Supporting Information for:

“Intermolecular Insertion Reactions of Azides Into 9-Borafluorenes to Generate 9,10-B,N-Phenanthrenes”

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**EXPERIMENTAL SECTION**

**General Considerations.** All manipulations were performed under an inert atmosphere in a nitrogen-filled MBraun Unilab glove box. Solvents were purchased from commercial sources as anhydrous grade, dried further using a JC Meyer Solvent System with dual columns packed with solvent-appropriate drying agents and stored over molecular sieves. 9,9-dimethyl-9-stannafluorene and 3Ph were prepared according to the literature procedures.$^1$ 2’-2’-dibromobiphenyl was purchased from Ark Pharm, boron trichloride in hexanes (1M) from Acros Organics, triethylphosphine oxide from Alfa Aesar, dichlorophenylborane from Beantown Chemicals, azidobenzene from Enamine, and 1-azidoadamantane and phenyllithium in dibutyl ether (1.8 M) from Sigma Aldrich, respectively. All reagents were used as received. CDCl$_3$ for NMR spectroscopy was purchased from Cambridge Isotope Laboratories and dried by stirring for 3 days over CaH$_2$, distilled, and stored over 4 Å molecular sieves. Multinuclear NMR spectra were recorded on Bruker 400 or 600 MHz spectrometers. FT-IR spectra were recorded on a Bruker Alpha ATR FT-IR spectrometer on solid samples. High resolution mass spectra (HRMS) were collected at the University of Texas at Austin Mass Spectrometry Center on a Micromass Autospec Ultima spectrometer using CI. Melting points were measured with a Thomas Hoover Uni-melt capillary melting point apparatus and are uncorrected. UV-Vis spectra were recorded using an Agilent 8453 UV-Vis spectrophotometer. Fluorescence spectra were recorded on a Cary Eclipse fluorescence spectrophotometer with excitation at the absorbance $\lambda_{\text{max}}$. Solutions were prepared in a N$_2$ filled glovebox and measured in screw capped quartz cuvettes for both UV-Vis and fluorescence. Single crystal X-ray diffraction data were collected on a Bruker Apex II-CCD detector using Mo-K$_{\alpha}$ radiation ($\lambda = 0.71073$ Å). Crystals were selected under paratone oil,
mounted on micromounts, and immediately placed in a cold stream of N₂. Structures were solved and refined using SHELXTL and figures produced using OLEX2.²,³
Note: The following synthesis is adapted from the previous preparation of 3Ph by Piers and coworkers.\textsuperscript{1} In our hands, this route was higher yielding than the prior synthesis for 3Cl by going through the corresponding 9,9-dimethyl-9-stannafluorene, an air-stable intermediate, instead of the lithiation route which was found to be exceedingly sensitive.\textsuperscript{4}

Synthesis of 3Cl: A solution of 9,9-dimethyl-9-stannafluorene (2.56 g, 8.51 mmol) in toluene (50 mL) was cooled to 0°C upon which BCl\textsubscript{3} in hexanes (1 M, 8.5 mL, 8.51 mmol) was added dropwise over 10 min. The reaction mixture was then stirred for 14 h at 23°C. The volatiles were removed \textit{in vacuo} to give an orange powder. The Me\textsubscript{2}SnCl\textsubscript{2} by-product was removed by sublimation (40°C, 0.2 Torr) and the resultant yellow residue was crystallized in \textit{n}-pentane to give bright yellow crystals of 3Cl.

\textbf{Yield}: 1.24 g, 73%

\textbf{\textsuperscript{1}H NMR} (600 MHz, CDCl\textsubscript{3}): $\delta$ 7.55 (d, $J$ = 12.0 Hz, 2H), 7.38-7.34 (m, 4H), 7.15 (td, $J$ = 12.0, 6.0 Hz, 2H)

\textbf{\textsuperscript{11}B(\textsuperscript{1}H) NMR} (193 MHz, CDCl\textsubscript{3}): $\delta$ 63.8 (br)

The spectroscopic data matches the literature values.\textsuperscript{4,5}
Synthesis of 8Cl: A cold (-35 °C) solution of azidobenzene (0.152 g, 1.27 mmol) in n-pentane (2 mL) was added dropwise to a n-pentane solution (2 mL) of 3Cl (0.253 g, 1.27 mmol) and stirred for 3 h, after which the solvent was removed in vacuo. The residue was washed with hexanes (3 x 2 mL) and dried in vacuo to give 8Cl as a yellow powder. Single crystals for X-ray diffraction studies were grown from a n-pentane solution of 8Cl by vapor diffusion into toluene.

Yield: 0.272 g, 74%

m.p. 92-94°C

$^1$H NMR (400 MHz, CDCl$_3$): δ 8.54-8.41 (m, 2H), 8.39 (d, $J = 8.0$ Hz, 1H), 7.82 (td, $J = 8.0, 1.2$ Hz, 1H), 7.61-7.55 (m, 4H), 7.52-7.48 (m, 1H), 7.31-7.29 (m, 2H), 7.25-7.23 (m, 1H), 6.82-6.78 (m, 1H)

$^{13}$C{$^1$H} NMR (151 MHz, CDCl$_3$): δ 143.00, 141.95, 139.08, 135.14, 132.32, 129.97, 129.21, 128.26, 127.86, 126.99, 124.19, 123.67, 122.32, 122.22, 118.90

$^{11}$B{$^1$H} NMR (193 MHz, CDCl$_3$): δ 35.5 (br)

FT-IR (cm$^{-1}$ (ranked intensity)): 1591(12), 1481(7), 1444(9), 1363(8), 1281(15), 1259(3), 1170(11), 950(6), 752(1), 739(13), 721(4), 698(2), 598(5), 560(10), 429(14)

HRMS (Cl$^+$) for C$_{18}$H$_{13}$BCIN [M$^+$], calcd: 289.0829; found 289.0829

UV-Vis (CH$_2$Cl$_2$) $\lambda_{\text{max}}$ (329 nm): $\varepsilon = 11,100$ Lmol$^{-1}$ cm$^{-1}$, (318 nm): $\varepsilon = 7,700$ Lmol$^{-1}$ cm$^{-1}$; Fluorescence (CH$_2$Cl$_2$) $\lambda_{\text{em}}$ 352 nm; Stokes shift (CH$_2$Cl$_2$) 23 nm (2,000 cm$^{-1}$).
Synthesis of 9Ph: A solution of azidobenzene (0.145 g, 1.22 mmol) in toluene (1 mL) was added to a toluene solution (1 mL) of 3Ph (0.293 g, 1.22 mmol) and stirred for 2 d at 23°C. The solvent was removed in vacuo to yield a yellow residue. The residue was washed with n-pentane (3 x 2 mL) and dried in vacuo to give 9Ph as a yellow powder (the estimated purity by 1H NMR 90%). Single crystals for X-ray diffraction studies were grown from a dichloromethane solution of 9Ph by vapor diffusion into toluene.

**Yield:** 0.312 g, 71%

**m.p.** 120-121°C

**1H NMR** (600 MHz, C₆D₆): δ 8.31 (d, J = 12.0 Hz, 1H), 8.27 (d, J = 6.0 Hz, 1H), 7.71-7.68 (m, 2H), 7.52 (t, J = 6.0, 1H), 7.29 (t, J = 6.0, 1H), 7.24-7.19 (m, 6H), 7.16-7.15 (m, 2H), 7.09 (t, J = 6.0, 2H), 7.04-6.99 (m, 2H)

**13C{1H} NMR** (151 MHz, CDCl₃): 148.24, 138.89, 138.74, 138.48, 137.63, 133.02, 131.90, 131.41, 130.91, 129.73, 129.22, 128.49, 127.92, 127.24, 126.92, 126.53, 124.09, 123.83, 123.34, 122.93, 122.15, 121.94, 119.01, 116.49

**11B{1H} NMR** (193 MHz, CDCl₃): δ 36.9 (br)

**FT-IR** (cm⁻¹ (ranked intensity)): 1598(13), 1481(7), 1429(9), 1291(11), 1229(3), 1140(12), 1002(4), 771(8), 745(1), 718(5), 705(2), 685(6), 638(15), 564(14), 516(10)

**HRMS (Cl⁺) for C_{24}H_{18}BN₃ [M⁺], calcd 359.1593; found 359.1597**

**UV-Vis** (CH₂Cl₂) λ_{max} (319 nm): ε = 24,300 L mol⁻¹ cm⁻¹;
Fluorescence (CH$_2$Cl$_2$) $\lambda_{em}$ 357 nm; Stokes shift (CH$_2$Cl$_2$) 38 nm (3,400 cm$^{-1}$).
Synthesis of 10Cl: A solution of 1-azidoadamantane (0.026 g, 0.15 mmol) in toluene (1 mL) was added to a toluene solution (1 mL) of 3Cl (0.029 g, 0.15 mmol) in a pressure tube and heated for 2 d at 110˚C, upon which the solvent was removed in vacuo. The yellow residue was washed with acetonitrile (3 x 2 mL) and dried in vacuo to give 10 as an off-white powder. Single crystals for X-ray diffraction studies were grown from a dichloromethane solution of 10Cl by vapor diffusion into hexanes.

**Yield:** 0.028 g, 54%

**m.p.** 117-118˚C

**1H NMR** (400 MHz, CDCl₃): δ 8.22 (d, J = 8.0 Hz, 1H), 8.14 (d, J = 8.0 Hz, 1H), 8.07 (dd, J = 8.0, 1.6 Hz, 1H), 7.73-7.66 (m, 2H), 7.46 (t, J = 8.0 Hz, 1H), 7.27-7.22 (m, 1H), 7.18 (m, 1H), 2.50 (s, 6H), 2.19 (s, 3H), 1.73 (q, J = 12.0 Hz, 6H)

**13C{1H} NMR** (151 MHz, CDCl₃): δ 140.00, 139.33, 133.65, 132.05, 128.01, 126.49, 125.26, 124.75, 123.73, 121.79, 61.28, 43.14, 36.48, 30.92

**11B{1H} NMR** (193 MHz, CDCl₃): δ 40.0 (br)

**FT-IR** (cm⁻¹(rank intensity)): 2905(4), 1597(9), 1478(11), 1441(14), 1333(15), 1304(6), 1230(2), 1176(12), 1137(13), 1065(7), 948(8), 888(10), 759(5), 741(1), 616(3)

**HRMS** (Cl⁺) for C₂₂H₂₃BClN [M⁺], calcd 347.1612; found 347.1608

**UV-Vis** (CH₂Cl₂) λₘₐₓ (328 nm): ε = 3,700 Lmol⁻¹ cm⁻¹;

**Fluorescence** (CH₂Cl₂) λₑₘ 353 nm; Stokes shift (CH₂Cl₂) 25 nm (2,200 cm⁻¹).
Synthesis of 10Ph: A solution of 1-azidoadamantane (0.037 g, 0.21 mmol) in toluene (1 mL) was added to a toluene solution (1 mL) of 3Ph (0.050 g, 0.21 mmol) in a pressure tube and heated for 5 d at 110˚C, after which the solvent was removed in vacuo. The yellow residue was washed with acetonitrile (3 x 2 mL) and dried in vacuo to give 10Ph as an off-white powder. Single crystals for X-ray diffraction studies were grown from a dichloromethane solution of 10Ph by vapor diffusion into hexanes.

Yield: 0.052 g, 64%

m.p. 178-179˚C.

$^1$H NMR (600 MHz, CDCl$_3$): δ 8.26 (d, $J = 12.0$ Hz, 1H), 8.21 (d, $J = 12.0$ Hz, 1H), 8.06 (d, $J = 6.0$ Hz, 1H), 7.89 (d, $J = 12.0$ Hz, 1H), 7.65 (t, $J = 6.0$ Hz, 2H), 7.59 (d, $J = 12.0$ Hz, 2H), 7.43 (t, $J = 6.0$ Hz, 2H), 7.39-7.36 (m, 2H), 7.32 (t, $J = 6.0$ Hz, 1H), 7.22 (t, $J = 6.0$ Hz, 1H), 2.26 (s, 6H), 2.01 (s, 3H), 1.54 (q, $J = 12.0$ Hz, 6H);

$^{13}$C($^1$H) NMR (151 MHz, CDCl$_3$): δ 145.02, 141.06, 139.03, 137.10, 135.54, 132.60, 131.07, 130.40, 128.27, 127.32, 127.16, 125.92, 125.41, 124.67, 123.51, 121.63, 121.19, 61.74, 44.72, 36.38, 30.79;

$^{11}$B($^1$H) NMR (193 MHz, CDCl$_3$): δ 42.1 (br);

FT-IR (cm$^{-1}$(ranked intensity)): 2903(3), 1596(10), 1482(6), 1427(8), 1305(12), 1257(2), 1062(5), 936(14), 906(9), 785(13), 745(1), 729(7), 704(4), 632(11), 580(15);

HRMS (Cl$^+$) for C$_{28}$H$_{28}$BN [M$^+$], calcd 389.2314; found 389.2315

UV-Vis (CH$_2$Cl$_2$) $\lambda_{\text{max}}$ (331 nm): $\varepsilon = 8,200$ Lmol$^{-1}$ cm$^{-1}$;
**Fluorescence** (CH$_2$Cl$_2$) $\lambda_{em}$ 357 nm; Stokes shift (CH$_2$Cl$_2$) 26 nm (2,200 cm$^{-1}$).
Synthesis of 8Ph: To a solution of 8Cl (0.298 g, 1.03 mmol) in toluene (5 mL) was added a solution of phenyllithium in dibutyl ether (1.9 M, 0.59 mL, 1.13 mmol) at -78 °C. The reaction was stirred at this temperature for 1 h upon which the cold bath was removed and the solution warmed to 23°C and stirred 3 h. The volatiles were removed in vacuo and the resultant orange residue was washed with hexanes (3 x 10 mL), filtered, and dried in vacuo to give 8Ph as a yellow powder. Single crystals for X-ray diffraction studies were grown from a dichloromethane solution of 8Ph by vapor diffusion into toluene.

**Yield:** 0.248 g, 73%

m.p 176-178°C.

**1H NMR** (600 MHz, CDCl$_3$): δ 8.58-8.55 (m, 2H), 7.87 (d, $J = 6.0$ Hz, 1H), 7.78 (t, $J = 6.0$ Hz, 1H), 7.45 (t, $J = 6.0$ Hz, 1H), 7.33-7.30 (m, 4H), 7.25-7.24 (m, 3H), 7.18 (m, 3H), 7.13 (d, $J = 6.0$ Hz, 2H), 6.94-6.91 (m, 1H)

**13C{1H} NMR** (151 MHz, CDCl$_3$): δ 144.29, 142.00, 138.89, 137.64, 133.02, 131.42, 129.73, 129.23, 127.92, 126.96, 126.93, 126.43, 124.22, 124.09, 121.98, 121.94, 119.01

**11B{1H} NMR** (193 MHz, CDCl$_3$): δ 39.3 (br)

**FT-IR** (cm$^{-1}$ (ranked intensity)): 1594(8), 1552(13), 1483(5), 1427(10), 1352(7),1323(9), 1298(3), 1023(14), 751(2), 742(15), 724(4), 697(1), 653(11), 619(6), 577(12)

**HRMS** (Cl$^+$) for C$_{24}$H$_{18}$BN [$M^+$], calcd 331.1532; found 331.1534

**UV-Vis** (CH$_2$Cl$_2$) $\lambda_{\text{max}}$ (331 nm): $\epsilon = 12,500$ Lmol$^{-1}$ cm$^{-1}$, (319 nm): $\epsilon = 11,300$ Lmol$^{-1}$ cm$^{-1}$;

**Fluorescence** (CH$_2$Cl$_2$) $\lambda_{\text{em}}$ 355 nm; Stokes shift (CH$_2$Cl$_2$) 24 nm (2,100 cm$^{-1}$).
Figure S-1: $^1\text{H}$ NMR spectrum of $3\text{Cl}$ in CDCl$_3$. 

![NMR spectrum of 3Cl in CDCl3](image)
Figure S-2: $^{11}\text{B}^1\text{H}$ NMR spectrum of 3Cl in CDCl$_3$. 
Figure S-3: $^1$H NMR spectrum of 8Cl in CDCl$_3$. 

![NMR Spectrum of 8Cl in CDCl3](image)
Figure S-4: Expansion of $^1$H NMR spectrum of 8Cl in CDCl$_3$ (aryl region).
Figure S-5: $^{13}$C-{'H} NMR spectrum of 8Cl in CDCl$_3$. 
Figure S-6: Expansion of $^{13}$C{^1H} NMR spectrum of 8Cl in CDCl₃ (aryl region).
Figure S-7: $^{11}$B{$^1$H} NMR spectrum of 8Cl in CDCl$_3$. 
Figure S-8: FT-IR spectrum of 8Cl.
Figure S-9: $^1$H NMR spectrum of 9Ph in C$_6$D$_6$. 

![1H NMR spectrum of 9Ph in C$_6$D$_6$.]
Figure S-10: Expansion of $^1$H NMR spectrum of 9Ph in C$_6$D$_6$ (aryl region).
Figure S-11: $^{13}$C$^1$H NMR spectrum of 9Ph in CDCl$_3$. 

![NMR Spectrum](image)

**9Ph**
Figure S-12: Expansion of $^{13}$C($^1$H) NMR spectrum of 9Ph in CDCl$_3$ (aryl region).
Figure S-13: $^{11}\text{B}^{(1)}\text{H}$ NMR spectrum of 9Ph in CDCl$_3$. 
Figure S-14: FT-IR spectrum of 9Ph.
Figure S-15: $^1$H NMR spectrum of 10Cl in CDCl$_3$ (*grease).
Figure S-16: Expansion of $^1$H NMR spectrum of 10Cl in CDCl$_3$ (aryl region).
Figure S-17: $^{13}$C($^1$H) NMR spectrum of 10Cl in CDCl$_3$ (*grease).
Figure S-18: Expansion of $^{13}\text{C}^{[1\text{H}]}$ NMR spectrum of $10\text{Cl}$ in CDCl$_3$ (aryl region).
Figure S-19: $^{11}$B{$^1$H} NMR spectrum of 10Cl in CDCl$_3$. 

![NMR Spectrum](image)

10Cl
Figure S-20: FT-IR spectrum of 10Cl.
Figure S-21: $^1$H NMR spectrum of 10Ph in CDCl$_3$ (*grease).
Figure S-22: Expansion of $^1$H NMR spectrum of 10Ph in CDCl$_3$ (aryl region).
Figure S-23: $^{13}\text{C}[^1\text{H}]$ NMR spectrum of 10Ph in CDCl$_3$ (*grease).
Figure S-24: Expansion of $^{13}$C($^1$H) NMR spectrum of 10Ph in CDCl$_3$ (aryl region).
Figure S-25: $^{11}$B$^1$H NMR spectrum of 10Ph in CDCl$_3$. 
Figure S-26: FT-IR spectrum of 10Ph.
Figure S-27: $^1$H NMR spectrum of 8Ph in CDCl$_3$ (*CH$_2$Cl$_2$).
Figure S-28: Expansion of $^1$H NMR spectrum of 8Ph in CDCl$_3$ (aryl region).
Figure S-29: $^{13}$C\textsuperscript{1H} NMR spectrum of 8Ph in CDCl$_3$. 
Figure S-30: Expansion of $^{13}$C{H} NMR spectrum of 8Ph in CDCl$_3$ (aryl region).
Figure S-31: $^{11}\text{B}^{(1)}\text{H}$ NMR spectrum of 8Ph in CDCl$_3$. 

8Ph
Figure S-32: FT-IR spectrum of 8Ph.
Gutmann-Beckett Studies

For the Gutmann–Beckett studies, samples were prepared in a 1:1 stoichiometric ratio of Lewis acid/Et₃PO. Subsequent $^{31}$P{¹H} NMR spectroscopy was done in C₆D₆. Samples were prepared in a glovebox under a nitrogen atmosphere. Single crystals for X-ray diffraction studies were grown from a dichloromethane solution of the adduct by vapor diffusion into hexanes.

$^{31}$P{¹H} NMR (600 MHz, CDCl₃): δ 7.68 (d, J = 6.0 Hz, 2H), δ 7.25 (d, J = 6.0 Hz, 1H), 7.11-7.00 (m, 12H), 6.91-6.86 (m, 8H), 6.79 (t, J = 6.0 Hz, 2H), 1.72 (dq, J = 18.0, 6.0 Hz, 6H), 1.04 (dt, J = 18.0, 6.0 Hz, 9H)

$^{31}$P{¹H} NMR (243 MHz, C₆D₆): δ 76.6 (br)

$^{11}$B{¹H} NMR (193 MHz, C₆D₆): δ 7.4 (br)

$^{1}$H NMR (600 MHz, CDCl₃): δ 7.84 (d, J = 6.0 Hz, 2H), 7.81 (d, J = 6.0 Hz, 2H), 7.67 (d, J = 6.0 Hz, 2H), 7.42-7.39 (m, 2H), 7.35-7.32 (m, 2H), 7.27-7.23 (m, 3H), 0.85-0.82 (m, 6H), 0.40-0.28 (m, 9H)

$^{31}$P{¹H} NMR (243 MHz, C₆D₆): δ 74.1 (br)

$^{11}$B{¹H} NMR (193 MHz, C₆D₆): δ 6.0 (br)
Figure S-33: $^1$H NMR spectrum of 1Ph·OPEt$_3$ in CDCl$_3$ (CH$_2$Cl$_2$).
Figure S-34: Expansion of $^1$H NMR spectrum of 1Ph·OPEt$_3$ in CDCl$_3$ ($^*_{\text{CH}_2\text{Cl}_2}$ aryl region).
Figure S-35: $^{31}$P NMR spectrum of $\text{1Ph-OPe}_3$ in $\text{C}_6\text{D}_6$. 
Figure S-36: $^{11}$B($^1$H) NMR spectrum of $1$Ph·OPEt$_3$ in C$_6$D$_6$. 

$1$Ph·OPEt$_3$
Figure S-37: $^1$H NMR spectrum of 3Ph$^\text{OP}$$\text{Et}_3$ in C$_6$D$_6$. 

3Ph$^\text{OP}$$\text{Et}_3$
Figure S-38: Expansion of $^1$H NMR spectrum of 3Ph·OPe₃ in C₆D₆ (aryl region).
Figure S-39: $^{31}$P NMR spectrum of 3Ph·OPEt$_3$ in C$_6$D$_6$. 
Figure S-40: $^{11}$B{H} NMR spectrum of $3\text{Ph}^\cdot\text{OPEt}_3$ in C$_6$D$_6$. 

![NMR spectrum of 3Ph·OPEt₃ in C₆D₆.](image)

3Ph·OPEt₃
UV-Vis and Fluorescence Studies

Figure S-41: Normalized absorption spectra of 8Cl, 8Ph, 9Ph, 10Cl, and 10Ph, in CH₂Cl₂ under an N₂ atmosphere (spectra have their respective λ<sub>max</sub> listed above their respective peaks).
Figure S-42: Normalized emission spectra of **8Cl**, **8Ph**, **9Ph**, **10Cl**, and **10Ph** in CH$_2$Cl$_2$ under an N$_2$ atmosphere (all emission spectra excited at their respective $\lambda_{\text{max}}$ and correspondingly labeled).
X-ray crystallographic details

Table S-1: Crystallographic data for 8-10, 1Ph·OPEt<sub>3</sub>, and 3Ph·OPEt<sub>3</sub>.

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<th>Compounds</th>
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<th>9Ph</th>
<th>10Cl</th>
<th>10Ph</th>
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<td>C&lt;sub&gt;28&lt;/sub&gt;H&lt;sub&gt;28&lt;/sub&gt;BN</td>
<td>C&lt;sub&gt;24&lt;/sub&gt;H&lt;sub&gt;18&lt;/sub&gt;BN</td>
<td>C&lt;sub&gt;40&lt;/sub&gt;H&lt;sub&gt;40&lt;/sub&gt;BOP</td>
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<td>P21/c</td>
<td>P21/c</td>
<td>I41/a</td>
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</tr>
<tr>
<td>V (Å&lt;sup&gt;3&lt;/sup&gt;)</td>
<td>1462.5(2)</td>
<td>909.5(2)</td>
<td>1751.1(3)</td>
<td>2112.6(3)</td>
<td>7122.0(13)</td>
<td>3146.2(2)</td>
<td>2108.8(3)</td>
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<tr>
<td>Z</td>
<td>4</td>
<td>2</td>
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<td>4</td>
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<td>D&lt;sub&gt;c&lt;/sub&gt; (mg m&lt;sup&gt;-3&lt;/sup&gt;)</td>
<td>1.315</td>
<td>1.312</td>
<td>1.319</td>
<td>1.224</td>
<td>1.236</td>
<td>1.221</td>
<td>1.179</td>
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<td>Radiation, λ (Å)</td>
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<tr>
<td>Temp (K)</td>
<td>150(2)</td>
<td>150(2)</td>
<td>150(2)</td>
<td>150(2)</td>
<td>150(2)</td>
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<tr>
<td>R&lt;sub&gt;1&lt;/sub&gt;[I &gt; 2σ(I)]&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.0481</td>
<td>0.0640</td>
<td>0.0433</td>
<td>0.0499</td>
<td>0.0928</td>
<td>0.0445</td>
<td>0.0492</td>
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<tr>
<td>wR&lt;sub&gt;2&lt;/sub&gt;(F&lt;sup&gt;2&lt;/sup&gt;)&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.1053</td>
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<td>0.1221</td>
<td>0.1109</td>
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<tr>
<td>GOF (S)&lt;sup&gt;a&lt;/sup&gt;</td>
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<td>1.153</td>
<td>1.147</td>
<td>1.042</td>
<td>1.221</td>
<td>1.110</td>
<td>1.025</td>
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<sup>a</sup> R<sub>1</sub>[I > 2σ(I)] = Σ||F<sub>o</sub>| - |F<sub>c</sub>||/ Σ |F<sub>o</sub>; wR<sub>2</sub>(F<sup>2</sup>) [all data] = [w(F<sub>o</sub><sup>2</sup> - F<sub>c</sub><sup>2</sup>)<sup>2</sup>]<sup>1/2</sup>; S(all data) = [w(F<sub>o</sub><sup>2</sup> - F<sub>c</sub><sup>2</sup>)<sup>2</sup>]/(n - p)<sup>1/2</sup> (n = no. of data; p = no. of parameters varied; w = 1/[2(F<sub>o</sub><sup>2</sup> + (aP)<sup>2</sup> + bP)] where P = (F<sub>o</sub><sup>2</sup> + 2F<sub>c</sub><sup>2</sup>)/3 and a and b are constants suggested by the refinement program.
Figure S-43: Solid-state structure of 8Ph. Thermal ellipsoids are drawn at the 50% probability level and hydrogen atoms have been omitted for clarity.

Note: Similar boron heterocycles bearing phenyl groups on boron and nitrogen atoms within the ring have shown disorder. Therefore, the bond distances and bond angles are not discussed in detail. However, the structure confirms the identity of 8Ph. The disorder was modeled using EADP on both boron and nitrogen atoms.
Figure S-44: Solid-state structures of 1Ph·OPEt₃ and 3Ph·OPEt₃. Thermal ellipsoids are drawn at the 50% probability level and hydrogen atoms have been omitted for clarity.
References


