Supporting Information

Expression of hyperconjugative stereoelectronic interactions in borazines

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1. General Remarks

Thin layer chromatography (TLC) was conducted on pre-coated aluminum sheets with 0.20 mm Merck Millipore Silica gel 60 with fluorescent indicator F254. TLC plates were visualized by exposure to ultraviolet light (254 or 366 nm).

Column chromatography was carried out using Merck Gerduran silica gel 60 (particle size 40-63 µm).

Melting points (MP) were measured on a Leica Galen III microscope equipped with a heating block and a Hg thermometer (T_{max} = 200 °C) on a microscope slide under air. According to the limitations of the apparatus, the compounds which did not melt or decompose (dec) up to 200 °C are presented as "> 200 °C".

Nuclear magnetic resonance (NMR) characterizations were performed at the NMR centre of the Faculty of Chemistry, University of Vienna. NMR spectra were recorded on Bruker spectrometers AV III HD 700, AV III 600 or AV NEO 400. ^{1}H NMR spectra were obtained at 700.4, 600.2 or 400.2 MHz, ^{13}C NMR spectra at 176.1, 150.9 or 100.6 MHz, ^{11}B NMR spectra at 192.6 in quartz NMR tube, ^{29}Si spectra at 119.3 MHz. All spectra were obtained at room temperature. Carbon spectra were acquired with a complete decoupling for the proton. Proton and carbon chemical shifts are reported in parts per million (ppm, δ scale) according to tetramethylsilane ($\delta_H = \delta_C = 0$ ppm) using the solvent residual signal as an internal reference ($CDCl_3$: δ_H = 7.27 ppm, δ_C = 77.00 ppm; CD_2Cl_2: δ_H = 5.32 ppm, δ_C = 54.00 ppm). Boron chemical shifts are reported in ppm, referenced to the external standard boron signal of $BF_3{\cdot}Et_2O$ (δ_B = 0 ppm). Silicon chemical shifts are reported in ppm, referenced external to tetramethylsilane (δ_{Si} = 0 ppm). Coupling constants (J) are given in Hz. Resonance multiplicity is described as s (singlet), d (doublet), dd (doublet of doublets), t (triplet), q (quartet), p (pentet), m (multiplet) and bs (broad signal). Solid-state $^{1}H \rightarrow {}^{13}C$ cross-polarization and magic angle spinning (CPMAS) NMR spectra were recorded on Bruker spectrometers AV III HD 500.

Infrared spectra (IR) were recorded on a Bruker Alpha FT-IR spectrometer in ATR mode. Selected absorption bands are reported in wavenumbers (cm^{-1}).

High-resolution mass spectrometry (HRMS) analyses were performed at the Mass Spectrometry Centre of the Faculty of Chemistry, University of Vienna. MALDI mass spectra were obtained on a Bruker Autoflex Speed MALDItimsTOF (matrix: 2-[(2E)-3-(4-tert-butylphenyl)-2-methylprop-2-enylidene]malononitrile (DCTB)) mass spectrometer.

X-ray measurements of **1a**, **3b** and **2e** were performed at the Centre for X-ray Structure Analysis of the Faculty of Chemistry, University of Vienna. X-ray intensity data were measured at 100 K for **1a** and **2e** and at 293 K for **3b**, on a STOE Stadivari diffractometer equipped with dual radiation source Mo and Cu Kα, and a Dectris EIGER2 R 500K detector. The structures were solved ab initio and refined by full-matrix least-squares techniques. Hydrogen atoms were inserted at calculated positions using AFIX instructions, while all other atoms were refined with anisotropic displacement parameters. The following softwares were used: STOE software package for collecting crystal data and image processing, STOE LANA for scaling and absorption correction,[1] SHELXT-2018/2 for structure solution,[2] SHELXL-2018/3 for structure refinement,[3] SHELXLE version 1378 and OLEX2-1.5 as graphical user interfaces.[4,5] X-ray data for **1b** and **2a** were collected at Cardiff University. The single crystals were mounted in paratone and analysed on an Agilent SuperNova Dual three-circle

diffractometer using Mo Kα (λ = 0.71073 Å) radiation and a CCD detector. Measurements were made at 150 K and 293 K for **1b** and **2a**, respectively, with temperatures maintained using an Oxford Cryostream. Data were collected, integrated and corrected for absorption using a numerical absorption correction based on gaussian integration over a multifaceted crystal model within CrysAlisPro.[6] The structures were solved by direct methods and refined by full-matrix least-squares techniques within SHELXL-2018/3.[3] Hydrogen atoms were inserted at calculated positions using AFIX instructions, while all other atoms were refined with anisotropic displacement parameters. Data collections for **3a** were performed at the XRD1 beamline of the Elettra Synchrotron, Trieste (Italy).[7] The crystals were dipped in NHV oil (Jena Bioscience, Jena, Germany) and mounted on the goniometer head with nylon loops (MiTeGen, Ithaca, USA). Complete datasets were collected at 100 K (nitrogen stream supplied through an Oxford Cryostream 700). Data were acquired using a monochromatic wavelength of 0.70 Å through the rotating crystal method on a Pilatus 2M hybrid-pixel area detector (DECTRIS Ltd., Baden-Daettwil, Switzerland). The diffraction data were indexed and integrated using XDS.[8] The structure was solved with Olex2[2] by using ShelXT[3] structure solution program by Intrinsic Phasing and refined with the ShelXL[4] refinement package using least-squares minimization. In the last cycles of refinement, non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in calculated positions, and a riding model was used for their refinement.
Single crystals suitable for X-ray diffraction of **1a**, **1b**, **2a**, and **2e** were grown by vapor diffusion CH_2Cl_2/MeOH. Single crystals suitable for X-ray diffraction were grown by slow evaporation, **3a** from CH_2Cl_2, and **3b** from CH_3CN. Crystal data collection parameters and structure refinement details are given in Tables S1–S6. Structures have been deposited in the Cambridge Structural Database (CSD) with the following deposition numbers: **1a** (2261150), **1b** (2280128), **2a** (2280127), **2e** (2307378), **3a** (2284380), **3b** (2261151). These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service via www.ccdc.cam.ac.uk/structures. Bond lengths and angles for the measured crystal structures have been reported in the manuscript as average values, together with the corresponding standard deviations. For **2a**, a single molecule from the asymmetric unit has been taken into account for statistics, due to disorder and relative restraints applied on bond lengths during refinement.

Density functional calculations were performed using the Gaussian 09 software package.[9] All structures were optimised without symmetry restraints and the nature of each stationary point verified by a frequency calculation to ascertain that there were no imaginary frequencies. The PBE functional[10,11] was used along with the def2-TZVP basis set on all centres.[12,13] Implicit solvent (chloroform) was used in all calculations. Natural bonding orbital analyses were calculated using NBO version 6[14] invoked via the Gaussian interface. Variations in the NBO contributions with torsion angle were undertaken by optimising the structure whilst freezing one N–B–C–H and N–B–C–C torsion angles. NMR calculations were undertaken with the Gauge-independent atomic orbital method as part of the Gaussian program.

TGA Analysis. All the thermogravimetric analyses were performed with a TGA 550 instrument manufactured by TA instruments, under a N_2 flow of 60 mL min^{-1} and with the following method: equilibration from room temperature to 100 °C, isothermal heating at 100 °C for 30 minutes, then ramp from 100 °C to 800 °C (heating rate of 10 °C min^{-1}).

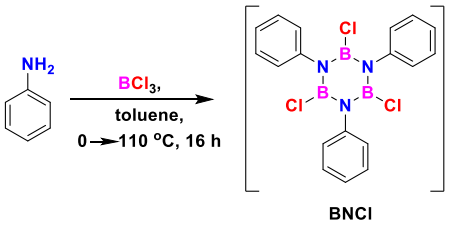
SEM images were recorded with a Zeiss Supra 55 VP instrument (Carl Zeiss, DE) with an acceleration voltage of 5 kV. The sample was prepared by drop-casting dispersion (1 mg/mL in THF) onto a Si substrate (1 cm^2) and, subsequently, sputter coated with Au (Emitech K575X Peltier cooled) for 60 s at 60 mA before fixation on Al support.

2. Materials and methods

Chemicals were purchased from Sigma Aldrich, Acros Organics, Thermo Fisher Scientific and BLDpharm and used without further purification. Aniline was distilled over CaH_2 and stored in an argon-filled glove box. Anhydrous toluene and tetrahydrofuran (THF) were dried on a MBraun SPS-800 solvent purification system, degassed, and stored over activated 4 Å molecular sieves. Deuterated solvents were purchased from Eurisotop. Anhydrous conditions were achieved by drying glassware in oven at 120 °C for at least 12 h and by flaming the reaction vessels with a heat gun under vacuum and purging with argon. The inert atmosphere was maintained using argon-filled balloons equipped with a syringe and needle that was used to penetrate the silicon septa used to close the flask's necks. Addition of liquid reagents was performed using argon-purged plastic syringes. Alternative to the use of Schlenk line techniques, inert conditions were achieved by using an argon filled MBraun LabStar glove box when stated. Degassing of solutions was performed by bubbling argon or freeze-pump-thaw procedure: solutions were frozen in liquid nitrogen and kept under vacuum for 10–15 min before thawing. 0 °C baths were prepared using ice/water.

3. Synthetic procedures and spectral data

3.1 2,4,6-trichloro-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**BNCl**)



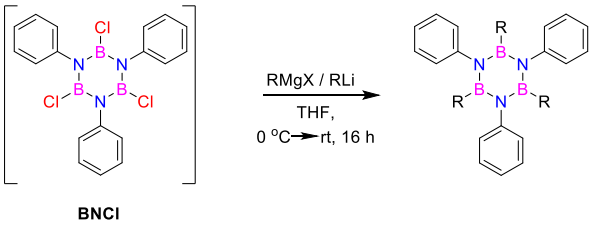
Scheme S1: Synthesis of trichloroborazole.

In a glove box, to a 100 mL Schlenk tube, aniline (2 mL, 21.91 mmol) was added in toluene (10 mL). The Schlenk tube was removed from the glove box and the solution cooled to 0 °C. Subsequently, a solution of BCl_3 (28.48 mL, 1 M solution in heptane, 28.48 mmol) was added dropwise. The septum was replaced with an oven-dried condenser topped with a $CaCl_2$ tube and the resulting mixture refluxed for 16 h. Afterward, the reaction solution was cooled to room temperature and the suspension purged with Ar. The solvent was evaporated under vacuum giving a white solid, which was further dried under vacuum for additional 4 h at rt (2.61 g, 91% yield) and stored in the glove box. The purity of **BNCl** was checked by ^{1}H and ^{11}B NMR.

^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.41 (t, J = 7.3 Hz, 6H), 7.32 (t, J = 7.3 Hz, 3H), 7.16 (d, J = 7.3 Hz, 6H). $^{13}C\{^{1}H\}$ NMR (150 MHz, CD_2Cl_2) δ 144.7, 129.5, 128.8, 127.1. ^{11}B NMR (193 MHz, CD_2Cl_2) δ 31.6.

**Note: The product is highly hygroscopic and should be handled under inert atmosphere.*

3.2 General procedure I: *Preparation of B,B',B''-trialkyl borazines*



Scheme S2: Synthesis of B,B',B''-trialkyl borazines.

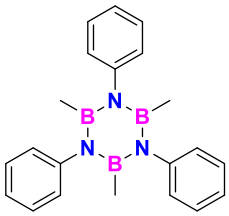
In a glove box, to a Schlenk tube, **BNCl** (1 eq.) was dissolved in THF. The Schlenk tube was removed from the glove box and the resulting solution cooled to 0 °C. Subsequently, a solution of alkyl lithium/Grignard (3.9 eq.) was slowly added dropwise. The solution was stirred at room temperature for 12-16 h and quenched by dropwise addition of water (1 mL) at 0 °C and extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4 and

the solvents evaporated in vacuo. The product was purified by silica gel column chromatography using mixtures of heptane/CH_2Cl_2 as eluent.

3.3 General procedure II: *Preparation of alkylmagnesium bromides*

A 50 mL Schlenk tube was charged with preactivated magnesium (1 eq.) and a catalytic amount of iodine. Subsequently, dry THF was added, and the solution was cooled to 0 °C. Alkyl bromide (1 eq.) was slowly added drop by drop. The solution was then subjected to reflux conditions until the complete dissolution of magnesium occurred.

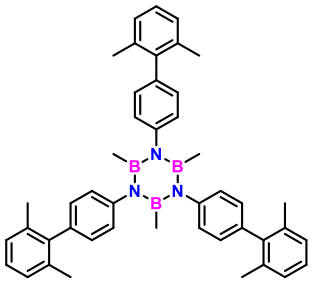
3.4 2,4,6-trimethyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**1a**)



Synthesized in accordance with general procedure I, using **BNCl** (0.20 g, 0.49 mmol), THF (2 mL) and a solution of methylmagnesium bromide (0.63 mL, 3M solution in Et_2O, 1.89 mmol). The product was purified by silica gel column chromatography (heptane) affording **1a** as a white solid (0.13 g, 0.36 mmol, 74% yield).

MP > 200 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.32 (t, J = 7.6 Hz, 6H), 7.19 (t, J = 7.6 Hz, 3H), 7.04 (d, J = 7.6 Hz, 6H), -0.18 (s, 9H). ^{13}C{^{1}H} NMR (176 MHz, CD_2Cl_2) δ 149.3, 129.2, 128.8, 125.3, 2.2 (broad due to ^{11}B-induced quadrupolar relaxation). ^{11}B NMR (193 MHz, CD_2Cl_2) δ 35.9. IR (cm^{-1}): 3067, 3036, 3022, 1592, 1485, 1449, 1365, 1316, 1273, 1186, 1153, 1071, 1027, 879, 770, 722, 696, 582, 563, 508. HRMS (MALDI-timsTOF) m/z calcd for $[C_{21}H_{24}B_3N_3]^+$: 351.2255 $[M]^+$; found: 351.2250. For crystal structure: CCDC 2261150 (Table S1 and Figure S52).

3.5 1,3,5-tris(2',6'-dimethyl-[1,1'-biphenyl]-4-yl)-2,4,6-trimethyl-1,3,5,2,4,6-triazatriborinane (**1b**)

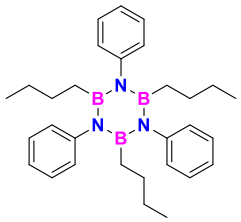


A 50 mL Schlenk tube was charged with 2',6'-dimethyl-[1,1'-biphenyl]-4-amine (0.20 g, 1.01 mmol) and toluene (5 mL). The solution cooled to 0 °C. Subsequently, a solution of BCl_3 (1.22 mL, 1 M solution in heptane, 1.22 mmol) was added dropwise. The septum was replaced with an oven-dried condenser topped with a $CaCl_2$ tube and the resulting mixture refluxed for 16 h. Afterward, the reaction solution was cooled to rt and the suspension purged with Ar. The solvent was evaporated under vacuum giving a white solid, in the same Schlenk tube THF (5 mL) added. The resulting solution cooled to 0 °C, and a solution of MeMgBr (1.35 mL, 3M solution in Et_2O, 4.06 mmol) slowly added dropwise. The solution stirred at rt for 16 h. The mixture quenched by dropwise addition of water (1 mL) at 0 °C and extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4 and the solvents evaporated in vacuo. The product purified by silica gel column chromatography using a mixture of heptane/CH_2Cl_2 (4:1) as eluent affording **1b** as a white solid (0.15 g, 0.71 mmol, 70% yield).

MP > 200 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.19-7.17 (m, 3H), 7.14-7.11 (m, 18H), 2.07 (s, 18H), 0.03 (s, 9H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 147.2, 141.7, 137.4, 136.2, 129.3, 128.2, 127.2, 126.9, 20.7, 1.8 (broad due to ^{11}B-induced quadrupolar relaxation). ^{11}B NMR (193 MHz, $CDCl_3$) δ 37.4. IR (cm^{-1}): 3032, 3019, 2969, 2942, 2914, 1509, 1466, 1434, 1401, 1370, 1317, 1273, 1198, 1168, 1098, 1004, 885, 836, 763, 626, 578, 521, 463. HRMS (MALDI-timsTOF) m/z calcd for $[C_{45}H_{48}B_3N_3]^+$: 663.4143 $[M]^+$; found: 663.4135. For crystal structure: CCDC 2280128 (Table S2 and Figure S53).

**Note: The 2',6'-dimethyl-[1,1'-biphenyl]-4-amine was synthesised according to literature procedure.*[15]

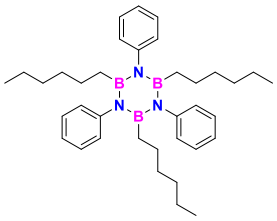
3.6 2,4,6-tributyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2a**)



Synthesized in accordance with general procedure I, using **BNCl** (0.20 g, 0.49 mmol), THF (2 mL) and a butyl lithium (0.95 mL, 2M solution in hexane, 1.89 mmol). The product was purified by silica gel column chromatography (heptane) affording **2a** as a white solid (0.14 g, 0.31 mmol, 63% yield).

MP 122–124 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.30 (t, J = 7.6 Hz, 6H), 7.18 (t, J = 7.6 Hz, 3H), 7.10 (d, J = 7.6 Hz, 6H), 0.87-0.83 (m, 6H), 0.76-0.72 (m, 6H), 0.42 (t, J = 7.5 Hz, 9H), 0.31 (m, 6H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 147.5, 128.8, 128.1, 124.8, 26.5, 25.7, 15.9 (broad due to ^{11}B-induced quadrupolar relaxation), 13.2. ^{11}B NMR (193 MHz, $CDCl_3$) δ 35.6. IR (cm^{-1}): 3081, 3061, 3023, 2955, 2924, 2853, 1595, 1488, 1449, 1431, 1368, 1269, 1219, 1202, 1154, 1085, 1069, 1027, 992, 889, 801, 762, 739, 698, 566, 524. HRMS (MALDI-timsTOF) m/z calcd for $[C_{30}H_{42}B_3N_3]^+$: 477.3667 $[M]^+$; found: 477.3658. For crystal structure: CCDC 2280127 (Table S3 and Figure S54). Solid-state ^{1}H → ^{13}C CPMAS NMR (126 MHz) δ 147.53, 127.97, 125.96, 124.95, 28.62, 26.61, 16.11, 12.95.

3.7 2,4,6-trihexyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2b**)

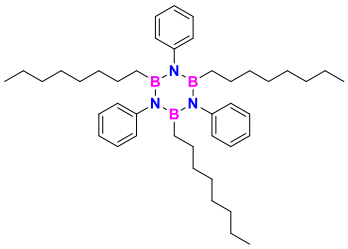


Synthesized in accordance with general procedure I, using **BNCl** (0.20 g, 0.49 mmol), THF (2 mL) and *n*-hexylmagnesium bromide (3.84 mL, 0.5 M solution in THF, 1.92 mmol). The product was purified by silica gel column chromatography (heptane) affording **2b** as a colorless liquid (0.18 g, 0.33 mmol, 68% yield).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.30 (t, J = 7.3 Hz, 6H), 7.19 (t, J = 7.3 Hz, 3H), 7.09 (d, J = 7.3 Hz, 6H), 1.04-0.95 (m, 6H), 0.92-0.83 (m, 6H), 0.81-0.76 (m, 6H), 0.72 (m, 15H), 0.33-0.29 (m, 6H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 147.5, 128.8, 128.1, 124.8, 32.4, 30.8, 24.1, 22.2, 16.3 (broad due to ^{11}B-induced quadrupolar relaxation), 14.0. ^{11}B NMR (193 MHz,

CD_2Cl_2) δ 35.6. IR (cm^{-1}): 3083, 3062, 3033, 2953, 2923, 2854, 1596, 1489, 1431, 1371, 1286, 1207, 1191, 1169, 1154, 1102, 1071, 1026, 1002, 986, 894, 872, 837, 769, 749, 723, 698, 618, 565, 527. HRMS (LD-timsTOF) m/z calcd for $[C_{36}H_{54}B_3N_3]^+$: 561.4608 $[M]^+$; found: 561.4600.

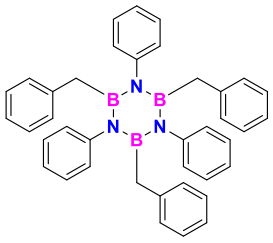
3.8 2,4,6-trioctyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2c**)



Synthesized in accordance with general procedure I, using **BNCl** (0.20 g, 0.49 mmol), THF (2 mL) and *n*-octylmagnesium bromide (3.79 mL, 0.5 M solution in THF, 1.89 mmol). The product was purified by silica gel column chromatography (heptane) affording **2c** as a colorless liquid (0.20 g, 0.31 mmol , 64% yield).

^1H NMR (600 MHz, $CDCl_3$) δ 7.29 (t, J = 7.7 Hz, 6H), 7.17 (t, J = 7.7 Hz, 3H), 7.09 (d, J = 7.7 Hz, 6H), 1.23-1.17 (m, 6H), 1.09-1.04 (m, 6H), 0.99-0.94 (m, 6H), 0.87-0.83 (m, 15H), 0.81-0.76 (m, 6H), 0.72-0.67 (m, 6H), 0.31-0.28 (m, 6H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 147.5, 129.0, 128.1, 124.8, 32.7, 31.8, 28.8, 28.5, 24.2, 22.6, 16.3 (broad due to ^{11}B-induced quadrupolar relaxation), 14.1. ^{11}B NMR (192 MHz, $CDCl_3$) δ 36.2. IR (cm^{-1}): 3084, 3063, 3034, 2953, 2921, 2852, 1597, 1489, 1432, 1373, 1196, 1108, 1071, 1026, 1003, 750, 721, 699, 565, 528. HRMS (MALDI-timsTOF) m/z calcd for $[C_{42}H_{66}B_3N_3]^+$: 645.5550 $[M]^+$; found: 645.5546.

3.9 2,4,6-tribenzyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2d**)

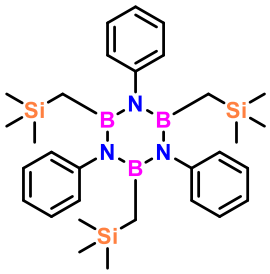


Synthesized in accordance with general procedure I, using **BNCl** (0.50 g, 1.21 mmol), THF (5 mL) and BnMgCl (2.43 mL, 2M solution in THF, 4.85 mmol). The product was purified by silica gel column chromatography (heptane/CH_2Cl_2 4:1) affording **2d** as a white solid (0.49 g, 0.86 mmol, 71% yield).

MP 73–75 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.10-7.05 (m, 9H), 6.95 (m, 9H), 6.85 (d, J = 7.7 Hz, 6H), 6.45 (m, 6H), 2.05 (s, 6H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 146.5, 140.5, 129.1,

128.9, 128.3, 127.5, 124.9, 123.8, 24.6 (broad due to ^{11}B-induced quadrupolar relaxation). ^{11}B NMR (193 MHz, $CDCl_3$) δ 35.8. IR (cm^{-1}): 3077, 3057, 3022, 1596, 1490, 1450, 1415, 1370, 1226, 1197, 1168, 1071, 1027, 809, 770, 760, 727, 694, 566, 525, 464. HRMS (MALDI-timsTOF) m/z calcd for $[C_{39}H_{36}B_3N_3]^+$: 579.3201 $[M]^+$; found: 579.3198.

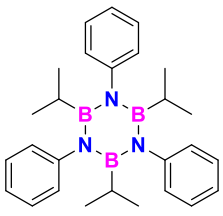
3.10 1,3,5-triphenyl-2,4,6-tris((trimethylsilyl)methyl)-1,3,5,2,4,6-triazatriborinane (**2e**)



Synthesized in accordance with general procedure I, using **BNCl** (0.20 g, 0.485 mmol), THF (2 mL) and (Trimethylsilyl)methyllithium (0.27 mL, 0.7 M solution in pentane, 1.94 mmol). The product was purified by reprecipitation from dichloromethane and methanol affording **2e** as a white solid (0.16 g, 0.30 mmol, 61% yield).

MP 172–174 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32 (t, J = 7.6 Hz, 6H), δ 7.17 (t, J = 7.6 Hz, 3H), 7.07 (d, J = 7.6 Hz, 6H), 0.02 (s, 6H), -0.42 (s, 27H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 149.2, 129.8, 128.7, 124.9, 6.75 (broad due to ^{11}B-induced quadrupolar relaxation), 1.19. ^{11}B NMR (193 MHz, $CDCl_3$) δ 36.2. ^{29}Si NMR (119 MHz, $CDCl_3$) δ 2.8. IR (cm^{-1}): 3064, 2949, 2893, 1596, 1488, 1449, 1391, 1347, 1244, 1195, 1071, 1027, 897, 832, 762, 700, 643, 546, 512. HRMS (ESI) m/z calcd for $[C_{30}H_{49}B_3Si_3N_3]^+$: 568.3525 $[M+H]^+$; found: 568.3524. For crystal structure: CCDC 2307378 (Table S4 and Figure S55).

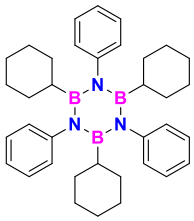
3.11 2,4,6-triisopropyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**3a**)



Synthesized in accordance with general procedure I, using **BNCl** (0.30 g, 0.73 mmol), THF (3 mL) and isopropylmagnesium chloride (2.84 mL, 1 M solution in THF, 2.84 mmol). The product was purified by silica gel column chromatography (heptane) affording **3a** as a white solid (0.22 g, 0.50 mmol, 69% yield).

MP 193–195 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.28 (t, J = 7.9 Hz, 6H), 7.20 (t, J = 7.9 Hz, 3H), 7.14 (d, J = 7.9 Hz, 6H), 0.95 (sept, J = 7.7 Hz, 3H), 0.35 (d, J = 7.7 Hz, 18H). ^{13}C{^{1}H} NMR (150 MHz, CD_2Cl_2) δ 147.6, 130.6, 128.4, 125.7, 19.3, 15.7 (broad due to ^{11}B-induced quadrupolar relaxation). ^{11}B NMR (193 MHz, CD_2Cl_2) δ 35.6. IR (cm^{-1}): 2970, 2938, 2923, 2863, 1595, 1489, 1466, 1449, 1388, 1367, 1327, 1302, 1249, 1146, 1068, 1032, 1024, 915, 900, 775, 732, 700, 564, 518. HRMS (MALDI-timsTOF) m/z calcd for $[C_{27}H_{36}B_3N_3]^+$: 435.3193 $[M]^+$; found: 435.3181. For crystal structure: CCDC 2284380 (Table S5 and Figure S56).

3.12 2,4,6-tricyclohexyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**3b**)



Synthesized in accordance with general procedure I, using **BNCl** (0.50 g, 1.25 mmol), THF (5 mL) and CyMgBr (4.98 mL, 1 M solution in THF, 4.98 mmol). The product was purified by silica gel column chromatography (heptane:CH_2Cl_2 4:1) affording **3b** as a white solid (0.44 g, 0.80 mmol, 64% yield).

MP 193–195 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.28 (t, J = 7.9 Hz, 6H), 7.20 (t, J = 7.9 Hz, 3H), 7.09 (d, J = 7.9 Hz, 6H), 1.27-1.22 (m, 15H), 0.70-0.61 (m, 6H), 0.53-0.47 (m, 6H), 0.37-0.31 (m, 6H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 147.3 (broad), 129.8 (broad), 127.7, 125.1, 29.7 (broad due to ^{11}B-induced quadrupolar relaxation), 28.7, 28.3, 26.7. ^{11}B NMR (192 MHz, $CDCl_3$) δ 35.0. IR (cm^{-1}): 2916, 2848, 1594, 1491, 1447, 1380, 1339, 1296, 1268, 1224, 1160, 1070, 1024, 1006, 905, 885, 774, 729, 700, 546. HRMS (MALDI-timsTOF) m/z calcd for $[C_{36}H_{48}B_3N_3]^+$: 555.4139 $[M]^+$; found: 555.4150. For crystal structure: CCDC 2261151 (Table S6 and Figure S57).

4. Spectroscopic Characterization

4.1 Characterization of 2,4,6-trichloro-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**BNCl**)

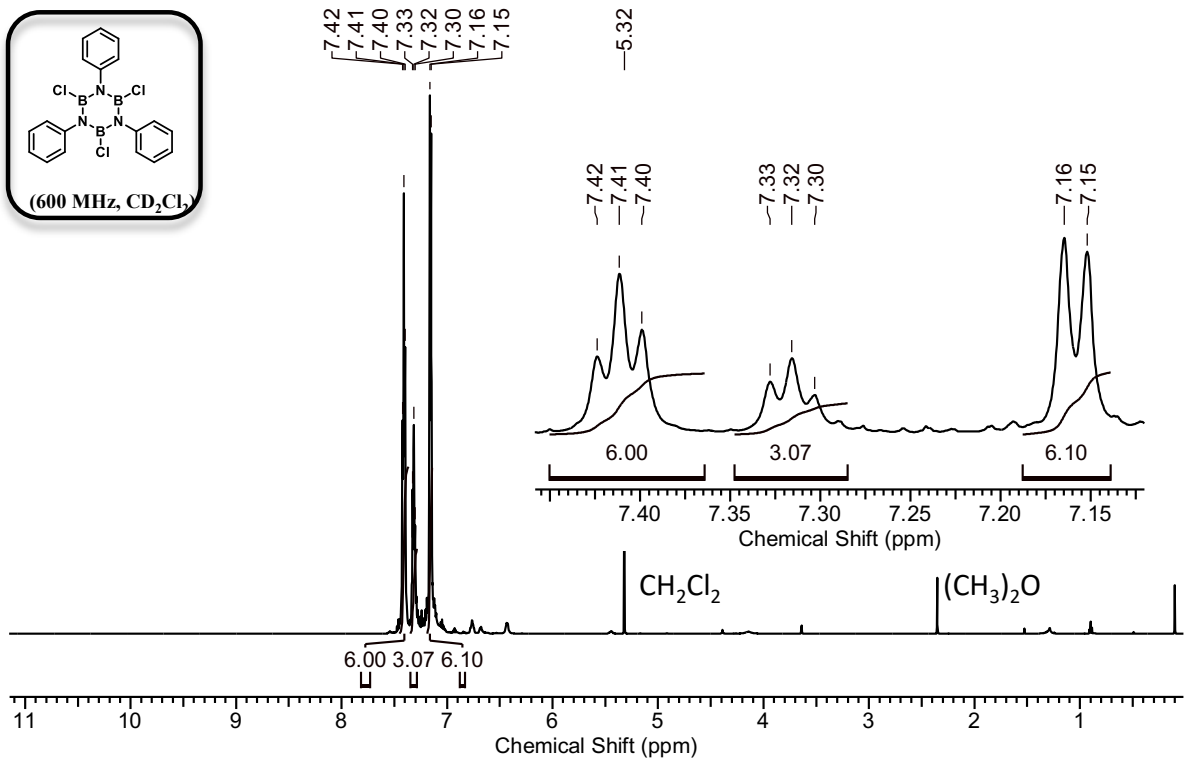


Figure S1. 600 MHz ^{1}H-NMR of **BNCl** in CD_2Cl_2.

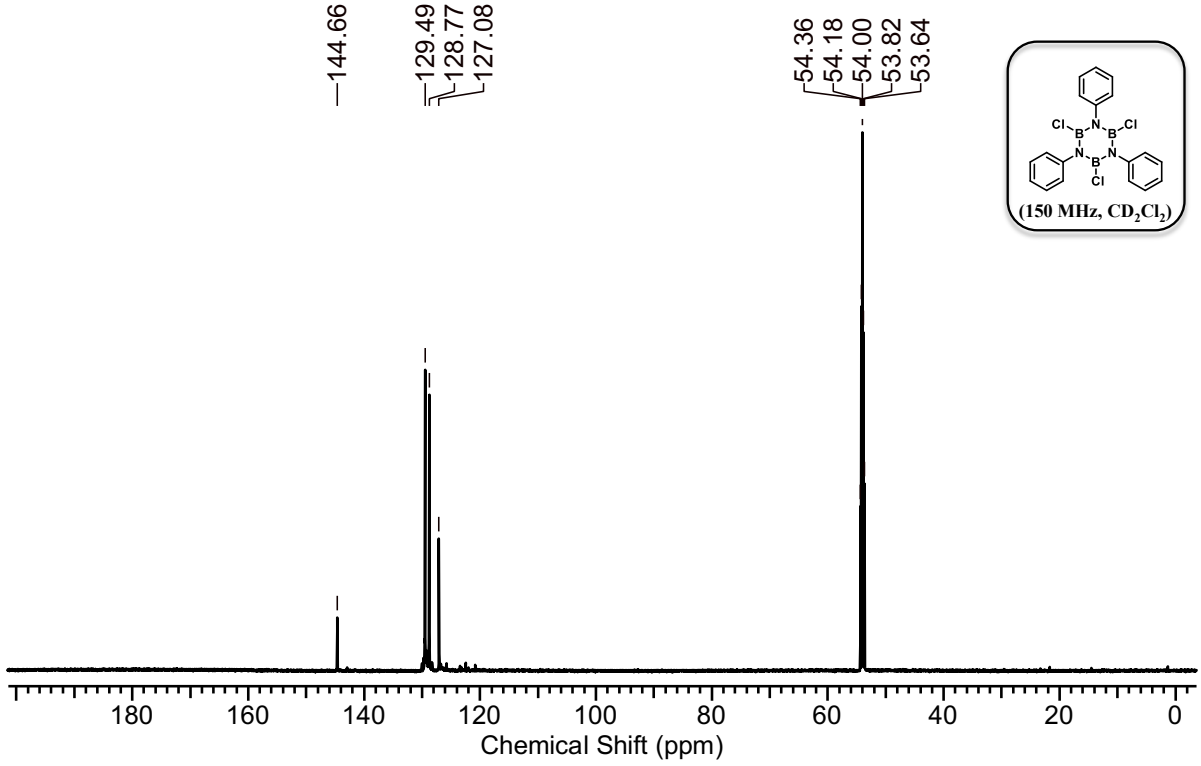


Figure S2. 150 MHz ^{13}C{^{1}H}-NMR of **BNCl** in CD_2Cl_2.

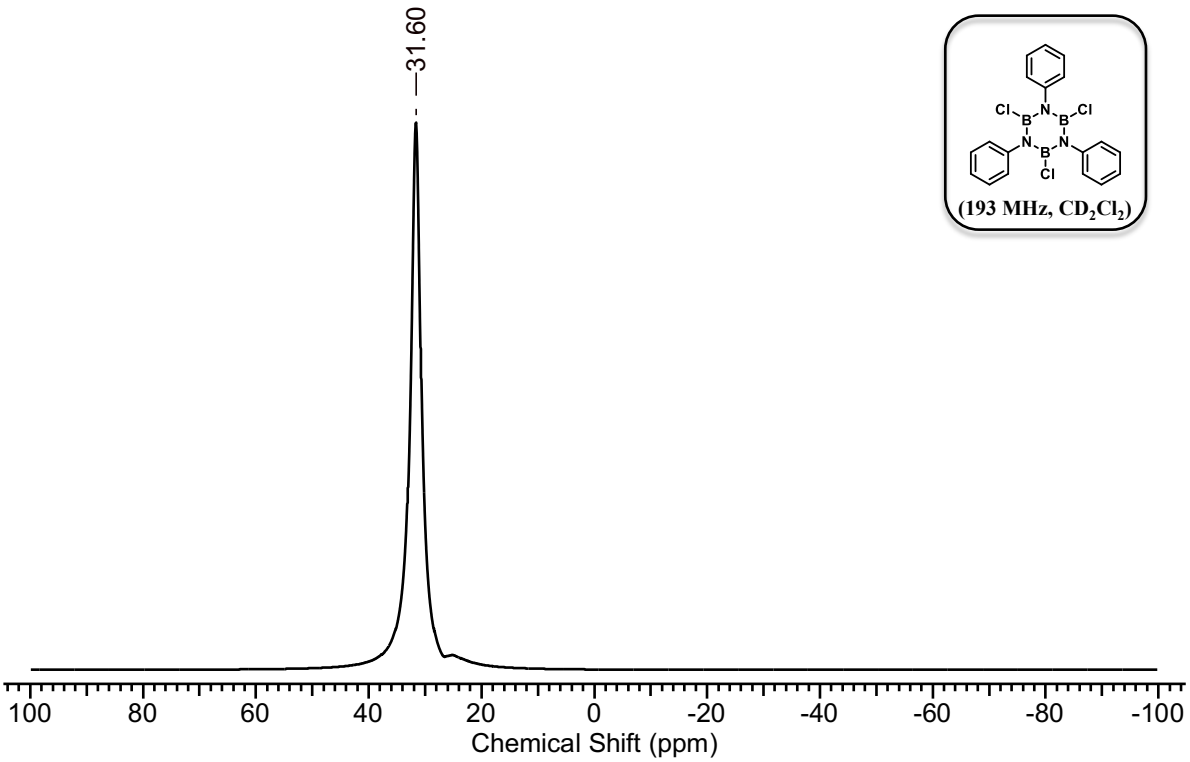


Figure S3. 193 MHz ^{11}B-NMR of **BNCl** in CD_2Cl_2.

4.2 Characterization of 2,4,6-trimethyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**1a**)

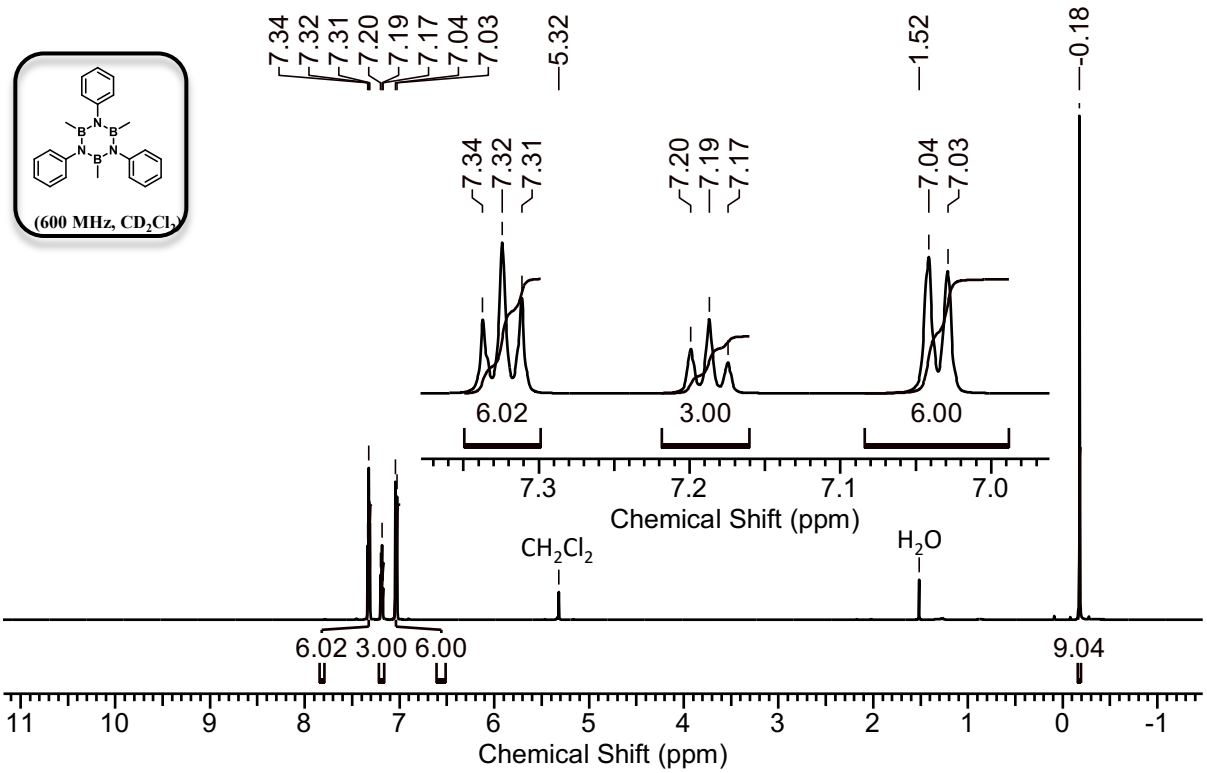


Figure S4. 600 MHz ^{1}H-NMR of **1a** in CD_2Cl_2.

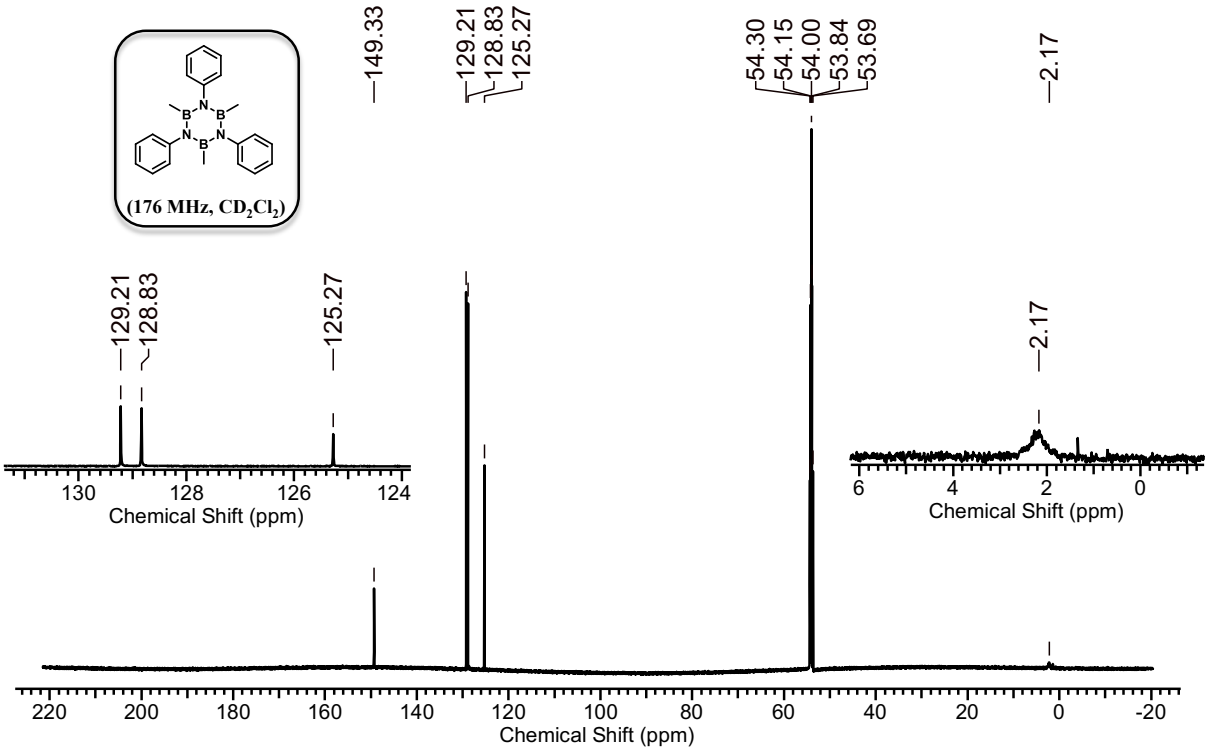


Figure S5. 176 MHz ^{13}C{^{1}H}-NMR of **1a** in CD_2Cl_2.

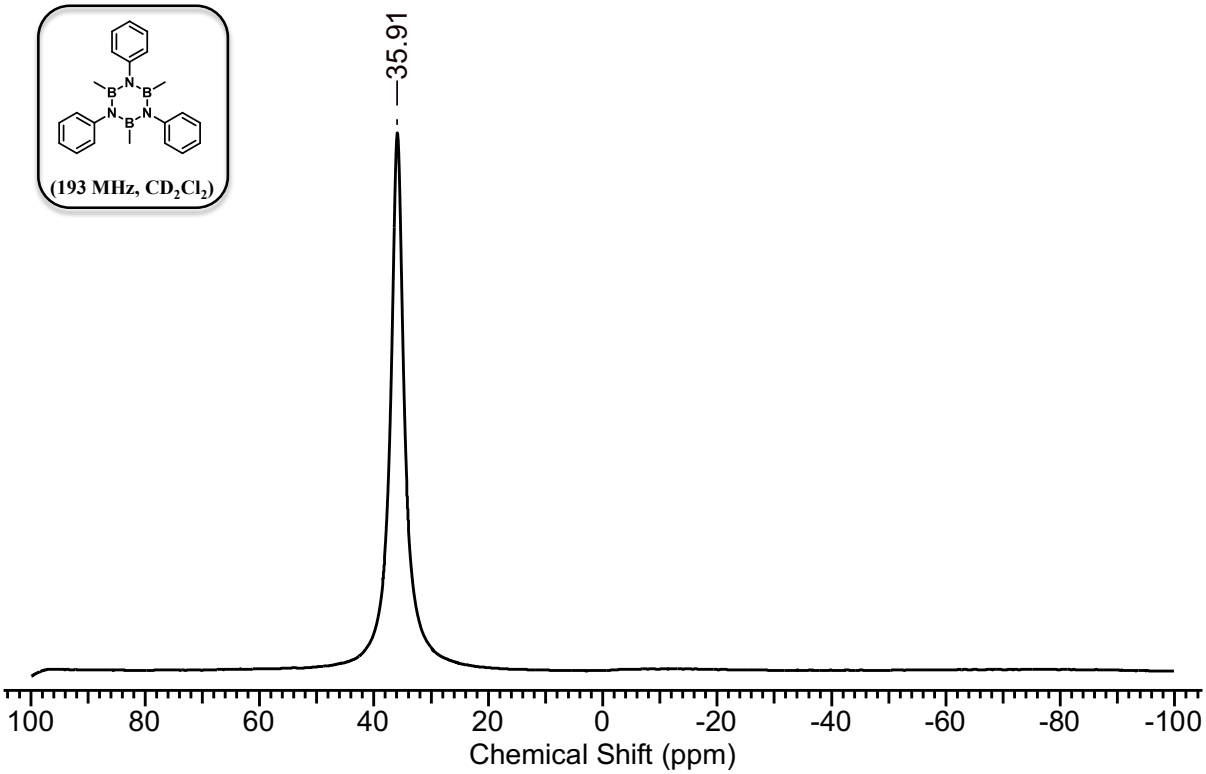


Figure S6. 193 MHz ^{11}B-NMR of **1a** in CD_2Cl_2.

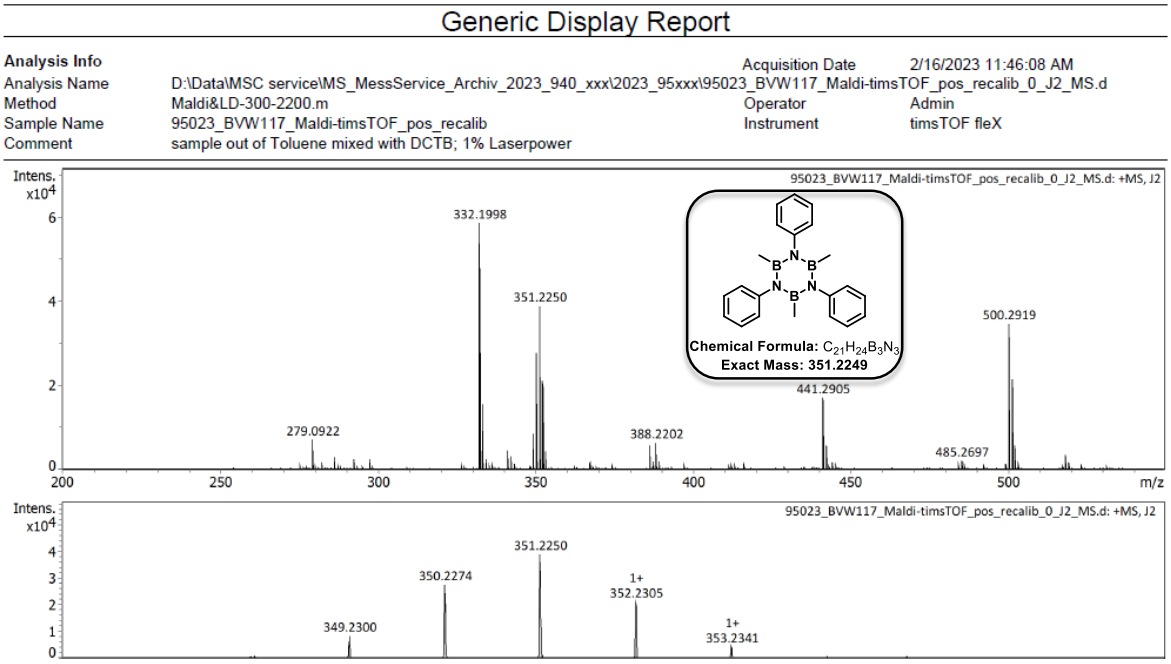


Figure S7. HRMS (MALDI-timsTOF, matrix: DCTB) spectrum of **1a**.

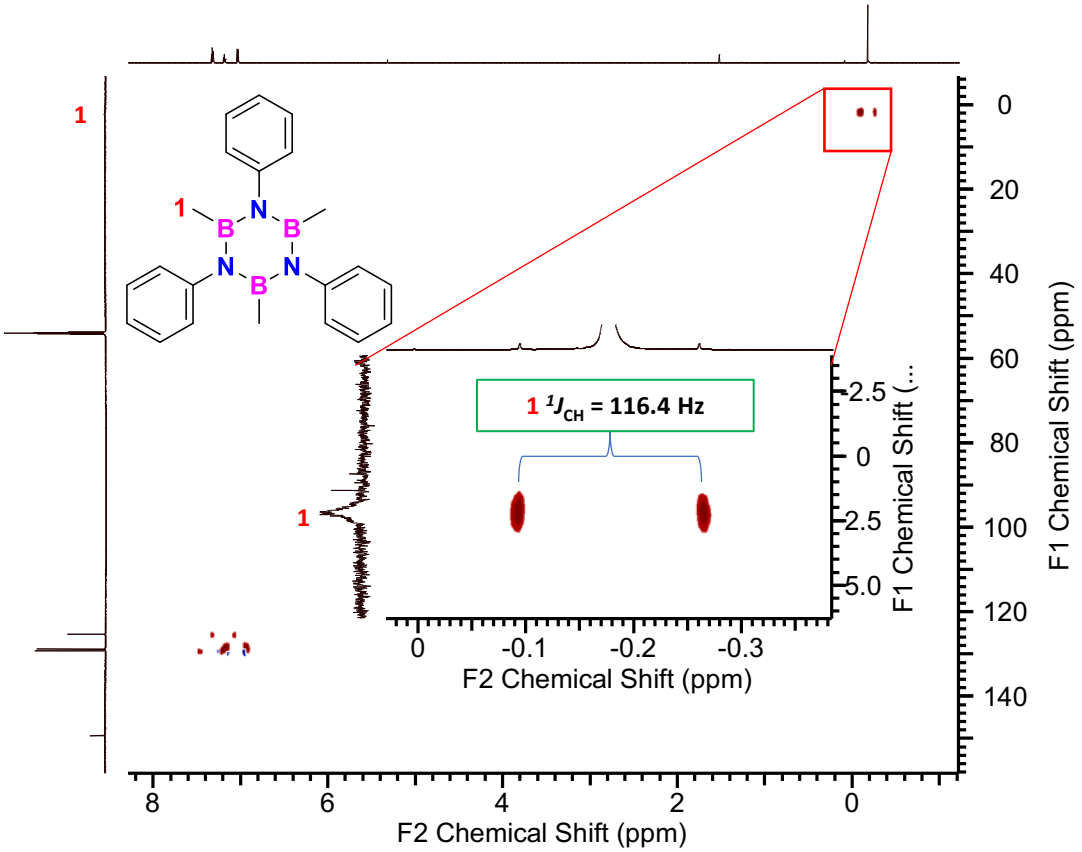


Figure S8. ^{1}H-^{13}C coupled HSQC NMR of **1a** in CD_2Cl_2.

4.3 Characterization of 1,3,5-tris(2',6'-dimethyl-[1,1'-biphenyl]-4-yl)-2,4,6-trimethyl-1,3,5,2,4,6-triazatriborinane (**1b**)

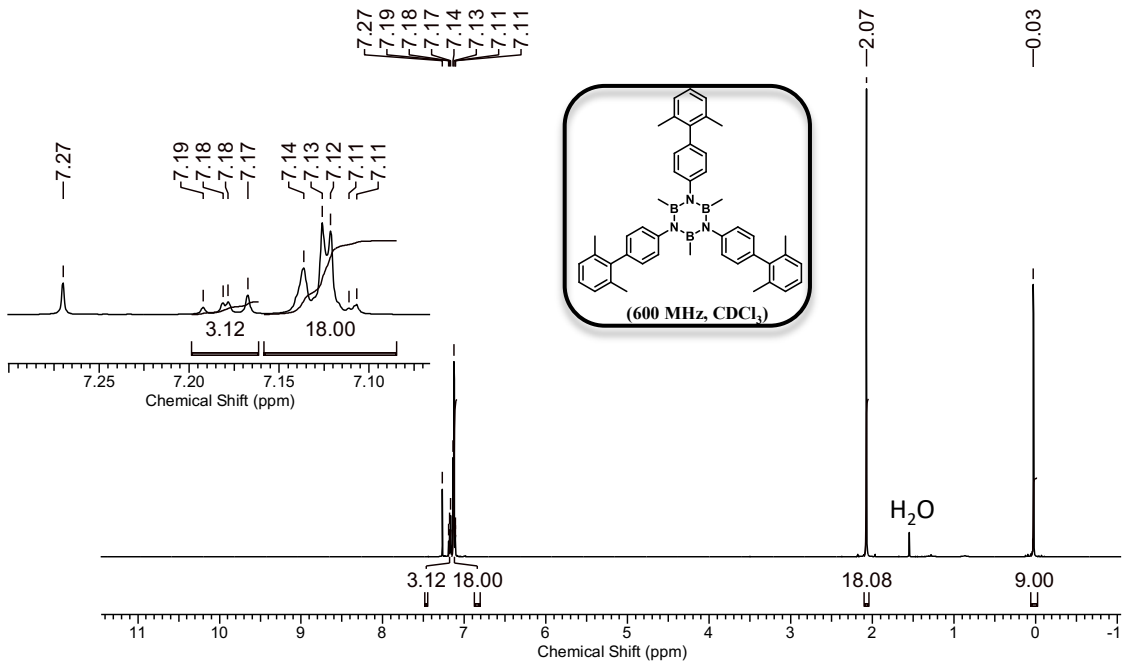


Figure S9. 600 MHz ^{1}H-NMR of **1b** in $CDCl_3$.

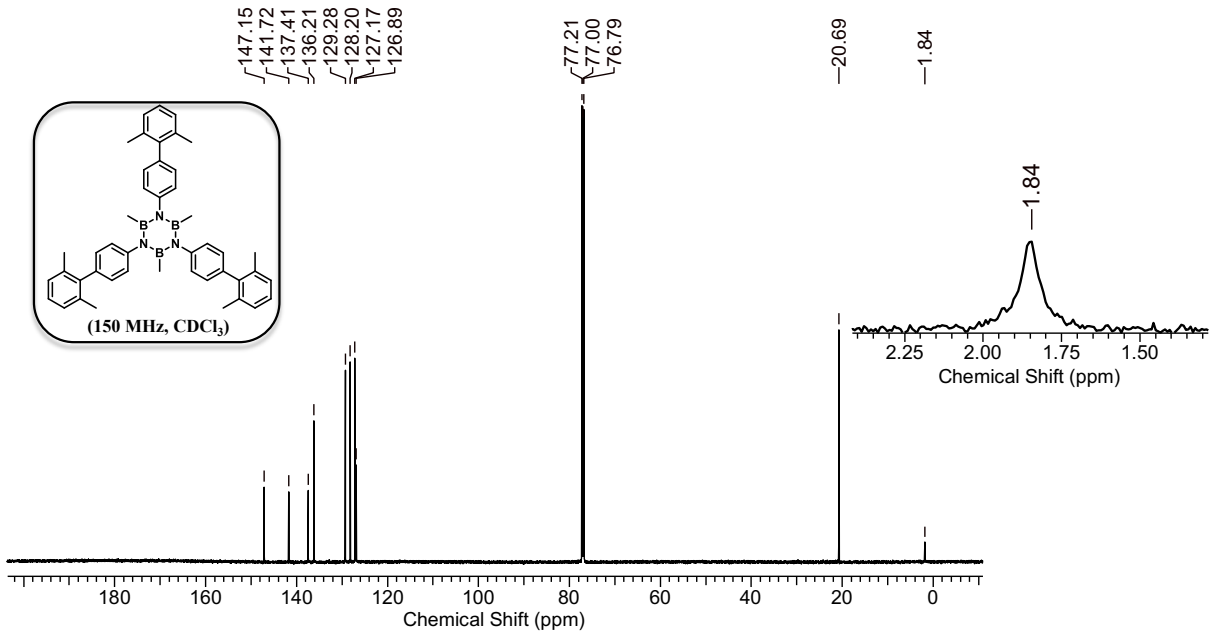


Figure S10. 150 MHz $^{13}C\{^{1}H\}$-NMR of **1b** in $CDCl_3$.

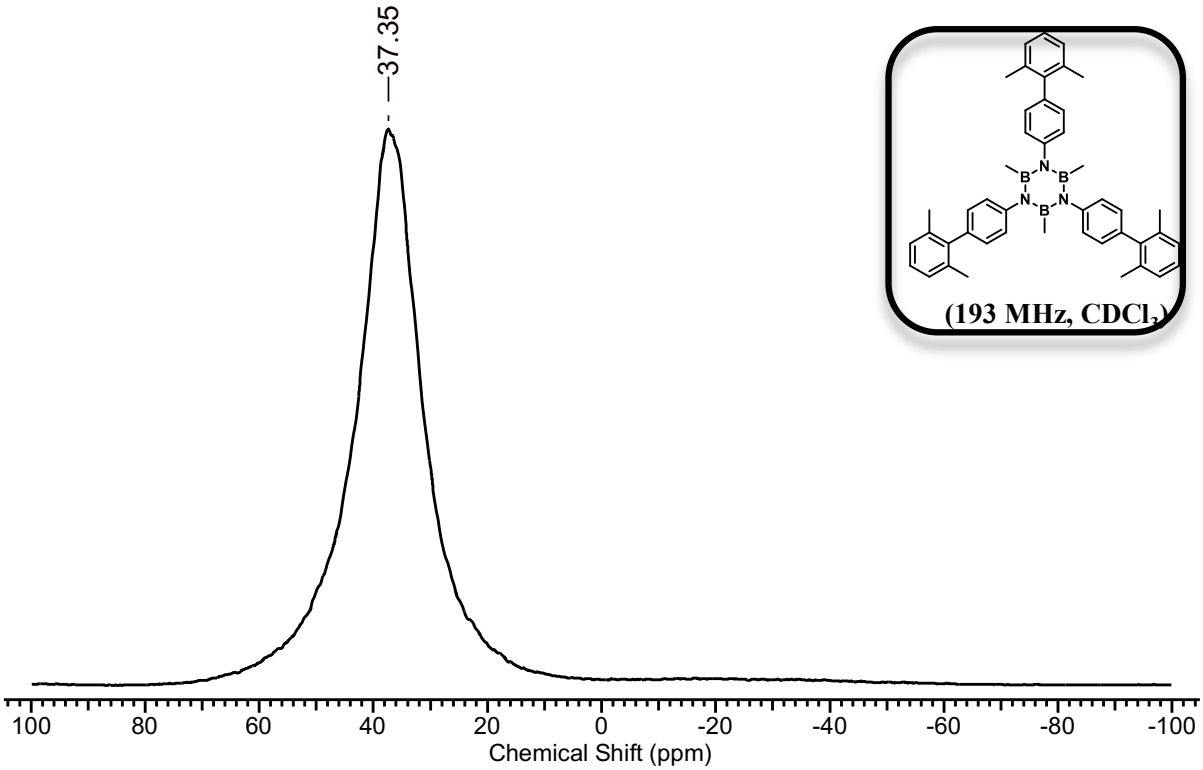


Figure S11. 193 MHz ^{11}B-NMR of **1b** in $CDCl_3$.

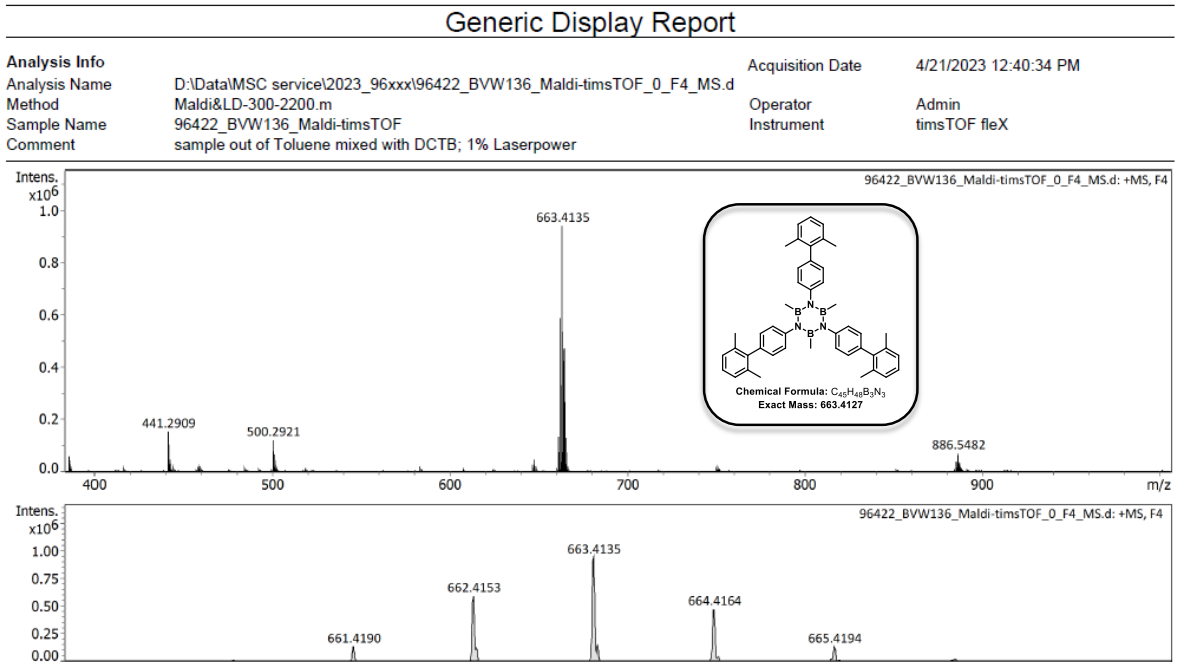


Figure S12. HRMS (MALDI-timsTOF, matrix: DCTB) spectrum of **1b**.

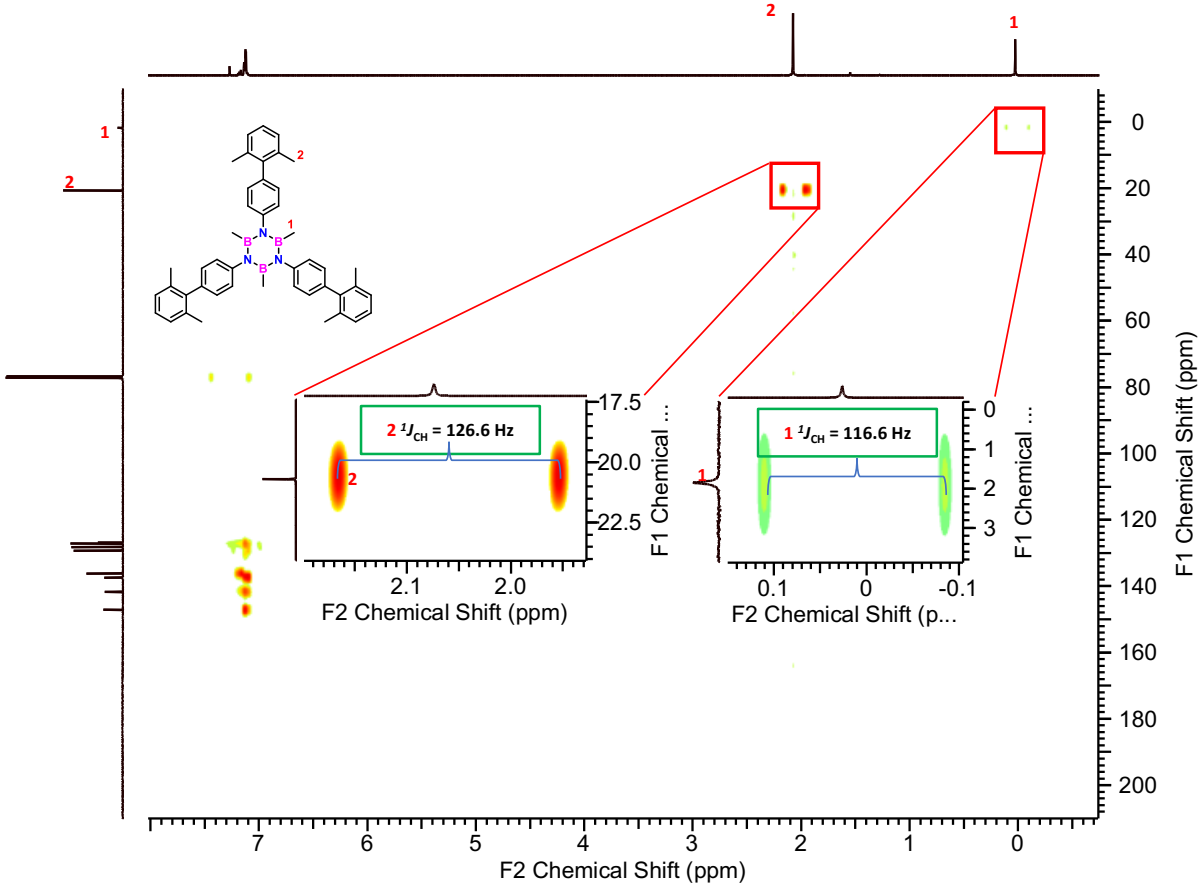


Figure S13. ^{1}H-^{13}C coupled HSQC NMR of **1b** in $CDCl_3$.

4.4 Characterization of 2,4,6-tributyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2a**)

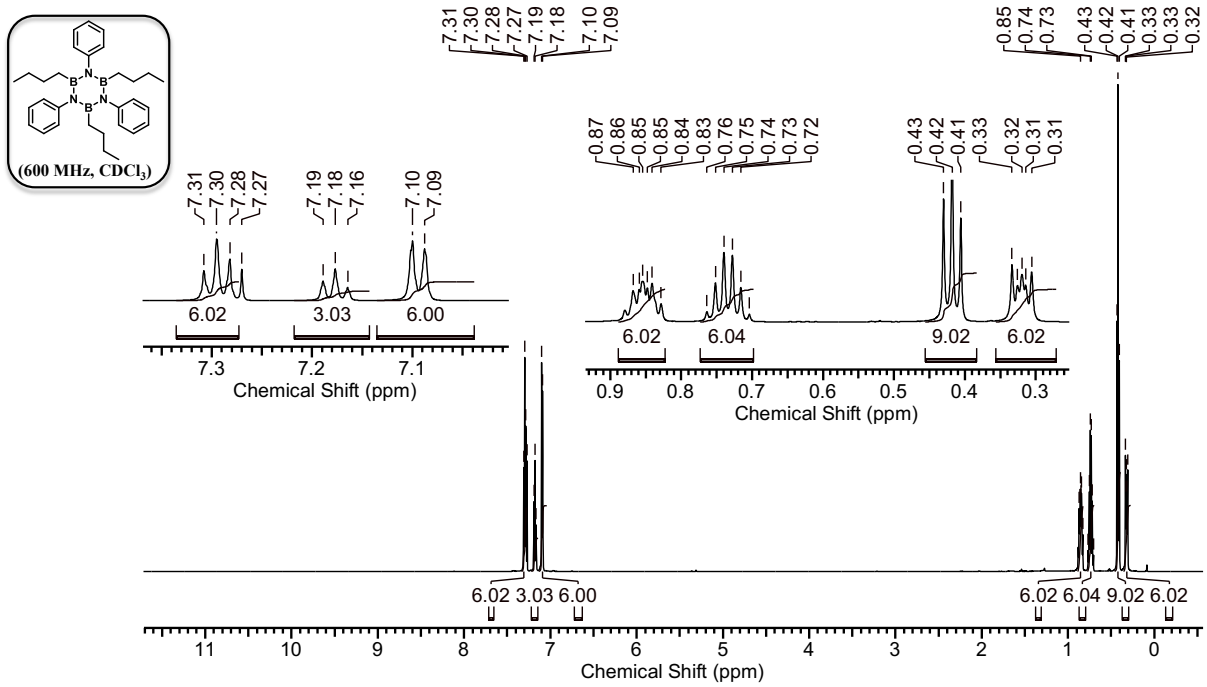


Figure S14. 600 MHz ^{1}H-NMR of **2a** in $CDCl_3$.

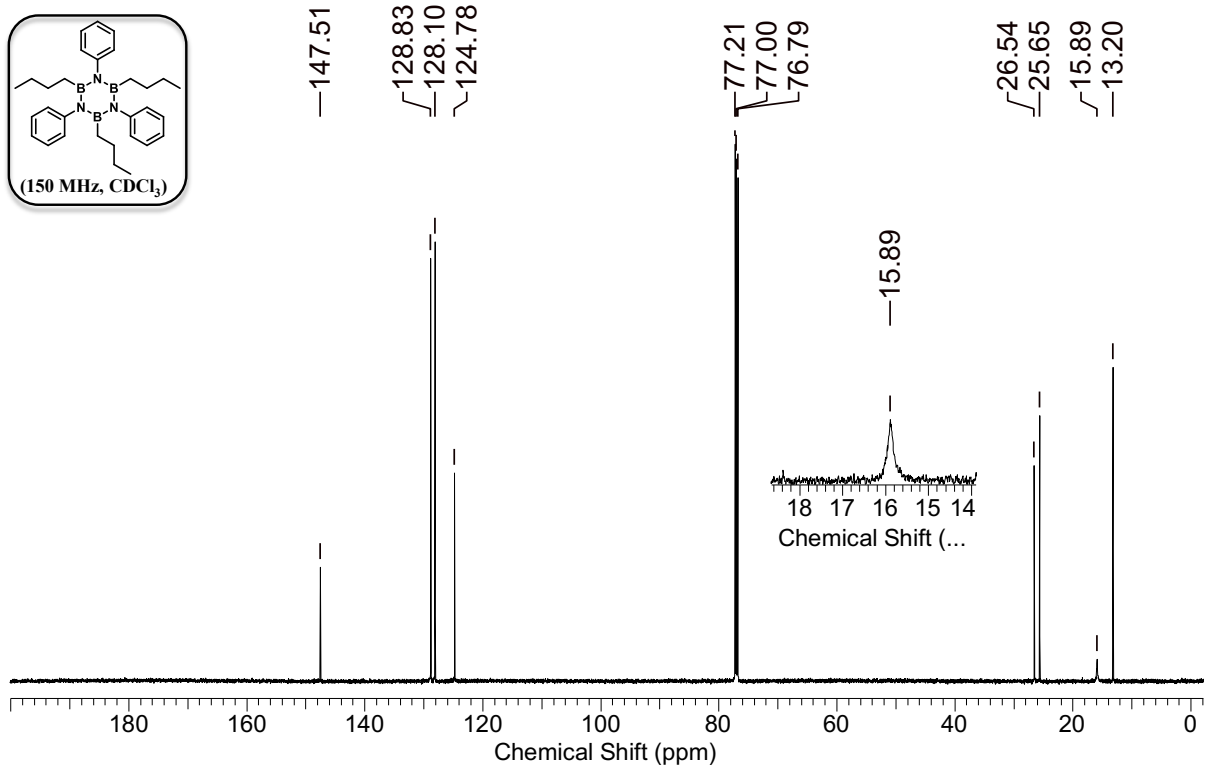


Figure S15. 150 MHz $^{13}C\{^{1}H\}$-NMR of **2a** in $CDCl_3$.

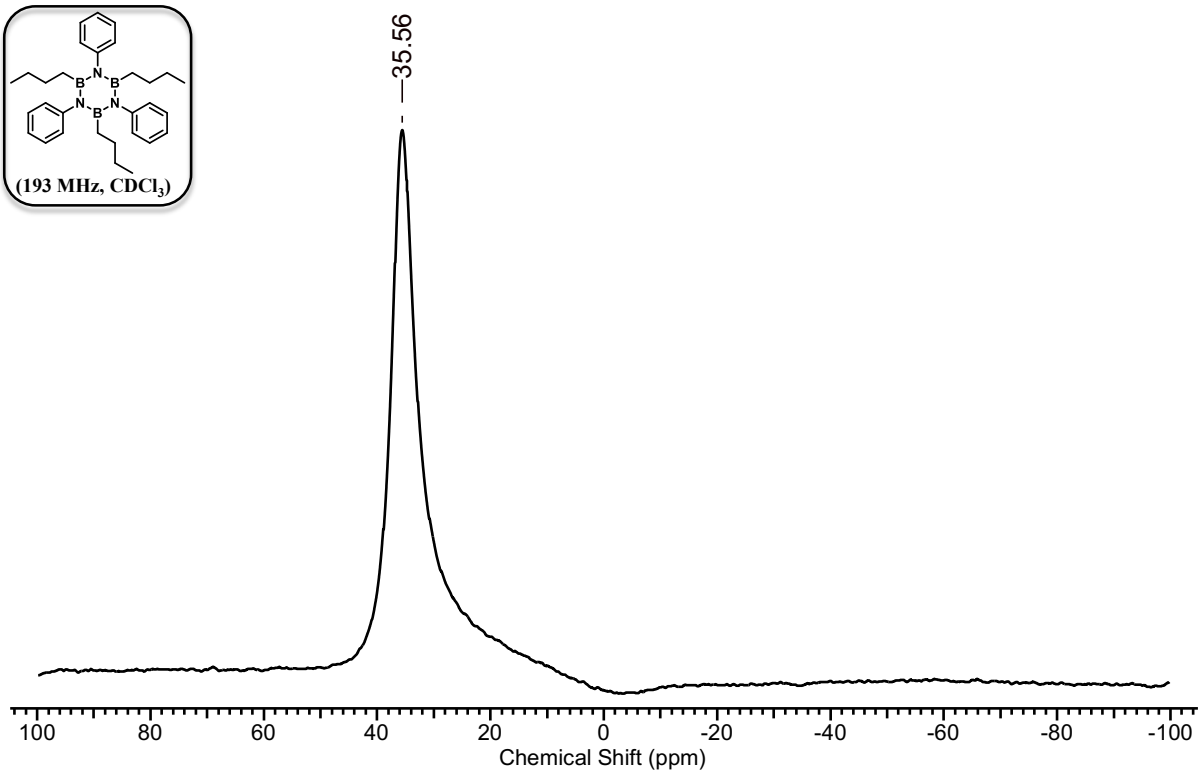


Figure S16. 193 MHz ^{11}B-NMR of **2a** in $CDCl_3$.

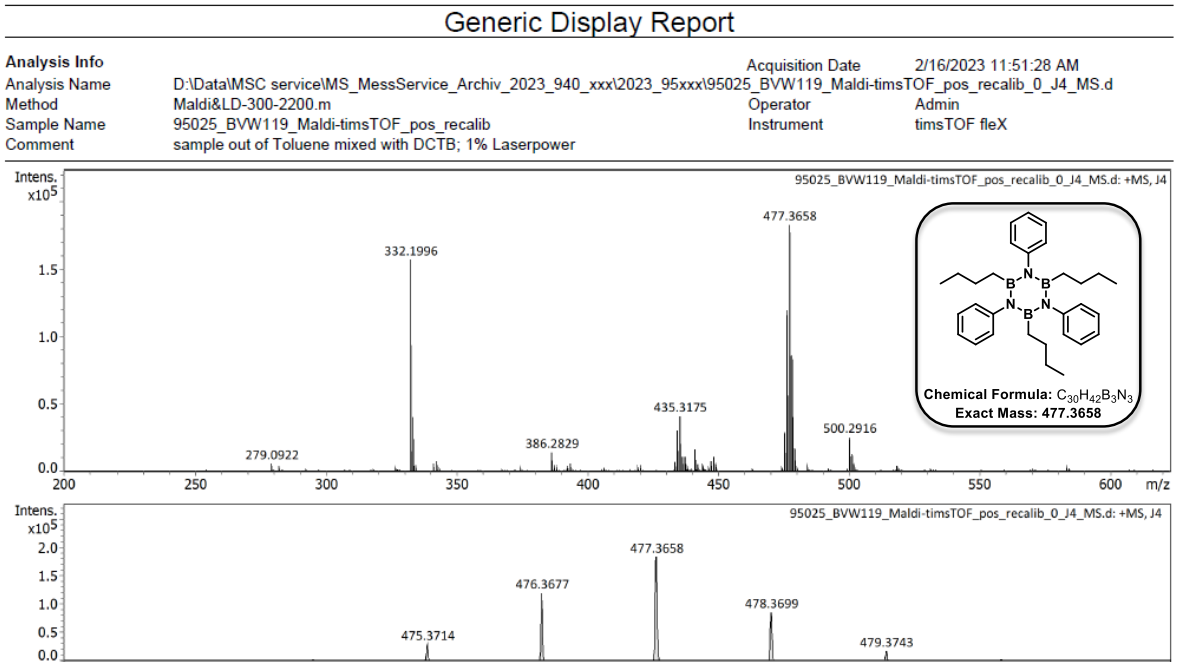
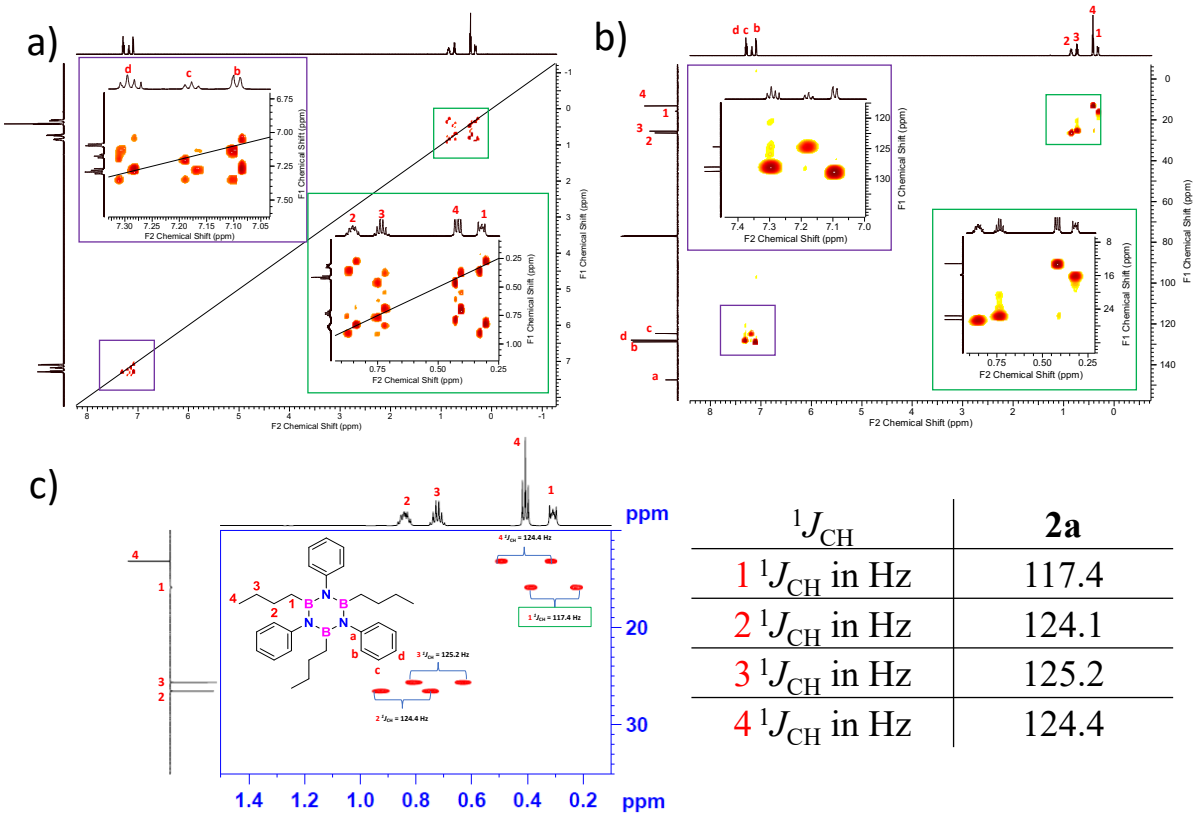


Figure S17. HRMS (MALDI-timsTOF, matrix: DCTB) spectrum of **2a**.



$^1J_{CH}$	**2a**
1 $^1J_{CH}$ in Hz	117.4
2 $^1J_{CH}$ in Hz	124.1
3 $^1J_{CH}$ in Hz	125.2
4 $^1J_{CH}$ in Hz	124.4

Figure S18. a) ^{1}H-^{1}H COSY, b) ^{1}H-^{13}C HSQC, c) ^{1}H-^{13}C coupled HSQC NMR of **2a** in $CDCl_3$ and corresponding coupling constants.

4.5 Characterization of 2,4,6-trihexyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2b**)

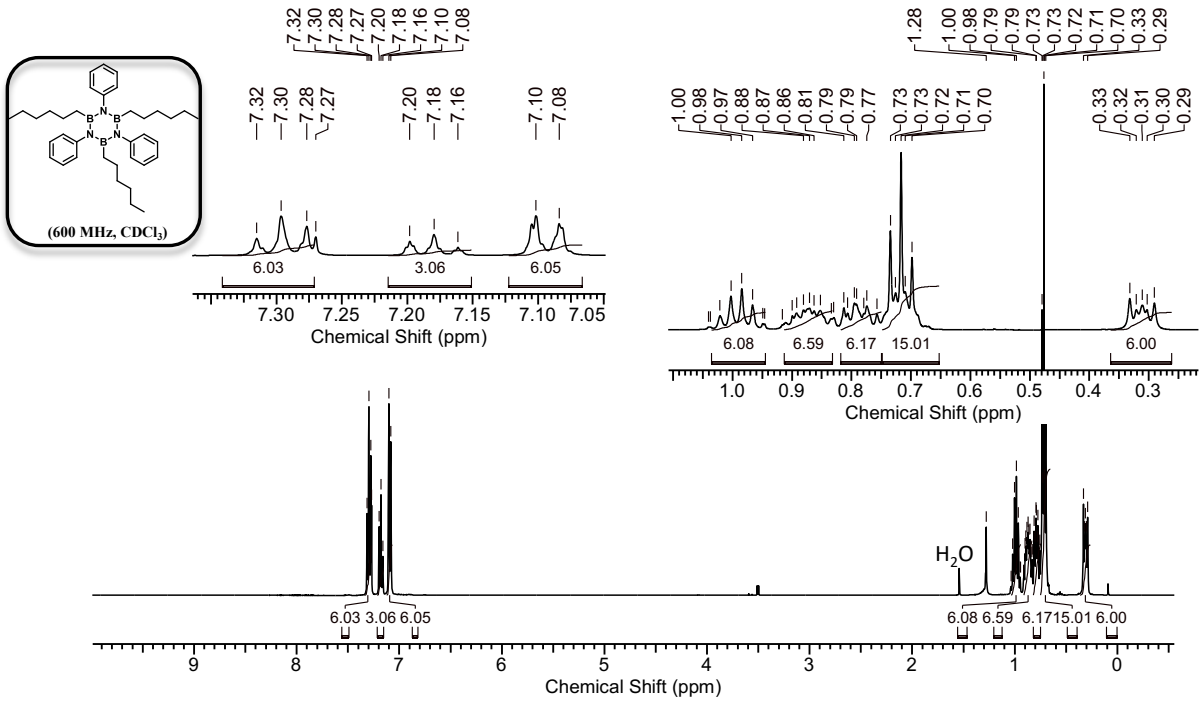


Figure S19. 600 MHz ^{1}H-NMR of **2b** in $CDCl_3$.

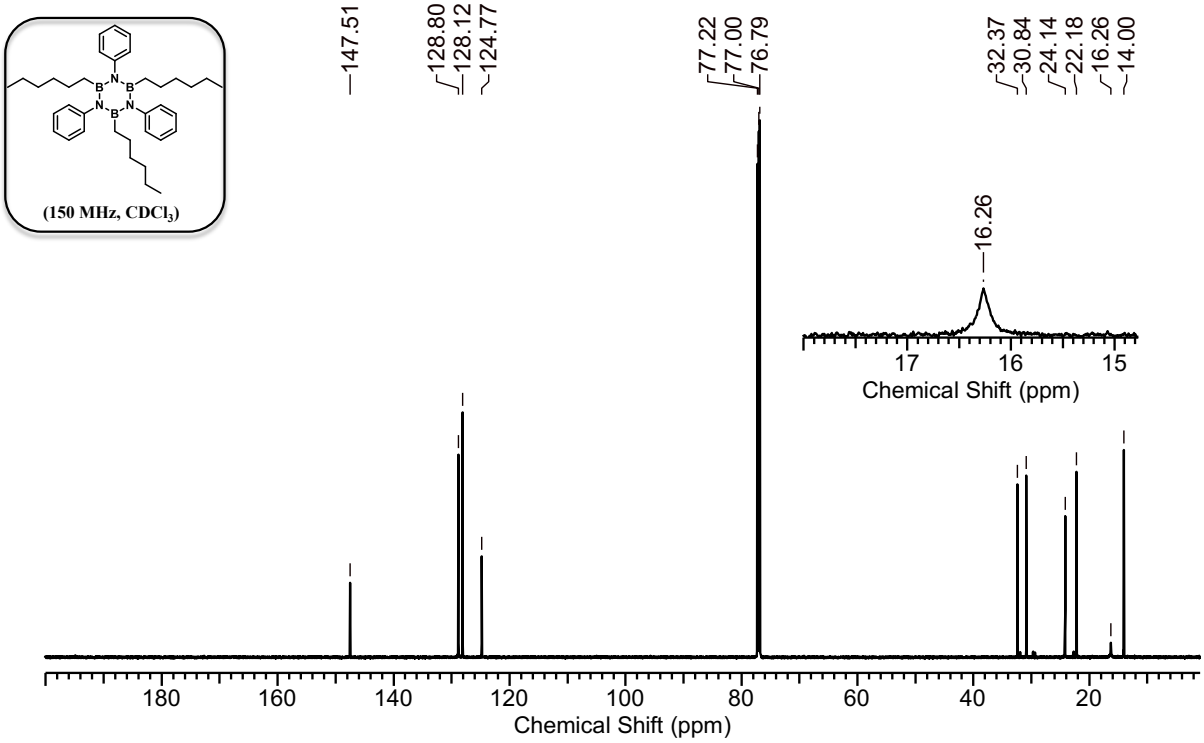


Figure S20. 150 MHz ^{13}C{^{1}H}-NMR of **2b** in $CDCl_3$.

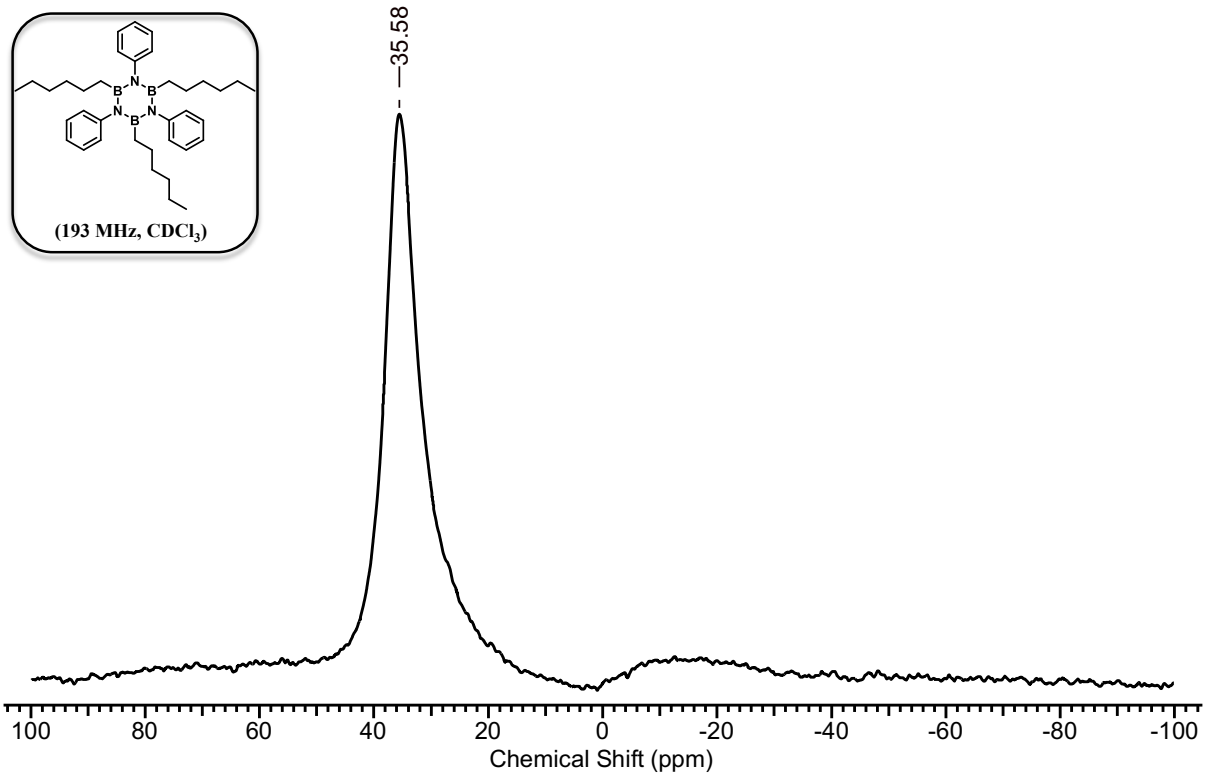


Figure S21. 193 MHz ^{11}B-NMR of **2b** in $CDCl_3$.

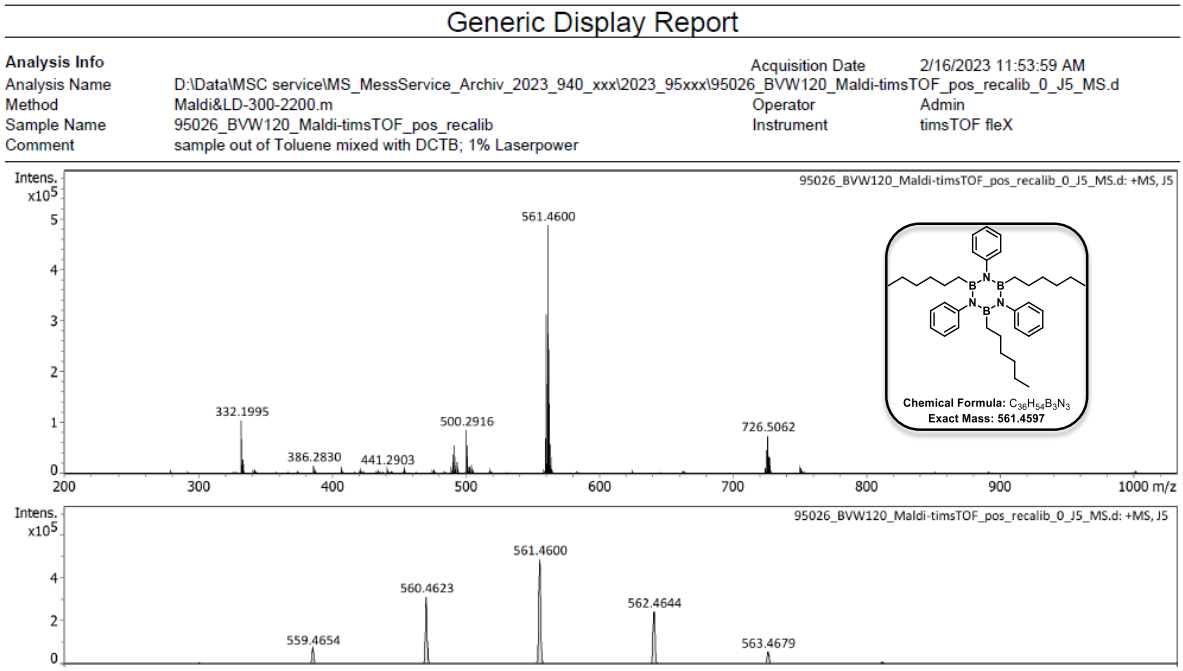
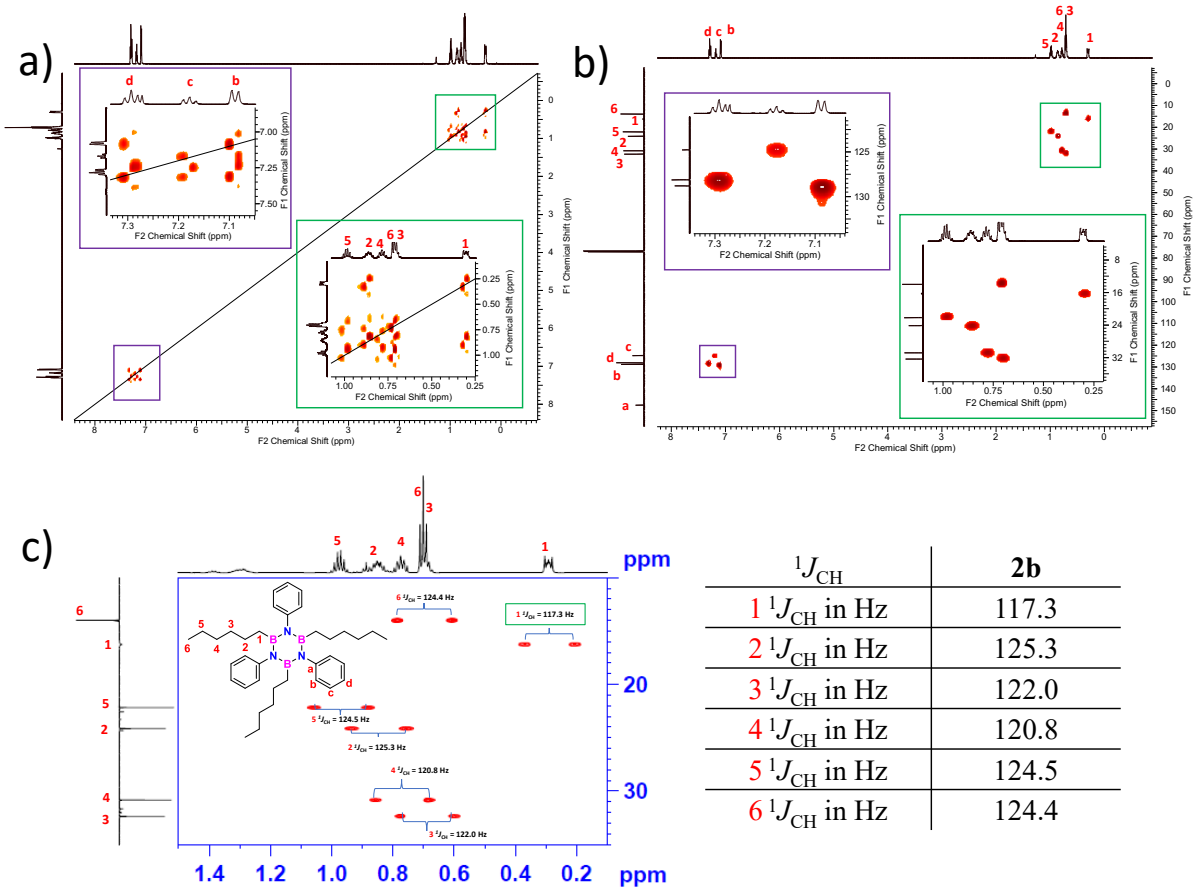


Figure S22. HRMS (MALDI-timsTOF, matrix: DCTB) spectrum of **2b**.



$^{1}J_{CH}$	**2b**
1 $^{1}J_{CH}$ in Hz	117.3
2 $^{1}J_{CH}$ in Hz	125.3
3 $^{1}J_{CH}$ in Hz	122.0
4 $^{1}J_{CH}$ in Hz	120.8
5 $^{1}J_{CH}$ in Hz	124.5
6 $^{1}J_{CH}$ in Hz	124.4

Figure S23. a) ^{1}H-^{1}H COSY, b) ^{1}H-^{13}C HSQC, c) ^{1}H-^{13}C coupled HSQC NMR of **2b** in $CDCl_3$ and corresponding coupling constants.

4.6 Characterization of 2,4,6-trioctyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2c**)

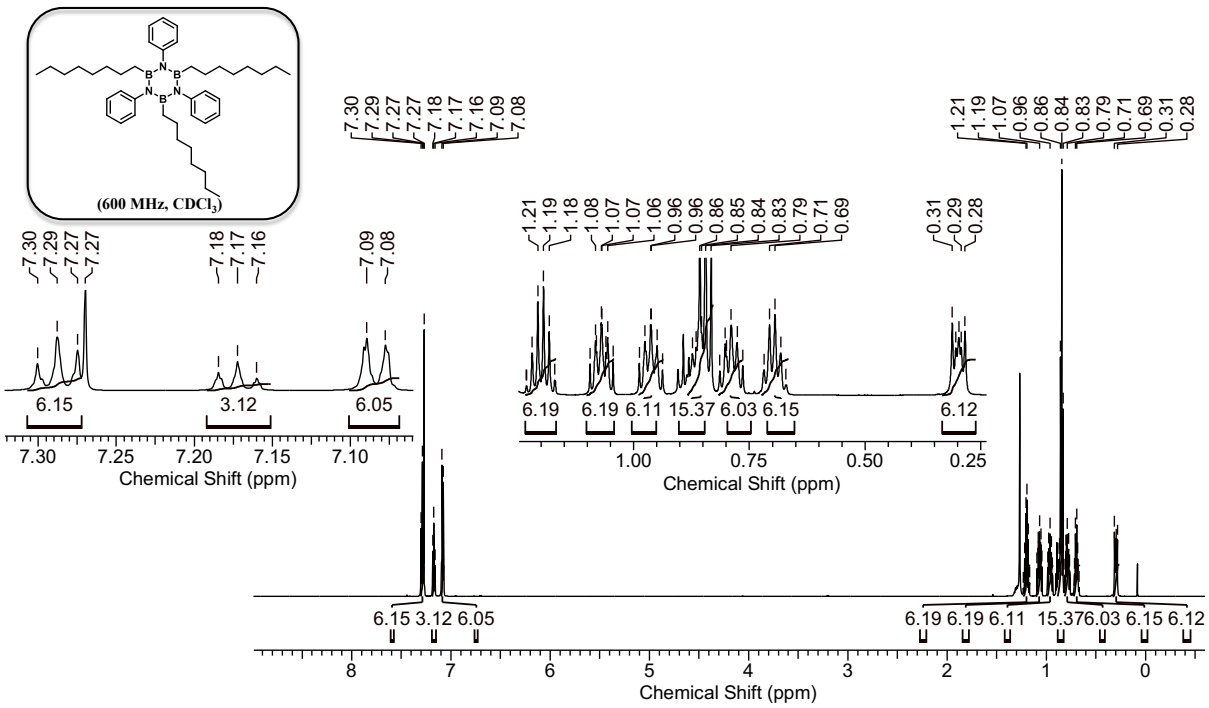


Figure S24. 600 MHz ^{1}H-NMR of **2c** in $CDCl_3$.

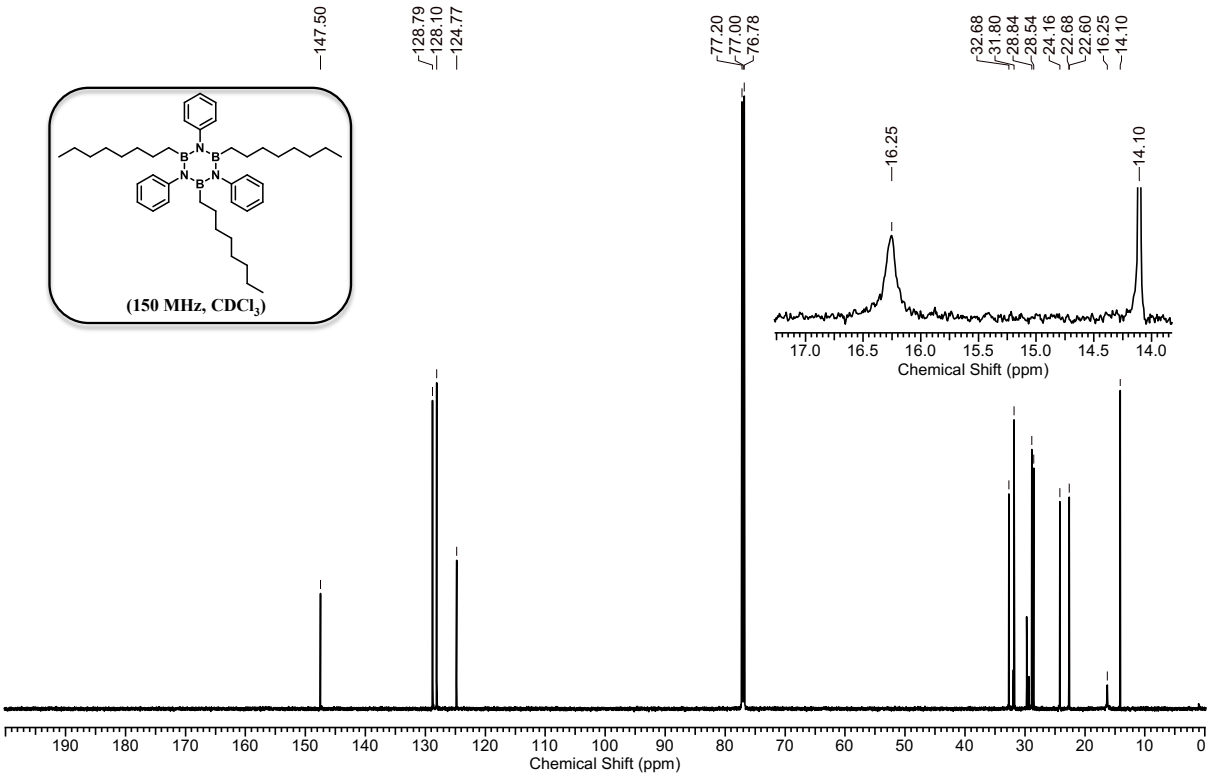


Figure S25. 150 MHz ^{13}C{^{1}H}-NMR of **2c** in $CDCl_3$.

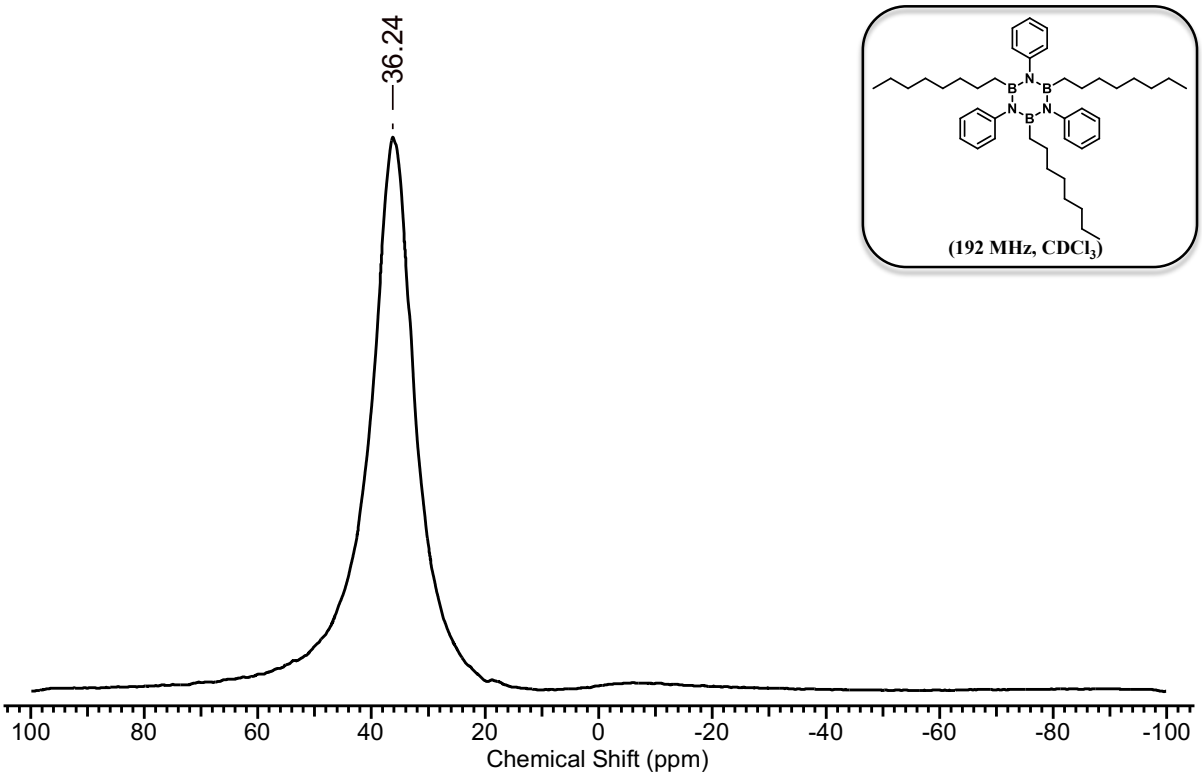


Figure S26. 193 MHz ^{11}B-NMR of **2c** in $CDCl_3$.

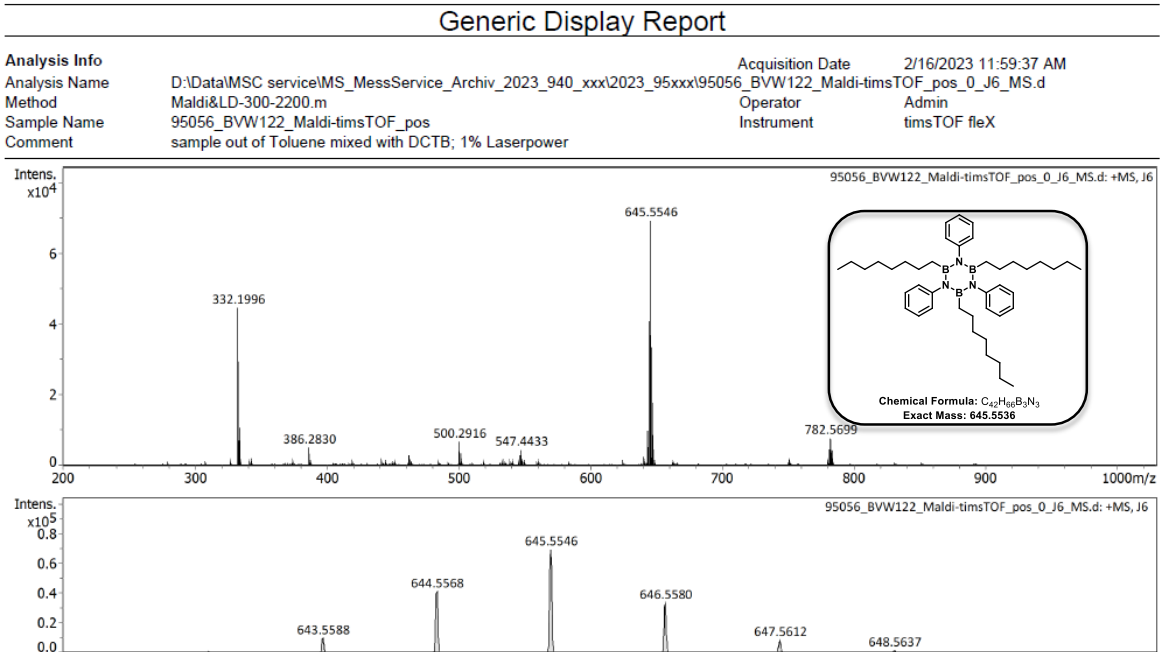
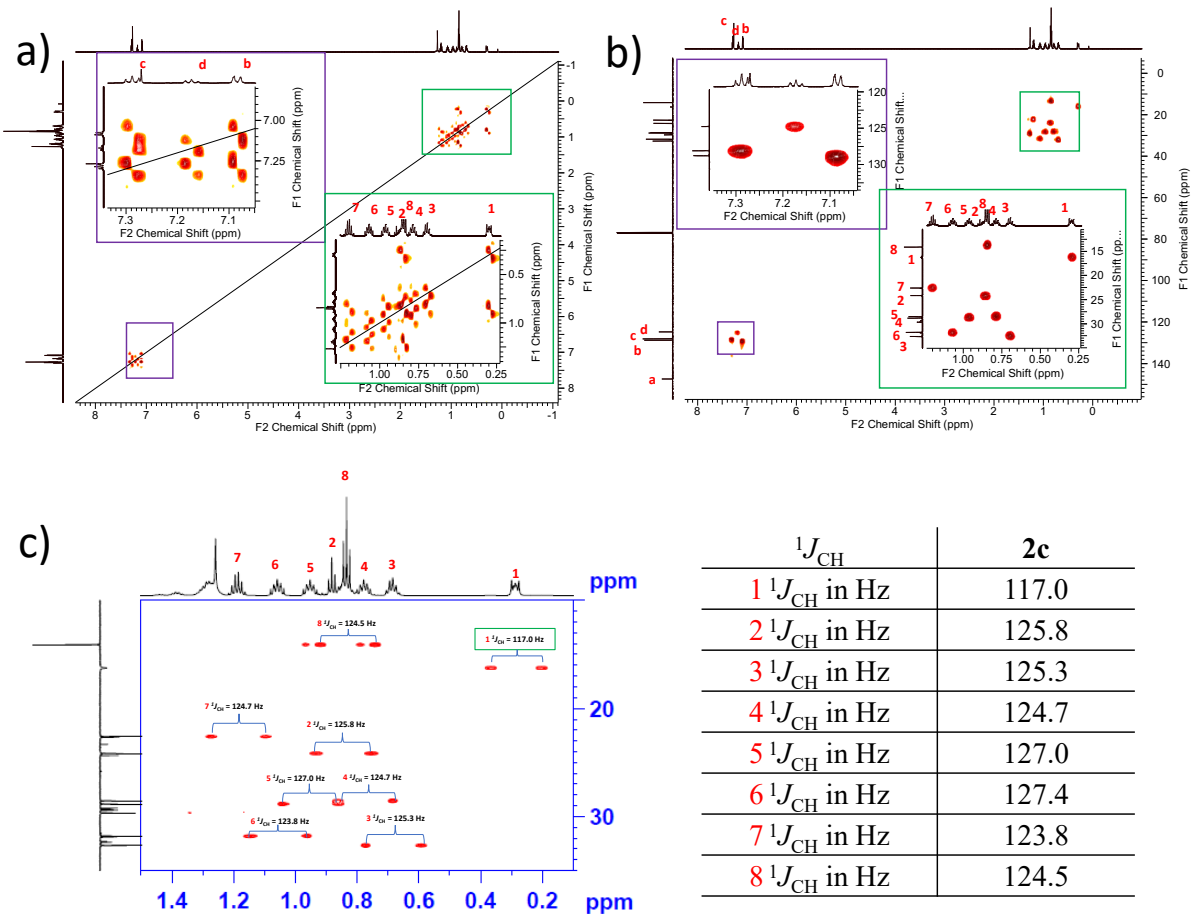


Figure S27. HRMS (MALDI-timsTOF, matrix: DCTB) spectrum of **2c**.



$^{1}J_{CH}$	**2c**
1 $^{1}J_{CH}$ in Hz	117.0
2 $^{1}J_{CH}$ in Hz	125.8
3 $^{1}J_{CH}$ in Hz	125.3
4 $^{1}J_{CH}$ in Hz	124.7
5 $^{1}J_{CH}$ in Hz	127.0
6 $^{1}J_{CH}$ in Hz	127.4
7 $^{1}J_{CH}$ in Hz	123.8
8 $^{1}J_{CH}$ in Hz	124.5

Figure S28. a) ^{1}H-^{1}H COSY, b) ^{1}H-^{13}C HSQC, c) ^{1}H-^{13}C coupled HSQC NMR of **2c** in $CDCl_3$ and corresponding coupling constant.

4.7 Characterization of 2,4,6-tribenzyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2d**)

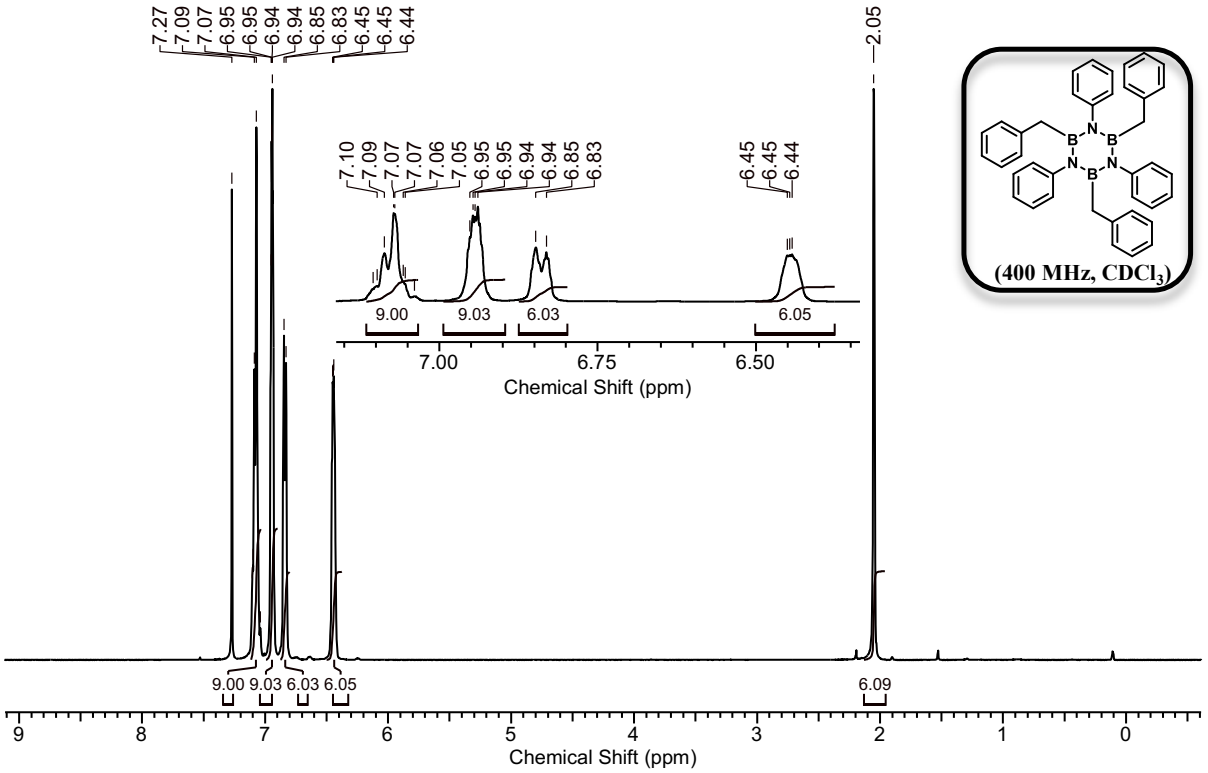


Figure S29. 400 MHz ^{1}H-NMR of **2d** in $CDCl_3$.

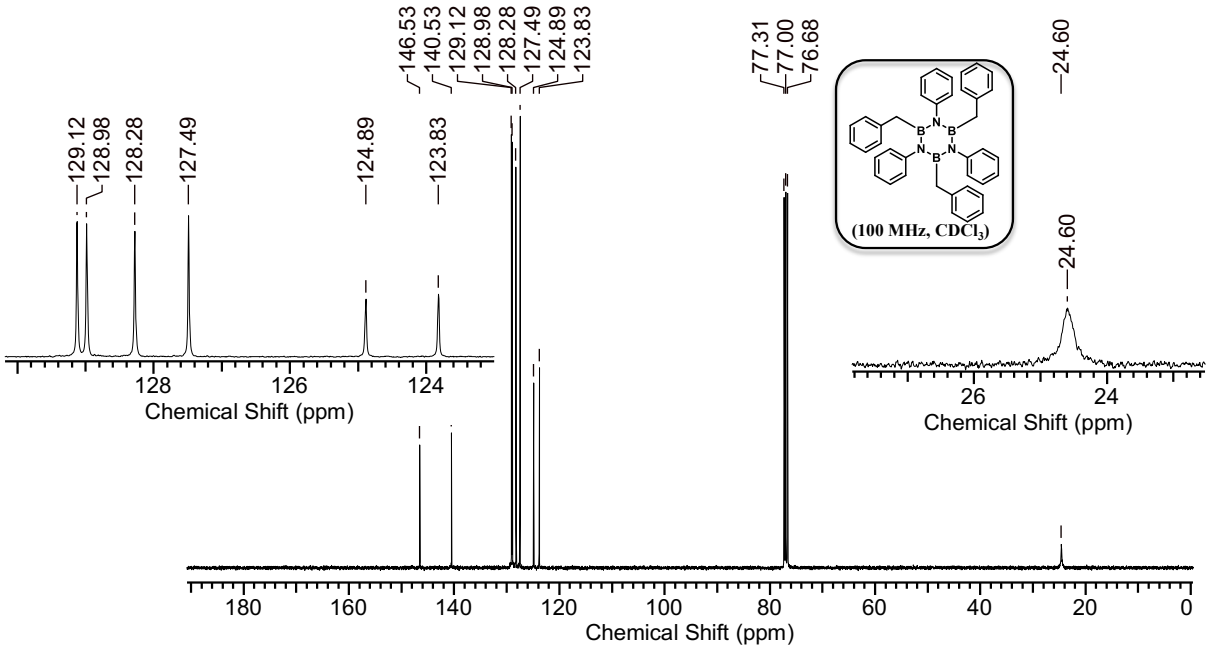


Figure S30. 100 MHz ^{13}C{^{1}H}-NMR of **2d** in $CDCl_3$.

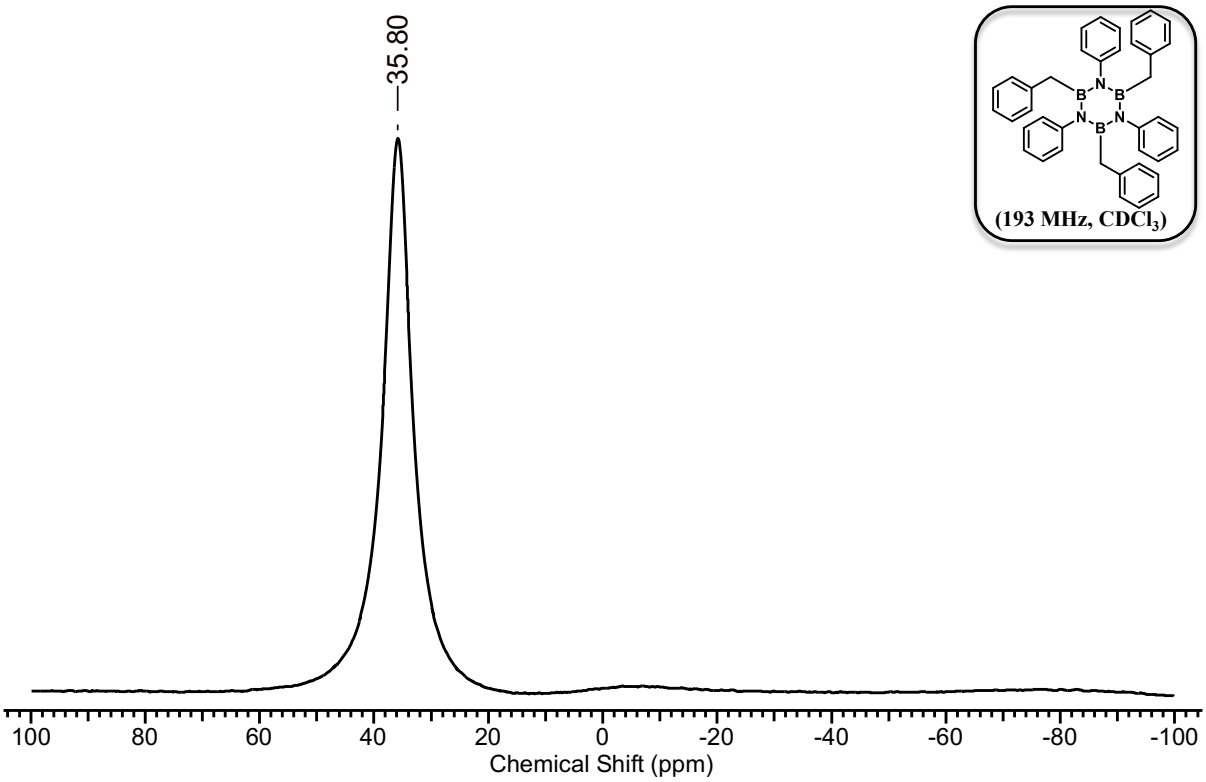


Figure S31. 193 MHz ^{11}B-NMR of **2d** in $CDCl_3$.

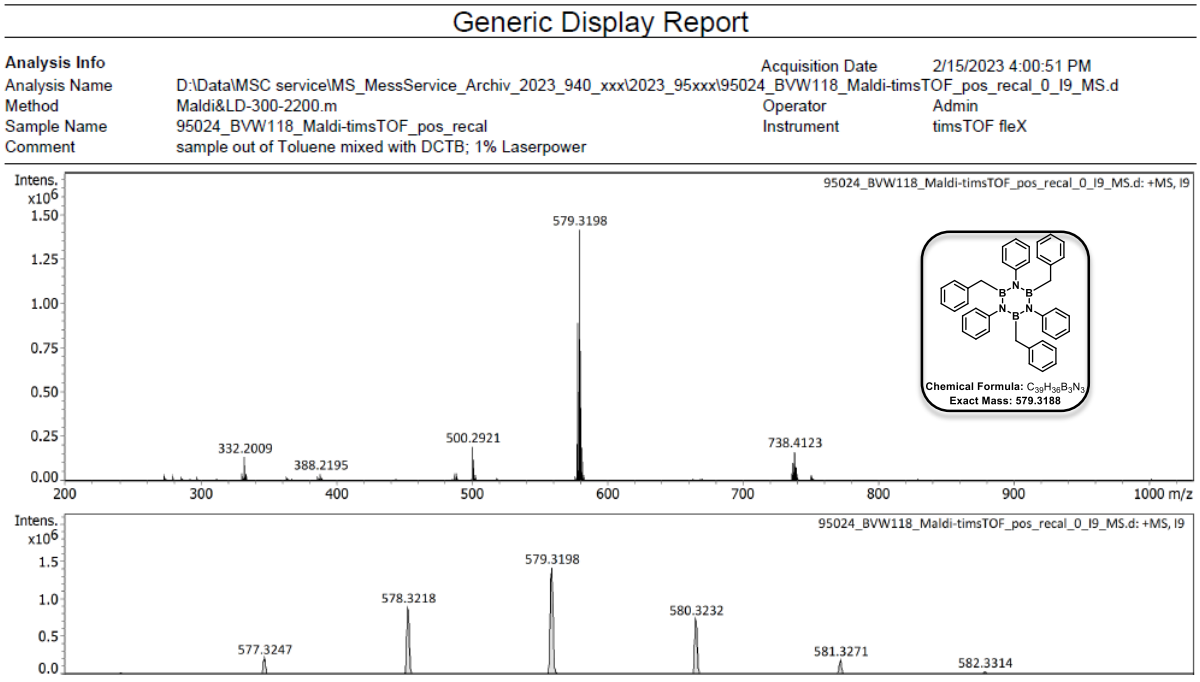


Figure S32. HRMS (MALDI-timsTOF, matrix: DCTB) spectrum of **2d**.

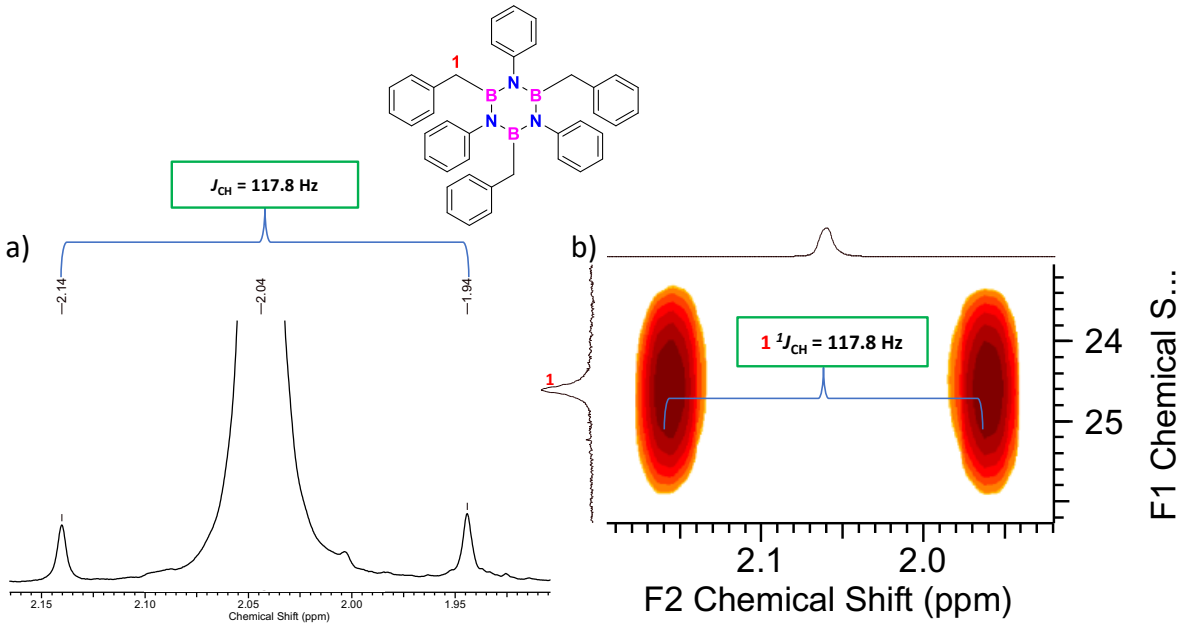


Figure S33. a) $^{1}J_{CH}$ derived from ^{13}C satellite peaks in ^{1}H NMR. b) ^{1}H-^{13}C coupled HSQC NMR of **2d** in $CDCl_3$.

4.8 Characterization of 1,3,5-triphenyl-2,4,6-tris((trimethylsilyl)methyl)-1,3,5,2,4,6-triazatriborinane (**2e**)

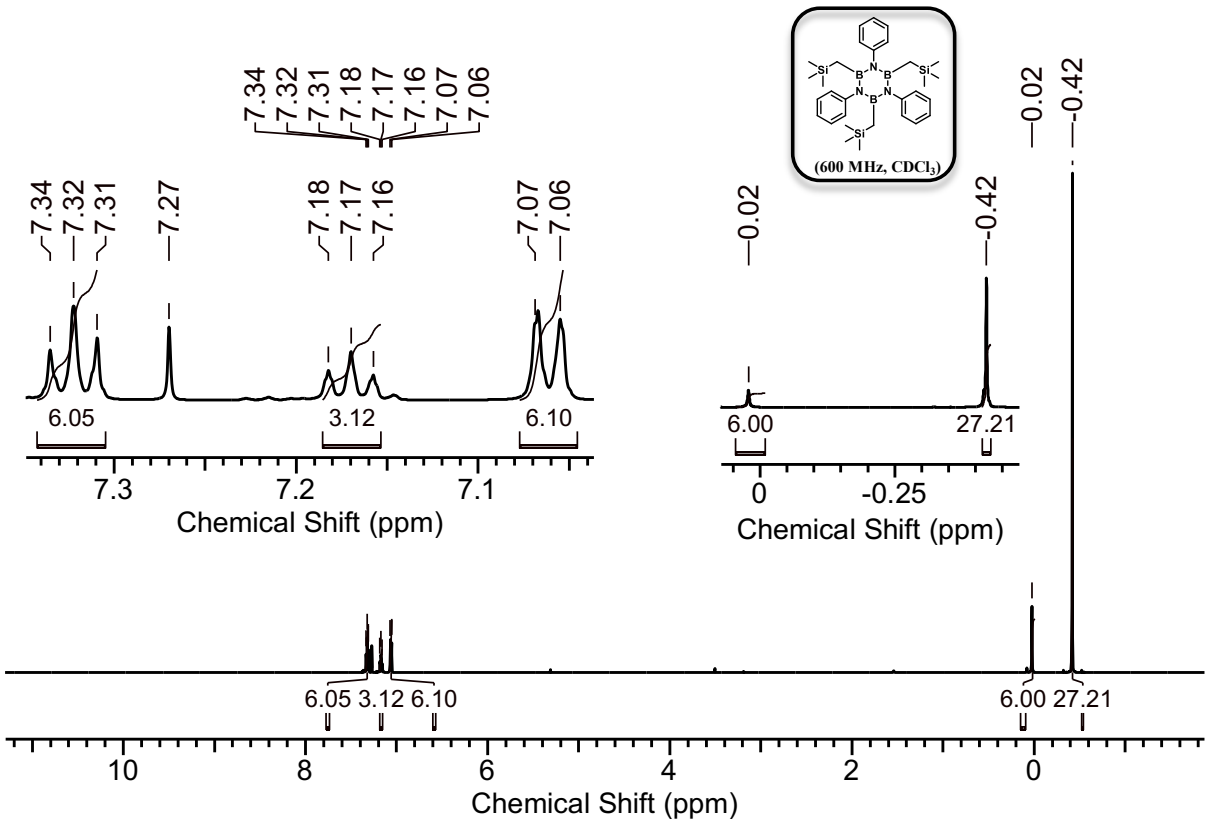


Figure S34. 600 MHz ^{1}H-NMR of **2e** in $CDCl_3$.

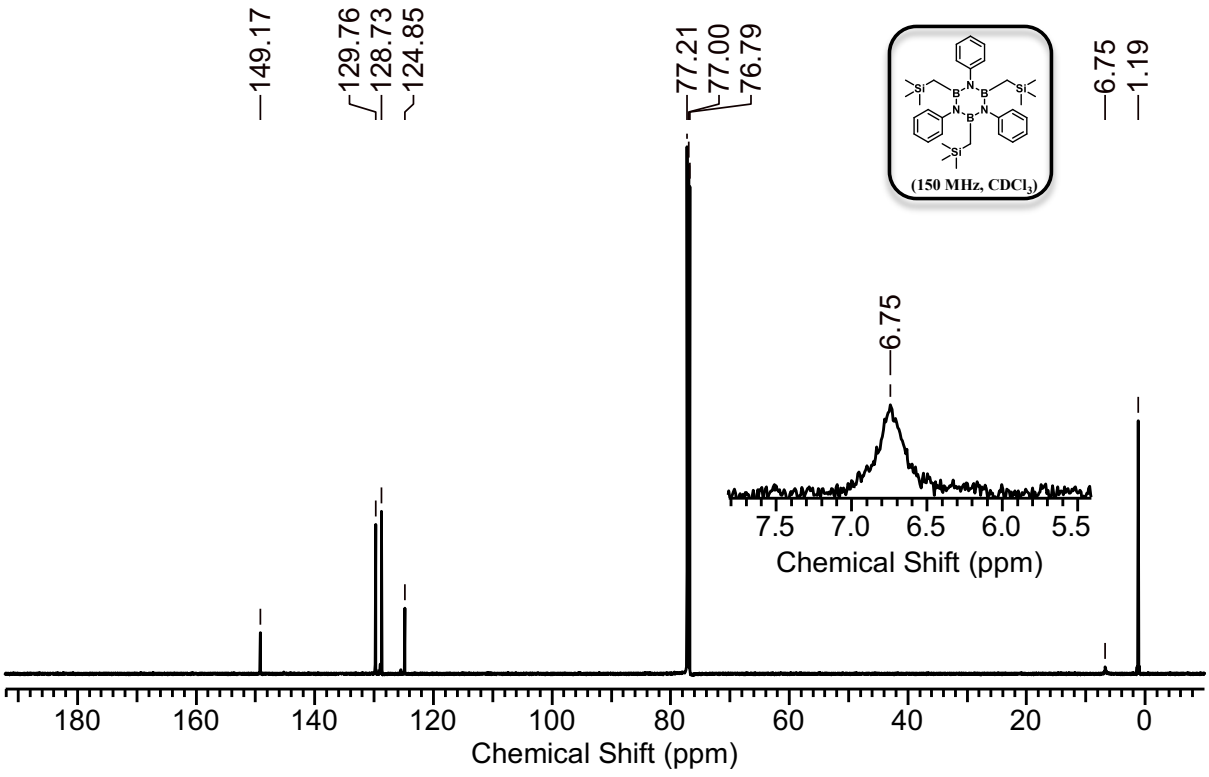


Figure S35. 150 MHz ^{13}C{^{1}H}-NMR of **2e** in $CDCl_3$.

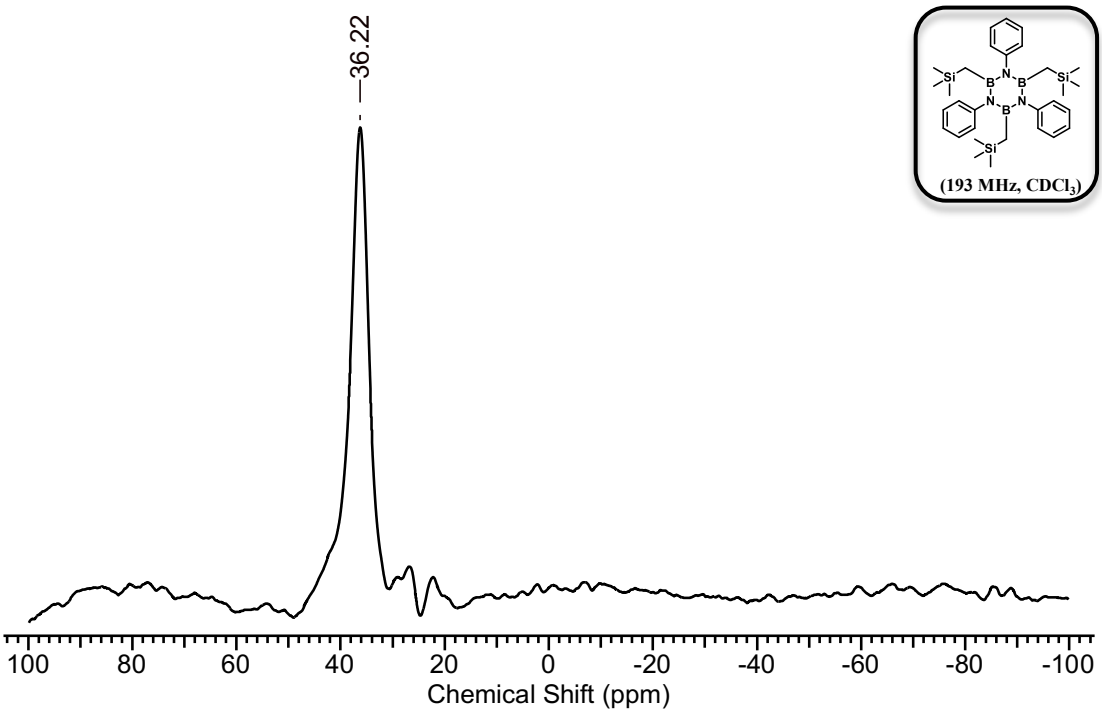


Figure S36. 193 MHz ^{11}B-NMR of **2e** in $CDCl_3$.

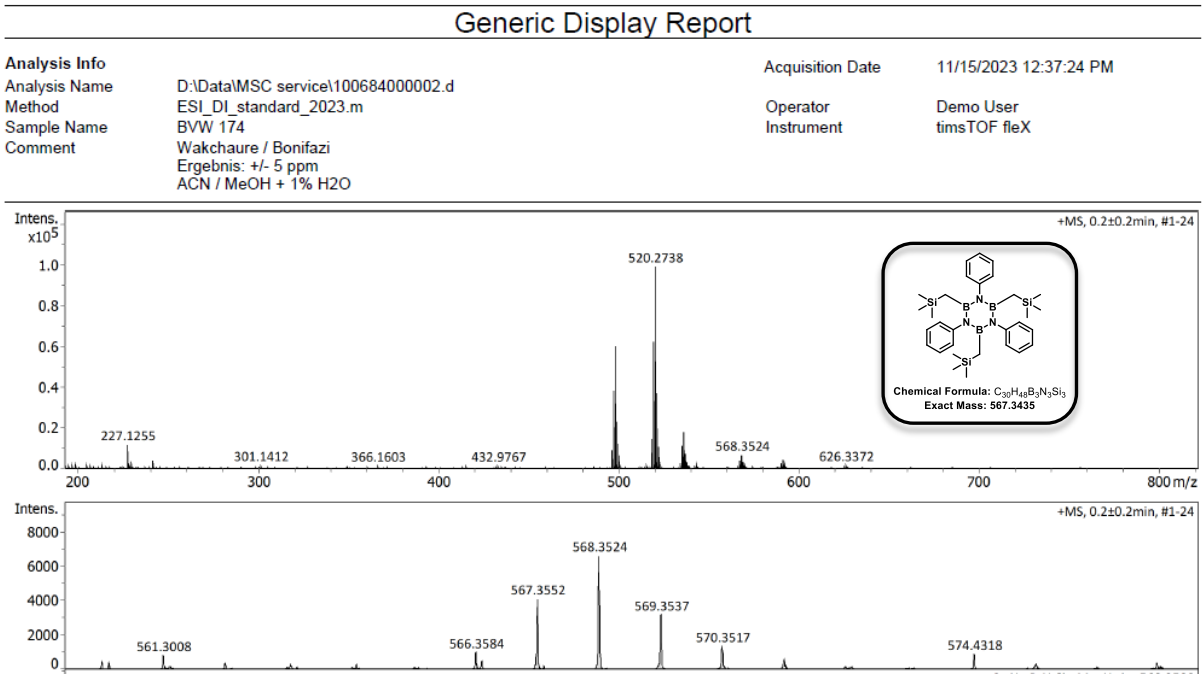


Figure S37. HRMS (ESI) spectrum of **2e**.

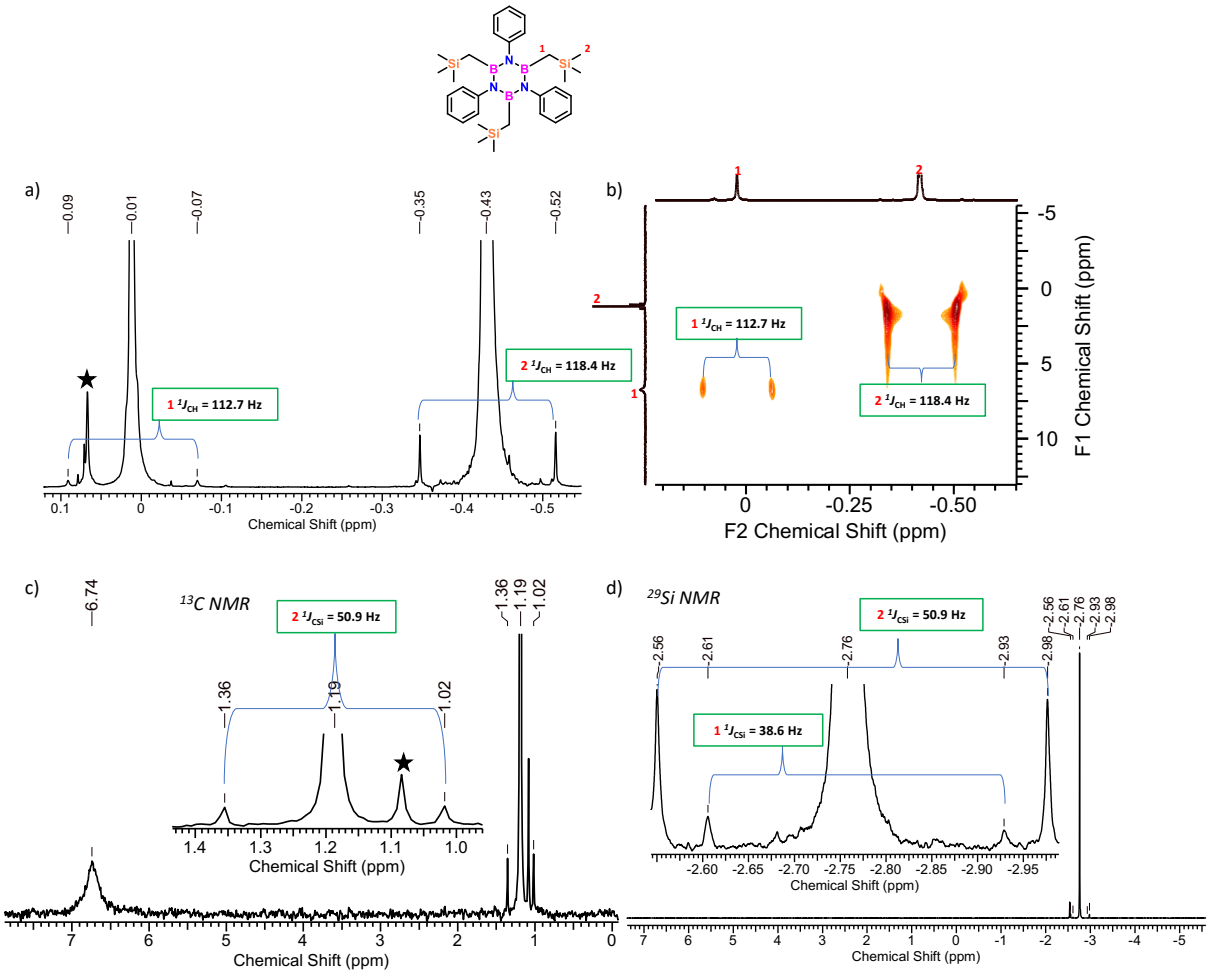


Figure S38. a) $^1J_{CH}$ derived from ^{13}C satellite peaks in ^1H NMR. b) ^1H-^{13}C coupled HSQC NMR of **2e** in $CDCl_3$. $^1J_{CSi}$ derived from c) ^{29}Si satellite peaks in ^{13}C NMR and d) ^{13}C satellite peaks in ^{29}Si NMR (^{29}Si spectra recorded with high concentration (~80 mM)). (*vacuum grease).

4.9 Characterization of 2,4,6-triisopropyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**3a**)

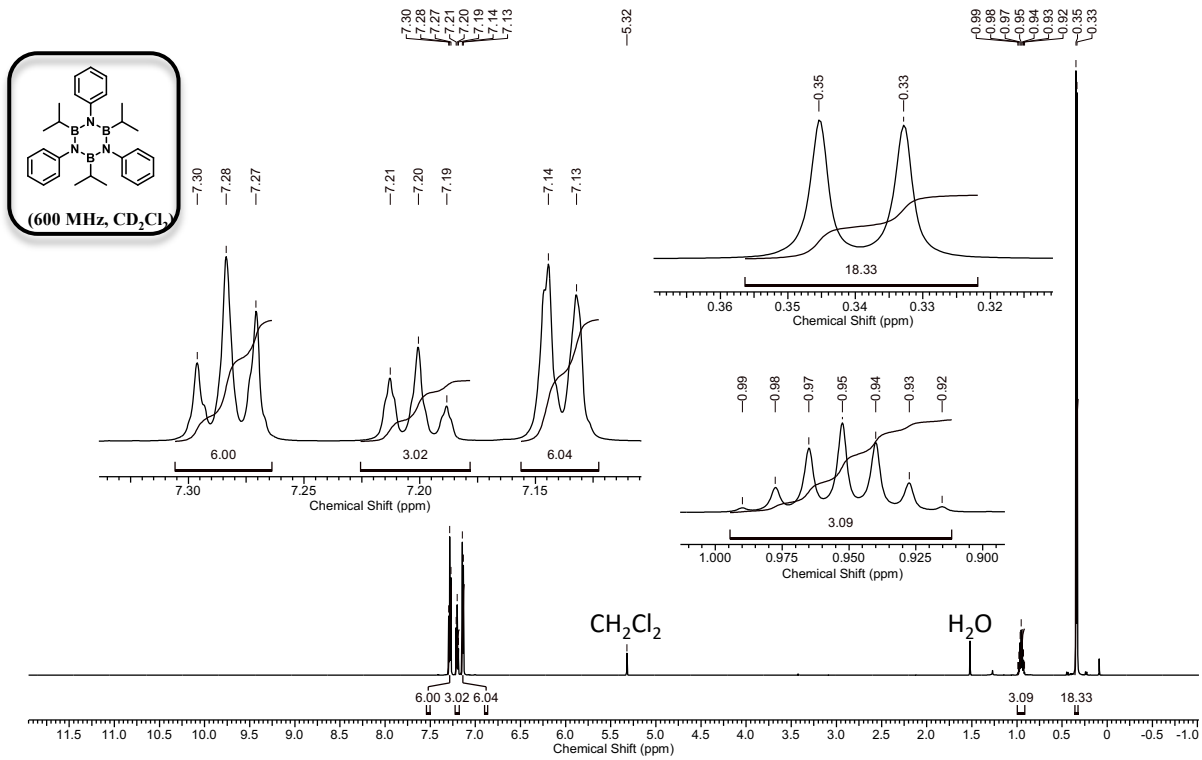


Figure S39. 600 MHz ^{1}H-NMR of **3a** in CD_2Cl_2.

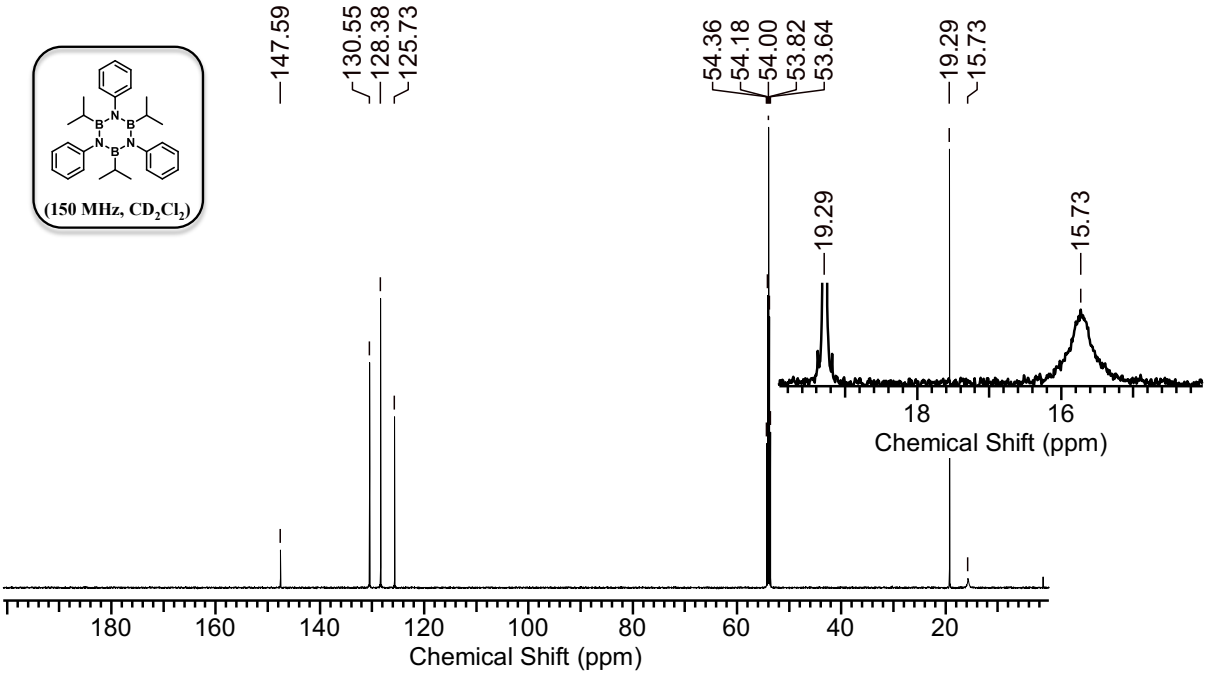


Figure S40. 150 MHz ^{13}C{^{1}H}-NMR of **3a** in CD_2Cl_2.

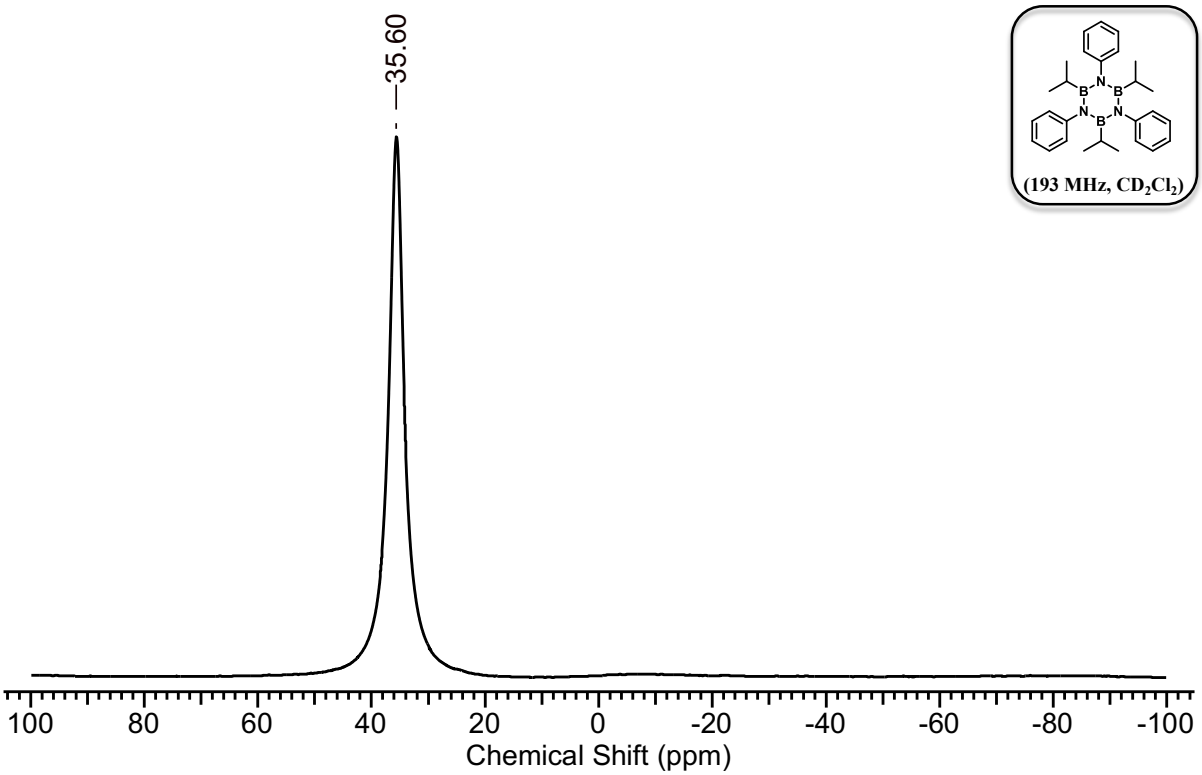


Figure S41. 193 MHz ^{11}B-NMR of **3a** in CD_2Cl_2.

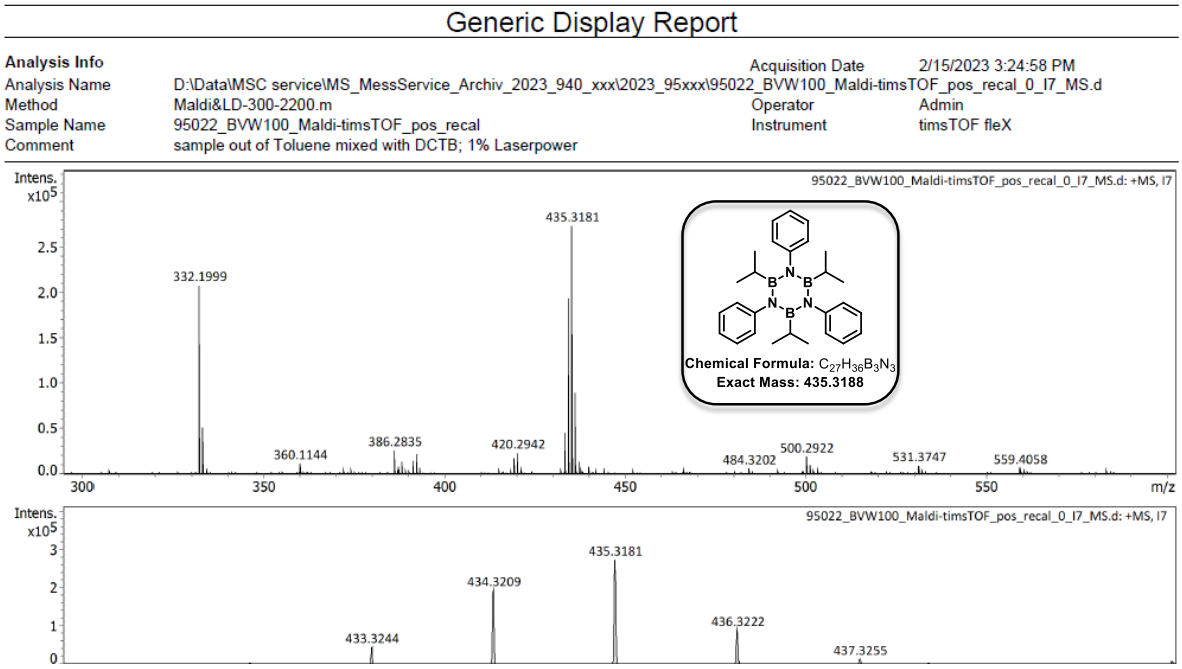


Figure S42. HRMS (MALDI-tims TOF, matrix: DCTB) spectrum of **3a**.

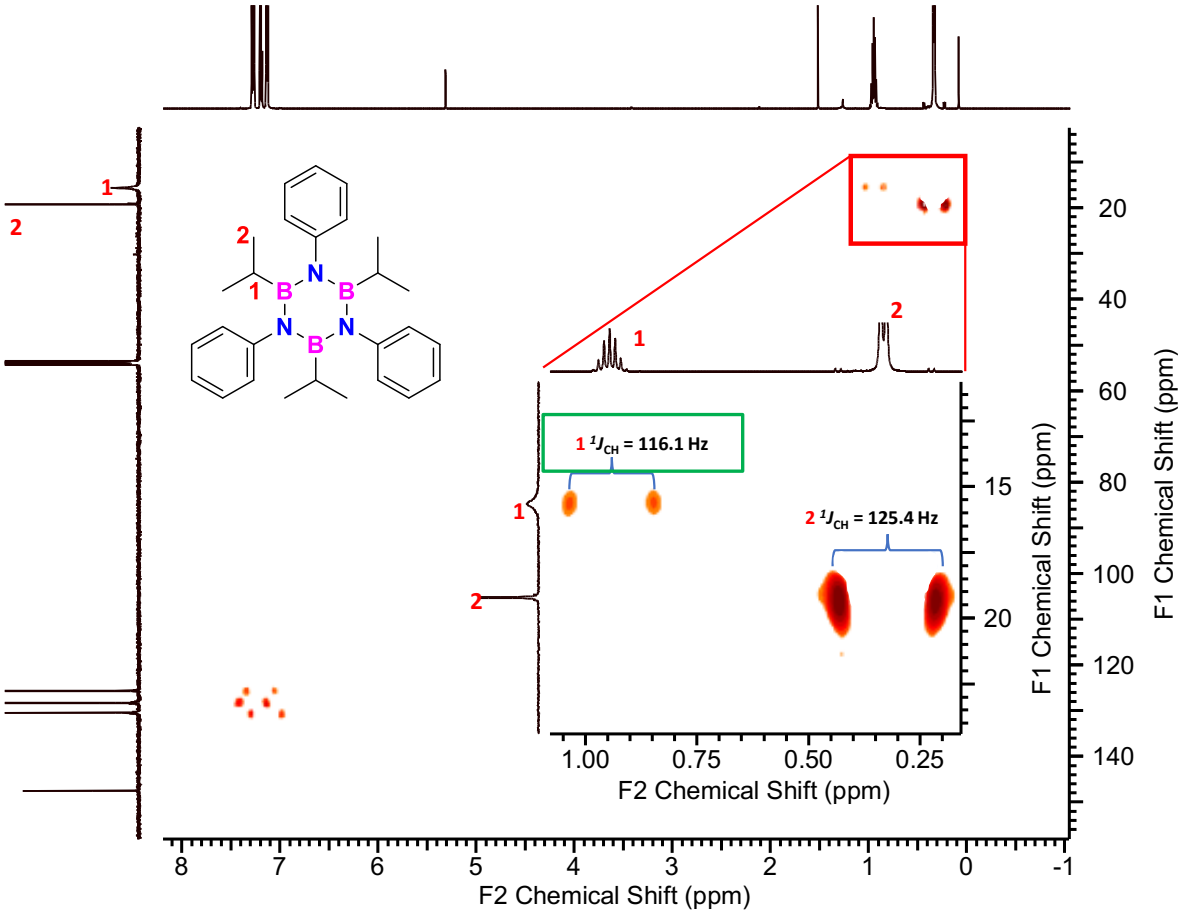


Figure S43. ^{1}H-^{13}C coupled HSQC NMR of **3a** in CD_2Cl_2.

4.10 Characterization of 2,4,6-tricyclohexyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**3b**)

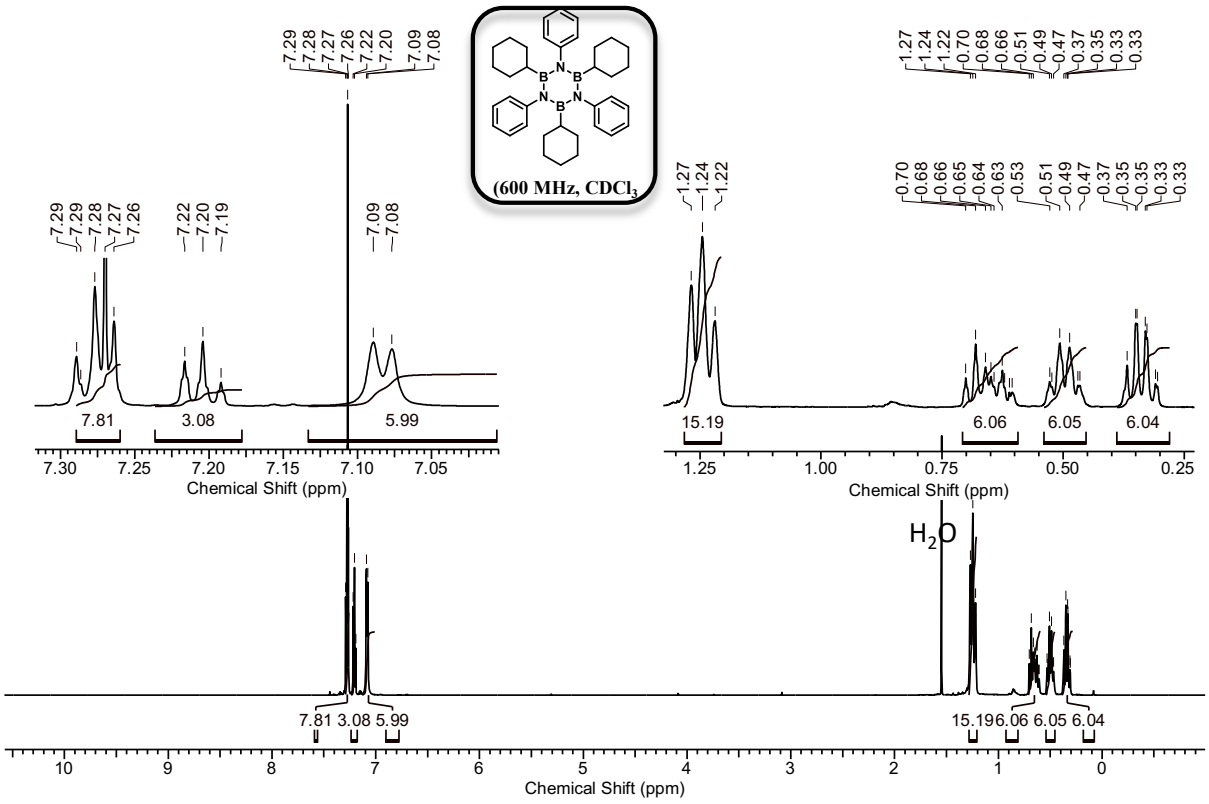


Figure S44. 600 MHz ^{1}H-NMR of **3b** in $CDCl_3$.

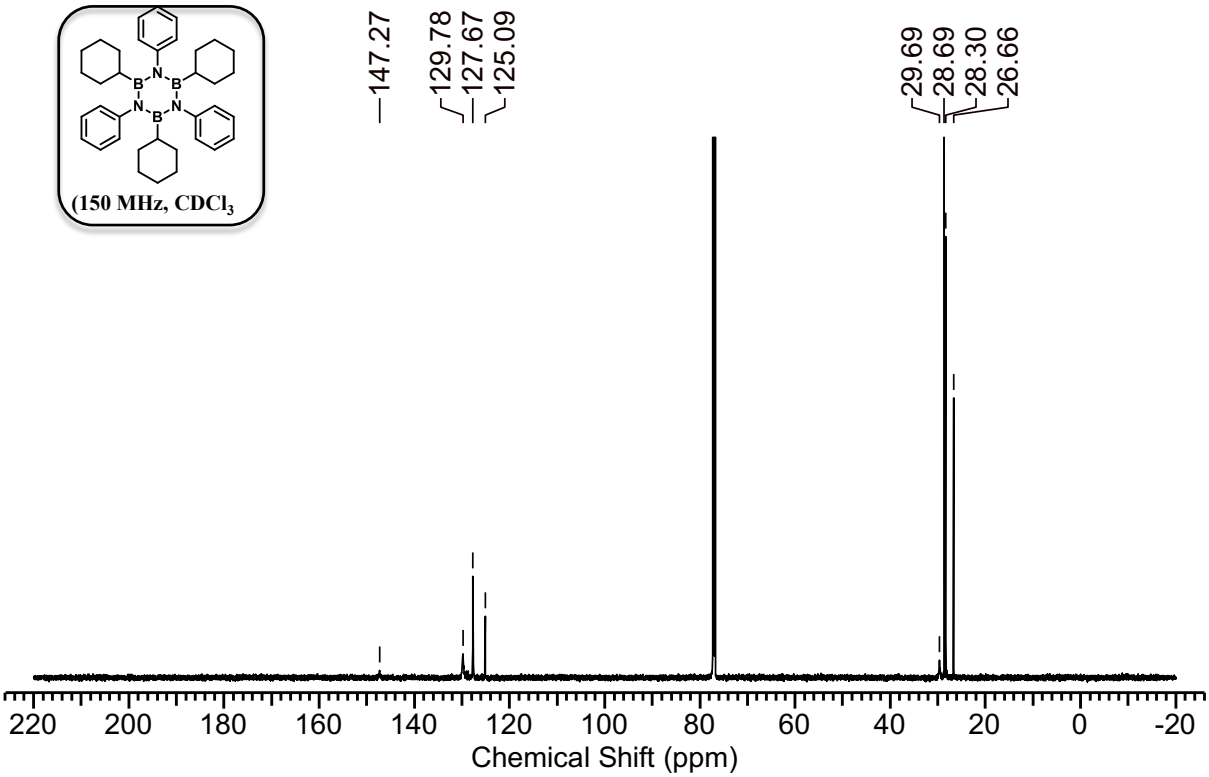


Figure S45. 150 MHz $^{13}C\{^{1}H\}$-NMR of **3b** in $CDCl_3$.

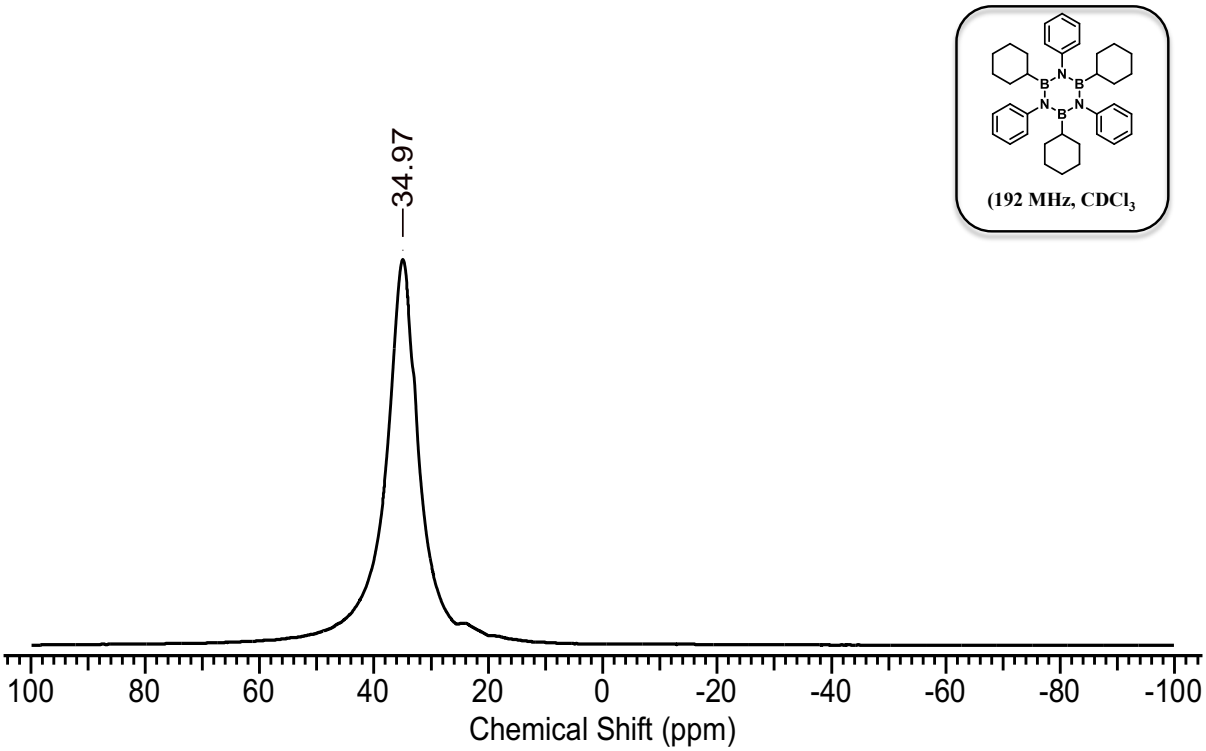


Figure S46. 193 MHz ^{11}B-NMR of **3b** in $CDCl_3$.

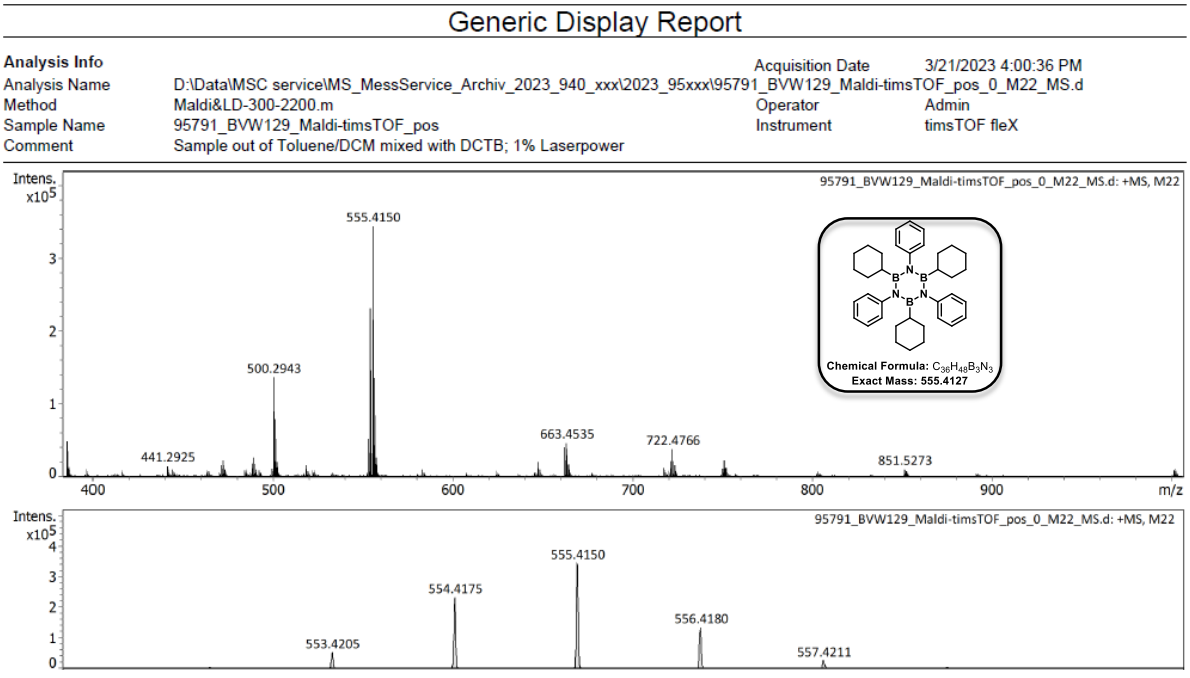
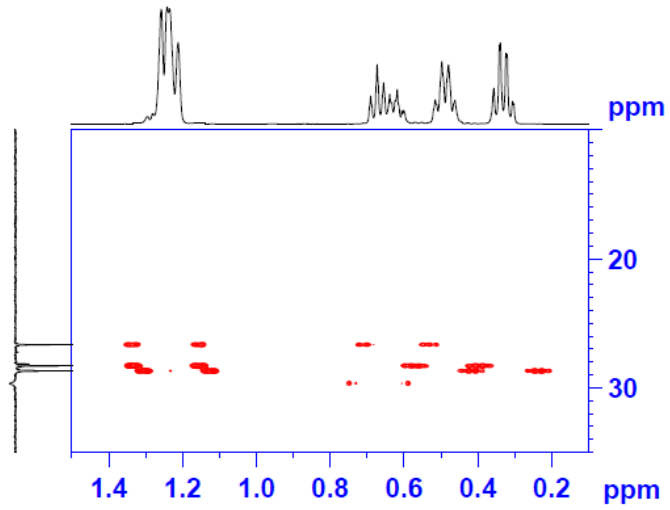


Figure S47. HRMS (MALDI-timsTOF, matrix: DCTB) spectrum of **3b**.



$^{1}J_{CH}$	**3b**
1 $^{1}J_{CH}$ in Hz	112.3
2 $^{1}J_{CH}$ in Hz	126.0/125.5
3 $^{1}J_{CH}$ in Hz	125.8/121.9
4 $^{1}J_{CH}$ in Hz	127.5/120.9

Figure S48. ^{1}H-^{13}C coupled HSQC NMR of **3b** in $CDCl_3$.

5. Thermal analysis

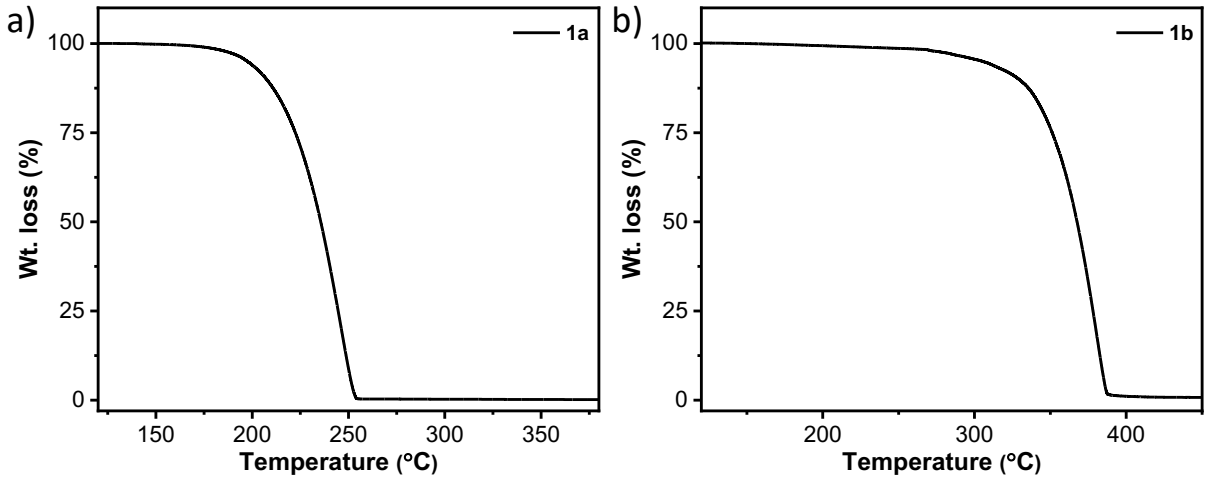


Figure S49. Thermogravimetric analysis (TGA) at a heating rate of 10 °C.min^{-1} under N_2 atmosphere of a) **1a**, and b) **1b**.

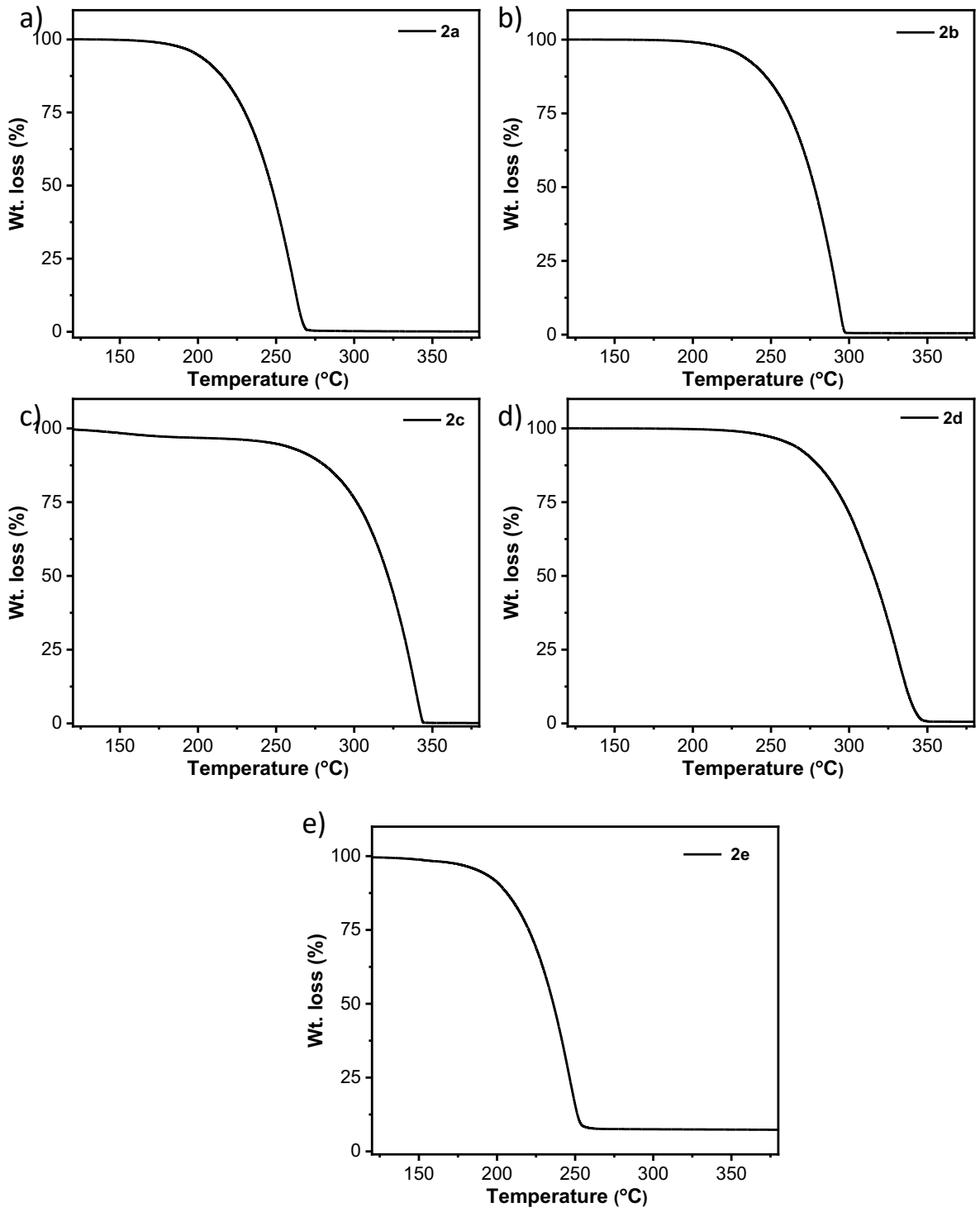


Figure S50. Thermogravimetric analysis (TGA) at a heating rate of 10 °C.min^{-1} under N_2 atmosphere of a) **2a**, b) **2b**, c) **2c**, d) **2d**, and e) **2e**.

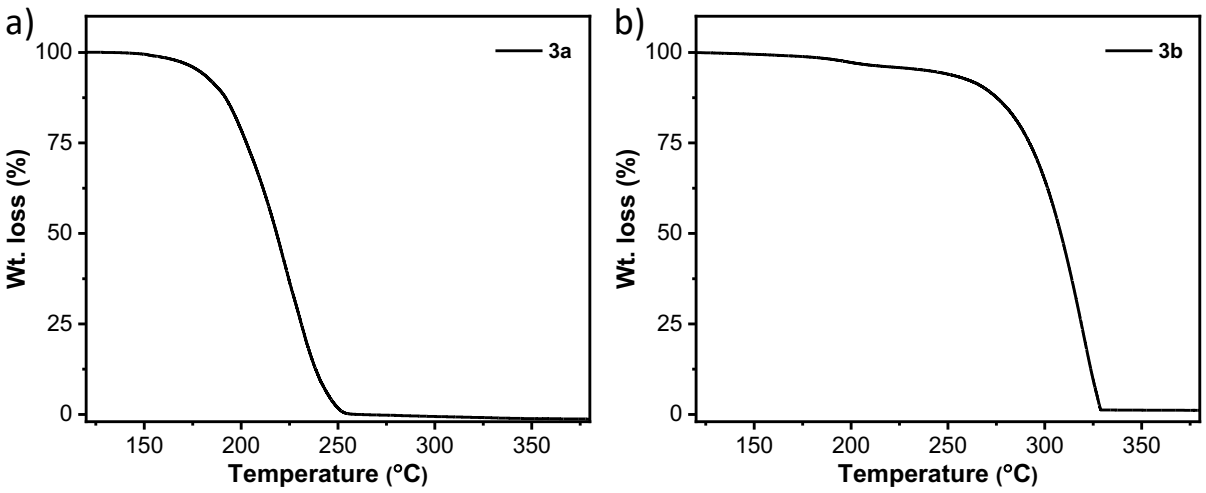


Figure S51. Thermogravimetric analysis (TGA) at a heating rate of 10 °C.min^{-1} under N_2 atmosphere of a) **3a**, and b) **3b**.

6. Crystallographic data

Table S1. Crystal data and structure refinement for **1a** (2261150).

Empirical formula	$C_{21}H_{24}B_3N_3$	
Formula weight	350.86	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 15.180(4) Å	α = 90°
	b = 14.833(3) Å	β = 123.148(16)°
	c = 10.438(3) Å	γ = 90°
Volume	1967.8(8) $Å^3$	
Z	4	
Density (calculated)	1.184 mg/m^3	
Absorption coefficient	0.068 mm^{-1}	
F(000)	744.0	
Crystal size	0.59 × 0.25 × 0.07 mm^3	
	Data collection	
Temperature	100 K	
Wavelength	0.71073 Å	
Theta range for data collection	4.22 to 50.056°	
Index ranges	$-17 \leq h \leq 18$, $-17 \leq k \leq 15$, $-12 \leq l \leq 12$	
Reflections collected	8927	
Independent reflections	1734 [R_{int} = 0.0789, R_{sigma} = 0.0794]	
Completeness to theta = 25.028°	99.1%	
	Refinement	
Absorption correction	multi-scan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1734/0/127	
Goodness-of-fit on F^2	0.911	
Final R indices [I>2sigma(I)]	R_1 = 0.0423, wR_2 = 0.0922	
R indices (all data)	R_1 = 0.0812, wR_2 = 0.1016	
Largest diff. peak and hole	0.18 and -0.25 $e \cdot Å^{-3}$	

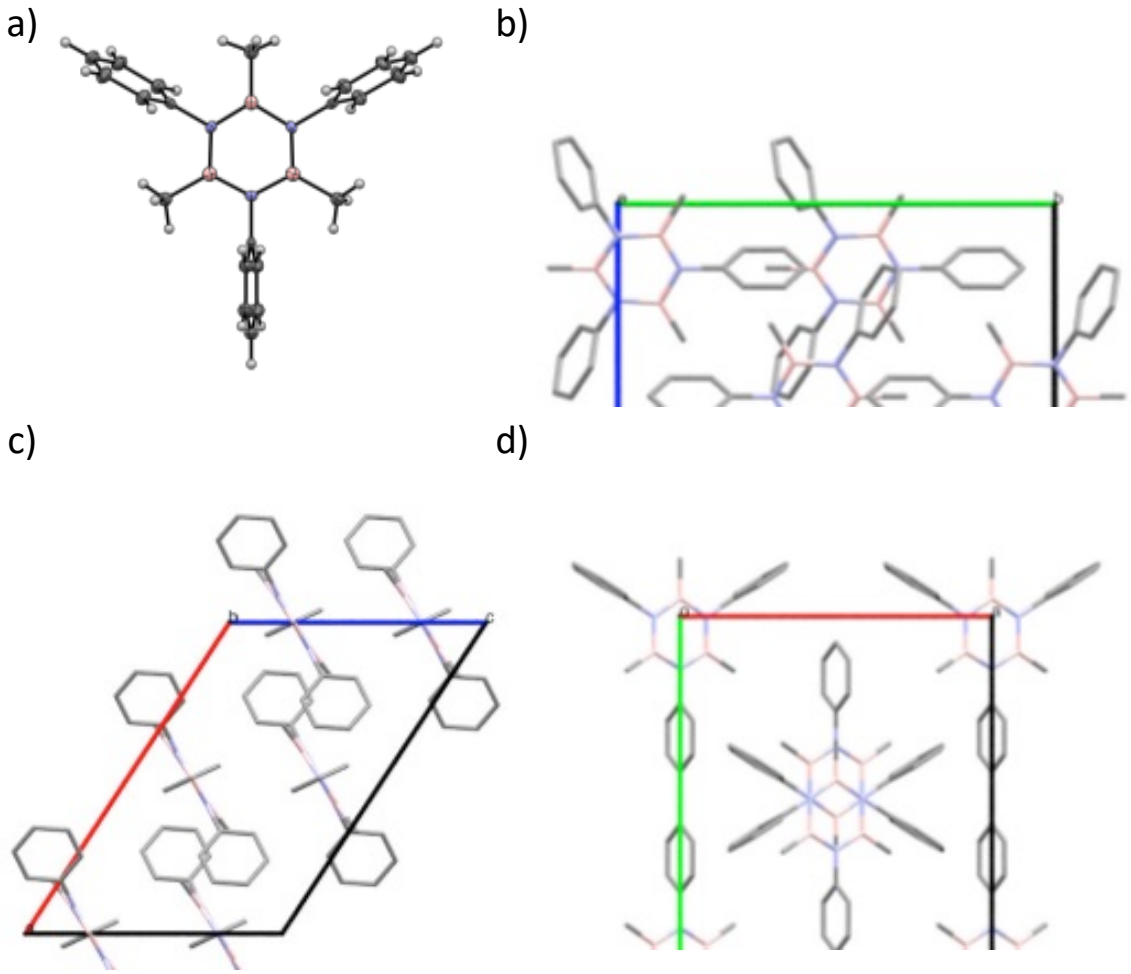


Figure S52. ORTEP representation (50% probability ellipsoids) and crystal packing views along crystallographic a, b and c axes of borazine **1a** (in b), c) and d) hydrogens omitted for clarity).

Table S2. Crystal data and structure refinement for **1b** (2280128).

Empirical formula	$C_{45}H_{48}B_3N_3$
Formula weight	663.29
Crystal system	Monoclinic
Space group	*C*2/*c*
Unit cell dimensions	a = 16.8926(9) Å α = 90°
	b = 16.5689(7) Å β = 115.765(7)°
	c = 15.7562(9) Å γ = 90°
Volume	3971.6(4) $Å^3$
Z	4
Density (calculated)	1.109 mg/m^3
Absorption coefficient	0.063 mm^{-1}
F(000)	1416.0
Crystal size	0.572 × 0.242 × 0.177 mm^3
	Data collection
Temperature	150(2) K
Wavelength	0.71073 Å
Theta range for data collection	7.272 to 59.296°
Index ranges	$-19 \leq h \leq 22$, $-16 \leq k \leq 22$, $-21 \leq l \leq 14$
Reflections collected	9679
Independent reflections	4704 [R_{int} = 0.0187, R_{sigma} = 0.0262]
Completeness to theta = 25.242°	99.7%
	Refinement
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4704/0/239
Goodness-of-fit on F^2	1.098
Final R indices [I>2sigma(I)]	R_1 = 0.0556, wR_2 = 0.1455
R indices (all data)	R_1 = 0.0697, wR_2 = 0.1544
Largest diff. peak and hole	0.24 and -0.24 $e \cdot Å^{-3}$

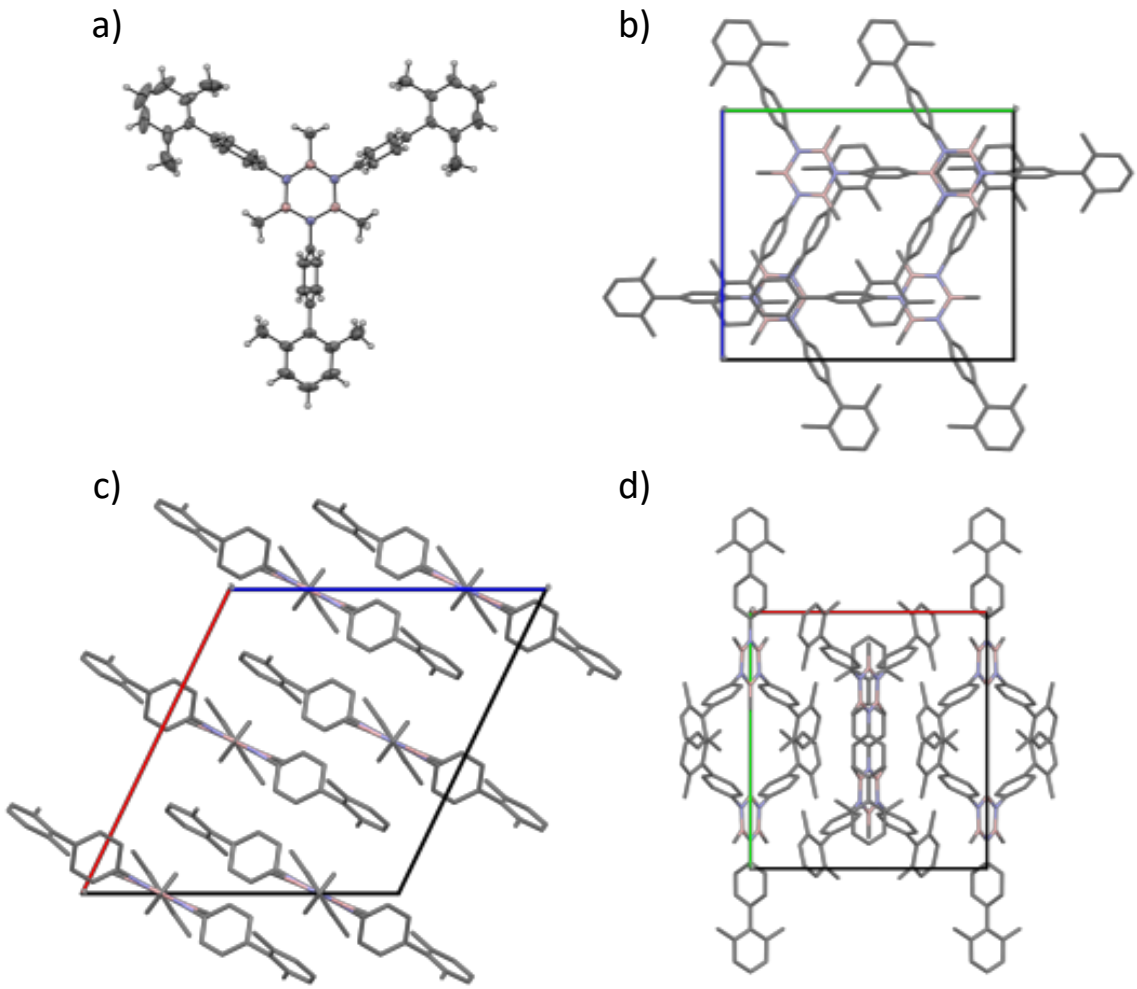


Figure S53. ORTEP representation (50% probability ellipsoids) and crystal packing views along crystallographic a, b and c axes of borazine **1b** (in b), c) and d) hydrogens omitted for clarity).

Table S3. Crystal data and structure refinement for **2a** (2280127).

Empirical formula	$C_{30}H_{42}B_3N_3$	
Formula weight	477.09	
Crystal system	Monoclinic	
Space group	*Cc*	
Unit cell dimensions	a = 12.5368(5) Å	α = 90°
	b = 21.2761(9) Å	β = 97.436(4)°
	c = 22.3298(11) Å	γ = 90°
Volume	5906.0(5) $Å^3$	
Z	8	
Density (calculated)	1.073 mg/m^3	
Absorption coefficient	0.061 mm^{-1}	
F(000)	2064.0	
Crystal size	0.444 × 0.062 × 0.029 mm^3	
	Data collection	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Theta range for data collection	6.72 to 50.05°	
Index ranges	$-11 \leq h \leq 14$, $-20 \leq k \leq 25$, $-25 \leq l \leq 26$	
Reflections collected	12149	
Independent reflections	7772 [R_{int} = 0.0290, R_{sigma} = 0.0422]	
Completeness to theta = 25.025°	99.6%	
	Refinement	
Absorption correction	multi-scan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7772/652/711	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R_1 = 0.0524, wR_2 = 0.1300	
R indices (all data)	R_1 = 0.0689, wR_2 = 0.1416	
Largest diff. peak and hole	0.22 and -0.31 $e \cdot Å^{-3}$	

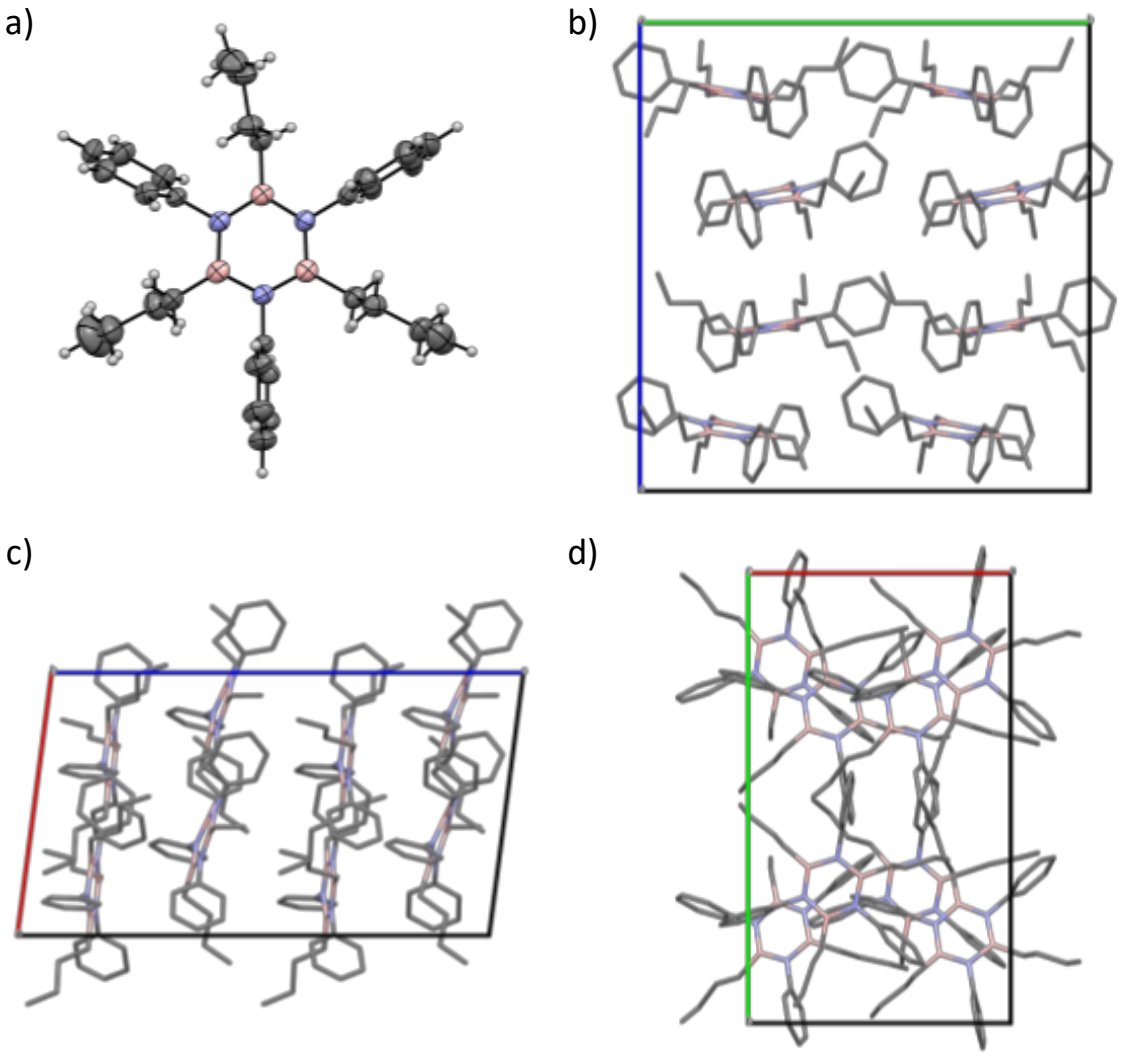


Figure S54. ORTEP representation (50% probability ellipsoids) and crystal packing views along crystallographic a, b and c axes of borazine **2a** (in b), c) and d) hydrogens omitted for clarity).

Table S4. Crystal data and structure refinement for **2e** (2307378).

Empirical formula	$C_{30}H_{48}B_3N_3Si_3$
Formula weight	567.41
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 25.4466(18) Å α = 90°
	b = 11.0925(4) Å β = 116.552(5)°
	c = 27.4043(18) Å γ = 90°
Volume	6919.5(8) $Å^3$
Z	8
Density (calculated)	1.089 mg/m^3
Absorption coefficient	0.160 mm^{-1}
F(000)	2448
Crystal size	0.70 × 0.307 × 0.07 mm^3
	Data collection
Temperature	100 K
Wavelength	0.71073 Å
Theta range for data collection	2.875 to 25.025°
Index ranges	$-30 \le h \le 30$, $-13 \le k \le 9$, $-32 \le l \le 32$
Reflections collected	170431
Independent reflections	12209 [R_{int} = 0.1825, R_{sigma} = 0.1128]
Completeness to theta = 25.025°	99.9%
	Refinement
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12209/0/721
Goodness-of-fit on F^2	0.920
Final R indices [I>2sigma(I)]	R_1 = 0.0417, wR_2 = 0.0917
R indices (all data)	R_1 = 0.1112, wR_2 = 0.1067
Largest diff. peak and hole	0.352 and -0.459 $e \cdot Å^{-3}$

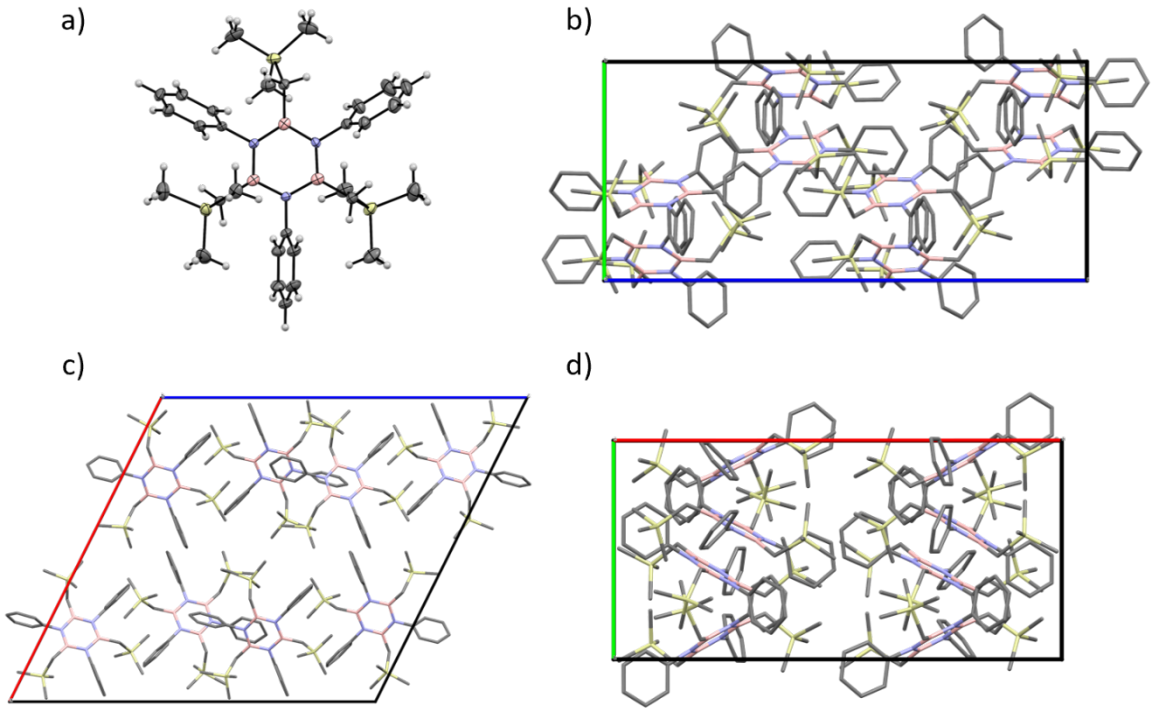


Figure S55. ORTEP representation (50% probability ellipsoids) and crystal packing views along crystallographic a, b and c axes of borazine **2e** (in b), c) and d) hydrogens omitted for clarity).

Table S5. Crystal data and structure refinement for **3a** (2284380).

Empirical formula	$C_{27}H_{36}B_3N_3$	
Formula weight	435.02	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 6.1370(12) Å	α = 74.71(3)°
	b = 22.026(4) Å	β = 89.58(3)°
	c = 29.481(6) Å	γ = 89.48(3)°
Volume	3843.9(14) $Å^3$	
Z	6	
Density (calculated)	1.128 mg/m^3	
Absorption coefficient	0.062 mm^{-1}	
F(000)	1404.0	
Crystal size	0.1 × 0.05 × 0.02 mm^3	
	Data collection	
Temperature	100(2) K	
Wavelength	0.700 Å (Synchrotron)	
Theta range for data collection	1.41 to 51.83°	
Index ranges	$-7 \le h \le 6$, $-27 \le k \le 27$, $-36 \le l \le 36$	
Reflections collected	47301	
Independent reflections	15362 [R_{int} = 0.0517, R_{sigma} = 0.0509]	
Completeness to theta = 24.835°	98.0%	
	Refinement	
Absorption correction	multi-scan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15362/0/911	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R_1 = 0.1302, wR_2 = 0.3758	
R indices (all data)	R_1 = 0.1579, wR_2 = 0.3936	
Largest diff. peak and hole	0.63 and -0.47 $e \cdot Å^{-3}$	

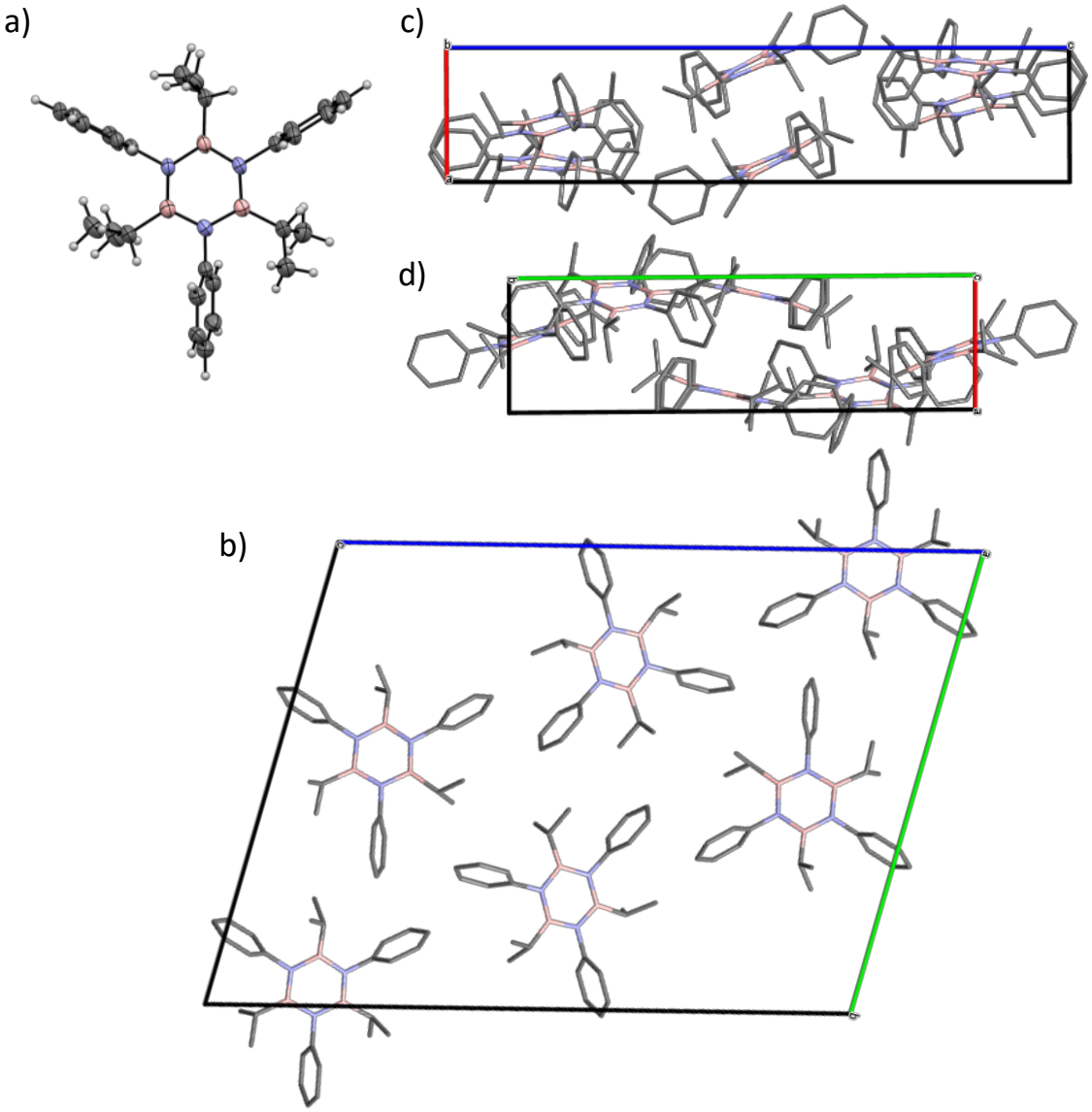


Figure S56. ORTEP representation (50% probability ellipsoids) and crystal packing views along crystallographic a, b and c axes of borazine **3a** (in b), c) and d) hydrogens omitted for clarity).

Table S6. Crystal data and structure refinement for **3b** (2261151).

Empirical formula	$C_{36}H_{48}B_3N_3$
Formula weight	555.20
Crystal system	Orthorhombic
Space group	*Pna*2$_1$
Unit cell dimensions	a = 11.8518(8) Å α = 90°
	b = 12.9244(10) Å β = 90°
	c = 21.2118(19) Å γ = 90°
Volume	3249.2(4) Å^3
Z	4
Density (calculated)	1.135 mg/m^3
Absorption coefficient	0.064 mm^{-1}
F(000)	1200.0
Crystal size	0.3 × 0.26 × 0.18 mm^3
	Data collection
Temperature	293 K
Wavelength	0.71073 Å
Theta range for data collection	4.664 to 50.054°
Index ranges	$-14 \leq h \leq 14$, $-12 \leq k \leq 15$, $-25 \leq l \leq 24$
Reflections collected	31179
Independent reflections	5613 [R_{int} = 0.1050, R_{sigma} = 0.0791]
Completeness to theta = 25.027°	99.6%
	Refinement
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5613/775/424
Goodness-of-fit on F^2	0.893
Final R indices [I>2sigma(I)]	R_1 = 0.0532, wR_2 = 0.1214
R indices (all data)	R_1 = 0.0987, wR_2 = 0.1370
Largest diff. peak and hole	0.22 and -0.22 e·Å^{-3}

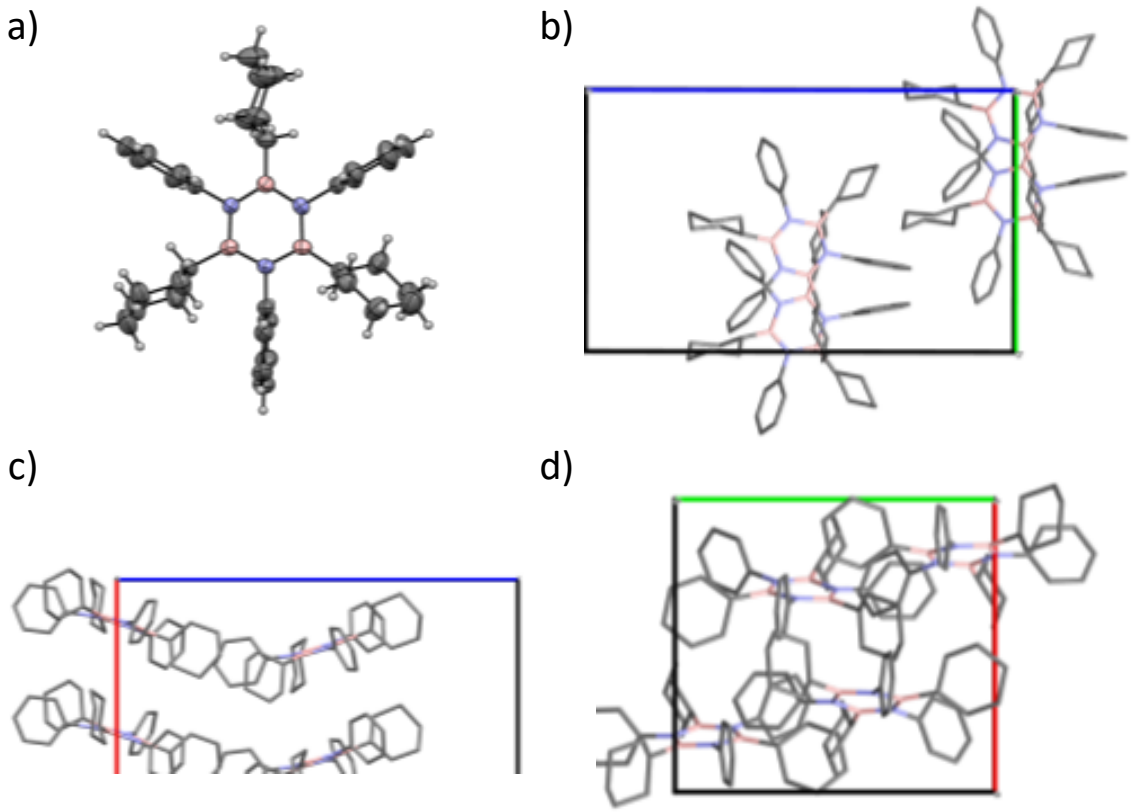


Figure S57. ORTEP representation (50% probability ellipsoids) and crystal packing views along crystallographic a, b and c axes of borazine **3b** (in b), c) and c) hydrogens omitted for clarity).

7. Computational Studies

7.1 Donor-acceptor interactions derived from natural bonding orbital analyses.

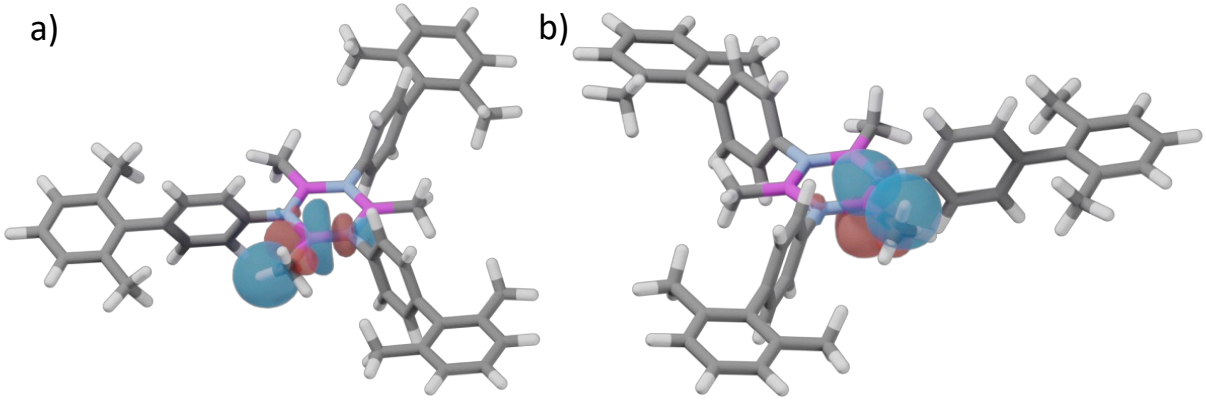


Figure S58. a) $\sigma_{C\text{-}H} \rightarrow \sigma^*_{B-N}$ and b) $\sigma_{C\text{-}H} \rightarrow \pi^*_{B=N}$ donor-acceptor interactions derived from natural bonding orbital analyses of **1b**. Orbitals associated with only one B-methyl component are shown for clarity. *PBE/def2-TZVP*.

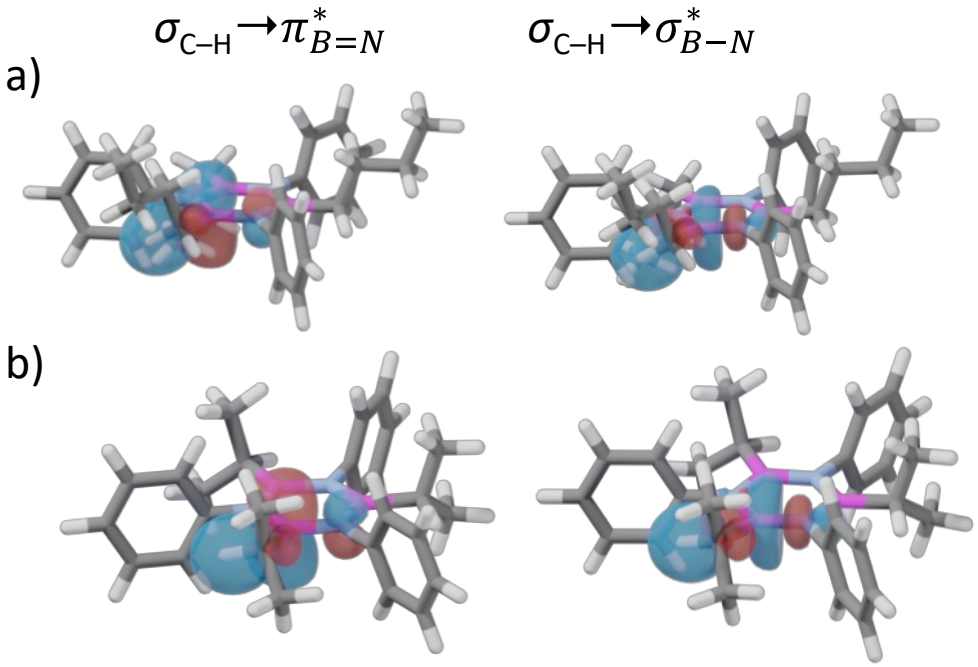


Figure S59. NBO analyses (PBE/def2-TZVP, orbitals with only one B are shown for clarity) for: $\sigma_{C-H} \rightarrow \pi^*_{B=N}$ and $\sigma_{C-H} \rightarrow \sigma^*_{B-N}$ in a) **2a**, b) **3a**.

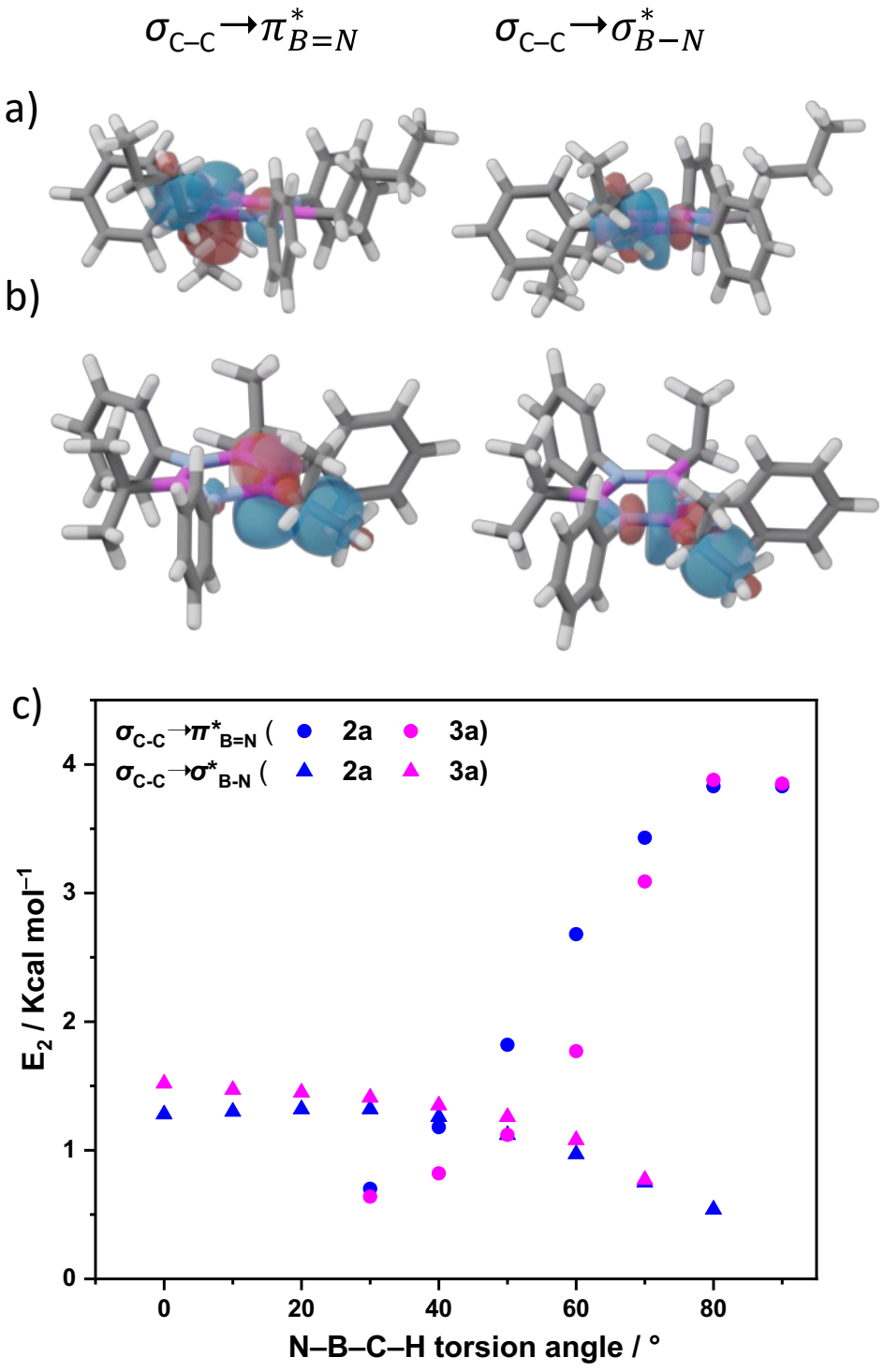


Figure S60. NBO analyses (PBE/def2-TZVP, orbitals with only one B are shown for clarity) for: $\sigma_{C-C} \rightarrow \pi^*_{B=N}$; $\sigma_{C-C} \rightarrow \sigma^*_{B-N}$ in a) **2a**, b) **3a**, c) Energies for the $\sigma_{C-C} \rightarrow \pi^*_{B=N}$ and $\sigma C-C \rightarrow \sigma^*_{B-N}$ interactions upon rotation of the B–alkyl group.

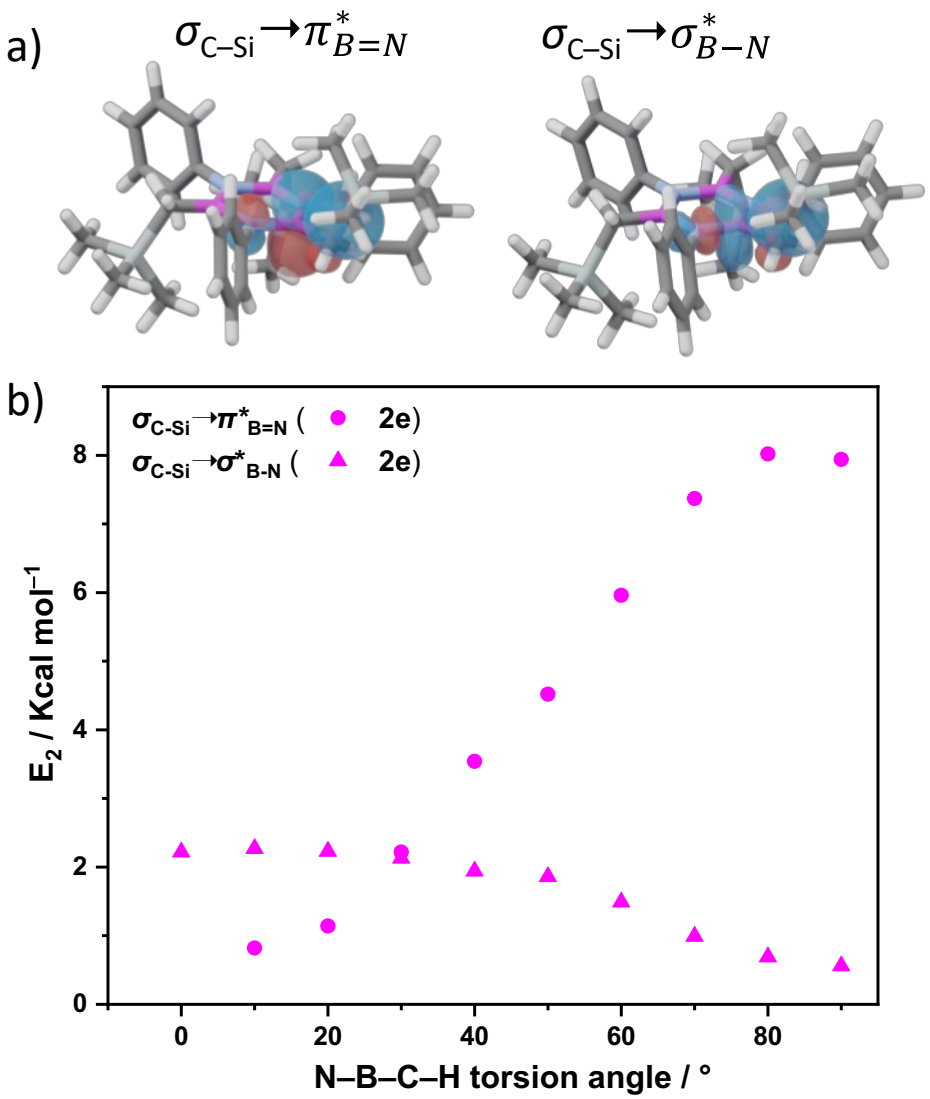


Figure S61. NBO analyses (PBE/def2-TZVP, orbitals with only one B are shown for clarity) for: a) $\sigma_{C-Si} \rightarrow \pi^*_{B=N}$ and $\sigma_{C-Si} \rightarrow \sigma^*_{B-N}$ in **2e**. b) Energies for the $\sigma_{C-Si} \rightarrow \pi^*_{B=N}$ and $\sigma_{C-Si} \rightarrow \sigma^*_{B-N}$ interactions upon rotation of the B–alkyl group.

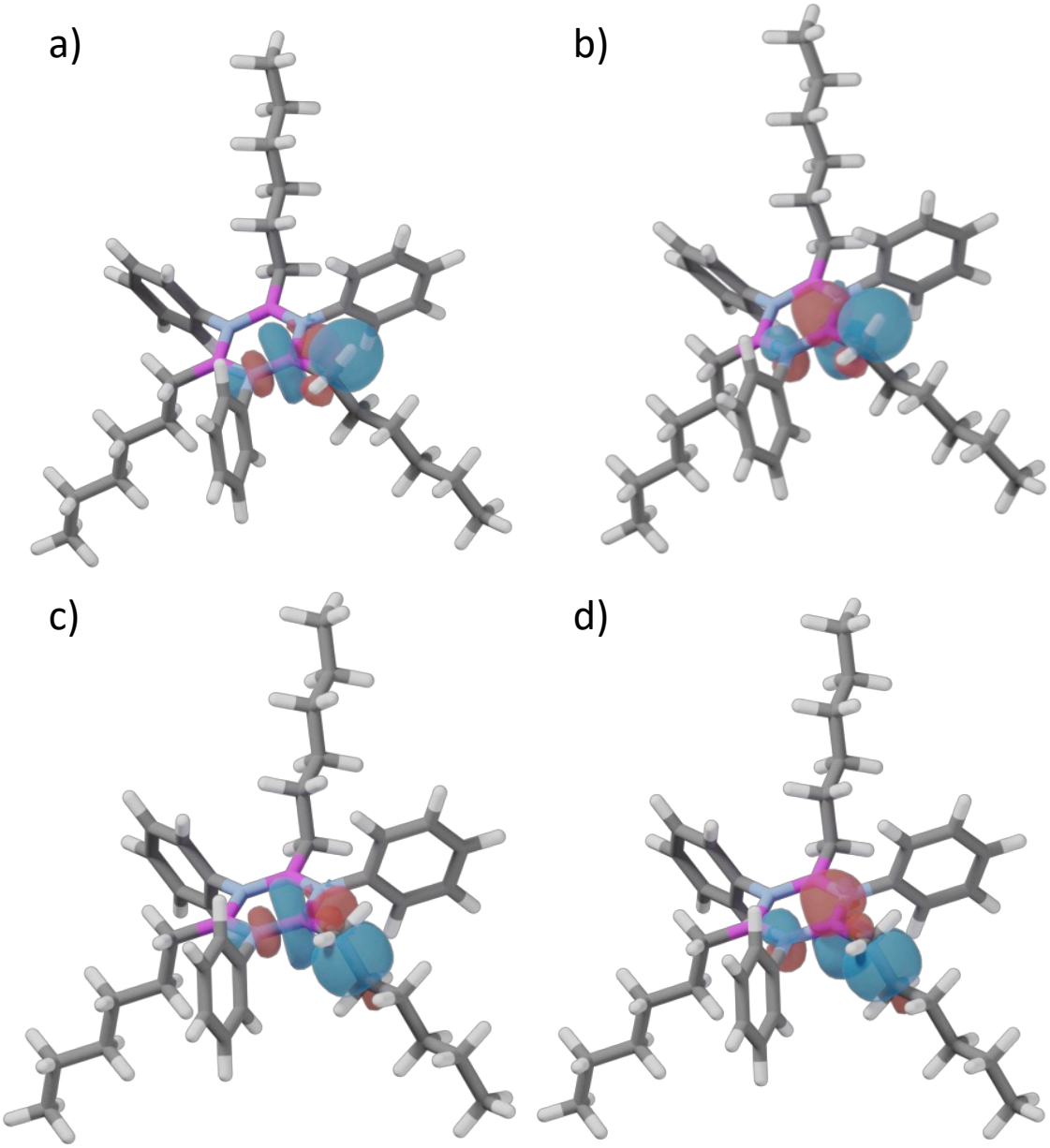


Figure S62. a) $\sigma_{C\text{-}H} \rightarrow \sigma^*_{B-N}$, b) $\sigma_{C\text{-}H} \rightarrow \pi^*_{B=N}$, c) $\sigma_{C\text{-}C} \rightarrow \sigma^*_{B-N}$ and d) $\sigma_{C\text{-}C} \rightarrow \pi^*_{B=N}$ donor-acceptor interactions derived from natural bonding orbital analyses of **2b**. Orbitals associated with only one B-hexyl component are shown for clarity. *PBE/def2-TZVP*.

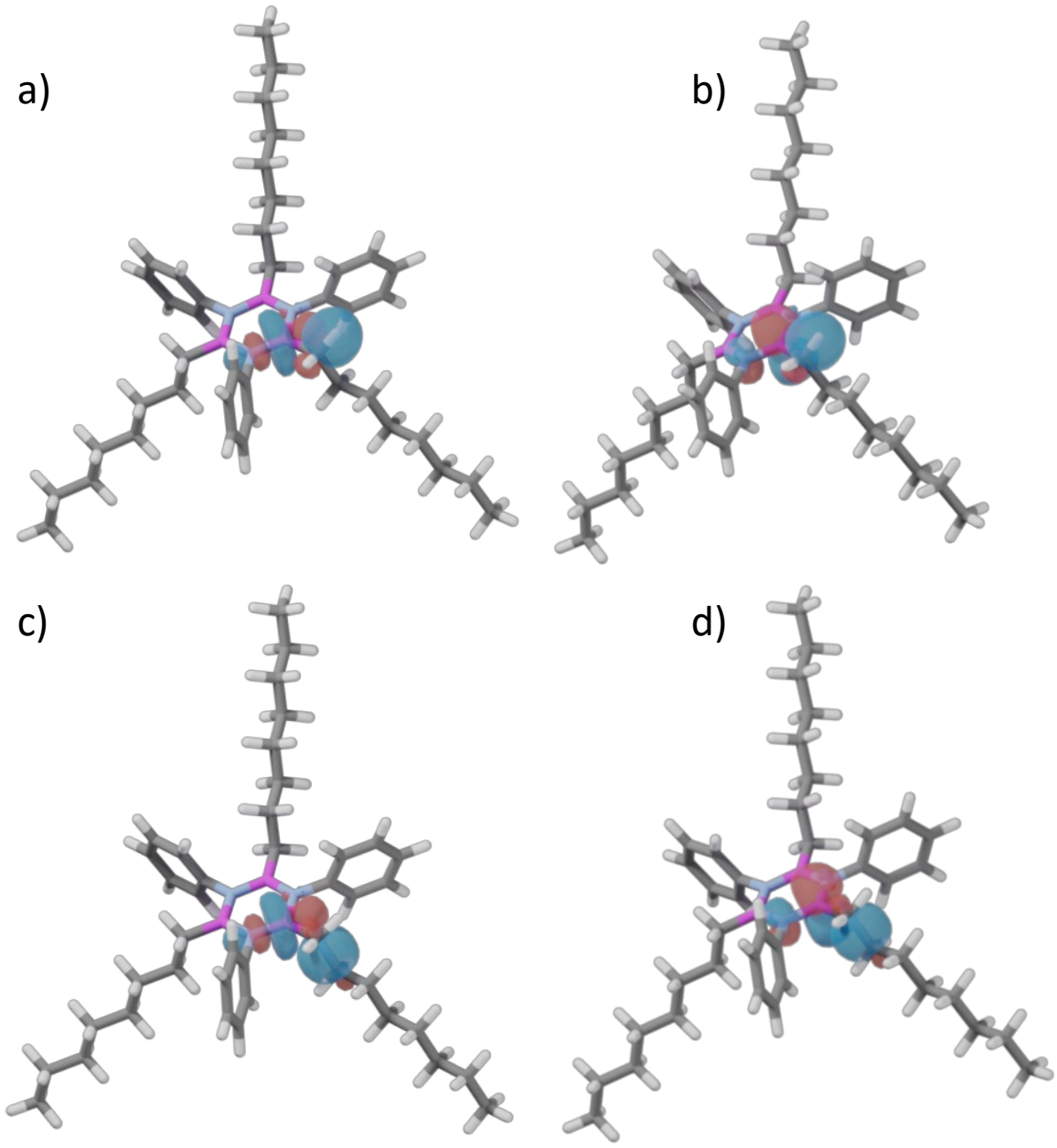


Figure S63. a) $\sigma_{C\text{-}H} \rightarrow \sigma^*_{B-N}$, b) $\sigma_{C\text{-}H} \rightarrow \pi^*_{B=N}$, c) $\sigma_{C\text{-}C} \rightarrow \sigma^*_{B-N}$ and d) $\sigma_{C\text{-}C} \rightarrow \pi^*_{B=N}$ donor-acceptor interactions derived from natural bonding orbital analyses of **2c**. Orbitals associated with only one B-octyl component are shown for clarity. *PBE/def2-TZVP*.

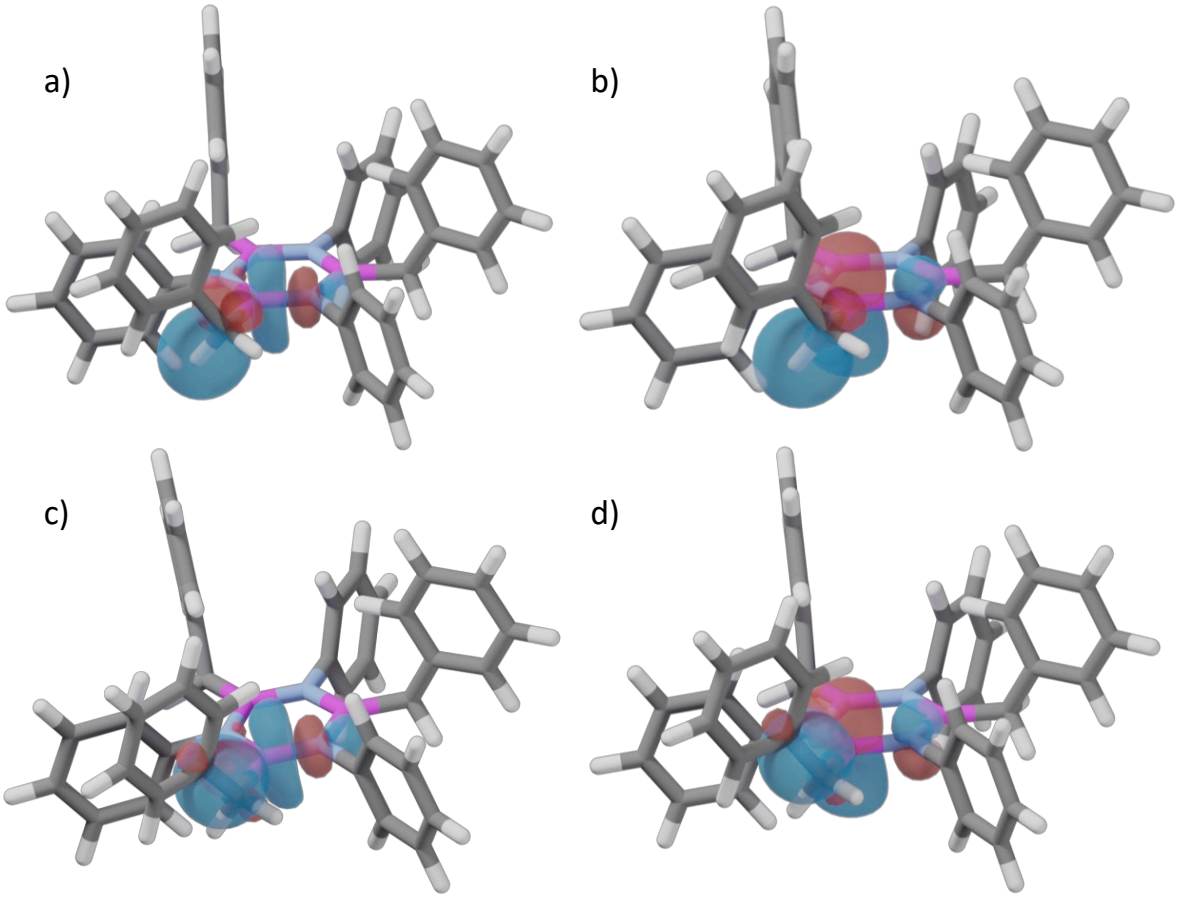


Figure S64. a) $\sigma_{C\text{-}H} \rightarrow \sigma^*_{B-N}$, b) $\sigma_{C\text{-}H} \rightarrow \pi^*_{B=N}$, c) $\sigma_{C\text{-}C} \rightarrow \sigma^*_{B-N}$ and d) $\sigma_{C\text{-}C} \rightarrow \pi^*_{B=N}$ donor-acceptor interactions derived from natural bonding orbital analyses of **2d**. Orbitals associated with only one B-benzyl component are shown for clarity. *PBE/def2-TZVP*.

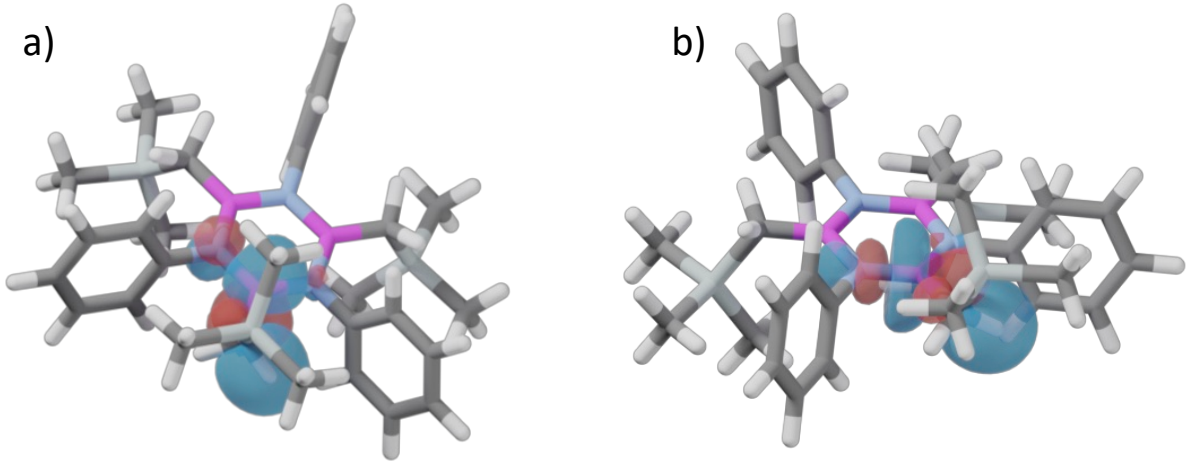


Figure S65. a) $\sigma_{C\text{-}H} \rightarrow \sigma^*_{B-N}$, b) $\sigma_{C\text{-}H} \rightarrow \pi^*_{B=N}$ donor-acceptor interactions derived from natural bonding orbital analyses of **2e**. Orbitals associated with only one B-benzyl component are shown for clarity. *PBE/def2-TZVP*.

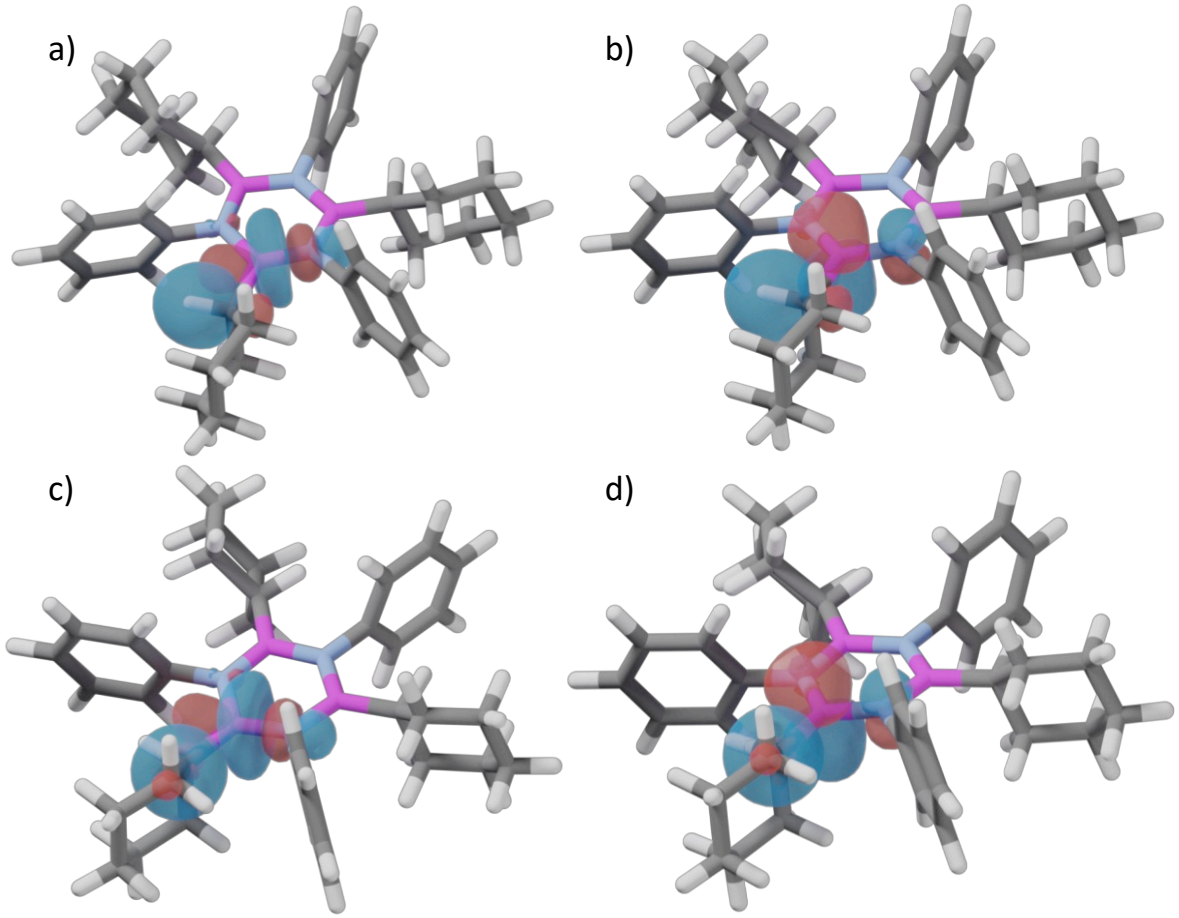


Figure S66. a) $\sigma_{C\text{-}H} \rightarrow \sigma^*_{B-N}$, b) $\sigma_{C\text{-}H} \rightarrow \pi^*_{B=N}$, c) $\sigma_{C\text{-}C} \rightarrow \sigma^*_{B-N}$ and d) $\sigma_{C\text{-}C} \rightarrow \pi^*_{B=N}$ donor-acceptor interactions derived from natural bonding orbital analyses of **3b**. Orbitals associated with only one B-cyclohexyl component are shown for clarity. *PBE/def2-TZVP*.

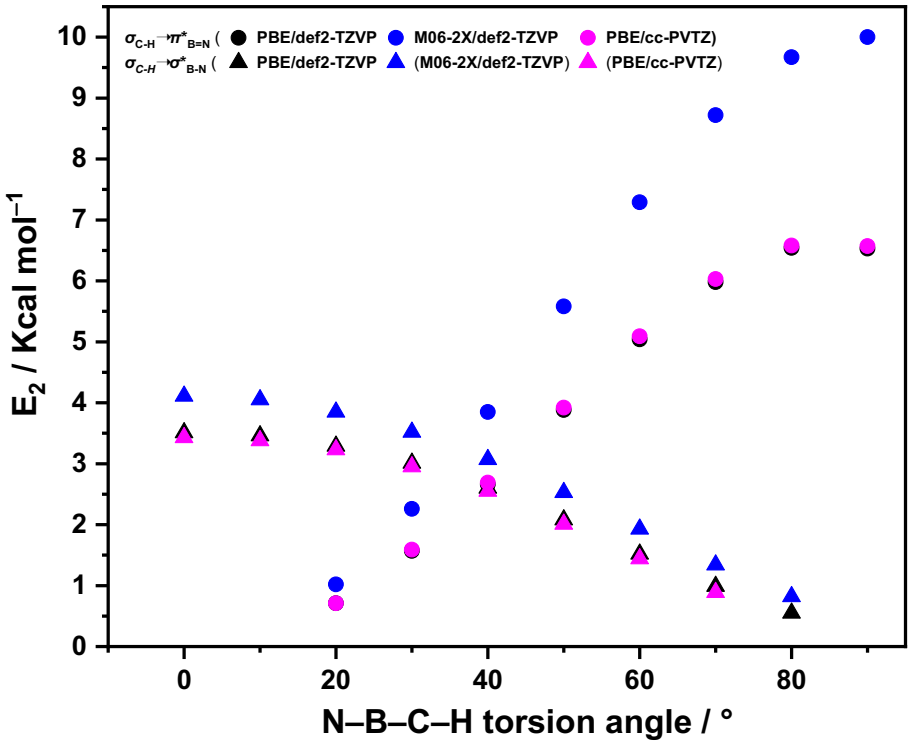


Figure S67: Comparison of energy variations for **1a** through alterations in the basis set and calculation function, depicting the $\sigma_{C-H} \rightarrow \pi^*_{B=N}$ and $\sigma_{C-H} \rightarrow \pi^*_{B-N}$ interactions upon rotation of the B–alkyl group.

7.2.1 Table S7. Calculated coupling constants (Hz) $^1J_{CH}$. *PBE/def2-TZVP*.

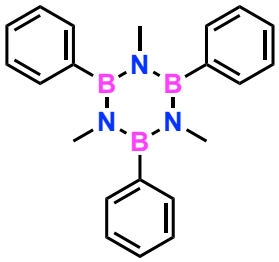
	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
1a	101							
	109							
	109							
1b	101							
	109							
	109							
2a	106	113	113	114				
	106	113	113	112				
				112				
2b	106	113	112	111	112	113		
	107	113	112	111	112	112		
						113		
2c	107	113	112	111	112	112	112	114
	107	113	112	111	112	112	112	113
								113
2d	104							
	108							
2e	106	111						
	106	109						
		109						
		111						
		109						
		109						
		109						
		109						
		109						
3a		112						
		112						
		114						
		114						
		114						
		114						
3b	102	112	115	116	102			
		114	111	110				
		114	115					
		114	111					

7.2.2 Table S8. Calculated coupling constants (Hz) $^1J_{CSi}$. *PBE/def2-TZVP*.

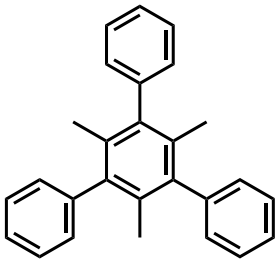
	C_1	C_2
2e	24	36

7.2.3 Table S9. Calculated coupling constants (Hz) $^{1}J_{CH}$. *PBE/def2-TZVP.*

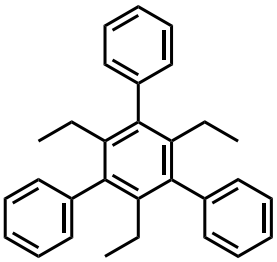
	C_1	C_2
$\mathbf{4_{Me}}$	113	
	115	
	115	
$\mathbf{4_{Et}}$	114	115
	115	115
	116	



3



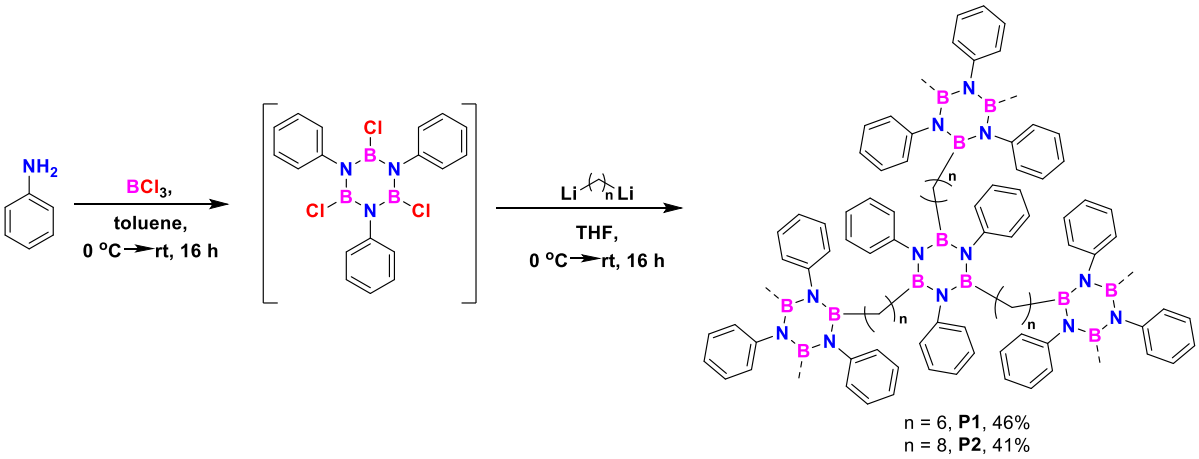
4_{Me}



4_{Et}

8. Polymer Synthetic Procedures and Characterization Data

8.1 General procedure III: *Preparation of BN alkyl polymer.*



Scheme S3: Synthetic protocols followed to prepare alkyl borazines polymers **P1** and **P2**.

In a glove box, to a Schlenk tube, **BNCl** (1 eq.) was dissolved in THF. The Schlenk tube was removed from the glove box and the resulting solution cooled to 0 °C. Subsequently, a solution of dilithioalkane (1.5 eq.) was slowly added dropwise. The solution was stirred at room temperature for 12-16 h and quenched by dropwise addition of water (0.2 mL) at 0 °C. Form precipitate was filtered and purify by Soxhlet extraction with THF.

8.2 General procedure IV: *Preparation of* dilithioalkane.

A 50 mL Schlenk tube was charged with diiodo alkane, subsequently dry diethyl ether was added, and the solution was cooled to -78 °C. 1.7 M t-BuLi in pentane was slowly added drop by drop. The reaction mixture was stirred for 0.5 h at -78 °C and warmed to 25 °C. After this the solvent were removed by vacuum under inert condition. The solid was dissolved in dry THF and used for the reaction.

8.4 Synthesis of BN Polymer **P1**

Synthesized in accordance with general procedure III, using **BNCl** (0.5 g, 1.21 mmol), THF (2 mL) and a 1,6-dilithiohexane (1.82 mL, 1M solution in THF, 1.82 mmol, *general procedure IV*). The product was purified purify by Soxhlet extraction with THF affording **P1** as off white solid (0.26 g, 46% yield).

Solid-state $^{1}H \rightarrow {}^{13}C$ CPMAS NMR (126 MHz) δ 147.60, 128.56, 124.92, 32.27, 25.00, 16.92.

8.5 Synthesis of BN Polymer **P2**

Synthesized in accordance with general procedure III, using **BNCl** (0.5 g, 1.21 mmol), THF (2 mL) and a 1,8-dilithiooctane (1.82 mL, 1M solution in THF, 1.82 mmol, *general procedure IV*). The product was purified purify by Soxhlet extraction with THF affording **P2** as off white solid (0.25 g, 41% yield).

Solid-state $^{1}H \rightarrow {}^{13}C$ CPMAS NMR (126 MHz) δ 147.23, 128.60, 125.49, 36.92, 33.94, 32.34, 29.18, 24.93, 14.37.

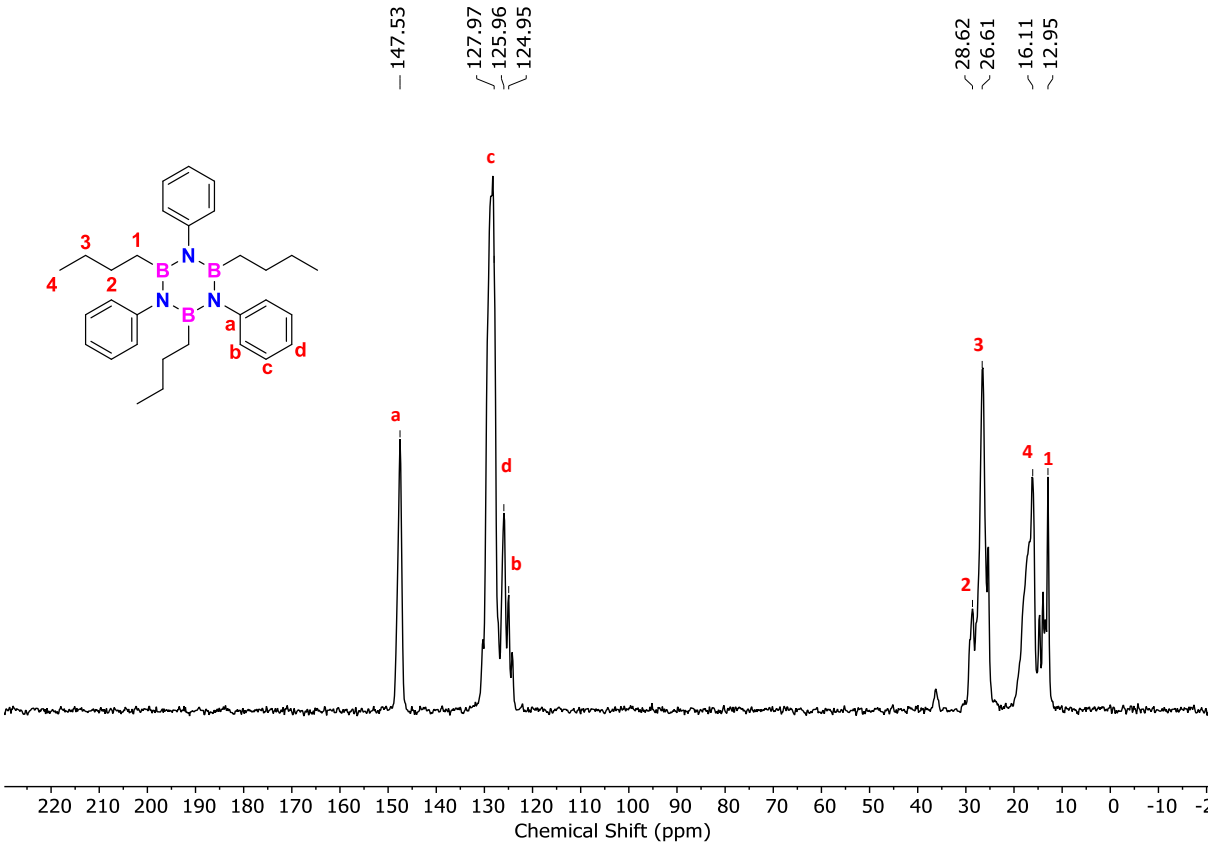


Figure S68. Solid-state $^{1}H \rightarrow {}^{13}C$ CPMAS NMR spectra recorded for **2a**.

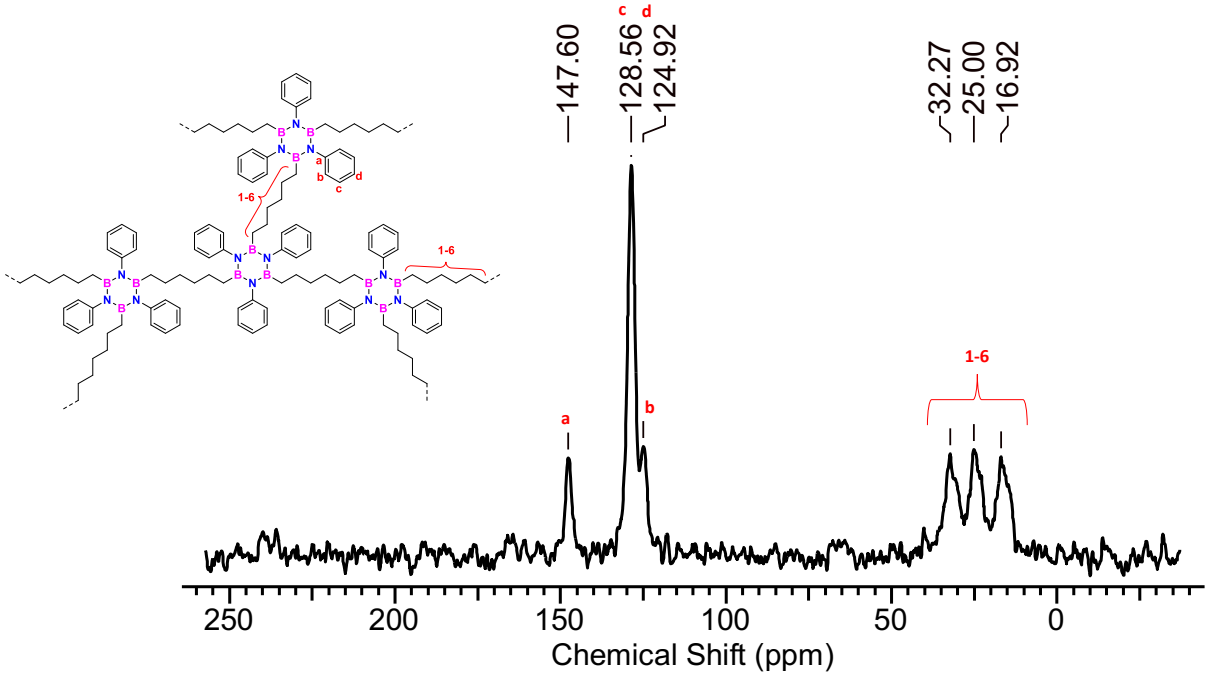


Figure S69. Solid-state $^{1}H \rightarrow {}^{13}C$ CPMAS NMR spectra recorded for **P1**.

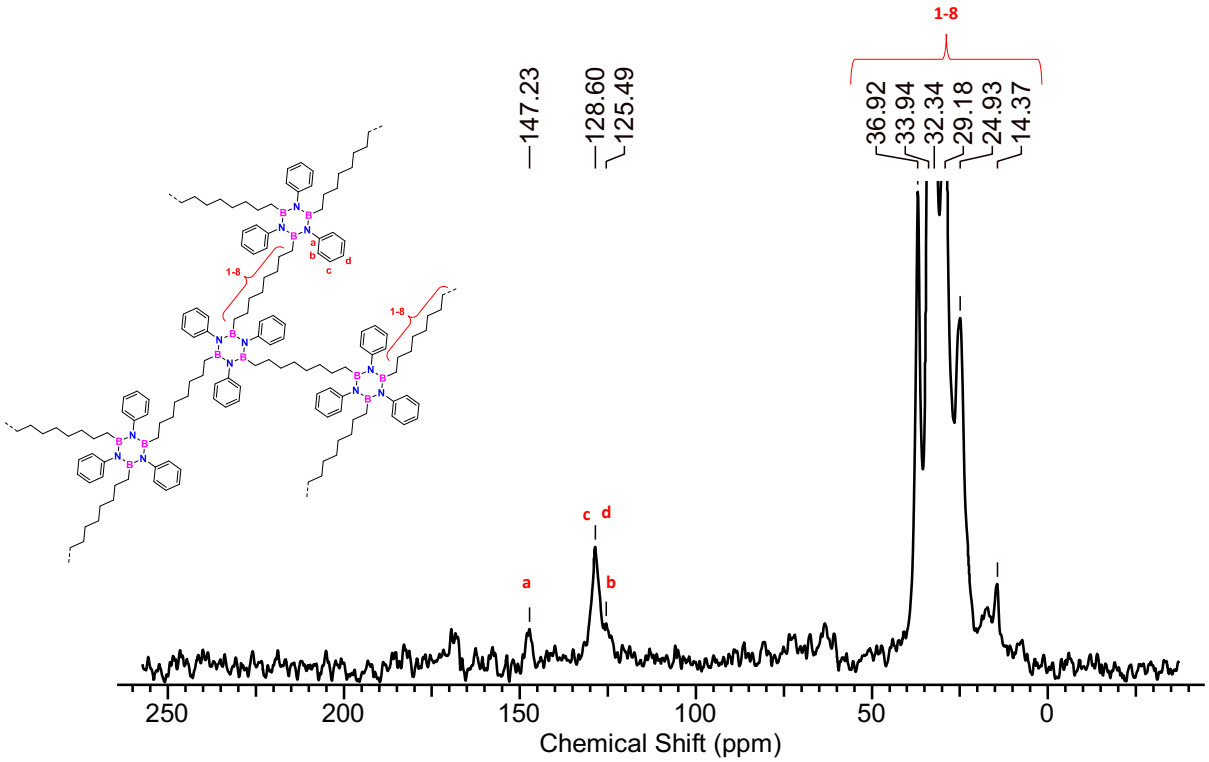


Figure S70. Solid-state $^{1}H \rightarrow {}^{13}C$ CPMAS NMR spectra recorded for **P2**.

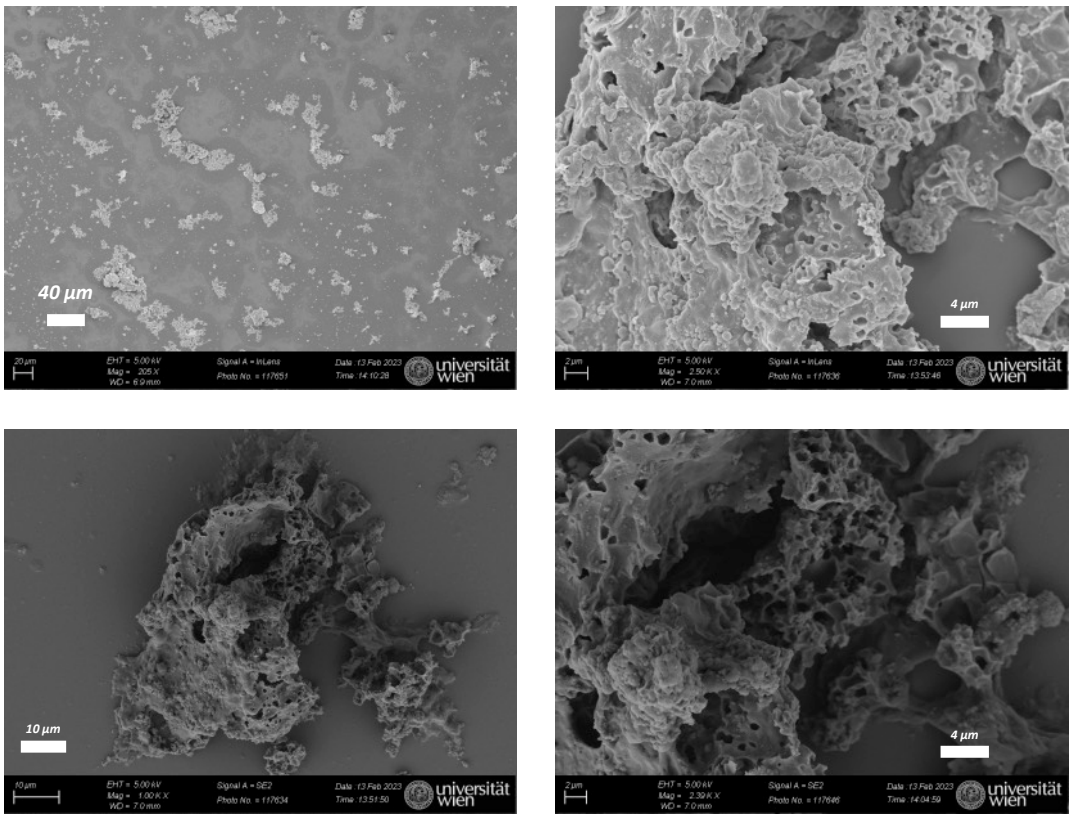


Figure S71: SEM images taken with different magnifications of a BN-polymer **P1**.

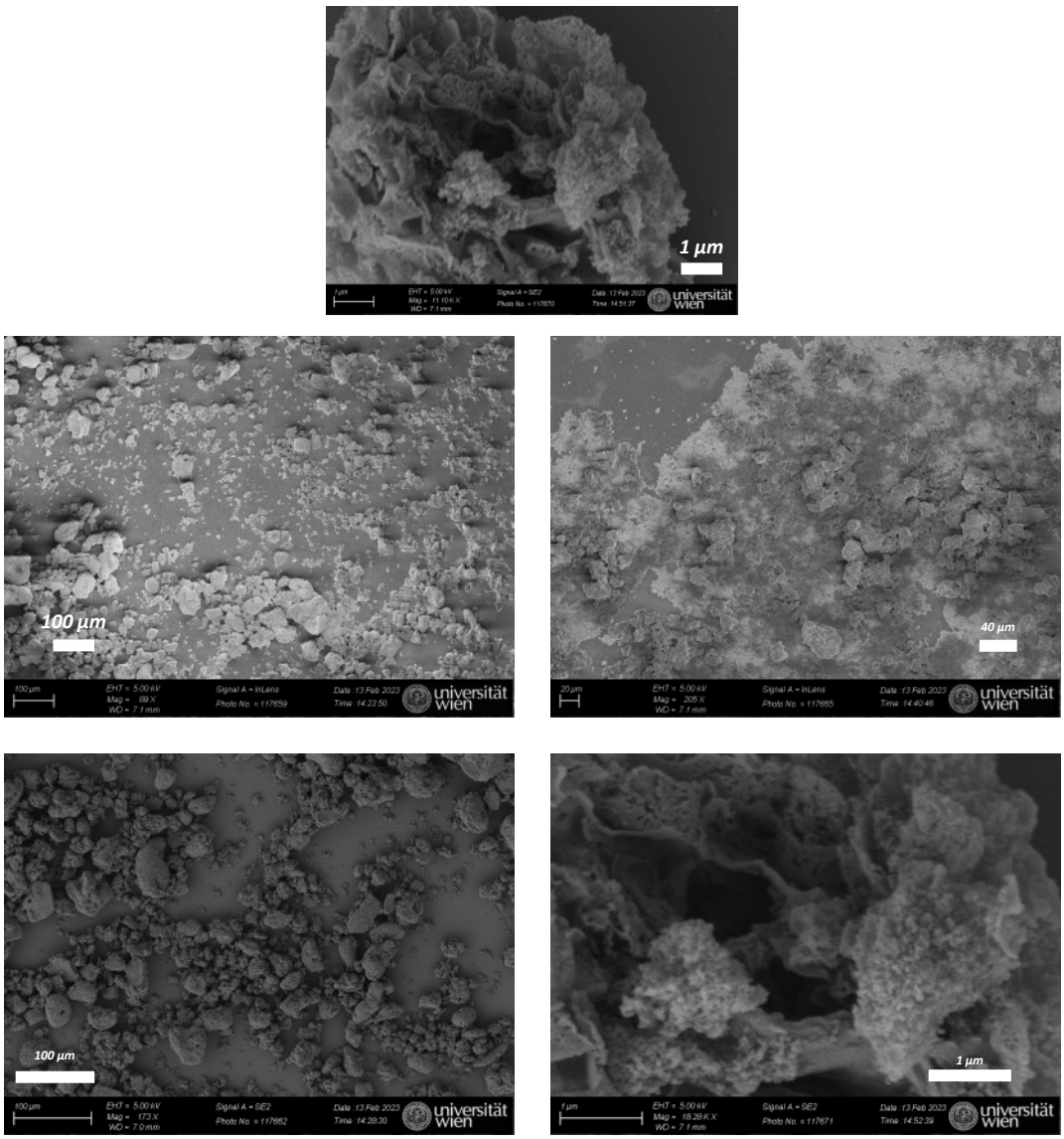


Figure S72: SEM images taken with different magnifications of a BN-polymer **P2**.

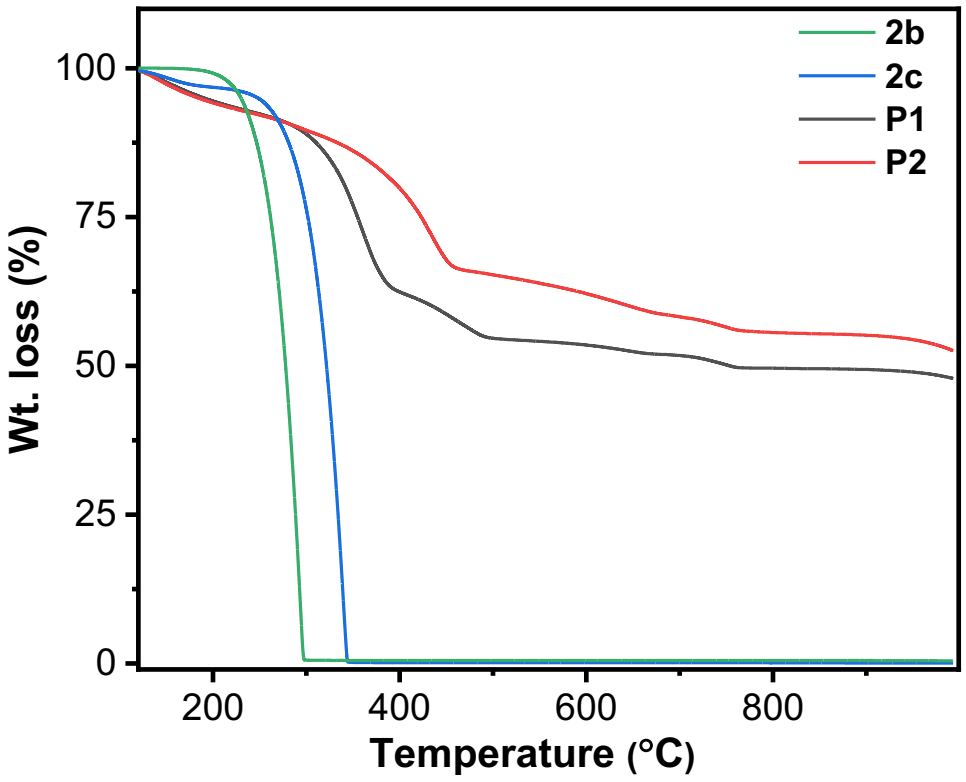


Figure S73. Thermogravimetric analysis at a heating rate of 10 °C.min^{-1} under N_2 atmosphere of **2b**, **2c**, **P1** and **P2**.

9. Cartesian coordinates of calculated structures

9.1 2,4,6-trimethyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**1a**)

N	-0.446080733139	-0.504810672969	-0.027528081632
N	1.694095378821	0.733467922917	0.001187132410
N	-0.448011918677	1.968385819796	-0.023439500221
B	1.005154607533	-0.544109701561	-0.015678901823
B	-1.207612662281	0.731203725295	-0.019468433622
B	1.003167653341	2.009979931181	-0.011373527781
C	3.132303951547	0.734414906153	0.046414922467
C	3.881968323737	0.737347456061	-1.136839261793
C	3.798915120829	0.732463225782	1.277210661087
C	5.277901319248	0.738379254617	-1.088626183242
H	3.360224600939	0.738886653827	-2.096001137605
C	5.195545626525	0.733487739495	1.324631387749
H	3.213240087805	0.730192247252	2.198707374891
C	5.940010298064	0.736460371270	0.142351157805

H	5.850196993237	0.740712956202	-2.018319445897
H	5.702879870291	0.731985554968	2.291313859799
H	7.030651177532	0.737287050076	0.179594375187
C	-1.165099593697	-1.750485420290	-0.040767540153
C	-1.697465674482	-2.247464709315	-1.236849087469
C	-1.342568460373	-2.480758233968	1.140905522683
C	-2.397582974199	-3.456295931340	-1.250632618778
H	-1.555922730120	-1.678994274869	-2.158211356255
C	-2.041276296517	-3.690373373964	1.125976967511
H	-0.930254628457	-2.090997143331	2.073721162145
C	-2.571897484644	-4.182568892262	-0.069523251845
H	-2.807150346968	-3.832187857339	-2.190233188894
H	-2.172579471956	-4.249305581974	2.054544208671
H	-3.118281544862	-5.127148180938	-0.080627425236
C	-1.168894665166	3.213016408796	-0.032644507887
C	-1.347823258987	3.938997870220	1.151453676044
C	-1.701606039977	3.713296848408	-1.227201419201
C	-2.048297917945	5.147630303920	1.140415497418
H	-0.935285726307	3.546646652430	2.083083809280
C	-2.403485464708	4.921142021013	-1.237097734304
H	-1.558918322242	3.148183330818	-2.150451004726
C	-2.579245137087	5.643123854978	-0.053575059347
H	-2.180741905822	5.703191434882	2.070842156963
H	-2.813303957145	5.299632924067	-2.175544903504
H	-3.127009833173	6.586934386411	-0.061637093256
C	-2.789188190313	0.730083684541	0.000213757724
H	-3.202589980451	1.620597842857	0.493849710214
H	-3.190900288274	0.733257542770	-1.027851447857
H	-3.201623430847	-0.163975403794	0.488161717269
C	1.793255756578	3.379743083720	0.000631885481
H	1.240183897588	4.189827013169	-0.494568218551
H	1.964283619691	3.713187534709	1.039172372092
H	2.785887365475	3.298328654167	-0.462974277354
C	1.798014904193	-1.912301718950	-0.008354139560
H	1.977293237437	-2.244536543856	1.029185684303
H	1.243763196394	-2.723997982010	-0.499459489733
H	2.787375262011	-1.828576834038	-0.478614061666

9.2 1,3,5-tris(2',6'-dimethyl-[1,1'-biphenyl]-4-yl)-2,4,6-trimethyl-1,3,5,2,4,6-triazatriborinane (**1b**)

C	2.703850950466	0.955863571256	0.018154019330
C	3.355675324059	1.185021896083	-1.198184314737
H	2.822821964032	0.996324249132	-2.132451506004
C	4.672578749794	1.649597725409	-1.221110470316
H	5.165822785986	1.822951344499	-2.180307688575
C	5.373689383873	1.897802116398	-0.031449618975
C	4.711607401553	1.665273030380	1.184193097020
H	5.235971104182	1.850943642635	2.124383947849
C	3.395410570364	1.200899820665	1.210348190243

H	2.892991114275	1.024277395456	2.163660626140
C	6.783459864142	2.394844157438	-0.057515322862
C	7.853129158661	1.471726541820	-0.073344885592
C	9.168307145418	1.956822570469	-0.097856482889
H	9.996741812186	1.244384755565	-0.110144106338
C	9.427294881147	3.326883765075	-0.106537765749
H	10.456899797066	3.689851744077	-0.125695431631
C	8.366486451391	4.231663778607	-0.090642125974
H	8.565050186850	5.306166957988	-0.097383624392
C	7.037858662643	3.784728313095	-0.066050615102
C	7.599136596270	-0.014587503289	-0.063817957034
H	8.545074860379	-0.571854719763	-0.077622872798
H	7.032678851735	-0.322655347737	0.828262603710
H	7.003016620620	-0.329147672359	-0.933996904390
C	5.907990699251	4.783144077092	-0.049243457470
H	6.295266169999	5.810461898106	-0.062112079329
H	5.242753944621	4.656342651241	-0.916935268522
H	5.277335430564	4.665733851762	0.845231606816
C	-0.523293150124	-2.816490393088	0.024318768834
C	-0.424787103812	-3.556859485529	-1.159188387315
H	-0.147364659927	-3.048301549393	-2.084758402735
C	-0.681040074579	-4.929317543146	-1.161020439875
H	-0.599637112987	-5.491031516723	-2.094427348678
C	-1.043524963165	-5.600167636605	0.017122938027
C	-1.140418845796	-4.849609916618	1.198901100740
H	-1.420101402869	-5.348653438308	2.129566305877
C	-0.883761179311	-3.477179057940	1.204133584322
H	-0.959703494432	-2.907278604817	2.132435921109
C	-1.318182701801	-7.069741539193	0.013339118444
C	-2.625921765308	-7.538925404960	-0.244120749514
C	-2.864147947753	-8.920539340220	-0.243065335056
H	-3.874999608801	-9.285015095770	-0.441460350426
C	-1.833425033899	-9.825769905355	0.006636254656
H	-2.034081924975	-10.899051383128	0.004060918034
C	-0.545481508526	-9.355226901502	0.259621579282
H	0.265212765843	-10.061250190002	0.455401776243
C	-0.268455865294	-7.980884042043	0.267329401450
C	-3.757502789574	-6.580324998660	-0.516779636233
H	-4.697124902313	-7.123573608904	-0.682728986625
H	-3.907693760924	-5.882490576295	0.321048417880
H	-3.558423135462	-5.961103781206	-1.404793776157
C	1.132799088802	-7.497079126854	0.543336067014
H	1.812713373006	-8.343807969876	0.705553160917
H	1.525444040692	-6.896489153297	-0.291296905884
H	1.170223598990	-6.852133372700	1.434562781873
C	-2.177029668850	1.863559989967	0.024758359409
C	-2.566385068150	2.500553252172	-1.158961696231
H	-2.031659826885	2.278571601829	-2.084739658149
C	-3.627946665507	3.407405161030	-1.160736025898
H	-3.918137148203	3.894860449975	-2.094319702999

C	-4.330598438399	3.702496726349	0.017676767430
C	-3.933611031394	3.058585570262	1.199665517870
H	-4.464034986879	3.271877102037	2.130559875587
C	-2.871707741905	2.152043253827	1.204848830938
H	-2.572050047651	1.661715763284	2.133336013334
C	-5.467466462696	4.673378514679	0.013921442975
C	-5.222760706475	6.042099267937	0.265584086124
C	-6.301624220075	6.937422970148	0.257713606807
H	-6.114126158013	7.996322272754	0.451630450705
C	-7.599620079733	6.494117237050	0.006916343922
H	-8.429945273484	7.203171017167	0.004183154894
C	-7.833250931950	5.141920964087	-0.240424243923
H	-8.848953427563	4.790253133172	-0.437140470295
C	-6.780016342482	4.216561467386	-0.241301319609
C	-3.828243923003	6.546262160913	0.539275795983
H	-3.831029577582	7.632260282505	0.700956784761
H	-3.392605419471	6.068444071856	1.430085041477
H	-3.146648655460	6.325311561503	-0.296254535596
C	-7.058590204189	2.759436624407	-0.511345448114
H	-8.130823329104	2.591929941650	-0.678103485772
H	-6.513813460566	2.400654874832	-1.397970636977
H	-6.738305450824	2.123709024000	0.328167314606
N	-0.259584706364	-1.402786500479	0.028810985958
N	-1.083640759875	0.929406683035	0.029172777516
N	1.347449265581	0.476739734081	0.039424933880
B	-1.388354890376	-0.489949526612	0.010303365349
B	0.271281511056	1.450837693521	0.042572868530
B	1.122160216354	-0.957220645709	0.042141172584
C	-2.879169443813	-1.016577250892	-0.035701375066
H	-2.963289034450	-1.993285653273	-0.532198173591
H	-3.274086318986	-1.154698269223	0.985738050823
H	-3.557534826984	-0.310262894496	-0.534236168253
C	2.325455099676	-1.983429542787	0.047333269512
H	2.062522316110	-2.940265826627	0.518997137344
H	2.629554873224	-2.221511530404	-0.987003418967
H	3.219004429585	-1.581268181094	0.544319148781
C	0.562861359049	3.005191631305	0.047820254238
H	1.509893269484	3.253705343497	0.546375353891
H	0.651954334476	3.380981666818	-0.986526106024
H	-0.243557839080	3.584796713075	0.517766841093

9.3 2,4,6-tributyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2a**)

N	-1.298988868069	-0.707261506820	-0.115527866925
N	0.214660373250	1.176702441374	0.413194024440
N	1.152067194901	-1.048794685479	-0.123868305179
B	-1.144890304390	0.693452779316	0.240797425602
B	-0.176441182130	-1.612793694832	-0.295208830533
B	1.389135413830	0.340360061011	0.232169802464
C	0.407475889619	2.551101945686	0.797102111467
C	0.461179257557	2.903434579483	2.152423903714

C	0.543680059157	3.552266308012	-0.171942381448
C	0.647928711823	4.234434810017	2.531387036063
H	0.354875969062	2.122088744549	2.907685784698
C	0.730600069713	4.884467741122	0.207883401752
H	0.502171944954	3.280167812773	-1.228135101961
C	0.783425266136	5.230565862374	1.560135184659
H	0.687629664102	4.493488249946	3.591174892144
H	0.835256153790	5.654285205763	-0.559121527060
H	0.929369826041	6.270745770118	1.856125813014
C	-2.630430819110	-1.227737747717	-0.286238270076
C	-3.376607591676	-1.649987502838	0.821601438646
C	-3.197764237841	-1.320627212538	-1.563661450937
C	-4.668517671062	-2.155150866521	0.654691515672
H	-2.936590127329	-1.575606109555	1.818060162595
C	-4.488826453755	-1.827917155007	-1.730411408580
H	-2.615383678892	-0.995486890079	-2.428047561156
C	-5.229414949532	-2.246508468624	-0.621871593876
H	-5.238146389535	-2.478877396863	1.527941053094
H	-4.916578285867	-1.895634482308	-2.732547114615
H	-6.238138428261	-2.642003932890	-0.752114032496
C	2.289338760521	-1.913265111949	-0.302976309005
C	2.801119316758	-2.156537869847	-1.584071511499
C	2.899048826579	-2.524428078577	0.800254063783
C	3.903182934427	-2.997287500731	-1.758960130311
H	2.324043297419	-1.683785201363	-2.444856108680
C	4.002508341498	-3.363363612347	0.625197860329
H	2.502793617773	-2.333506797017	1.799558273802
C	4.508523105651	-3.603403224586	-0.654995671141
H	4.289422807761	-3.178441262730	-2.763865755885
H	4.467765098354	-3.831277572639	1.494929515810
H	5.369814126189	-4.259467582344	-0.791597814195
C	-0.392185461525	-3.153363523573	-0.612227862399
H	-1.304914803965	-3.297505008107	-1.213172308087
H	0.442329720339	-3.540965876065	-1.219133588224
C	2.857837961376	0.922453111852	0.389516120319
H	3.530462887553	0.150863569295	0.799268795560
H	2.862505184032	1.752834255830	1.114727199842
C	-2.397437057590	1.654723486020	0.407419897399
H	-3.252615590132	1.096014591295	0.822373155139
H	-2.170078649567	2.454069307761	1.131878588009
C	3.468146986688	1.434511804769	-0.933627713502
H	3.485978355620	0.617418852674	-1.675550277266
H	2.822487754719	2.220910207512	-1.361729764393
C	4.886074443292	1.990028463618	-0.772632205450
H	4.868931964510	2.807609565636	-0.031191894912
H	5.532404133953	1.203853480814	-0.345349932682
C	5.488564141825	2.495893915100	-2.083595358976
H	6.505634740693	2.888752491194	-1.937308833111
H	5.546896438977	1.689379543050	-2.831204081436
H	4.877945378793	3.304110159818	-2.515774702313

C	-2.853346273493	2.315360612380	-0.912085780820
H	-3.098827354411	1.534963677935	-1.653117196569
H	-2.020178608930	2.895701227865	-1.345221075615
C	-4.064291334241	3.237186036994	-0.742125926755
H	-4.898048536494	2.657244442068	-0.309806552702
H	-3.819343322259	4.018240537010	-0.001571482973
C	-4.514290114717	3.889718223607	-2.049497603966
H	-4.795873920475	3.130574836366	-2.795955107902
H	-5.384221309916	4.545512544877	-1.896776584300
H	-3.708890091663	4.500628575567	-2.486495404972
C	-0.509342210214	-4.025256181929	0.657475714658
H	0.399465796494	-3.908642746448	1.273333499170
H	-1.347515473969	-3.665223852620	1.279290552974
C	-0.717552329277	-5.512171134314	0.356106460518
H	-1.626407097492	-5.629235612816	-0.259280775480
H	0.120545799885	-5.872651246592	-0.265237319916
C	-0.833164739266	-6.372695779772	1.614511371068
H	-0.981923915008	-7.434264589229	1.367278955926
H	0.075919321090	-6.298296668670	2.231642679232
H	-1.683134834654	-6.053194806115	2.237640646718

9.4 2,4,6-trihexyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2b**)

N	0.724356255433	1.237285330023	0.029205353580
N	-1.354423066875	0.000354809655	-0.489035374517
N	0.723786237985	-1.237542462903	0.029183064930
B	-0.686749581652	1.279483174290	-0.316540387940
B	1.468491975771	-0.000301531941	0.194398739857
B	-0.687338911604	-1.279084128975	-0.316563219252
C	-2.744966053005	0.000678699186	-0.863174508667
C	-3.110772191741	0.000773360587	-2.215992517777
C	-3.748679907147	0.000903954792	0.112779039048
C	-4.457369383455	0.001087542464	-2.585773117256
H	-2.327414614950	0.000597805293	-2.976636993658
C	-5.096503541220	0.001218526104	-0.257826684262
H	-3.466480693828	0.000831446663	1.167152166648
C	-5.455962894037	0.001311425655	-1.607615156183
H	-4.726682059718	0.001157608149	-3.643747516183
H	-5.868071855846	0.001391600156	0.514555211927
H	-6.508361259822	0.001557061944	-1.896322790944
C	1.424151598766	2.483227195232	0.204042322400
C	1.935045264785	3.174517960869	-0.902016488124
C	1.605594838476	3.020540620275	1.484975572028
C	2.615246845002	4.382738683057	-0.729763052510
H	1.791507836990	2.758472344289	-1.901184763318
C	2.287800346721	4.227560498799	1.657060696209
H	1.210797077745	2.480394748825	2.347787583237
C	2.794814812618	4.913578716698	0.550291331595
H	3.006636577675	4.910419967565	-1.601666427823

H	2.422805579852	4.632501063109	2.661868170170
H	3.327113523531	5.856733343462	0.684584593763
C	1.423007624743	-2.483809693365	0.203997171639
C	1.604200323988	-3.021231852007	1.484920251927
C	1.933585680750	-3.175313726423	-0.902074041799
C	2.285849617536	-4.228569097266	1.656983212594
H	1.209649007223	-2.480921368491	2.347741926545
C	2.613230593275	-4.383850839604	-0.729842794960
H	1.790242256687	-2.759182300360	-1.901234436208
C	2.792550960232	-4.914798800428	0.550201544857
H	2.420665870096	-4.633591648239	2.661783015844
H	3.004379510458	-4.911695028827	-1.601755631571
H	3.324415066580	-5.858201042848	0.684477486321
C	3.029009564708	-0.000663731206	0.486134828745
H	3.309266421505	0.881365971304	1.084750383256
H	3.308857499632	-0.882825544945	1.084746943712
C	-1.468060444744	-2.652724714154	-0.472731700367
H	-0.799686131968	-3.423719525132	-0.890510811508
H	-2.296409364378	-2.539764813269	-1.191457708755
C	-1.466838814468	2.653485781720	-0.472683793088
H	-0.798105895371	3.424184569947	-0.890435299806
H	-2.295230712864	2.540923969926	-1.191422669841
C	-2.049542627861	-3.191265941501	0.853147285212
H	-1.237259468087	-3.320243128348	1.589079834009
H	-2.737896795723	-2.445165664795	1.286372641673
C	-2.792553860317	-4.520487782477	0.693378994533
H	-3.605886236123	-4.393255496426	-0.043624311528
H	-2.103831146825	-5.268765398244	0.261416277296
C	-3.373299633402	-5.061352123792	2.001456658384
H	-2.559190161733	-5.186655849684	2.738351079318
H	-4.060839360483	-4.311657391359	2.433675021856
C	-2.048090894045	3.192259535182	0.853201613815
H	-1.235758098732	3.320846055503	1.589147677604
H	-2.736792059173	2.446463366703	1.286399224496
C	-2.790491642447	4.521825400347	0.693457852742
H	-2.101420913116	5.269798868991	0.261523397772
H	-3.603872556260	4.394984341499	-0.043559328987
C	-3.371006943267	5.062921705413	2.001541888681
H	-2.556849870332	5.187833778709	2.738450214405
H	-4.058895379003	4.313530540991	2.433731856713
C	3.884127278954	-0.000859914800	-0.800916545191
H	3.629815700785	-0.882561888378	-1.414404908174
H	3.630225002848	0.880961991672	-1.414401984181
C	5.391007779527	-0.001210236028	-0.529350637997
H	5.647553341885	0.881322837456	0.083921060517
H	5.647143403952	-0.883864085710	0.083918604787
C	6.243613801989	-0.001406516713	-1.799838995156
H	5.984710432038	-0.883580336105	-2.413227371556
H	5.985120223026	0.880889118506	-2.413224994529
C	-4.112890338185	6.392451148622	1.843389566189

H	-4.925739676162	6.267327720285	1.107081888078
H	-3.425396030295	7.140682152774	1.412104197378
C	-4.688963788612	6.923483416243	3.156357905887
H	-5.215385831166	7.878381972958	3.011427900971
H	-5.405392365842	6.210089006639	3.592807871890
H	-3.894075208775	7.089893038276	3.900083221796
C	-4.115793461802	-6.390537818922	1.843279691531
H	-3.428647358221	-7.139072146724	1.411965744878
H	-4.928595242359	-6.265023314753	1.106986075581
C	-4.692092375421	-6.921340536489	3.156241906637
H	-5.408188619835	-6.207629713872	3.592719964875
H	-5.218953249635	-7.875994339356	3.011294109876
H	-3.897270124892	-7.088133209641	3.899952307127
C	7.750609562363	-0.001756885093	-1.531558464454
H	8.008858411972	0.879501423465	-0.919027704452
H	8.008448994848	-0.883136575197	-0.919029870787
C	8.591929920473	-0.001950750321	-2.808276933141
H	9.668866867979	-0.002201172433	-2.584291892588
H	8.378658042656	-0.889676369829	-3.424007996386
H	8.379070472764	0.885875347103	-3.424005841909

9.5 2,4,6-trioctyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2c**)

N	0.706508030933	1.237145240134	0.027318387506
N	-1.382067687651	-0.000051766820	-0.449109812689
N	0.706258585615	-1.237637790332	0.027400956337
B	-0.710700828065	1.279170179871	-0.292811587224
B	1.452673212494	-0.000316303722	0.184393071217
B	-0.710958379392	-1.279398465878	-0.292727891775
C	-2.779775358581	0.000077203319	-0.795210947594
C	-3.172871857088	0.000075126481	-2.140337912998
C	-3.763330813013	0.000204719406	0.201007041602
C	-4.526634059097	0.000199525690	-2.482790007915
H	-2.405049840103	-0.000024927919	-2.916661166672
C	-5.118398939214	0.000329193689	-0.142265602526
H	-3.459235582682	0.000205318437	1.249271234640
C	-5.505144919373	0.000327297419	-1.484510903908
H	-4.817367600155	0.000196486543	-3.535079268584
H	-5.874210151024	0.000427854561	0.645541480541
H	-6.563194625447	0.000424444469	-1.751773919415
C	1.410061418462	2.483478829674	0.183624064717
C	1.904039350924	3.166666384364	-0.935118703167
C	1.611746492695	3.029680470485	1.457762301681
C	2.587273469278	4.375764015765	-0.782139901487
H	1.744885405945	2.743415032055	-1.928887753332
C	2.297009851241	4.237609109413	1.610545159463
H	1.230340584764	2.495972583858	2.330546273504
C	2.786831102580	4.915590164147	0.491179407059
H	2.965224235818	4.897069204572	-1.663752575473

H	2.447909548253	4.649560305805	2.610230598044
H	3.321412414258	5.859467753824	0.610535744928
C	1.409561739736	-2.484102406698	0.183787977217
C	1.611136306724	-3.030262069482	1.457961713180
C	1.903404927954	-3.167460515611	-0.934910095761
C	2.296158226018	-4.238317690399	1.610823271110
H	1.229836327384	-2.496421528065	2.330710837540
C	2.586397368408	-4.376684716592	-0.781852510090
H	1.744337225088	-2.744241153647	-1.928706583742
C	2.785845392256	-4.916468739373	0.491501829636
H	2.446974570882	-4.650234503523	2.610535456378
H	2.964245361099	-4.898122067421	-1.663431078466
H	3.320238101228	-5.860445340614	0.610919698065
C	3.015214971028	-0.000464819586	0.465322431372
H	3.297362915517	0.881480887399	1.063290734996
H	3.297182688107	-0.882421227013	1.063359894266
C	-1.493393930436	-2.652820430163	-0.441183152297
H	-0.832354777663	-3.421098171825	-0.875324156355
H	-2.334307481928	-2.536159220107	-1.144607961478
C	-1.492859108083	2.652740357257	-0.441357077029
H	-0.831671391344	3.420850421489	-0.875568349636
H	-2.333809586148	2.536197497202	-1.144757406864
C	-2.051602289120	-3.200346745468	0.891036782883
H	-1.225922790381	-3.337603801516	1.610406915558
H	-2.729813450165	-2.456274827896	1.343423822693
C	-2.800858014030	-4.526245068304	0.732785962661
H	-3.629308831116	-4.389088539113	0.014651326831
H	-2.123179705864	-5.270865562582	0.277681871961
C	-3.354980985251	-5.081521059793	2.046614066718
H	-2.524890284890	-5.218669755873	2.763030609358
H	-4.029582093012	-4.334500624346	2.502761770278
C	-2.050929728265	3.200481969202	0.890832141761
H	-1.225207877220	3.337626322915	1.610175269712
H	-2.729282981377	2.456582635860	1.343289745802
C	-2.799919191696	4.526520389183	0.732494778012
H	-2.122099257765	5.270967981704	0.277318743707
H	-3.628413096572	4.389476687784	0.014388317843
C	-3.353901492575	5.082010545858	2.046291664732
H	-2.523767668755	5.219046744401	2.762679770064
H	-4.028644085316	4.335162152103	2.502511808467
C	3.867982644375	-0.000602945618	-0.822974454713
H	3.613116731930	-0.882570224762	-1.435854792153
H	3.613298100624	0.881368505141	-1.435924091121
C	5.374775630448	-0.000747282300	-0.550919406729
H	5.630347329962	0.881749676984	0.062825627526
H	5.630165727266	-0.883248586484	0.062894974821
C	6.230099812934	-0.000885166948	-1.819727069368
H	5.972229434211	-0.883166938658	-2.433099674152
H	5.972410943149	0.881401380616	-2.433169082708
C	-4.104044182885	6.406393827119	1.885437387357

H	-4.935578315164	6.268811152232	1.170889835313
H	-3.430322386105	7.152273577260	1.426399590362
C	-4.655316343286	6.966233880821	3.198412416330
H	-5.328880859706	6.220922554117	3.659083467252
H	-3.824089376051	7.105752491854	3.913227142599
C	-4.105388344340	-6.405764923670	1.885846552892
H	-3.431807446484	-7.151816939152	1.426881939053
H	-4.936878774014	-6.268069652939	1.171269829568
C	-4.656802900653	-6.965390790819	3.198853104655
H	-5.330227007126	-6.219907280776	3.659450823280
H	-3.825620064354	-7.105021469383	3.913697264472
C	7.735871013401	-0.001029297278	-1.545332659935
H	7.993620317117	0.880956573290	-0.931632025351
H	7.993438808454	-0.883019864853	-0.931562575104
C	8.593610570658	-0.001167463808	-2.812396476397
H	8.337054822044	-0.883196807643	-3.426870982609
H	8.337236309916	0.880866226260	-3.426940488910
C	-5.406416160948	8.289975340444	3.036873068360
H	-6.237346934909	8.149454921177	2.323854861355
H	-4.733385701300	9.033442646398	2.575491429783
C	-5.950895349741	8.841102608166	4.355002204691
H	-6.484908185993	9.791332116253	4.207420117183
H	-6.652805894023	8.132544262882	4.821816459397
H	-5.137885101390	9.023211057991	5.075059953986
C	-5.408166634719	-8.288993061942	3.037400640460
H	-4.735276080768	-9.032632567438	2.576092462269
H	-6.239052946097	-8.148360613161	2.324352706773
C	-5.952786836724	-8.839906906351	4.355560743778
H	-6.654564738354	-8.131170161746	4.822303599639
H	-6.486988292584	-9.790040097869	4.208041174245
H	-5.139829604759	-9.022123098877	5.075651093553
C	10.099252246310	-0.001311544819	-2.537420472797
H	10.354695103326	0.879979900515	-1.923688559561
H	10.354513743239	-0.882607150217	-1.923619079365
C	10.946472154040	-0.001448901192	-3.810162976842
H	12.022310936307	-0.001550546910	-3.581117259787
H	10.736223856644	-0.889200893205	-4.426867523184
H	10.736406511294	0.886297682636	-4.426937547728

9.6 2,4,6-tribenzyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**2d**)

N	1.416734000000	0.129983000000	-0.906346000000
N	-0.833699000000	1.164254000000	-0.896982000000
N	-0.604430000000	-1.301384000000	-0.907122000000
B	0.606836000000	1.335482000000	-0.899535000000
B	0.844757000000	-1.202971000000	-0.901546000000
B	-1.473462000000	-0.139673000000	-0.901879000000
C	-1.671089000000	2.336252000000	-0.981484000000
C	-2.068407000000	2.817964000000	-2.235711000000
C	-2.087053000000	3.009378000000	0.172147000000

C	-2.867418000000	3.959298000000	-2.334052000000
H	-1.739387000000	2.293448000000	-3.135208000000
C	-2.882331000000	4.153744000000	0.072415000000
H	-1.791399000000	2.628803000000	1.150413000000
C	-3.276060000000	4.632137000000	-1.179360000000
H	-3.168375000000	4.324746000000	-3.317695000000
H	-3.198670000000	4.669311000000	0.980865000000
H	-3.898265000000	5.525443000000	-1.255237000000
C	2.848993000000	0.270009000000	-1.011068000000
C	3.443939000000	0.389360000000	-2.274149000000
C	3.659066000000	0.279889000000	0.129191000000
C	4.829942000000	0.512930000000	-2.394217000000
H	2.810051000000	0.377757000000	-3.163237000000
C	5.045661000000	0.400722000000	0.007868000000
H	3.199451000000	0.199211000000	1.114762000000
C	5.636042000000	0.517381000000	-1.252469000000
H	5.280573000000	0.602032000000	-3.384525000000
H	5.665505000000	0.406246000000	0.906199000000
H	6.719274000000	0.611618000000	-1.345369000000
C	-1.197539000000	-2.612499000000	-1.010419000000
C	-1.573726000000	-3.326545000000	0.132001000000
C	-1.409277000000	-3.181423000000	-2.273387000000
C	-2.164119000000	-4.587204000000	0.012979000000
H	-1.396944000000	-2.894121000000	1.117480000000
C	-1.995109000000	-4.443760000000	-2.391050000000
H	-1.116256000000	-2.621657000000	-3.164047000000
C	-2.377336000000	-5.150154000000	-1.247318000000
H	-2.455816000000	-5.131294000000	0.913012000000
H	-2.156748000000	-4.874099000000	-3.381226000000
H	-2.838196000000	-6.135109000000	-1.338717000000
C	1.760579000000	-2.507883000000	-0.921124000000
H	1.421732000000	-3.175677000000	-1.730399000000
H	2.793507000000	-2.223985000000	-1.183735000000
C	-3.061388000000	-0.284078000000	-0.932700000000
H	-3.464925000000	0.330138000000	-1.754816000000
H	-3.324971000000	-1.325254000000	-1.183089000000
C	1.278072000000	2.781321000000	-0.926587000000
H	2.004068000000	2.824957000000	-1.755609000000
H	0.509042000000	3.534553000000	-1.166286000000
C	-3.792147000000	0.094570000000	0.341541000000
C	-5.036741000000	0.742767000000	0.288568000000
C	-3.271721000000	-0.216436000000	1.608613000000
C	-5.736956000000	1.066159000000	1.452721000000
H	-5.459027000000	1.003418000000	-0.685203000000
C	-3.967595000000	0.102960000000	2.777484000000
H	-2.300525000000	-0.711799000000	1.683899000000
C	-5.205374000000	0.747219000000	2.705321000000
H	-6.701364000000	1.573499000000	1.380950000000
H	-3.538188000000	-0.149985000000	3.749266000000
H	-5.749714000000	1.000120000000	3.617056000000

C	1.806454000000	-3.312040000000	0.365189000000
C	1.917218000000	-4.711917000000	0.329143000000
C	1.777063000000	-2.692565000000	1.625340000000
C	2.002372000000	-5.463956000000	1.502382000000
H	1.934247000000	-5.218456000000	-0.639217000000
C	1.861777000000	-3.439223000000	2.803758000000
H	1.680025000000	-1.605848000000	1.688677000000
C	1.975997000000	-4.830244000000	2.748176000000
H	2.085714000000	-6.551241000000	1.443382000000
H	1.836383000000	-2.930232000000	3.769682000000
H	2.040684000000	-5.415743000000	3.667109000000
C	1.985720000000	3.216887000000	0.342632000000
C	3.159258000000	3.986096000000	0.279914000000
C	1.480749000000	2.899757000000	1.614423000000
C	3.803631000000	4.422316000000	1.439301000000
H	3.576314000000	4.240287000000	-0.697803000000
C	2.119288000000	3.335273000000	2.778671000000
H	0.574240000000	2.295047000000	1.698508000000
C	3.285837000000	4.099359000000	2.696911000000
H	4.716758000000	5.016140000000	1.360008000000
H	1.703914000000	3.072710000000	3.753983000000
H	3.788775000000	4.437939000000	3.604554000000

9.7 1,3,5-triphenyl-2,4,6-tris((trimethylsilyl)methyl)-1,3,5,2,4,6-triazatriborinane (**2e**)

N	0.717712343900	1.239257707977	0.117758791345
N	-1.426480599853	-0.002693599560	0.055075078943
N	0.717779814175	-1.244899382553	0.117647515236
B	-0.739507224538	1.281281565451	0.090137303613
B	1.481917257118	-0.002827644815	0.091754381522
B	-0.739491839560	-1.286706862639	0.091941495028
C	-2.858191806081	-0.003024266721	-0.084551987446
C	-3.434824263794	-0.002736990300	-1.362863750000
C	-3.697403799628	-0.003588886418	1.034997659558
C	-4.822684190576	-0.003082520903	-1.516643853669
H	-2.780710871946	-0.002163927478	-2.237162673238
C	-5.087112712213	-0.004127349384	0.881905261677
H	-3.255612029740	-0.003446987587	2.032468970120
C	-5.655436963726	-0.003835984695	-0.393742959448
H	-5.254851042077	-0.002790450643	-2.519219635890
H	-5.727101113480	-0.004637833018	1.766523109548
H	-6.740139726226	-0.004205724669	-0.512920744599
C	1.440519430833	2.480913463778	0.146359268840
C	1.529326101131	3.287512222321	-0.996558744818
C	2.079810732459	2.903441541829	1.320395293335
C	2.235988916039	4.492394640082	-0.964417726889
H	1.038331627583	2.962817992396	-1.915917419314
C	2.794650270684	4.103235154578	1.350415297903
H	2.017340540970	2.277404113166	2.212593864974
C	2.873830761521	4.904604664462	0.208409348941

H	2.292962968408	5.107819080396	-1.864370552549
H	3.287423869124	4.414304402082	2.273604701396
H	3.428826140609	5.843826150249	0.232257191101
C	1.440345666400	-2.486755117129	0.141215072333
C	2.085314375287	-2.912028234111	1.311135853841
C	1.522659475697	-3.291413070513	-1.003613427164
C	2.799236289171	-4.112567328780	1.335179638718
H	2.027938869494	-2.287848158160	2.204985876789
C	2.228277412316	-4.497013578626	-0.977395653990
H	1.027445527648	-2.964487120657	-1.919930033828
C	2.871804454727	-4.911941026378	0.191357367978
H	3.296423773198	-4.425788326446	2.255270773614
H	2.280052454637	-5.110760176755	-1.878807855980
H	3.426013530140	-5.851729938439	0.210670471550
C	3.054295544233	-0.002878007369	-0.008069229371
H	3.482191764325	-0.887486407731	0.486370115073
H	3.482051978363	0.881814782119	0.486356246487
C	-1.541614580648	-2.643515545316	0.096860867464
H	-1.007107472522	-3.413659527921	-0.480121261204
H	-2.523480413170	-2.507282683720	-0.382170508146
C	-1.541309149472	2.638322398381	0.090378081631
H	-1.004767093061	3.406829077002	-0.486937106608
H	-2.521506719423	2.501156391391	-0.391827226447
Si	-1.917628801395	3.481299671255	1.769079485377
Si	-1.910038894236	-3.481635127860	1.779617102367
Si	3.811498360908	-0.003753443443	-1.768449770586
C	-3.782024292397	3.758653115184	1.916864067083
H	-4.146736067366	4.396195682460	1.096758959382
H	-4.335565362350	2.809124333990	1.874085800514
H	-4.029736115068	4.257273060356	2.866767031000
C	-1.335244150269	2.462684496988	3.252633213898
H	-1.577324385226	2.986530509971	4.190423744851
H	-1.817784702645	1.474856968441	3.288121371733
H	-0.247348465521	2.302893435277	3.229282735154
C	-1.067571026386	5.168163875403	1.821398302543
H	0.022519972271	5.072438977286	1.709229774777
H	-1.435193085603	5.813690925283	1.008861096116
H	-1.269944420111	5.679714631771	2.775194844357
C	4.903258507550	1.525305230828	-1.974370247032
H	4.324185260555	2.450848304957	-1.838921501828
H	5.717237509859	1.525796941273	-1.233152711590
H	5.359768145432	1.550274358188	-2.976011665407
C	4.892799078293	-1.539796206541	-1.977591838999
H	5.706709815660	-1.547254232657	-1.236325644765
H	4.307696701109	-2.461839442468	-1.844081833890
H	5.349193223709	-1.565598312417	-2.979271732982
C	2.494065239003	0.002520708087	-3.125519674877
H	1.852012010099	0.893374701187	-3.061254367554
H	2.969650216201	0.002154534242	-4.118578158365
H	1.845350291626	-0.883711429219	-3.063864431475

C	-1.057928573405	-5.167510584962	1.833997611768
H	-1.428343895449	-5.816368697256	1.025387782315
H	0.031541216723	-5.070957079761	1.716677199048
H	-1.255526868556	-5.675904385650	2.790480273038
C	-3.773271325725	-3.761064246113	1.936896662271
H	-4.328809886613	-2.812810221531	1.892724650411
H	-4.140265584036	-4.402594732577	1.120935357631
H	-4.015906541002	-4.256437696704	2.889802534945
C	-1.320558337755	-2.457193353259	3.256381823079
H	-0.233144049778	-2.295338804392	3.225062202797
H	-1.804236857907	-1.469966844634	3.291679979219
H	-1.555370788652	-2.978238069209	4.197561855717

9.8 2,4,6-triisopropyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**3a**)

N	0.561445000000	1.313899000000	-0.054821000000
N	-1.419330000000	-0.170530000000	-0.055009000000
N	0.856651000000	-1.143794000000	-0.055185000000
B	-0.895429000000	1.185397000000	-0.043670000000
B	1.473733000000	0.182197000000	-0.044084000000
B	-0.579607000000	-1.368003000000	-0.044081000000
C	-2.849009000000	-0.356649000000	-0.085427000000
C	-3.506896000000	-0.548031000000	-1.308220000000
C	-3.595089000000	-0.379686000000	1.098255000000
C	-4.887983000000	-0.743390000000	-1.347214000000
H	-2.922793000000	-0.539533000000	-2.230550000000
C	-4.979365000000	-0.570833000000	1.059052000000
H	-3.083236000000	-0.253672000000	2.053719000000
C	-5.631338000000	-0.750820000000	-0.162929000000
H	-5.386164000000	-0.888147000000	-2.307735000000
H	-5.548414000000	-0.583423000000	1.990623000000
H	-6.711786000000	-0.901055000000	-0.192709000000
C	1.115234000000	2.645017000000	-0.085309000000
C	1.277577000000	3.310907000000	-1.307979000000
C	1.469511000000	3.302169000000	1.098283000000
C	1.799505000000	4.604436000000	-1.346895000000
H	0.991928000000	2.801285000000	-2.230278000000
C	1.996864000000	4.596261000000	1.059159000000
H	1.323086000000	2.795745000000	2.053725000000
C	2.166231000000	5.251262000000	-0.162716000000
H	1.922548000000	5.108630000000	-2.307310000000
H	2.271533000000	5.094854000000	1.990694000000
H	2.576873000000	6.261860000000	-0.192522000000
C	1.732995000000	-2.288650000000	-0.085373000000
C	2.126344000000	-2.922686000000	1.098489000000
C	2.228262000000	-2.762697000000	-1.307958000000
C	2.984790000000	-4.025370000000	1.059770000000
H	1.761132000000	-2.542386000000	2.053862000000
C	3.088942000000	-3.860364000000	-1.346450000000
H	1.928669000000	-2.261649000000	-2.230532000000

C	3.467397000000	-4.499829000000	-0.161981000000
H	3.280463000000	-4.511308000000	1.991566000000
H	3.463974000000	-4.219273000000	-2.306807000000
H	4.138523000000	-5.359799000000	-0.191455000000
C	3.076511000000	0.282119000000	0.039017000000
H	3.436825000000	-0.719965000000	-0.241345000000
C	3.815748000000	1.251722000000	-0.901483000000
H	3.479751000000	1.153952000000	-1.945031000000
H	3.689173000000	2.302680000000	-0.610376000000
H	4.896557000000	1.033684000000	-0.880608000000
C	3.547925000000	0.491866000000	1.495920000000
H	3.103644000000	-0.242732000000	2.184723000000
H	4.643585000000	0.387637000000	1.562188000000
H	3.290607000000	1.495591000000	1.863814000000
C	-1.783187000000	2.523545000000	0.040322000000
H	-1.095785000000	3.336534000000	-0.241026000000
C	-1.294472000000	-2.805911000000	0.039832000000
H	-2.342686000000	-2.617180000000	-0.239930000000
C	-2.993667000000	2.678989000000	-0.898618000000
H	-2.742871000000	2.435197000000	-1.942198000000
H	-3.840750000000	2.045235000000	-0.605280000000
H	-3.344078000000	3.724428000000	-0.878645000000
C	-2.198599000000	2.826909000000	1.497802000000
H	-2.657083000000	3.827444000000	1.564587000000
H	-2.937929000000	2.101496000000	1.866921000000
H	-1.339113000000	2.810429000000	2.185178000000
C	-0.824947000000	-3.931414000000	-0.900307000000
H	-0.741015000000	-3.591911000000	-1.943922000000
H	0.147973000000	-4.348135000000	-0.608672000000
H	-1.554827000000	-4.757841000000	-0.879512000000
C	-1.347299000000	-3.318213000000	1.497080000000
H	-1.984710000000	-4.215383000000	1.564315000000
H	-0.348890000000	-3.596218000000	1.864452000000
H	-1.761485000000	-2.565999000000	2.185625000000

9.9 2,4,6-tricyclohexyl-1,3,5-triphenyl-1,3,5,2,4,6-triazatriborinane (**3b**)

N	0.495855966954	1.365228351116	0.234035018952
N	-1.617340903423	0.065196386565	0.252072449518
N	0.561220163766	-1.102576171902	0.155652799468
B	-0.967271729788	1.367781611896	0.208654477727
B	1.302165549340	0.154269281794	0.219513384970
B	-0.895475129556	-1.197402655167	0.174486585123
C	-3.050981795360	0.024236405900	0.392741736860
C	-3.891471237347	-0.011948824406	-0.725175275681
C	-3.620291386748	0.020544390243	1.672827458051
C	-5.279649250438	-0.050734807701	-0.565334264985
H	-3.452518383494	-0.008441696244	-1.723786694707
C	-5.005799609924	-0.017971645389	1.833317935913
H	-2.962938104953	0.047996747538	2.543846533695

C	-5.842017975016	-0.053788752795	0.713504016406
H	-5.923300044338	-0.078303308121	-1.446706644689
H	-5.434106756966	-0.020181170074	2.837443792221
H	-6.925886340450	-0.083914689466	0.837091617537
C	1.162919464951	2.642300309455	0.277183311388
C	1.629125971906	3.247833037110	-0.895254655311
C	1.321772823106	3.312299878621	1.498165611173
C	2.260043936916	4.494348299842	-0.845967491589
H	1.484895291175	2.740375863557	-1.850486052980
C	1.947607290313	4.558660657519	1.547011730054
H	0.950267907696	2.843117947228	2.411289849131
C	2.423812151453	5.153493794809	0.374583573711
H	2.619703636349	4.953420523564	-1.768899243701
H	2.066053318651	5.066428144612	2.506149097420
H	2.914823616461	6.127337164658	0.412111456890
C	1.317446063226	-2.328888005735	0.096075207538
C	1.667275775530	-3.004849761189	1.273592814321
C	1.711264050170	-2.863256888401	-1.136469230684
C	2.396904936904	-4.193705405309	1.218113523725
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C	2.441899157772	-4.053566344504	-1.191440702022
H	1.438814981637	-2.340266971149	-2.054984096350
C	2.787573638888	-4.723489854580	-0.015438412239
H	2.661462366422	-4.708419601669	2.143834405597
H	2.741127221832	-4.458199369613	-2.160279102139
H	3.357756053239	-5.652893555279	-0.059067972064
C	2.906490062429	0.099377779935	0.235936489306
C	3.532928524777	0.317404580015	-1.166236929353
C	3.674212791032	0.940735301548	1.280272616704
H	3.147679897764	-0.948234893366	0.491605980112
C	5.031431372560	-0.011989698959	-1.172336154491
H	3.392660072802	1.367902974809	-1.471563408121
H	3.015081636081	-0.298972773743	-1.919605613125
C	5.167106148817	0.585016519070	1.285122210807
H	3.570608165485	2.014719926705	1.062997770056
H	3.247888471408	0.785345488236	2.285585292005
C	5.790648609933	0.779309425127	-0.101549097271
H	5.459202956380	0.187600967694	-2.168944366802
H	5.160824916470	-1.093299237496	-0.984873079392
H	5.700262933669	1.197892273665	2.030628979982
H	5.291280128265	-0.468475287996	1.595590693608
H	6.853098991451	0.486019842460	-0.090775593900
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C	-1.568543766902	-2.647800782013	0.031762240093
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C	-1.990006342870	-2.932276898729	-1.434815325808
H	-0.748962398207	-3.360606190627	0.232119373064
C	-3.041500751663	-4.568055713065	0.793350542159
H	-3.611181798738	-2.490661472481	0.807725242618
H	-2.412183268877	-2.898512072161	2.034693182851

C	-2.360492172503	-4.406852898189	-1.640482267805
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C	-2.101015259066	2.995139724562	-1.461566757290
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H	-0.961189244796	3.541113253966	0.242514545597
C	-2.560469389786	4.436458071689	-1.718666490853
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H	-1.244595435508	2.757710643026	-2.114911919521
C	-3.348652753462	4.607428469664	0.681792054379
H	-3.781000564314	2.498164944064	0.728264194071
H	-2.661131568853	3.013104337189	1.989336805822
C	-3.710118262567	4.840902110858	-0.789369106734
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H	-1.705915144051	5.117837548171	-1.556011542736
H	-4.204336870422	4.863791910426	1.328093425906
H	-2.523796036191	5.285939007749	0.966296931882
H	-3.983333996497	5.895529755586	-0.956776502407
H	-4.604689532091	4.241568577955	-1.038227928864

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