

**Generation of a series of B<sub>n</sub> fused oligo-naphthalenes (n = 1 to 3) from a B<sub>1</sub>-Polycyclic Aromatic Hydrocarbon.**

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## General Considerations

Unless otherwise stated, all manipulations were carried out using standard Schlenk techniques under argon, or in a MBraun UniLab glovebox, under an atmosphere of argon (< 0.1 ppm O<sub>2</sub>/H<sub>2</sub>O). All solvents were distilled from appropriate drying agents: dichloromethane (CaH<sub>2</sub>); 1,2-dichloroethane (CaH<sub>2</sub>); THF (potassium); toluene (potassium); and triethylamine (CaH<sub>2</sub>). All solvents were stored over 3 Å molecular sieves with the exception of toluene, which was stored over a potassium mirror. Unless otherwise stated all compounds were purchased from commercial sources and used as received. Solvents for column chromatography were of technical grade and used without further purification. Column chromatography was performed on silica gel (230-400 mesh).

NMR spectra were recorded on Bruker AvanceIII-400, Bruker AvanceII-500 or Bruker Ascend-400 spectrometers. Chemical shifts are reported as dimensionless  $\delta$  values and are frequency referenced relative to residual protio impurities in the NMR solvents for <sup>1</sup>H and <sup>13</sup>C{<sup>1</sup>H}, while <sup>11</sup>B shifts are referenced relative to external BF<sub>3</sub>-etherate. Coupling constants J are given in Hertz (Hz) as positive values regardless of their real individual signs. The multiplicity of the signals are indicated as “s”, “d”, “t”, “q”, “pent”, “sept” or “m” for singlet, doublet, triplet, quartet, pentet, septet or multiplet, respectively. Broad features in the <sup>11</sup>B NMR spectra are due to boron present in borosilicate glass. Carbon atoms directly bonded to boron are not always observed in the <sup>13</sup>C{<sup>1</sup>H} NMR spectra due to quadrupolar relaxation leading to signal broadening.

GCMS analysis was performed on an Agilent Technologies 7890A GC system equipped with an Agilent Technologies 5975C inertXL EI/CI MSD with triple axis detector. The column employed was an Agilent J&W HP-5ms ((5%-Phenyl)-methylpolysiloxane) of dimensions: length, 30 m; internal diameter, 0.250 mm; film, 0.25  $\mu$ m. MALDI-TOF analyses were performed using a Shimadzu Axima Confidence spectrometer using a 4k PPG as a calibration reference. 1  $\mu$ L of a solution of dopant NaI in THF (10 mg mL<sup>-1</sup>) was spotted onto a well of the MALDI plate and the solvent left to evaporate. Solutions were made up to 10 mg mL<sup>-1</sup> in DCM. A solution of matrix dithranol was made up to 10 mg mL<sup>-1</sup> in THF. 2  $\mu$ L of sample solution and 20  $\mu$ L of matrix solution were thoroughly mixed and 1  $\mu$ L of this solution was spotted onto a well with no dopant and 1  $\mu$ L spotted by a layered method with the NaI. The solvent was allowed to evaporate before being placed in the spectrometer. Samples were run in positive polarity mode in either linear or reflection mode. High resolution mass spectra (HRMS) were recorded on a Waters QTOF mass spectrometer.

Cyclic voltammetry was performed using a CH-Instrument 1110C Electrochemical/Analyzer potentiostat under a nitrogen flow. Measurements were made using a 1 mM analyte solution with 0.1 M tetra<sup>n</sup>butylammonium hexafluorophosphate (Fluka  $\geq$ 99.0 %) as the supporting electrolyte in THF that had been dried and degassed prior to use and obtained from a dry solvent system. A glassy carbon electrode served as the working electrode and a platinum wire as the counter electrode. An Ag/AgNO<sub>3</sub> non-aqueous reference electrode was used. All scans were calibrated against the ferrocene/ferrocenium (Fc/Fc<sup>+</sup>) redox couple, which in this work is taken to be 4.8 eV below vacuum.<sup>1</sup> The half-wave potential of the ferrocene/ferrocenium (Fc/Fc<sup>+</sup>) redox couple ( $E_{1/2, Fc, Fc^+}$ ) was estimated from  $E_{1/2, Fc, Fc^+} = (E_{ap} + E_{cp})/2$ , where  $E_{ap}$  and  $E_{cp}$  are the anodic and cathodic peak potentials, respectively.

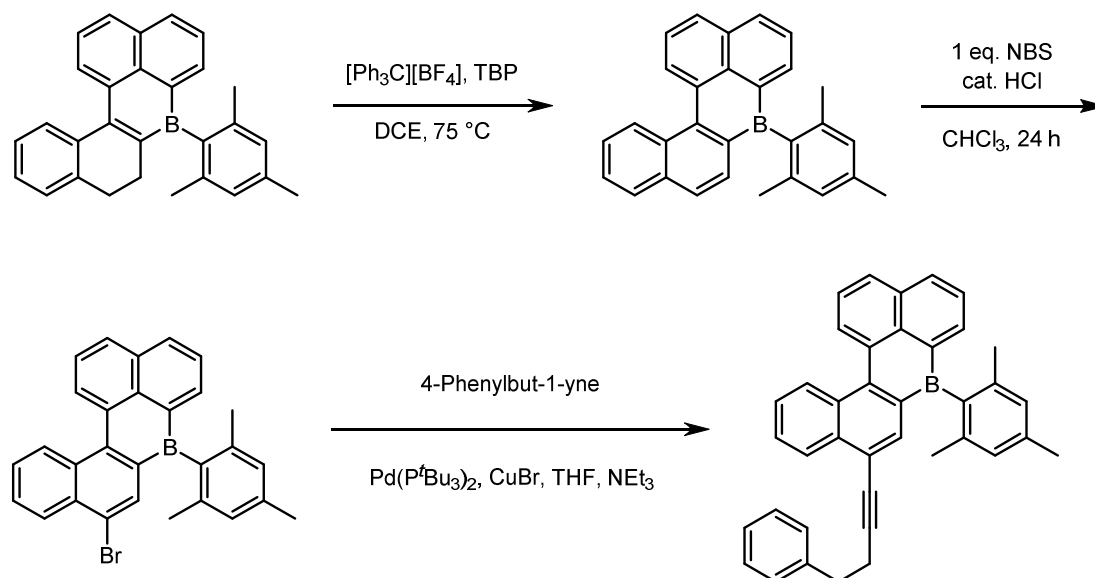
All calculations were performed using the Gaussian09 series of programs.<sup>2</sup> Geometries were optimized with the DFT method using M06-2X functional<sup>3</sup> and 6-311G(d,p) as a basis set. All geometry optimizations were full, with no restrictions. In all cases, structures were confirmed as minima by frequency analysis and the absence of imaginary frequencies. Solvent effects of the dichloromethane were introduced using the self-consistent field approach, by means of the integral equation formalism polarizable continuum model (IEFPCM).<sup>4</sup> Full Cartesian coordinates and energies of the optimised structures are provided below.

## Synthetic Procedures

Compounds **G** and **H** were prepared according to literature methods.<sup>5</sup>

Note, the separation of **G** and **1** from Ph<sub>3</sub>CH can be problematic on scale resulting in significantly lower yields, therefore in the reactions reported herein Ph<sub>3</sub>CH is not separated from **G** or **1**. In contrast **2** can be readily separated from Ph<sub>3</sub>CH by column chromatography.

### Synthesis of 9-bromo-7-mesityl-7H-dinaphtho[1,8-bc:1',2'-e]borinine (**2**)



To a mixture of **H** (0.631 g, 1.64 mmol), tri-*tert*-butylpyridine (0.814 g, 3.29 mmol) and trityl tetrafluoroborate (1.085 g, 3.29 mmol) was added dry 1,2-dichloroethane (15 mL) to give a dark brown suspension which was refluxed at 75 °C for 24 hours. Once cool all volatiles were removed *in vacuo* and the residue containing **2** and triphenylmethane (generated as a side product from trityl tetrafluoroborate) was taken up in 50:50 DCM:Hexane and filtered through a silica plug. NMR spectroscopy confirmed full conversion of **H** to **G**.

In a 100 mL round-bottomed flask crude **G** and a small excess of N-bromosuccinimide (0.380 g, 2.14 mmol) were dissolved in wet chloroform (20 mL) and catalytic HCl (60 μL, 1.0 M in diethyl ether, 0.06 mmol) was added. The golden solution darkens slightly and was stirred at ambient temperature for 18 hours. Volatiles were removed *in vacuo* and the residue was taken up in hexane and filtered. NMR spectroscopy confirmed >95% conversion of **G** to **1** (minor double bromination product also observed, with meta C-H mesityl bromination at ca. 5% in addition).

In a Schlenk crude **1** was taken up in THF (15 mL) and triethylamine (4 mL). To the solution was added CuBr (7 mg, 0.05 mmol) and bis(tri-*tert*-butylphosphine)palladium(0) (13 mg, 0.025 mmol) to give a yellow solution. Under argon flow was added 4-phenylbut-1-yne (0.50 mL, 3.6 mmol) to form a bright yellow solution which darkens to red/black within 5 minutes. The mixture was stirred at ambient temperature for 72 hours after which NMR spectroscopy revealed full conversion **2**. The product was purified by flash column chromatography using a DCM:petrol eluent (10:90) to yield analytically pure product **2** at R<sub>f</sub> = 0.24 as a yellow solid (0.540 g, 1.06 mmol, 64% with respect to **1**).

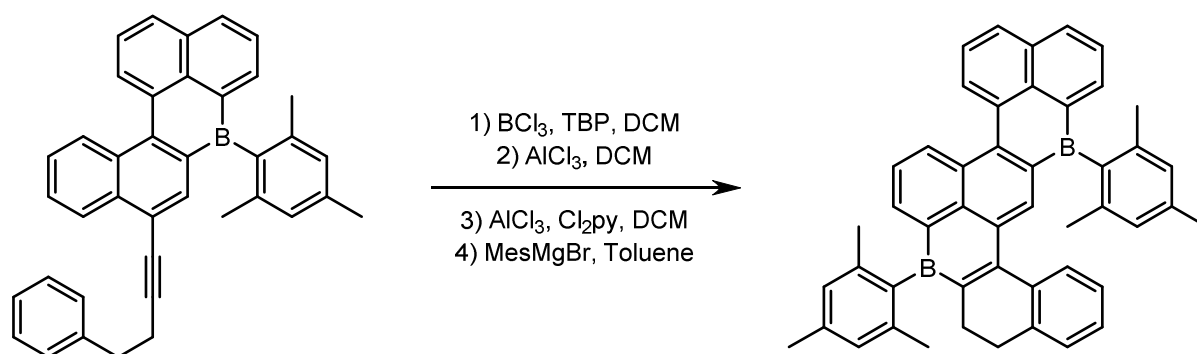
Data for **1** / Ph<sub>3</sub>CH mixture:

<sup>1</sup>H NMR (400MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ = 8.71 (d, 8.3 Hz, 1H), 8.59 (dd, 7.5, 1.2 Hz, 1H), 8.49 (dd, 8.5, 1.5 Hz, 1H), 8.36 (dd, 8.1, 1.5 Hz, 1H), 8.25 (dd, 6.8, 1.5 Hz, 1H), 8.16 (dd, 8.2, 1.2 Hz, 1H), 8.15 (s, 1H), 7.86 – 7.64 (m, 4H), 7.38 – 7.15 (m, 15H, Ph<sub>3</sub>CH aromatic H), 7.03 (s, 2H), 5.61 (s, 1H, Ph<sub>3</sub>C-H), 2.49 (s, 3H), 2.04 (s, 6H). <sup>11</sup>B NMR (128MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ = 57.9 (ν<sub>2</sub> = 1858 Hz). <sup>13</sup>C{<sup>1</sup>H} NMR (101MHz, CDCl<sub>3</sub>) δ = 143.6, 142.0, 138.9, 137.0, 136.4, 136.0, 135.8, 134.2, 132.6, 132.2, 131.9, 131.3, 131.0, 130.8, 128.4, 127.5, 127.1, 126.4, 126.3, 125.2, 122.1, 23.4, 21.3.

Data for **2**: <sup>1</sup>H NMR (400MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ = 8.67 (m, 1H), 8.59 (dd, 7.4, 1.4 Hz, 1H), 8.38 – 8.31 (m, 2H), 8.17 – 8.11 (m, 2H), 7.84 (s, 1H), 7.80 (dd, 8.0 Hz, 7.6 Hz, 1H), 7.73 (dd, 8.0 Hz, 6.8 Hz, 1H), 7.69-7.63 (m, 2H), 7.35-7.27 (m, 4H), 7.23 (m, 1H), 6.99 (s, 2H), 3.00 (t, 7.2 Hz, 2H), 2.86 (t, 7.1 Hz, 2H), 2.43 (s, 3H), 1.96 (s, 6H). <sup>11</sup>B NMR (128MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ = 58.4 (ν<sub>2</sub> = 1727 Hz). <sup>13</sup>C{<sup>1</sup>H} NMR (101MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ = 144.1, 142.2, 141.3, 139.3, 137.8, 137.5, 137.1, 136.9, 134.7, 133.2, 132.6, 132.0, 131.3, 131.3, 131.0, 129.2, 128.9, 128.3, 127.5, 127.1, 126.9, 126.9, 126.6, 125.8, 120.4, 95.7, 80.1, 35.6, 23.7, 22.5, 21.6. HRMS (APCI) Calculated for C<sub>39</sub>H<sub>32</sub>B<sup>+</sup> ([M+H]<sup>+</sup>) 511.2592. Found 511.2584.

Note present in **2** is a ca. 5% impurity derived from the bromination at the meta mesityl C-H position

#### Synthesis of **4**

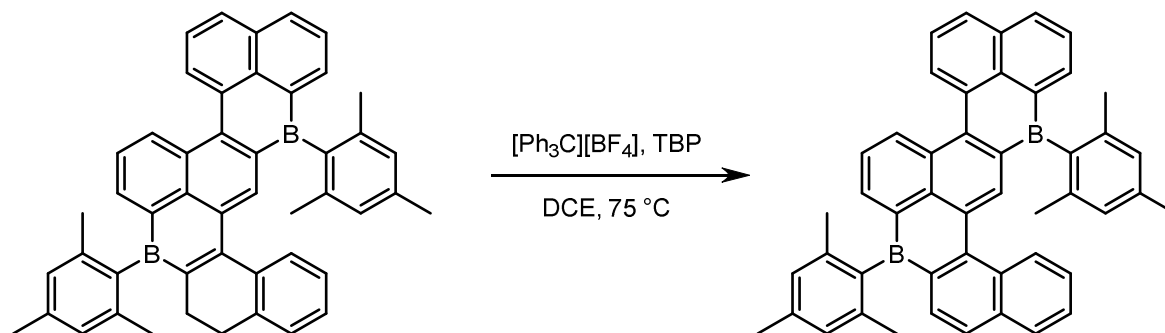


A Schlenk was charged with **2** (0.155 g, 0.303 mmol) and tri-*tert*-butylpyridine (78.8 mg, 0.318 mmol) and then dry DCM was added (4 mL) and BCl<sub>3</sub> (0.45 mL, 1.0 M in DCM, 0.45 mmol) to give a yellow solution. This was stirred at ambient temperature for 1 hour then all volatiles were removed *in vacuo*. To the residue was added AlCl<sub>3</sub> (43 mg, 0.32 mmol) and DCM (4 mL) to give a green solution which changes to yellow then orange within 5 minutes. The mixture was stirred at ambient temperature for 20 minutes then all volatiles were removed *in vacuo*. To the residue was added AlCl<sub>3</sub> (43 mg, 0.32 mmol), 2,6-dichloropyridine (48 mg, 0.32 mmol) and DCM (4 mL) to give a dark orange suspension. The mixture was stirred at ambient temperature for 1 hour then all volatiles were removed *in vacuo*. The residue was taken up in toluene (3 mL) and MesMgBr (3.0 mL, 1.0 M in THF, 3.0 mmol) was added dropwise to give an orange suspension. The mixture was stirred at ambient temperature for 18 hours then all volatiles were removed *in vacuo*. The product was purified by flash column chromatography using a DCM:petrol eluent (7:93 to 15:85) to yield analytically pure product **4** (at R<sub>f</sub> = 0.21 in 15:85 DCM:petrol) as an orange solid (0.144 g, 0.225 mmol, 74% with respect to **2**).

<sup>1</sup>H NMR (400MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ = 8.94 (dd, 8.4 Hz, 1.4 Hz, 1H), 8.49 (s, 1H), 8.46 (dd, 7.5 Hz, 1.1 Hz, 1H), 8.41 (dd, 8.0 Hz, 1.4 Hz, 1H), 8.22 (dd, 8.2 Hz, 1.1 Hz, 1H), 8.19 (ddd, 6.9 Hz, 2.5 Hz, 1.4 Hz, 2H), 7.90 (dd, 7.8 Hz, 7.5 Hz, 1H), 7.83 (dd, 8.4 Hz, 6.8 Hz, 1H), 7.78 (dd, 8.1 Hz, 6.8 Hz, 1H), 7.53 (dd, 7.7 Hz, 1.4 Hz, 1H), 7.33 (dd, 7.5 Hz, 1.7 Hz, 1H), 7.29 (td, 7.3 Hz, 1.4 Hz, 1H), 7.23 (dd, 7.4 Hz, 1.8 Hz, 1H), 6.93 (s, 2H), 6.91 (s, 2H), 2.74 (dd, 7.6 Hz, 6.9 Hz, 2H), 2.47 (dd, 7.6 Hz, 6.8 Hz, 2H), 2.37 (s, 3H), 2.33 (s, 3H), 2.06 (s, 6H), 2.04 (s, 6H). <sup>11</sup>B NMR (128MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ = 59.4 (ν<sub>2</sub> = 2367 Hz). <sup>13</sup>C{<sup>1</sup>H} NMR

(101MHz, CD<sub>2</sub>Cl<sub>2</sub>)  $\delta$  = 152.3, 147.5, 142.8, 142.5, 142.5, 140.4, 139.3, 138.9, 138.9, 137.7, 137.6, 137.0, 136.0, 134.9, 133.3, 132.6, 132.6, 131.8, 131.5, 130.2, 129.7, 128.6, 127.9, 127.5, 127.4, 127.1, 126.3, 126.3, 126.0, 29.6, 28.3, 23.7, 23.3, 21.5. Two carbon resonances cannot be observed due to overlap. HRMS (APCI) Calculated for C<sub>48</sub>H<sub>41</sub>B<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>) 639.3389. Found 639.3371.

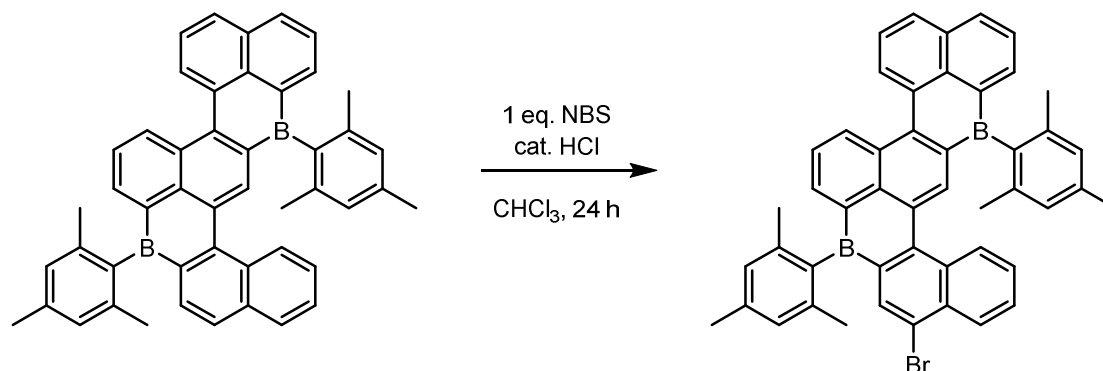
### Synthesis of 5



A Schlenk was charged with **4** (0.208 g, 0.326 mmol), tri-*tert*-butylpyridine (0.159 g, 0.643 mmol) and trityl tetrafluoroborate (0.215 g, 0.651 mmol) and dry 1,2-dichloroethane (15 mL) was added to give a bright orange solution which was refluxed at 75 °C for 24 hours. All volatiles were removed *in vacuo* and the product was purified by flash column chromatography using a petrol then 18:82 DCM:Petrol eluent to yield analytically pure product **5** (at R<sub>f</sub> = 0.46 in 18:82 DCM:petrol) as an orange solid (0.201 g, 0.316 mmol, 97% with respect to **4**).

<sup>1</sup>H NMR (400MHz, CD<sub>2</sub>Cl<sub>2</sub>)  $\delta$  = 9.04 (dd, 8.4 Hz, 1.4 Hz, 1H), 8.71 (s, 1H), 8.61 (d, 8.7 Hz, 1H), 8.54 (dd, 7.4 Hz, 1.2 Hz, 1H), 8.43 (dd, 8.1 Hz, 1.5 Hz, 1H), 8.30 – 8.22 (m, 3H), 7.92 (m, 2H), 7.86 (dd, 8.4 Hz, 6.8 Hz, 1H), 7.81 (dd, 8.1 Hz, 6.7 Hz, 1H), 7.77 (d, 1.4 Hz, 2H), 7.60 (ddd, 8.1 Hz, 6.8 Hz, 1.2 Hz, 1H), 7.49 (8.4 Hz, 6.8 Hz, 1.4 Hz, 1H), 6.98 (s, 2H), 6.92 (s, 2H), 2.41 (s, 3H), 2.32 (s, 3H), 2.11 (s, 6H), 2.00 (s, 6H). <sup>11</sup>B NMR (128MHz, CD<sub>2</sub>Cl<sub>2</sub>)  $\delta$  = 61.2 ( $\nu_{1/2}$  = 1691 Hz). <sup>13</sup>C{<sup>1</sup>H} NMR (101MHz, CD<sub>2</sub>Cl<sub>2</sub>)  $\delta$  = 146.9, 144.8, 142.6, 142.5, 140.8, 139.4, 139.4, 139.2, 138.2, 137.6, 137.4, 137.1, 137.1, 137.0, 133.3, 133.1, 132.6, 132.5, 131.7, 131.3, 130.7, 130.4, 130.3, 128.7, 127.9, 127.5, 127.5, 127.2, 127.1, 126.4, 126.3, 125.9, 23.7, 23.7, 21.6, 21.5. HRMS (APCI) Calculated for C<sub>48</sub>H<sub>39</sub>B<sub>2</sub><sup>+</sup> ([M+H]<sup>+</sup>) 637.3232. Found 637.3221.

### Synthesis of 6



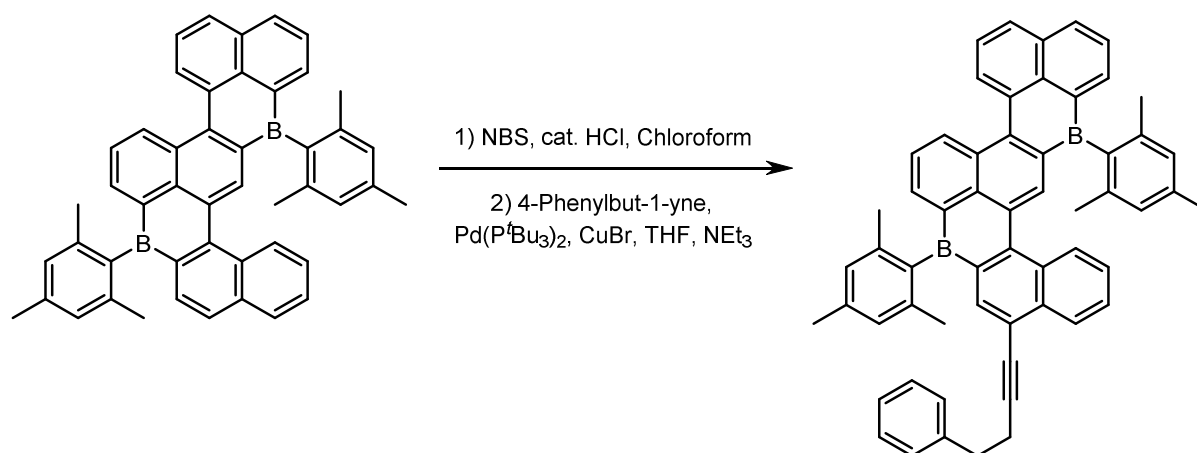
In a 100 mL round-bottomed flask **5** (90 mg, 0.14 mmol) and N-bromosuccinimide (26 mg, 0.15 mmol) were dissolved in wet chloroform (25 mL) and catalytic HCl (30  $\mu$ L, 1.0 M in diethyl ether, 0.03

mmol) was added. The mixture was stirred at ambient temperature for 18 hours then volatiles were removed *in vacuo*. The product was extracted in hexane and filtered through glass wool to give an orange solution. The product was purified by flash column chromatography using a DCM:petrol eluent (7:93 to 20:80) to yield product **6** (at  $R_f = 0.68$  in 20:80 DCM:petrol) as an orange solid (70 mg, 0.098 mmol, 70% with respect to **5**).

A minor amount ca. 5% of bromination at the mesityl meta C-H position is again observed.

$^1\text{H}$  NMR (400MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta = 9.06$  (dd, 8.3 Hz, 1.5 Hz, 1H), 8.65 (s, 1H), 8.62 (d, 8.7 Hz, 1H), 8.54 (dd, 7.7 Hz, 1.2 Hz, 1H), 8.44 (dd, 8.1 Hz, 1.5 Hz, 1H), 8.39 (dd, 8.7 Hz, 1.2 Hz, 1H), 8.31 (dd, 6.9 Hz, 1.4 Hz, 1H), 8.26 (m, 2H), 8.04 (s, 1H), 7.94 (dd, 8.2 Hz, 7.8 Hz, 1H), 7.89 (dd, 8.4 Hz, 6.9 Hz, 1H), 7.82 (dd, 8.0 Hz, 6.7 Hz, 1H), 7.74 (ddd, 8.3 Hz, 6.7 Hz, 1.2 Hz, 1H), 7.57 (ddd, 8.4 Hz, 6.8 Hz, 1.4 Hz, 1H), 7.01 (s, 2H), 6.93 (s, 2H), 2.44 (s, 3H), 2.32 (s, 3H), 2.11 (s, 6H), 2.02 (s, 6H).  $^{11}\text{B}$  NMR (128MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta = 57.8$  ( $\nu_{1/2} = 2982$  Hz).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta = 147.4, 144.8, 142.9, 142.7, 141.5, 139.8, 139.4, 139.2, 137.7, 137.6, 137.2, 137.1, 137.0, 136.5, 136.1, 133.4, 132.9, 132.5, 132.4, 131.9, 131.4, 130.3, 129.8, 129.3, 127.7, 127.6, 127.5, 127.2, 126.6, 126.6, 126.3, 122.4, 23.8, 23.7, 21.6, 21.5$ . HRMS (APCI) Calculated for  $\text{C}_{48}\text{H}_{38}\text{B}_2\text{Br}^+$  ( $[\text{M}+\text{H}]^+$ ) 715.2338. Found 715.2370.

### Synthesis of **7**

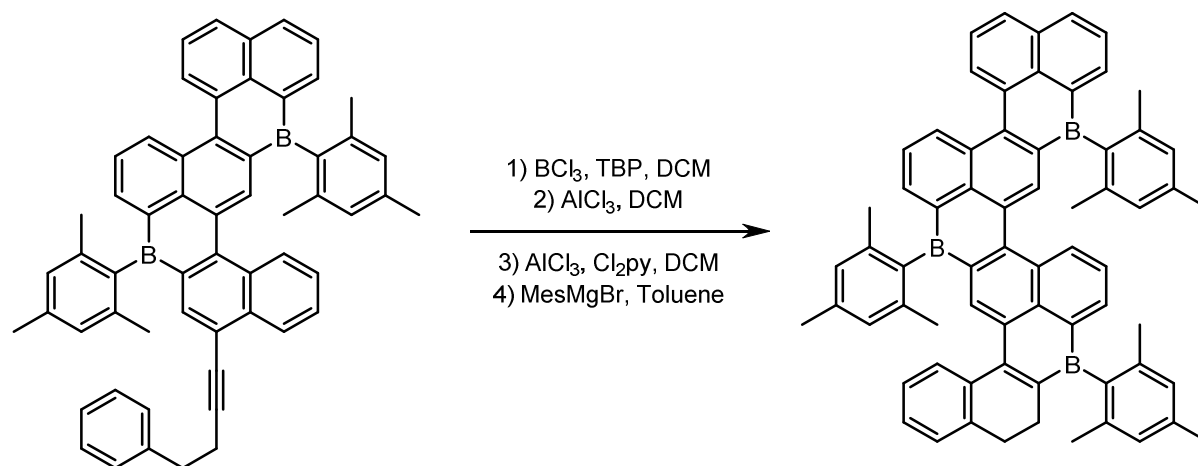


In a 100 mL round-bottomed flask **5** (0.200 g,  $3.15 \times 10^{-4}$  mol) and N-bromosuccinimide (77.0 mg,  $4.33 \times 10^{-4}$  mol) were dissolved in wet chloroform (15 mL) and catalytic HCl (30  $\mu\text{L}$ , 1.0 M in diethyl ether, 0.03 mmol) was added. The orange solution was stirred at ambient temperature for 18 hours. Volatiles were removed *in vacuo* and the residue was taken up in hexane and filtered. NMR spectroscopy confirmed full conversion of **5** to **6**. In a Schlenk crude **6** was taken up in THF (10 mL) and triethylamine (3 mL). To the solution was added CuBr (4 mg,  $3 \times 10^{-5}$  mol) and bis(*tri-tert*-butylphosphine)palladium(0) (6 mg,  $1 \times 10^{-5}$  mol) to give an orange solution. Under argon flow was added 4-phenylbut-1-yne (0.25 mL, 1.8 mmol) to form a dark red solution. The mixture was heated to 60  $^\circ\text{C}$  for 48 hours after which TLC revealed full consumption of **6**. The product was purified by flash column chromatography using a DCM:petrol eluent (12:88 to 20:80) to yield analytically pure product **7** (at  $R_f = 0.34$  in 20:80 DCM:petrol) as a red solid (70.4 mg,  $9.21 \times 10^{-5}$  mol, 29% with respect to **5**).

$^1\text{H}$  NMR (400MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta = 9.03$  (dd, 8.4, 1.3 Hz, 1H), 8.66 (s, 1H), 8.59 (d, 8.6 Hz, 1H), 8.52 (d, 7.4 Hz, 1H), 8.42 (dd, 8.1, 1.3 Hz, 1H), 8.31 – 8.21 (m, 4H), 7.91 (dd, 7.8, 7.4 Hz, 1H), 7.87 (s, 1H), 7.86 (dd, 8.4, 6.7 Hz, 1H), 7.80 (dd, 8.0, 6.8 Hz, 1H), 7.62 (ddd, 8.1, 6.7, 1.1 Hz, 1H), 7.51 (ddd, 8.4, 6.7, 1.3 Hz, 1H), 7.36 – 7.19 (m, 5H), 7.02 (s, 2H), 6.93 (s, 2H), 2.99 (t, 7.2 Hz, 2H), 2.85 (t, 7.2 Hz, 2H), 2.45 (s, 3H), 2.33 (s, 3H), 2.11 (s, 6H), 2.01 (s, 6H).  $^{11}\text{B}$  NMR (128MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta = 62.1$  ( $\nu_{1/2} = 3006$  Hz).  $^{13}\text{C}\{^1\text{H}\}$

NMR (101MHz, CD<sub>2</sub>Cl<sub>2</sub>)  $\delta$  = 147.1, 144.6, 142.6, 141.3, 141.3, 140.6, 139.7, 139.6, 139.4, 139.2, 137.6, 137.6, 137.5, 137.2, 137.1, 137.1, 135.3, 135.0, 134.8, 134.4, 133.3, 132.5, 132.4, 131.8, 131.1, 131.0, 130.3, 130.0, 129.3, 128.9, 128.4, 127.5, 127.5, 127.2, 127.0, 126.8, 126.5, 126.3, 126.2, 120.4, 95.7, 80.2, 35.6, 23.7, 23.6, 22.6, 21.6, 21.6. HRMS (APCI) Calculated for C<sub>58</sub>H<sub>46</sub>B<sub>2</sub>K<sup>+</sup> ([M+K]<sup>+</sup>) 803.3417. Found 803.3387.

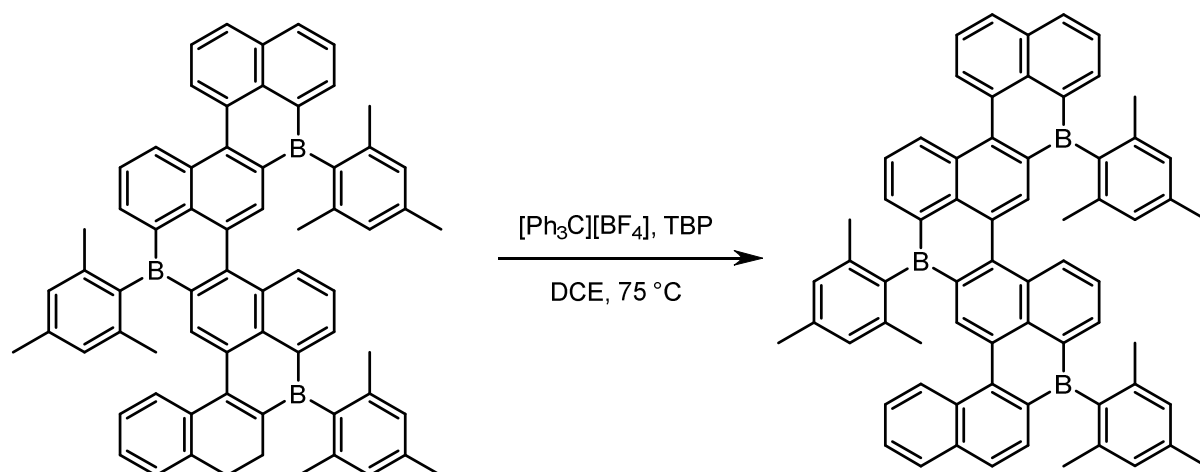
### Synthesis of **8**



A Schlenk was charged with **7** (52.9 mg, 6.92 x 10<sup>-5</sup> mol) and tri-*tert*-butylpyridine (18 mg, 7.3 x 10<sup>-5</sup> mol) and dry DCM (2 mL) and BCl<sub>3</sub> (0.12 mL, 1.0 M in DCM, 0.12 mmol) were added to give an orange/red solution. This was stirred at ambient temperature for 40 min. then all volatiles were removed *in vacuo*. To the residue was added AlCl<sub>3</sub> (10 mg, 7.5 x 10<sup>-5</sup> mol) and DCM (2 mL) and the mixture was stirred at ambient temperature for 30 minutes. All volatiles were removed *in vacuo* and to the residue was added AlCl<sub>3</sub> (10 mg, 7.5 x 10<sup>-5</sup> mol), 2,6-dichloropyridine (17 mg, 0.11 mmol) and DCM (2 mL) to give a dark red suspension. The mixture was stirred at ambient temperature for 1 hour then all volatiles were removed *in vacuo*. The residue was taken up in toluene (2.5 mL) and MesMgBr (0.5 mL, 1.0 M in THF, 0.5 mmol) was added dropwise to give a pink/red suspension. The mixture was stirred at ambient temperature for 18 hours then all volatiles were removed *in vacuo*. The product was purified by preparative thin layer chromatography using a DCM:petrol eluent (20:80) to yield analytically pure product **8** at R<sub>f</sub> = 0.38 as a red solid (42.3 mg, 4.73 x 10<sup>-5</sup> mol, 68% with respect to **7**).

<sup>1</sup>H NMR (400MHz, CD<sub>2</sub>Cl<sub>2</sub>)  $\delta$  = 9.07 (dd, 8.4, 1.3 Hz, 1H), 8.86 (dd, 8.4, 1.4 Hz, 1H), 8.58 – 8.54 (m, 2H), 8.52 (s, 1H), 8.44 (dd, 8.6, 1.4 Hz, 1H), 8.33 (dd, 6.9, 1.3 Hz, 1H), 8.30 – 8.23 (m, 2H), 8.16 (dd, 6.8, 1.3 Hz, 1H), 7.97 – 7.82 (m, 2H), 7.82 (dd, 8.1, 6.8 Hz, 1H), 7.71 (dd, 8.3, 6.8 Hz, 1H), 7.52 (dd, 7.6, 1.3 Hz, 1H), 7.37 – 7.28 (m, 2H), 7.24 (ddd, 7.4, 7.3, 1.9 Hz, 1H), 6.96 (s, 2H), 6.93 (s, 2H), 6.91 (s, 2H), 2.74 (t, 7.1 Hz, 2H), 2.50 – 2.44 (m, 2H), 2.38 (s, 3H), 2.36 (s, 3H), 2.28 (s, 3H), 2.13 (s, 6H), 2.12 (s, 6H), 2.03 (s, 6H). <sup>11</sup>B NMR (128MHz, CD<sub>2</sub>Cl<sub>2</sub>)  $\delta$  = 60.0 ( $\nu_{1/2}$  = 3184 Hz). <sup>13</sup>C{<sup>1</sup>H} NMR (101MHz, CD<sub>2</sub>Cl<sub>2</sub>)  $\delta$  = 152.3, 147.9, 147.8, 145.2, 144.4, 142.9, 142.8, 142.8, 142.4, 141.8, 140.5, 140.2, 139.6, 139.3, 139.1, 138.9, 138.7, 137.7, 137.5, 137.4, 137.2, 136.9, 135.7, 135.3, 135.1, 134.9, 134.4, 133.3, 132.5, 132.4, 132.0, 131.5, 130.4, 130.3, 130.0, 129.6, 128.5, 127.9, 127.5, 127.5, 127.3, 127.2, 126.7, 126.3, 125.9, 125.9, 29.6, 28.2, 23.7, 23.7, 23.3, 21.6, 21.5, 21.5. HRMS (APCI) Calculated for C<sub>67</sub>H<sub>56</sub>B<sub>3</sub><sup>+</sup> ([M+H]<sup>+</sup>) 893.4656. Found 893.4645.

## Synthesis of 9



A Schlenk was charged with **8** (24.2 mg,  $2.71 \times 10^{-5}$  mol), tri-*tert*-butylpyridine (15 mg,  $6.1 \times 10^{-5}$  mol) and trityl tetrafluoroborate (19 mg,  $5.8 \times 10^{-5}$  mol) and dry 1,2-dichloroethane (0.5 mL) was added to give a dark red suspension which was refluxed at 75 °C for 72 hours. Once cool all volatiles were removed *in vacuo* and the product was purified by preparative thin layer chromatography using a DCM:petrol eluent (20:80) to yield product **9** at  $R_f = 0.35$  as a red solid (13.6 mg,  $1.52 \times 10^{-5}$  mol, 56% with respect to **8**).

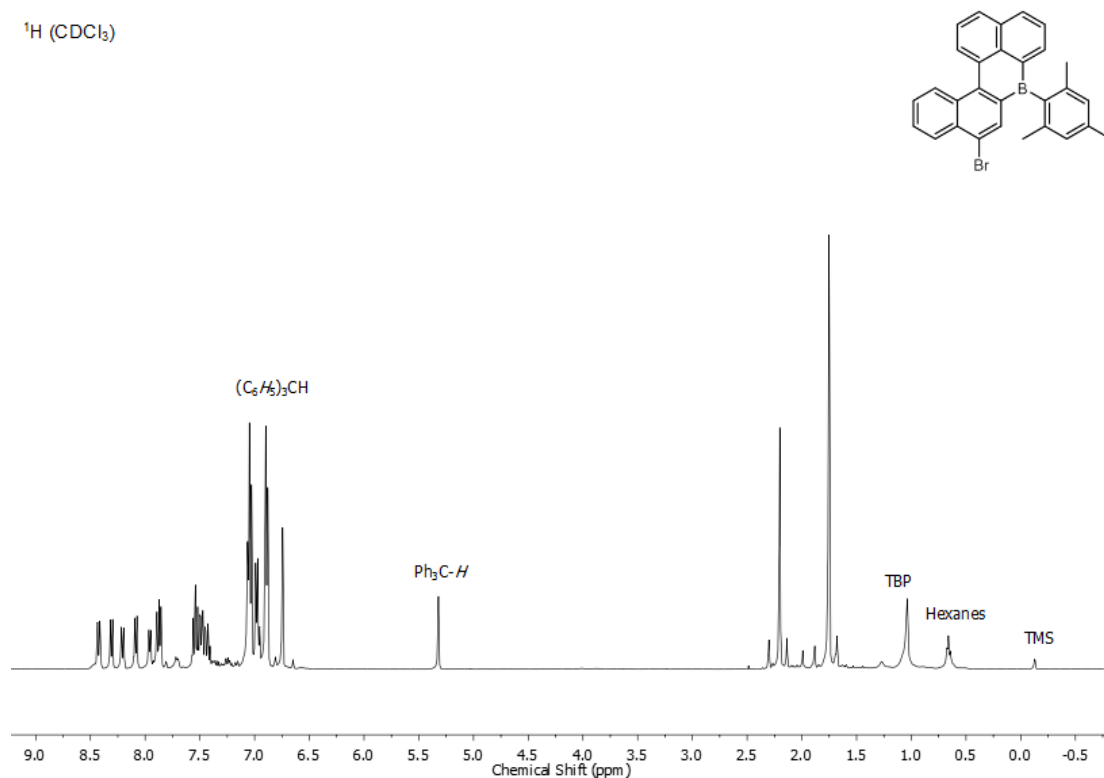
$^1\text{H}$  NMR (400MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta = 9.11$  (dd, 8.4, 1.4 Hz, 1H), 8.96 (dd, 8.4, 1.4 Hz, 1H), 8.77 (s, 1H), 8.61 (s, 1H), 8.60 – 8.57 (m, 2H), 8.45 (dd, 8.1, 1.5 Hz, 1H), 8.39 (dd, 6.9, 1.3 Hz, 1H), 8.30 – 8.22 (m, 3H), 7.99 – 7.90 (m, 3H), 7.82 (dd, 8.1, 6.8 Hz, 1H), 7.78 – 7.71 (m, 3H), 7.60 (ddd, 8.0, 6.7, 1.1 Hz, 1H), 7.49 (ddd, 8.3, 6.8, 1.4 Hz, 1H), 6.98 (s, 2H), 6.97 (s, 2H), 6.91 (s, 2H), 2.42 (s, 3H), 2.35 (s, 3H), 2.27 (s, 3H), 2.16 (s, 6H), 2.14 (s, 6H), 1.99 (s, 6H).  $^{11}\text{B}$  NMR (128MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta = 62.6$  ( $\nu_{1/2} = 2689$  Hz).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta = 147.8, 147.3, 144.9, 143.8, 142.9, 142.8, 142.8, 142.6, 141.0, 140.2, 139.9, 139.6, 139.4, 139.3, 139.2, 139.2, 138.2, 137.7, 137.6, 137.4, 137.3, 137.2, 136.8, 136.2, 135.3, 135.0, 134.5, 134.4, 133.4, 133.1, 132.6, 132.5, 132.0, 131.3, 130.8, 130.5, 130.5, 130.4, 130.1, 128.6, 127.9, 127.5, 127.4, 127.2, 127.2, 126.7, 126.4, 126.1, 125.9, 23.7, 23.7, 23.7, 21.6, 21.6, 21.5$ . HRMS (APCI) Calculated for  $\text{C}_{67}\text{H}_{54}\text{B}_3^+$  ( $[\text{M}+\text{H}]^+$ ) 891.4499. Found 891.4508.



## NMR Spectra and Mass Spectra

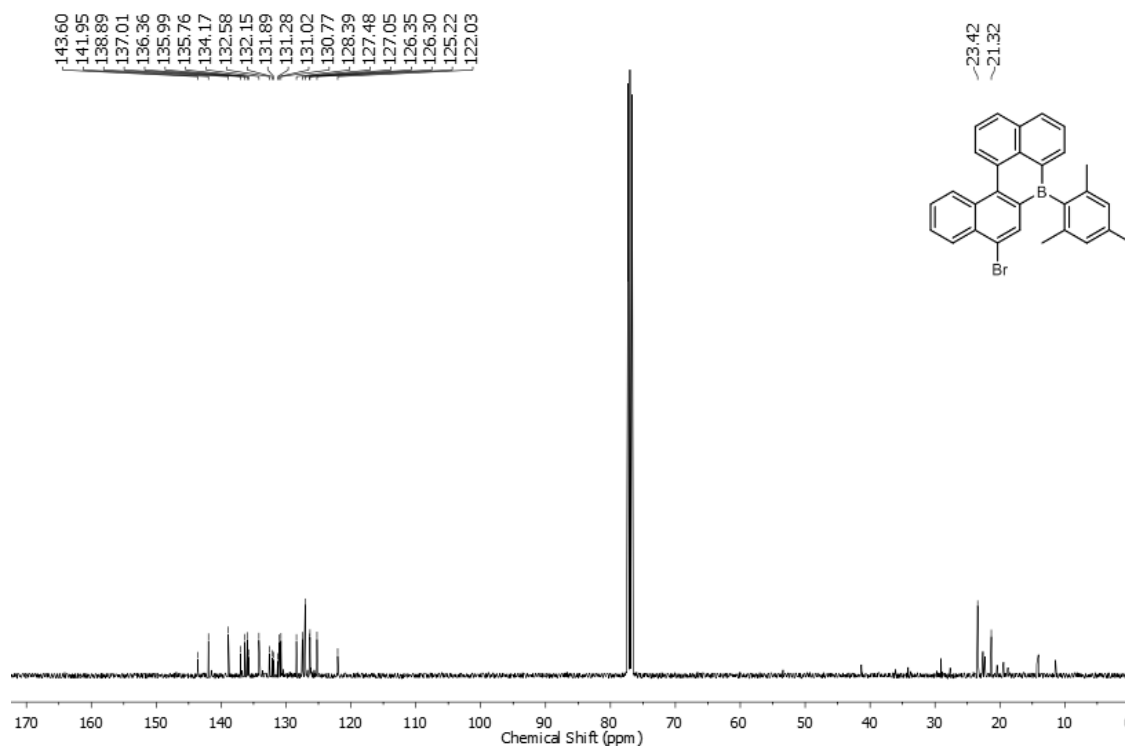
Crude 9-bromo-7-mesityl-7H-dinaphtho[1,8-bc:1',2'-e]borinine (**1**) without purification of  $\text{Ph}_3\text{CH}$

$^1\text{H}$  ( $\text{CDCl}_3$ )

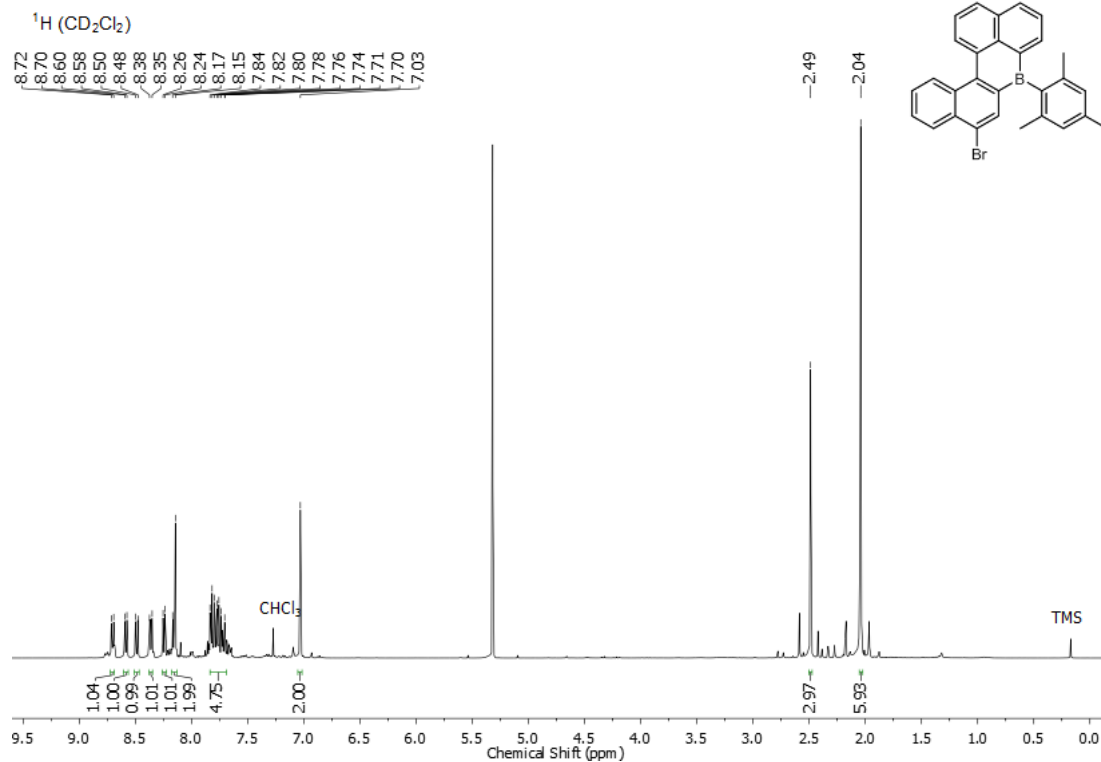


A number of the small resonances between 1.5 and 2.5 ppm are Mes- $\text{CH}_3$  resonances for the minor product from bromination at the meta C-H position of mesityl.

$^{13}\text{C}\{^1\text{H}\}$  ( $\text{CDCl}_3$ )



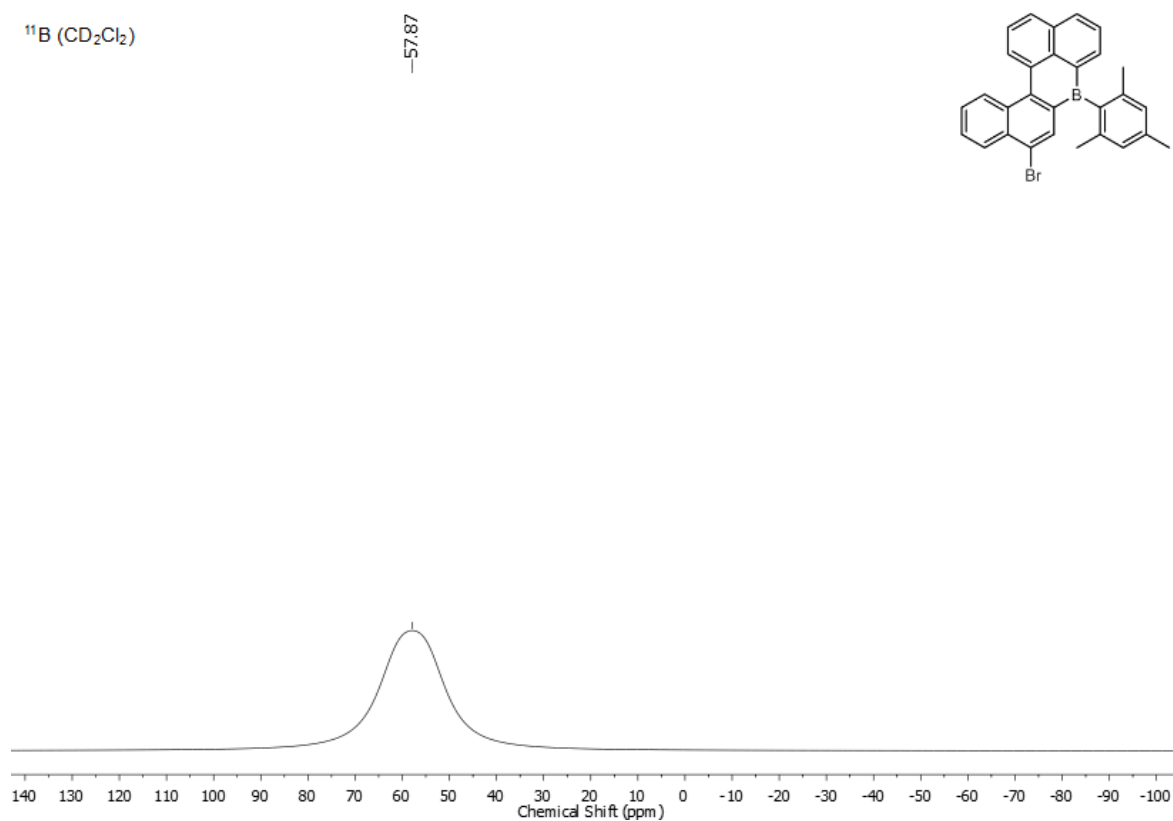
Crude 9-bromo-7-mesityl-7H-dinaphtho[1,8-bc:1',2'-e]borinine (1) (after purification to remove all Ph<sub>3</sub>CH)



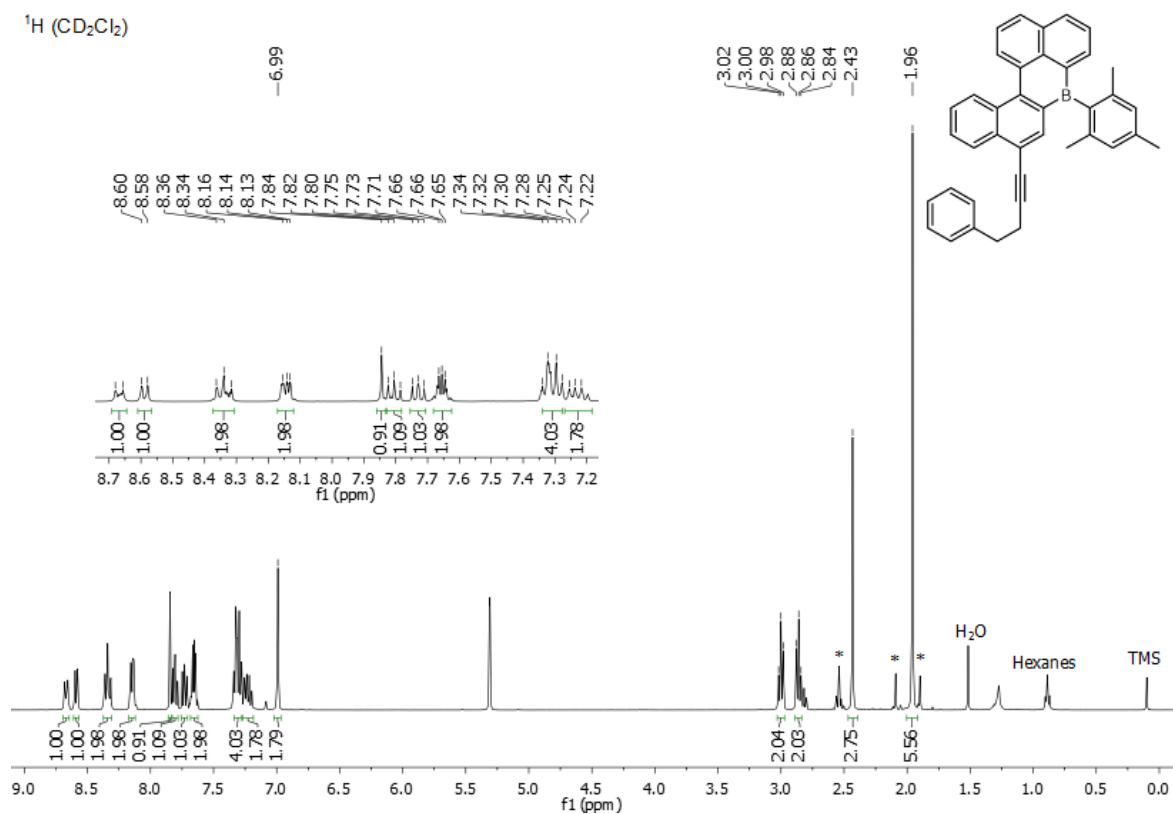
A number of the small resonances between 1.5 and 2.5 ppm are Mes-CH<sub>3</sub> resonances for the minor product from bromination at the meta C-H position of mesityl.

<sup>11</sup>B (CD<sub>2</sub>Cl<sub>2</sub>)

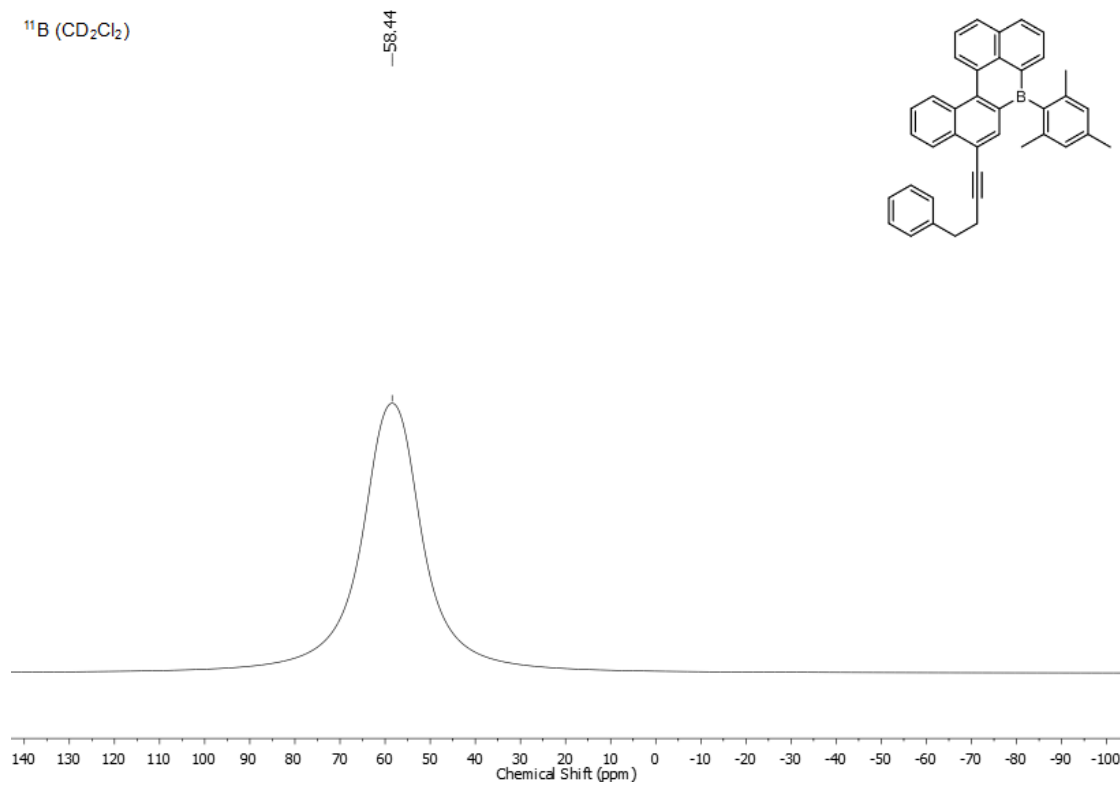
-57.87



## Compound 2

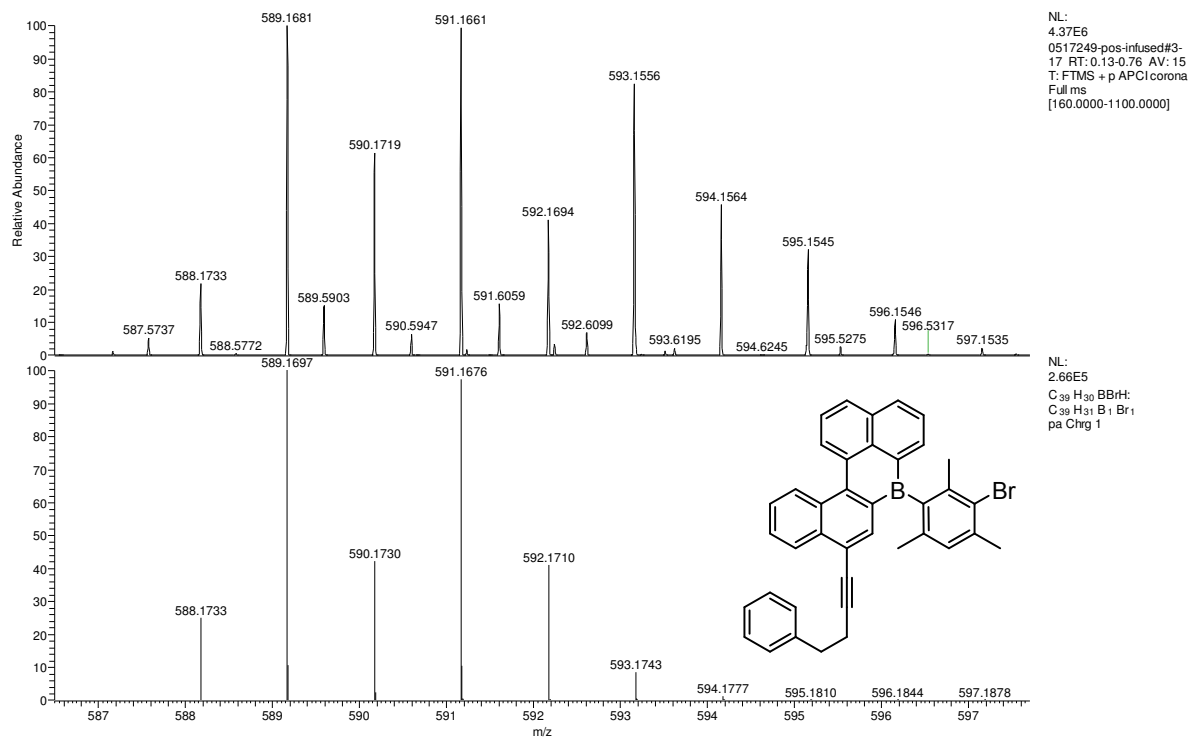


\*Small resonances between 1.5 and 2.5 ppm are Mes-CH<sub>3</sub> resonances for the minor product derived from the double bromination product **2-Br**.

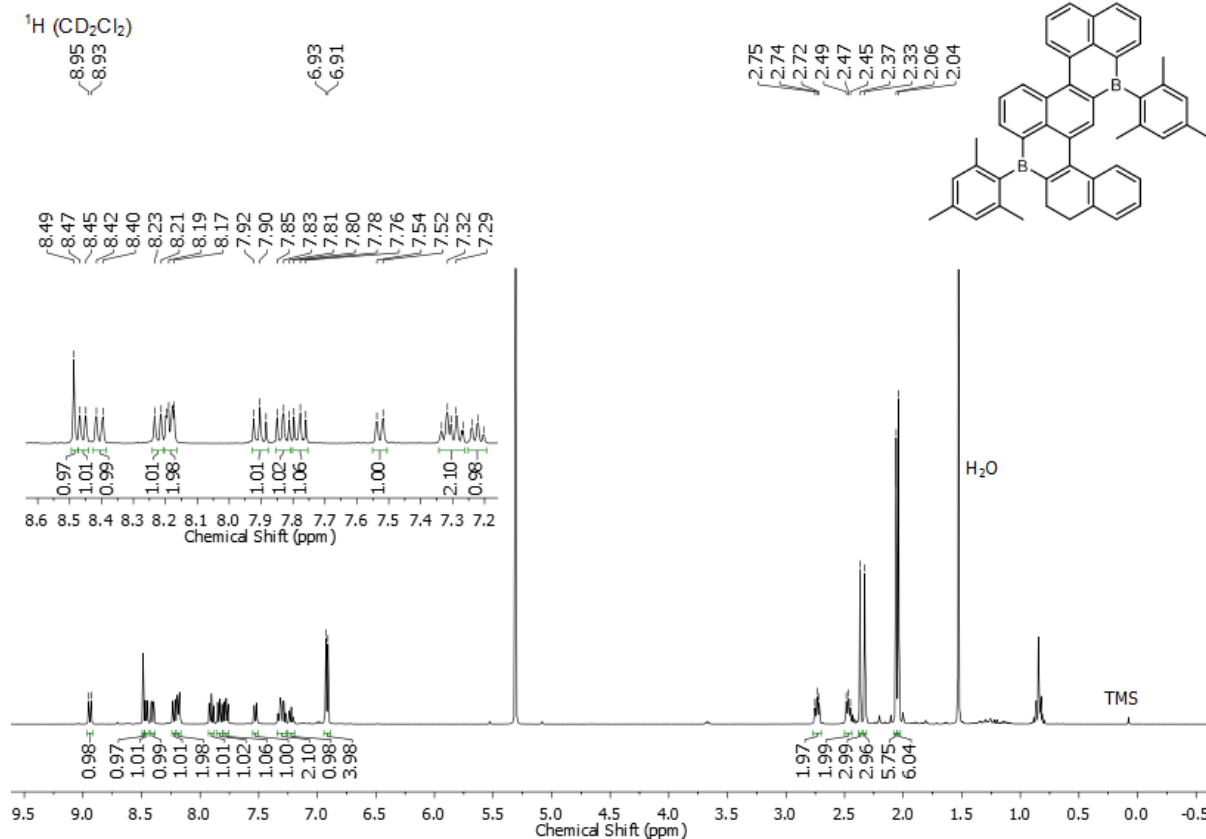




The mass spectra indicate the presence of the desired product plus the brominated analogue. The position of bromination is from the combined NMR spectra (3 minor Mes methyl peaks and from X-ray diffraction studies, see later).

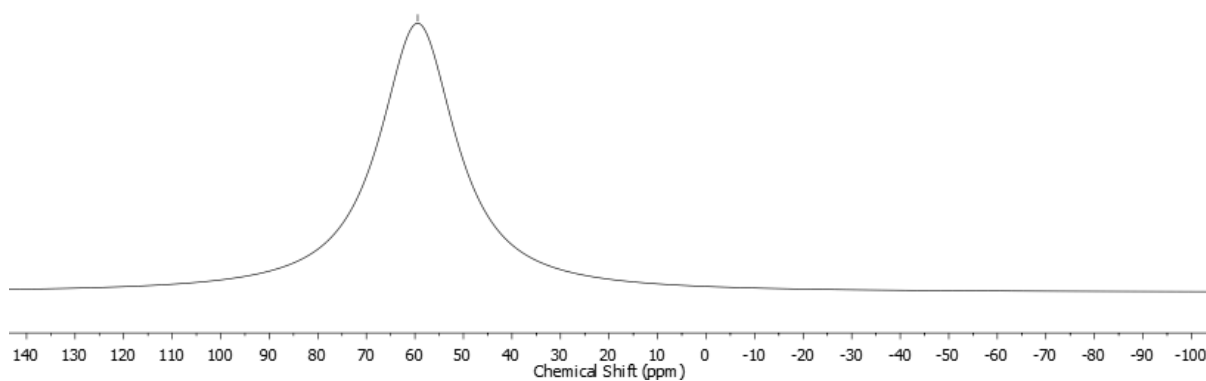
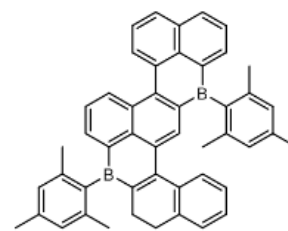


#### Compound 4



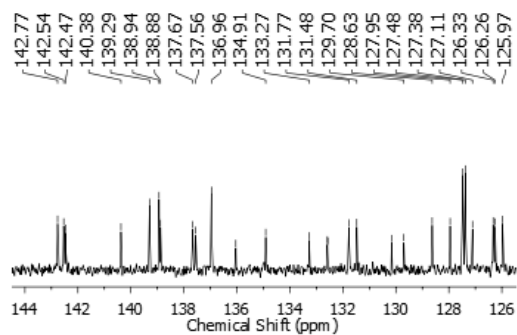
$^{11}\text{B}$  ( $\text{CD}_2\text{Cl}_2$ )

-59.43

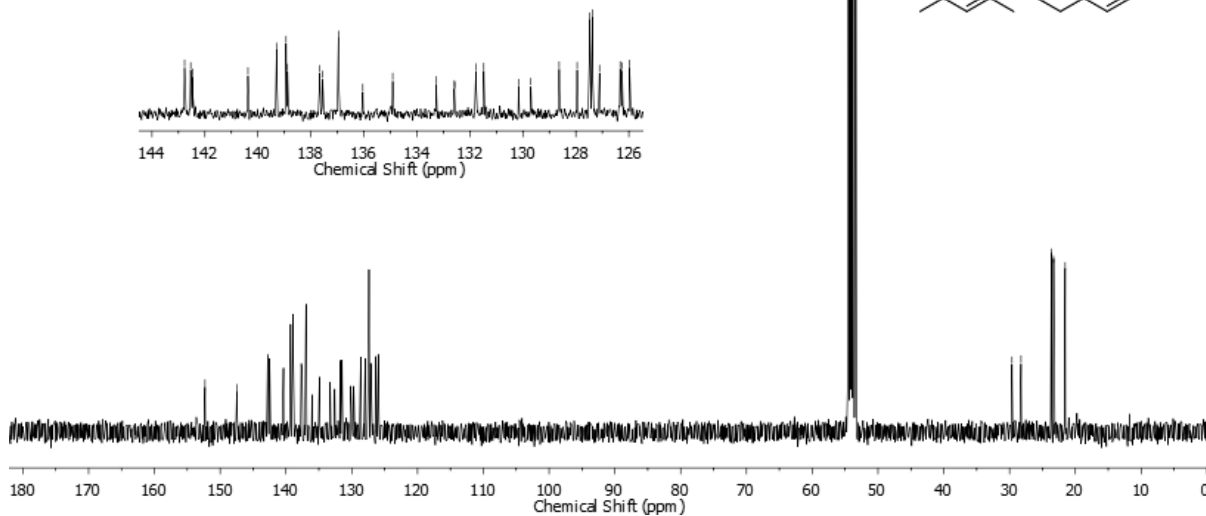
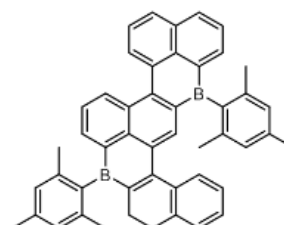


$^{13}\text{C}\{^1\text{H}\}$  ( $\text{CD}_2\text{Cl}_2$ )

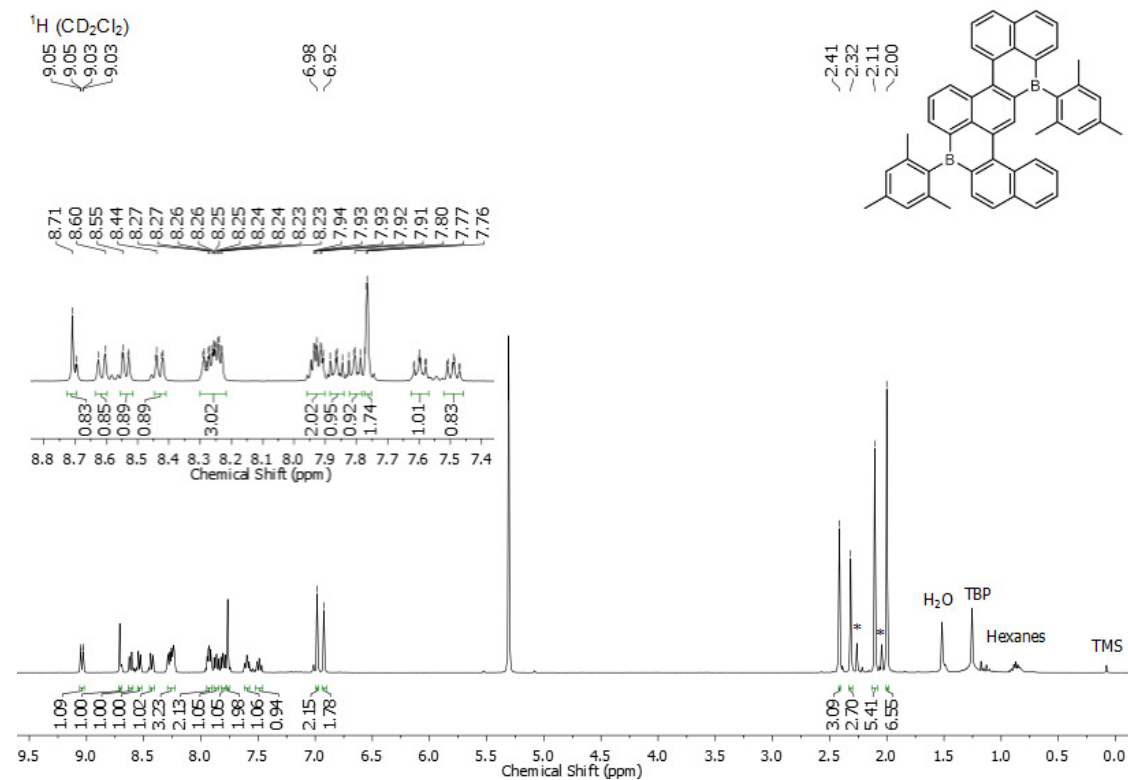
-152.30  
-147.47



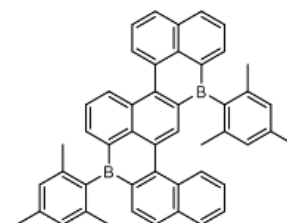
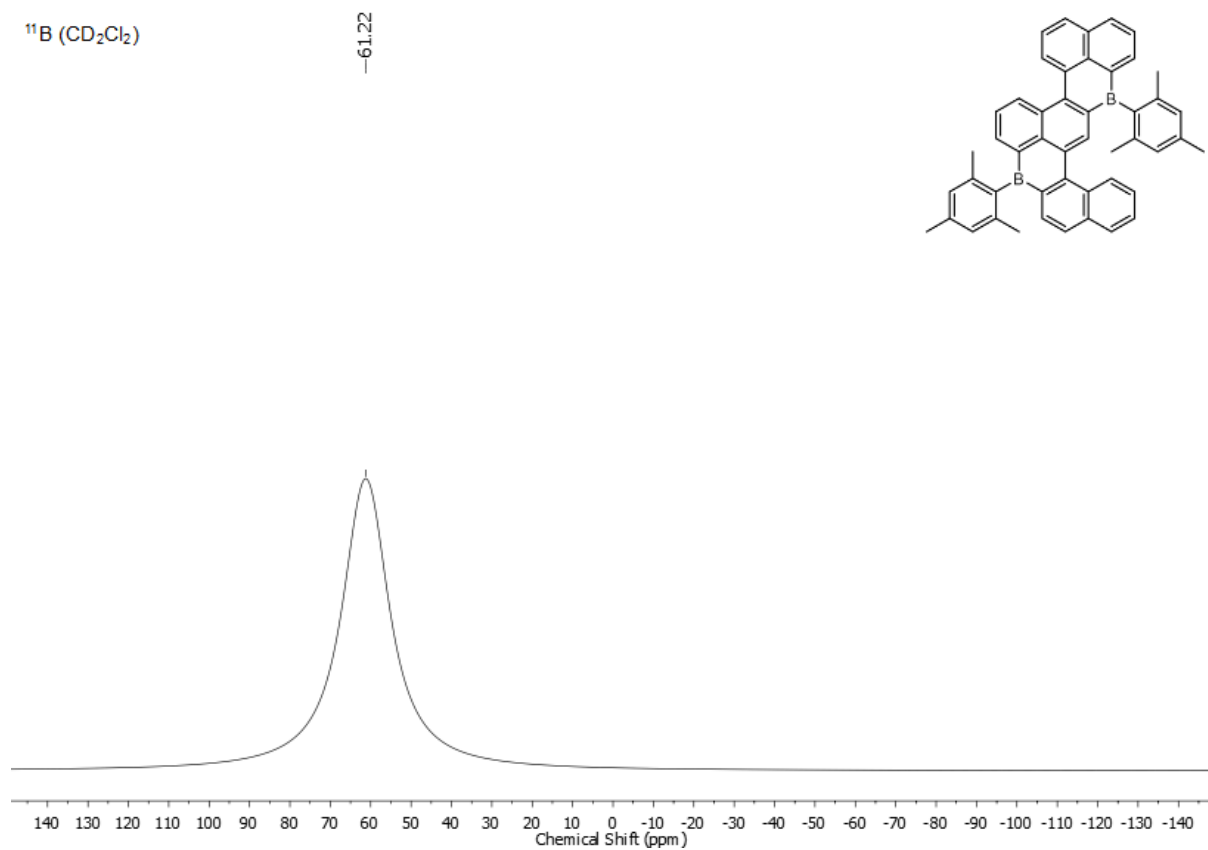
29.63  
28.26  
23.66  
23.31  
21.54



## Compound 5



\*Small resonances between 1.5 and 2.5 ppm are Mes-CH<sub>3</sub> resonances for the minor brominated product.

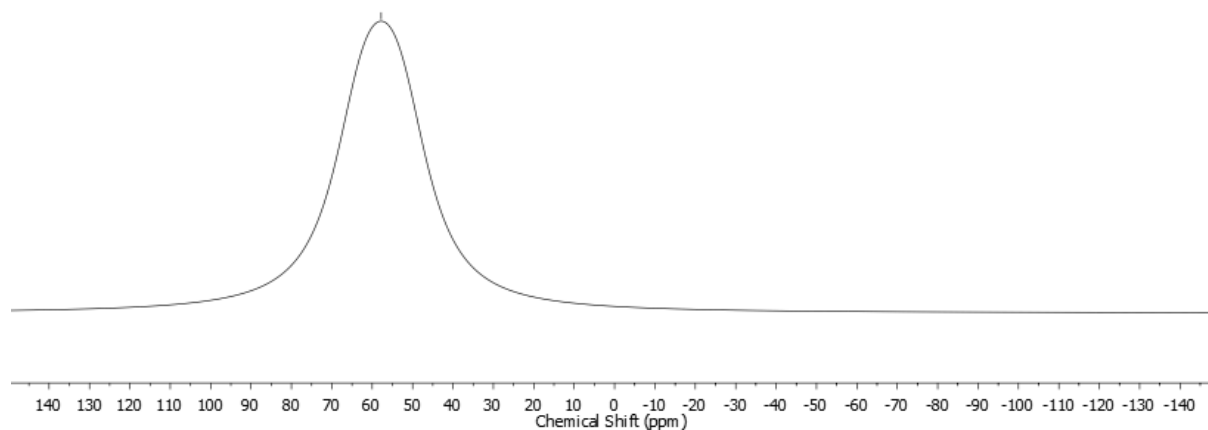
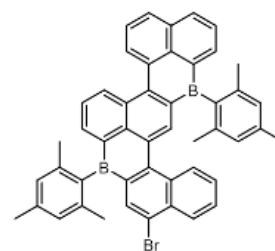






$^{11}\text{B}$  ( $\text{CD}_2\text{Cl}_2$ )

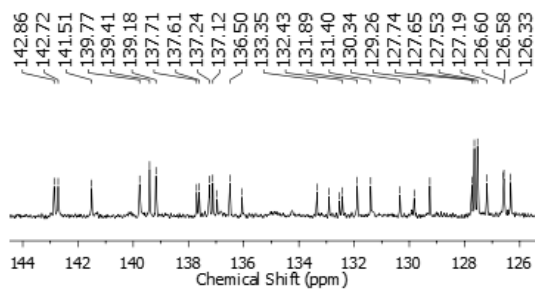
-57.79



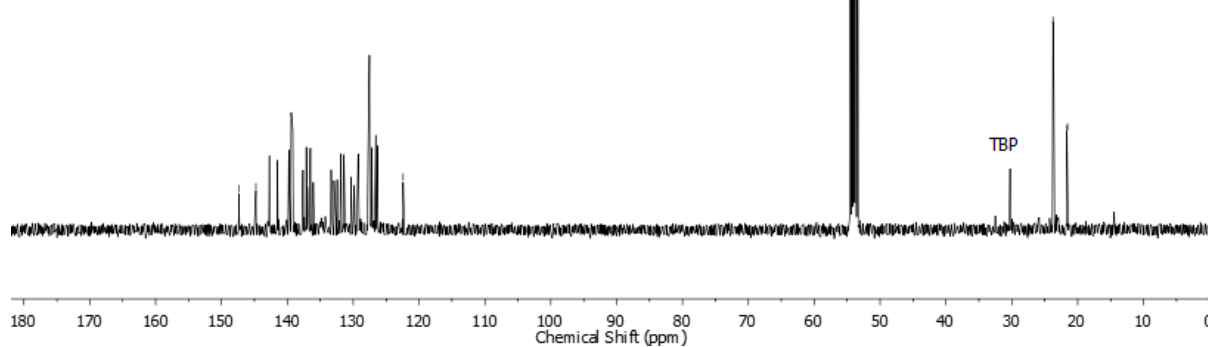
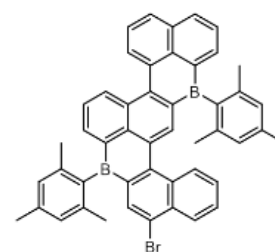
$^{13}\text{C}\{^1\text{H}\}$  ( $\text{CD}_2\text{Cl}_2$ )

-147.37  
-144.78

-122.41



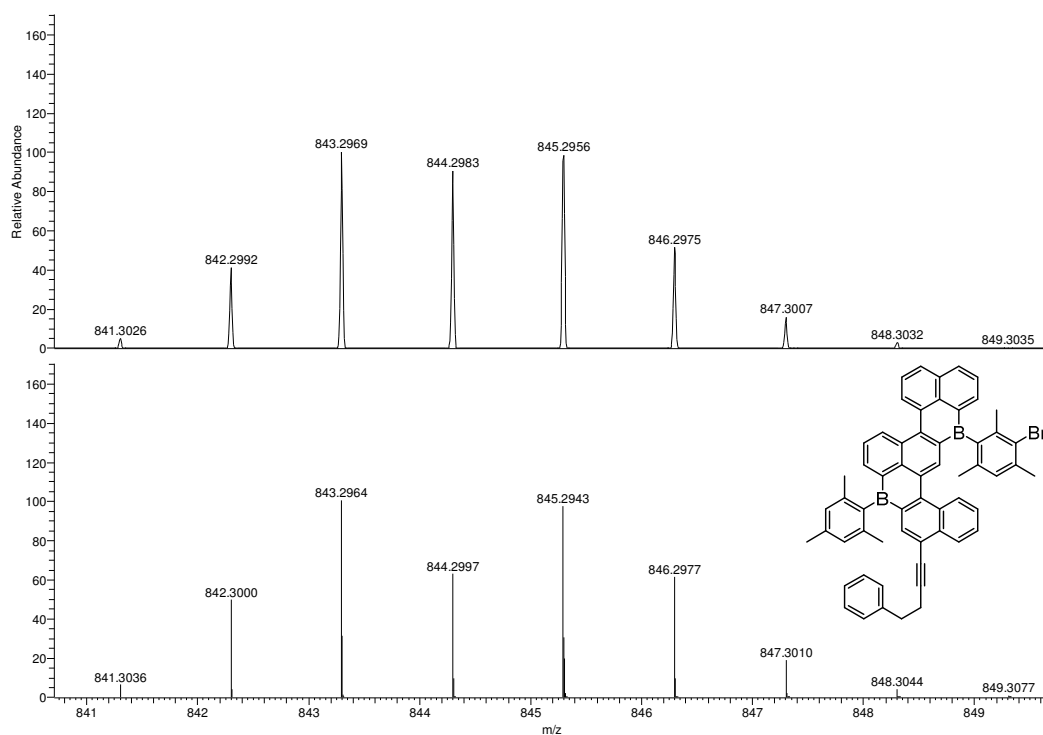
23.75  
23.67  
21.63  
21.53



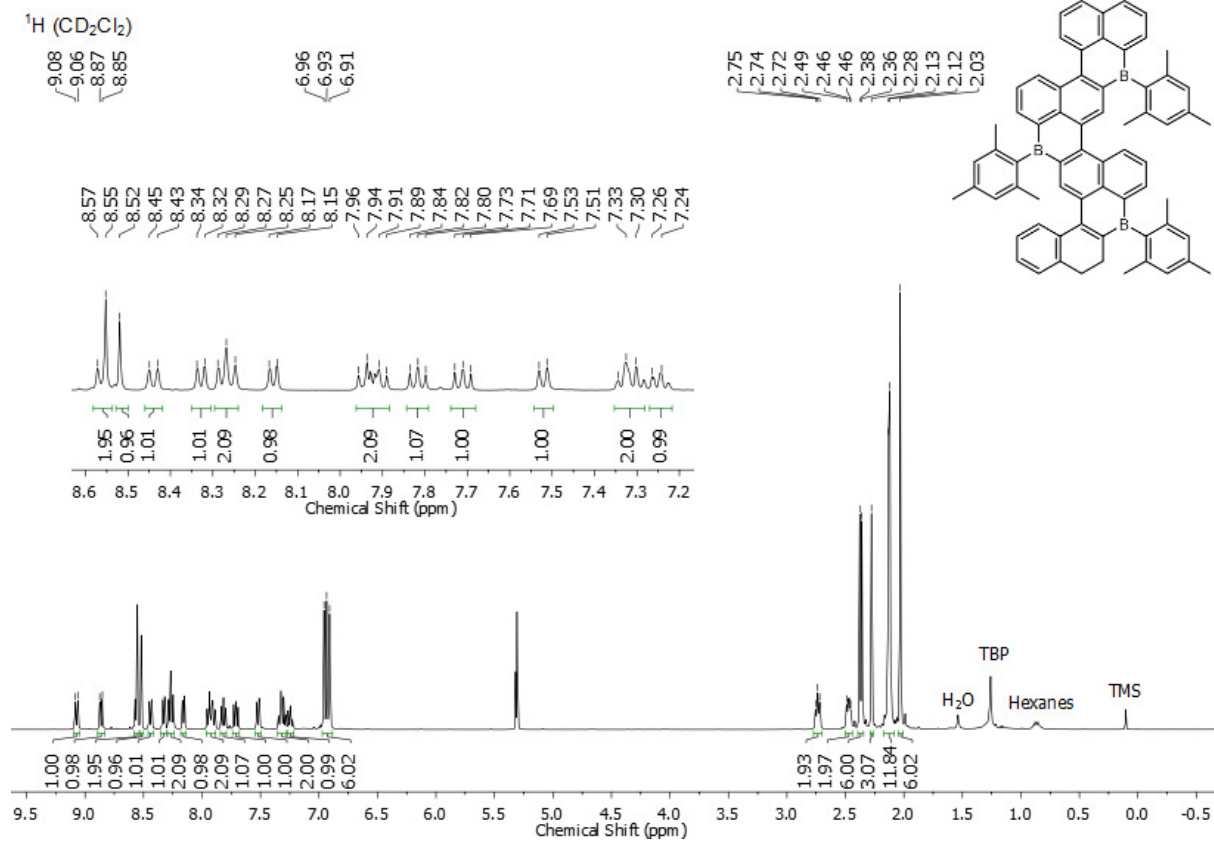
Again minor resonances for a second product containing different Mes methyls are observed in the  $^1\text{H}$  NMR spectrum which are attributed to a mesityl brominated by-product.





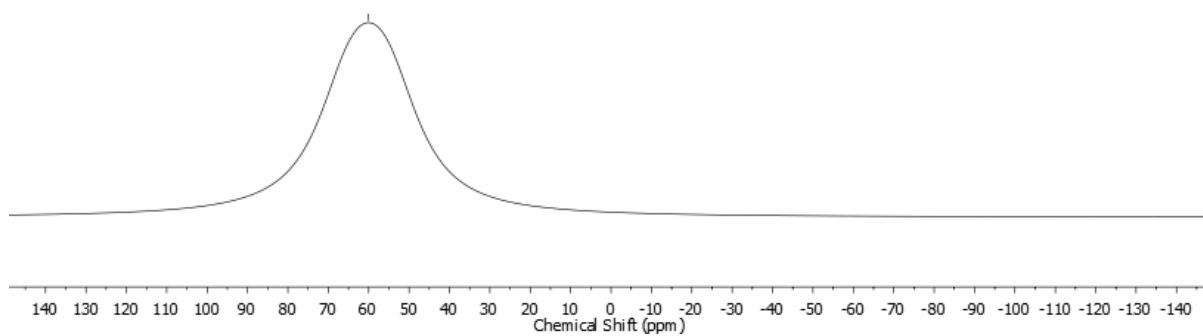
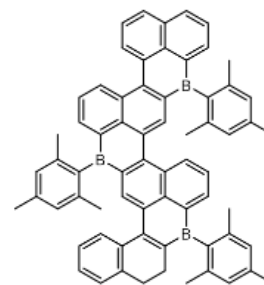


### Compound 8

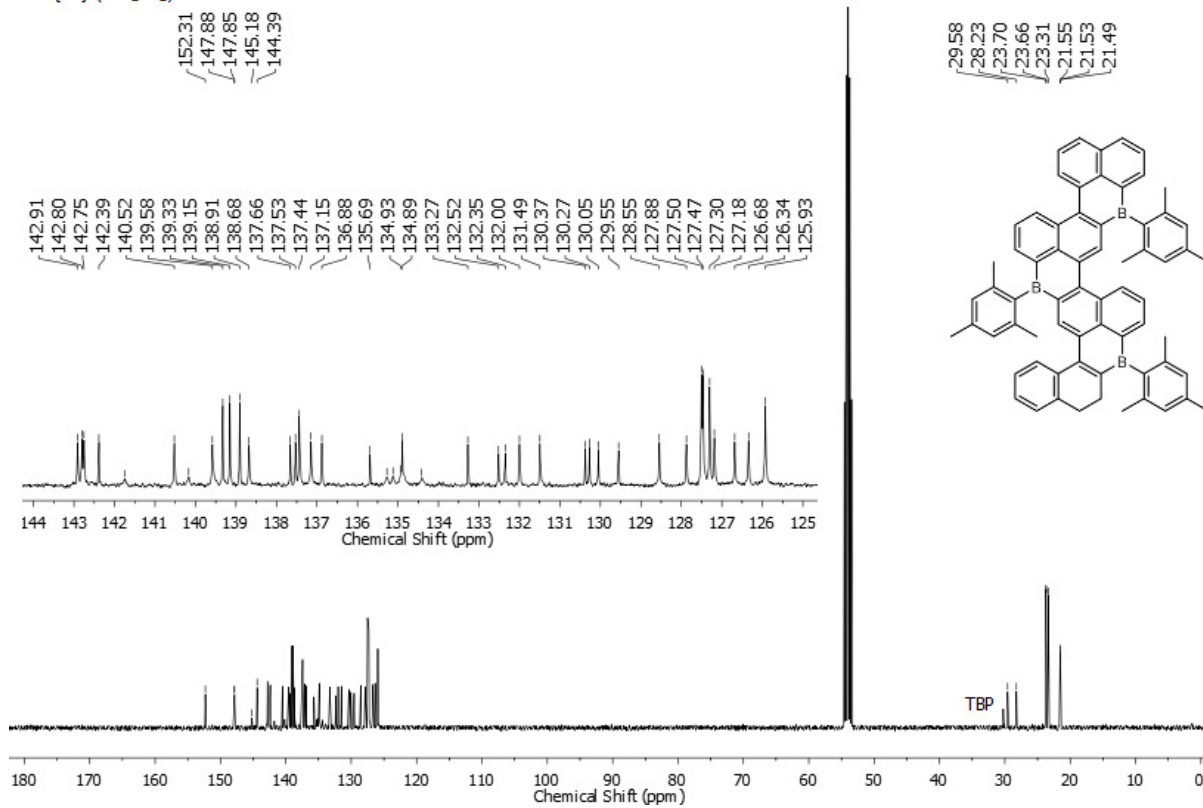


$^{11}\text{B}$  ( $\text{CD}_2\text{Cl}_2$ )

-60.05

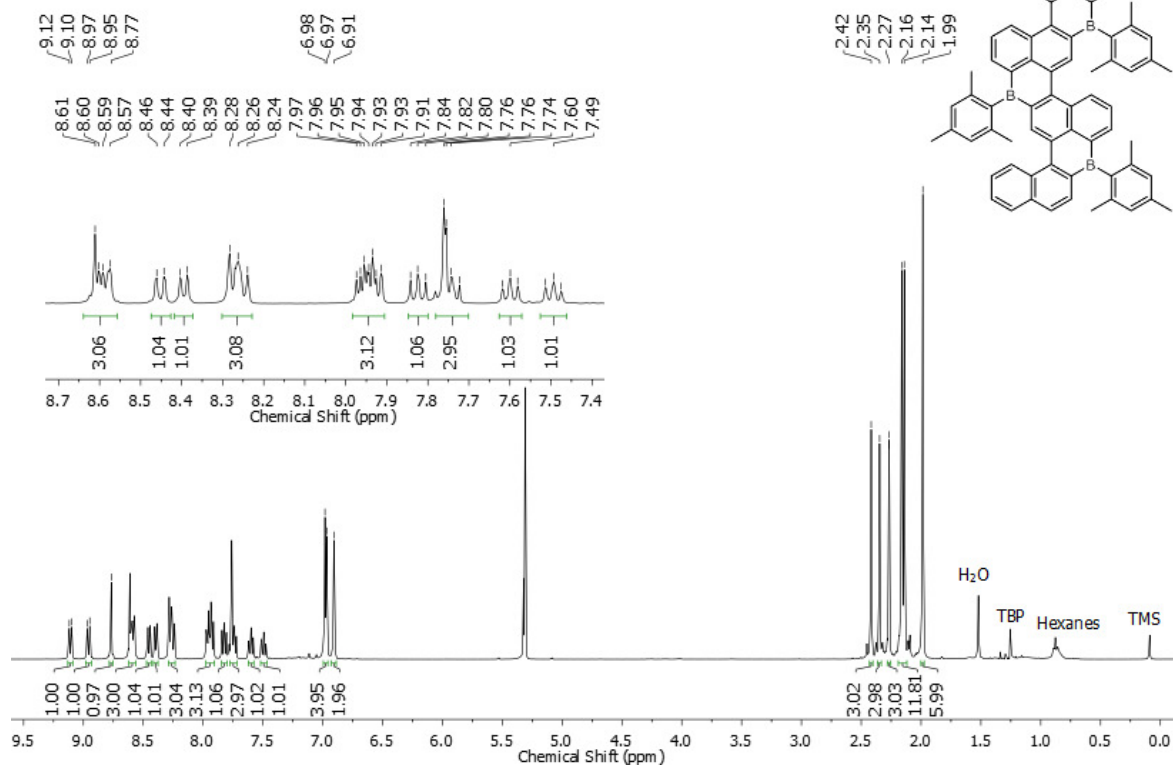


$^{13}\text{C}\{^1\text{H}\}$  ( $\text{CD}_2\text{Cl}_2$ )

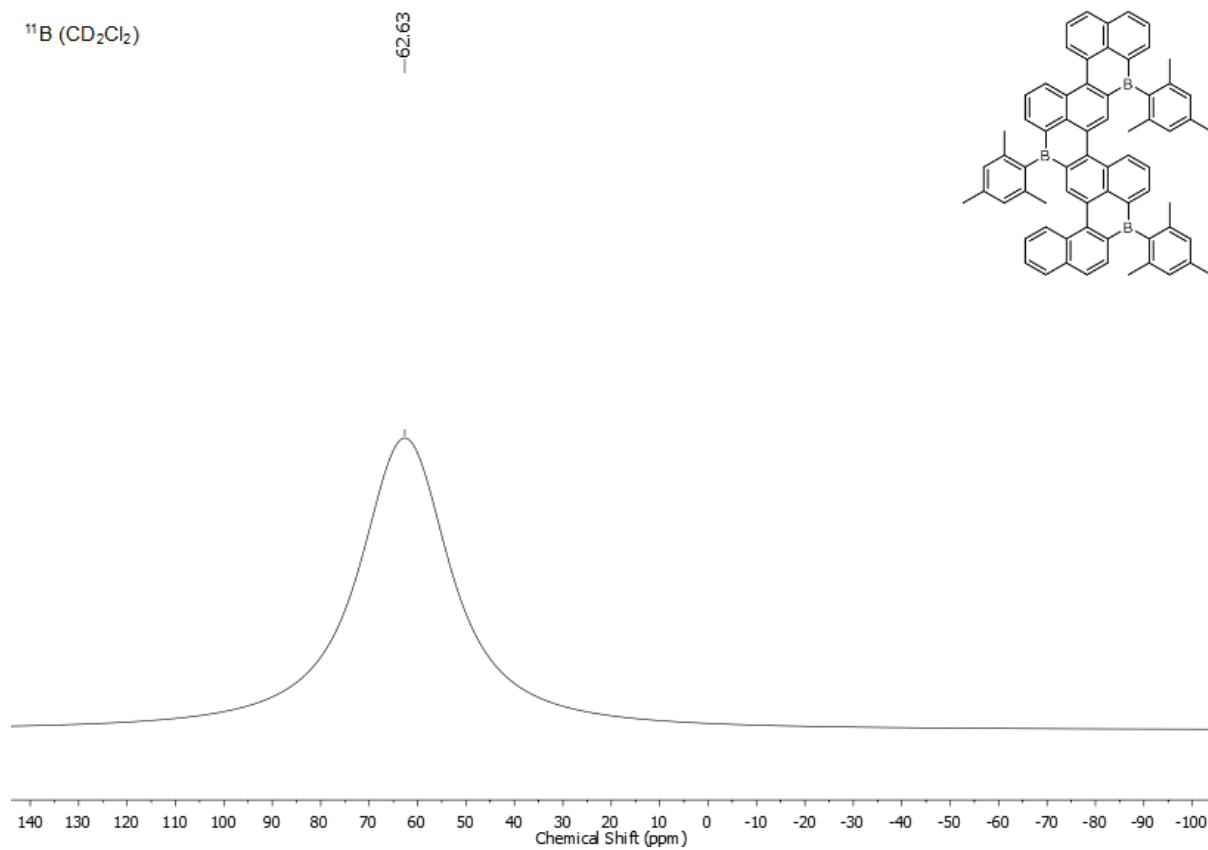


# Compound 9

$^1\text{H}$  ( $\text{CD}_2\text{Cl}_2$ )



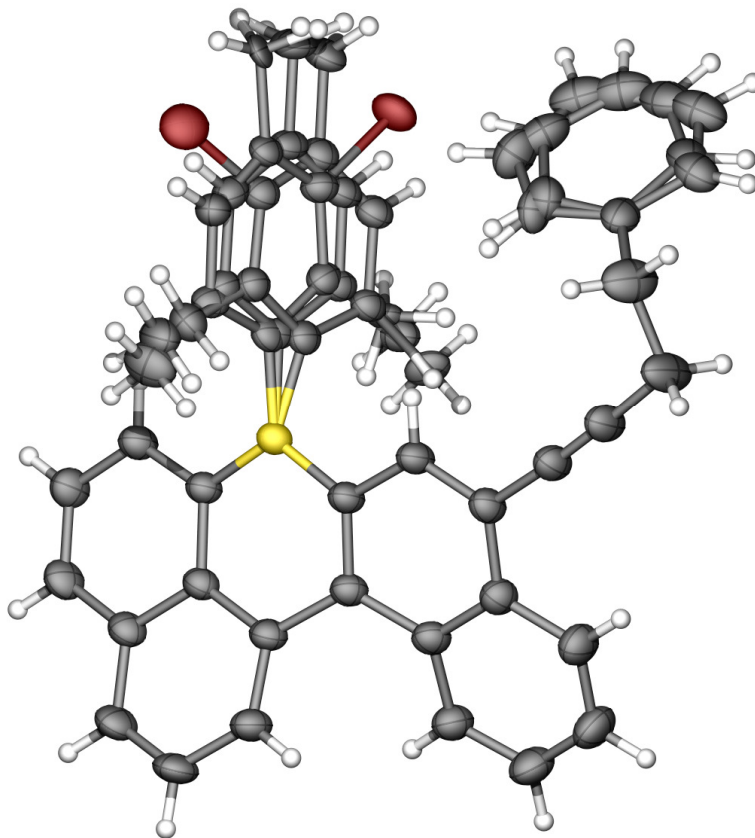
$^{11}\text{B}$  ( $\text{CD}_2\text{Cl}_2$ )





0.0279(10) (Br3). Further flat and sadi restraints were introduced in order to refine sensible geometries around the mesityl C-B bond. The thermal parameters for all disordered components were restrained in order to refine sensible thermal ellipsoids.

The molecular structure of compound **2** also presents disorder on the phenyl ring next to the -CH<sub>2</sub>CH<sub>2</sub>- moiety (thermal parameters for these were restrained using RIGU and SIMU).



**Figure S1** Representation of the asymmetric unit of **2** in the crystal. (carbon = grey, boron = yellow, bromine = brown and hydrogen = white; image produced using POV-ray).<sup>14</sup>

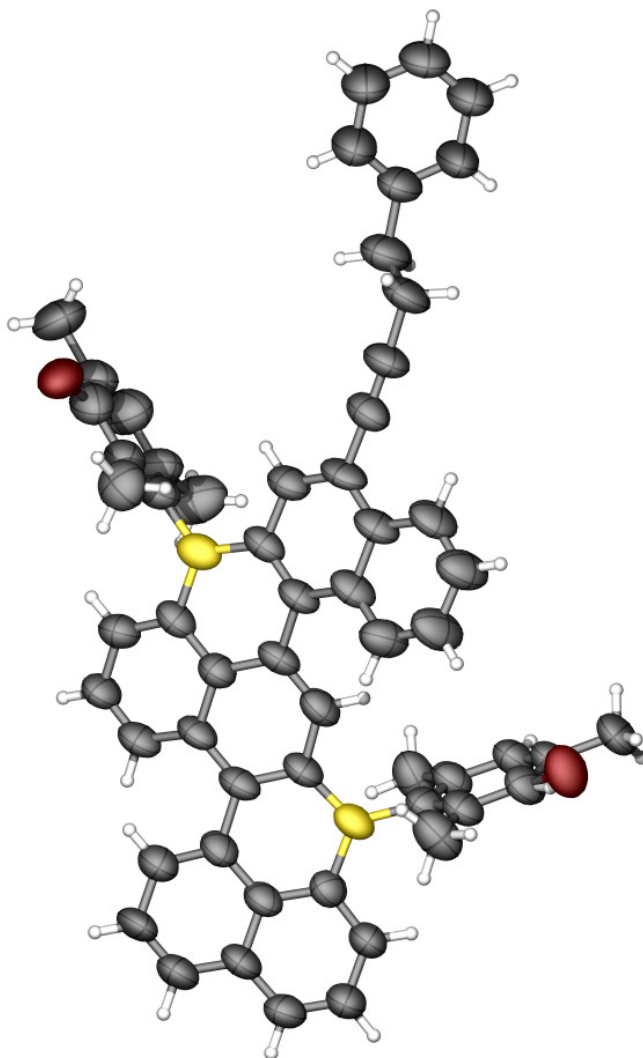
### Compound 7

The data collected for compound **7** was found to contain significant electron density at the meta-position of two of the mesityl rings. This was assigned as traces of bromine, based on data from mass spectrometry. The bromine occupancies were freely refined to 0.085(3) (Br2) and 0.044(3) (Br1)

Crystals of the sample are very weakly diffracting, therefore the data were truncated accordingly. Despite best efforts, better data could not be obtained using a synchrotron source.



There is a solvent void present in the structure with poorly defined features in the electron density map, which was modelled using a solvent mask calculated using Olex2. The solvent void was calculated to contain 50.4 electrons and so has been assigned as CH<sub>2</sub>Cl<sub>2</sub>.



**Figure S2** Representation of the asymmetric unit of 1mji7 in the crystal. (carbon = grey, boron = yellow, bromine = brown and hydrogen = white; image produced using POV-ray<sup>3</sup>)

**Table S1** Crystal Structure Refinement Data

	<b>2</b>	<b>7</b>
Empirical Formula	C <sub>39</sub> H <sub>30.89</sub> BBr <sub>0.11</sub>	C <sub>58</sub> H <sub>45.87</sub> B <sub>2</sub> Br <sub>0.13</sub>
Fw/g mol <sup>-1</sup>	518.93	774.82
Temperature/K	150.00(10)	150.0(2)
Crystal system, Space Group	Monoclinic, P2 <sub>1</sub> /n	Monoclinic, P2 <sub>1</sub> /c
a /Å	10.71416(15)	17.5450(17)
b /Å	18.5823(3)	12.6207(12)
c /Å	14.07156(18)	22.2518(14)
α /°	90	90
β /°	95.4564(12)	94.451(9)
γ /°	90	90
Vol /Å <sup>3</sup>	2788.87(7)	4912.4(8)
Z, calc density /g.cm <sup>-3</sup>	4, 1.236	4, 1.048
Abs coeff /mm <sup>-1</sup>	0.694	0.559
F(000)	1095.0	1634.0
Crystal, colour	Block, yellow	Plate, Red
Crystal dimensions /mm <sup>3</sup>	0.347 × 0.164 × 0.133	0.161 × 0.058 × 0.007
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2θ range for data collection /deg	7.904 to 154.82	5.052 to 108.478
Index ranges	-13 ≤ h ≤ 13, -23 ≤ k ≤ 23, -17 ≤ l ≤ 17	-18 ≤ h ≤ 14, -13 ≤ k ≤ 13, - 23 ≤ l ≤ 23
Reflections collected/unique	36142	35475
Independent reflections	5791 [R <sub>int</sub> = 0.0567, R <sub>sigma</sub> = 0.0257]	5986 [R <sub>int</sub> = 0.1607, R <sub>sigma</sub> = 0.1028]
Data/restraint/parameters	5791/1241/593	5986/6/561
Goodness-of-fit on F <sup>2</sup>	1.169	0.946
Final R indices [F <sup>2</sup> < 2θ(F <sup>2</sup> )]	R <sub>1</sub> = 0.0599, wR <sub>2</sub> = 0.1453	R <sub>1</sub> = 0.0816, wR <sub>2</sub> = 0.2117
R indices (all data)	R <sub>1</sub> = 0.0619, wR <sub>2</sub> = 0.1464	R <sub>1</sub> = 0.1672, wR <sub>2</sub> = 0.2687
Largest diff peak and hole /e Å <sup>-3</sup>	0.23, -0.20	0.41, -0.20

## Photophysical Properties

Table S2 Summary of photophysical data.

Compound	$\lambda_{\text{max,abs}}$ (nm) <sup>a</sup>	$\epsilon \times 10^{-3}$ (M <sup>-1</sup> cm <sup>-1</sup> ) <sup>a</sup>	$\lambda_{\text{max,em}}$ (nm) <sup>a</sup>	Stoke shift (nm)	PLQY (%) <sup>b</sup>	Band-gap (eV) <sup>a</sup>
<b>G</b> <sup>5</sup>	351, 367, 420	16.1, 12.9, 4.1	516 <sup>d</sup>	94	16	2.61
<b>4</b>	378, 404, 427, 474	15.1, 12.8, 10.4, 10.4	554	80	30	2.31
<b>5</b>	388, 406 (s), 486	9.6, 8.6, 10.9	569	83	49	2.27
<b>8</b>	322, 513	41.6, 21.8	611	98	34	2.12
<b>9</b>	326, 522	48.0, 23.8	623	101	34	2.08
<b>J</b> <sup>5</sup>	318, 353, 487	46.5, 12.5, 21.5	592 <sup>e</sup>	105	23	2.31

<sup>a</sup>Measured at  $1 \times 10^{-5}$  M in toluene, <sup>b</sup>absolute quantum yield values measured using an integrating sphere at  $0.2 \times 10^{-5}$  M in toluene (estimated error  $\pm 10\%$ ), <sup>s</sup>Shoulder,  $\lambda_{\text{ex}}$  (nm): <sup>d</sup>351, <sup>e</sup>487

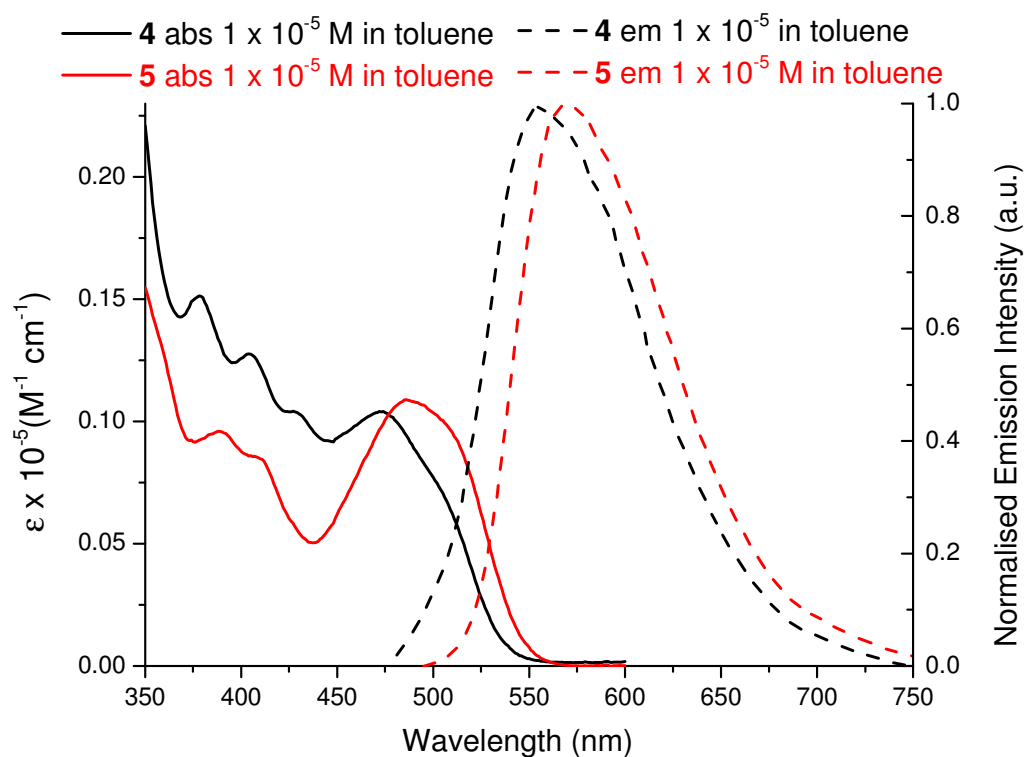
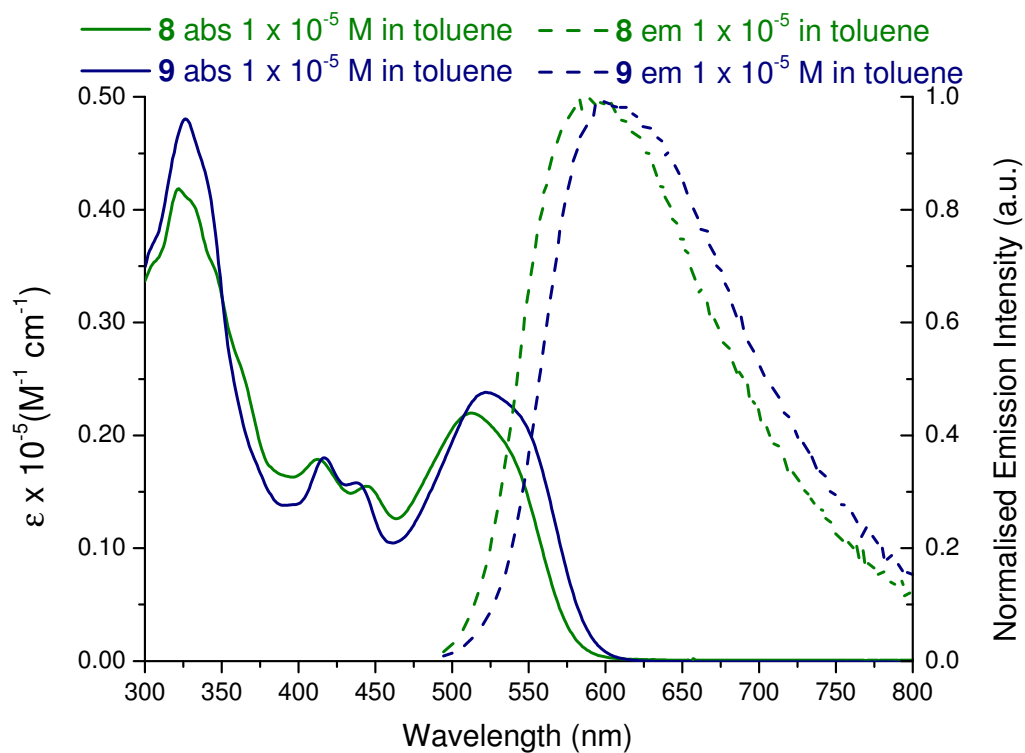


Figure S3 Absorbance and emission spectra of **4** and **5** in toluene ( $1 \times 10^{-5}$  M).



**Figure S4** Absorbance and emission spectra of **8** and **9** in toluene ( $1 \times 10^{-5}$  M).

**Table S3** Summary of photophysical data in varying solvents.

Compound	$\lambda_{\text{max}_{\text{abs}}}$ (nm) <sup>a</sup>	$\lambda_{\text{max}_{\text{em}}}$ (nm) <sup>a</sup>	PLQY (%) <sup>b</sup>
<b>8 (toluene)</b>	322, 513	611	34
<b>8 (MeCN)</b>	319, 509	625	31
<b>9 (toluene)</b>	326, 522	623	34
<b>9 (MeCN)</b>	323, 519	626	29

<sup>a</sup>Measured at  $1 \times 10^{-5}$  M, <sup>b</sup>absolute quantum yield values measured using an integrating sphere (estimated error  $\pm 10\%$ )

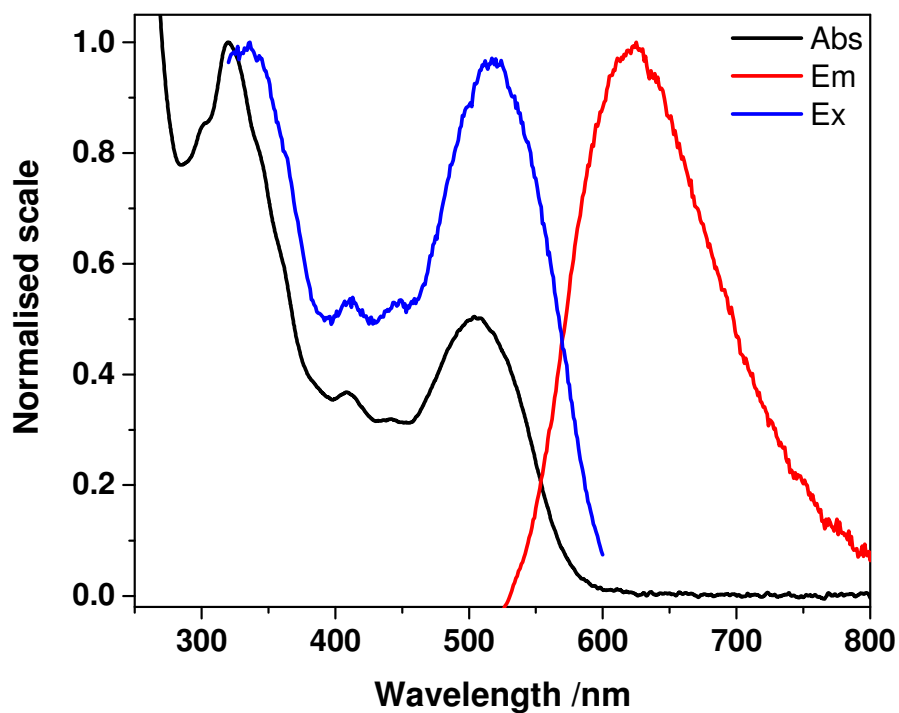


Figure S5 Absorbance, excitation and emission spectra of **8** in MeCN.

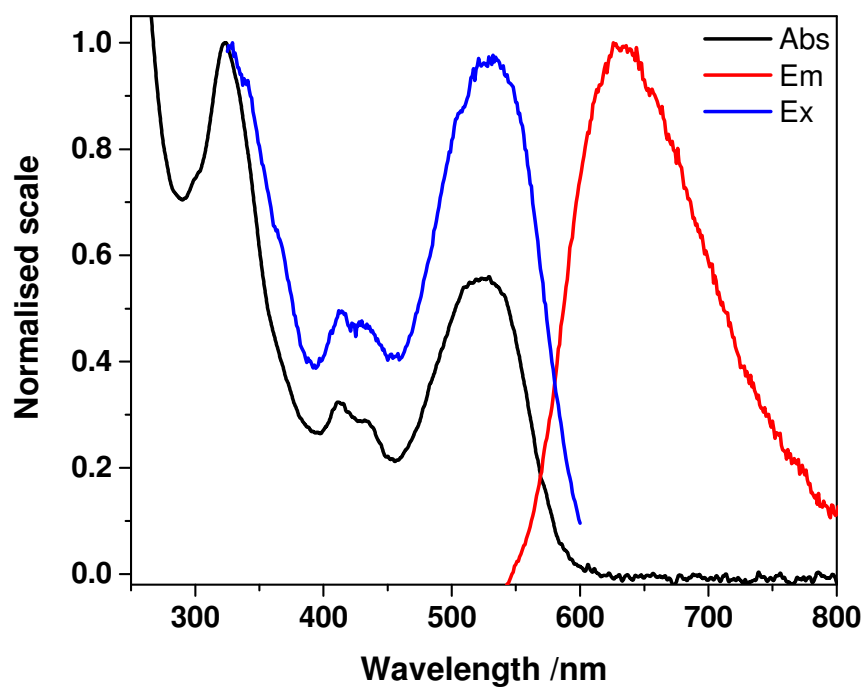


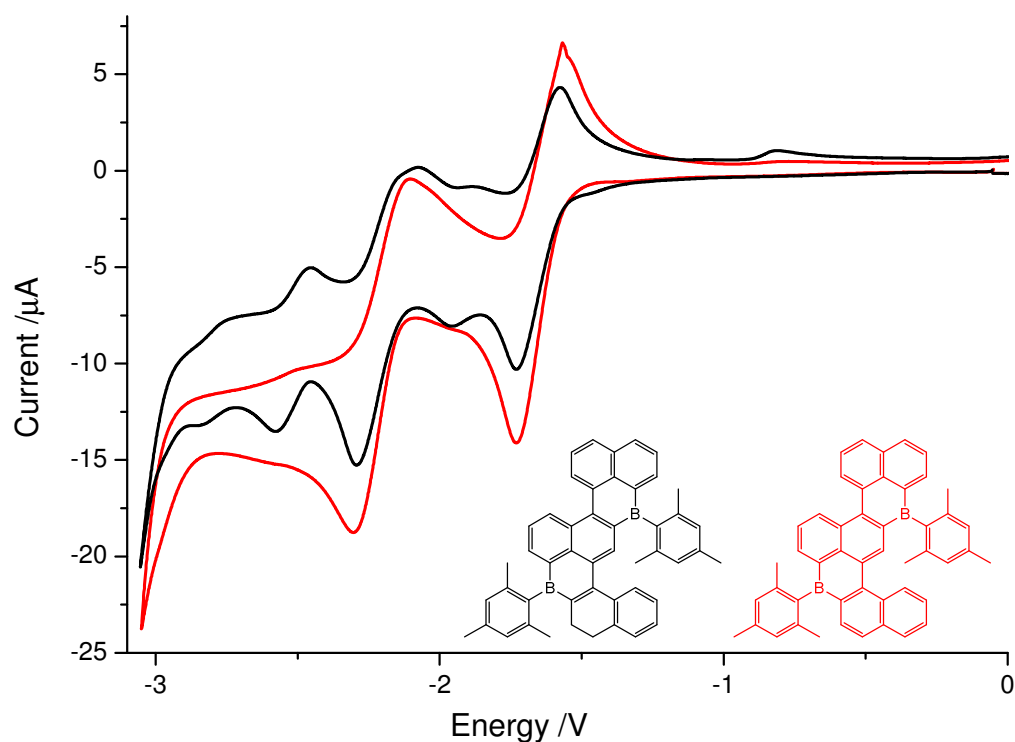
Figure S6 Absorbance, excitation and emission spectra of **9** in MeCN.

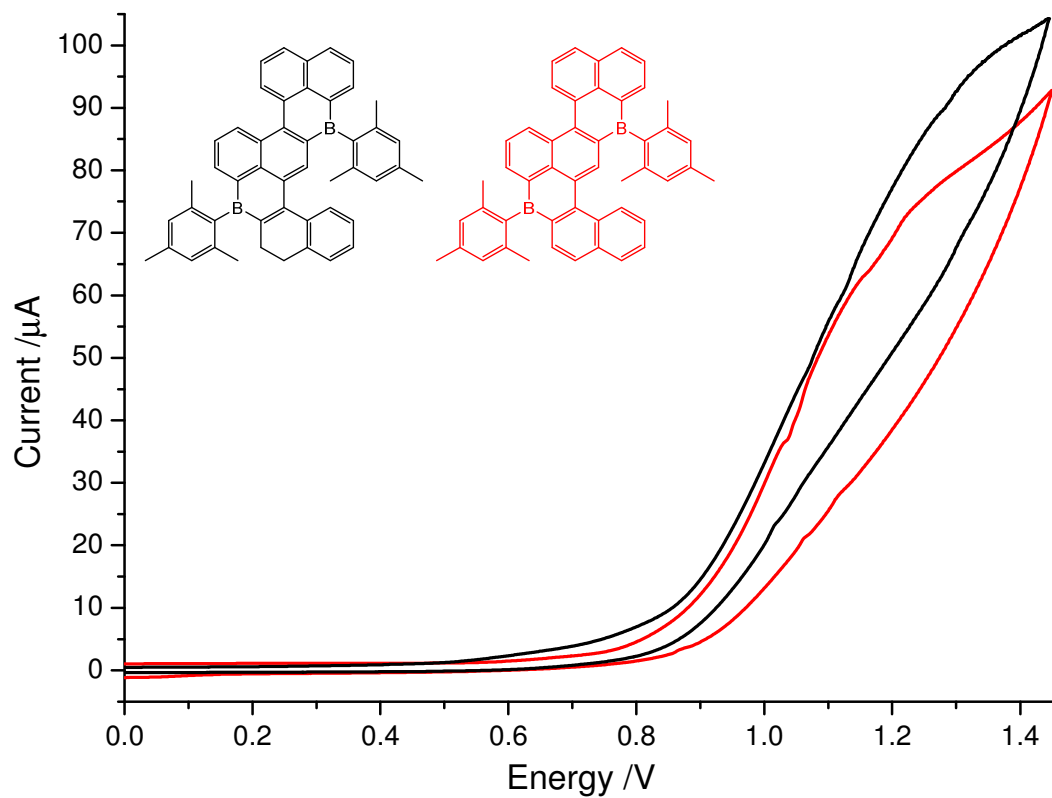
## Electrochemical Properties

**Table S4** Summary of cyclic voltammetry results

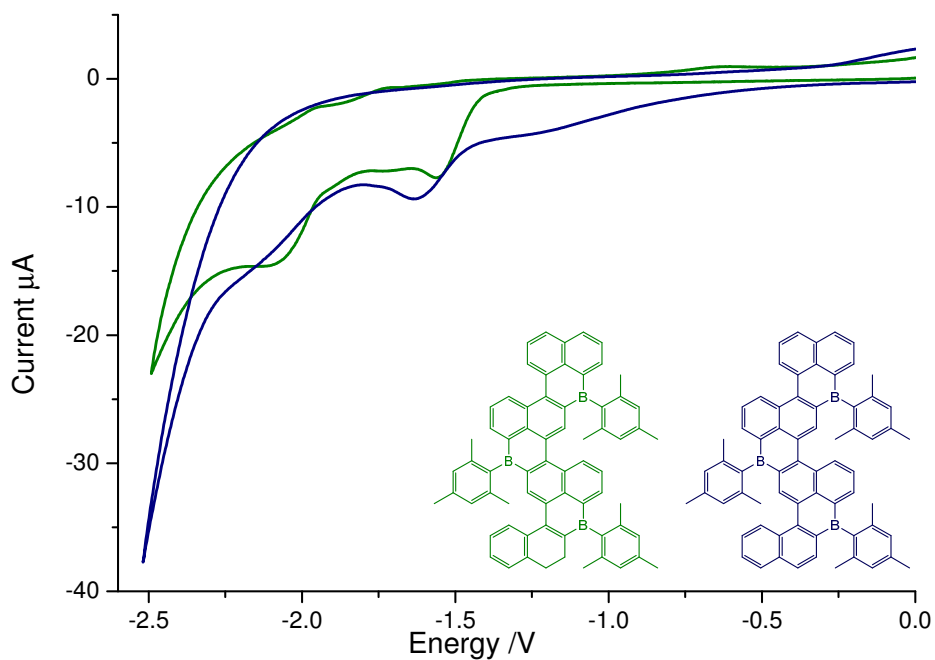
Compound	First Reduction				Second Reduction	Oxidation	
	$E_{pa}$ (V)	$E_{1/2}$ (V)	$E_{onset}$ (V)	$E_{LUMO}$ (eV)	$E_{pa}$ (V)	$E_{onset}$ (V)	$E_{HOMO}$ (eV)
<b>G</b> <sup>5</sup>	-2.00	-1.92	-1.85	-2.95	-2.65	–	–
<b>4</b>	-1.73	-1.65	-1.57	-3.23	-1.96	0.85	-5.65
<b>5</b>	-1.73	-1.65	-1.58	-3.22	-2.30	0.88	-5.68
<b>8</b>	-1.56	–	-1.41	-3.39	-2.12	0.89	-5.69
<b>9</b>	-1.63	–	-1.39	-3.42	–	0.90	-5.70
<b>J</b> <sup>5</sup>	-1.46	-1.39	-1.32	-3.48	-1.93	–	–

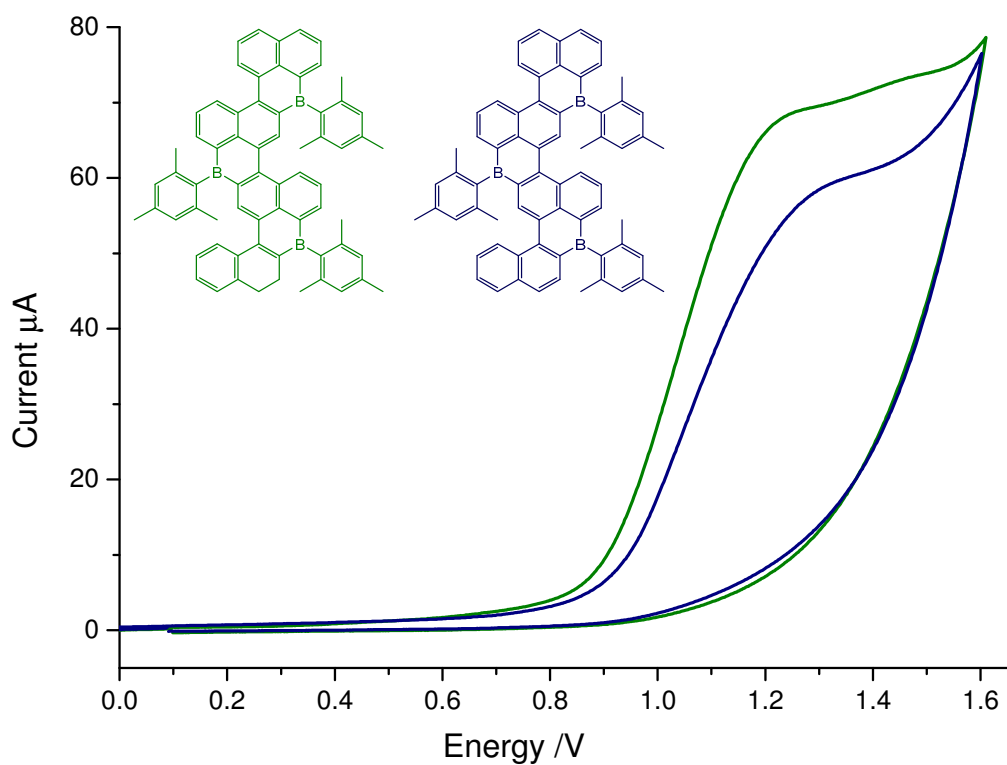
Measured in THF (1 mM) with [<sup>n</sup>Bu<sub>4</sub>N][PF<sub>6</sub>] (0.1 M) as the supporting electrolyte at a scan rate of 50 mV/s. Potentials are given relative to the Fc/Fc<sup>+</sup> redox couple.  $E_{LUMO} = -4.8$  eV – (onset of first reduction) as Fc/Fc<sup>+</sup> is taken to be  $-4.8$  eV vs vacuum level.<sup>1</sup> No oxidation waves are observed within the potential window on THF for **G** and **J**.<sup>5</sup> Oxidation waves for **4**, **5**, **8** and **9** were unstable with cycling. The first reduction wave of each compound was reversible to at least 10 cycles, except for compound **9** which was unstable with cycling





**Figure S7** Cyclic Voltammetry plots of **5** and **6**. Measured in THF (1 mM), with  $[\text{Bu}_4\text{N}][\text{PF}_6]$  (0.1 M) as the supporting electrolyte at a scan rate of 50 mV/s.



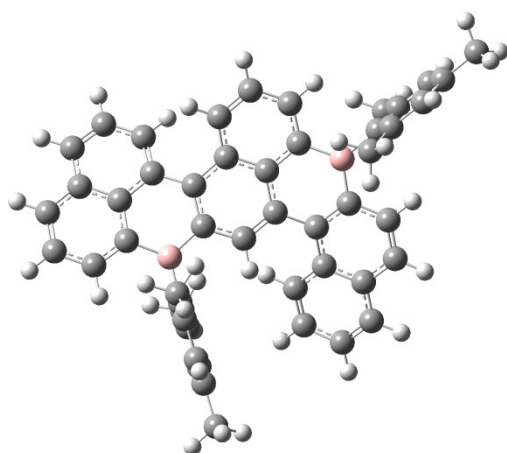


**Figure S8** Cyclic Voltammetry plots of **9** and **10**. Measured in THF (1 mM), with  $[\text{nBu}_4\text{N}][\text{PF}_6]$  (0.1 M) as the supporting electrolyte at a scan rate of 50 mV/s.



## Optimised Structure Coordinates

### Compound 5

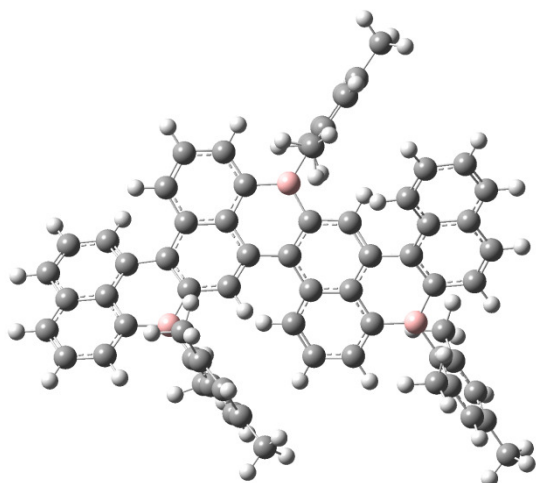


E(RM062X) = -1901.49419560

C	3.626200	9.485300	15.514700
C	4.001300	8.607700	14.439200
C	6.361700	6.756400	18.704800
C	6.639900	6.347900	20.036900
C	7.186400	6.274700	17.643000
C	5.050800	7.750500	14.690300
H	5.536700	7.241100	13.866400
C	2.860500	10.657600	15.241900
C	3.428100	8.743700	13.082900
C	5.217700	7.585900	18.450500
C	4.949600	8.097600	17.091100
C	4.115100	9.245900	16.835100
C	7.445000	5.864000	14.942800
C	8.283200	5.483200	17.947600
H	8.888900	5.095200	17.133500
C	3.177500	7.934400	10.764600
C	2.606400	11.556400	16.268300
H	2.044100	12.458900	16.046800
C	2.837800	9.951800	12.703100
C	5.533800	7.468900	15.991300
C	3.867900	10.234800	17.822500
H	4.329100	10.135100	18.795400
C	7.458500	4.179200	13.201300
H	7.010400	3.299800	12.745900
C	2.713900	9.223900	10.386200
C	8.590200	6.436700	14.369400
C	1.725900	12.330100	13.418300
C	4.325700	7.795400	19.490200
H	3.386000	8.296100	19.297900
C	3.119200	11.357000	17.556500
H	2.968200	12.101700	18.328400
C	8.595800	4.742900	12.622800
C	7.797300	5.570500	20.295500
H	8.013400	5.293400	21.322100

C	9.149300	5.870800	13.222400
H	10.030000	6.328800	12.781300
C	2.491200	10.172000	11.338700
H	2.062100	11.131500	11.066900
C	3.481500	7.658900	12.129800
C	6.880700	4.721000	14.346500
C	4.584700	7.351400	20.802000
H	3.860700	7.552400	21.581900
C	8.616100	5.155300	19.275200
H	9.491300	4.553200	19.486600
C	5.742900	6.678100	21.083400
H	5.969300	6.354000	22.093300
C	0.323900	12.407400	13.467800
C	3.288100	6.903500	9.797000
H	3.081300	7.146300	8.760300
C	9.204000	7.672700	14.983900
H	8.460400	8.468900	15.087600
H	10.024400	8.053100	14.374400
H	9.592300	7.462300	15.984900
C	2.457700	13.462600	13.025700
C	3.739900	6.302500	12.477400
H	3.838200	6.026900	13.517300
C	-0.317900	13.598100	13.131800
H	-1.403200	13.644100	13.166200
C	9.203400	4.136600	11.383500
H	8.446300	3.991400	10.609600
H	9.639700	3.158300	11.601900
H	9.989700	4.774200	10.977900
C	5.667400	4.066700	14.964300
H	5.931100	3.576700	15.906800
H	5.240300	3.313200	14.300800
H	4.889300	4.800400	15.196400
B	6.741300	6.520800	16.186900
C	3.618800	5.625700	10.161400
H	3.696300	4.845000	9.414100
C	0.400400	14.729800	12.747400
C	-0.478500	11.196800	13.882100
H	-0.220800	10.328600	13.267600
H	-1.549900	11.376400	13.785900
H	-0.269800	10.929000	14.922500
C	3.811400	5.318300	11.525200
H	3.999900	4.294400	11.826500
B	2.476100	10.994400	13.784000
C	3.965300	13.397000	12.964600
H	4.295600	12.584200	12.310300
H	4.387800	13.204200	13.955800
H	4.389800	14.329500	12.590900
C	1.790000	14.642300	12.697500
H	2.367100	15.511400	12.393200
C	-0.309800	16.018300	12.418400
H	-1.253700	15.827300	11.904700
H	0.306300	16.656800	11.783600
H	-0.539100	16.577200	13.330100
H	2.494400	9.412900	9.341000

Compound 9



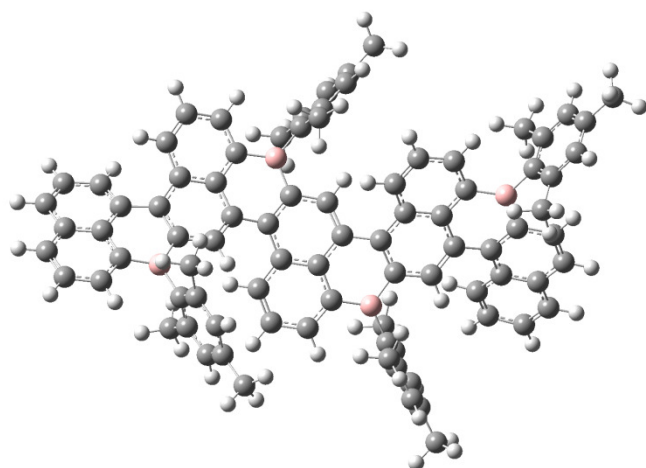
E(RM062X) = -2659.33491548

C	3.725300	9.580200	15.539900
C	4.071800	8.705500	14.451800
C	6.350100	6.703500	18.715700
C	6.634300	6.314300	20.059700
C	7.067000	6.104700	17.636300
C	5.083300	7.800600	14.691300
H	5.543900	7.277600	13.861400
C	2.989500	10.775700	15.285300
C	3.505500	8.881900	13.097400
C	5.269500	7.615500	18.449100
C	5.007500	8.131600	17.095500
C	4.207100	9.308700	16.856200
C	7.338800	5.752000	14.930600
C	8.015100	5.128900	17.909700
H	8.534900	4.658300	17.080100
C	3.229300	8.116200	10.767100
C	2.743200	11.657300	16.328600
H	2.200200	12.574800	16.121400
C	2.961800	10.116700	12.734300
C	5.553000	7.482400	15.988600
C	3.973000	10.283500	17.861000
H	4.430100	10.159700	18.832900
C	7.272800	4.113300	13.147100
H	6.780100	3.271900	12.666200
C	2.819100	9.428700	10.406200
C	8.517400	6.276100	14.377300
C	1.914600	12.513000	13.486600
C	4.387500	7.843300	19.484400
H	3.435300	8.320000	19.280600
C	3.239900	11.420800	17.616600
H	3.093600	12.149800	18.404700
C	8.442800	4.628300	12.589200
C	7.575900	5.272200	20.263200
H	7.716500	4.876500	21.259600
C	9.052800	5.709700	13.219900

H	9.960700	6.129400	12.796000
C	2.629200	10.370400	11.372100
H	2.237900	11.349500	11.113800
C	3.517400	7.809100	12.129000
C	6.717800	4.656700	14.303400
C	4.663500	7.504400	20.830300
C	8.261400	4.697200	19.218900
H	8.956500	3.888600	19.408500
C	5.873000	6.883100	21.145500
C	0.515300	12.627800	13.534500
C	3.299900	7.095100	9.785600
H	3.107100	7.360400	8.751700
C	9.188200	7.465400	15.023200
H	8.517900	8.330700	15.038300
H	10.094400	7.750000	14.487400
H	9.457800	7.247900	16.060900
C	2.678100	13.631700	13.114900
C	3.715000	6.438400	12.458700
H	3.796200	6.144200	13.495300
C	-0.093000	13.841100	13.217400
H	-1.176700	13.916400	13.250300
C	9.028600	4.018000	11.341500
H	8.259900	3.875600	10.578800
H	9.463700	3.037900	11.554800
H	9.812800	4.650700	10.924300
C	5.468400	4.053400	14.900600
H	5.709100	3.488500	15.806800
H	4.979700	3.373300	14.201300
H	4.748200	4.824400	15.191300
B	6.668600	6.431700	16.181800
C	3.573800	5.799300	10.133200
H	3.620200	5.026300	9.375500
C	0.656900	14.959100	12.854100
C	-0.321400	11.433500	13.927900
H	-0.079500	10.565400	13.306800
H	-1.386900	11.641000	13.823400
H	-0.129800	11.149300	14.967200
C	3.747100	5.465000	11.493200
H	3.888200	4.429700	11.780900
B	2.625600	11.150400	13.831800
C	4.183600	13.526200	13.056600
H	4.493700	12.712900	12.393200
H	4.597800	13.309900	14.046400
H	4.634100	14.451500	12.695700
C	2.043700	14.834600	12.805500
H	2.645000	15.692600	12.516600
C	-0.016600	16.272500	12.546600
H	-0.972300	16.116400	12.043300
H	0.611200	16.898400	11.910700
H	-0.216700	16.828600	13.466900
H	2.611000	9.641400	9.363100
C	6.312500	6.816300	22.553500
C	5.367300	6.987200	23.620700
C	7.653100	6.701500	22.886100
C	4.013800	7.366700	23.368000
C	5.806200	6.842200	24.964500

C	8.088300	6.599700	24.222000
H	8.401800	6.711100	22.105200
C	3.144500	7.511300	24.438200
C	4.864600	6.963900	26.017900
C	7.178500	6.624300	25.244400
H	9.146500	6.497100	24.427500
C	3.553300	7.279300	25.764500
H	2.123700	7.827600	24.242200
H	5.209500	6.820100	27.036600
H	7.495500	6.520400	26.276200
H	2.846300	7.381300	26.578500
B	3.605100	7.752900	21.932300
C	2.197600	8.351900	21.565000
C	2.049900	9.734600	21.360000
C	1.088000	7.511500	21.371100
C	0.815800	10.250800	20.966300
C	-0.134800	8.056100	20.982800
C	-0.290400	9.425800	20.775500
H	0.716800	11.320300	20.800500
H	-0.982800	7.395300	20.825200
C	1.230600	6.019600	21.560100
H	1.495400	5.777900	22.593500
H	0.304900	5.498000	21.315000
H	2.024500	5.619200	20.921800
C	3.215000	10.666100	21.598300
H	3.030000	11.653200	21.171900
H	3.393900	10.791700	22.670800
H	4.141000	10.273600	21.167500
C	-1.625600	10.001300	20.378200
H	-1.502200	10.915900	19.796100
H	-2.201500	9.288800	19.785700
H	-2.217200	10.250300	21.263900

**Compound 10**



E(RM062X) = -3417.17570568

C	3.612900	9.521700	15.569900
C	3.893100	8.620600	14.482800
C	6.244300	6.582600	18.683800
C	6.553200	6.190300	20.021300
C	6.903000	5.947800	17.588400
C	4.882500	7.683600	14.694800
H	5.291400	7.136100	13.852900
C	2.895500	10.732100	15.331100
C	3.282400	8.797500	13.155100
C	5.196900	7.539900	18.443800
C	4.906500	8.049400	17.094000
C	4.140400	9.252800	16.868900
C	7.118200	5.605700	14.876800
C	7.812800	4.930300	17.840100
H	8.289600	4.435600	16.998700
C	2.905100	8.030800	10.823700
C	2.726100	11.637600	16.369500
H	2.198700	12.566600	16.172100
C	2.731200	10.029300	12.804400
C	5.389200	7.366900	15.977100
C	3.981900	10.249400	17.867200
H	4.474900	10.124500	18.821200
C	7.011200	3.983100	13.080700
H	6.503900	3.150800	12.599600
C	2.629500	9.387100	10.431100
C	8.295000	6.122500	14.312500
C	1.771500	12.455700	13.521900
C	4.364100	7.820800	19.506900
H	3.427300	8.336900	19.330800
C	3.276200	11.406900	17.636300
H	3.188000	12.151900	18.418000
C	8.179800	4.490300	12.512500
C	7.446900	5.103500	20.203900
H	7.596900	4.706400	21.198500
C	8.809300	5.560000	13.143900
H	9.716400	5.973300	12.712000
C	2.404700	10.286700	11.450600
H	1.973800	11.255400	11.226400
C	3.213300	7.730400	12.185400
C	6.477500	4.522300	14.249300
C	4.674500	7.488500	20.846500
C	8.072800	4.490400	19.143800
H	8.732700	3.649700	19.318600
C	5.861300	6.809100	21.126000
C	0.387800	12.631700	13.696900
C	2.763500	6.972200	9.877700
C	8.987000	7.299000	14.959400
H	8.328300	8.173000	14.985400
H	9.891900	7.575100	14.417000
H	9.263000	7.071700	15.993200
C	2.522700	13.493300	12.944500
C	3.316800	6.364300	12.555100
H	3.429900	6.108100	13.599100

C	-0.216600	13.821200	13.294900
H	-1.288800	13.942000	13.424500
C	8.744900	3.882800	11.253900
H	7.964000	3.739900	10.503900
H	9.185400	2.903300	11.458700
H	9.521100	4.517400	10.824700
C	5.230300	3.928700	14.860300
H	5.475400	3.369600	15.768800
H	4.732800	3.246200	14.169900
H	4.516400	4.705600	15.151300
B	6.481800	6.287500	16.144000
C	2.935200	5.659700	10.295500
H	2.802700	4.859600	9.572900
C	0.519700	14.854000	12.716000
C	-0.440700	11.524200	14.303900
H	-0.304500	10.586900	13.755400
H	-1.502800	11.771400	14.293300
H	-0.144400	11.335900	15.340100
C	3.203800	5.349100	11.634400
H	3.272200	4.317000	11.956800
B	2.460900	11.090300	13.894400
C	4.018700	13.353200	12.788300
H	4.296800	12.359600	12.425300
H	4.519000	13.488900	13.752500
H	4.419300	14.096100	12.096400
C	1.890100	14.671300	12.547000
H	2.479700	15.462500	12.091400
C	-0.147400	16.142000	12.306300
H	-1.168900	15.964900	11.965400
H	0.404200	16.633600	11.503500
H	-0.196400	16.836800	13.149600
C	6.349900	6.739000	22.517300
C	5.457700	6.978600	23.616700
C	7.693900	6.553900	22.800700
C	4.119100	7.431600	23.409400
C	5.939700	6.828800	24.945200
C	8.174200	6.446500	24.120500
H	8.411600	6.510000	21.992400
C	3.301000	7.639600	24.509100
C	5.048000	7.019000	26.031200
C	7.307600	6.537500	25.176100
H	9.232100	6.287000	24.288000
C	3.747000	7.403100	25.822400
H	2.293300	8.011900	24.346600
H	5.423700	6.872100	27.038500
H	7.658700	6.430500	26.196500
H	3.078900	7.556200	26.660800
B	3.679700	7.823500	21.984600
C	2.309800	8.524700	21.658800
C	2.264200	9.913700	21.449200
C	1.134300	7.771600	21.498400
C	1.063700	10.521800	21.083400
C	-0.052400	8.407100	21.137200
C	-0.106900	9.783900	20.924400
H	1.043400	11.595100	20.914500
H	-0.953500	7.814000	21.006300

C	1.167600	6.273900	21.692600
H	1.459500	6.016300	22.714800
H	0.193600	5.825800	21.493500
H	1.897900	5.810200	21.021700
C	3.503700	10.753300	21.650700
H	3.372500	11.759600	21.250200
H	3.738300	10.843200	22.716000
H	4.378900	10.304400	21.171400
C	-1.403700	10.457600	20.554800
H	-1.223300	11.385900	20.010700
H	-2.022800	9.807600	19.934200
H	-1.979400	10.704900	21.451200
C	2.412200	9.761600	9.017100
C	2.536000	11.130700	8.571000
C	2.059800	8.776600	8.091100
C	3.208300	12.151200	9.301800
C	2.036400	11.475400	7.281600
C	1.623100	9.153600	6.788100
C	3.270800	13.441700	8.841100
H	3.723700	11.901000	10.218000
C	2.085400	12.823600	6.844800
C	1.545900	10.461100	6.414400
H	1.328700	8.368000	6.099100
C	2.670200	13.794000	7.613600
H	3.801600	14.191300	9.416300
H	1.669500	13.064900	5.872600
H	1.167300	10.747800	5.439300
H	2.708700	14.819500	7.266300
B	2.254600	7.287900	8.453800
C	1.968500	6.145100	7.408300
C	0.656600	5.674400	7.223000
C	3.007200	5.583700	6.649700
C	0.406400	4.661600	6.299700
C	2.727300	4.574400	5.727600
C	1.431500	4.100600	5.538500
H	-0.610200	4.300000	6.170100
H	3.539500	4.148100	5.145100
C	-0.473900	6.268100	8.029500
H	-0.273900	6.189300	9.102600
H	-0.597700	7.331800	7.803100
H	-1.418500	5.764200	7.822300
C	4.424400	6.071300	6.838300
H	4.480600	7.159500	6.735500
H	4.792600	5.823300	7.838400
H	5.099900	5.626000	6.107000
C	1.134300	3.027500	4.522000
H	0.396500	2.318800	4.903300
H	0.727100	3.463800	3.605600
H	2.036800	2.475600	4.255600



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