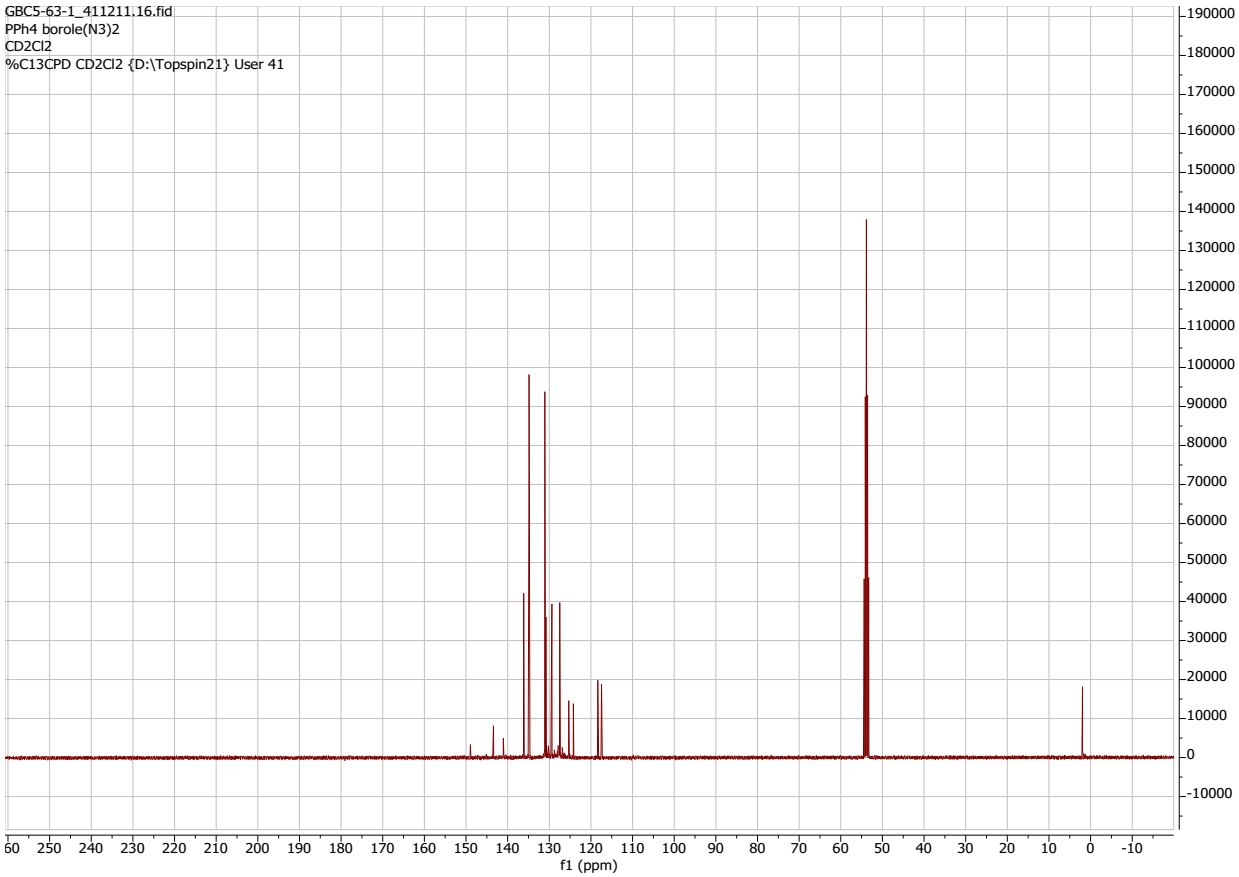


Figure S30 : $^{13}C\{^{1}H\}$ NMR spectrum of **[PPh$_4$][5]**in CD_2Cl_2. The signal near 0 ppm belongs to excess $TMNN_3$.

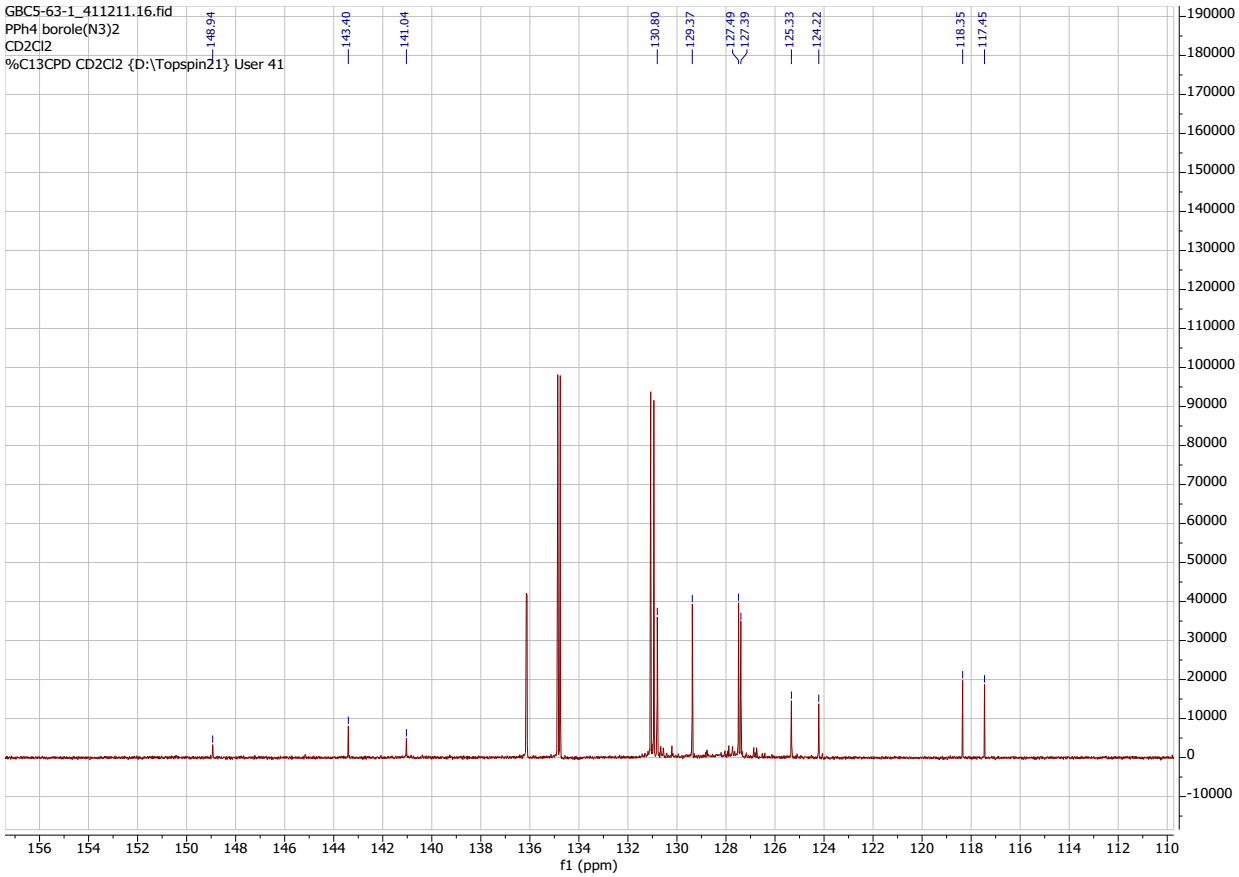


Figure S31 : Extended aromatic region of the ^{13}C NMR spectrum of **[PPh_4][5]** in CD_2Cl_2.

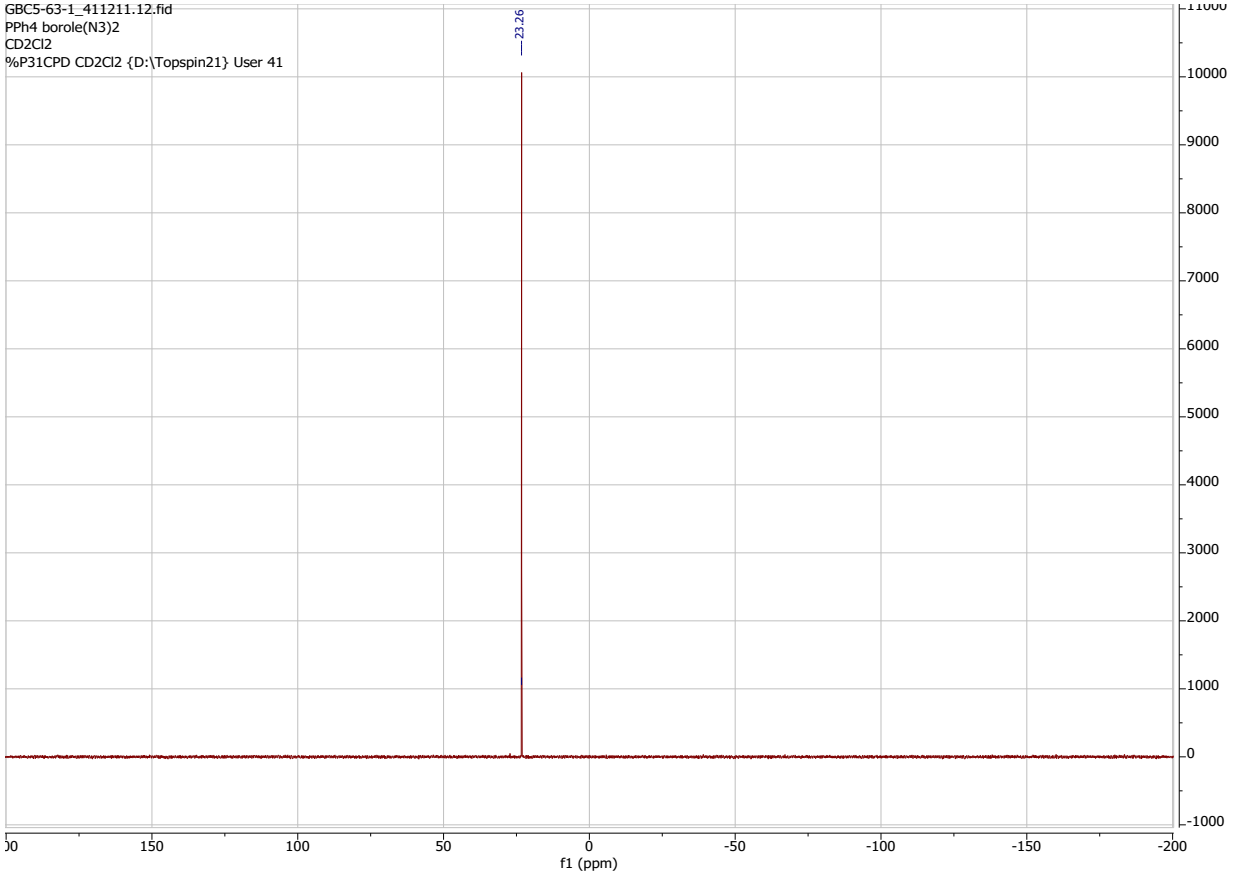


Figure S32 : $^{31}P\{^{1}H\}$ NMR spectrum of **[PPh_4][5]** in CD_2Cl_2.

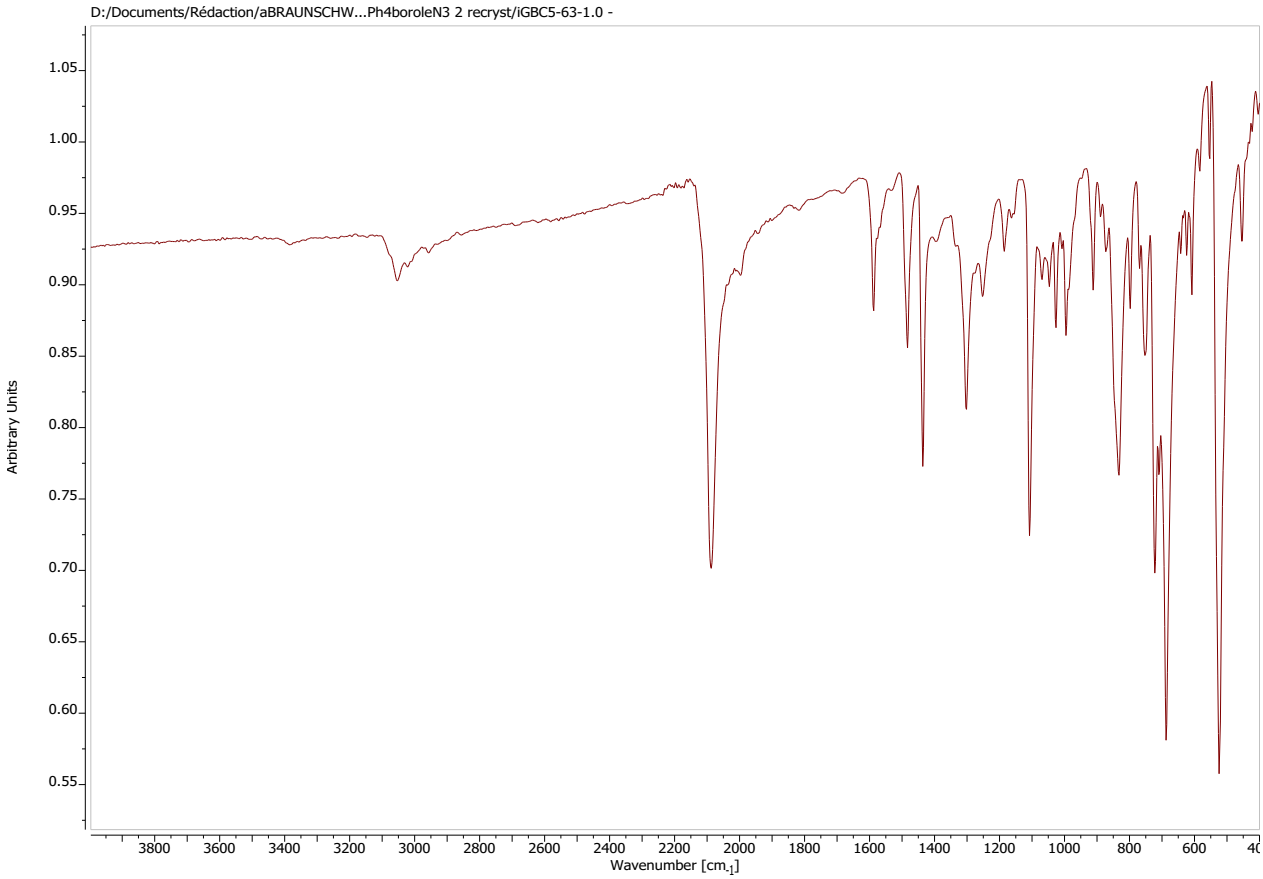
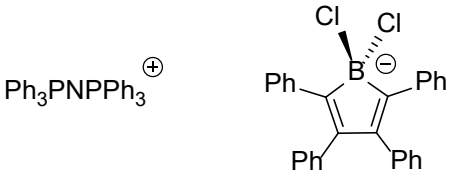


Figure S33 : ATR IR spectrum of **[PPh_4][5]**.

<u>Synthesis of [PPN][borolate(Cl_2)] ([PPN][6]</u>:



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1 (112 mg; 0.279 mmol) and [PPN]Cl (140 mg; 0.243 mmol) were dissolved in dichloromethane, yielding a dark brown/orange solution. The mixture was left standing overnight and the volatiles were removed *in vacuo*, yielding the crude compound as a brownish-yellow foam-like solid (210 mg; 0.215 mmol, 77 mol% recovered yield based on **1**). Crystals suitable for X-ray crystallography could be found directly in the isolated material (see Crystal Structure Determinations).

Upon standing for several months, samples contained traces of BCl_4^- (very sharp signal at 7.1 ppm in ^{11}B NMR spectroscopy)

The compound was found to be too sensitive for HRMS conditions, which yielded, among other signals, peaks consistent with the composition chloroborole+H_2O+OH^- (437.1488 (calculated for $[C_{28}H_{23}BClO_2]^-$: 437.14798).

^{1}H NMR (CD_2Cl_2): δ = 7.67 (m, 6H, PPN), 7.51 (2x m, 24H, PPN), 7.43 (m, 4H, C_6H_5), 7.06 (m, 4H, C_6H_5), 6.94 (2x m, 12H, C_6H_5).

^{11}B NMR (CD_2Cl_2): δ = 7.24 ppm.

^{13}C NMR (CD_2Cl_2): δ = 152.7 (C_q, C_B, 2C), 145.4 (C_q, 2C), 143.1 (C_q, 2C), 140.6 (C_q, 2C), 134.12 (m, *C*H, 6C, PPN), 132.5 (m, *C*H, 12C, PPN), 130.8 (*C*H, 4C), 130.0 (*C*H, 4C), 129.8 (m, *C*H, 12C, PPN), 127.4 (dd, J= 108 Hz; J= 2Hz, *C*-P, 6C, PPN), 127.2 (*C*H, 4C), 127.1 (*C*H, 4C), 125.2 (*C*H, 2C), 124.2 (*C*H, 2C).

^{31}P NMR (CD_2Cl_2): δ = 21.1 ppm

HRMS-ESI: $[PPN]^+$ 538.1836 (calculated 538.1848)

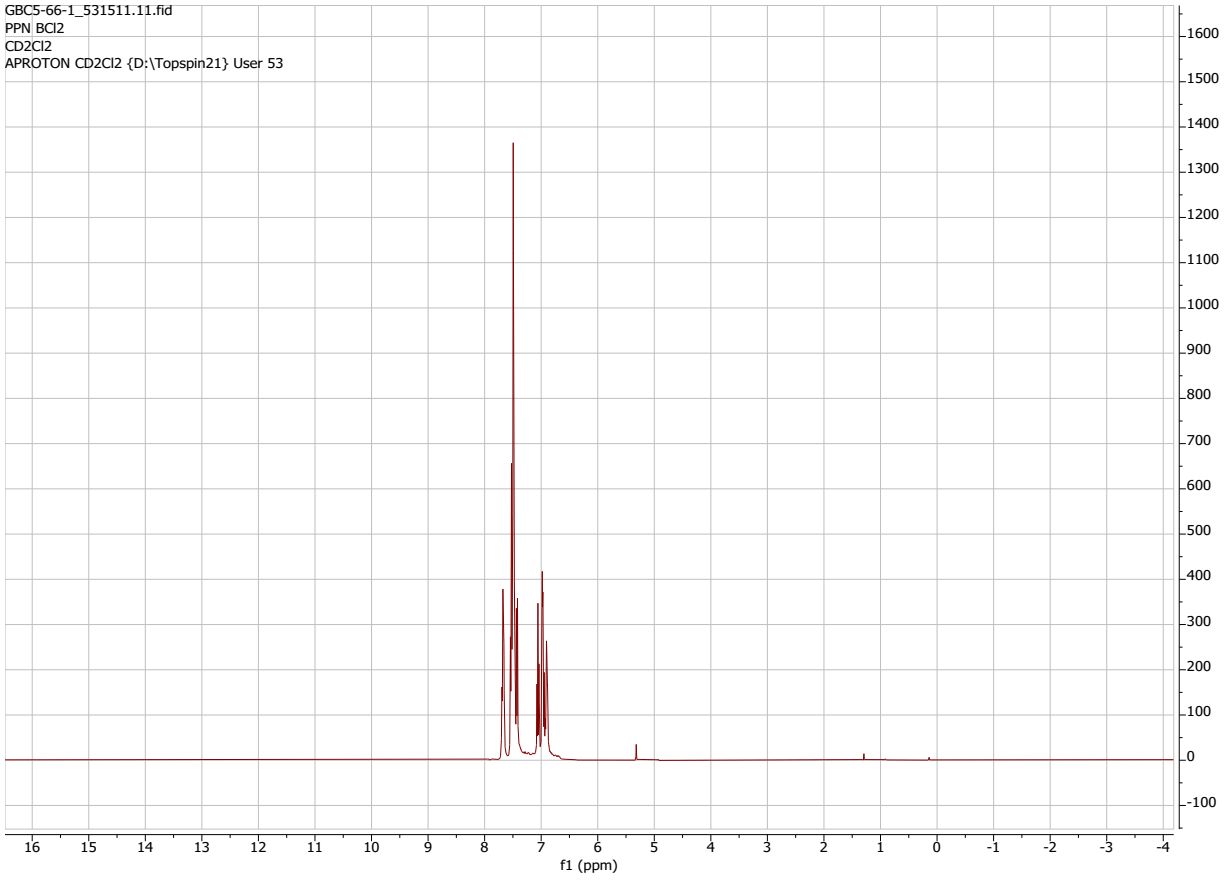


Figure S34 : ^{1}H NMR spectrum of **[PPN][6]** in CD_2Cl_2.

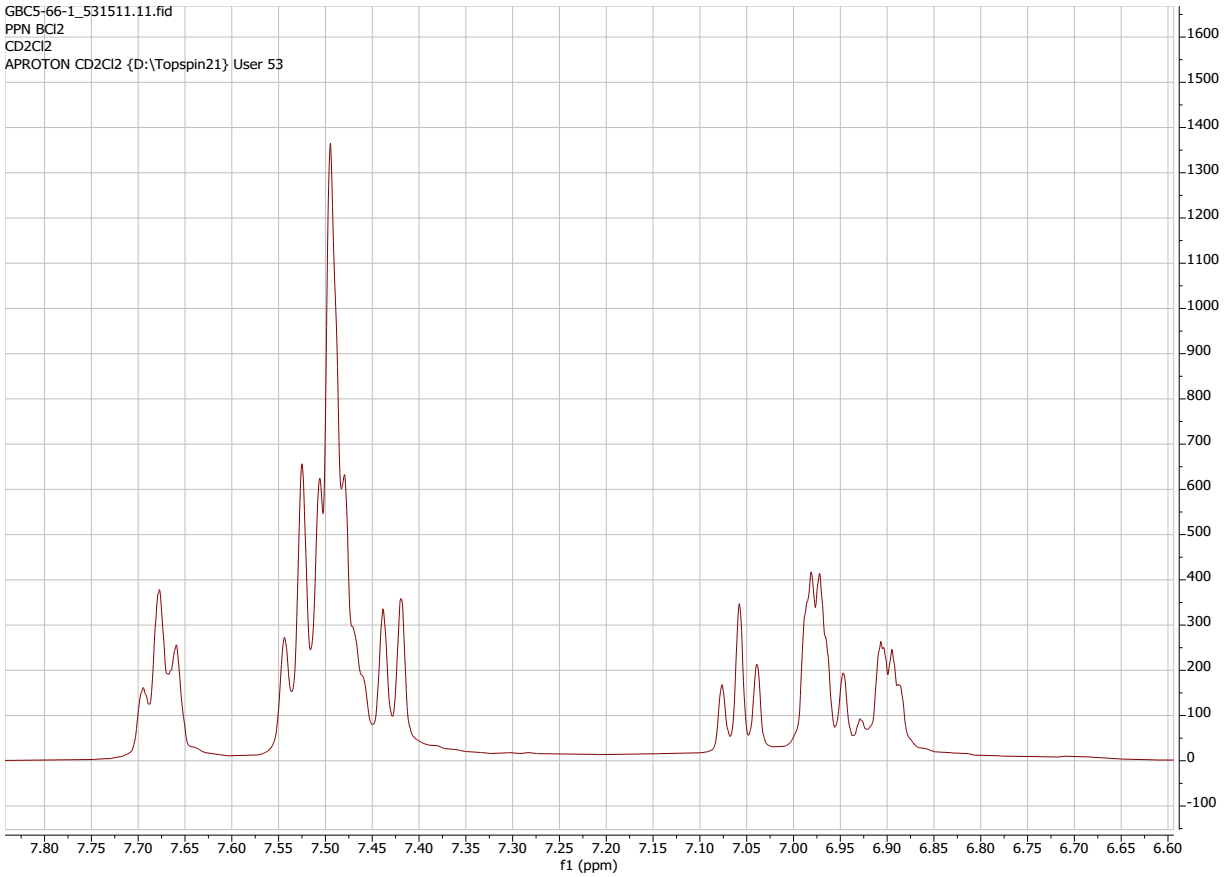


Figure S35 :Extended aromatic region of the ^{1}H NMR spectrum of **[PPN][6]** in CD_2Cl_2.

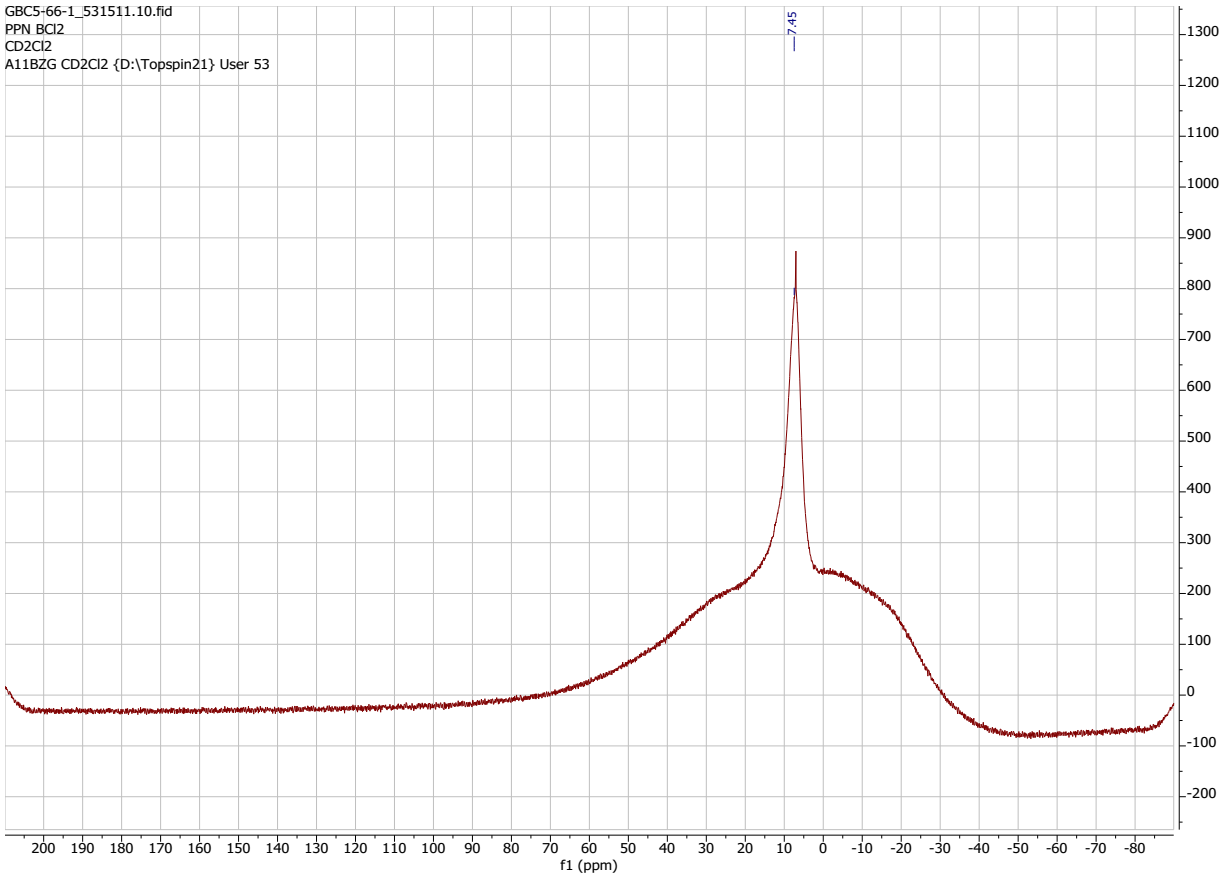


Figure S36 : ^{11}B NMR spectrum of **[PPN][6]** in CD_2Cl_2.

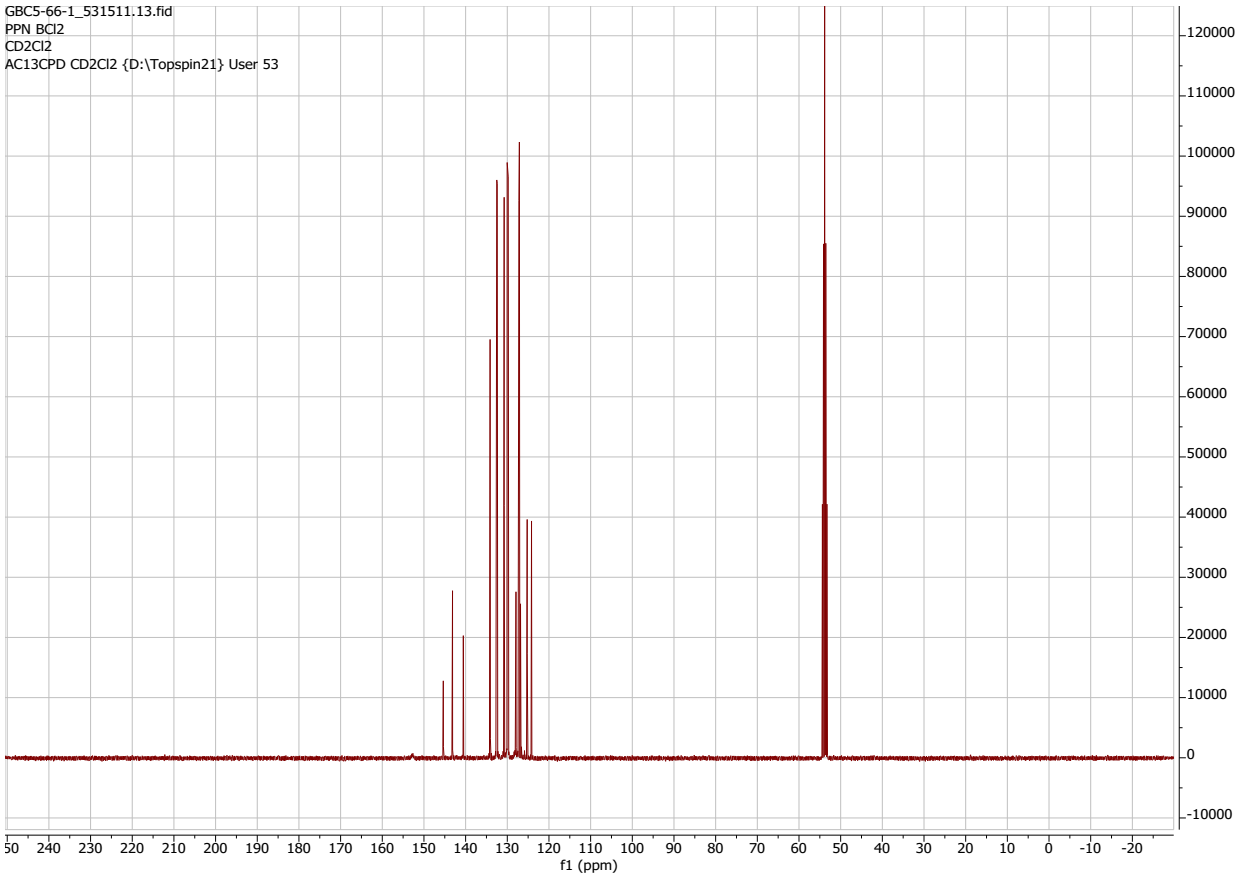


Figure S37 : $^{13}C\{^{1}H\}$ NMR spectrum of **[PPN][6]** in CD_2Cl_2.

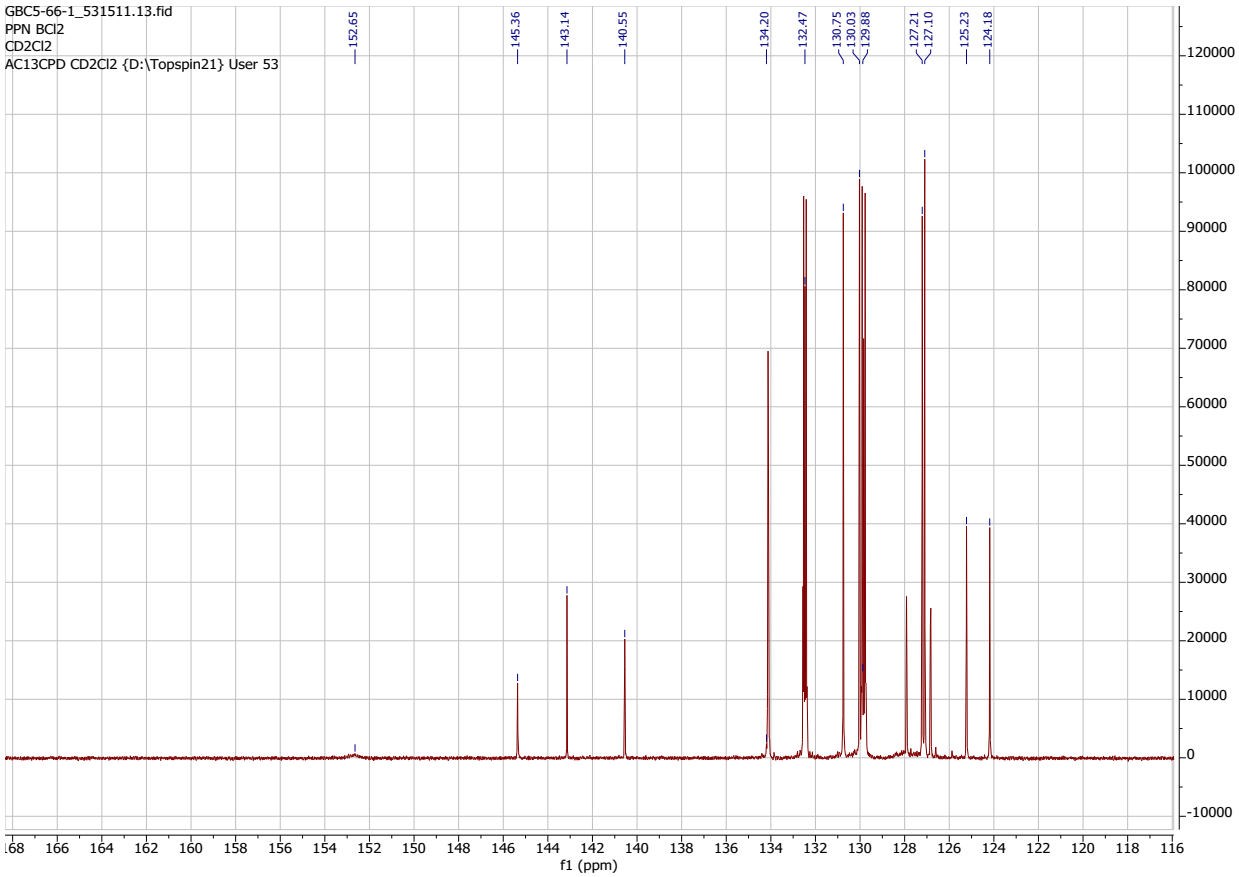


Figure S38 : Extended aromatic region of the ^{13}C NMR spectrum of **[PPN][6]** in CD_2Cl_2.

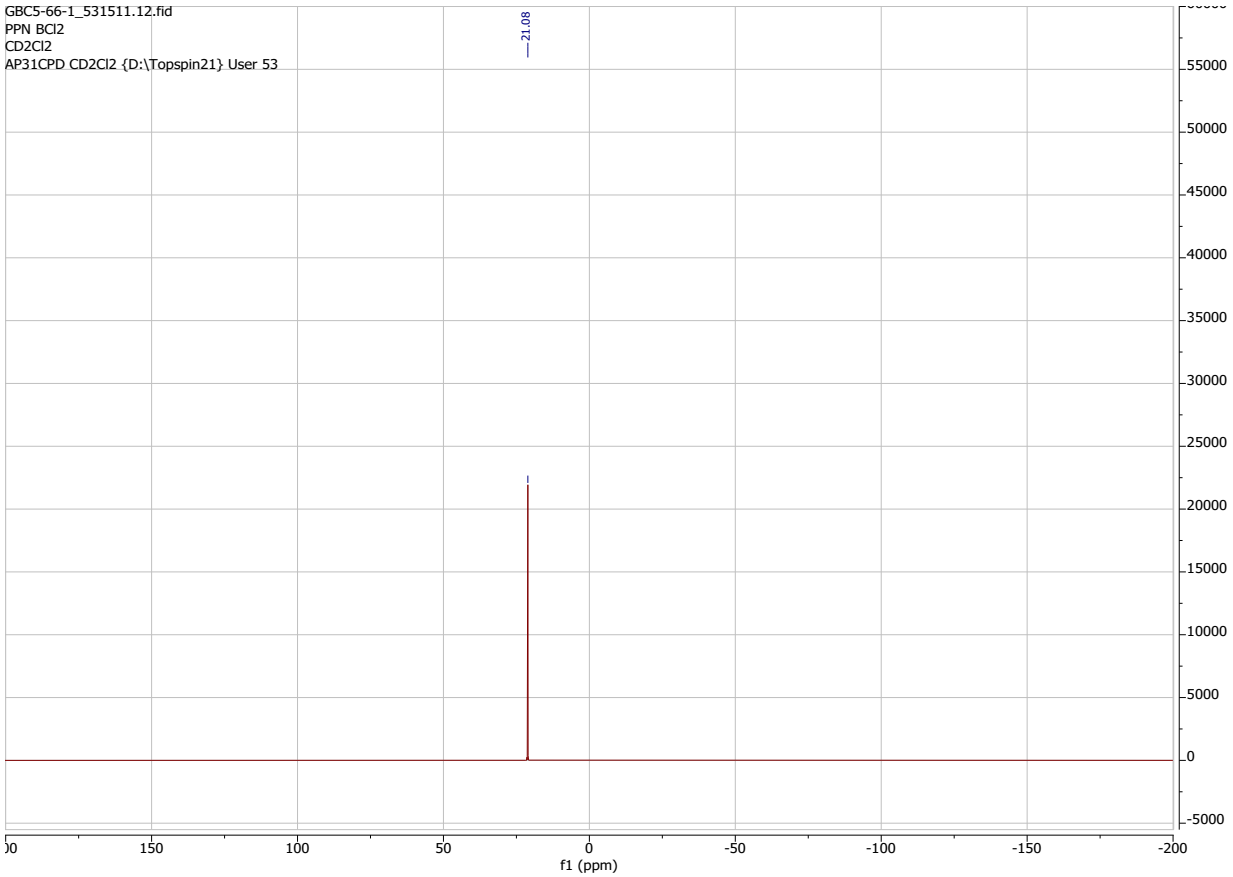


Figure S39 : $^{31}P\{^{1}H\}$ NMR spectrum of **[PPN][6]** in CD_2Cl_2.

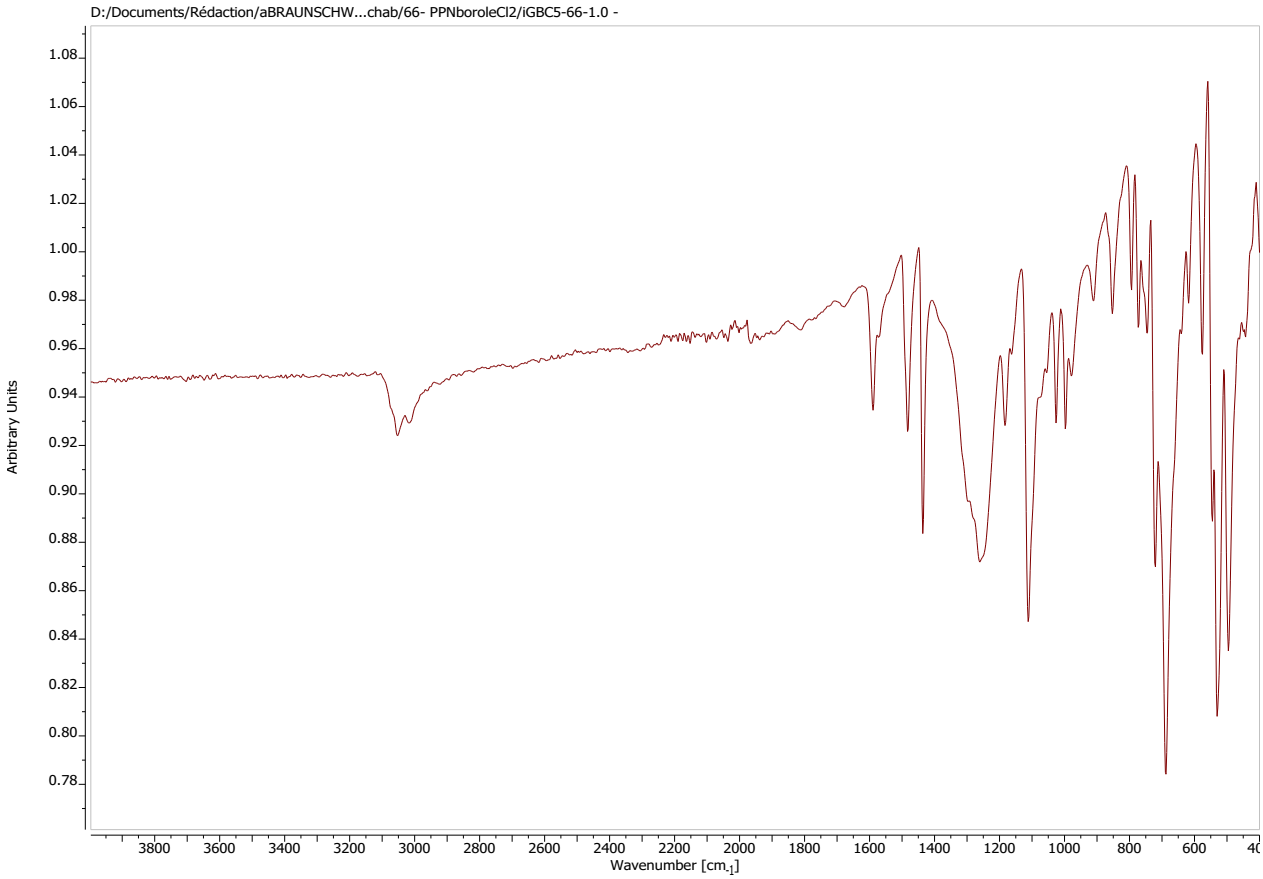
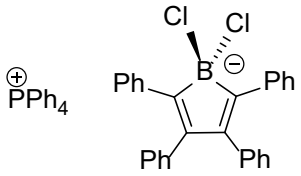


Figure S40 : ATR IR spectrum of **[PPN][6]**.

Synthesis of [PPh_4][borolate(Cl_2)] ([PPh_4][6])



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A dichloromethane solution of [PPh_4]Cl (106 mg ; 0.283 mmol) was added to a solution of **1** (114 mg; 0.283 mmol) in the same solvent, which gave a bright orange solution, that progressively turns to bright yellow. The volatiles were removed *in vacuo*, yielding the compound as a bright yellow, foam-like solid (163 mg; 0.210 mmol, 74 mol% recovered yield based on **1**).

The compound was found to be too sensitive for HRMS-ESI conditions.

^{1}H NMR (CD_2Cl_2): δ = 7.89 (m, 4H, PPh_4^+), 7.73 (m, 8H, PPh_4^+), 7.59 (m, 8H, PPh_4^+), 7.37 (m, 4H, C_6H_5), 6.9 (4 x m, 16H, C_6H_5).

^{11}B NMR (CD_2Cl_2): δ = 7.1 ppm.

^{13}C{^{1}H} NMR (CD_2Cl_2): δ =152.5 (very broad, C_q, C_B, 2C), 145.4 (C_q, 2C), 143.2 (C_q, 2C), 140.5(C_q, 2C), 136.1 (d, J= 3.6 Hz, *C*H, 4C, PPh_4^+), 134.7 (d, J= 10 Hz, *C*H, 8C, PPh_4^+), 131.0 (d, J= 12 Hz, *C*H, 8C, PPh_4^+), 130.7 (*C*H, 4C), 130.0 (*C*H, 4C), 127.2 (*C*H, 4C), 127.1 (*C*H, 4C), 125.3 (*C*H, 2C), 124.2 (*C*H, 2C), 117.8 (d, J= 90 Hz, *C*-P, 4C, PPh_4^+).

^{31}P{^{1}H} NMR (CD_2Cl_2): δ = 23.1 ppm.

HRMS-ESI: $[PPh_4]^+$ 339.1288 (calculated 339.1308).

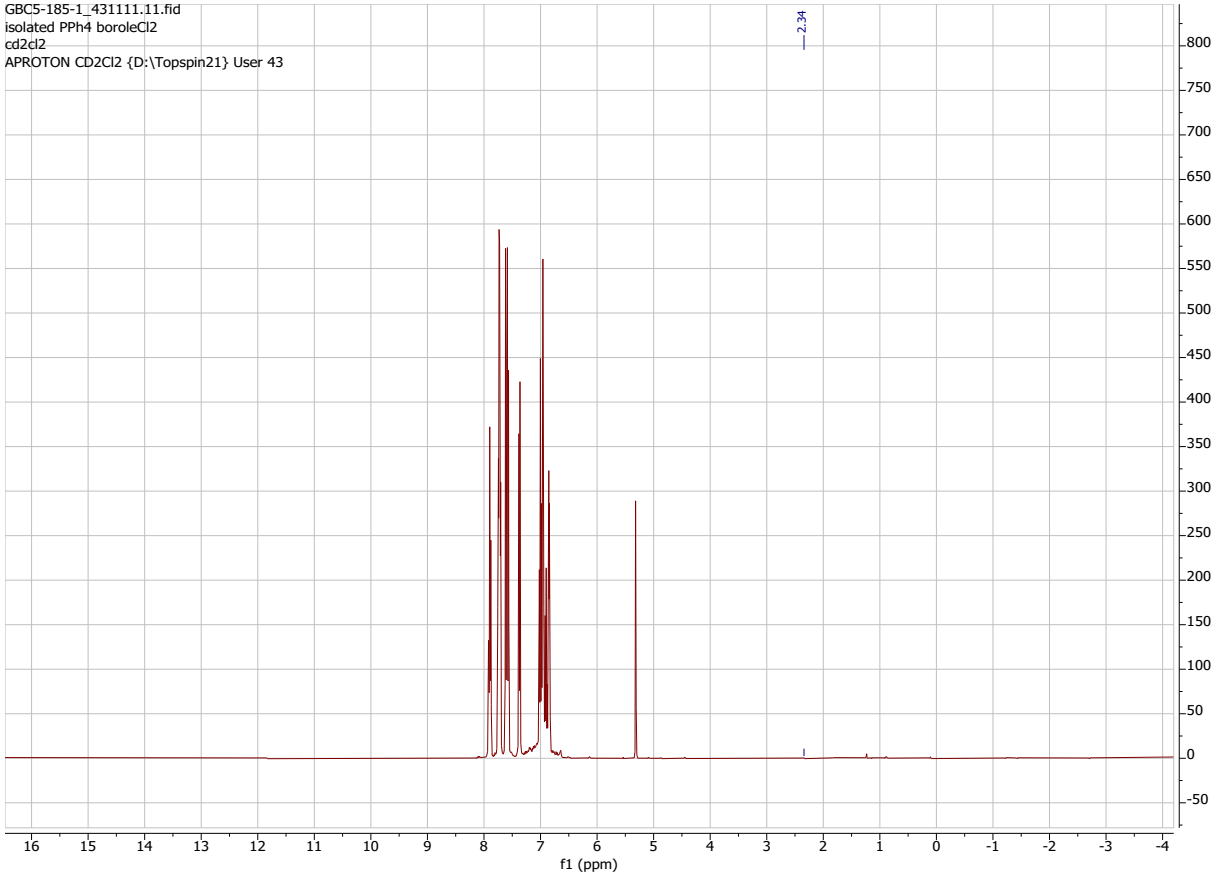

Figure S41 : ^{1}H NMR spectrum of **[PPh_4][6]** in CD_2Cl_2.

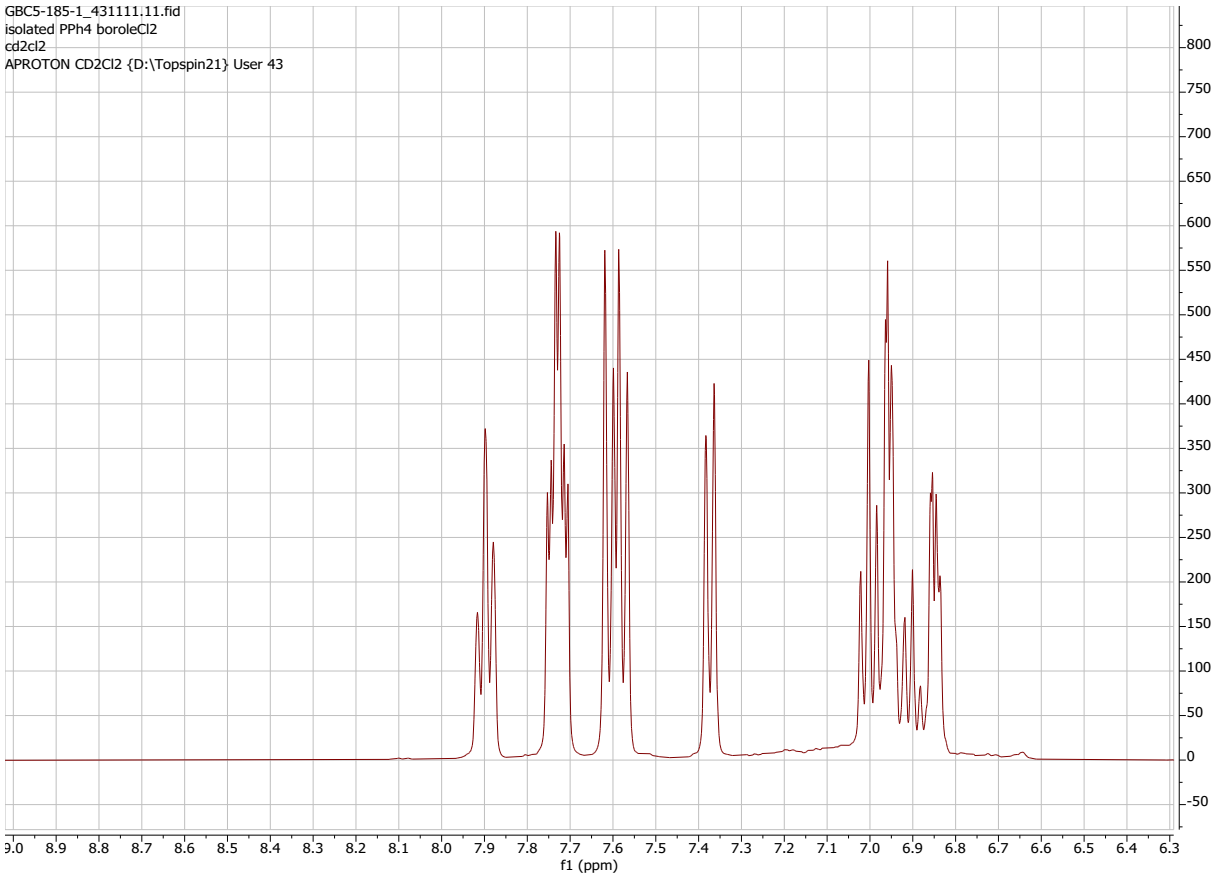

Figure S42 : Extended aromatic region of the ^{1}H NMR spectrum of **[PPh_4][6]** in CD_2Cl_2.

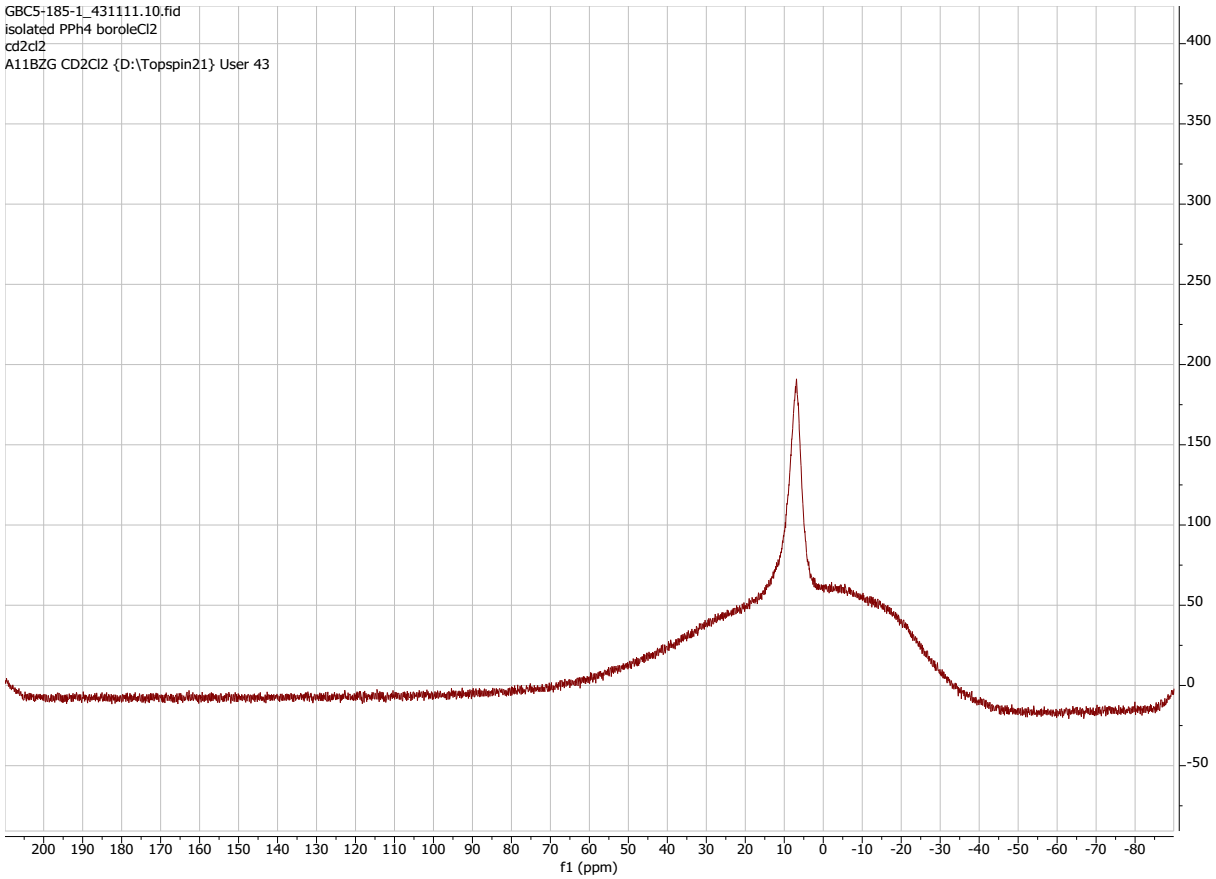

Figure S43 : ^{11}B NMR spectrum of **[PPh_4][6]** in CD_2Cl_2.

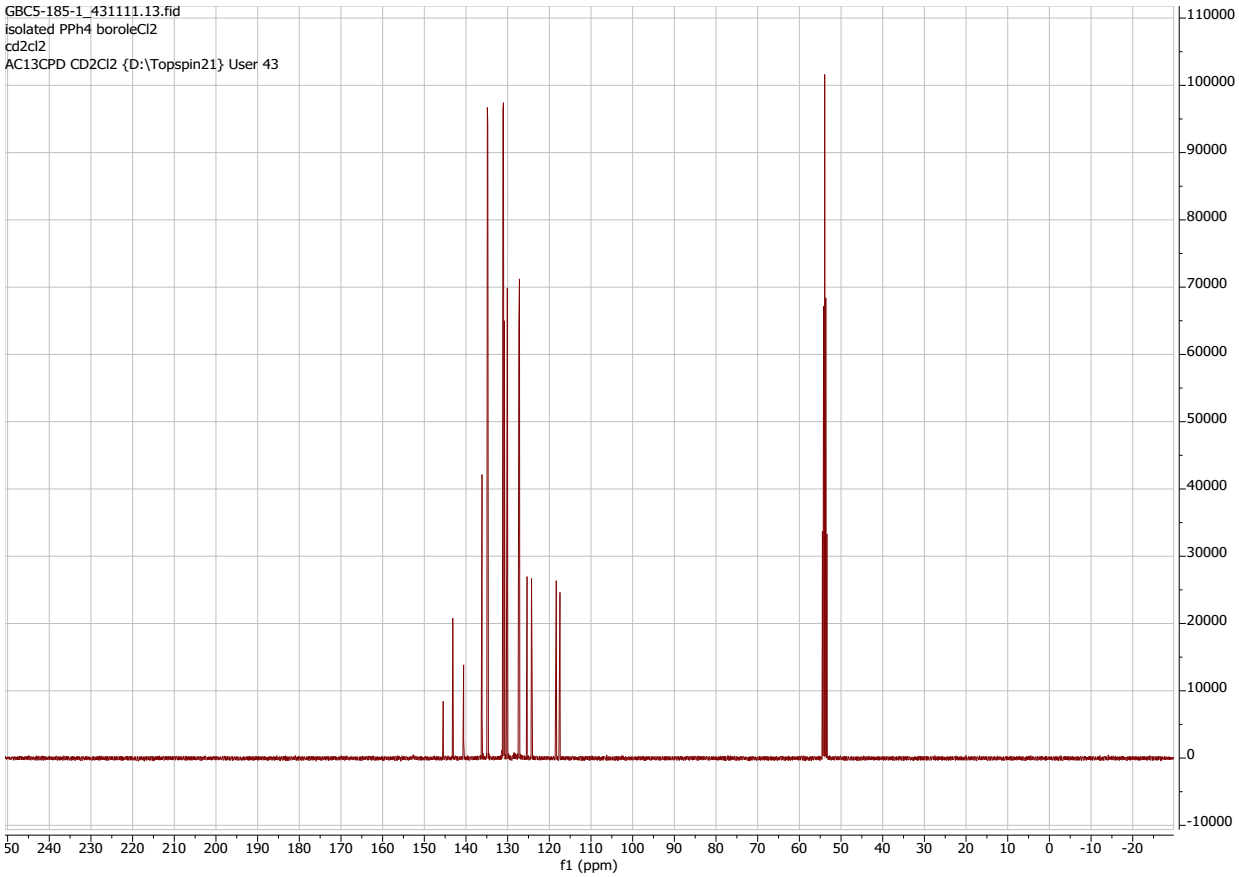

Figure S44 : $^{13}C\{^{1}H\}$ NMR spectrum of **[PPh_4][6]** in CD_2Cl_2.

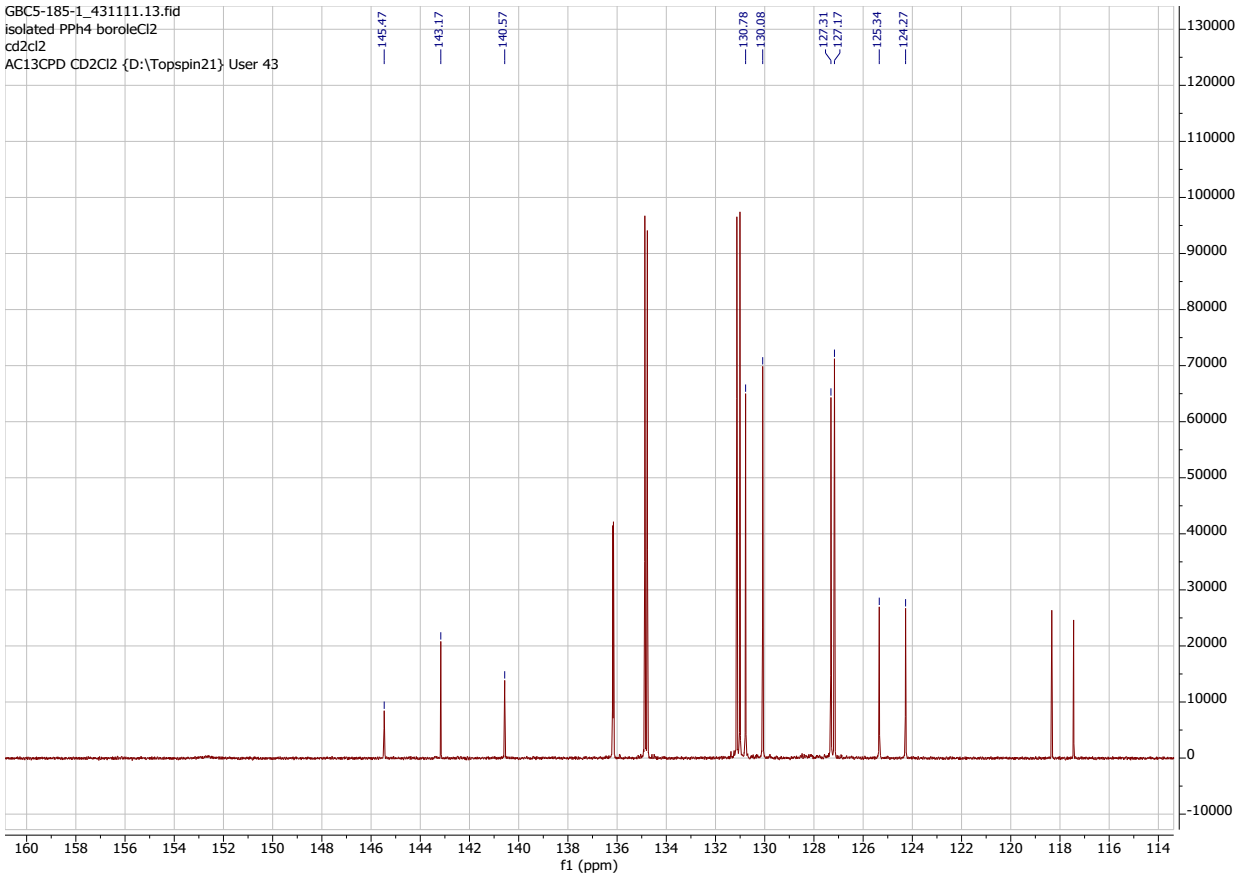

Figure S45 : Extended aromatic region of the ^{13}C NMR spectrum of **[PPh_4][6]** in CD_2Cl_2.

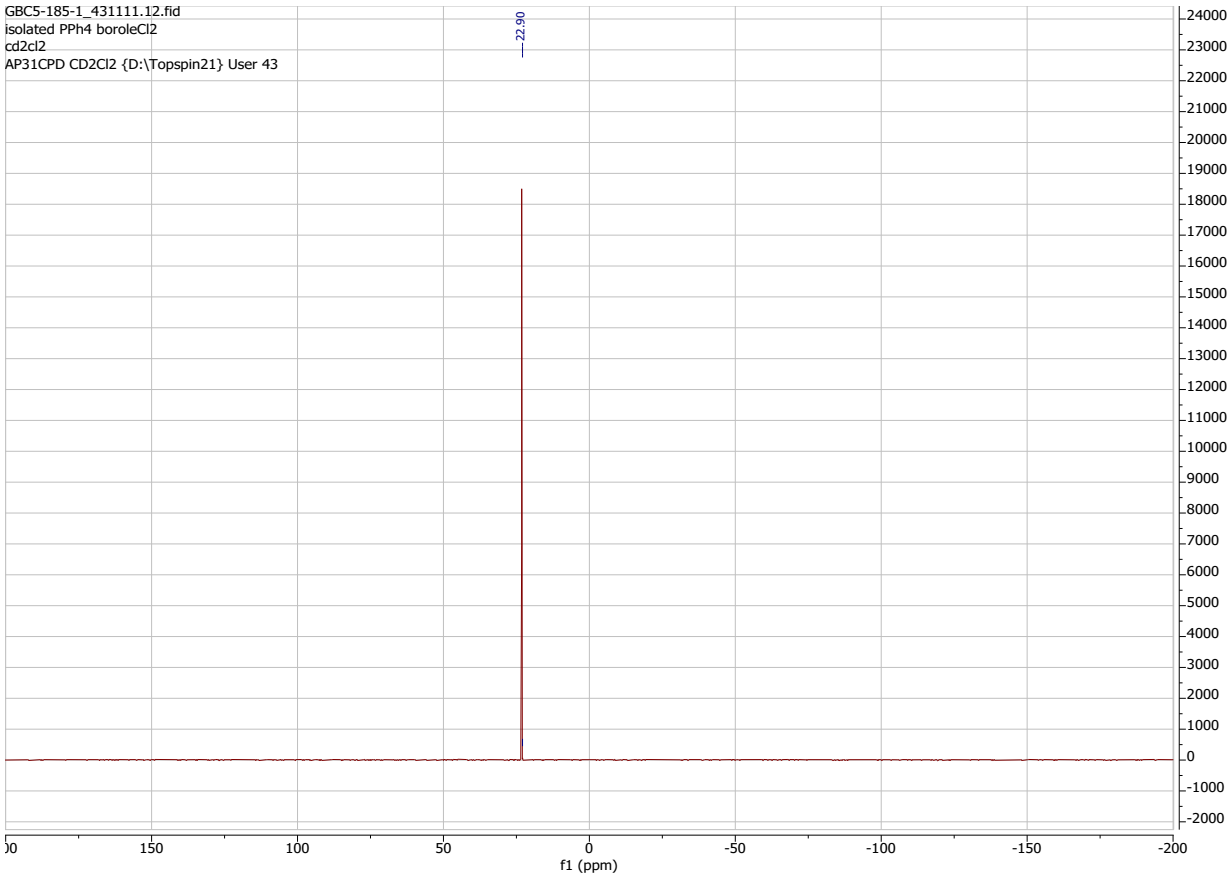

Figure S46 : $^{31}P\{^{1}H\}$ NMR spectrum of **[PPh_4][6]** in CD_2Cl_2.

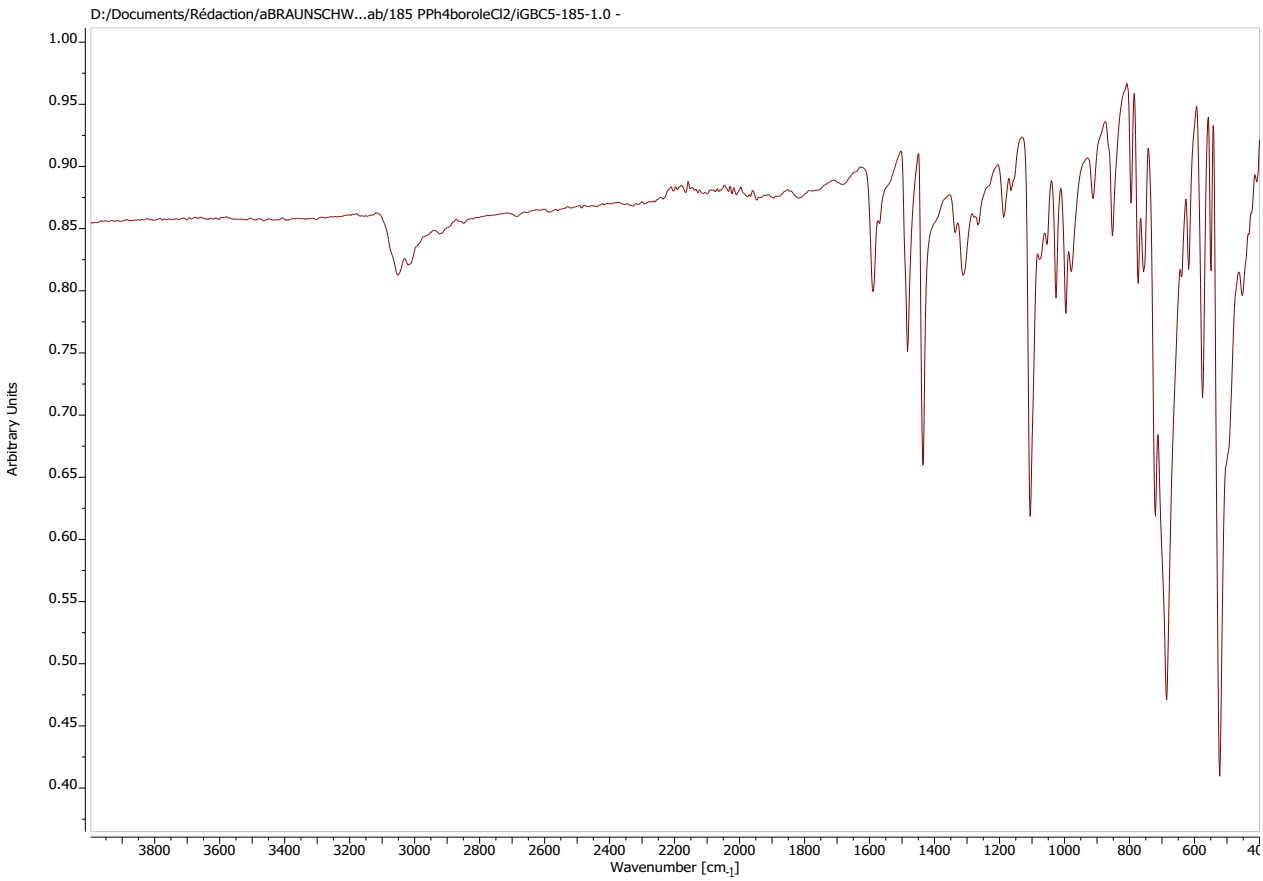

Figure S47 : ATR IR spectrum of **[PPh_4][6].**

Photolysis experiments

The photolysis of salts of **4-mix** and of isolated **5** yield intractable mixtures displaying a very broad ^{11}B signal at 28 ppm. These photolysis products appear to be different in nature than those formed by spontaneous decomposition of **2** (^{11}B NMR signals at 38 and 10 ppm). These photolysis mixtures displayed strong MS signals for masses 777.3474 and 396.1789, corresponding to formulae **[2+BC_4Ph_4+H]$^+$** (calculated 777.3481) and $[HN_2BC_4Ph_4]^+$ (calculated 396.17979). The following gives further details on these photolysis experiments.

A dichloromethane solution of the **[PPh_4][4-mix]** mixture of salts was photolyzed overnight, after which time the only initial species remaining was residual **6** at *ca* 7 ppm in the ^{11}B NMR spectrum. The resulting solution displayed a broad singlet at *ca* 28 ppm in ^{11}B NMR spectroscopy and produced, among other LIFDI-HRMS signals, a peak corresponding to the mass of **2**+C_4Ph_4B+H^+.

LIFDI-HRMS : 777.3474 (777.3481 predicted for $C_{56}H_{40}B_2N_3+H^+$)

A sample of **[PPh_4][5]** in dichloromethane was photolyzed for two days, during which time N_2 evolution could be detected by ^{14}N NMR spectroscopy. The main new product(s) appeared as a broad singlet at 28 ppm in the ^{11}B NMR spectrum of the mixture.

A CD_2Cl_2 solution of the **[PPh_4][4-mix]** mixture of salts was prepared *in situ* from **1** (49 mg; 0.12 mmol) and [PPh_4]N_3 (46 mg; 0.12 mmol). The orange solution was photolyzed for several days, after which time some prismatic crystals could be found near the surface of the solution, which were analyzed by X-ray diffraction and shown to be of trimer **7** (see Crystal Structure Determinations). The structural model is that of a non-planar borazine-like species that can be described as the trimer of 3,4,5,6-tetraphenyl-1,2-azaborine. DFT computations reveal that the borazine core is indeed distorted in the optimized structure of **7**. This distortion is a direct consequence of steric demands of the peripheral aryl groups featuring large R = Ph substituents. Similar distortions are found for the model system where these substituents are replaced by R = Me groups, while a planar B_3N_3 ring is found only for R = H (see Figure S59).

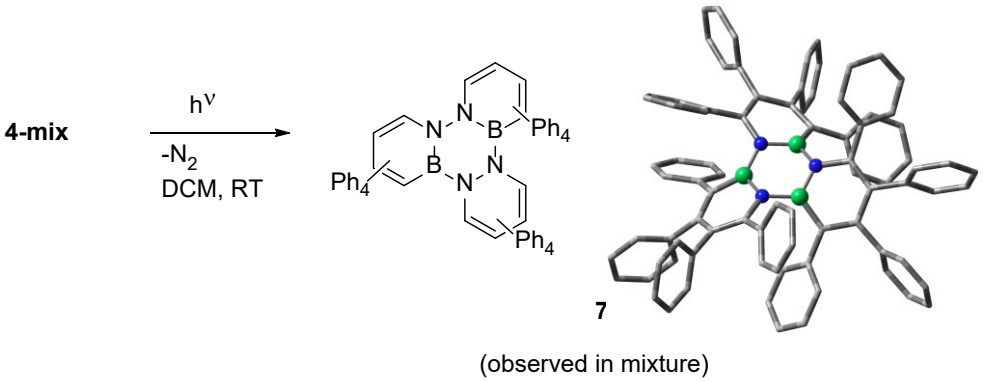

Figure S48: Photolysis experiments on **4-mix** led, on one occasion, to the detection of **7** by X-ray crystallography. (Right) Optimized geometry for 7.

Crystal Structure Determinations

The crystal data of **[PPh$_4$][5], [PPN][6]** and trimer **7** were collected on a BRUKER D8 QUEST diffractometer with a CMOS area detector and multi-layer mirror monochromated Mo$_{K\alpha}$ radiation. The crystal data of **[PPh$_4$][4-mix]** were collected on a BRUKER X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated Mo$_{K\alpha}$ radiation.
The crystal data of **3a** and **3b** were collected on a RIGAKU SYNERGY DUALFLEX HYPIX diffractometer with a CMOS area detector and multi-layer mirror monochromated Cu$_{K\alpha}$ radiation.

The structures were solved using the intrinsic phasing method,[5] refined with the SHELXL program[6] and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealized geometric positions and depicted (unless otherwise mentioned) as spheres of arbitrary radius. Ellipsoids are represented at the 50% probability level.
Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication numbers 2143487-2143492. CCDC. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Crystal structure determination of 3a

Single crystals suitable for X-Ray diffraction were grown via gas phase diffusion of pentane into a saturated solution of **3a** in CH_2Cl_2.
The structure displayed a N_3/Cl substitutional disorder that was modeled as a two-part disorder with refined N3:Cl ratios of 0.93 : 0.07. U_{ij} displacement parameters of "overlapping" atoms Cl1 and N1were restrained to approximate isotropic behavior with the ISOR keyword and displacement parameters were constrained to be similar with the EADP keyword.
Crystal data for GuBC268_GuBC: $C_{46}H_{53}BCl_{0.07}N_{2.78}P$; M_r = 689.22, colorless block, dimensions 0.149 x 0.081 x 0.034 mm^3; Monoclinic space group $P2_1/n$, a = 13.05170(10) Å, b = 16.9298(2) Å, c = 17.5029(2) Å, β = 95.6750(10)°, V = 3848.53(7) Å^3; Z = 4; ρ_{calcd} = 1.190 g·cm^{-3}; μ = 0.937

mm^{-1}; F(000) = 1479; T = 100(2) K; R_1 = 0.0418, wR^2 = 0.1080; 8073 independent reflections [2θ≤154.952°] and 464 parameters, Highest peak 0.33 (e·Å^{-3}) at 0.9042 0.1958 0.0569 [0.99 Å from B1] Deepest hole -0.37 (e·Å^{-3}) at 0.9082 0.1928 0.1131 [0.66 Å from P1].

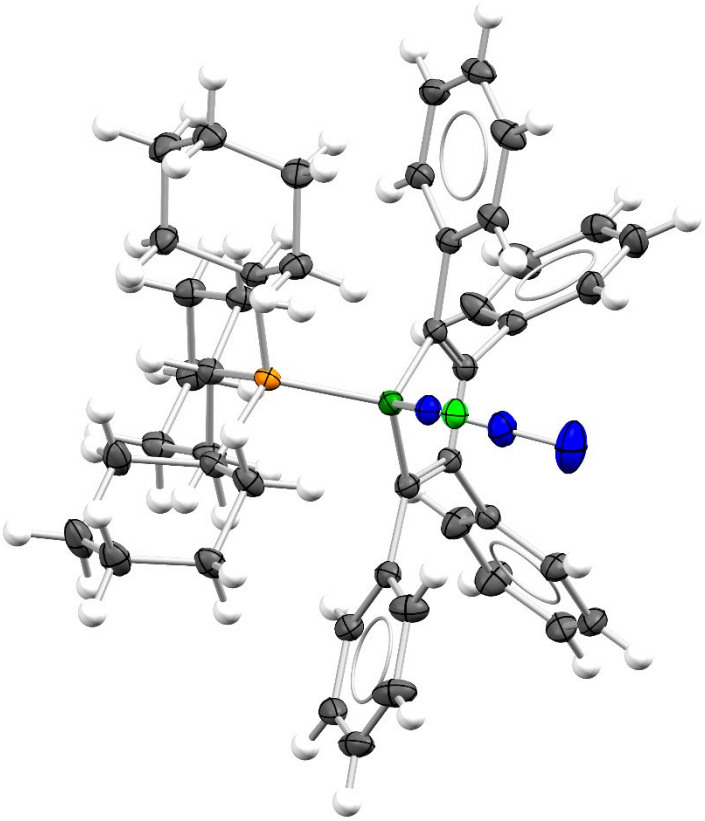

Figure S49 : Solid-state structure of **3a**, showing the minor substitutional N_3/Cl disorder.

Crystal structure determination of 3b

Single crystals suitable for X-Ray diffraction were grown via gas-phase diffusion of pentane into a saturated solution of **3b** in benzene.

The structure displayed an N_3/Cl substitutional disorder that was modeled as a two-part disorder with refined N_3:Cl ratios of 0.97 : 0.03. U_{ij} displacement parameters of "overlapping" atoms Cl1 and N1 had their displacement parameters constrained to be similar with the EADP keyword.

Crystal data for GuBC268_GuBC: $C_{33}H_{25}BCl_{0.03}N_{3.92}$; M_r = 1291.55(9); colorless to pale yellow prism, dimensions 0.315 x 0.239 x 0.181 mm^3; Triclinic space group $P\bar{1}$, a = 10.1028(4)Å, b = 10.3516(4)Å, c = 14.1317(3)Å, α = 76.623(3) °; β = 78.356(3) °; γ = 64.759(4) °,

V = 1291.55(9) Å^3; Z = 2; ρ_{calcd} = 1.255 g·cm^{-3}; μ = 0.600 mm^{-1}; F(000) = 512; T = 100(2) K; R_1 = 0.0421, wR^2 = 0.1164; 5395 independent reflections [2θ≤155.016°] and 347 parameters; Highest peak 0.26 (e·Å^{-3}) at 0.5469 0.5194 0.2100 [0.81 Å from B1], Deepest hole -0.21(e·Å^{-3}) at 0.7018 0.8816 0.3018 [0.69 Å from H6_3]

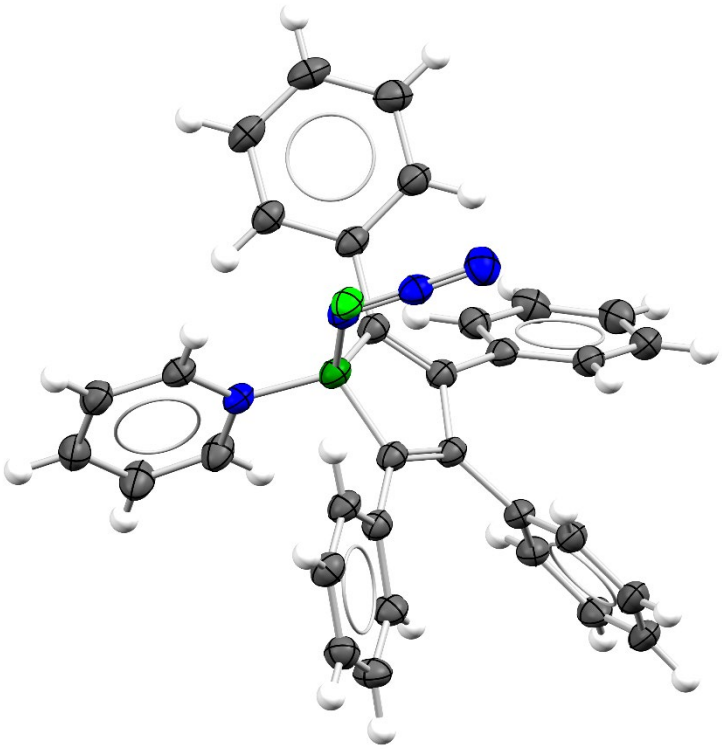

Figure S50 : Solid-state structure of **3b**, showing the minor substitutional N_3/Cl disorder.

Crystal structure determination for [PPh_4][4-mix]

Crystals suitable for X-ray diffraction were obtained from the slow evaporation of the dichloromethane/pentane extract of the crude isolated compound.

The mixture of compounds co-crystallized with one molecule of dichloromethane per asymmetric unit. The compound appears as a borolate anion with a boron atom in a roughly tetrahedral coordination environment with N_3:Cl substitutional disorders at two coordination sites. The substitutional disorders were treated as two independent two-part disorders with refined Cl:N3 ratios of 0.88: 0.12 and 0.87: 0.13. The B1-N1 distance was restrained to 1.5 Å with the DFIX

keyword. Displacement parameters within azide groups were restrained to similar values with the RIGU keyword and U_{ij} displacement parameters were restrained to approximate isotropic behavior with the ISOR keyword. Although the model strongly supports the presence of a mixture of chloride-azide-substituted borole-based anions, the poorly-behaved N-N distances only allows the use of this structure as a strictly qualitative proof of connectivity.
The dichloromethane disorder was treated as a two-part disorder with a refined ratio of 0.86 : 0.14. Interatomic distances were restrained to be similar between dichloromethane molecules with SADI and SAME keywords. Displacement parameters within dichloromethane molecules were restrained to similar values with the RIGU and SIMU keywords.

Crystal data for GuBC063_GuBC: $C_{53}H_{42}BCl_{3.75}N_{0.74}P$; M_r = 864.07; orange prism, dimensions 0.234×0.207×0.143 mm^3; Monoclinic space group $P2_1/n$, a = 18.758(2) Å, b = 12.3357(14) Å, c = 18.957(2) Å, β = 91.531(4)°, V = 4385.1(9) Å^3; Z = 4; ρ_{calcd} = 1.309 g·cm^{-3}; μ = 0.329 mm^{-1}; F(000) = 1796; T = 103(2) K; R_1 = 0.0480, wR^2 = 0.0963; 8972 independent reflections [2θ≤52.744°] and 616 parameters; Highest peak 0.51 (e·Å^{-3}) at 0.4991 0.8343 0.1452 [0.46 Å from N1]; Deepest hole -0.35 (e·Å^{-3}) at 0.3862 0.4230 0.1907 [0.51 Å from P1].

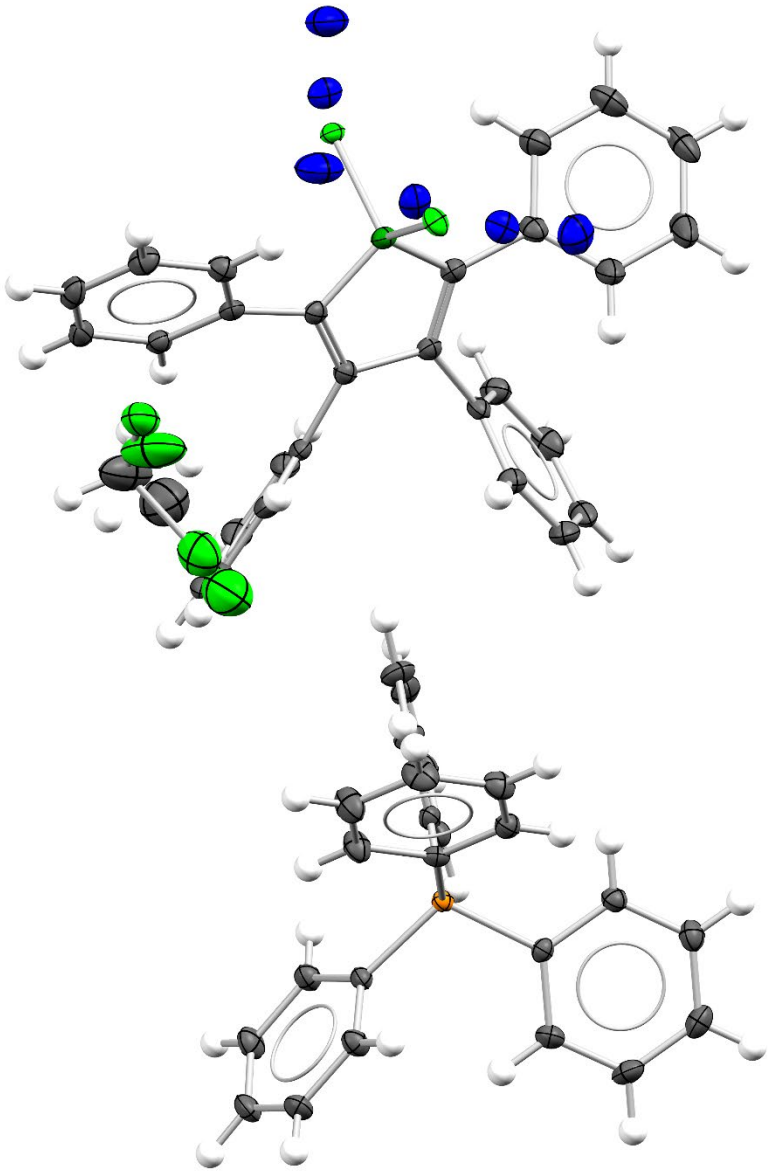

Figure S51 : Solid-state structure of **[PPh_4][4-mix]**, showing the extensive substitutional disorders. Note that the constitution of the particular crystal from which this model was derived does not necessarily reflect the respective occupancies of the N_3 and Cl ligands in the mixture.

Crystal structure determination for [PPh_4][5]

Crystals suitable for X-ray diffraction were obtained from the slow evaporation of a benzene extract of the material resulting from the treatment of *in situ*-generated **3a** with [PPh_4]N_3 in dichloromethane.

One azide group was found to be disordered over two orientations related by a rotation about the B-N bond. This was modeled as a two part disorder with a refined ratio of 0.76 : 0.24. N-N distances between orientations were restrained to similar values with the use of the SADI keyword, while displacement parameters were restrained to similar values with the SIMU keyword.

Crystal data for GuBC058_GuBC: $C_{52}H_{40}BN_6P$; M_r = 790.68, yellow prism, dimensions 0.36×0.142×0.111 mm^3; Monoclinic space group $P2_1/n$, a = 10.3755(7) Å, b = 17.1250(9) Å, c = 23.2382(12) Å, β = 93.498(2)°, V = 4121.3(4) $Å^3$; Z = 4, ρ_{calcd} = 1.274 $g \cdot cm^{-3}$; μ = 0.112 mm^{-1}; $F(000)$ = 1656; T = 100(2) K; R_1 = 0.0825, wR^2 = 0.1489; 8167 independent reflections [2θ≤52.744°] and 561 parameters; Highest peak 0.44 ($e \cdot Å^{-3}$) at 0.7374 0.3221 0.2213 [1.02 Å from P1]; Deepest hole -0.40 ($e \cdot Å^{-3}$) at 0.6971 0.3142 0.1613 [0.72 Å from P1].

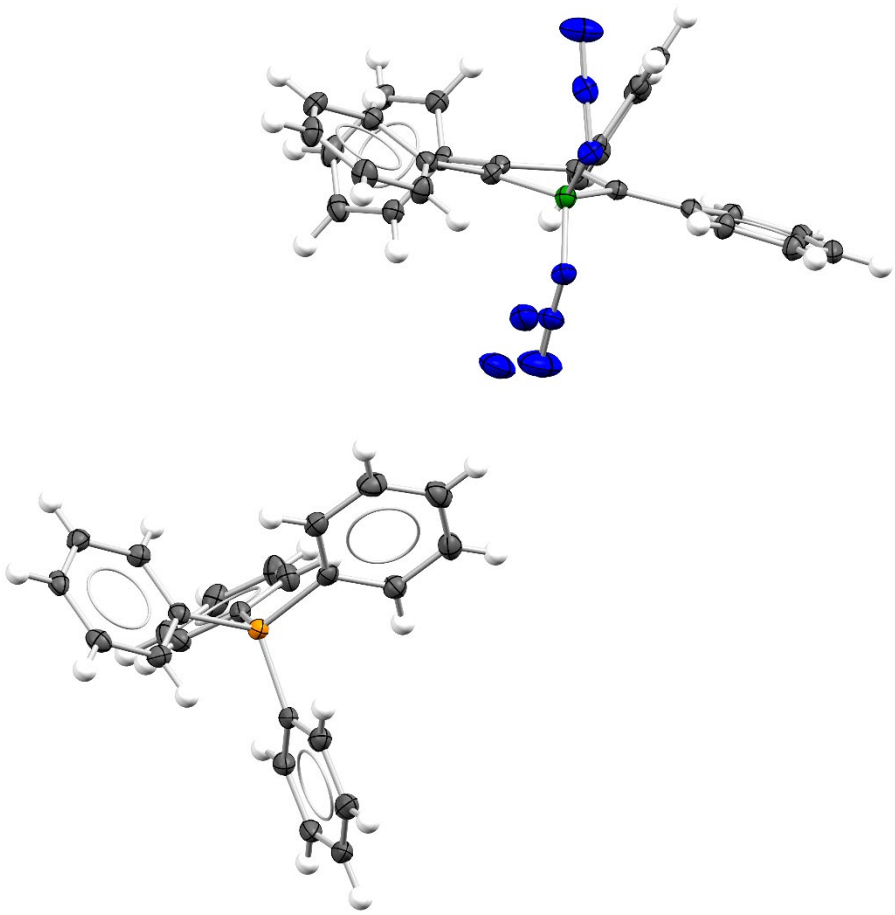

Figure S52 : Solid-state structure of the **[PPh$_4$][5]**, showing the conformational disorder for one of the azide substituents.

Crystal structure determination of [PPN][6]

Crystals suitable for X-ray crystallography could be found directly in the isolated material.

The salt co-crystallized with one dichloromethane molecule, which was heavily disordered over several orientations. This could be modeled as a four-part disorder with refined ratios 0.390: 0.383 : 0.152: 0.073. Interatomic distances within dichloromethane molecules were restrained to similar values for all dichloromethane molecules with the SADI key word. Displacement parameters for dichloromethane atoms were restrained to similar values with the SIMU keyword.

Crystal data for GuBC108_GuBC: $C_{65}H_{52}BCl_4NP_2$; M_r = 1061.48; colorless prism, dimensions 0.297×0.245×0.182 mm^3; Triclinic space group $P\bar{1}$, a = 11.4915(6) Å, b = 13.6720(7) Å, c = 17.9784(8) Å, α = 81.894(2)°, β = 75.6420(10)°, γ = 85.430(2)°, V = 2706.1(2) Å^3; Z = 2; ρ_{calcd} = 1.303 g·cm^{-3}; μ = 0.320 mm^{-1}; F(000) = 1104; T = 100(2) K; R_1 = 0.0679, wR^2 = 0.1600; 11075 independent reflections [2θ≤52.742°] and 743 parameters; Highest peak 0.90 (e·Å^{-3}) at 0.0129 0.7748 0.1663 [0.90 Å from N1_2]; Deepest hole -0.57 (e·Å^{-3}) at 0.5080 0.8234 0.4745 [0.65 Å from CL1A_4].

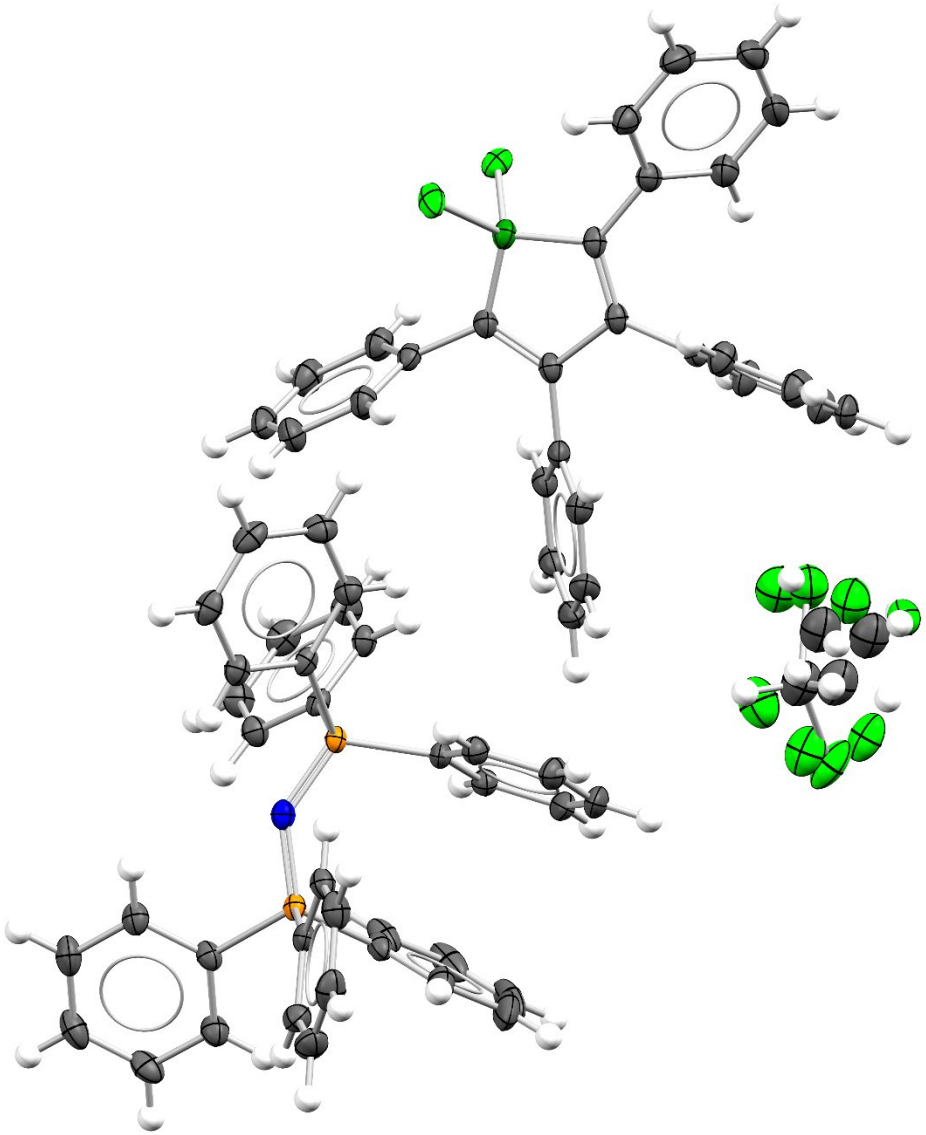

Figure S53 : Solid-state structure of the **[PPN][6]**, showing the co-crystallized dichloromethane molecule in its two disordered orientations.

Crystal structure determination of Azaborinine trimer 7

Crystals suitable for X-ray diffraction were obtained near the surface of a solution containing the photolysis products of **[PPh_4][4-mix]** in CD_2Cl_2 in an NMR tube.

The crystals diffracted weakly. The crystal yielding a more complete dataset bore a disordered dichloromethane solvate molecule in addition to having its main residue disordered about a C_2 rotation axis. Despite this, the model supports the existence of trimer **7**. The unusual, distorted nature of the BNBNBN ring in **7** is supported by computational calculations (see below).

The disorder on the main residue was approximated by treating two of the most heavily disordered aryl moieties as separate "independent" disorders and the central BNBNBN ring as a third disorder.

The BNBNBN ring was treated as a two-part disorder with occupancy constrained to 0.5 about a symmetry element (Part -1 instruction). B-N distances were restrained to similar values with SADI constraints. The displacement parameters of atoms N1 >B3 were restrained to similar value with similarity constraint simu and their U_{ij} displacement parameters were restrained to approximate isotropic behavior with the ISOR keyword.

The two disordered aryl groups (and RESI_1/RESI_2; RESI_3/RESI_4) were treated similarly: they were modeled as two-part disorders (refined ratios of 0.52:0.48 and 0.59:0.41, respectively) distances and displacement parameters were restrained to similar values with keywords SAME, SIMU and RIGU and U_{ij} displacement parameters were restrained to approximate isotropic behavior with the ISOR keyword.

The dichloromethane molecule was disordered over two orientations that were modeled as a two-part disorder with a refined ratio 0.59:0.61.
The displacement parameters of atoms C4 > Cl1a were restrained to similar value with similarity constraint simu and their U_{ij} displacement parameters were restrained to approximate isotropic behavior with the ISOR keyword. Interatomic distances in dichloromethane molecules were restrained to similar value between both with the SADI restraint.

Crystal data for GuBC010_LF: $C_{86}H_{64}B_3Cl_4N_3$; M_r = 1313.63; yellow prism, dimensions 0.166 mm x 0.214 mm x 0.218 mm^3; Monoclinic space group *C*2/*c*, *a* = 29.7421(11) Å, *b* = 15.8764(7) Å, *c* = 16.4574(7) Å, β = 118.2850(10)°, *V* = 6843.3(5) Å^3; *Z* = 4; ρ_{calcd} = 1.275 g·cm^{-3}; μ = 0.223 mm^{-1}; *F*(000) = 2736; *T* = 100(2) K; R_1 = 0.0940, wR^2 = 0.2331; 6273 independent reflections [2θ≤50.68°] and 609 parameters; Highest peak 0.87 (e·Å^{-3}) at 0.0534 0.5251 0.0879 [0.84 Å from C4_1], Deepest hole -1.03 (e·Å^{-3}) at 0.1468 0.6584 0.0725 [0.48 Å from CL1A].

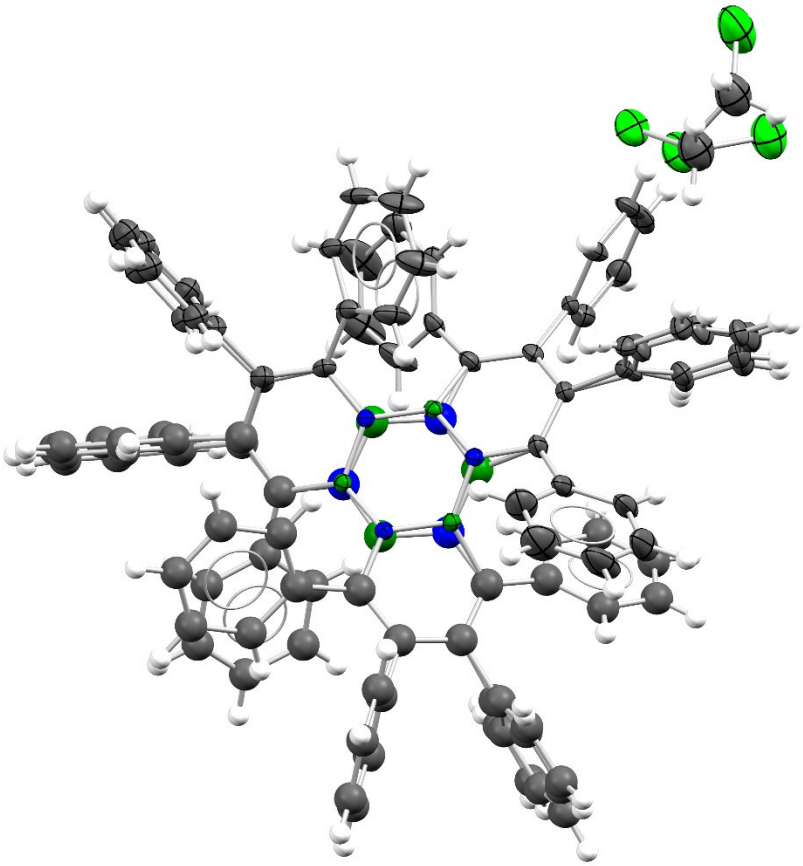

Figure S54 : Complete model for the solid-state structure of trimer **7**, showing the conformationally-disordered molecule as well as the disordered co-crystallized dichloromethane molecule.

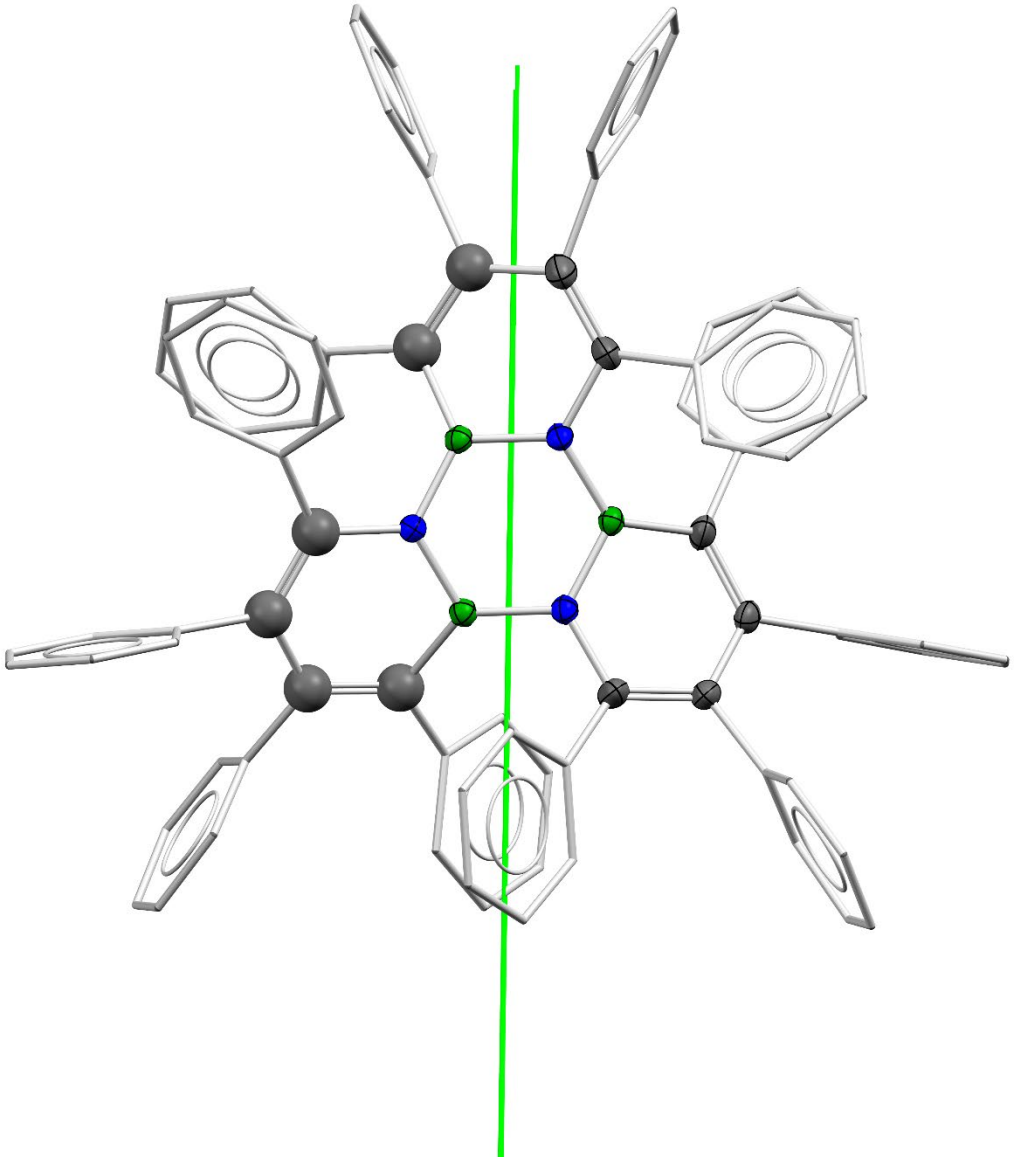

Figure S55 : Depiction of the asymmetric unit in the solid-state structure of trimer **7** showing how the whole molecule is generated by the application of a two-fold rotation axis going through its center. Ellipsoids for peripheral aryl groups are omitted for clarity.

Computational Details

Geometry optimizations and Hessian calculations were performed at the ωB97XD[7]/6-31+G** level of theory. All optimized geometries were characterized as either minimum energy structures (only positive eigenvalues) or transition states (one negative eigenvalue) by vibrational frequency calculations. Solvation corrections were included using the solvent model based on density (SMD)[8] method at the ωB97XD/6-311++G** level. A concentration correction of $\Delta G^{0\rightarrow *}$ = 1.89 kcal mol^{-1} was also included in the free energies of all species in order to account for the change in standard states in going from gas phase (1 atm) to the condensed phase (1 M) and to properly describe associative/dissociative steps.[9, 10] Wiberg bond indexes (WBI)[11] were obtained for selected bonds. In order to investigate the antiaromaticity of the compounds, we performed calculations based on the nucleus-independent chemical shift (NICS)[12-14] approach. Optical HOMO-LUMO gaps were obtained from TDDFT computations. WBI calculations were done in Multiwfn 3.8.[15] [15] All geometry optimizations, vibrational frequencies, TDDFT, and NICS calculations were performed in Gaussian 16, revision C.01.[16]

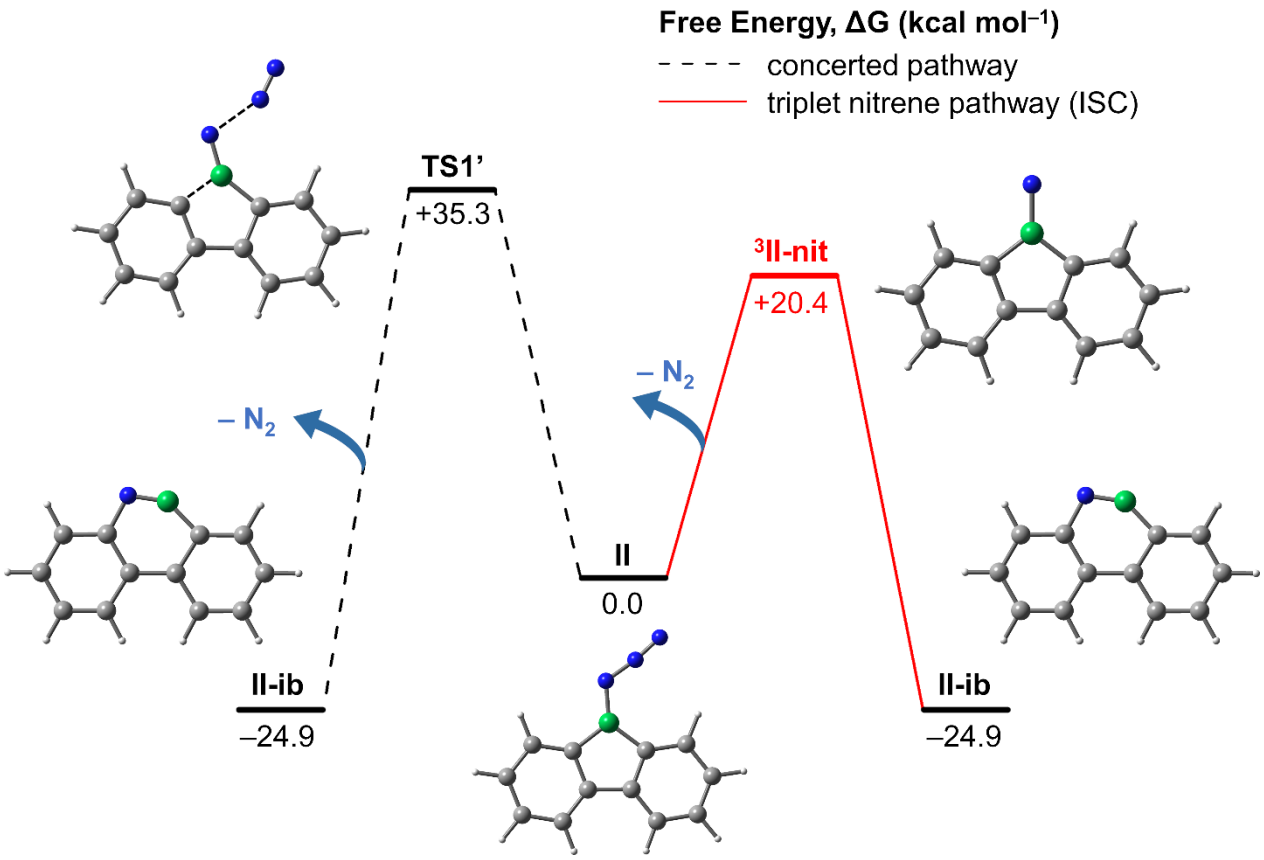

Figure S56 : Comparison of the free energy profile of the nitrogen insertion step for **2** (black curve) and the azidoborafluorene (red curve). Level of theory: ωB97XD/6-311++G**+SMD from optimized structures at the ωB97XD/6-31+G**.

Our computations (Figure S57) reveal that **2** (FA = 82.0 kcal mol^{-1}) has a larger Lewis acidity than azidoborafluorene **II** (FA = 75.5 kcal mol^{-1}). The computed FA value for the parent borole $C_4H_4BN_3$ (FA = 71.9 kcal mol^{-1}) indicates that the Lewis acidity of **2** is enhanced by the presence of Ph substituents as a consequence of their inductive electron withdrawing effects. Our calculations also show that **2** has smaller optical HOMO-LUMO (HL) and adiabatic singlet-triplet (ST) gaps (2.37 eV and 20.7 kcal mol^{-1}, respectively) in comparison to those of azidoborafluorene **II** (3.38 eV and 54.9 kcal mol^{-1}). We attribute these differences to the smaller antiaromaticity of the latter due to its extended π-conjugation (as depicted in its HOMO, see Figure S57), which confers extra stabilization to the molecule and lowers its HOMO energy by 0.64 eV. In contrast, the LUMO of azidoborafluorene is not π extended and has additional nodal planes, which increases its energy in comparison to that of 2 by 0.37 eV. The smaller LUMO energy of **2** also reflects its

higher Lewis acidity, as observed in the FIA computations. Further nucleus independent chemical shift (NICS) calculations indeed reveal that the antiaromaticity of **2** (NICS(1): +6.3 ppm; $NICS_{zz}(1)$: +22.6 ppm) is larger than that of azidoborafluorene (NICS(1): +4.6 ppm; $NICS_{zz}(1)$: +20.7 ppm), supporting its description as less antiaromatic. These results provide further rationales for the observed stability differences between **2** and the azidoborafluorene **II**.

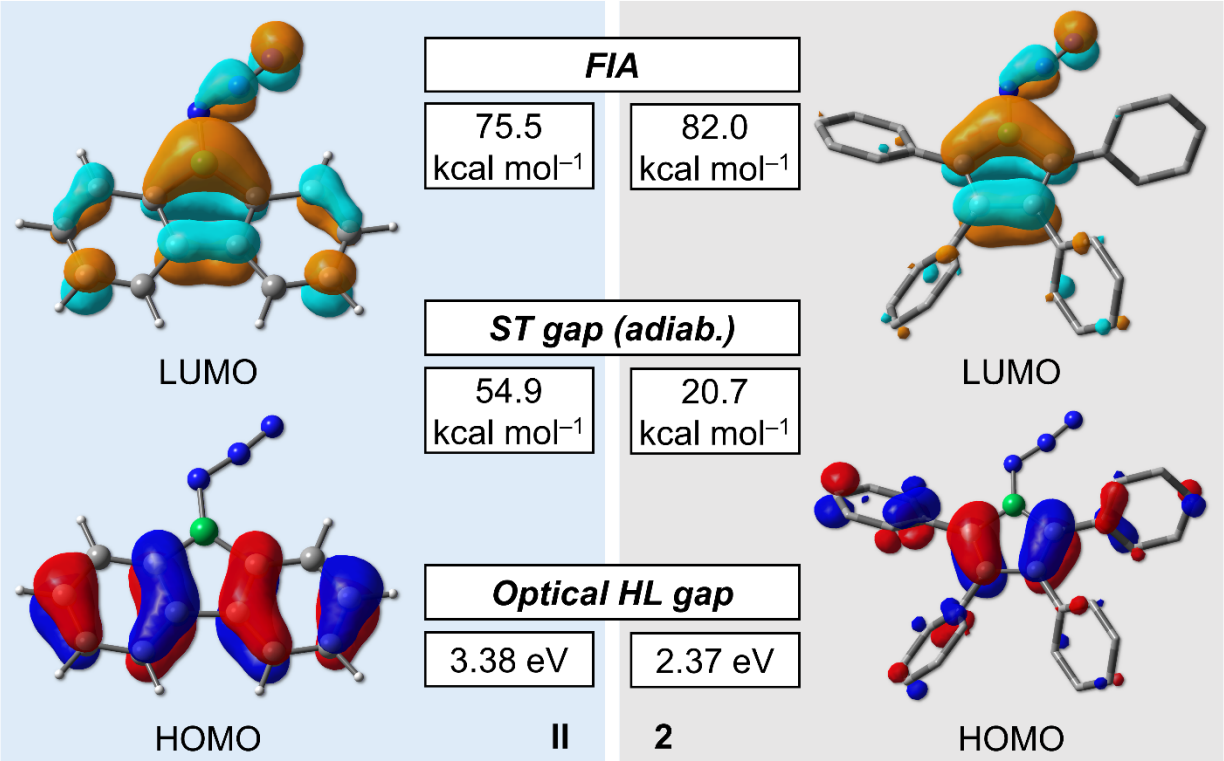

Figure S57 : Computed fluoride ion affinity (FIA), adiabatic singlet-triplet gap (ST gap), and optical HOMO-LUMO gap (HL gap) of the azidoborafluorene **II** and the borole azide **2**. Their corresponding Canonical Kohn-Sham molecular orbitals (isosurface: 0.03 a.u.) are also shown. Level of theory: ωB97XD/6-31+G**.

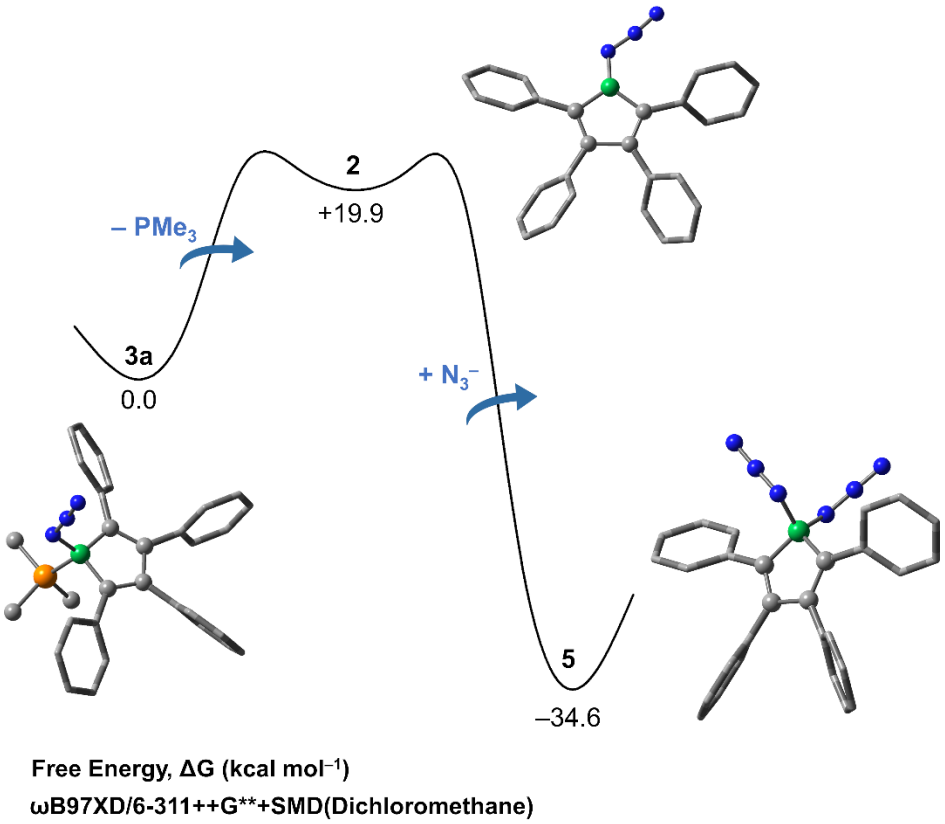

Figure S58 : Free energy profile of the formation of **5** from **3a** following the dissociative pathway. **2** is characterized as a shallow minimum energy structure. Level of theory: ωB97XD/6-311++G**+SMD from optimized structures at the ωB97XD/6-31+G**.

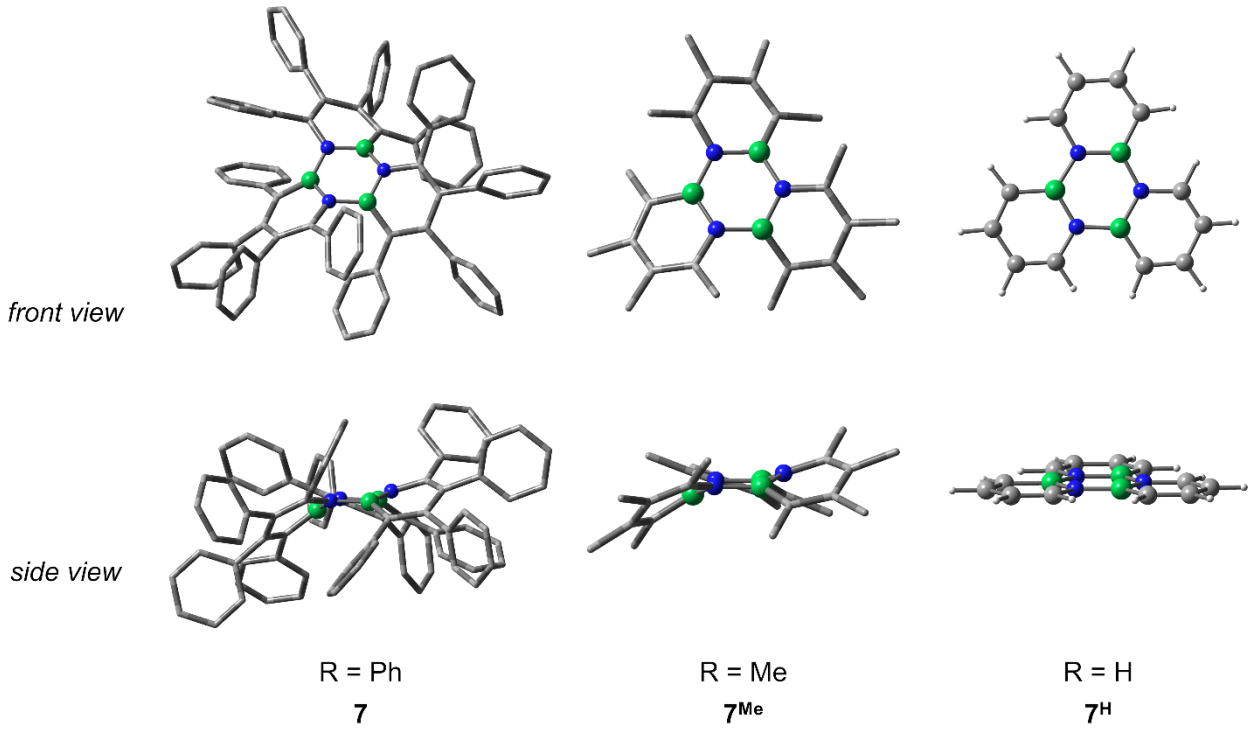

Figure S59 : Front and side views of the optimized structures of the trimer **7** and its corresponding model systems $\mathbf{7^{Me}}$ and $\mathbf{7^{H}}$. Level of theory: ωB97XD/6-31+G**.

Cartesian Coordinates

Coordinates in angstrom from optimizations at the ωB97XD/6-31+G** level of theory.

1 (E: -1563.78328407 hartree)

C	1.266404000	-0.982420000	-0.030838000
C	0.766201000	0.275971000	-0.010246000
C	-0.766195000	0.275967000	0.010185000
C	-1.266390000	-0.982427000	0.030808000
C	2.688008000	-1.375244000	0.029016000
C	3.186747000	-2.350422000	-0.844032000
C	3.564317000	-0.805035000	0.962917000
C	4.526242000	-2.728353000	-0.801131000
H	2.520545000	-2.809857000	-1.568169000
C	4.900883000	-1.185827000	1.009660000
H	3.191029000	-0.056947000	1.655473000
C	5.388735000	-2.146499000	0.124931000
H	4.894889000	-3.481052000	-1.491268000
H	5.563246000	-0.732392000	1.740735000
H	6.432280000	-2.443327000	0.161573000
C	1.549260000	1.529551000	-0.002587000
C	1.308779000	2.526127000	0.950989000
C	2.557210000	1.731301000	-0.953211000
C	2.069329000	3.691246000	0.961654000
H	0.524580000	2.387593000	1.688881000
C	3.307793000	2.901990000	-0.950179000
H	2.751006000	0.960743000	-1.692950000
C	3.068010000	3.884257000	0.009347000
H	1.875886000	4.452226000	1.711083000
H	4.083711000	3.045422000	-1.695535000
H	3.655818000	4.796857000	0.013736000
C	-1.549263000	1.529543000	0.002559000
C	-2.557205000	1.731268000	0.953197000
C	-1.308812000	2.526132000	-0.951012000
C	-3.307806000	2.901946000	0.950187000
H	-2.750982000	0.960699000	1.692929000
C	-2.069383000	3.691239000	-0.961656000
H	-0.524626000	2.387616000	-1.688919000
C	-3.068051000	3.884226000	-0.009332000
H	-4.083718000	3.045357000	1.695555000
H	-1.875964000	4.452227000	-1.711082000
H	-3.655874000	4.796817000	-0.013705000
C	-2.687994000	-1.375258000	-0.029004000
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C	-4.526210000	-2.728345000	0.801219000
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C	-5.388721000	-2.146524000	-0.124846000
H	-4.894843000	-3.481022000	1.491388000
H	-5.563264000	-0.732467000	-1.740690000
H	-6.432266000	-2.443355000	-0.161459000
B	0.000009000	-1.910346000	-0.000026000
Cl	0.000016000	-3.663814000	-0.000067000

2 (E: -1267.73348825 hartree)

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C	1.245568000	-1.019986000	0.013313000
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C	-3.334463000	-1.730756000	1.029105000
C	-3.537056000	-0.384193000	-0.955221000
C	-4.709992000	-1.945296000	1.028066000
H	-2.720675000	-2.168740000	1.812841000
C	-4.911376000	-0.599328000	-0.959176000
H	-3.080142000	0.227610000	-1.727235000
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H	-5.160987000	-2.555898000	1.804182000
H	-5.522162000	-0.156750000	-1.740076000
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H	-3.637691000	3.614695000	1.607209000
H	-3.006589000	5.264878000	-0.139324000
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C	2.823302000	1.537811000	-0.962365000
C	1.686860000	2.473173000	0.946494000
C	3.694515000	2.622060000	-0.975291000
H	2.927013000	0.745069000	-1.696936000
C	2.565119000	3.552472000	0.940015000
H	0.899919000	2.423203000	1.692932000
C	3.569569000	3.631808000	-0.022449000
H	4.474205000	2.676734000	-1.728607000

H	2.459884000	4.335517000	1.684361000
H	4.250492000	4.477189000	-0.031288000
C	2.609169000	-1.578766000	0.082850000
C	2.958939000	-2.674552000	-0.717941000
C	3.575227000	-1.058312000	0.956374000
C	4.241124000	-3.214996000	-0.668975000
H	2.217996000	-3.102347000	-1.386223000
C	4.853869000	-1.602111000	1.010140000
H	3.318350000	-0.221179000	1.597838000
C	5.194679000	-2.679785000	0.193805000
H	4.493498000	-4.058906000	-1.303866000
H	5.586443000	-1.184113000	1.693935000
H	6.193591000	-3.102828000	0.235680000
B	-0.117653000	-1.809714000	-0.004024000
N	-0.193219000	-3.231431000	-0.133698000
N	-1.255136000	-3.861652000	-0.233730000
N	-2.124878000	-4.569850000	-0.345278000

3a (E: -1728.83621426 hartree)

C	-1.265387000	-0.448298000	0.258963000
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C	1.238374000	-0.473444000	0.264544000
C	-2.699090000	-0.803712000	0.251125000
C	-3.220008000	-1.675271000	1.219968000
C	-3.565516000	-0.355218000	-0.757549000
C	-4.553361000	-2.072367000	1.187496000
H	-2.574852000	-2.040490000	2.011396000
C	-4.898259000	-0.756690000	-0.795987000
H	-3.188109000	0.314907000	-1.522684000
C	-5.399274000	-1.618638000	0.176875000
H	-4.932408000	-2.739970000	1.955469000
H	-5.546030000	-0.392735000	-1.588018000
H	-6.438263000	-1.932018000	0.149518000
C	-1.518121000	2.070150000	0.060993000
C	-1.885551000	2.645024000	-1.158910000
C	-1.877210000	2.722113000	1.243241000
C	-2.600432000	3.838388000	-1.200230000
H	-1.608342000	2.149419000	-2.086521000
C	-2.591985000	3.916963000	1.206679000
H	-1.593557000	2.283236000	2.195157000
C	-2.955794000	4.478737000	-0.014746000
H	-2.880187000	4.268383000	-2.157365000
H	-2.865614000	4.408856000	2.134991000
H	-3.513003000	5.409912000	-0.043471000
C	1.552353000	2.031802000	0.094660000
C	1.478701000	2.917717000	-0.985547000

C	2.431135000	2.327218000	1.142864000
C	2.267855000	4.063922000	-1.022117000
H	0.804178000	2.704842000	-1.808728000
C	3.219012000	3.473644000	1.110055000
H	2.495284000	1.643915000	1.984302000
C	3.141065000	4.346041000	0.026290000
H	2.198769000	4.738261000	-1.870374000
H	3.895281000	3.685526000	1.932548000
H	3.754631000	5.241261000	-0.000096000
C	2.663304000	-0.855246000	0.192633000
C	3.518680000	-0.308406000	-0.778050000
C	3.184205000	-1.842764000	1.042380000
C	4.840417000	-0.727980000	-0.891783000
H	3.139296000	0.457020000	-1.448447000
C	4.508510000	-2.258509000	0.934527000
H	2.544070000	-2.290003000	1.795147000
C	5.343007000	-1.706317000	-0.035244000
H	5.479971000	-0.287747000	-1.651088000
H	4.888584000	-3.018380000	1.610881000
H	6.374471000	-2.033503000	-0.121910000
B	-0.022491000	-1.483220000	0.334714000
N	-0.036441000	-2.607198000	1.393266000
N	-0.013041000	-2.288776000	2.570151000
N	0.005955000	-2.075981000	3.689216000
P	-0.043325000	-2.468373000	-1.374024000
C	-0.079676000	-1.331017000	-2.791348000
C	-1.493781000	-3.554814000	-1.536216000
H	0.777611000	-0.656473000	-2.723283000
H	-0.996040000	-0.737929000	-2.743829000
H	-0.044325000	-1.879749000	-3.735675000
H	-1.514206000	-4.233698000	-0.680100000
H	-1.450088000	-4.130972000	-2.464362000
H	-2.404488000	-2.950842000	-1.515014000
C	1.409833000	-3.539198000	-1.604544000
H	2.313362000	-2.925509000	-1.642127000
H	1.319050000	-4.125946000	-2.522681000
H	1.487979000	-4.209009000	-0.744641000

4 (E: -1728.05165270 hartree)

C	-1.252736000	-0.555444000	0.096957000
C	-0.613135000	0.636253000	0.036223000
C	0.877272000	0.464278000	-0.022329000
C	1.227665000	-0.842923000	-0.023428000
C	-2.716074000	-0.741800000	0.037162000
C	-3.359640000	-1.627591000	0.914749000
C	-3.501794000	-0.080750000	-0.920599000
C	-4.737027000	-1.820923000	0.855105000

H	-2.762250000	-2.167081000	1.642536000
C	-4.877622000	-0.276798000	-0.983289000
H	-3.019903000	0.591277000	-1.624099000
C	-5.505325000	-1.145027000	-0.091039000
H	-5.210057000	-2.513232000	1.546285000
H	-5.460857000	0.247075000	-1.736062000
H	-6.579362000	-1.302119000	-0.141247000
C	-1.257063000	1.973019000	0.007273000
C	-0.946128000	2.908541000	-0.988333000
C	-2.200271000	2.330752000	0.978853000
C	-1.564903000	4.154947000	-1.019079000
H	-0.209497000	2.652667000	-1.744286000
C	-2.821188000	3.576105000	0.950703000
H	-2.449048000	1.612559000	1.754366000
C	-2.506644000	4.495327000	-0.049206000
H	-1.307972000	4.863345000	-1.801848000
H	-3.553957000	3.828551000	1.712175000
H	-2.989133000	5.468511000	-0.071208000
C	1.802932000	1.623791000	-0.052909000
C	2.782246000	1.732727000	-1.047968000
C	1.722613000	2.637838000	0.910275000
C	3.660455000	2.812302000	-1.073663000
H	2.854610000	0.950142000	-1.797335000
C	2.599013000	3.718892000	0.887361000
H	0.961595000	2.574389000	1.682543000
C	3.573281000	3.811679000	-0.105398000
H	4.416018000	2.872268000	-1.852188000
H	2.517926000	4.492776000	1.645645000
H	4.256717000	4.655983000	-0.125582000
C	2.604998000	-1.368738000	0.001122000
C	2.948844000	-2.457441000	-0.814964000
C	3.593855000	-0.843817000	0.847231000
C	4.241753000	-2.974027000	-0.813641000
H	2.181147000	-2.893562000	-1.446710000
C	4.884567000	-1.363509000	0.853670000
H	3.340086000	-0.022247000	1.509739000
C	5.219147000	-2.427606000	0.016919000
H	4.484240000	-3.814249000	-1.459110000
H	5.631123000	-0.938344000	1.519463000
H	6.226927000	-2.834218000	0.021889000
B	-0.125933000	-1.728467000	0.071335000
N	-0.273554000	-2.704213000	-1.116166000
N	-1.187072000	-3.500693000	-1.177961000
N	-1.995359000	-4.295809000	-1.320808000
Cl	-0.104784000	-2.722206000	1.728609000

5 (E: -1431.99161963 hartree)

C	-1.247681000	0.593264000	-0.064716000
C	-0.750064000	-0.664779000	-0.034529000
C	0.750042000	-0.664793000	0.034537000
C	1.247682000	0.593241000	0.064726000
C	-2.677767000	0.954785000	-0.052077000
C	-3.148197000	1.973255000	-0.895835000
C	-3.596619000	0.343662000	0.815854000
C	-4.490218000	2.342573000	-0.893423000
H	-2.439663000	2.474184000	-1.548508000
C	-4.936868000	0.716466000	0.822322000
H	-3.247952000	-0.428668000	1.494610000
C	-5.393464000	1.714868000	-0.037290000
H	-4.829173000	3.134445000	-1.555954000
H	-5.626514000	0.229079000	1.506470000
H	-6.439267000	2.009723000	-0.029650000
C	-1.539754000	-1.921531000	-0.060869000
C	-1.364794000	-2.912082000	0.914047000
C	-2.485414000	-2.145742000	-1.069262000
C	-2.118307000	-4.082333000	0.889361000
H	-0.627285000	-2.760180000	1.696773000
C	-3.240443000	-3.314567000	-1.097004000
H	-2.629784000	-1.382739000	-1.828297000
C	-3.060805000	-4.289501000	-0.116715000
H	-1.965838000	-4.836053000	1.656922000
H	-3.972378000	-3.463380000	-1.886073000
H	-3.648179000	-5.203223000	-0.137697000
C	1.539708000	-1.921560000	0.060874000
C	2.485362000	-2.145793000	1.069267000
C	1.364729000	-2.912105000	-0.914045000
C	3.240368000	-3.314634000	1.097006000
H	2.629747000	-1.382796000	1.828304000
C	2.118219000	-4.082371000	-0.889362000
H	0.627224000	-2.760187000	-1.696772000
C	3.060712000	-4.289561000	0.116714000
H	3.972299000	-3.463464000	1.886075000
H	1.965736000	-4.836086000	-1.656925000
H	3.648068000	-5.203295000	0.137694000
C	2.677774000	0.954737000	0.052086000
C	3.148222000	1.973200000	0.895844000
C	3.596616000	0.343601000	-0.815846000
C	4.490249000	2.342496000	0.893432000
H	2.439696000	2.474140000	1.548517000
C	4.936871000	0.716383000	-0.822315000
H	3.247935000	-0.428722000	-1.494603000
C	5.393484000	1.714777000	0.037298000
H	4.829218000	3.134362000	1.555962000

H	5.626508000	0.228984000	-1.506464000
H	6.439292000	2.009614000	0.029658000
B	0.000010000	1.638387000	0.000009000
N	-0.023629000	2.532242000	1.288419000
N	-0.901269000	3.352111000	1.463416000
N	-1.675967000	4.156240000	1.712274000
N	0.023667000	2.532253000	-1.288392000
N	0.901357000	3.352063000	-1.463410000
N	1.676184000	4.156032000	-1.712385000

6 (E: -2024.10875403 hartree)

C	-1.249017000	-0.821731000	0.052866000
C	-0.749668000	0.436695000	0.027007000
C	0.749667000	0.436700000	-0.026991000
C	1.249024000	-0.821723000	-0.052853000
C	-2.681985000	-1.169011000	-0.012880000
C	-3.222598000	-2.139083000	0.844069000
C	-3.537766000	-0.573531000	-0.952441000
C	-4.573286000	-2.473040000	0.786492000
H	-2.566831000	-2.630368000	1.555276000
C	-4.886295000	-0.910102000	-1.014242000
H	-3.131997000	0.159252000	-1.643028000
C	-5.414882000	-1.858233000	-0.139230000
H	-4.968176000	-3.224328000	1.465504000
H	-5.525691000	-0.432517000	-1.752131000
H	-6.467934000	-2.122657000	-0.186206000
C	-1.542859000	1.690924000	0.030568000
C	-1.345116000	2.680933000	-0.940817000
C	-2.517146000	1.913164000	1.011890000
C	-2.103114000	3.848441000	-0.938377000
H	-0.587931000	2.530027000	-1.704580000
C	-3.277070000	3.079133000	1.016922000
H	-2.679253000	1.150941000	1.768064000
C	-3.073772000	4.053753000	0.041017000
H	-1.932581000	4.601360000	-1.702976000
H	-4.031282000	3.225906000	1.785145000
H	-3.664790000	4.965403000	0.044456000
C	1.542848000	1.690935000	-0.030559000
C	2.517125000	1.913182000	-1.011890000
C	1.345107000	2.680944000	0.940826000
C	3.277041000	3.079156000	-1.016930000
H	2.679231000	1.150960000	-1.768065000
C	2.103097000	3.848457000	0.938379000
H	0.587930000	2.530033000	1.704596000
C	3.073745000	4.053775000	-0.041023000
H	4.031246000	3.225934000	-1.785159000
H	1.932565000	4.601376000	1.702979000

H	3.664757000	4.965430000	-0.044467000
C	2.681994000	-1.168998000	0.012890000
C	3.222604000	-2.139081000	-0.844049000
C	3.537779000	-0.573509000	0.952443000
C	4.573292000	-2.473037000	-0.786473000
H	2.566834000	-2.630373000	-1.555248000
C	4.886307000	-0.910080000	1.014244000
H	3.132012000	0.159280000	1.643024000
C	5.414891000	-1.858220000	0.139240000
H	4.968179000	-3.224333000	-1.465478000
H	5.525705000	-0.432488000	1.752126000
H	6.467943000	-2.122644000	0.186215000
B	0.000007000	-1.852248000	0.000000000
Cl	0.139351000	-2.949605000	1.545970000
Cl	-0.139331000	-2.949562000	-1.546008000

7 (E: -3475.21807543 hartree)

C	5.018051000	1.139681000	0.747604000
C	3.670096000	0.564210000	0.461321000
C	1.169078000	3.272881000	-1.113672000
C	4.764187000	-1.112853000	-1.066393000
C	2.401366000	-1.413939000	-0.294681000
C	0.023899000	2.786897000	-0.292229000
C	3.327007000	3.576738000	1.319715000
C	2.534638000	2.476421000	1.658125000
C	7.545451000	2.212111000	1.312134000
C	-1.192409000	3.429581000	-0.278864000
C	1.606965000	4.603041000	-1.093816000
C	4.727374000	-1.038102000	-2.460031000
C	3.179608000	-3.693739000	-1.098103000
C	2.995967000	-4.833345000	-1.872716000
C	2.685742000	5.015708000	-1.867373000
C	3.292335000	4.734971000	2.086938000
C	5.923491000	-1.577808000	-0.442092000
C	5.830360000	-1.419431000	-3.218906000
C	0.927191000	-3.935564000	-2.706550000
C	1.860959000	2.368863000	-1.931359000
C	1.866754000	-4.962867000	-2.679656000
C	-1.419838000	4.680334000	-1.066616000
C	1.119714000	-2.792459000	-1.935915000
C	6.982283000	-1.886218000	-2.589698000
C	1.705635000	2.568006000	2.784387000
C	7.024264000	-1.966749000	-1.198781000
C	3.364958000	4.103641000	-2.673484000
C	2.947448000	2.775522000	-2.700659000
C	2.464900000	4.816614000	3.205089000
C	-1.815428000	7.063511000	-1.202509000

C	1.669482000	3.727316000	3.552581000
C	-1.600539000	5.917138000	-0.444080000
C	-1.463816000	4.609308000	-2.460248000
C	-1.861826000	6.985122000	-2.593402000
C	-1.686395000	5.753768000	-3.220880000
C	-3.345847000	-3.567973000	-1.065958000
C	-2.374454000	-2.746627000	-0.279581000
C	-3.409965000	0.955149000	1.661775000
C	-1.521667000	-4.915046000	0.747256000
C	-0.221286000	-2.800465000	0.876629000
C	-2.314090000	1.591874000	0.878942000
C	-4.789077000	-0.907077000	-1.094625000
C	-3.417873000	-0.622766000	-1.115022000
C	-5.125241000	-5.100708000	-2.590091000
C	-2.324026000	2.895113000	0.462567000
C	-4.759822000	1.088917000	1.325338000
C	-1.809304000	-5.341540000	2.045142000
C	1.436070000	-4.668589000	1.319130000
C	2.456445000	-5.217332000	2.086654000
C	-5.743497000	0.479123000	2.094712000
C	-5.685171000	-0.178976000	-1.868827000
C	-1.408472000	-5.870097000	-0.267207000
C	-1.974605000	-6.695360000	2.328412000
C	2.393329000	-3.308699000	3.552966000
C	-3.072103000	0.192880000	2.788236000
C	2.939899000	-4.541746000	3.205329000
C	-3.496686000	3.774675000	0.747747000
C	1.371331000	-2.760714000	2.784456000
C	-1.858067000	-7.639871000	1.311517000
C	-2.979883000	0.426619000	-1.934570000
C	-1.574473000	-7.222313000	0.011642000
C	-5.397737000	-0.276650000	3.213127000
C	-4.055933000	-0.418668000	3.558611000
C	-5.233869000	0.863628000	-2.676509000
C	-5.469214000	4.971674000	0.010486000
C	-3.874541000	1.164202000	-2.704715000
C	-4.380372000	4.152516000	-0.267334000
C	-3.722886000	4.238200000	2.045104000
C	-5.689852000	5.427019000	1.309881000
C	-4.813514000	5.057494000	2.327350000
H	3.005497000	6.052709000	-1.828839000
H	0.371281000	-2.004025000	-1.962769000
H	1.112236000	5.317804000	-0.446281000
H	3.821081000	-0.691010000	-2.948385000
H	7.842748000	-2.186425000	-3.179581000
H	1.089338000	1.718434000	3.064229000
H	7.918802000	-2.327605000	-0.700622000

H	4.045951000	-3.624490000	-0.450353000
H	3.950549000	3.538099000	0.435032000
H	8.523971000	2.628764000	1.530317000
H	3.905996000	5.582792000	1.798871000
H	5.963143000	-1.630090000	0.641824000
H	5.786637000	-1.358371000	-4.302006000
H	0.038331000	-4.022587000	-3.324982000
H	3.732773000	-5.630062000	-1.834485000
H	1.554012000	1.325984000	-1.958525000
H	1.719364000	-5.856536000	-3.278334000
H	-1.308374000	3.650633000	-2.947195000
H	-1.715562000	5.684001000	-4.303943000
H	4.212705000	4.424218000	-3.271258000
H	1.021810000	3.777270000	4.422441000
H	3.469296000	2.050146000	-3.318397000
H	2.438727000	5.724116000	3.800477000
H	-2.033106000	7.879341000	-3.184613000
H	-1.953022000	8.018932000	-0.705685000
H	-1.576923000	5.978999000	0.639800000
H	2.759651000	-2.772851000	4.423206000
H	2.884617000	-6.172293000	1.798398000
H	1.091936000	-5.188955000	0.433835000
H	-5.161286000	-1.692224000	-0.446543000
H	-5.815679000	-5.695211000	-3.180299000
H	-6.785166000	0.585097000	1.808216000
H	-5.040228000	1.647065000	0.440616000
H	-6.743387000	-0.419320000	-1.829821000
H	-1.892942000	-4.603448000	2.838039000
H	-1.181808000	-5.546140000	-1.278370000
H	-2.192375000	-7.011457000	3.344080000
H	-1.481757000	-7.951810000	-0.787139000
H	-5.934857000	1.437481000	-3.274913000
H	-4.978956000	5.404959000	3.342643000
H	-3.506363000	1.977266000	-3.323970000
H	0.942980000	-1.802595000	3.064522000
H	-6.147370000	5.254772000	-0.788751000
H	-6.540276000	6.065995000	1.527141000
H	-4.212563000	3.793329000	-1.278093000
H	-1.987046000	-8.695569000	1.529608000
H	-1.922947000	0.680643000	-1.963097000
H	-3.773194000	-1.003306000	4.428606000
H	-2.027640000	0.085661000	3.066650000
H	-6.169001000	-0.753421000	3.810261000
H	3.738844000	-4.972595000	3.800963000
H	-3.041795000	3.942981000	2.838467000
C	-5.214887000	-5.098815000	-1.199104000
C	-4.145827000	-4.335205000	-3.218982000

C	-4.327384000	-4.340712000	-0.441987000
C	-3.263770000	-3.571463000	-2.459675000
C	5.531306000	1.103822000	2.045483000
C	6.786075000	1.638243000	2.328887000
C	7.041975000	2.248967000	0.012301000
C	5.788222000	1.715985000	-0.266678000
C	-1.345594000	-3.459996000	0.461057000
C	-2.424862000	-1.371943000	-0.293278000
C	0.878375000	-3.432707000	1.657727000
C	2.536743000	1.207950000	0.877145000
C	3.566795000	-0.682974000	-0.280213000
C	2.248333000	-2.647867000	-1.117323000
H	-4.391766000	-4.350413000	0.641960000
H	-5.974120000	-5.694003000	-0.701196000
H	-4.071958000	-4.326244000	-4.302130000
H	-2.510699000	-2.959054000	-2.947709000
H	7.168719000	1.607679000	3.344550000
H	4.934190000	0.661863000	2.838311000
H	7.627119000	2.694505000	-0.786395000
H	5.394308000	1.750327000	-1.277822000
B	1.201925000	-0.784437000	0.432250000
B	-1.279590000	-0.648082000	0.433183000
B	0.078986000	1.433044000	0.433820000
N	-1.184439000	0.800486000	0.696599000
N	1.286215000	0.626027000	0.695237000
N	-0.100213000	-1.426389000	0.695092000

7^{Me} (E: -1175.00396662 hartree)

C	-3.076564000	-2.108311000	-0.273619000
C	-0.820659000	-2.729628000	0.482118000
C	-1.953544000	2.075143000	0.482252000
C	-1.524112000	3.377412000	0.403947000
C	3.687366000	-0.368954000	0.403101000
C	2.067866000	-1.909632000	-0.586760000
C	0.619714000	2.745784000	-0.586819000
C	-0.288021000	3.718805000	-0.272925000
C	3.364516000	-1.610311000	-0.273203000
C	2.774520000	0.654227000	0.481661000
C	-2.687343000	-0.835756000	-0.587305000
C	-2.163264000	-3.008426000	0.403342000
B	-0.360626000	-1.399666000	-0.125318000
B	1.392841000	0.387529000	-0.125852000
B	-1.031426000	1.012250000	-0.125365000
N	0.339031000	1.398635000	-0.359816000
N	-1.380237000	-0.405797000	-0.359862000
N	1.041883000	-0.992577000	-0.359659000
C	-2.747086000	-4.276479000	0.983626000

C	0.115419000	-3.637579000	1.256258000
C	-4.475143000	-2.587132000	-0.593048000
C	-3.606674000	0.103105000	-1.336843000
C	-3.207791000	1.717409000	1.256050000
C	-2.330744000	4.516583000	0.984580000
C	-0.003956000	5.169563000	-0.592229000
C	1.892425000	3.072947000	-1.336173000
C	3.092369000	1.919242000	1.255324000
C	5.077594000	-0.240144000	0.982755000
C	4.478548000	-2.582145000	-0.591954000
C	1.713924000	-3.175777000	-1.335151000
H	-3.710359000	-4.091118000	1.467397000
H	-2.084249000	-4.734503000	1.717936000
H	-2.921089000	-5.019912000	0.195650000
H	1.114207000	-3.203658000	1.342312000
H	0.224940000	-4.626559000	0.794436000
H	-0.246562000	-3.796630000	2.278356000
H	-4.933286000	-2.009870000	-1.397391000
H	-5.141776000	-2.515666000	0.276206000
H	-4.475274000	-3.633518000	-0.911704000
H	-3.155777000	1.085284000	-1.474684000
H	-4.565897000	0.239367000	-0.830974000
H	-3.811357000	-0.305854000	-2.332787000
H	-3.329178000	0.635261000	1.343447000
H	-4.119415000	2.114704000	0.792958000
H	-3.166081000	2.111983000	2.277617000
H	-1.688700000	5.258415000	1.468106000
H	-3.058305000	4.171072000	1.719181000
H	-2.888180000	5.038778000	0.196906000
H	0.725340000	5.278072000	-1.396268000
H	0.390470000	5.711460000	0.277183000
H	-0.910173000	5.692352000	-0.911482000
H	2.518911000	2.191972000	-1.471829000
H	2.488544000	3.837500000	-0.831571000
H	1.640533000	3.452294000	-2.333038000
H	2.215764000	2.565030000	1.344086000
H	3.891261000	2.510639000	0.791240000
H	3.414928000	1.685615000	2.276303000
H	5.398320000	-1.166388000	1.468142000
H	5.143464000	0.564236000	1.715541000
H	5.808340000	-0.021077000	0.194171000
H	4.207078000	-3.269484000	-1.394396000
H	4.751598000	-3.193024000	0.278296000
H	5.384037000	-2.059121000	-0.912994000
H	0.637698000	-3.275831000	-1.472215000
H	2.075422000	-4.074339000	-0.828697000
H	2.169968000	-3.149532000	-2.331329000

7^{H} (E: -703.351031310 hartree)

C	-2.362402000	2.914992000	0.000298000
C	-2.950689000	0.553572000	-0.000191000
C	1.954988000	2.278584000	-0.000217000
C	3.280029000	1.949680000	-0.000124000
C	0.048583000	-3.815324000	0.000175000
C	-1.756666000	-2.209588000	-0.000132000
C	2.791917000	-0.416493000	0.000120000
C	3.705704000	0.588143000	0.000064000
C	-1.343402000	-3.503240000	0.000008000
C	0.995896000	-2.832189000	0.000163000
C	-1.035413000	2.626144000	0.000273000
C	-3.328589000	1.865476000	0.000044000
B	-1.461594000	0.229699000	-0.000179000
B	0.531887000	-1.380595000	-0.000040000
B	0.929741000	1.151047000	-0.000114000
N	1.428996000	-0.205424000	-0.000038000
N	-0.536537000	1.340356000	-0.000041000
N	-0.892462000	-1.134775000	-0.000204000
H	-4.381765000	2.139968000	-0.000002000
H	-3.745833000	-0.186518000	-0.000357000
H	-2.673828000	3.952954000	0.000537000
H	-0.306693000	3.426001000	0.000479000
H	1.712137000	3.337349000	-0.000390000
H	4.044400000	2.724431000	-0.000256000
H	4.760285000	0.338693000	0.000161000
H	3.120016000	-1.447592000	0.000219000
H	2.034346000	-3.150924000	0.000324000
H	0.337389000	-4.864664000	0.000272000
H	-2.086655000	-4.291870000	0.000024000
H	-2.813689000	-1.978212000	-0.000245000

2-ib (E: -1158.28724802 hartree)

C	-1.499783000	-1.467708000	-0.029675000
C	-0.718892000	-0.283919000	-0.004664000
C	0.715565000	-0.273765000	0.019891000
C	1.454460000	-1.477743000	0.022523000
C	-2.975734000	-1.557393000	-0.065859000
C	-3.631324000	-2.424501000	0.816557000
C	-3.743851000	-0.827518000	-0.981125000
C	-5.018000000	-2.548811000	0.797522000
H	-3.047287000	-2.993682000	1.535183000
C	-5.128991000	-0.951905000	-1.000432000
H	-3.253833000	-0.157884000	-1.679645000
C	-5.772526000	-1.809762000	-0.110219000
H	-5.507541000	-3.221818000	1.494621000

H	-5.707586000	-0.376529000	-1.716385000
H	-6.853782000	-1.903448000	-0.126500000
C	-1.447097000	1.024820000	0.005891000
C	-1.345513000	1.910692000	-1.069120000
C	-2.255402000	1.362354000	1.092803000
C	-2.040480000	3.115813000	-1.055875000
H	-0.713146000	1.656558000	-1.914215000
C	-2.944968000	2.571224000	1.110477000
H	-2.346709000	0.670306000	1.924881000
C	-2.840548000	3.450627000	0.035183000
H	-1.952271000	3.796519000	-1.896817000
H	-3.568127000	2.823203000	1.962820000
H	-3.379647000	4.392719000	0.046884000
C	1.429418000	1.039958000	0.004281000
C	2.221779000	1.395403000	-1.090407000
C	1.321645000	1.935433000	1.072449000
C	2.894100000	2.613920000	-1.117554000
H	2.318170000	0.703145000	-1.922109000
C	1.989678000	3.155716000	1.048001000
H	0.705287000	1.672630000	1.927215000
C	2.779602000	3.498984000	-0.047815000
H	3.508804000	2.871096000	-1.974700000
H	1.892807000	3.839455000	1.885768000
H	3.302141000	4.450323000	-0.067575000
C	2.944994000	-1.535131000	0.070628000
C	3.605301000	-2.434303000	-0.772654000
C	3.699611000	-0.760405000	0.957117000
C	4.993005000	-2.532438000	-0.756732000
H	3.018099000	-3.058173000	-1.439148000
C	5.086551000	-0.869402000	0.983484000
H	3.204217000	-0.071199000	1.631740000
C	5.738722000	-1.747939000	0.121101000
H	5.491968000	-3.226452000	-1.426084000
H	5.658060000	-0.264765000	1.680738000
H	6.821435000	-1.826019000	0.138081000
B	-0.476777000	-2.492814000	-0.031297000
N	0.817842000	-2.677961000	-0.034706000

II (E: -650.999523064 hartree)

C	2.265091000	1.674469000	-0.000099000
C	3.550353000	1.122322000	-0.000105000
C	3.715914000	-0.260774000	-0.000006000
C	2.609388000	-1.118150000	0.000032000
C	1.338040000	-0.564808000	0.000007000
C	1.156775000	0.835687000	0.000003000
C	-1.044062000	-0.331665000	0.000172000
C	0.021258000	-1.263413000	0.000060000

C	-2.356138000	-0.795725000	0.000162000
C	-2.609230000	-2.171948000	0.000014000
C	-1.550914000	-3.075738000	-0.000132000
C	-0.225006000	-2.627541000	-0.000107000
B	-0.382566000	1.092549000	0.000149000
N	-0.977232000	2.400710000	0.000365000
N	-3.298257000	2.829442000	-0.000513000
N	-2.203887000	2.552837000	0.000124000
H	2.134145000	2.753084000	-0.000292000
H	4.421667000	1.769671000	-0.000194000
H	4.717155000	-0.681223000	0.000017000
H	2.757099000	-2.194292000	0.000082000
H	-3.193699000	-0.103486000	0.000301000
H	-3.631675000	-2.536068000	0.000004000
H	-1.755161000	-4.142227000	-0.000270000
H	0.590108000	-3.345423000	-0.000239000

II-ib (E: -541.530157489 hartree)

C	2.909547000	1.003180000	0.000001000
C	3.624701000	-0.177158000	0.000000000
C	2.934115000	-1.397673000	0.000000000
C	1.552702000	-1.437798000	0.000000000
C	0.776787000	-0.258329000	0.000000000
C	1.507527000	0.976790000	0.000001000
C	-1.464185000	0.928014000	0.000001000
C	-0.703825000	-0.284835000	0.000000000
C	-2.868995000	0.874202000	0.000000000
C	-3.531297000	-0.337469000	-0.000001000
C	-2.801204000	-1.532940000	-0.000001000
C	-1.419129000	-1.498565000	0.000000000
N	-0.828747000	2.172439000	0.000000000
H	3.425966000	1.957278000	0.000001000
H	4.709391000	-0.162600000	0.000001000
H	3.490869000	-2.329570000	0.000000000
H	1.068163000	-2.406749000	-0.000001000
H	-3.408356000	1.815086000	0.000000000
H	-4.616646000	-0.361835000	-0.000001000
H	-3.315908000	-2.488139000	-0.000001000
H	-0.886769000	-2.442844000	-0.000001000
B	0.446810000	2.013558000	0.000000000

TS1 (E: -1267.67334623 hartree; im. freq. –302.6 cm^{-1})

C	1.295175000	-0.649320000	-0.111764000
C	0.582021000	0.500911000	-0.046861000
C	-0.901553000	0.244394000	-0.022909000
C	-1.210988000	-1.076583000	-0.058284000
C	2.758467000	-0.810047000	-0.095231000

C	3.385430000	-1.593280000	-1.073760000
C	3.552387000	-0.207805000	0.890792000
C	4.767792000	-1.760321000	-1.076527000
H	2.779532000	-2.063416000	-1.843911000
C	4.932451000	-0.377425000	0.890458000
H	3.078012000	0.399205000	1.655765000
C	5.545556000	-1.153527000	-0.093131000
H	5.236585000	-2.365182000	-1.846706000
H	5.532436000	0.097270000	1.660720000
H	6.623079000	-1.284792000	-0.091266000
C	1.157687000	1.864634000	0.003126000
C	0.780946000	2.766771000	1.004914000
C	2.101267000	2.266463000	-0.948759000
C	1.344499000	4.037641000	1.059441000
H	0.041341000	2.471880000	1.743068000
C	2.658046000	3.540649000	-0.899206000
H	2.398290000	1.572512000	-1.729121000
C	2.283045000	4.429255000	0.106571000
H	1.045010000	4.724915000	1.844456000
H	3.387034000	3.838582000	-1.646313000
H	2.717914000	5.423097000	0.146270000
C	-1.884239000	1.354394000	0.024873000
C	-2.852655000	1.395730000	1.033491000
C	-1.855271000	2.378028000	-0.928622000
C	-3.776336000	2.434825000	1.084590000
H	-2.881415000	0.601419000	1.773230000
C	-2.783139000	3.413962000	-0.881478000
H	-1.100326000	2.362947000	-1.709142000
C	-3.745543000	3.446096000	0.125907000
H	-4.522577000	2.453265000	1.872764000
H	-2.750525000	4.199661000	-1.629792000
H	-4.466652000	4.256597000	0.165040000
C	-2.550914000	-1.687267000	-0.131576000
C	-2.853777000	-2.836931000	0.609434000
C	-3.548229000	-1.144687000	-0.955119000
C	-4.120629000	-3.409538000	0.553435000
H	-2.084253000	-3.283565000	1.232865000
C	-4.812696000	-1.720792000	-1.015371000
H	-3.328691000	-0.267840000	-1.555157000
C	-5.107552000	-2.851701000	-0.256511000
H	-4.334311000	-4.297666000	1.140159000
H	-5.568381000	-1.286258000	-1.662602000
H	-6.094754000	-3.300697000	-0.304536000
B	0.234212000	-1.801462000	-0.046144000
N	0.138311000	-3.126360000	0.174397000
N	1.916544000	-3.870056000	0.357263000
N	2.555732000	-4.719555000	0.648824000

TS1' (E: -650.934259508 hartree; im. freq. –320.0 cm^{-1})

C	-2.076688000	-1.920331000	0.000081000
C	-3.415837000	-1.520291000	0.000045000
C	-3.747056000	-0.167161000	-0.000032000
C	-2.748475000	0.808054000	-0.000068000
C	-1.414034000	0.417831000	-0.000011000
C	-1.078790000	-0.955469000	0.000060000
C	0.968905000	0.511244000	-0.000018000
C	-0.211225000	1.283470000	-0.000038000
C	2.210614000	1.132209000	0.000022000
C	2.279924000	2.528206000	0.000024000
C	1.110522000	3.286771000	0.000017000
C	-0.143524000	2.671270000	0.000010000
B	0.532455000	-0.989179000	0.000027000
N	0.971798000	-2.263416000	-0.000098000
N	3.869804000	-2.816649000	0.000032000
N	2.910675000	-2.273473000	-0.000061000
H	-1.825900000	-2.975720000	0.000119000
H	-4.201598000	-2.269170000	0.000090000
H	-4.790333000	0.133064000	-0.000064000
H	-3.016286000	1.860846000	-0.000194000
H	3.125361000	0.546018000	0.000128000
H	3.245531000	3.023840000	0.000000000
H	1.174451000	4.370648000	0.000048000
H	-1.045452000	3.276307000	0.000074000

^{1}2-nit (E: -1158.18509728 hartree)

C	1.274194000	-1.102280000	0.021499000
C	0.748793000	0.148500000	-0.006471000
C	-0.748664000	0.148302000	0.006128000
C	-1.273747000	-1.102588000	-0.021950000
C	2.657913000	-1.587830000	0.092859000
C	2.935758000	-2.924805000	-0.223244000
C	3.729244000	-0.776599000	0.506714000
C	4.228047000	-3.432022000	-0.167663000
H	2.114281000	-3.581143000	-0.518084000
C	5.022374000	-1.283971000	0.566928000
H	3.551631000	0.252021000	0.795641000
C	5.281953000	-2.609081000	0.222979000
H	4.408765000	-4.471749000	-0.420904000
H	5.831359000	-0.638459000	0.894732000
H	6.292989000	-3.000712000	0.273378000
C	1.508039000	1.419615000	-0.084970000
C	1.432560000	2.366868000	0.940858000
C	2.287187000	1.696966000	-1.212903000
C	2.136191000	3.563965000	0.846384000

H	0.819647000	2.164034000	1.813827000
C	2.986403000	2.896100000	-1.309180000
H	2.348201000	0.960450000	-2.008699000
C	2.913789000	3.831893000	-0.278597000
H	2.072470000	4.290219000	1.650509000
H	3.589062000	3.099320000	-2.188865000
H	3.459281000	4.767389000	-0.353005000
C	-1.508304000	1.419166000	0.084795000
C	-2.287884000	1.695918000	1.212574000
C	-1.432861000	2.366731000	-0.940747000
C	-2.987512000	2.894801000	1.309007000
H	-2.348895000	0.959141000	2.008129000
C	-2.136895000	3.563578000	-0.846115000
H	-0.819639000	2.164347000	-1.813604000
C	-2.914893000	3.830927000	0.278728000
H	-3.590493000	3.097564000	2.188576000
H	-2.073182000	4.290089000	-1.650009000
H	-3.460706000	4.766227000	0.353257000
C	-2.657422000	-1.588300000	-0.092970000
C	-2.935044000	-2.925447000	0.222617000
C	-3.728980000	-0.776895000	-0.505871000
C	-4.227337000	-3.432692000	0.167363000
H	-2.113415000	-3.581893000	0.516756000
C	-5.022115000	-1.284296000	-0.565751000
H	-3.551536000	0.251912000	-0.794266000
C	-5.281461000	-2.609604000	-0.222385000
H	-4.407893000	-4.472555000	0.420157000
H	-5.831288000	-0.638647000	-0.892819000
H	-6.292501000	-3.001259000	-0.272523000
B	0.000340000	-2.074082000	-0.000765000
N	0.000604000	-3.392484000	-0.000293000

^{3}2-nit (E: -1158.19319947 hartree)

C	-1.241758000	-1.186054000	-0.023740000
C	-0.714417000	0.125307000	0.009515000
C	0.714508000	0.125367000	-0.009606000
C	1.241965000	-1.185932000	0.023649000
C	-2.640273000	-1.564157000	-0.100823000
C	-3.000900000	-2.857249000	0.334882000
C	-3.650606000	-0.734322000	-0.633855000
C	-4.321237000	-3.282254000	0.284346000
H	-2.222164000	-3.516450000	0.707764000
C	-4.964491000	-1.174526000	-0.703573000
H	-3.402185000	0.246716000	-1.019752000
C	-5.307401000	-2.442697000	-0.232393000
H	-4.579728000	-4.275791000	0.635946000
H	-5.725209000	-0.527524000	-1.128657000

H	-6.338721000	-2.778889000	-0.280122000
C	-1.497787000	1.381611000	0.094952000
C	-1.410161000	2.355946000	-0.904370000
C	-2.331376000	1.606827000	1.195642000
C	-2.153377000	3.528670000	-0.810521000
H	-0.758813000	2.192510000	-1.757457000
C	-3.064878000	2.784884000	1.294299000
H	-2.407454000	0.849458000	1.970277000
C	-2.980397000	3.747328000	0.289597000
H	-2.081601000	4.274690000	-1.595570000
H	-3.706606000	2.948889000	2.154176000
H	-3.556074000	4.664465000	0.364204000
C	1.497736000	1.381771000	-0.094924000
C	2.331123000	1.607274000	-1.195710000
C	1.410094000	2.355949000	0.904542000
C	3.064450000	2.785447000	-1.294296000
H	2.407192000	0.850025000	-1.970464000
C	2.153115000	3.528801000	0.810750000
H	0.758865000	2.192295000	1.757680000
C	2.979955000	3.747738000	-0.289448000
H	3.706030000	2.949678000	-2.154239000
H	2.081328000	4.274707000	1.595906000
H	3.555475000	4.664977000	-0.364010000
C	2.640475000	-1.564015000	0.100779000
C	3.001032000	-2.857267000	-0.334540000
C	3.650901000	-0.734077000	0.633494000
C	4.321343000	-3.282335000	-0.283937000
H	2.222255000	-3.516556000	-0.707192000
C	4.964766000	-1.174323000	0.703259000
H	3.402578000	0.247091000	1.019120000
C	5.307588000	-2.442665000	0.232470000
H	4.579746000	-4.276006000	-0.635221000
H	5.725545000	-0.527212000	1.128070000
H	6.338893000	-2.778894000	0.280252000
B	0.000138000	-2.180450000	-0.000158000
N	-0.000002000	-3.534599000	-0.000368000

TS2 (E: -1158.18366859 hartree; im. freq. –28.3 cm^{-1})

C	-1.265110000	-1.131240000	-0.031652000
C	-0.752234000	0.124814000	-0.002792000
C	0.743573000	0.133061000	-0.012114000
C	1.288224000	-1.109982000	0.011957000
C	-2.656160000	-1.602551000	-0.094560000
C	-2.975272000	-2.880670000	0.385244000
C	-3.687564000	-0.827957000	-0.650277000
C	-4.280168000	-3.358759000	0.347168000
H	-2.185021000	-3.506810000	0.794900000

C	-4.991685000	-1.308658000	-0.692869000
H	-3.467935000	0.150643000	-1.061207000
C	-5.297037000	-2.571328000	-0.188488000
H	-4.500147000	-4.350691000	0.728998000
H	-5.771856000	-0.694413000	-1.131789000
H	-6.315929000	-2.943751000	-0.225362000
C	-1.528389000	1.385337000	0.076681000
C	-1.423695000	2.360387000	-0.920551000
C	-2.366107000	1.619431000	1.172043000
C	-2.154231000	3.541495000	-0.830218000
H	-0.767086000	2.192264000	-1.768798000
C	-3.092420000	2.802566000	1.264449000
H	-2.450846000	0.862233000	1.945811000
C	-2.989624000	3.765953000	0.262355000
H	-2.066740000	4.289047000	-1.612294000
H	-3.740134000	2.971565000	2.118977000
H	-3.556435000	4.688939000	0.333802000
C	1.499282000	1.408281000	-0.074121000
C	2.295890000	1.692815000	-1.187803000
C	1.403056000	2.350492000	0.954527000
C	2.991961000	2.894894000	-1.267467000
H	2.373063000	0.959688000	-1.985272000
C	2.103584000	3.550608000	0.876593000
H	0.776031000	2.141755000	1.816047000
C	2.898907000	3.825907000	-0.234157000
H	3.608427000	3.104061000	-2.136094000
H	2.023655000	4.273361000	1.682412000
H	3.442247000	4.763601000	-0.295491000
C	2.681197000	-1.565989000	0.088690000
C	3.005826000	-2.876324000	-0.284448000
C	3.718572000	-0.744531000	0.564168000
C	4.311558000	-3.347049000	-0.228354000
H	2.207150000	-3.541355000	-0.621514000
C	5.025588000	-1.215233000	0.625405000
H	3.504179000	0.262619000	0.899931000
C	5.332561000	-2.512900000	0.221977000
H	4.528030000	-4.367808000	-0.526571000
H	5.807386000	-0.562540000	1.001360000
H	6.354063000	-2.876175000	0.273715000
B	-0.001989000	-2.093228000	-0.038919000
N	0.166763000	-3.395329000	-0.135037000

^{3}II-nit (E: -541.455399926 hartree)

C	-2.614645000	0.969611000	-0.000036000
C	-3.492767000	-0.120606000	0.000035000
C	-2.991421000	-1.418742000	0.000106000
C	-1.610440000	-1.660205000	0.000115000

C	-0.745192000	-0.579454000	0.000052000
C	-1.242079000	0.745740000	-0.000026000
C	1.242044000	0.745398000	-0.000044000
C	0.744992000	-0.579652000	0.000032000
C	2.614695000	0.969481000	-0.000089000
C	3.492764000	-0.120647000	-0.000052000
C	2.991250000	-1.418799000	0.000024000
C	1.610339000	-1.660376000	0.000063000
B	0.000199000	1.701308000	-0.000061000
N	0.000283000	3.155579000	-0.000141000
H	-3.005251000	1.983111000	-0.000086000
H	-4.565475000	0.044189000	0.000033000
H	-3.679028000	-2.259195000	0.000155000
H	-1.238829000	-2.680826000	0.000165000
H	3.005075000	1.983057000	-0.000145000
H	4.565522000	0.043869000	-0.000083000
H	3.678880000	-2.259237000	0.000049000
H	1.238896000	-2.681057000	0.000116000

$[2F]^-$ (E: -1367.69169305 hartree)

C	-1.273049000	-0.634066000	0.173509000
C	-0.625534000	0.549166000	0.075577000
C	0.868327000	0.363181000	0.044500000
C	1.213329000	-0.942440000	0.121000000
C	-2.732460000	-0.835352000	0.167852000
C	-3.294084000	-1.796405000	1.024224000
C	-3.596309000	-0.142690000	-0.696163000
C	-4.666423000	-2.027781000	1.042459000
H	-2.631201000	-2.365061000	1.669077000
C	-4.967490000	-0.378044000	-0.682365000
H	-3.182038000	0.582492000	-1.389574000
C	-5.512628000	-1.317161000	0.192666000
H	-5.074757000	-2.777847000	1.714489000
H	-5.612889000	0.170553000	-1.363566000
H	-6.583119000	-1.503729000	0.200490000
C	-1.250832000	1.893394000	0.001871000
C	-0.953440000	2.778713000	-1.042455000
C	-2.160478000	2.310134000	0.982101000
C	-1.553163000	4.033113000	-1.111604000
H	-0.242271000	2.476532000	-1.805706000
C	-2.762447000	3.563338000	0.915890000
H	-2.399687000	1.629974000	1.794174000
C	-2.461660000	4.432150000	-0.132357000
H	-1.307109000	4.702015000	-1.931752000
H	-3.469603000	3.861647000	1.685064000
H	-2.928992000	5.411585000	-0.184524000

C	1.798216000	1.516114000	-0.055860000
C	2.772589000	1.560127000	-1.060982000
C	1.729352000	2.586973000	0.844849000
C	3.657030000	2.630648000	-1.156118000
H	2.834932000	0.734094000	-1.763113000
C	2.612150000	3.659337000	0.752711000
H	0.971486000	2.575752000	1.622806000
C	3.581600000	3.686594000	-0.248759000
H	4.408215000	2.639427000	-1.941175000
H	2.539459000	4.478040000	1.463399000
H	4.269881000	4.523973000	-0.322899000
C	2.586446000	-1.470209000	0.198383000
C	2.929776000	-2.622667000	-0.527436000
C	3.574674000	-0.890947000	1.011281000
C	4.217391000	-3.148976000	-0.472648000
H	2.164542000	-3.094654000	-1.136356000
C	4.859881000	-1.420943000	1.071977000
H	3.325404000	-0.016324000	1.604190000
C	5.192524000	-2.550114000	0.324236000
H	4.458147000	-4.037581000	-1.050617000
H	5.604433000	-0.951063000	1.709575000
H	6.196184000	-2.964248000	0.370948000
B	-0.154879000	-1.832537000	0.195874000
N	-0.274857000	-2.735675000	-1.086968000
N	-1.133133000	-3.588251000	-1.151165000
N	-1.899640000	-4.427189000	-1.294092000
F	-0.234770000	-2.662913000	1.361249000

$[IIF]^-$ (E: -750.946926784 hartree)

C	2.377170000	1.481451000	0.179554000
C	3.625859000	0.905524000	-0.079812000
C	3.726030000	-0.461236000	-0.342492000
C	2.579968000	-1.259371000	-0.344902000
C	1.342932000	-0.674217000	-0.080326000
C	1.222710000	0.704515000	0.184888000
C	-0.998888000	-0.411277000	0.281798000
C	0.016502000	-1.339774000	-0.027645000
C	-2.308093000	-0.875383000	0.385553000
C	-2.605105000	-2.228177000	0.182197000
C	-1.588075000	-3.131043000	-0.127174000
C	-0.267339000	-2.688225000	-0.232637000
B	-0.341952000	1.078121000	0.446288000
N	-0.835974000	2.079289000	-0.673420000
N	-3.115403000	2.592913000	-0.961820000
N	-2.015569000	2.315037000	-0.786191000
H	2.307161000	2.549021000	0.377575000
H	4.522579000	1.521548000	-0.080019000

H	4.697314000	-0.906347000	-0.545892000
H	2.662171000	-2.324733000	-0.551281000
H	-3.110945000	-0.182572000	0.627971000
H	-3.631436000	-2.579024000	0.264396000
H	-1.822234000	-4.181306000	-0.285093000
H	0.524088000	-3.396315000	-0.470676000
F	-0.601373000	1.673527000	1.723065000

$C_4H_4BN_3$ (E: -343.756645385 hartree)

C	-1.418397000	-1.216267000	-0.000315000
C	-2.423425000	-0.325412000	0.000295000
C	-1.918427000	1.095945000	0.000234000
C	-0.576383000	1.160307000	-0.000373000
B	-0.101845000	-0.349460000	0.000632000
N	1.228376000	-0.883408000	0.000025000
H	-1.556959000	-2.290765000	-0.000764000
H	-3.485796000	-0.553755000	0.000242000
H	-2.598065000	1.944199000	0.000093000
H	-0.020022000	2.091012000	-0.000950000
N	2.203398000	-0.117316000	-0.000408000
N	3.166778000	0.467749000	0.000266000

$[C_4H_4BN_3F]^-$ (E: -443.698447358 hartree)

C	1.460459000	-0.882695000	-0.699424000
C	2.363145000	0.108187000	-0.593028000
C	1.868904000	1.221941000	0.268729000
C	0.635366000	0.979657000	0.746637000
B	0.139569000	-0.474470000	0.171316000
N	-1.110666000	-0.326805000	-0.802096000
H	1.644439000	-1.775334000	-1.296696000
H	3.345753000	0.139971000	-1.067213000
H	2.470587000	2.112528000	0.459512000
H	0.114968000	1.687288000	1.391693000
N	-2.113412000	0.221921000	-0.417518000
N	-3.104675000	0.730157000	-0.132371000
F	-0.215506000	-1.414618000	1.198060000

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