

Supporting Information

Double Boron–Oxygen-Fused Polycyclic Aromatic Hydrocarbons: Skeletal Editing and Applications in Organic Optoelectronic Materials

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Methods

Synthesis and Structure Characterization. Unless noted, all commercial reagents were purchased and used as received without further purification. ^1H NMR spectra were recorded at 400 or 500 MHz, and ^{13}C NMR spectra were recorded at 100 or 150 MHz NMR instruments in CDCl_3 or $\text{DMSO-}d_6$ solutions and chemical shifts were referenced to tetramethylsilane (TMS) or residual protiated solvent. If CDCl_3 was used as solvent, ^1H and ^{13}C NMR spectra were recorded with TMS ($\delta = 0.00$ ppm) and CDCl_3 ($\delta = 77.00$ ppm) as internal references, respectively. If $\text{DMSO-}d_6$ was used as solvent, ^1H and ^{13}C NMR spectra were recorded with TMS ($\delta = 0.00$ ppm) and $\text{DMSO-}d_6$ ($\delta = 39.52$ ppm) as internal references, respectively. The following abbreviations (or combinations thereof) were used to explain ^1H NMR multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, m = multiplet, br = broad. All of the new compounds were analyzed for HRMS on a Waters mass spectrometer using electrospray ionization in positive ion mode of ESI-Q-TOF.

X-ray Crystallography. X-ray diffraction data were collected at 170 K on a Bruker D8 Venture diffractometer using graphite-monochromated $\text{Mo-K}\alpha$ radiation ($\lambda = 0.71073$ Å) from a rotating anode generator.

Quantum Chemical Calculations. The theoretical calculations were performed using Gaussian 09. The molecular geometries of ground states (S_0) were optimized with the density functional theory (DFT) method. The DFT calculations were performed using a B3LYP function with a basis set of 6-31G(d) for C, H, O and B atoms.

Electrochemistry. Cyclic voltammetry and different pulsed voltammetry were performed using a CH1760E electrochemical analyzer according previous report. 0.1 M tetra-*n*-butylammonium hexafluorophosphate was used as the supporting electrolyte, anhydrous *N,N*-dimethylformamide, was used as the solvents for the E_{ox} and E_{red} measurements, and the solutions were bubbled with nitrogen for 15 min prior to the test. Silver wire, platinum wire and glassy carbon were used as pseudoreference electrode, counter electrode, and working electrode respectively. Scan rate was 300 mV/s. The redox potentials are based on the values measured from different pulsed voltammetry and are reported relative to an internal reference ferrocenium/ferrocene ($\text{Cp}_2\text{Fe}/\text{Cp}_2\text{Fe}^+$). The reversibility of reduction or oxidation was determined using CV. As defined, if the magnitudes of the peak anodic and the peak cathodic current have an equal magnitude as scan speeds of 100 mV/s or slower, then

the process is considered reversible; if the magnitudes of the peak anodic and the peak cathodic currents are not equal, but the return sweeps are nonzero, the process is considered quasi-reversible; otherwise, the process is considered irreversible.

Photophysical Measurements. The absorption spectra were measured on an Agilent 8453 UV–VS Spectrometer. Steady state emission experiments and lifetime measurements were performed on a Horiba Jobin Yvon FluoroLog-3 spectrometer. Low temperature (77 K) emission spectra and lifetimes were measured in 2-MeTHF cooled with liquid nitrogen.

OLED Fabrication and Characterization. All devices were fabricated by vacuum thermal evaporation, and were tested outside glove box after encapsulation. Prior to deposition, the prepatterned ITO coated glass substrates were cleaned by subsequent sonication in deionized water, acetone, and isopropanol. The metal layer and organic layers were fabricated by vacuum thermal evaporation on the cleaned indium-tin-oxide (ITO) glass substrate under vacuum ($< 4 \times 10^{-4}$ Pa) with 4 Å/s deposition rate for aluminum cathode and 2 Å/s for organic layers. The device areas were 9 mm² (3 mm × 3 mm). The current density-voltage-luminance characteristics of OLEDs were measured using a Keithley 2400 Source meter and a Keithley 2000 Source multimeter equipped with a calibrated silicon photodiode. The electroluminescence (EL) spectra were recorded with a multichannel spectrometer (PMA12, Hamamatsu Photonics).

Estimation of experimental oscillator strength. The theoretical quantity of the oscillator strength f in the classical theory of light absorption is related to the extinction coefficient ε of absorption by the expression [N. J. Turro, V. Ramamurthy, J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules; University Science Books, 2009; pp195–200.]:

$$f \equiv 4.3 \times 10^{-9} \int \varepsilon \, d\bar{\nu} \quad (\text{S1})$$

Where ε is the experimental extinction coefficient and $\bar{\nu}$ is the energy of the absorption. With the assumption that the absorption spectrum is a smooth Gaussian curve which can be approximated by an isosceles triangle, we can have $\int \varepsilon \, d\bar{\nu} \sim \varepsilon_{\max} \Delta\bar{\nu}_{1/2}$, where $\varepsilon_{\max}$ is the value of ε at the absorption maximum and $\Delta\bar{\nu}_{1/2}$ is the full-width half-maximum (FWHM) of the absorption band.

With the experiment data extracted from the UV-Vis spectrum and **Equation S1**, the approximate of f can be obtained:

$$f \sim 4.3 \times 10^{-9} \varepsilon_{\max} \Delta\bar{\nu}_{1/2} \quad (\text{S2})$$

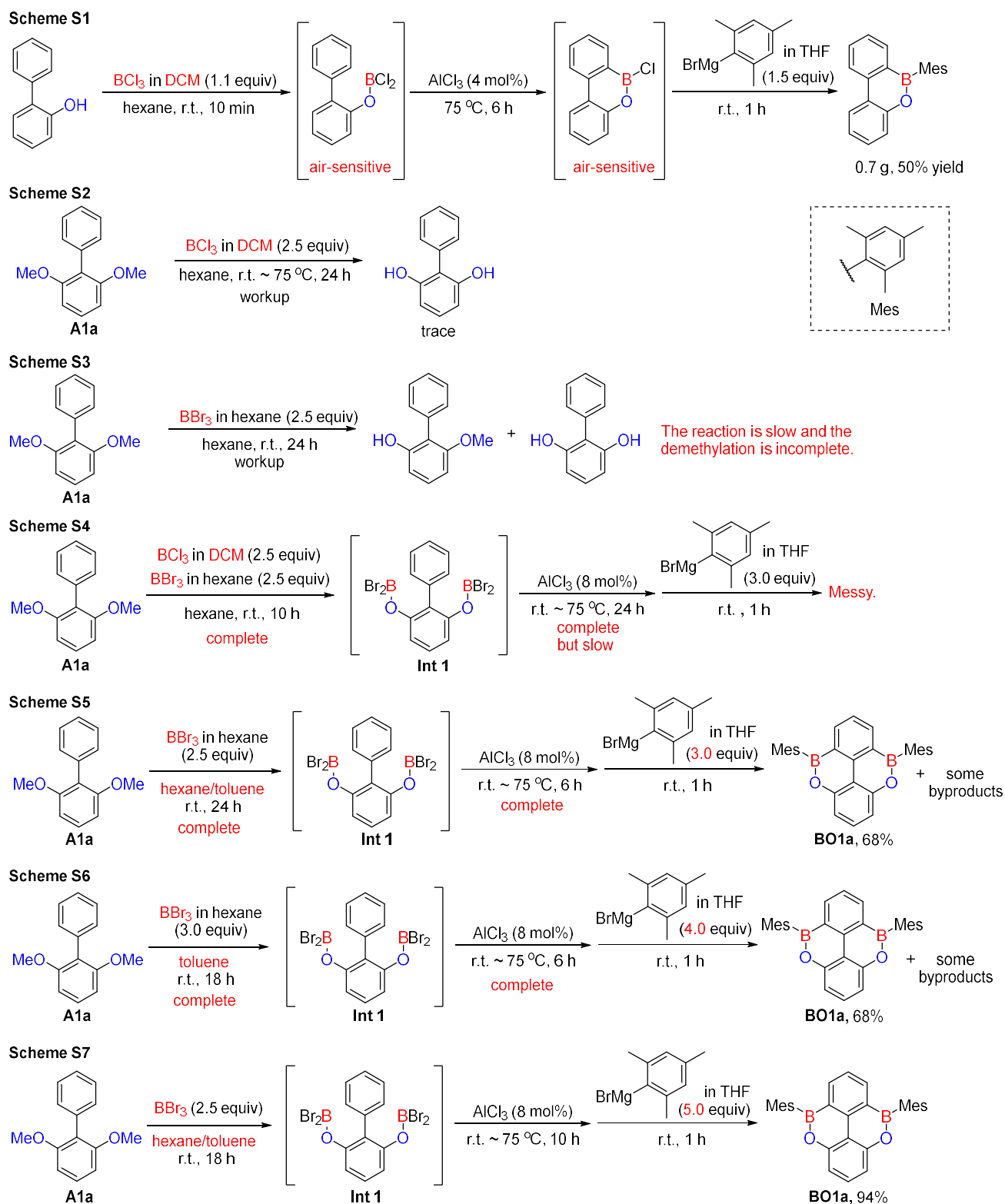


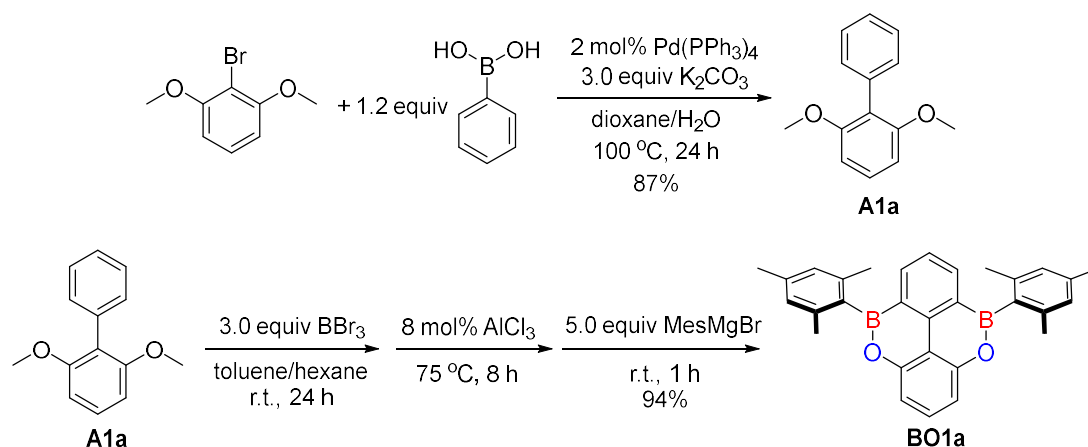
Fig. S1. Reaction condition optimization. Template reactions and selected optimization of reaction conditions

Reaction Condition Optimization. We initiated our examination by carrying out template reactions (see Supporting Information [Figure S1](#), [Scheme S1](#)). To our delight, [1,1'-Biphenyl]-2-ol smoothly transformed into 9,10-boroxarophenanthrene in hexane with 50% isolated yield using BCl₃-dichloromethane solution, AlCl₃ and mesitylmagnesium bromide (MesMgBr) as boron source, Lewis acid catalyst and nucleophilic reagent, respectively ([Scheme S1](#)). Then, we investigated the demethylation reaction of 2,6-dimethoxy-1,1'-biphenyl (**A1a**) using BCl₃-dichloromethane solution, however, only trace desired product [1,1'-biphenyl]-2,6-diol was obtained ([Scheme S2](#)), however, the demethylation reaction could be significantly improved through employing BBr₃-hexane solution, although the reaction proceeded slowly and the demethylation was incomplete ([Scheme S3](#)). After many optimized reactions, it was found that the demethylation could proceed completely by using a combine of 2.5 equiv BBr₃-dichloromethane and 2.5 equiv BBr₃-hexane solutions, however, this reaction system decelerated the followed electrophilic borylation and also made the final products messy ([Scheme S4](#)). This result revealed that the dichloromethane molecules had a great influence on the electrophilic borylation and nucleophilic substitution, which was unfavourable to the B–C bond formation owing to the strong coordination of the chlorine atoms. Thus, as might be expected, 68% isolated yield of **BO1a** could be obtained using only 2.5 equiv BBr₃-hexane solution as demethylation reagent ([Scheme S5](#)). Moreover, it was demonstrated that pure BBr₃ also accelerated the demethylation, and nonpolar solvents (hexane/toluene) improved the solubility of the intermediates and enhanced the reaction rate, additionally, the reaction time of the electrophilic borylation was also critical, carefully monitoring was necessary, prolonging the reaction time was not beneficial to the final product ([Schemes S5–S7](#)). Finally, 94% isolated yield of **BO1a** in gram scale could be achieved using 2.5 equiv pure BBr₃, 8 mol% AlCl₃ and 5.0 equiv MesMgBr for the corresponding demethylation, electrophilic borylation and nucleophilic substitution steps, respectively ([Scheme S7](#)). Notably, bulky Mes groups were incorporated to enhance molecular stability, which protected the boron from nucleophilic reagents. The attempt for the nucleophilic substitution of using (2,4,6-triisopropylphenyl)lithium was unsuccessful typically owing to its excessive steric hindrance.

General Experimental Procedure for the Synthesis of Dimethoxy Compounds and Double BO-Fused Polycyclic Aromatic Hydrocarbons (dBO-PAHs).

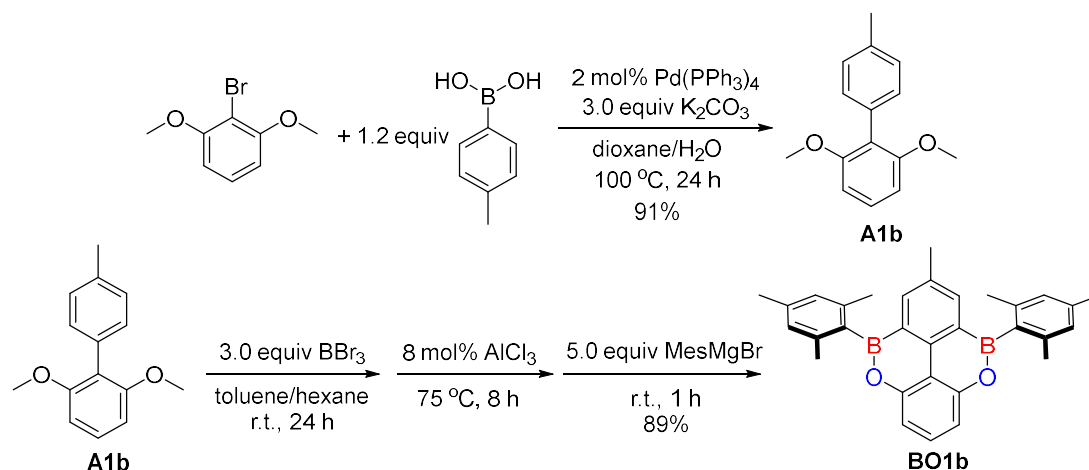
Aryl bromide or aryl iodide, aryl boronic acid and $\text{Pd}(\text{PPh}_3)_4$ were added to a dry three-necked flask equipped with a magnetic stir bar and a condensor. The flask was then evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then solvent dioxane and a solution of K_2CO_3 in H_2O were added under nitrogen atmosphere. The mixture was bubbled with nitrogen for 20 minutes and the flask was placed in oil bath (95 or 100 °C) and stirred for 24 hour until the starting material was consumed completely monitoring by TLC. Then the mixture was cooled down, diluted with ethyl acetate. The organic layer was then separated, and aqueous layer was extracted with ethyl acetate twice. The combined organic layer was dried over anhydrous Na_2SO_4 , filtered and concentrated under reduced pressure. The residue was purified through column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to afford the desired dimethoxy compound.

The dimethoxy compound was added to a dry three-necked flask equipped with a magnetic stir bar and a condensor. The flask was then evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then solvent toluene and *n*-hexane were added under nitrogen atmosphere, then BBr_3 was added dropwise. The mixture was stirred at room temperature for 18–40 hours monitoring by TLC until the demethylation was completely. Then AlCl_3 was added quickly, the flask was placed in oil bath (75 °C) and stirred for 8–10 hour, and then the mixture was cooled down to room temperature. Mesitylmagnesium bromide (MesMgBr) was then added dropwise, and the mixture was then stirred at room temperature for another 1–2 hours monitoring by TLC until the reaction was completely. The reaction mixture was concentrated under reduced pressure, and the residue was purified through column chromatography on silica gel using petroleum ether/dichloromethane as eluent to afford the desired double BO-fused polycyclic aromatic hydrocarbon.



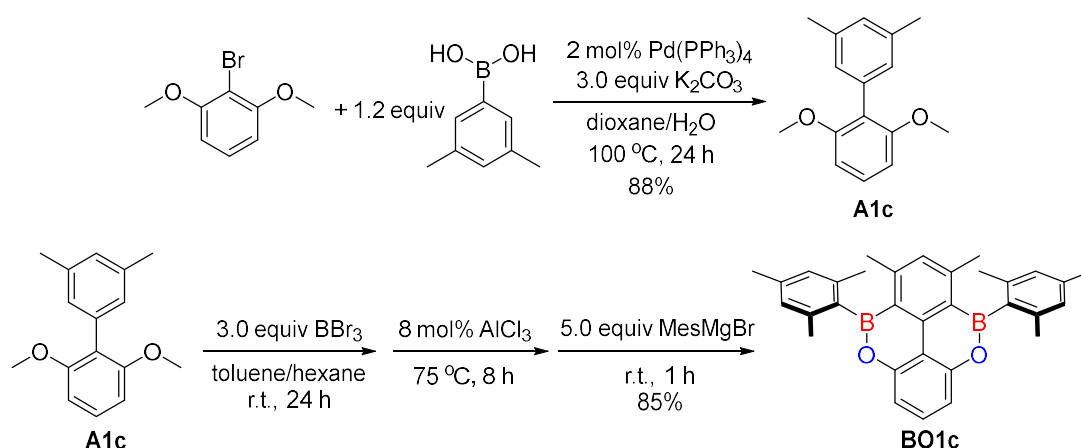
Synthesis of A1a: Following the general procedure, the reaction of 2-bromo-1,3-dimethoxybenzene (2.17 g, 10.00 mmol, 1.0 equiv), phenylboronic acid (1.46 g, 12.00 mmol, 1.2 equiv), Pd(PPh₃)₄ (213 mg, 0.20 mmol, 0.02 equiv) and K₂CO₃ (4.15 g, 30.00 mmol, 3.0 equiv, in 15 mL H₂) in dioxane (60 mL) at 100 °C for 24 hours afforded **A1a** (eluent: petroleum ether/ethyl acetate = 10:1–5:1) as a white solid 1.86 g in 87% yield. ¹H NMR (400 MHz, CDCl₃): δ (ppm) 3.78 (s, 6H), 6.71 (d, *J* = 8.4 Hz, 2H), 7.34 (t, *J* = 8.4 Hz, 2H), 7.37–7.49 (m, 4H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 55.81, 104.14, 119.49, 126.68, 127.59, 128.57, 130.83, 134.08, 157.60. The ¹H and ¹³C NMR data are agreement with the previous report (Truong, T.; Daugulis, O. Base-mediated intermolecular sp² C-H bond arylation via benzyne intermediates. *J. Am. Chem. Soc.* **2011**, *133*, 4243–4245).

Synthesis of BO1a: Following the general procedure, BBr₃ (1.16 mL, d = 2.6 g/mL, 12.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A1a** (857 mg, 4.00 mmol, 1.0 equiv) in toluene (40 mL) and *n*-hexane (40 mL) and stirred at room temperature for 24 hours, added AlCl₃ (42 mg, 0.32 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (20 mL, 1.0 M in THF, 20 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO1a** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.66 g in 94% yield. ¹H NMR (500 MHz, DMSO-*d*₆): δ (ppm) 2.15 (s, 12H), 2.33 (s, 6H), 6.95 (s, 4H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.75–7.79 (m, 2H), 8.08 (d, *J* = 7.0 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.31, 22.56, 112.91, 113.69, 126.80, 127.18, 127.43, 128.91, 133.89, 138.52, 140.09, 140.15, 141.65, 151.50. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 46.31. HRMS (ESI): calcd for C₃₀H₂₈[¹¹B]₂NaO₂⁺ [M+Na]⁺ 465.2168, found 465.2185.



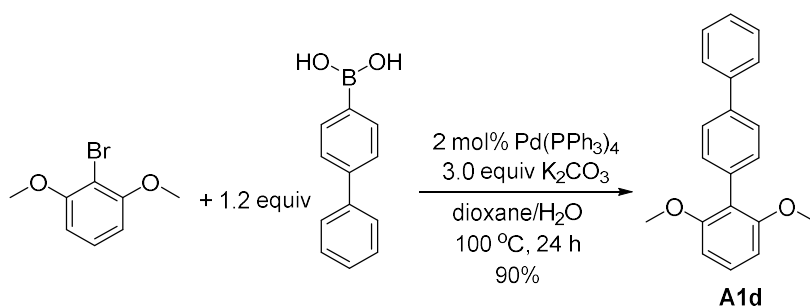
Synthesis of A1b: Following the general procedure, the reaction of 2-bromo-1,3-dimethoxybenzene (2.17 g, 10.00 mmol, 1.0 equiv), 4-methylphenylboronic acid (1.63 g, 12.00 mmol, 1.2 equiv), Pd(PPh₃)₄ (213 mg, 0.20 mmol, 0.02 equiv) and K₂CO₃ (4.15 g, 30.00 mmol, 3.0 equiv, in 15 mL H₂O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A1b** (eluent: petroleum ether/ethyl acetate = 10:1–5:1) as a white solid 2.08 g in 91% yield. ¹H NMR (500 MHz, DMSO-*d*₆): δ (ppm) 2.32 (s, 3H), 3.64 (s, 6H), 6.72 (d, *J* = 8.5 Hz, 2H), 7.10–7.03 (m, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.27 (t, *J* = 8.5 Hz, 1H). The ¹H NMR is in agreement with the previous report (Dai, J.-J.; Liu, J.-H.; Luo, D.-F.; Liu, L. Pd-catalysed decarboxylative Suzuki reactions and orthogonal Cu-based O-arylation of aromatic carboxylic acids. *Chem. Commun.* **2011**, 47, 677–679).

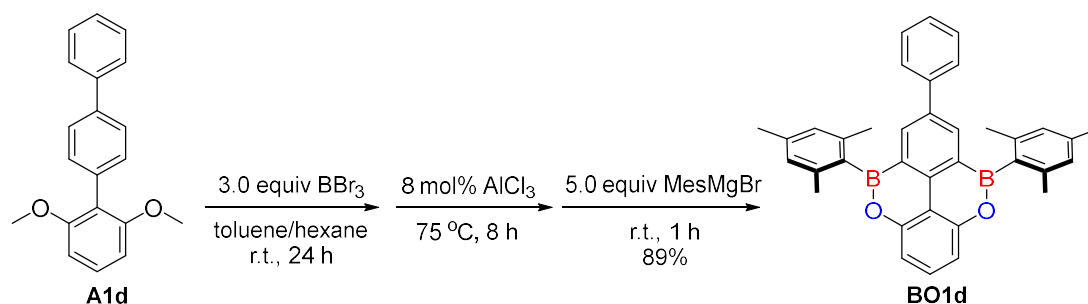
Synthesis of BO1b: Following the general procedure, BBr₃ (1.16 mL, d = 2.6 g/mL, 12.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A1b** (913 mg, 4.00 mmol, 1.0 equiv) in toluene (40 mL) and *n*-hexane (40 mL) and stirred at room temperature for 24 hours, added AlCl₃ (42 mg, 0.32 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (20 mL, 1.0 M in THF, 20 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO1b** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.62 g in 89% yield. m.p.: 276.2–277.9 °C. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.26 (s, 12H), 2.40 (s, 6H), 2.46 (s, 3H), 6.99 (s, 4H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.61–7.64 (m, 1H), 8.00 (s, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.33, 21.52, 22.57, 112.97, 113.56, 126.85, 127.41, 128.33, 134.11, 137.11, 137.79, 138.49, 140.20, 142.12, 151.28. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 49.59. HRMS (ESI): calcd for C₃₁H₃₁[¹¹B]₂O₂⁺ [M+H]⁺ 457.2505, found 457.2521.



Synthesis of A1c: Following the general procedure, the reaction of 2-bromo-1,3-dimethoxybenzene (2.17 g, 10.00 mmol, 1.0 equiv), 3,5-dimethylphenylboronic acid (1.80 g, 12.00 mmol, 1.2 equiv), Pd(PPh₃)₄ (213 mg, 0.20 mmol, 0.02 equiv) and K₂CO₃ (4.15 g, 30.00 mmol, 3.0 equiv, in 15 mL H₂O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A1c** (eluent: petroleum ether/ethyl acetate = 10:1–5:1) as a white solid 2.13 g in 88% yield. ¹H NMR (500 MHz, DMSO-*d*₆): δ (ppm) 2.26 (s, 6H), 3.63 (s, 6H), 6.70 (d, *J* = 8.5 Hz, 2H), 6.75 (s, 2H), 6.88 (s, 1H), 7.27 (t, *J* = 8.5 Hz, 1H).

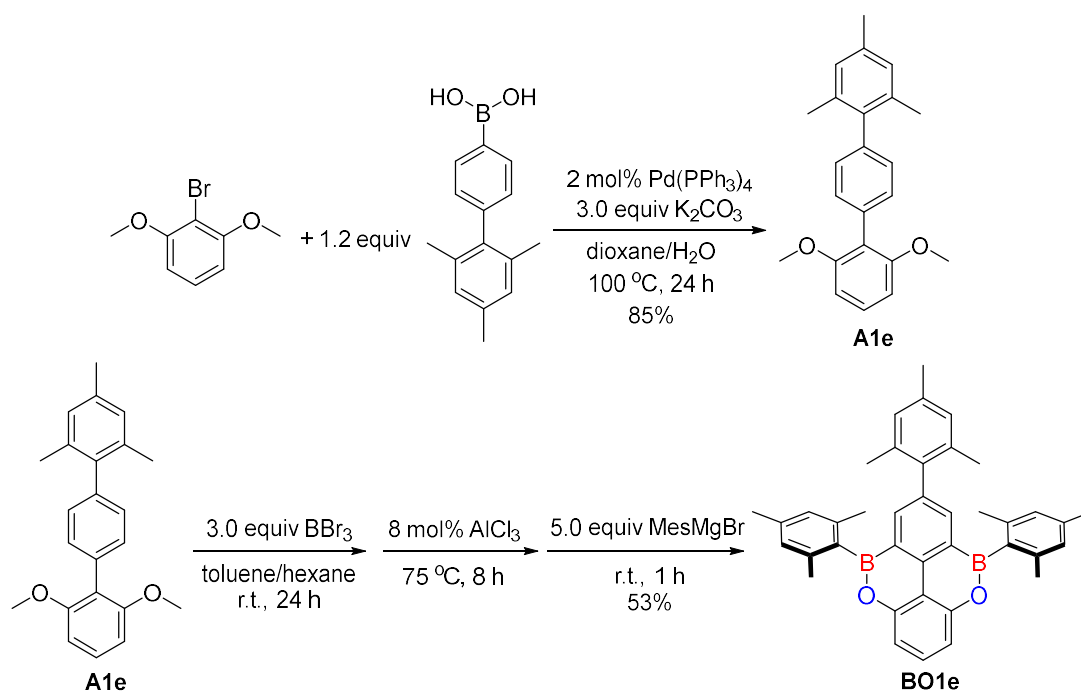
Synthesis of BO1c: Following the general procedure, BBr₃ (1.16 mL, *d* = 2.6 g/mL, 12.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A1c** (969 mg, 4.00 mmol, 1.0 equiv) in toluene (40 mL) and *n*-hexane (40 mL) and stirred at room temperature for 24 hours, added AlCl₃ (42 mg, 0.32 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (20 mL, 1.0 M in THF, 20 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO1c** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.62 g in 85% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.21 (s, 12H), 2.28 (s, 6H), 2.36 (s, 6H), 6.93 (s, 4H), 7.27 (s, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.57 (t, *J* = 8.0 Hz, 1H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.31, 22.13, 23.24, 112.87, 113.15, 123.50, 127.58, 128.67, 133.31, 137.94, 138.31, 139.30, 143.01, 151.45, 152.98. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 45.80. HRMS (ESI): calcd for C₃₂H₃₃[¹¹B]₂O₂⁺ [M+H]⁺ 471.2661, found 471.2677.





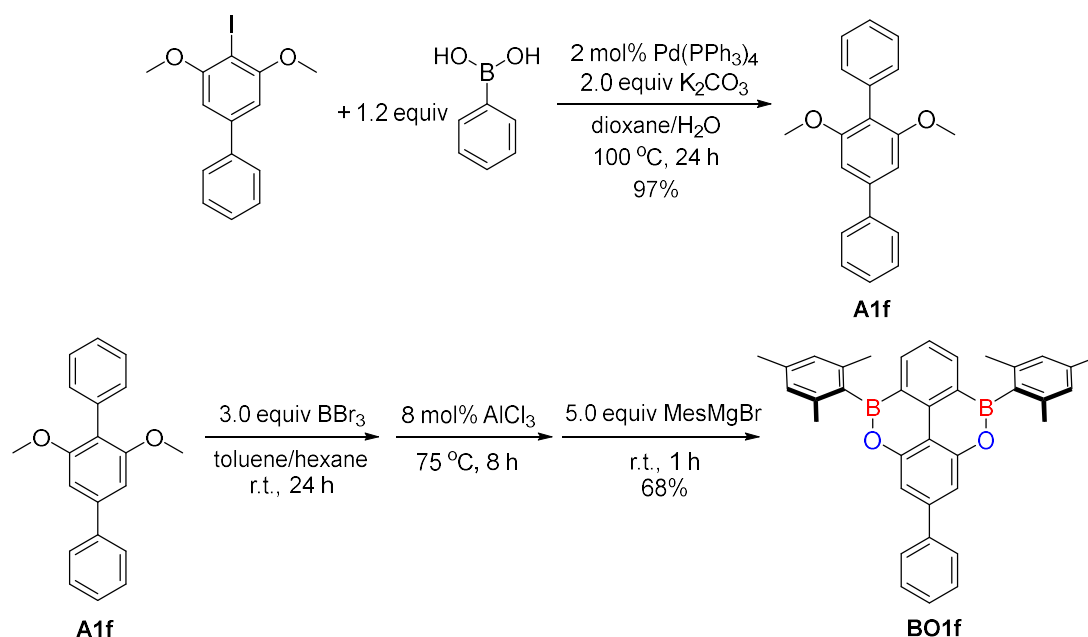
Synthesis of A1d: Following the general procedure, the reaction of 2-bromo-1,3-dimethoxybenzene (2.17 g, 10.00 mmol, 1.0 equiv), [1,1'-biphenyl]-4-ylboronic acid (2.38 g, 12.00 mmol, 1.2 equiv), Pd(PPh₃)₄ (213 mg, 0.20 mmol, 0.02 equiv) and K₂CO₃ (4.15 g, 30.00 mmol, 3.0 equiv, in 15 mL H₂O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A1d** (eluent: petroleum ether/ethyl acetate = 10:1–5:1) as a white solid 2.61 g in 90% yield. ¹H NMR (500 MHz, DMSO-*d*₆): δ (ppm) 3.68 (s, 6H), 6.76 (d, *J* = 8.5 Hz, 2H), 7.26–7.34 (m, 3H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.70 (d, *J* = 7.0 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 55.88, 104.18, 118.99, 126.41, 126.97, 127.11, 128.61, 128.68, 131.30, 133.07, 139.39, 141.24, 157.67. The ¹³C NMR is agreement with the previous reopr (Crowley, B. M.; Potteiger, C. M.; Deng, J. Z.; Prier, C. K.; Paone, D. V.; Burgey, C. S. Expanding the scope of the Cu assisted Suzuki–Miyaura reaction. *Tetrahedron Lett.* **2011**, 52, 5055–5059).

Synthesis of BO1d: Following the general procedure, BBr₃ (1.16 mL, d = 2.6 g/mL, 12.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A1d** (1.16 g, 4.00 mmol, 1.0 equiv) in toluene (40 mL) and *n*-hexane (40 mL) and stirred at room temperature for 24 hours, added AlCl₃ (42 mg, 0.32 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (20 mL, 1.0 M in THF, 20 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO1d** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.85 g in 89% yield. ¹H NMR (500 MHz, DMSO-*d*₆): δ (ppm) 2.20 (s, 12H), 2.33 (s, 6H), 6.96 (s, 4H), 7.36–7.40 (m, 1H), 7.45–7.48 (m, 2H), 7.51–7.53 (m, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.78 (t, *J* = 8.0 Hz, 1H), 8.20 (s, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.31, 22.65, 112.74, 113.71, 125.75, 127.53, 127.65, 128.79, 128.94, 129.54, 133.79, 138.53, 139.15, 140.16, 140.19, 140.30, 140.44, 151.45. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 48.79. HRMS (ESI): calcd for C₃₆H₃₃[¹¹B]₂O₂⁺ [M+H]⁺ 519.2661, found 519.2673.



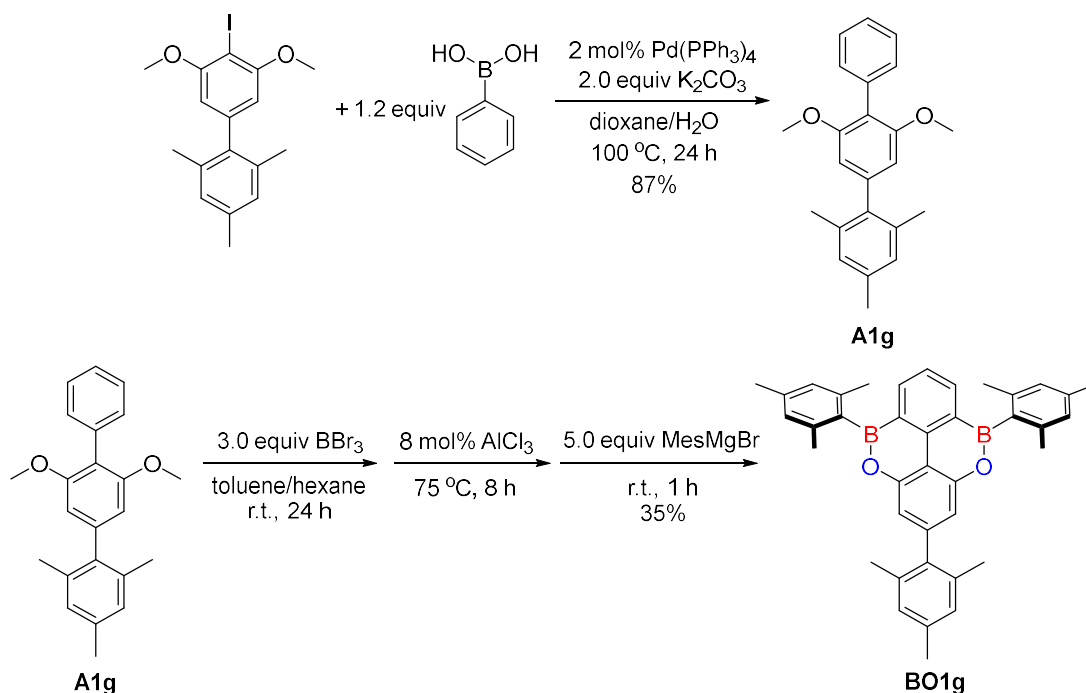
Synthesis of A1e: Following the general procedure, the reaction of 2-bromo-1,3-dimethoxybenzene (2.17 g, 10.00 mmol, 1.0 equiv), (2',4',6'-trimethyl-[1,1'-biphenyl]-4-yl)boronic acid (2.89 g, 12.00 mmol, 1.2 equiv), Pd(PPh₃)₄ (213 mg, 0.20 mmol, 0.02 equiv) and K₂CO₃ (4.15 g, 30.00 mmol, 3.0 equiv, in 15 mL H₂O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A1e** (eluent: petroleum ether/ethyl acetate = 10:1–5:1) as a white solid 2.83 g in 85% yield, which was directly used for the next step.

Synthesis of BO1e: Following the general procedure, BBr₃ (1.16 mL, d = 2.6 g/mL, 12.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A1e** (1.33 g, 4.00 mmol, 1.0 equiv) in toluene (40 mL) and *n*-hexane (40 mL) and stirred at room temperature for 24 hours, added AlCl₃ (42 mg, 0.32 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (20 mL, 1.0 M in THF, 20 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO1e** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.19 g in 53% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.18 (s, 3H), 2.28 (s, 12H), 2.31 (s, 6H), 2.38 (s, 6H), 6.97 (s, 4H), 7.12 (s, 2H), 7.49 (d, *J* = 8.5 Hz, 2H), 7.62–7.65 (m, 1H), 8.33 (s, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 15.13, 20.65, 21.32, 22.65, 112.83, 113.62, 126.96, 127.27, 127.49, 128.73, 133.98, 134.64, 136.90, 137.65, 138.47, 138.84, 140.26, 140.80, 151.41. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 47.17. HRMS (ESI): calcd for C₃₉H₃₉[¹¹B]₂O₂⁺ [*M*+*H*]⁺ 561.3131, found 561.3127.



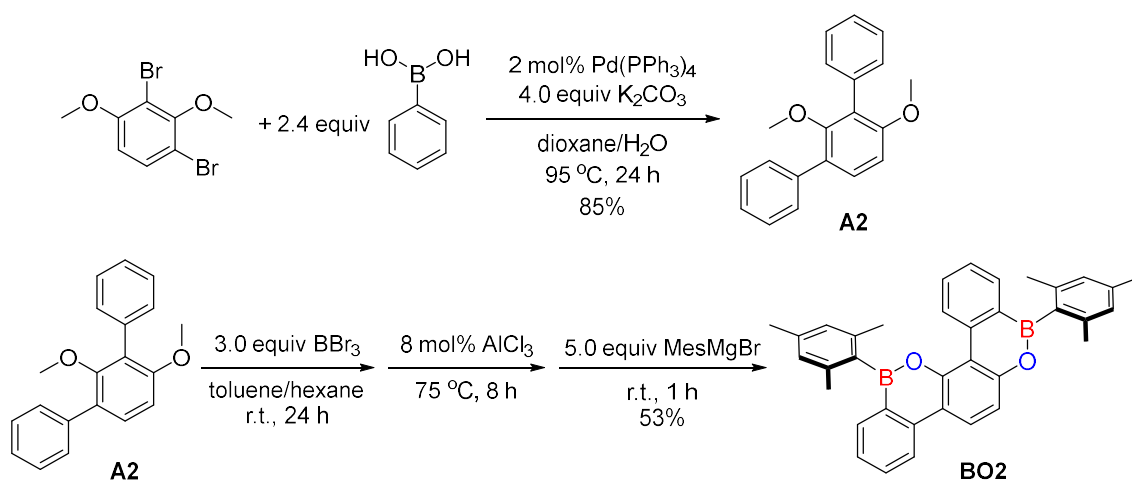
Synthesis of A1f: Following the general procedure, the reaction of 4-iodo-3,5-dimethoxy-1,1'-biphenyl (680 mg, 2.00 mmol, 1.0 equiv), phenylboronic acid (293 mg, 2.40 mmol, 1.2 equiv), Pd(PPh₃)₄ (46 mg, 0.04 mmol, 0.02 equiv) and K₂CO₃ (552 mg, 4.00 mmol, 2.0 equiv, in 5 mL H₂O) in dioxane (20 mL) at 100 °C for 24 hours afforded **A1f** (eluent: petroleum ether/ethyl acetate = 10:1) as a white solid 564 mg in 97% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 3.80 (s, 6H), 6.86 (s, 2H), 7.31–7.35 (m, 1H), 7.37–7.44 (m, 5H), 7.46–7.49 (m, 2H), 7.64–7.66 (m, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 55.96, 103.45, 118.52, 126.80, 127.17, 127.55, 127.66, 128.75, 130.92, 133.87, 141.51, 142.15, 157.79.

Synthesis of BO1f: Following the general procedure, BBr₃ (0.29 mL, d = 2.6 g/mL, 3.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A1f** (290 mg, 1.00 mmol, 1.0 equiv) in toluene (20 mL) and *n*-hexane (20 mL) and stirred at room temperature for 24 hours, added AlCl₃ (12 mg, 0.08 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (5 mL, 1.0 M in THF, 5.00 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO1f** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 355 mg in 68% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.26 (s, 12H), 2.38 (s, 6H), 6.97 (s, 4H), 7.41 (t, *J* = 6.0 Hz, 1H), 7.50 (t, *J* = 6.5 Hz, 2H), 7.61 (t, *J* = 6.0 Hz, 1H), 7.75 (s, 1H), 7.76 (s, 3H), 8.18 (d, *J* = 6.0 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.32, 22.58, 111.86, 112.31, 126.71, 127.16, 127.35, 127.44, 128.00, 129.02, 133.82, 138.54, 139.99, 140.07, 140.14, 141.74, 142.31, 151.69. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 46.99. HRMS (ESI): calcd for C₃₆H₃₃[¹¹B]₂O₂⁺ [*M*+*H*]⁺ 519.2661, found 519.2672.



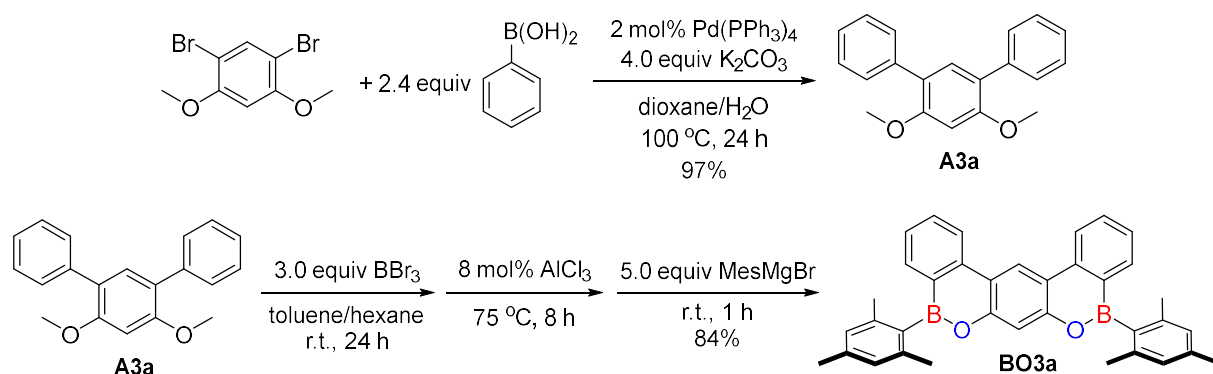
Synthesis of A1g: Following the general procedure, the reaction of 4'-iodo-3',5'-dimethoxy-2,4,6-trimethyl-1,1'-biphenyl (764 mg, 2.00 mmol, 1.0 equiv), phenylboronic acid (292 mg, 2.40 mmol, 1.2 equiv), Pd(PPh₃)₄ (46 mg, 0.04 mmol, 0.02 equiv) and K₂CO₃ (552 mg, 4.00 mmol, 2.0 equiv, in 5 mL H₂O) in dioxane (20 mL) at 100 °C for 24 hours afforded **A1g** (eluent: petroleum ether/ethyl acetate = 10:1) as a white solid 578 mg in 87% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.13 (s, 6H), 2.35 (s, 3H), 3.69 (s, 6H), 6.43 (s, 2H), 6.98 (s, 2H), 7.31–7.33 (m, 1H), 7.42 (d, *J* = 4.5 Hz, 4H).

Synthesis of BO1g: Following the general procedure, BBr₃ (0.29 mL, d = 2.6 g/mL, 3.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A1g** (332 mg, 1.00 mmol, 1.0 equiv) in toluene (20 mL) and *n*-hexane (20 mL) and stirred at room temperature for 24 hours, added AlCl₃ (12 mg, 0.08 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (5 mL, 1.0 M in THF, 5.00 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO1g** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 196 mg in 35% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.12 (s, 6H), 2.27 (s, 12H), 2.36 (s, 3H), 2.38 (s, 6H), 6.97 (s, 4H), 6.99 (s, 2H), 7.28 (s, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 8.18 (d, *J* = 7.0 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 20.88, 21.04, 21.31, 22.66, 111.34, 114.80, 126.70, 126.98, 127.44, 128.25, 133.90, 135.81, 136.96, 138.07, 138.54, 140.17, 140.24, 141.67, 142.62, 151.38. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 47.63. HRMS (ESI): calcd for C₃₉H₃₉[¹¹B]₂O₂⁺ [*M*+H]⁺ 561.3131, found 561.3147.



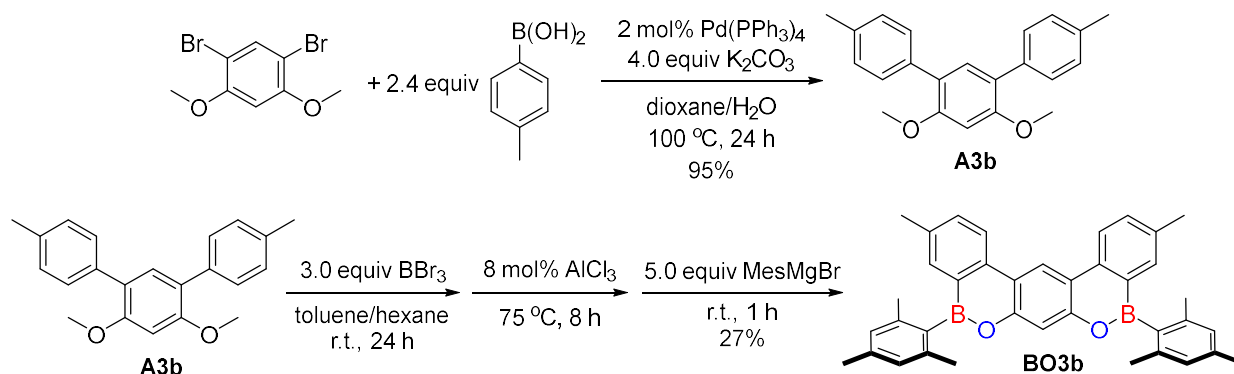
Synthesis of **A2:** Following the general procedure, the reaction of 1,3-dibromo-2,4-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), boronic acid (1.17 g, 9.60 mmol, 2.4 equiv), Pd(PPh₃)₄ (92 mg, 0.08 mmol, 0.02 equiv) and K₂CO₃ (2.21 g, 16.00 mmol, 4.0 equiv) in 10 mL H₂O in dioxane (40 mL) at 95 °C for 24 hours afforded **A2** (eluent: petroleum ether/ethyl acetate = 10:1–5:1) as a white solid 985 mg in 85% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 3.09 (s, 3H), 3.77 (s, 3H), 6.83 (d, *J* = 8.5 Hz, 1H), 7.29–7.36 (m, 3H), 7.38–7.44 (m, 6H), 7.56–7.58 (m, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 55.91, 60.37, 106.94, 125.03, 126.65, 126.91, 127.75, 128.07, 128.15, 129.13, 130.23, 130.62, 134.30, 138.67, 155.92, 157.15.

Synthesis of **BO2:** Following the general procedure, BBr₃ (0.58 mL, d = 2.6 g/mL, 6.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A2** (581 mg, 2.00 mmol, 1.0 equiv) in toluene (20 mL) and *n*-hexane (20 mL) and stirred at room temperature for 24 hours, added AlCl₃ (22 mg, 0.16 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (10 mL, 1.0 M in THF, 10 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO2** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 550 mg in 53% yield. m.p.: 277.1–278.2 °C. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.22 (s, 6H), 2.27 (s, 6H), 2.38 (s, 3H), 2.43 (s, 3H), 6.95 (s, 2H), 7.00 (s, 2H), 7.42–7.49 (m, 2H), 7.63 (d, *J* = 9.0 Hz, 1H), 7.71–7.74 (m, 1H), 7.83–7.86 (m, 3H), 8.41 (d, *J* = 8.0 Hz, 1H), 8.47 (d, *J* = 9.0 Hz, 1H), 9.61 (d, *J* = 8.0 Hz, 1H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.30, 21.36, 22.51, 22.78, 115.02, 116.47, 118.84, 121.78, 123.56, 126.91, 127.04, 127.33, 127.40, 128.00, 128.18, 129.79, 130.37, 133.57, 133.89, 134.27, 137.06, 137.23, 138.21, 138.31, 139.08, 140.18, 140.24, 150.49, 153.25. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 47.21. HRMS (ESI): calcd for C₃₆H₃₃[¹¹B]₂O₂⁺ [M+H]⁺ 519.2661, found 519.2655.



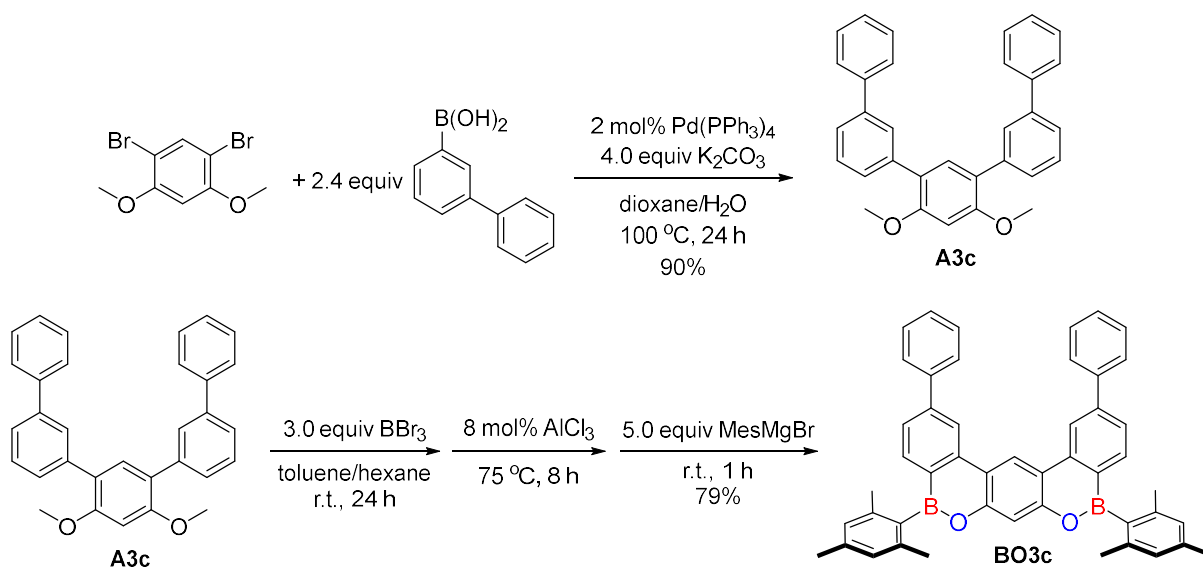
Synthesis of **A3a:** Following the general procedure, the reaction of 1,5-dibromo-2,4-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), boronic acid (1.17 g, 9.60 mmol, 2.4 equiv), $\text{Pd(PPh}_3)_4$ (92 mg, 0.08 mmol, 0.02 equiv) and K_2CO_3 (2.21 g, 16.00 mmol, 4.0 equiv, in 10 mL H_2O) in dioxane (40 mL) at $100\text{ }^\circ\text{C}$ for 24 hours afforded **A3a** (eluent: petroleum ether/ethyl acetate = 10:1–3:1) as a white solid 1.13 g in 97% yield. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 3.88 (s, 6H), 6.67 (s, 1H), 7.27–7.36 (m, 3H), 7.40 (t, $J = 7.5\text{ Hz}$, 4H), 7.55 (d, $J = 7.5\text{ Hz}$, 4H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 55.48, 111.14, 120.75, 127.49, 128.15, 128.49, 130.72, 130.75, 130.96, 138.11, 156.48. The ^1H NMR is agreement with the previous report (Ciana, C.-L.; Phipps, R. J.; Brandt, J. R.; Meyer, F.-M.; Gaunt, M. J. A highly *para*-selective copper(II)-catalyzed direct arylation of aniline and phenol derivatives. *Angew. Chem. Int. Ed.* **2011**, 50, 458–462).

Synthesis of **BO3a:** Following the general procedure, BBr_3 (0.87 mL, $d = 2.6\text{ g/mL}$, 9.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A3a** (871 mg, 3.00 mmol, 1.0 equiv) in toluene (30 mL) and *n*-hexane (30 mL) and stirred at room temperature for 24 hours, added AlCl_3 (32 mg, 0.24 mmol, 0.08 equiv) and stirred at $75\text{ }^\circ\text{C}$ for 8 hours, cooled down to room temperature, added MesMgBr (15 mL, 1.0 M in THF, 15 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO3a** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.30 g in 84% yield. ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ (ppm) 2.13 (s, 12H), 2.32 (s, 6H), 6.93 (s, 4H), 7.57 (t, $J = 7.5\text{ Hz}$, 2H), 7.67 (dd, $J = 8.0, 1.5\text{ Hz}$, 2H), 7.76 (s, 1H), 7.97 (td, $J = 7.5, 1.5\text{ Hz}$, 2H), 9.02 (d, $J = 8.0\text{ Hz}$, 2H), 9.58 (s, 1H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 21.28, 22.46, 111.29, 118.30, 119.56, 121.31, 127.18, 127.34, 128.88, 133.54, 134.09, 137.63, 138.40, 138.44, 140.06, 152.30. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 47.36. HRMS (ESI): calcd for $\text{C}_{36}\text{H}_{33}[^{11}\text{B}]_2\text{O}_2^+ [\text{M}+\text{H}]^+$ 519.2661, found 519.2671.



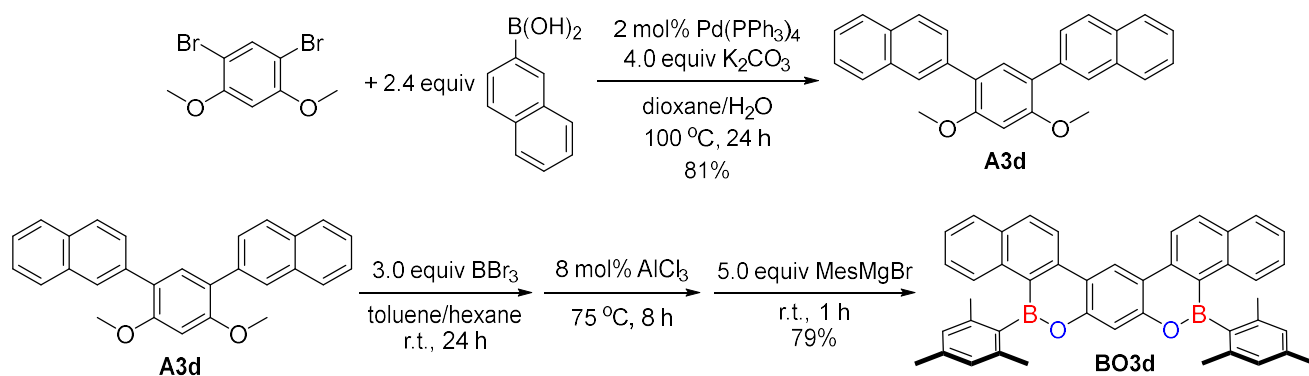
Synthesis of A3b: Following the general procedure, the reaction of 1,5-dibromo-2,4-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), 4-methylboronic acid (1.31 g, 9.60 mmol, 2.4 equiv), $\text{Pd(PPh}_3)_4$ (92 mg, 0.08 mmol, 0.02 equiv) and K_2CO_3 (2.21 g, 16.00 mmol, 4.0 equiv), in 10 mL H_2O in dioxane (40 mL) at $100\text{ }^\circ\text{C}$ for 24 hours afforded **A3b** (eluent: petroleum ether/ethyl acetate = 10:1–3:1) as a white solid 1.21 g in 95% yield. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 2.40 (s, 6H), 3.89 (s, 6H), 6.67 (s, 1H), 7.23 (d, $J = 8.0$ Hz, 4H), 7.31 (s, 1H), 7.44–7.46 (m, 4H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 21.13, 55.81, 96.23, 123.13, 128.73, 129.28, 132.66, 135.21, 136.15, 156.58.

Synthesis of BO3b: Following the general procedure, BBr_3 (0.87 mL, $d = 2.6\text{ g/mL}$, 9.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A3b** (955 mg, 3.00 mmol, 1.0 equiv) in toluene (30 mL) and *n*-hexane (30 mL) and stirred at room temperature for 24 hours, added AlCl_3 (32 mg, 0.24 mmol, 0.08 equiv) and stirred at $75\text{ }^\circ\text{C}$ for 8 hours, cooled down to room temperature, added MesMgBr (15 mL, 1.0 M in THF, 15 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO3b** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 443 mg in 27% yield. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 2.22 (s, 12H), 2.37 (s, 6H), 2.43 (s, 6H), 6.95 (s, 4H), 7.62 (s, 2H), 7.66 (s, 1H), 7.67 (dd, $J = 8.0, 1.5$ Hz, 2H), 8.42 (d, $J = 8.0$ Hz, 2H), 9.17 (s, 1H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 21.19, 21.30, 22.47, 111.05, 117.68, 119.58, 121.34, 127.32, 128.87, 134.37, 134.77, 135.99, 136.92, 137.42, 138.33, 140.12, 151.74. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 46.36. HRMS (ESI): calcd for $\text{C}_{38}\text{H}_{37}[^{11}\text{B}]_2\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 547.2974, found 547.2990.



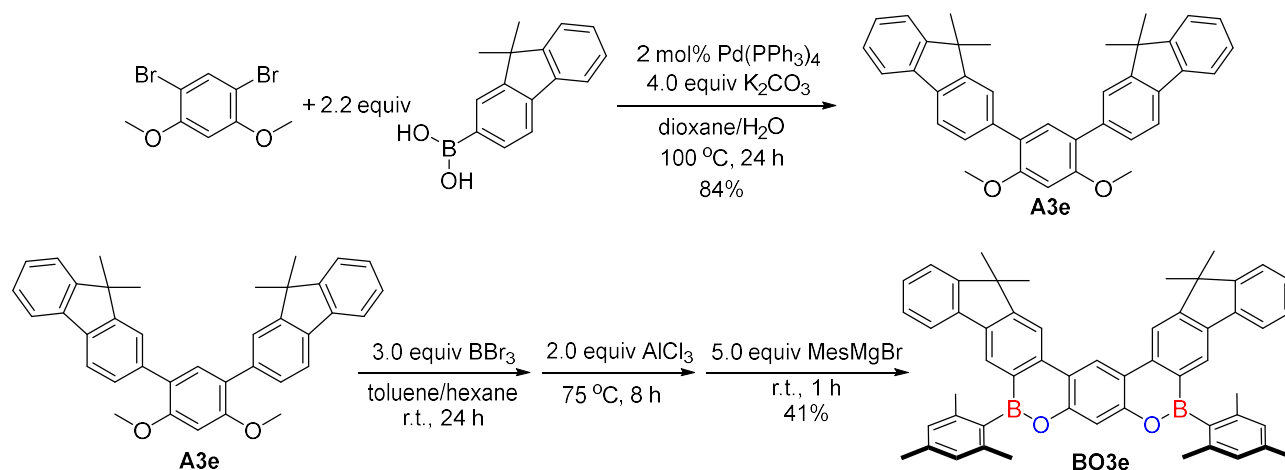
Synthesis of A3c: Following the general procedure, the reaction of 1,5-dibromo-2,4-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), [1,1'-biphenyl]-3-ylboronic acid (1.90 g, 9.60 mmol, 2.4 equiv), Pd(PPh₃)₄ (92 mg, 0.08 mmol, 0.02 equiv) and K₂CO₃ (2.21 g, 16.00 mmol, 4.0 equiv, in 10 mL H₂O) in dioxane (40 mL) at 100 °C for 24 hours afforded **A3c** (eluent: petroleum ether/ethyl acetate = 10:1–3:1) as a white solid 1.59 g in 90% yield. ¹H NMR (500 MHz, DMSO-*d*₆): δ (ppm) 3.90 (s, 6H), 6.91 (s, 1H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.40 (s, 1H), 7.43–7.55 (m, 8H), 7.57 (d, *J* = 7.5, 2H), 7.69 (d, *J* = 7.5, 4H), 7.75 (s, 2H).

Synthesis of BO3c: Following the general procedure, BBr₃ (0.87 mL, *d* = 2.6 g/mL, 9.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A3c** (1.33 g, 3.00 mmol, 1.0 equiv) in toluene (30 mL) and *n*-hexane (30 mL) and stirred at room temperature for 24 hours, added AlCl₃ (32 mg, 0.24 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (15 mL, 1.0 M in THF, 15 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO3c** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.59 g in 79% yield. ¹H NMR (500 MHz, DMSO-*d*₆): δ (ppm) 2.16 (s, 12H), 2.33 (s, 6H), 6.94 (s, 4H), 7.49–7.52 (m, 2H), 7.59–7.62 (m, 4H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.79 (s, 1H), 7.81 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.95–7.97 (m, 4H), 9.23 (s, 2H), 9.83 (s, 1H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.30, 22.52, 111.59, 118.22, 119.67, 120.07, 126.66, 127.38, 127.64, 127.79, 128.10, 129.02, 134.11, 138.16, 138.43, 138.88, 140.10, 141.23, 146.68, 152.66. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 47.62. HRMS (ESI): calcd for C₄₈H₄₁[¹¹B]₂O₂⁺ [*M*+H]⁺ 671.3287, found 671.3283.



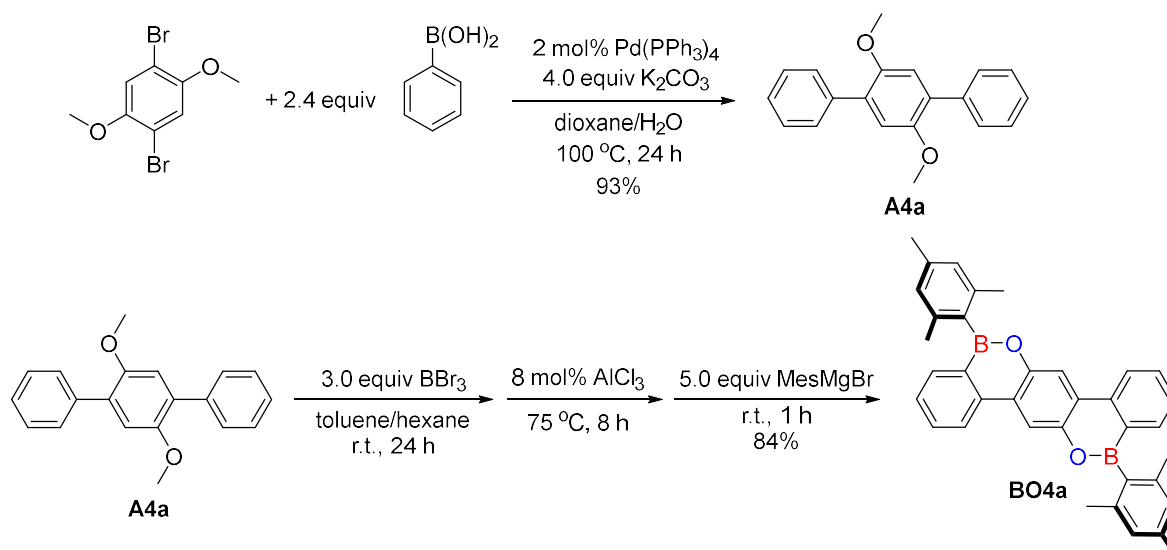
Synthesis of A3d: Following the general procedure, the reaction of 1,5-dibromo-2,4-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), naphthalen-2-ylboronic acid (1.65 g, 9.60 mmol, 2.4 equiv), Pd(PPh₃)₄ (92 mg, 0.08 mmol, 0.02 equiv) and K₂CO₃ (2.21 g, 16.00 mmol, 4.0 equiv, in 20 mL H₂O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A3d** (eluent: petroleum ether/ethyl acetate = 10:1–3:1) as a white solid 1.26 g in 81% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 3.91 (s, 6H), 6.73 (s, 1H), 7.43–7.54 (m, 4H), 7.54 (s, 1H), 7.74 (dd, *J* = 8.5, 1.0 Hz, 2H), 7.83–7.87 (m, 6H), 7.99 (s, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 56.00, 96.54, 123.41, 125.62, 125.87, 127.24, 127.55, 127.87, 128.03, 128.13, 132.29, 133.41, 133.52, 135.81, 157.18.

Synthesis of BO3d: Following the general procedure, BBr₃ (0.87 mL, d = 2.6 g/mL, 9.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A3d** (1.17 g, 3.00 mmol, 1.0 equiv) in toluene (40 mL) and *n*-hexane (40 mL) and stirred at room temperature for 24 hours, added AlCl₃ (32 mg, 0.24 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (15 mL, 1.0 M in THF, 15 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO3d** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.47 g in 79% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.19 (s, 12H), 2.42 (s, 6H), 7.00 (s, 4H), 7.32–7.35 (m, 2H), 7.49–7.52 (m, 2H), 7.77 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 2H), 8.25 (d, *J* = 8.5 Hz, 2H), 8.34 (d, *J* = 8.5 Hz, 2H), 8.75 (d, *J* = 9.0 Hz, 2H), 9.53 (s, 1H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.40, 22.08, 110.08, 119.72, 119.95, 120.00, 125.49, 126.10, 127.09, 127.75, 127.88, 128.59, 132.36, 134.87, 137.88, 138.29, 138.86, 139.18, 139.68, 152.47. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 45.48. HRMS (ESI): calcd for C₄₄H₃₆[¹¹B]₂NaO₂⁺ [M+Na]⁺ 641.2794, found 641.2783.



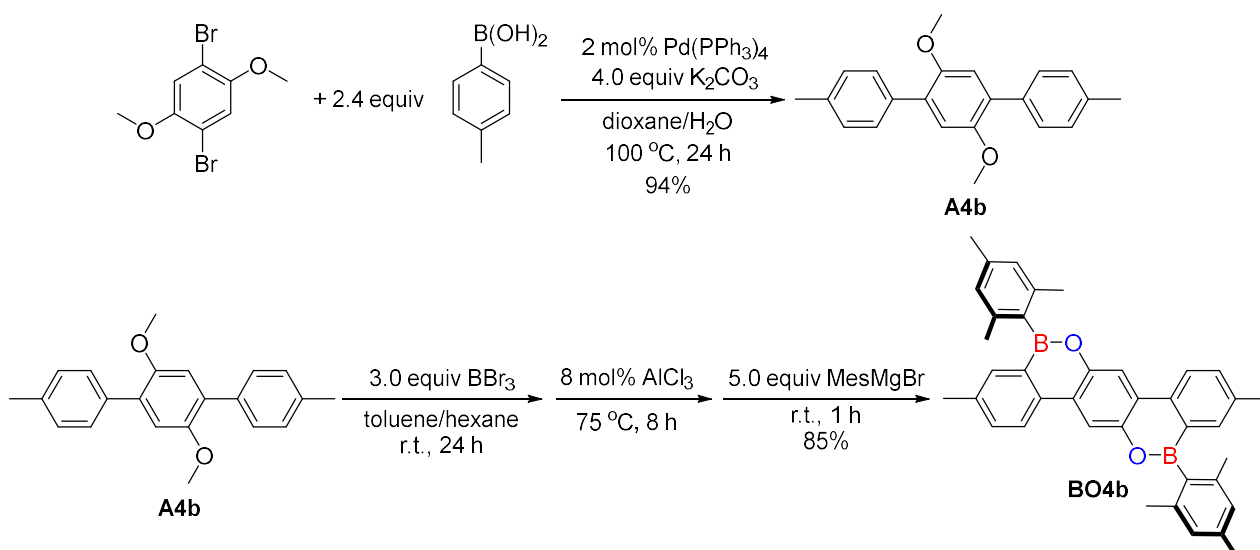
Synthesis of A3e: Following the general procedure, the reaction of 1,5-dibromo-2,4-dimethoxybenzene (1.26 g, 4.26 mmol, 1.0 equiv), (9,9-dimethyl-9H-fluoren-2-yl)boronic acid (2.23 g, 9.37 mmol, 2.2 equiv), Pd(PPh₃)₄ (100 mg, 0.087 mmol, 0.02 equiv) and K₂CO₃ (2.35 g, 17.03 mmol, 4.0 equiv, in 20 mL H₂O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A3e** (eluent: petroleum ether/ethyl acetate = 10:1–3:1) as a white solid 1.88 g in 84% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 1.52 (s, 12H), 3.92 (s, 6H), 6.71 (s, 1H), 7.29–7.35 (m, 4H), 7.43 (dd, *J* = 7.5, 1.0 Hz, 2H), 7.46 (s, 1H), 7.57 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.62 (d, *J* = 1.0 Hz, 2H), 7.73–7.77 (m, 4H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 55.91, 60.37, 106.94, 125.03, 126.65, 126.91, 127.75, 128.07, 128.15, 129.13, 130.23, 130.62, 134.30, 138.67, 155.92, 157.15. HRMS (ESI): calcd for C₃₈H₃₅O₂⁺ [M+H]⁺ 523.2632, found 523.2644.

Synthesis of BO3e: Following the general procedure, BBr₃ (0.29 mL, d = 2.6 g/mL, 3.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A3e** (523 mg, 1.0 mmol, 1.0 equiv) in toluene (20 mL) and *n*-hexane (20 mL) and stirred at room temperature for 24 hours, added AlCl₃ (267 mg, 2.0 mmol, 2.0 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (5 mL, 1.0 M in THF, 5.0 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO3e** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a yellow solid 306 mg in 41% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 1.75 (s, 12H), 2.27 (s, 12H), 2.41 (s, 6H), 7.02 (s, 4H), 7.33–7.38 (m, 4H), 7.52 (d, *J* = 5.5 Hz, 2H), 7.71 (s, 1H), 7.77 (dd, *J* = 5.5, 1.0 Hz, 2H), 8.15 (s, 2H), 8.55 (s, 2H), 9.31 (s, 1H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.35, 22.59, 27.59, 47.51, 111.34, 115.40, 117.90, 120.01, 120.71, 122.64, 127.23, 127.43, 127.83, 128.36, 128.73, 134.49, 138.01, 138.35, 138.38, 138.91, 140.25, 152.19, 153.45, 159.44. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 45.52. HRMS (ESI): calcd for C₅₄H₄₈[¹¹B]₂NaO₂⁺ [M+Na]⁺ 773.3733, found 773.3720.



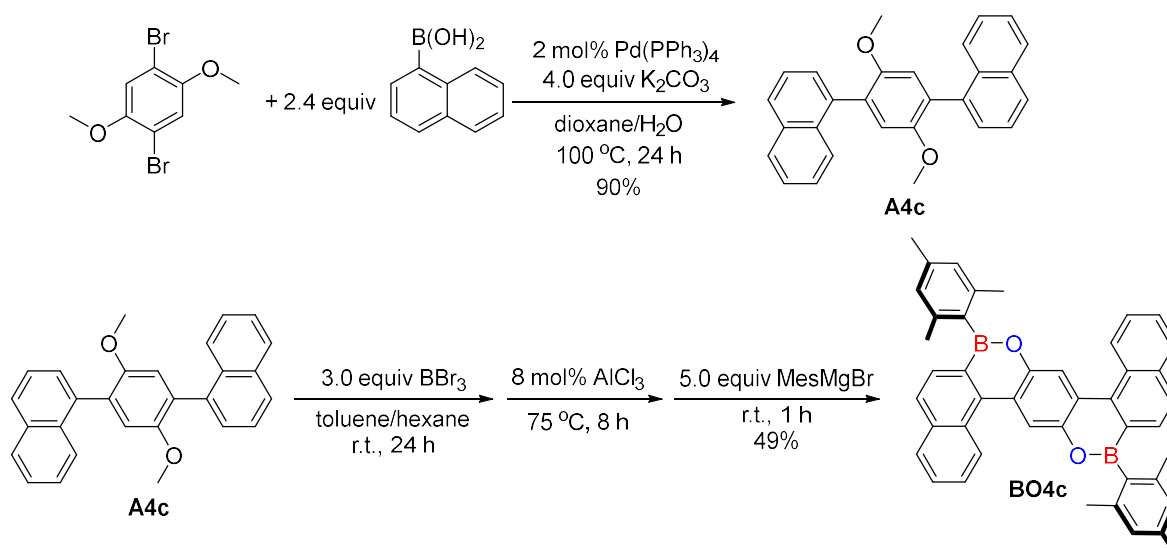
Synthesis of A4a: Following the general procedure, the reaction of 1,4-dibromo-2,5-dimethoxybenzene (2.37 g, 8.00 mmol, 1.0 equiv), boronic acid (2.34 g, 19.20 mmol, 2.4 equiv), $\text{Pd(PPh}_3)_4$ (185 mg, 0.16 mmol, 0.02 equiv) and K_2CO_3 (4.42 g, 32.00 mmol, 4.0 equiv, in 20 mL H_2O) in dioxane (80 mL) at $100\text{ }^\circ\text{C}$ for 24 hours afforded **A4a** (eluent: petroleum ether/ethyl acetate = 10:1–5:1) as a white solid 2.16 g in 93% yield. ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ (ppm) 3.76 (s, 6H), 7.03 (s, 2H), 7.34 (t, $J = 7.5\text{ Hz}$, 2H), 7.43 (t, $J = 7.5\text{ Hz}$, 4H), 7.56 (d, $J = 8.0$, 4H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 56.35, 114.73, 127.07, 128.05, 129.41, 130.36, 138.28, 150.59. The ^{13}C NMR is in agreement with the previous report (Bolligera, J. L.; Frech, C. M. Polyaromatic the 1,3-diaminobenzene-derived aminophosphine palladium pincer complex $\{\text{C}_6\text{H}_3\text{ACHTUNG TRENUNG}[\text{NHP}(\text{piperidiny})_2]_2\text{Pd}(\text{Cl})\}$ —a highly active Suzuki–Miyaura catalyst with excellent functional group tolerance. *Adv. Synth. Catal.* **2010**, 352, 1075–1080).

Synthesis of BO4a: Following the general procedure, BBr_3 (1.16 mL, $d = 2.6\text{ g/mL}$, 12.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A4a** (1.16 g, 4.00 mmol, 1.0 equiv) in toluene (30 mL) and *n*-hexane (30 mL) and stirred at room temperature for 24 hours, added AlCl_3 (42 mg, 0.32 mmol, 0.08 equiv) and stirred at $75\text{ }^\circ\text{C}$ for 8 hours, cooled down to room temperature, added MesMgBr (20 mL, 1.0 M in THF, 20 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO4a** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.74 g in 84% yield. m.p.: $>350\text{ }^\circ\text{C}$. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 2.24 (s, 12H), 2.39 (s, 6H), 6.96 (s, 4H), 7.49 (t, $J = 7.5\text{ Hz}$, 2H), 7.81–7.84 (m, 4H), 8.34 (d, $J = 8.0\text{ Hz}$, 2H), 8.45 (s, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 21.32, 22.47, 114.38, 121.99, 124.13, 127.35, 127.87, 129.33, 133.52, 137.44, 137.94, 138.37, 140.11, 141.79. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 44.68. HRMS (ESI): calcd for $\text{C}_{36}\text{H}_{33}[^{11}\text{B}]_2\text{O}_2^+ [\text{M}+\text{H}]^+$ 519.2661, found 519.2672.



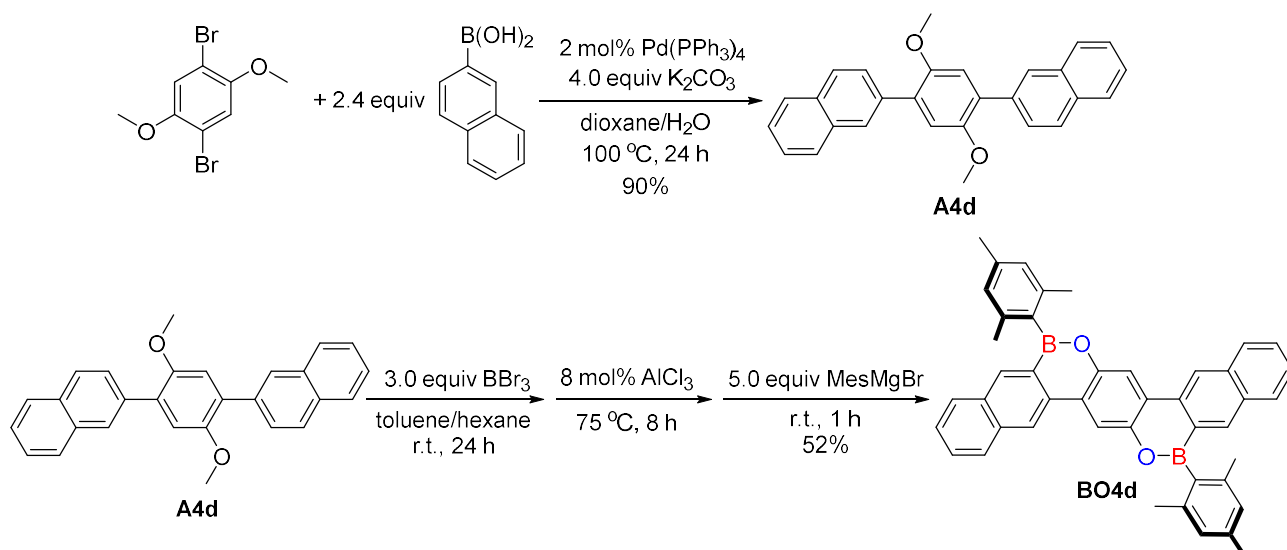
Synthesis of **A4b:** Following the general procedure, the reaction of 1,4-dibromo-2,5-dimethoxybenzene (2.37 g, 8.00 mmol, 1.0 equiv), 4-methylboronic acid (2.61 g, 19.20 mmol, 2.4 equiv), $\text{Pd(PPh}_3)_4$ (185 mg, 0.16 mmol, 0.02 equiv) and K_2CO_3 (4.42 g, 32.00 mmol, 4.0 equiv, in 20 mL H_2O) in dioxane (80 mL) at $100\text{ }^\circ\text{C}$ for 24 hours afforded **A4b** (eluent: petroleum ether/ethyl acetate = 10:1–5:1) as a white solid 2.40 g in 94% yield. ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ (ppm) 2.35 (s, 6H), 3.74 (s, 6H), 6.98 (s, 2H), 7.23 (d, $J = 8.0\text{ Hz}$, 4H), 7.45 (d, $J = 8.0\text{ Hz}$, 4H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 21.19, 56.35, 114.60, 128.81, 129.28, 130.11, 135.40, 136.78, 150.61.

Synthesis of **BO4b:** Following the general procedure, BBr_3 (1.16 mL, $d = 2.6\text{ g/mL}$, 12.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A4b** (1.27 g, 4.00 mmol, 1.0 equiv) in toluene (30 mL) and *n*-hexane (30 mL) and stirred at room temperature for 24 hours, added AlCl_3 (42 mg, 0.32 mmol, 0.08 equiv) and stirred at $75\text{ }^\circ\text{C}$ for 8 hours, cooled down to room temperature, added MesMgBr (20 mL, 1.0 M in THF, 20 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO4b** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.86 g in 85% yield. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 2.23 (s, 12H), 2.39 (s, 6H), 2.41 (s, 6H), 6.97 (s, 4H), 7.62–7.64 (m, 4H), 8.22 (d, $J = 8.0\text{ Hz}$, 2H), 8.38 (s, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 21.29, 21.33, 22.47, 113.98, 121.96, 123.83, 127.33, 129.32, 134.77, 135.55, 137.27, 137.69, 138.27, 140.15, 147.58. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 46.97. HRMS (ESI): calcd for $\text{C}_{38}\text{H}_{37}[^{11}\text{B}]_2\text{O}_2^+ [\text{M}+\text{H}]^+$ 547.2974, found 547.2992.



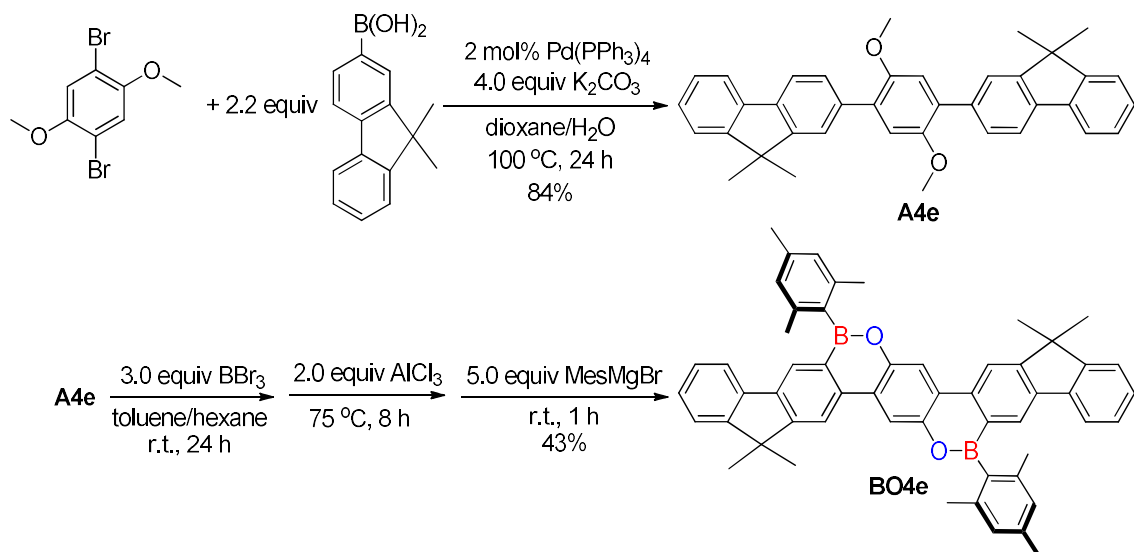
Synthesis of **A4c:** Following the general procedure, the reaction of 1,4-dibromo-2,5-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), naphthalen-1-ylboronic acid (1.66 g, 9.60 mmol, 2.4 equiv), $\text{Pd(PPh}_3)_4$ (92 mg, 0.08 mmol, 0.02 equiv) and K_2CO_3 (2.21 g, 16.00 mmol, 4.0 equiv, in 20 mL H_2O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A4c** (eluent: petroleum ether/ethyl acetate = 10:1–3:1) as a white solid 1.41 g in 90% yield. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 3.63 (s, 6H), 7.01 (d, J = 4.0 Hz, 2H), 7.46–7.60 (m, 8H), 7.76–7.81 (m, 2H), 7.90–7.94 (m, 4H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 55.91, 60.37, 106.94, 125.03, 126.65, 126.91, 127.75, 128.07, 128.15, 129.13, 130.23, 130.62, 134.30, 138.67, 155.92, 157.15. HRMS (ESI): calcd for $\text{C}_{28}\text{H}_{26}\text{NO}_2^+ [\text{M}+\text{NH}_4]^+$ 408.1958, found 408.1976.

Synthesis of **BO4c:** Following the general procedure, BBr_3 (0.58 mL, d = 2.6 g/mL, 6.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A4c** (781 mg, 2.00 mmol, 1.0 equiv) in toluene (30 mL) and *n*-hexane (30 mL) and stirred at room temperature for 24 hours, added AlCl_3 (22 mg, 0.16 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (10 mL, 1.0 M in THF, 10 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO4c** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 610 mg in 49% yield. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 2.22 (s, 12H), 2.38 (s, 6H), 6.97 (s, 4H), 7.69–7.74 (m, 4H), 7.77 (d, J = 8.0 Hz, 2H), 7.88 (d, J = 8.5 Hz, 2H), 8.00–8.02 (m, 2H), 8.97 (s, 2H), 9.15 (d, J = 7.0 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 21.32, 22.52, 119.87, 124.09, 126.88, 127.44, 127.94, 128.21, 128.42, 128.91, 129.02, 129.18, 131.29, 134.31, 137.09, 137.88, 138.52, 140.17, 148.42. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 45.44. HRMS (ESI): calcd for $\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{NaO}_2^+ [\text{M}+\text{Na}]^+$ 641.2794, found 641.2780.



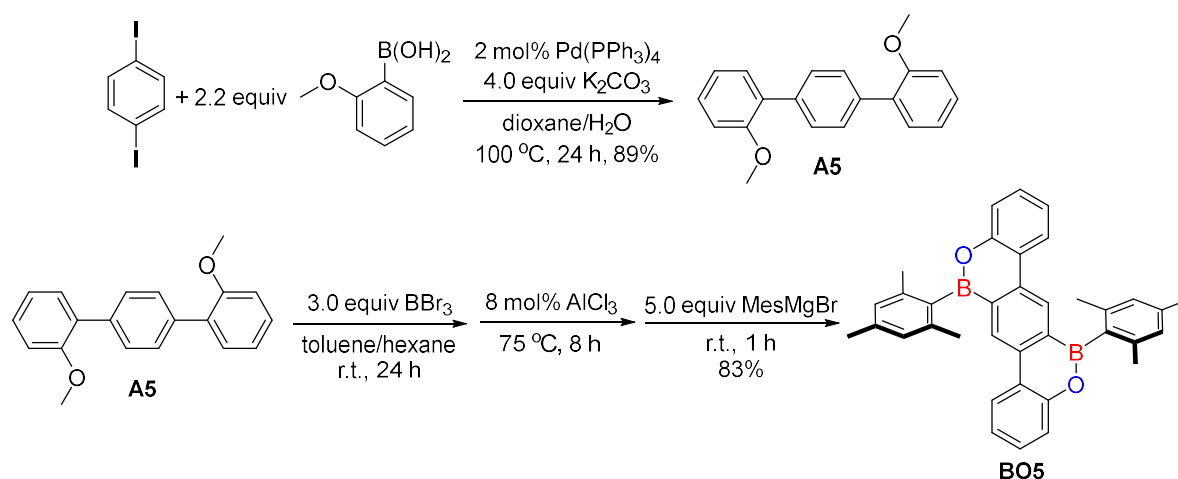
Synthesis of A4d: Following the general procedure, the reaction of 1,4-dibromo-2,5-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), naphthalen-2-ylboronic acid (1.65 g, 9.60 mmol, 2.4 equiv), $\text{Pd(PPh}_3)_4$ (92 mg, 0.08 mmol, 0.02 equiv) and K_2CO_3 (2.21 g, 16.00 mmol, 4.0 equiv, in 20 mL H_2O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A4d** (eluent: petroleum ether/ethyl acetate = 10:1–3:1) as a white solid 1.40 g in 90% yield. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 3.84 (s, 6H), 7.13 (s, 2H), 7.48–7.53 (m, 4H), 7.37 (dd, J = 8.5, 1.0 Hz, 2H), 7.87–7.92 (m, 6H), 8.05 (d, J = 0.5 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 56.62, 115.20, 125.92, 126.03, 127.39, 127.63, 127.92, 128.06, 128.14, 130.63, 132.56, 133.45, 135.99, 151.02. HRMS (ESI): calcd for $\text{C}_{28}\text{H}_{26}\text{NO}_2^+$ [$\text{M}+\text{NH}_4$] $^+$ 408.1958, found 408.1972.

Synthesis of BO4d: Following the general procedure, BBr_3 (0.29 mL, d = 2.6 g/mL, 3.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A4d** (390 mg, 1.00 mmol, 1.0 equiv) in toluene (20 mL) and *n*-hexane (20 mL) and stirred at room temperature for 24 hours, added AlCl_3 (12 mg, 0.08 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (5 mL, 1.0 M in THF, 5 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO4d** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 322 mg in 52% yield. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 2.29 (s, 12H), 2.43 (s, 6H), 7.02 (s, 4H), 7.53 (t, J = 7.0 Hz, 2H), 7.64 (d, J = 7.0 Hz, 2H), 7.93 (d, J = 8.0 Hz, 2H), 8.05 (d, J = 8.5 Hz, 2H), 8.41 (s, 2H), 8.58 (s, 2H), 8.76 (s, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 21.39, 22.54, 114.82, 120.79, 124.37, 126.28, 127.40, 128.37, 128.46, 128.99, 132.64, 133.40, 136.09, 138.41, 139.86, 140.25, 147.80. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 46.76. HRMS (ESI): calcd for $\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{O}_2^-$ [M] $^-$ 618.2907, found 618.2988.



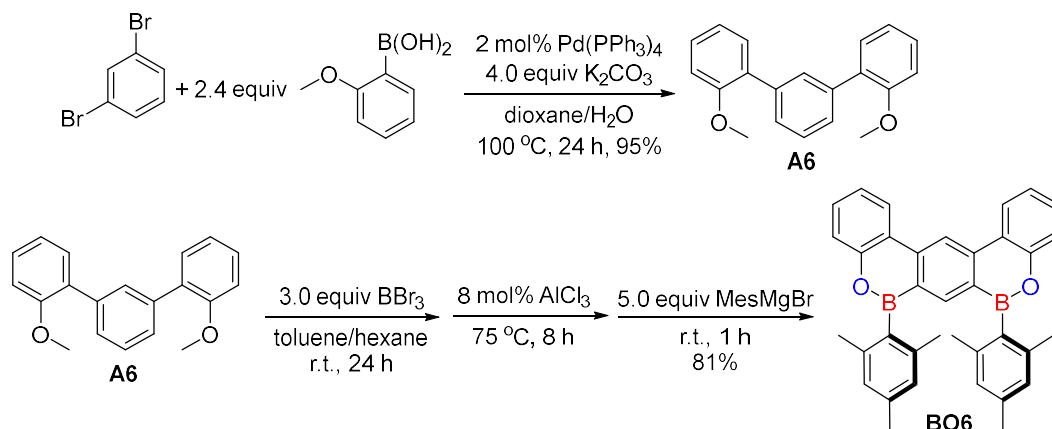
Synthesis of A4e: Following the general procedure, the reaction of 1,4-dibromo-2,5-dimethoxybenzene (1.26 g, 4.26 mmol, 1.0 equiv), (9,9-dimethyl-9H-fluoren-2-yl)boronic acid (2.23 g, 9.37 mmol, 2.2 equiv), Pd(PPh₃)₄ (98 mg, 0.085 mmol, 0.02 equiv) and K₂CO₃ (2.36 g, 17.04 mmol, 4.0 equiv, in 20 mL H₂O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A4e** (eluent: petroleum ether/ethyl acetate = 10:1–3:1) as a white solid 1.87 g in 84% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 1.24 (s, 12H), 3.85 (s, 6H), 7.08 (s, 2H), 7.31–7.37 (m, 4H), 7.46 (dd, *J* = 6.5, 1.5 Hz, 2H), 7.59 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.68 (d, *J* = 1.0 Hz, 2H), 7.76 (dd, *J* = 6.5, 1.5 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 24.81, 27.19, 46.89, 56.61, 75.01, 115.07, 119.59, 120.01, 122.54, 123.78, 126.94, 127.15, 128.31, 130.80, 137.27, 138.26, 139.02, 150.84, 153.39, 153.89. HRMS (ESI): calcd for C₃₈H₃₈NO₂⁺ [M+NH₄]⁺ 540.2897, found 540.2910.

Synthesis of BO4e: Following the general procedure, BBr₃ (0.29 mL, d = 2.6 g/mL, 3.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A4e** (523 mg, 1.00 mmol, 1.0 equiv) in toluene (20 mL) and *n*-hexane (20 mL) and stirred at room temperature for 24 hours, added AlCl₃ (267 mg, 2.00 mmol, 2.0 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (5 mL, 1.0 M in THF, 5 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO4e** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a slight yellow solid 325 mg in 43% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 1.62 (s, 12H), 2.29 (s, 12H), 2.43 (s, 6H), 7.00 (s, 4H), 7.31–7.36 (m, 4H), 7.47–7.49 (m, 2H), 7.76–7.77 (m, 2H), 8.14 (s, 2H), 8.42 (s, 2H), 8.56 (s, 2H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.38, 22.57, 27.39, 47.35, 114.21, 116.24, 120.79, 122.72, 124.31, 127.19, 127.42 (2C), 127.93, 128.44, 128.77, 137.49, 138.26, 138.37, 139.52, 140.17, 147.79, 153.57, 159.43. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 45.87. HRMS (ESI): calcd for C₅₄H₄₈[¹¹B]₂NaO₂ [M+Na]⁺ 773.3733, found 773.3712.



Synthesis of A5: Following the general procedure, the reaction of 1,4-diiodobenzene (6.60 g, 20.00 mmol, 1.0 equiv), 2-methoxyphenylboronic acid (6.69 g, 44.00 mmol, 2.2 equiv), $\text{Pd(PPh}_3)_4$ (462 mg, 0.40 mmol, 0.02 equiv) and K_2CO_3 (11.06 g, 80.00 mmol, 4.0 equiv, in 30 mL H_2O) in dioxane (120 mL) at $100\text{ }^\circ\text{C}$ for 24 hours afforded **A5** (eluent: petroleum ether/ethyl acetate = 10:1–3:1) as a white solid 5.17 g in 89% yield. ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ (ppm) 3.79 (s, 6H), 7.05 (t, $J = 7.5$ Hz, 2H), 7.13 (d, $J = 7.5$ Hz, 2H), 7.31–7.38 (m, 4H), 7.50 (s, 4H).

Synthesis of BO5: Following the general procedure, BBr_3 (1.16 mL, $d = 2.6\text{ g/mL}$, 12.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A5** (1.16 g, 4.00 mmol, 1.0 equiv) in toluene (40 mL) and *n*-hexane (40 mL) and stirred at room temperature for 24 hours, added AlCl_3 (21 mg, 0.16 mmol, 0.04 equiv) and stirred at $75\text{ }^\circ\text{C}$ for 8 hours, cooled down to room temperature, added MesMgBr (20 mL, 1.0 M in THF, 20 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO5** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.72 g in 83% yield. m.p.: $320.1\text{--}322.5\text{ }^\circ\text{C}$. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 2.26 (s, 12H), 2.43 (s, 6H), 7.01 (s, 4H), 7.29–7.33 (m, 2H), 7.45–7.48 (m, 2H), 7.55 (dd, $J = 8.5, 1.0$ Hz, 2H), 8.20 (dd, $J = 8.0, 1.5$ Hz, 2H), 8.74 (s, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 21.38, 22.64, 110.58, 122.87, 123.63, 123.83, 127.56, 129.20, 130.60, 136.54, 138.56, 140.26, 151.54. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 46.85. HRMS (ESI): calcd for $\text{C}_{36}\text{H}_{32}[^{11}\text{B}]_2\text{O}_2]^+ [\text{M}]^+$ 518.2583, found 518.2586.



Synthesis of A6: Following the general procedure, the reaction of 1,3-dibromobenzene (1.18 g, 5.00 mmol, 1.0 equiv), 2-methoxyphenylboronic acid (1.82 g, 12.00 mmol, 2.4 equiv), Pd(PPh₃)₄ (116 mg, 0.10 mmol, 0.02 equiv) and K₂CO₃ (2.76 g, 20.00 mmol, 4.0 equiv, in 20 mL H₂O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A6** (eluent: petroleum ether/ethyl acetate = 20:1–10:1) as a white solid 1.38 g in 95% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 3.82 (s, 6H), 6.99 (d, *J* = 8.0 Hz, 2H), 7.02–7.05 (m, 2H), 7.30–7.34 (m, 2H), 7.38 (d, *J* = 7.5, 2.0 Hz, 2H), 7.43–7.46 (m, 1H), 7.50–7.52 (m, 2H), 7.69 (t, *J* = 1.5 Hz, 1H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 55.48, 111.14, 120.75, 127.49, 128.15, 128.49, 130.72, 130.75, 130.96, 138.11, 156.48. The ¹H NMR and ¹³C NMR are agreement with the previous report (Shukla, R.; Lindeman, S. V.; Rathore, R. Terphenyl Crowns: A new family of receptors containing ethereal canopies that direct potassium cation onto benzenoid platforms for cation–π interactions. *Chem. Commun.* **2009**, 5600–5602).

Synthesis of BO6: Following the general procedure, BBr₃ (1.16 mL, d = 2.6 g/mL, 12.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A6** (581 mg, 2.00 mmol, 1.0 equiv) in toluene (30 mL) and *n*-hexane (30 mL) and stirred at room temperature for 24 hours, added AlCl₃ (42 mg, 0.32 mmol, 0.08 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (10 mL, 1.0 M in THF, 10 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO6** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 839 mg in 81% yield. m.p.: 271.8–272.9 °C. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.15 (s, 12H), 2.30 (s, 6H), 6.84 (s, 4H), 7.43–7.47 (m, 2H), 7.54–7.58 (m, 4H), 8.32 (s, 1H), 8.59 (d, *J* = 6.5 Hz, 2H), 9.26 (s, 1H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 21.21, 22.50, 113.80, 120.88, 122.93, 123.55, 124.00, 127.38, 128.03, 130.16, 133.79, 138.25, 140.02, 142.07, 148.71, 152.39. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 46.23. HRMS (ESI): calcd for C₃₆H₃₃[¹¹B]₂O₂⁺ [M+H]⁺ 519.2661, found 519.2676.

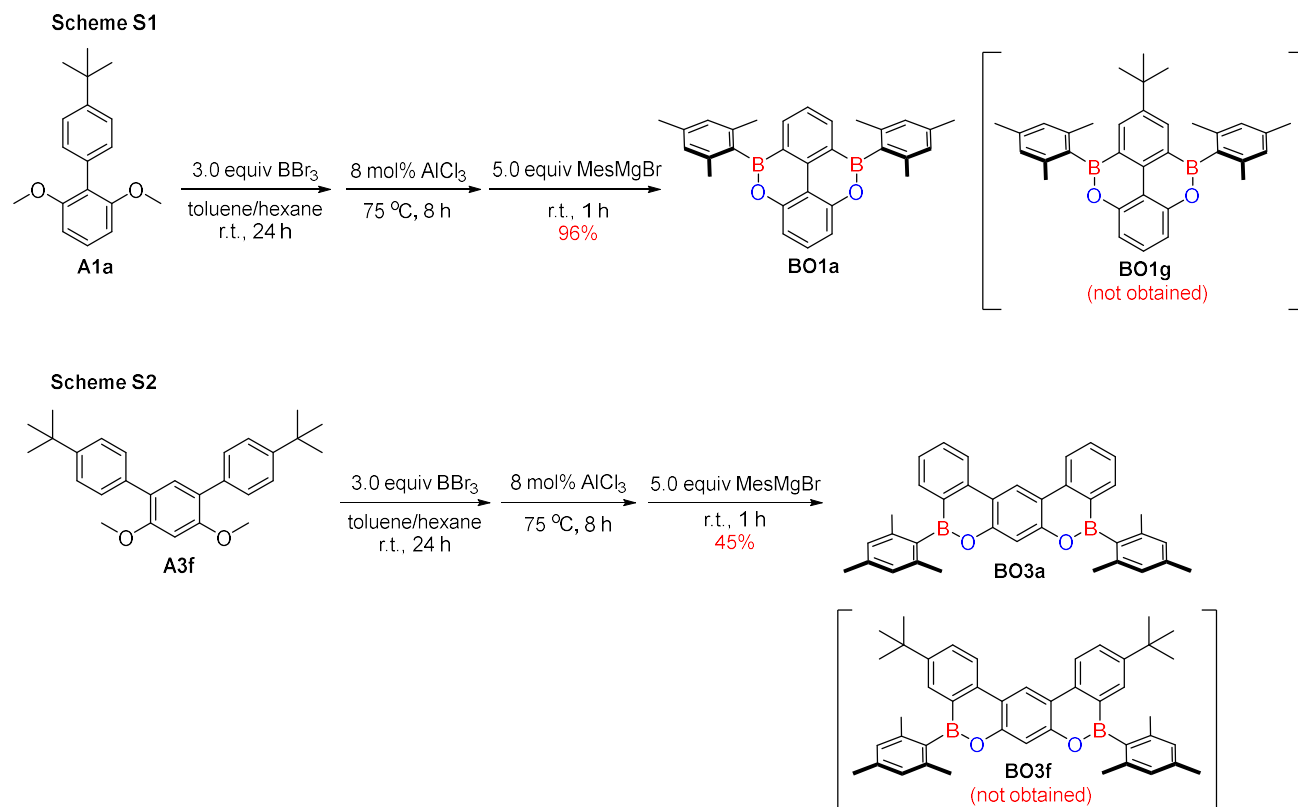


Fig. S2. AlCl₃ induced de-*tert*-butylation reactions. The observed de-*tert*-butylation reactions catalyzed by AlCl₃

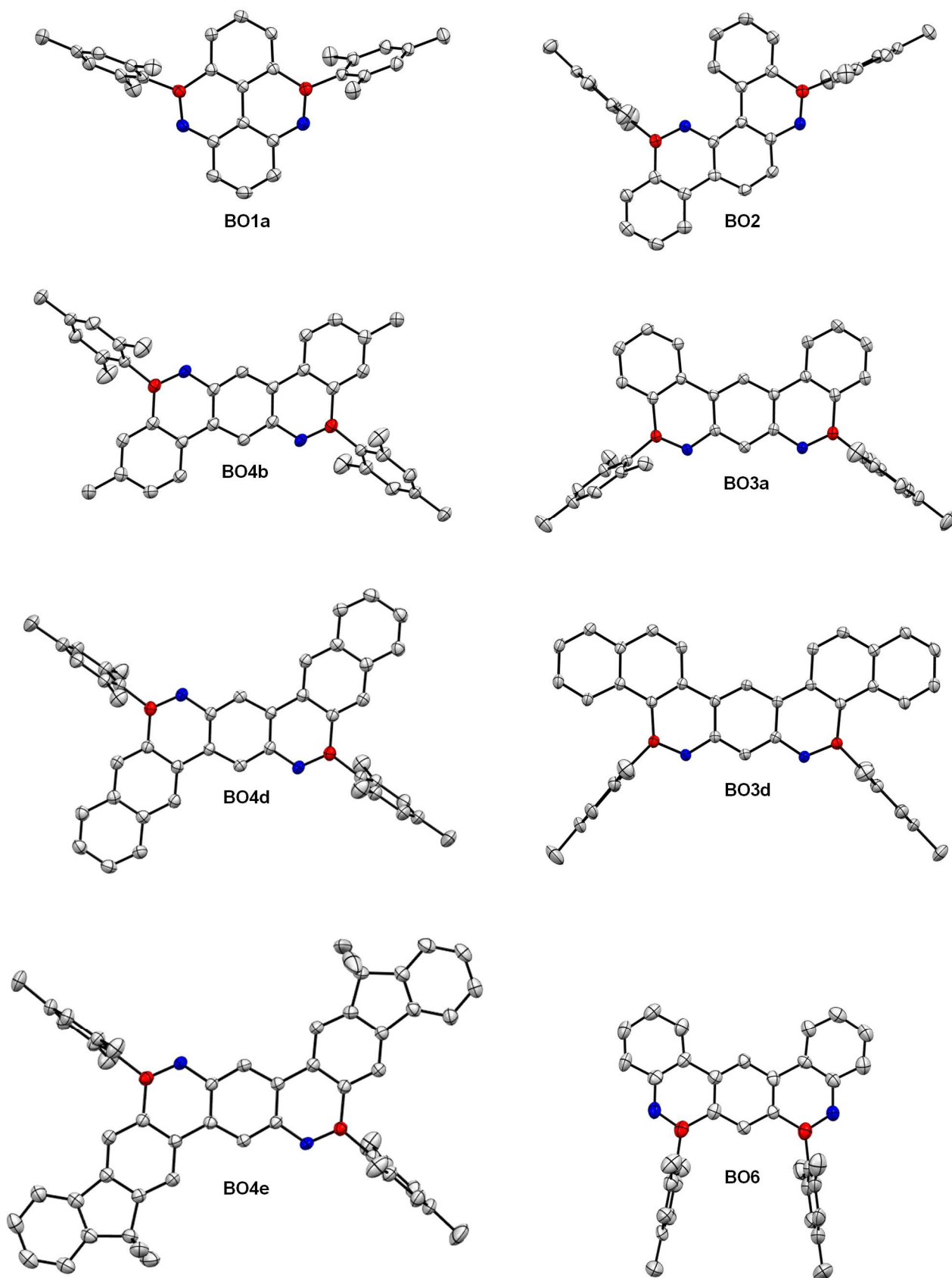
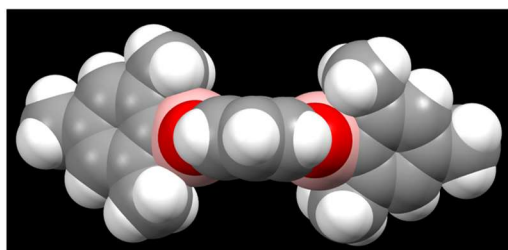
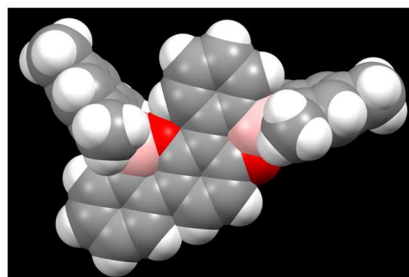


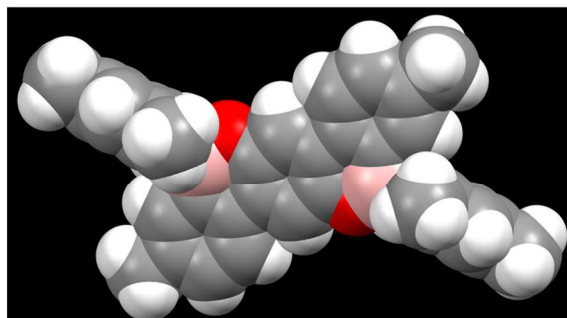
Fig. S3. Single crystal diffraction structures of BO-PAHs. ORTEP drawing of X-ray single crystal diffraction structures of **BO1a**, **BO2**, **BO3a**, **BO3d**, **BO4b**, **BO4d**, **BO4e** and **BO6**. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.



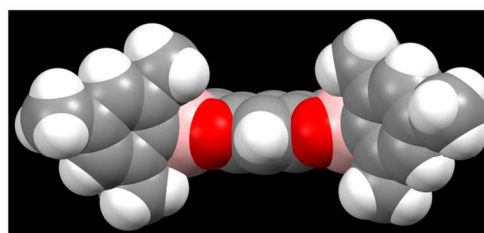
BO1a (top view)



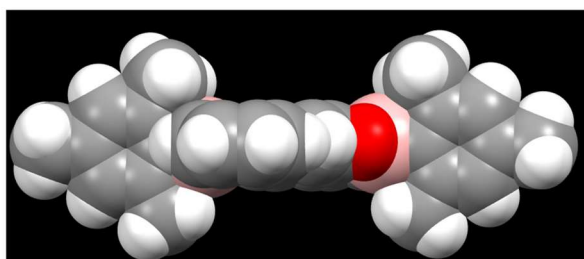
BO2 (front view)



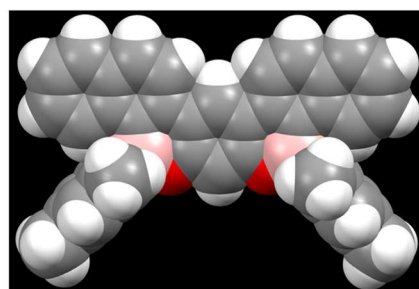
BO4b (front view)



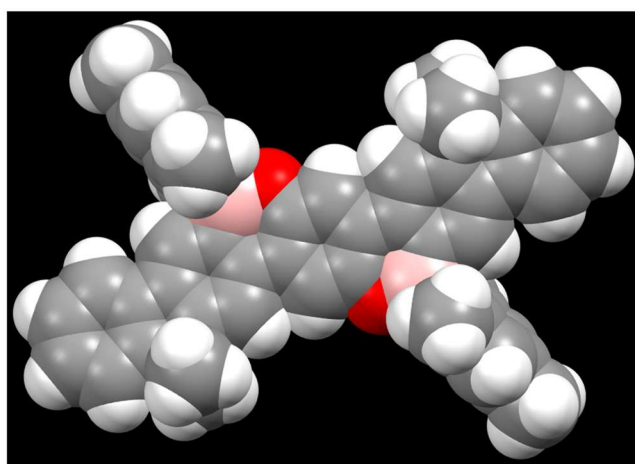
BO3a (bottom view)



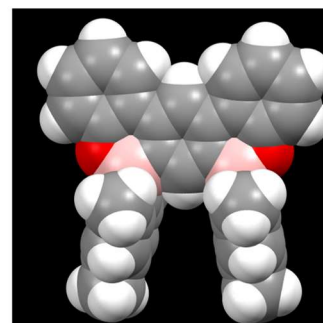
BO4d (top view)



BO3d (front view)



BO4e (front view)



BO6 (front view)

Fig. S4. Spacefill drawing of X-ray single crystal diffraction structures of **BO1a**, **BO2**, **BO3a**, **BO3d**, **BO4b**, **BO4d**, **BO4e** and **BO6**. B, pink; O, red.

Table S1. Crystal data and structure refinements for BO1a, BO2 and BO6

Compound	BO1a	BO2	BO6
CCDC number	1954663	1954662	2029823
Empirical formula	C ₃₀ H ₂₈ B ₂ O ₂	C ₃₆ H ₃₂ B ₂ O ₂	C ₃₆ H ₃₂ B ₂ O ₂
Formula weight	442.14	518.23	518.23
Temperature (K)	293(2) K	193(2)	192(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	monoclinic	orthorhombic	monoclinic
Space group	P 21/n	P 21 21 21	P c
<i>a</i> (Å)	12.3732(4)	8.0150(3)	19.776(2)
<i>b</i> (Å)	8.0799(3)	14.7515(6)	18.2753(15)
<i>c</i> (Å)	25.7096(10)	24.6982(8)	16.4263(15)
α (°)	90	90	90
β (°)	100.6030(10)	90	90.339(3)
γ (°)	90	90	90
Volume (Å ³)	2526.41(16)	2920.15(19)	5936.7(9)
<i>Z</i>	4	4	8
<i>F</i> (000)	936	1096	2192
Crystal size (mm ³)	0.200×0.150×0.120	0.200×0.160×0.130	0.180×0.140×0.100
θ (deg) for collection (°)	2.647 to 25.498	2.672 to 25.985	2.229 to 24.999
Index ranges	−14≤ <i>h</i> ≤14, −9≤ <i>k</i> ≤9, −31≤ <i>l</i> ≤31	−9≤ <i>h</i> ≤9, −18≤ <i>k</i> ≤14, −30≤ <i>l</i> ≤27	−23≤ <i>h</i> ≤22, −21≤ <i>k</i> ≤21, −19≤ <i>l</i> ≤19
Reflections collected	23738	14696	80398
Unique (<i>R</i> _{int})	4665 (0.0349)	5706 (0.0593)	19509 (0.1088)
Data / restraints / parameters	4665 / 0 / 314	5706 / 0 / 368	19509 / 2 / 1467
Goodness-of-fit on <i>F</i> ²	1.050	1.032	1.001
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0493 <i>wR</i> ₂ = 0.1275	<i>R</i> ₁ = 0.0483 <i>wR</i> ₂ = 0.1208	<i>R</i> ₁ = 0.0755 <i>wR</i> ₂ = 0.1898
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0722 <i>wR</i> ₂ = 0.1462	<i>R</i> ₁ = 0.0586 <i>wR</i> ₂ = 0.1313	<i>R</i> ₁ = 0.1119 <i>wR</i> ₂ = 0.2132
Largest diff. peak and hole (Å ^{−3})	0.155/−0.125	0.201/−0.178	0.203/−0.216

Table S2. Crystal data and structure refinements for BO3a and BO3d

Compound	BO3a	BO3d
CCDC number	1954665	1954664
Empirical formula	C ₃₆ H ₃₂ B ₂ O ₂	C ₄₄ H ₃₆ B ₂ O ₂
Formula weight	518.23	618.35
Temperature (K)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	monoclinic	monoclinic
Space group	C 2/c	C 2
<i>a</i> (Å)	34.7317(9)	30.8251(8)
<i>b</i> (Å)	7.7855(2)	7.5638(2)
<i>c</i> (Å)	24.5964(6)	17.0835(4)
α (°)	90	90
β (°)	98.6690(10)	92.9740(10)
γ (°)	90	90
Volume (Å ³)	6575.0(3)	3977.74(17)
<i>Z</i>	8	4
F(000)	2192	1304
Crystal size (mm ³)	0.200×0.170×0.130	0.200×0.120×0.100
θ (deg) for collection (°)	2.784 to 25.996	2.388 to 25.499
Index ranges	−42≤ <i>h</i> ≤42, −9≤ <i>k</i> ≤9, −30≤ <i>l</i> ≤30	−36≤ <i>h</i> ≤37, −9≤ <i>k</i> ≤9, −19≤ <i>l</i> ≤20
Reflections collected	37277	19699
Unique (Rint)	6409 (0.0395)	7366 (0.0322)
Data / restraints / parameters	6409 / 0 / 368	7366 / 1 / 440
Goodness-of-fit on F ²	1.028	1.012
Final R indices [<i>I</i> >2σ(<i>I</i>)]	R ₁ = 0.0587 wR ₂ = 0.1815	R ₁ = 0.0566 wR ₂ = 0.1508
R indices (all data)	R ₁ = 0.0793 wR ₂ = 0.2003	R ₁ = 0.0726 wR ₂ = 0.1641
Largest diff. peak and hole (Å ^{−3})	0.219/−0.205	0.213/−0.160

Table S3. Crystal data and structure refinements for BO4b, BO4d and BO4e·CH₂Cl₂

Compound	BO4b	BO4d	BO4e·CH₂Cl₂
CCDC number	1954661	1966566	1968761
Empirical formula	C ₃₈ H ₃₆ B ₂ O ₂	C ₄₄ H ₃₆ B ₂ O ₂	C ₅₅ H ₅₀ B ₂ Cl ₂ O ₂
Formula weight	546.29	618.35	835.47
Temperature (K)	192(2)	170	170
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	orthorhombic	monoclinic	monoclinic
Space group	P b c a	P2 ₁ -C	P2 ₁ /n
<i>a</i> (Å)	18.752(2)	7.3765(3)	14.345(6)
<i>b</i> (Å)	7.4170(10)	28.2294(12)	15.450(6)
<i>c</i> (Å)	21.713(2)	8.0685(3)	20.591(9)
α (°)	90	90	90
β (°)	90	95.884(2)	99.88(2)
γ (°)	90	90	90
Volume (Å ³)	3019.9(6)	1671.29(12)	4496(3)
<i>Z</i>	4	2	4
<i>F</i> (000)	1160	652.0	1760.0
Crystal size (mm ³)	0.180×0.150×0.120	0.15×0.05×0.03	0.39×0.23×0.19
θ (deg) for collection (°)	2.871 to 26.000	2.638 to 34.051	2.306 to 26.405
Index ranges	−23≤ <i>h</i> ≤18, −9≤ <i>k</i> ≤9, −26≤ <i>l</i> ≤25	−11≤ <i>h</i> ≤10, −40≤ <i>k</i> ≤40, −12≤ <i>l</i> ≤12	−17≤ <i>h</i> ≤17, −18≤ <i>k</i> ≤19, −25≤ <i>l</i> ≤25
Reflections collected	13983	39127	62483
Unique (<i>R</i> _{int})	2956 (0.0628)	5819 (0.0867)	9215 (0.0619)
Data / restraints / parameters	2956 / 0 / 195	5819 / 0 / 220	9215 / 99 / 588
Goodness-of-fit on <i>F</i> ²	1.027	1.022	1.024
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0537 w <i>R</i> ₂ = 0.1312	<i>R</i> ₁ = 0.0740 w <i>R</i> ₂ = 0.1696	<i>R</i> ₁ = 0.0735 w <i>R</i> ₂ = 0.2018
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0760 w <i>R</i> ₂ = 0.1487	<i>R</i> ₁ = 0.1644 w <i>R</i> ₂ = 0.2208	<i>R</i> ₁ = 0.1017 w <i>R</i> ₂ = 0.2315
Largest diff. peak and hole (Å ^{−3})	0.266/−0.184	0.34/−0.27	0.67/−0.87

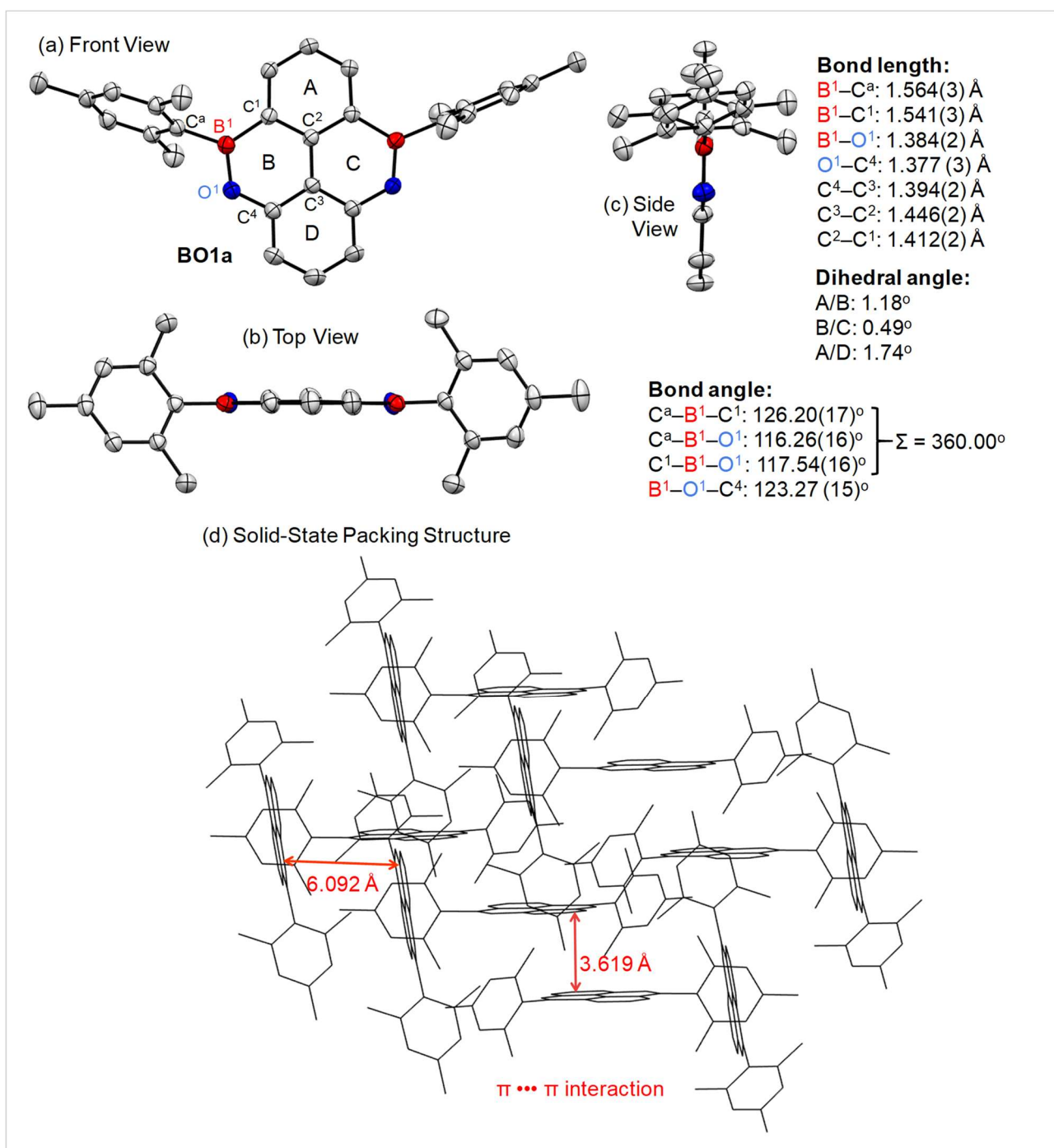


Fig. S5. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of BO1a. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.

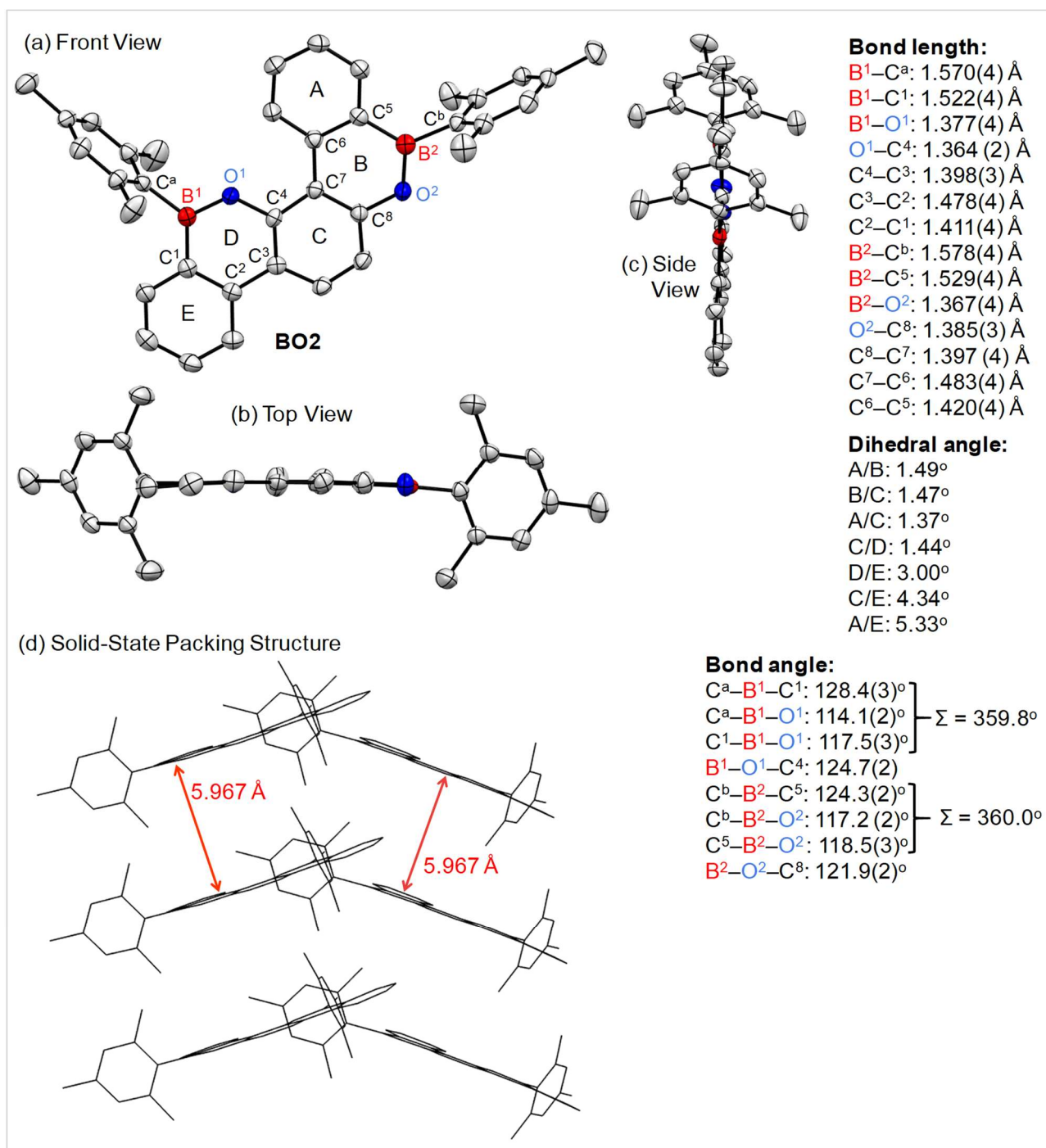


Fig. S6. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of BO2. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.

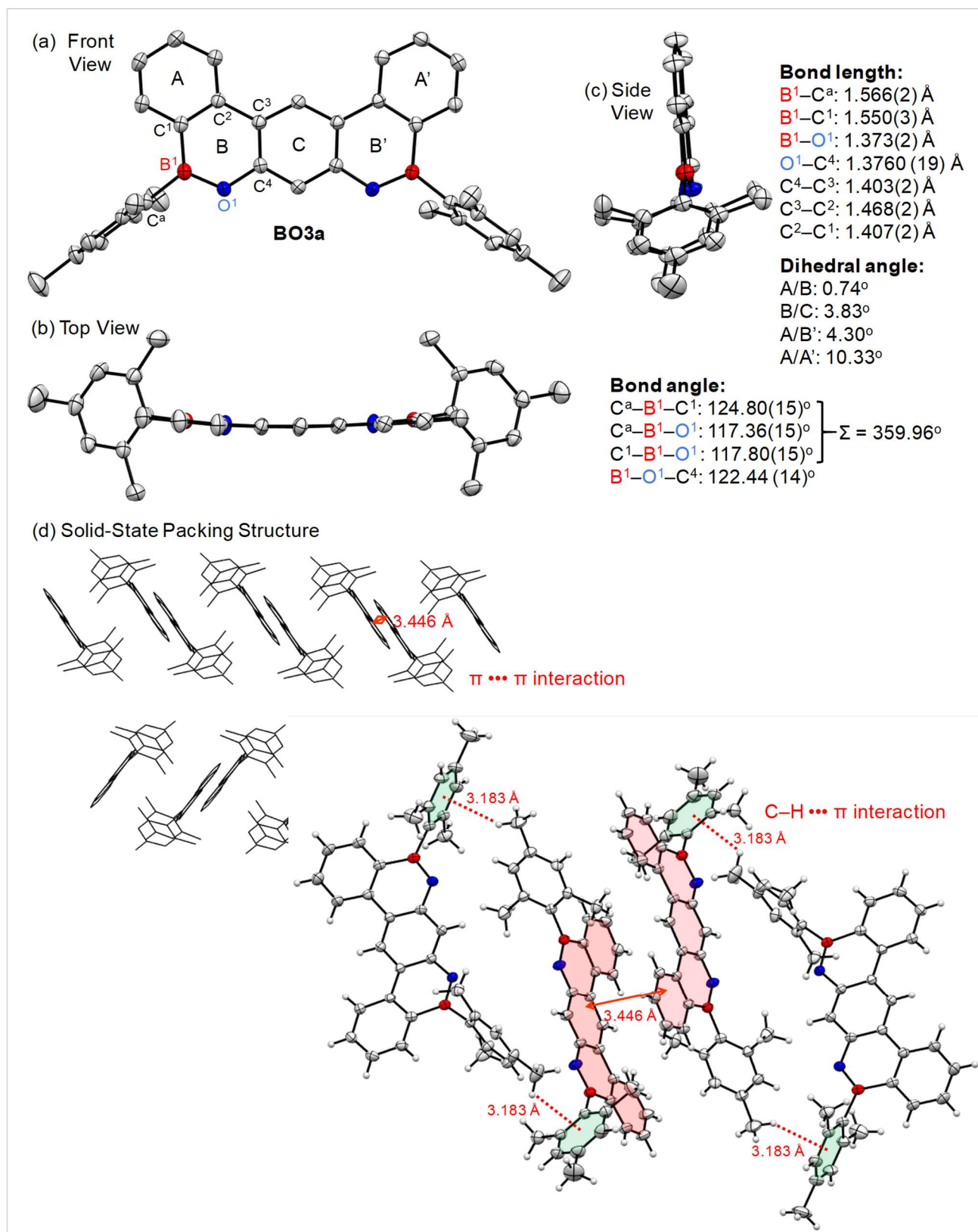


Fig. S7. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO3a**. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.

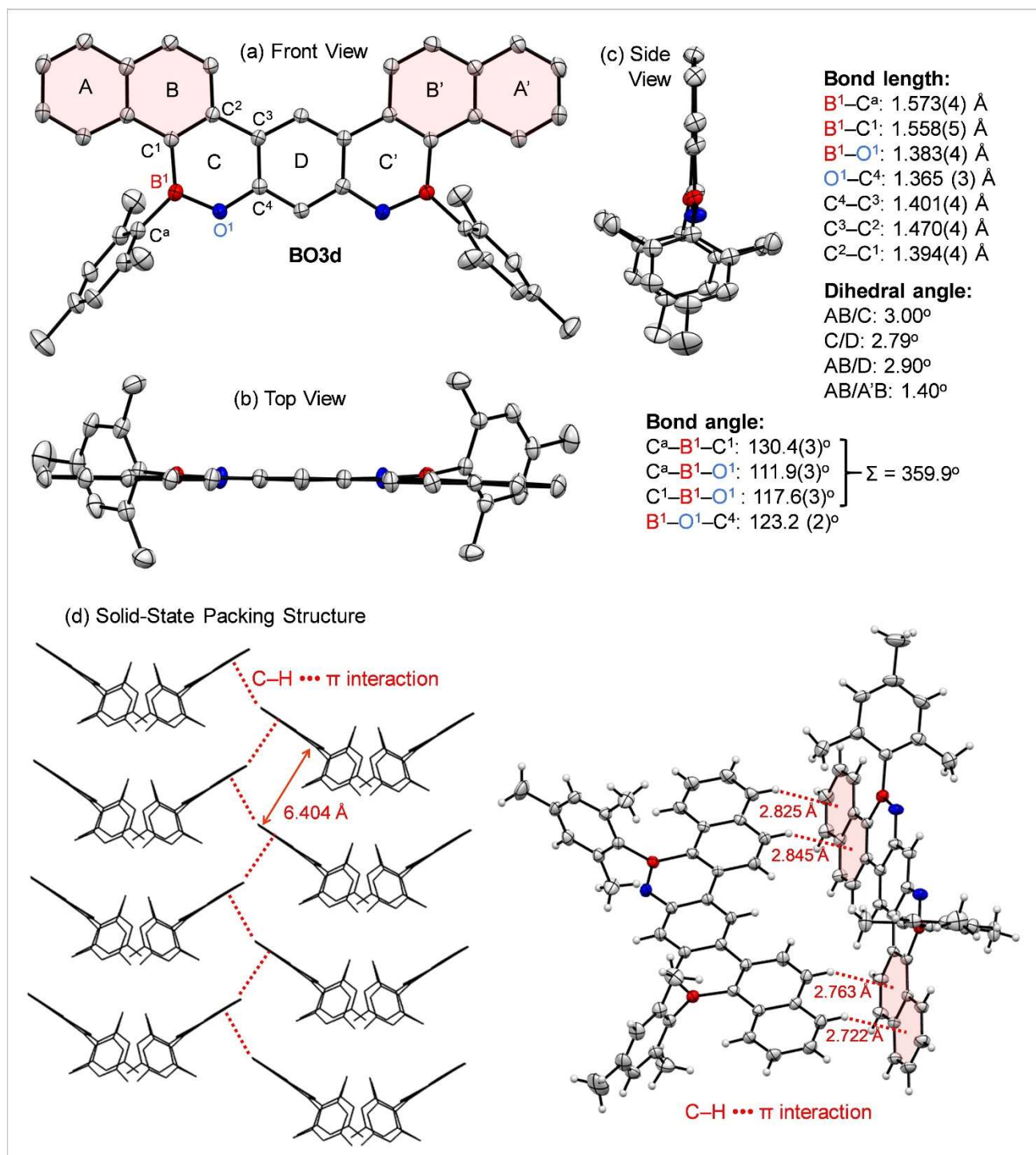


Fig. S8. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO3d**. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.

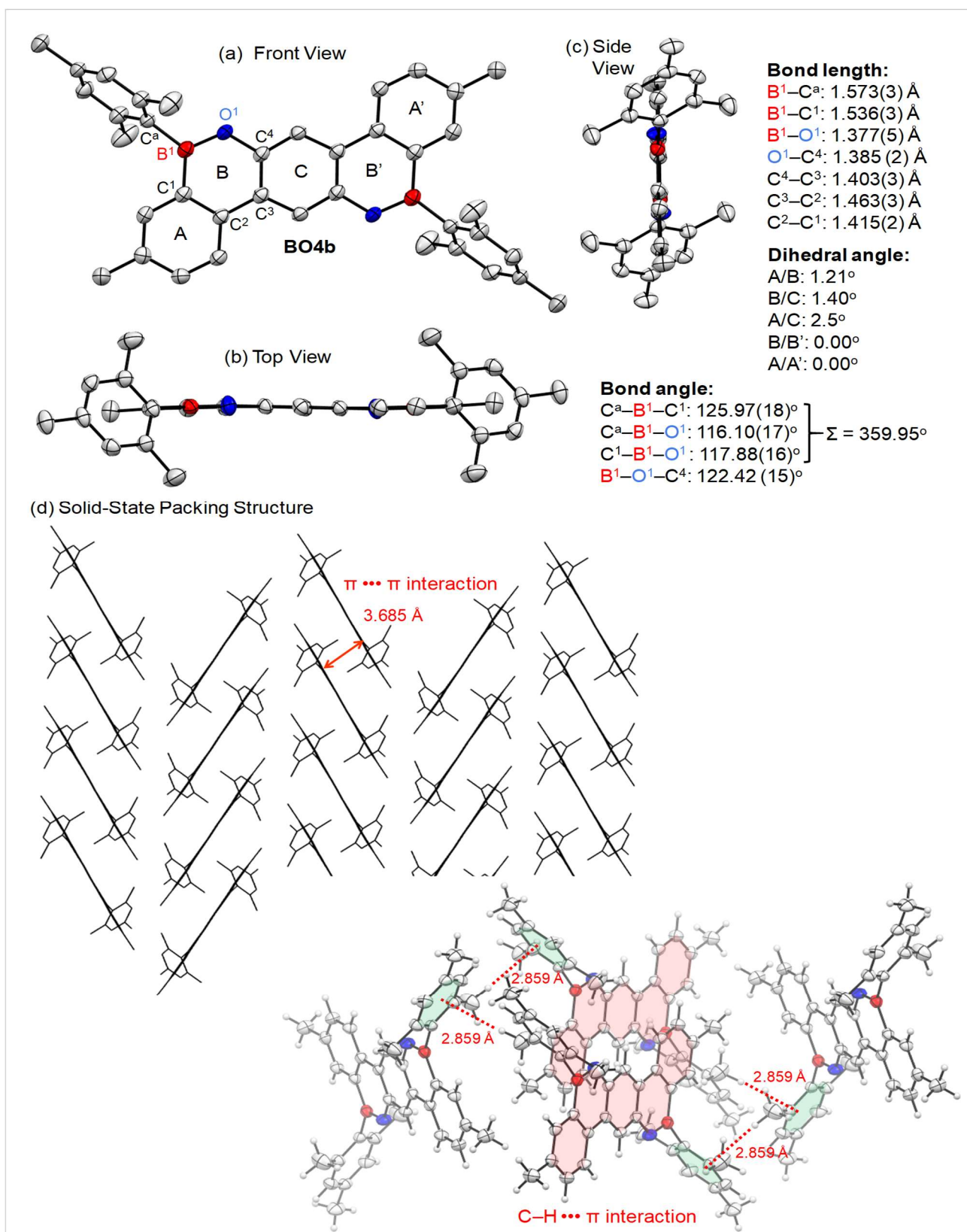


Fig. S9. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO4b**. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.

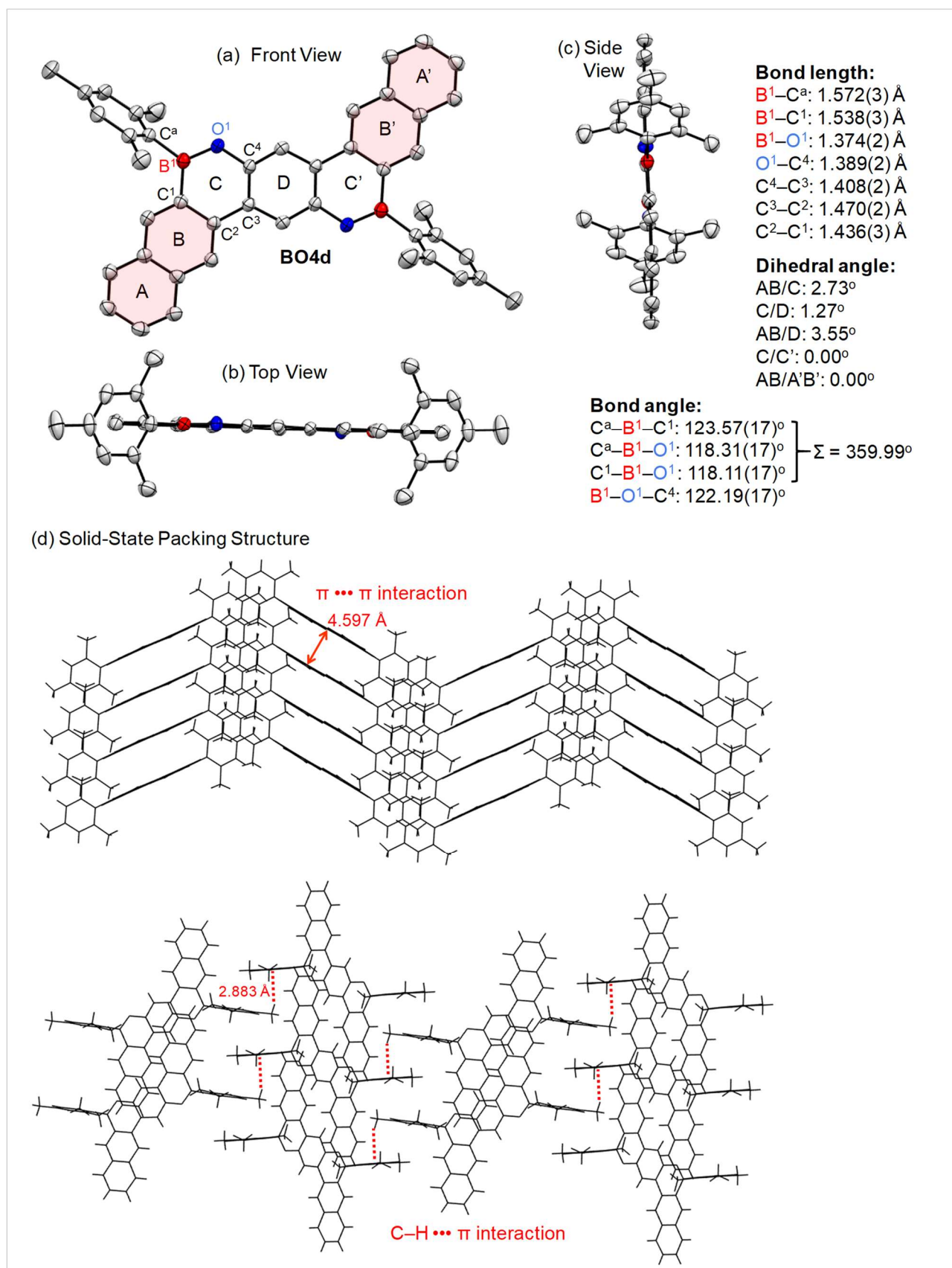


Fig. S10. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of BO4d. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.

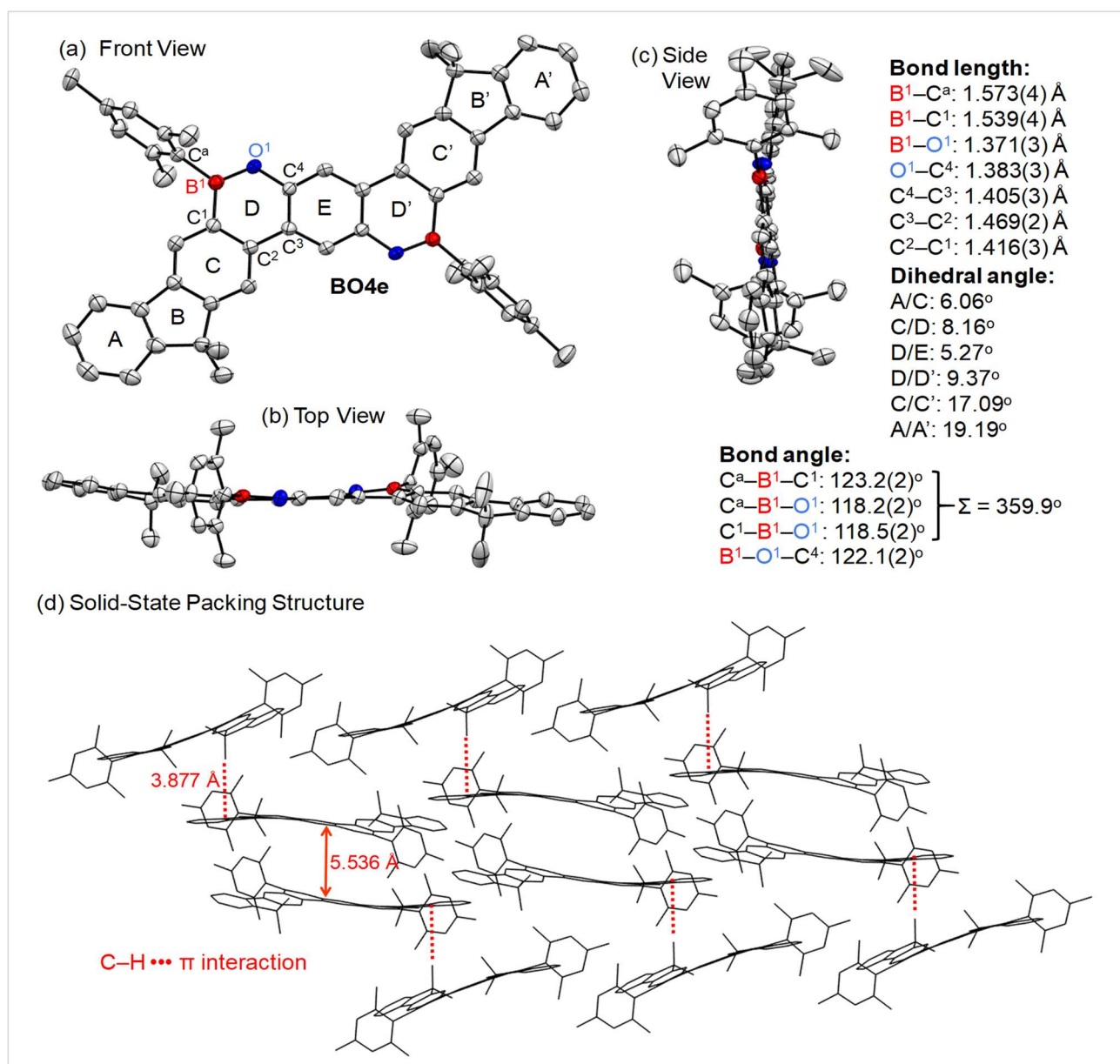


Fig. S11. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO4e**. Hydrogen atoms and solvent dichloromethane molecules were omitted for clarity. Ellipsoids are shown at the 50% probability level.

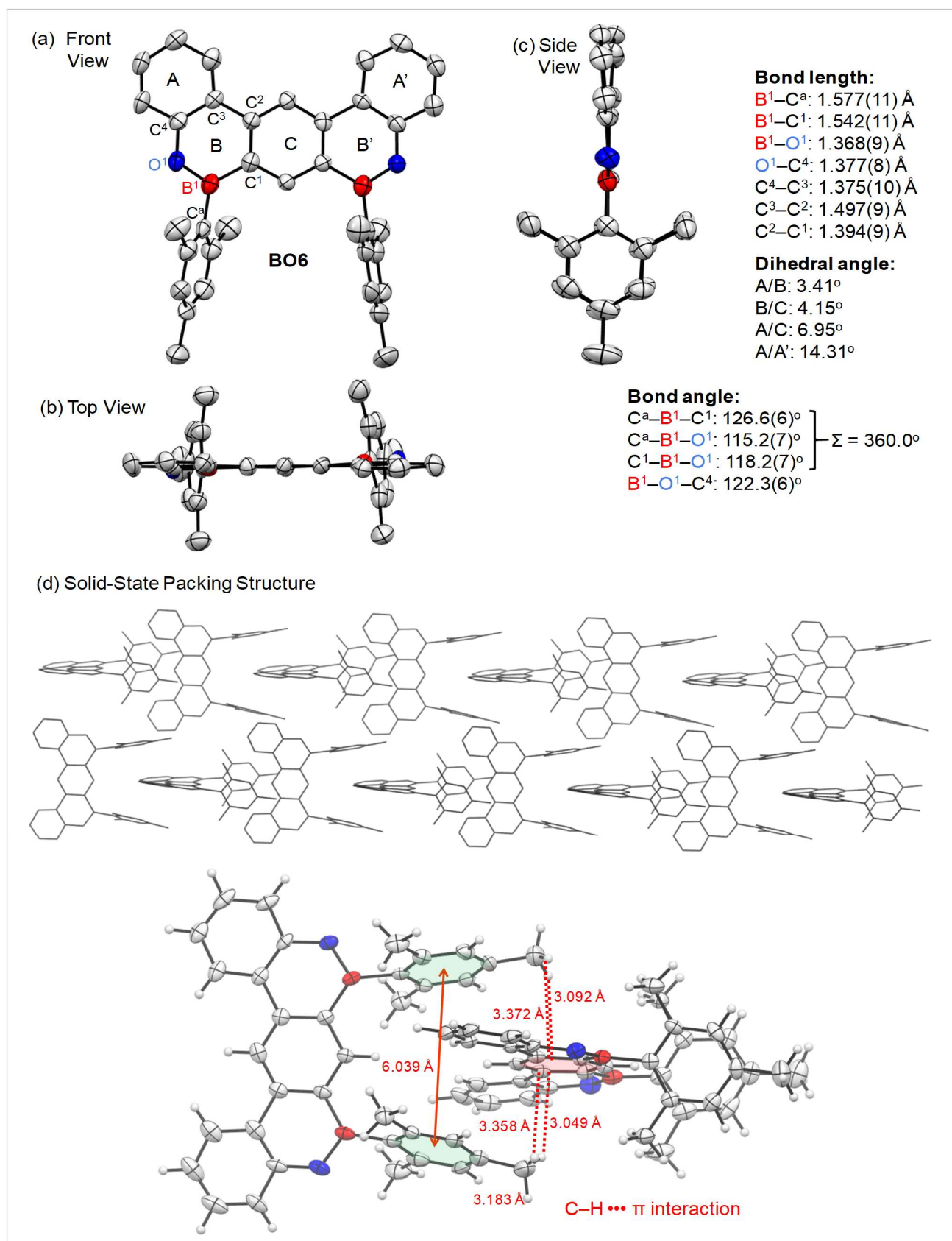


Fig. S12. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of BO6. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.

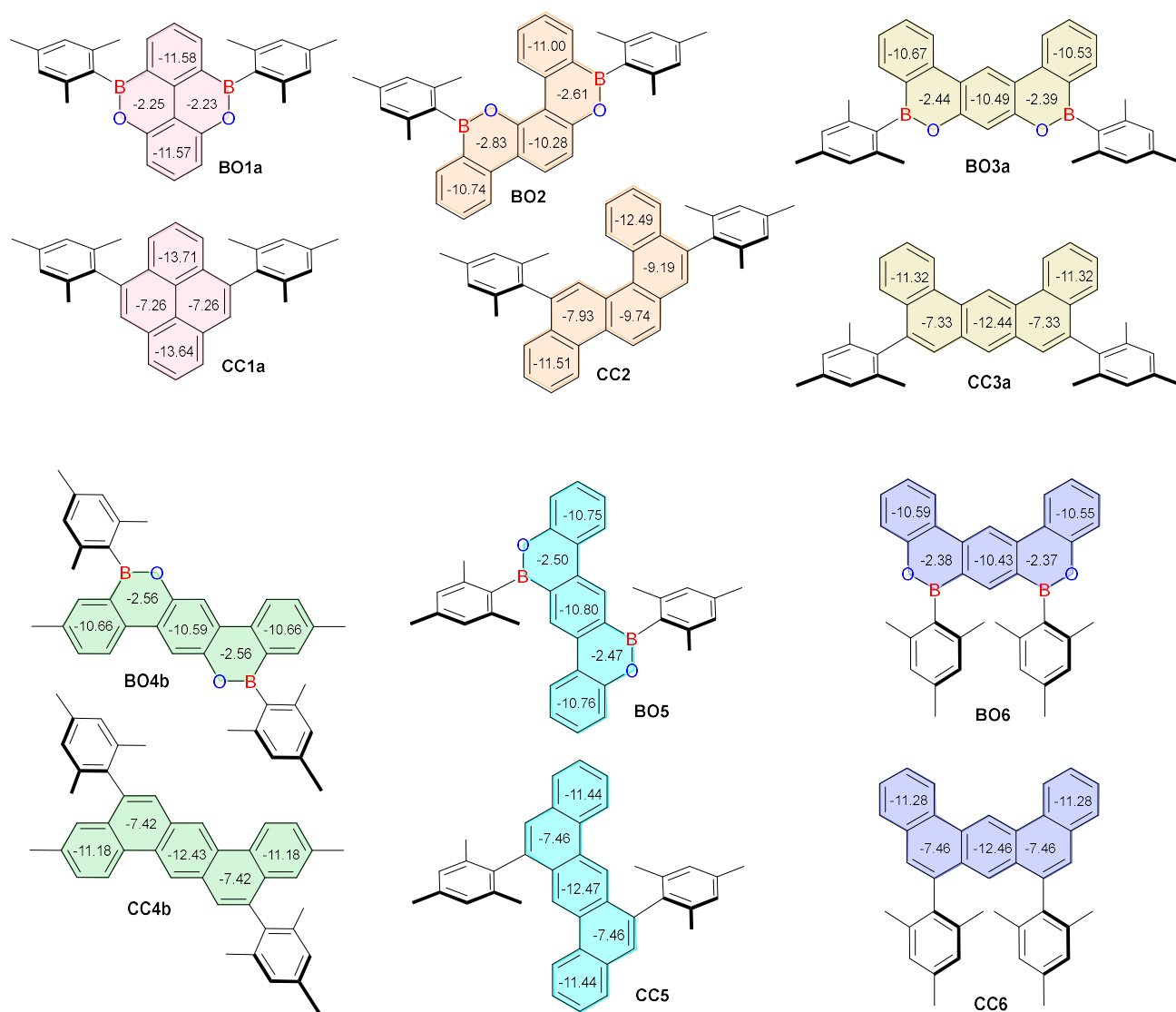


Fig. S13. NICS(1) values of dBO-PAHs. Comparison of the calculated NICS(1) values of dBO-PAHs **BO1a**, **BO2**, **BO3a**, **BO4b**, **BO5**, **BO6** and their corresponding PAH analogues **CC1a**, **CC2**, **CC3a**, **CC4b**, **CC5**, **CC6**. The calculations were performed at B3LYP/6-31G* level.

Table S4. Comparison of calculated HOMO and LUMO levels and energy gaps of the dBO-PAHs and their corresponding carbon analogues

BO-PAH	<i>cat.</i> HOMO/LUMO/ E_g [eV]	BO-PAH	<i>cat.</i> HOMO/LUMO/ E_g [eV]	BO-PAH	<i>cat.</i> HOMO/LUMO/ E_g [eV]
CC1a	−5.28/−1.47/3.81	CC2	−5.47/−1.28/4.19	CC4a	−5.32/−1.49/3.83
BO1a	−6.06/−1.50/4.56	BO2	−5.87/−1.32/4.55	BO4a	−5.82/−1.64/4.18
CC1b	−5.24/−1.44/3.80	CC3a	−5.38/−1.46/3.92	CC4b	−5.24/−1.41/3.83
BO1b	−6.02/−1.47/4.55	BO3a	−5.84/−1.45/4.39	BO4b	−5.65/−1.55/4.10
CC1c	−5.06/−1.41/3.65	CC3b	−5.27/−1.41/3.86	CC4c	−5.12/−1.76/3.36
BO1c	−6.02/−1.43/4.59	BO3b	−5.69/−1.38/4.31	BO4c	−5.49/−2.00/3.49
CC1d	−5.30/−1.50/3.80	CC3c	−5.31/−1.57/3.74	CC4d	−5.11/−1.75/3.36
BO1d	−5.90/−1.53/4.37	BO3c	−5.84/−1.57/4.27	BO4d	−5.45/−1.78/3.67
CC1e	−5.29/−1.50/3.79	CC3d	−5.12/−1.78/3.34	CC4e	−5.17/−1.52/3.65
BO1e	−6.04/−1.51/4.53	BO3d	−5.76/−1.78/3.98	BO4e	−5.38/−1.73/3.65
CC1f	−5.30/−1.51/3.39	CC3e	−5.18/−1.51/3.67	CC5	−5.31/−1.44/3.87
BO1f	−5.92/−1.53/4.39	BO3e	−5.47/−1.49/3.98	BO5	−5.76/−1.69/4.07
CC1g	−5.29/−1.49/3.80			CC6	−5.35/−1.45/3.90
BO1g	−6.05/−1.50/4.55			BO6	−5.99/−1.65/4.34

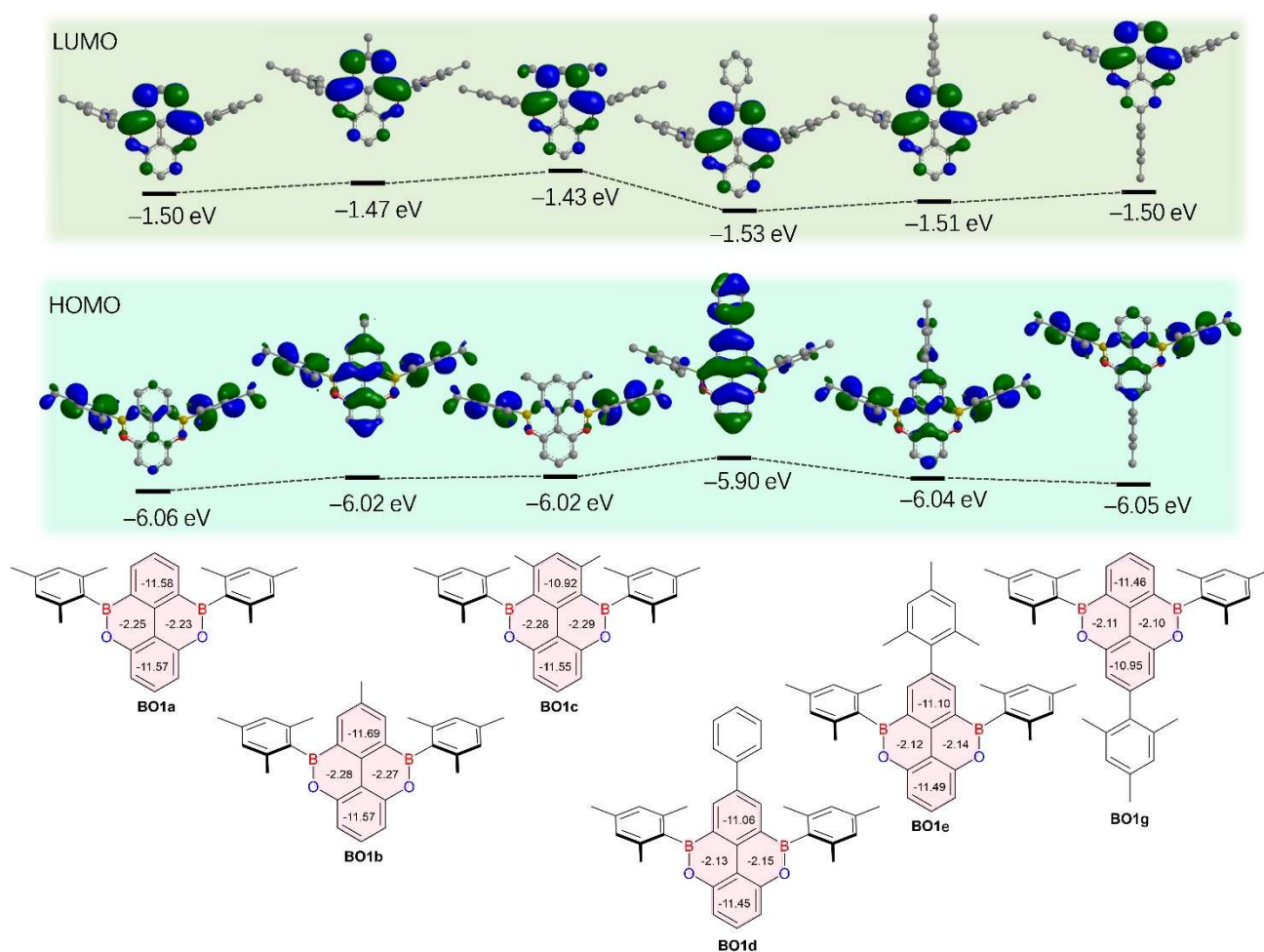


Fig. S14. Theoretical calculation. Comparison of frontier orbital distributions, energy levels and gaps, and NICS(1) values of dBO-PAHs **BO1a**, **BO1b**, **BO1c**, **BO1d**, **BO1e** and **BO1g**. The calculations were performed at B3LYP/6-31G(d) level.

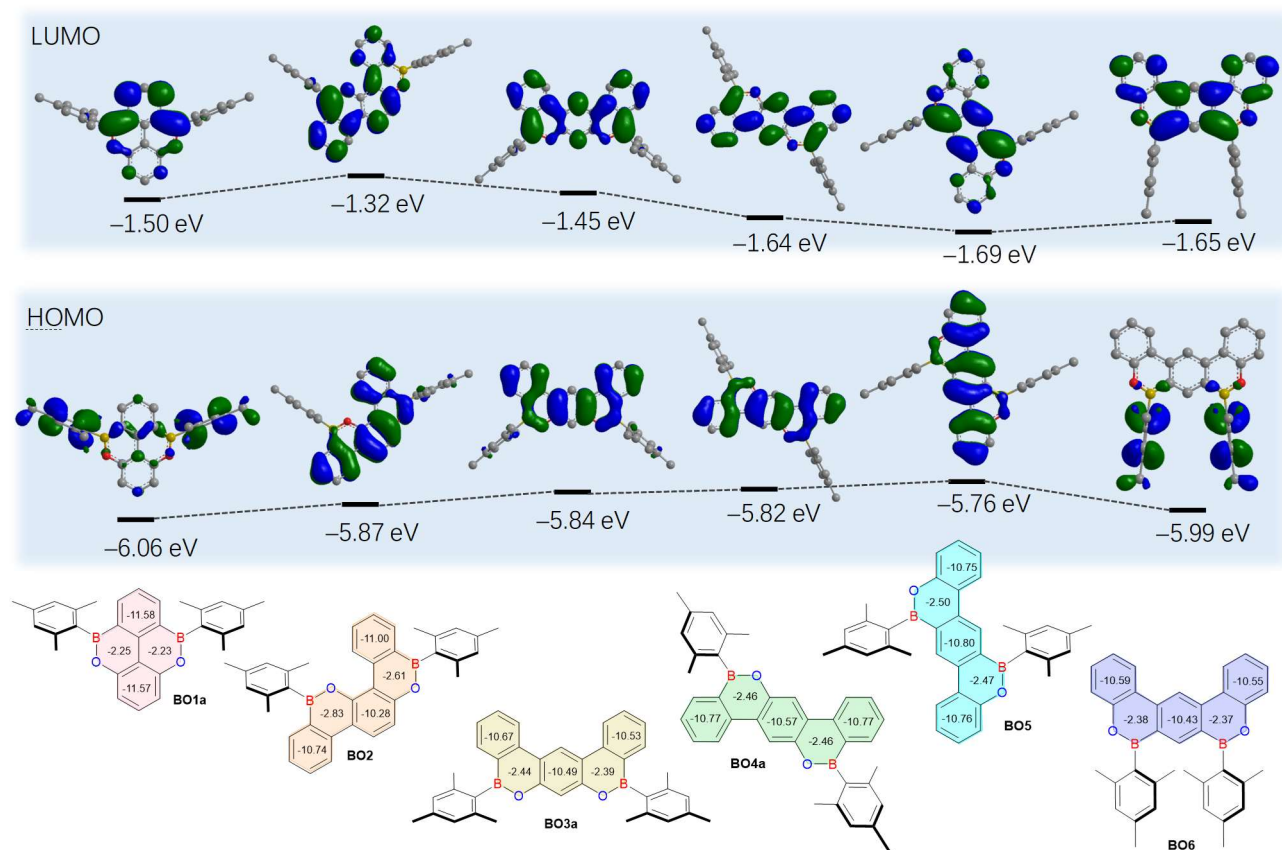


Fig. S15. Theoretical calculation. Comparison of frontier orbital distributions, energy levels and gaps, and NICS(1) values of dBO-PAHs **BO1a**, **BO2**, **BO3a**, **BO4a**, **BO5** and **BO6**. The calculations were performed at B3LYP/6-31G(d) level.

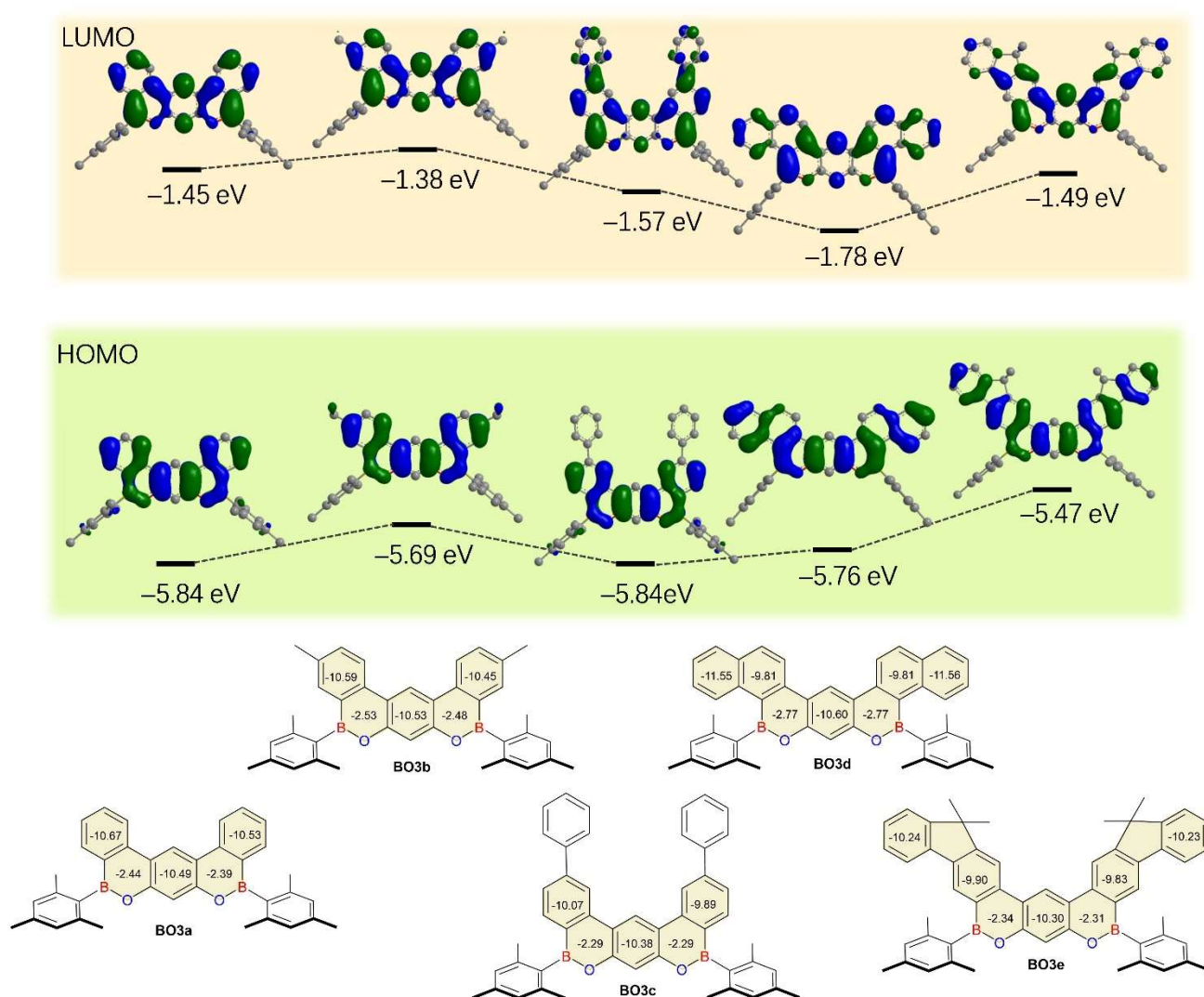


Fig. S16. Theoretical calculation. Comparison of frontier orbital distributions, energy levels and gaps, and NICS(1) values of dBO-PAHs **BO3a**, **BO3b**, **BO3c**, **BO3d** and **BO3e**. The calculations were performed at B3LYP/6-31G(d) level.

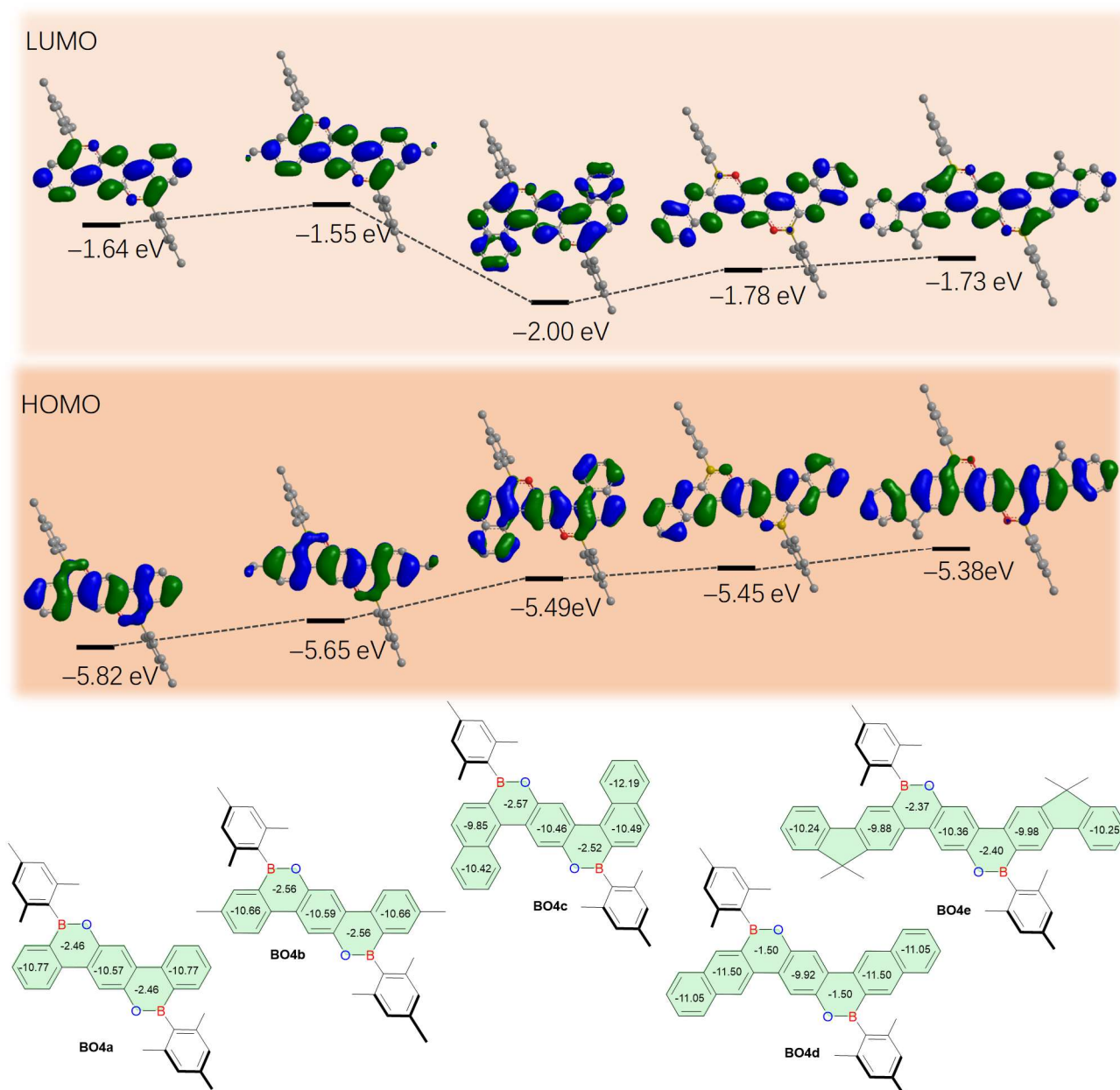


Fig. S17. Theoretical calculation. Comparison of frontier orbital distributions, energy levels and gaps, and NICS(1) values of dBO-PAHs **BO4a**, **BO4b**, **BO4c**, **BO4d** and **BO4e**. The calculations were performed at B3LYP/6-31G(d) level.

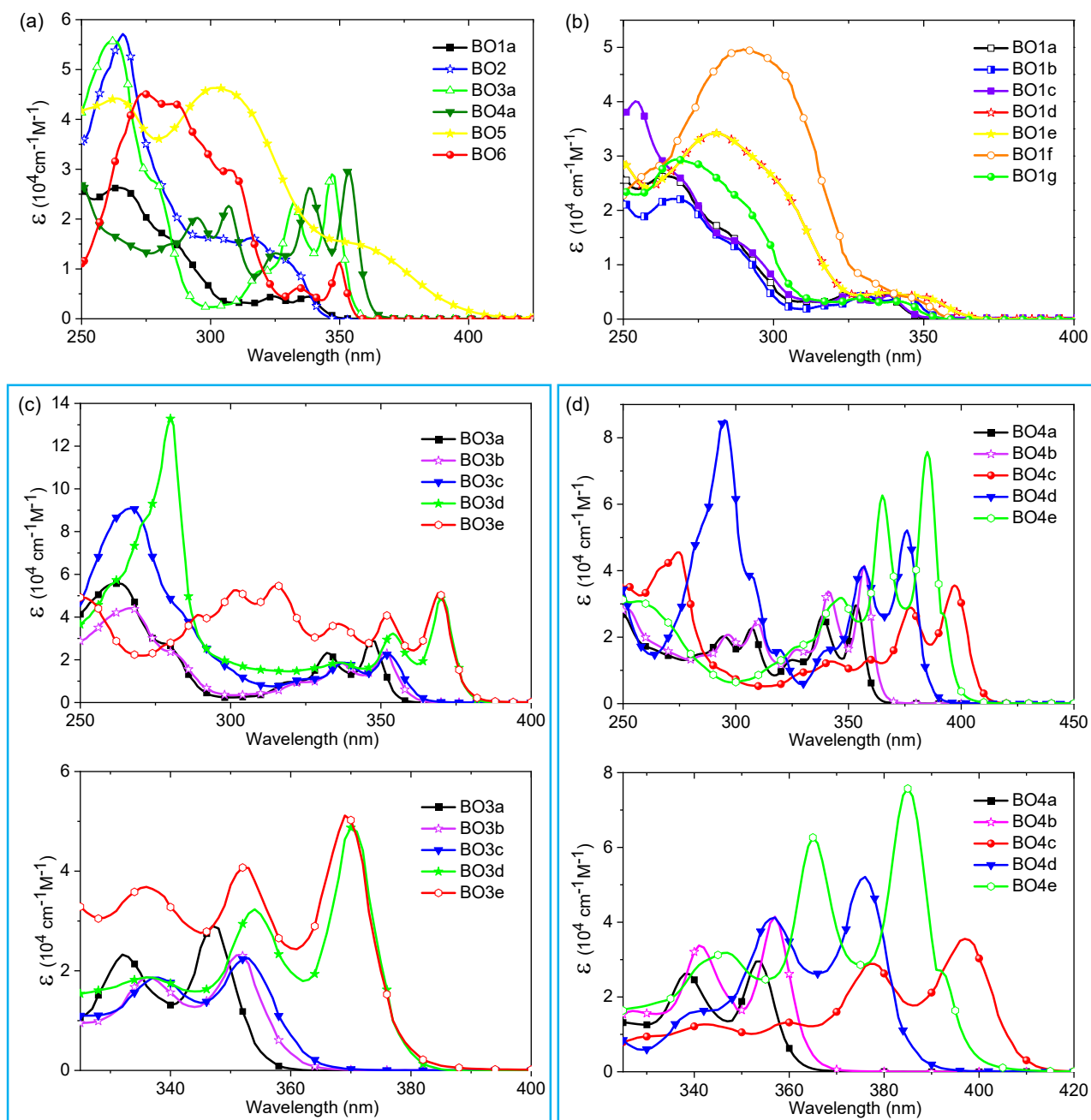


Fig. S18. Photophysical properties. Comparison of room-temperature absorption spectra for (a) BO1a, BO2, BO3a, BO4a, BO5 and BO6, (b) BO1 series, (c) BO3 series and (d) BO4 series in dichloromethane solution.

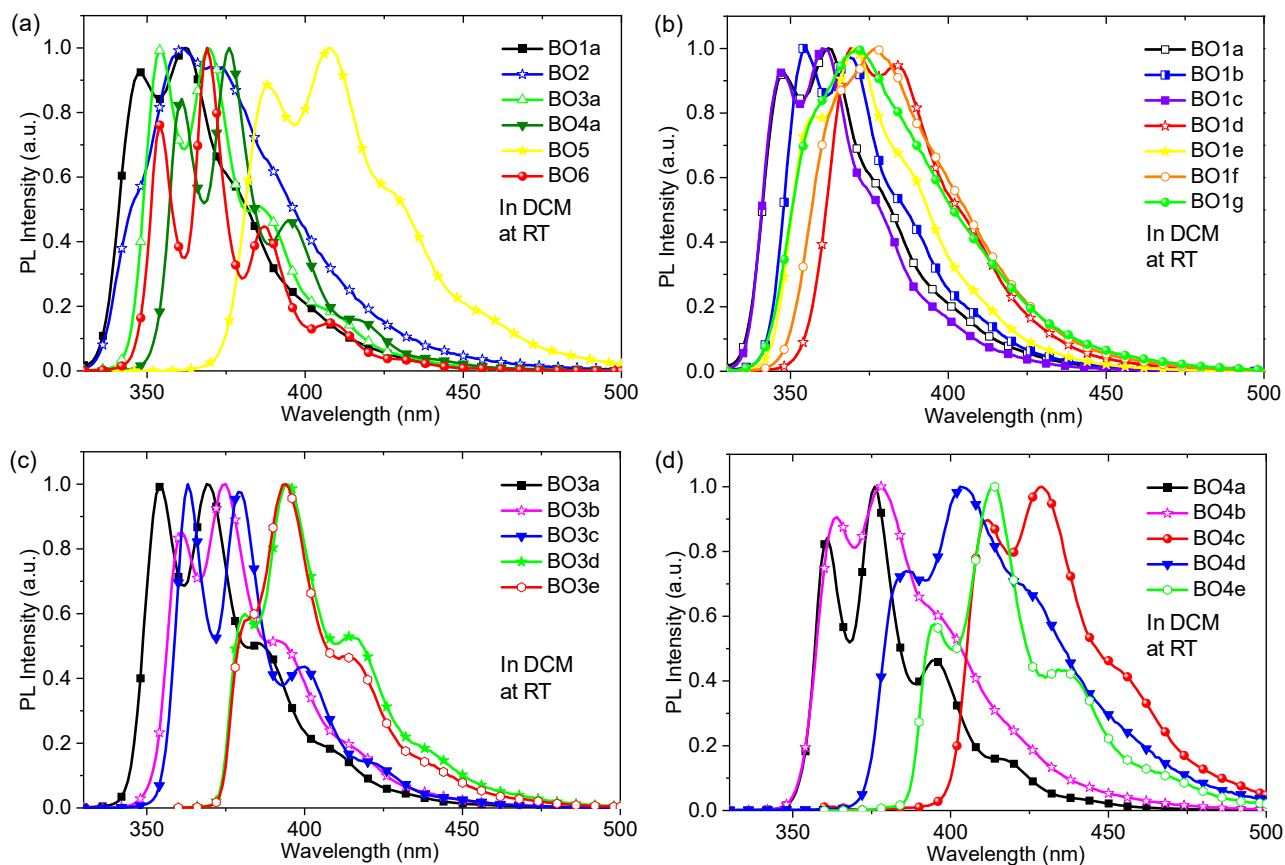


Fig. S19. Photophysical properties. Comparison of room-temperature (RT) PL spectra for (a) **BO1a**, **BO2**, **BO3a**, **BO4a**, **BO5** and **BO6**, (b) **BO1** series, (c) **BO3** series and (d) **BO4** series in dichloromethane solution.

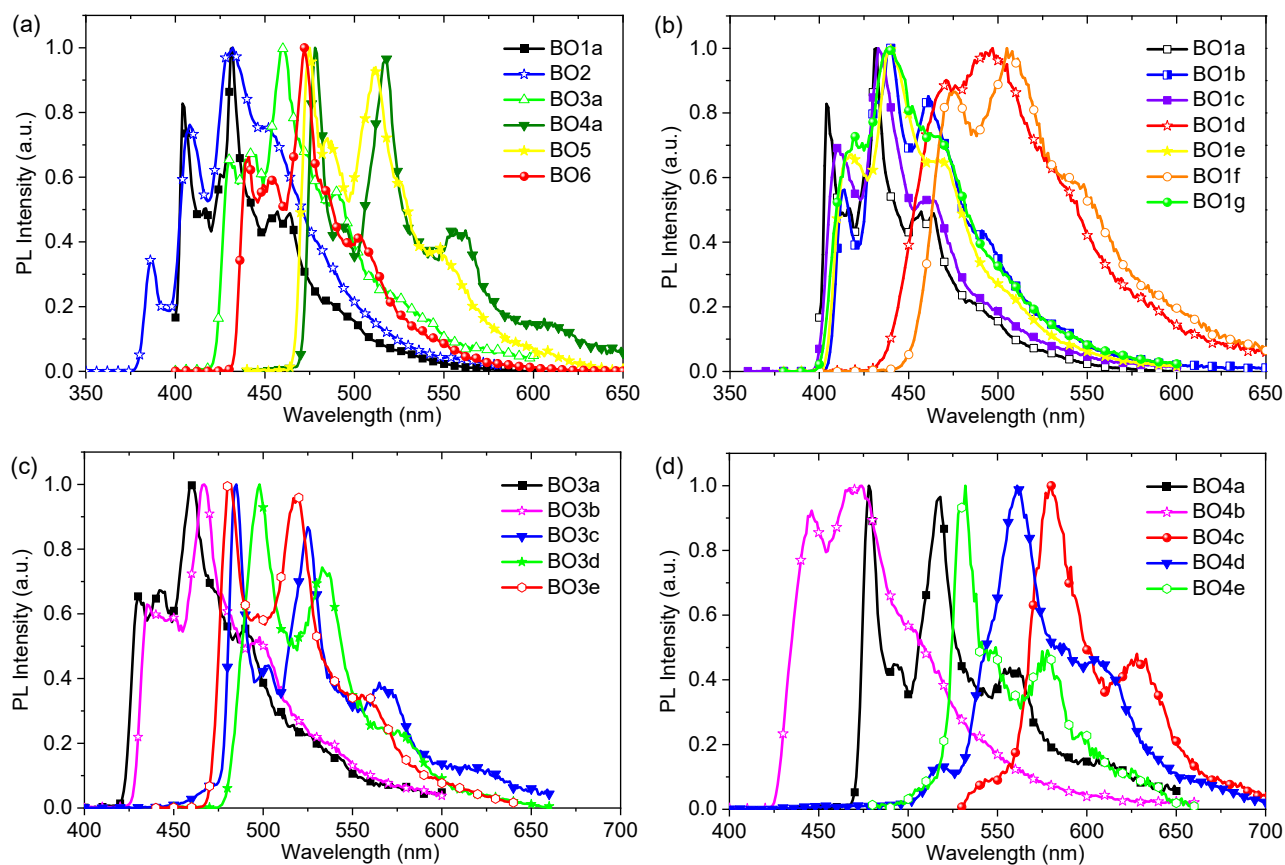


Fig. S20. Photophysical properties. Comparison of low-temperature (77 K) phosphorescent spectra for (a) **BO1a**, **BO2**, **BO3a**, **BO4a**, **BO5** and **BO6**, (b) **BO1** series, (c) **BO3** series and (d) **BO4** series in 2-MeTHF.

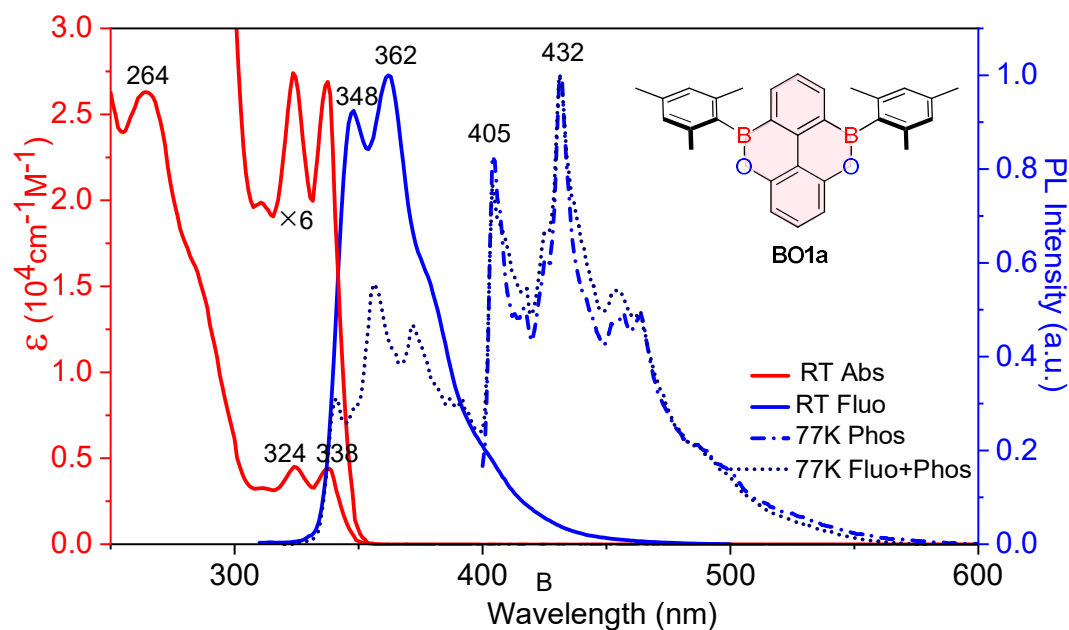


Fig. S21. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1a**. The chemical structure is shown in the inset.

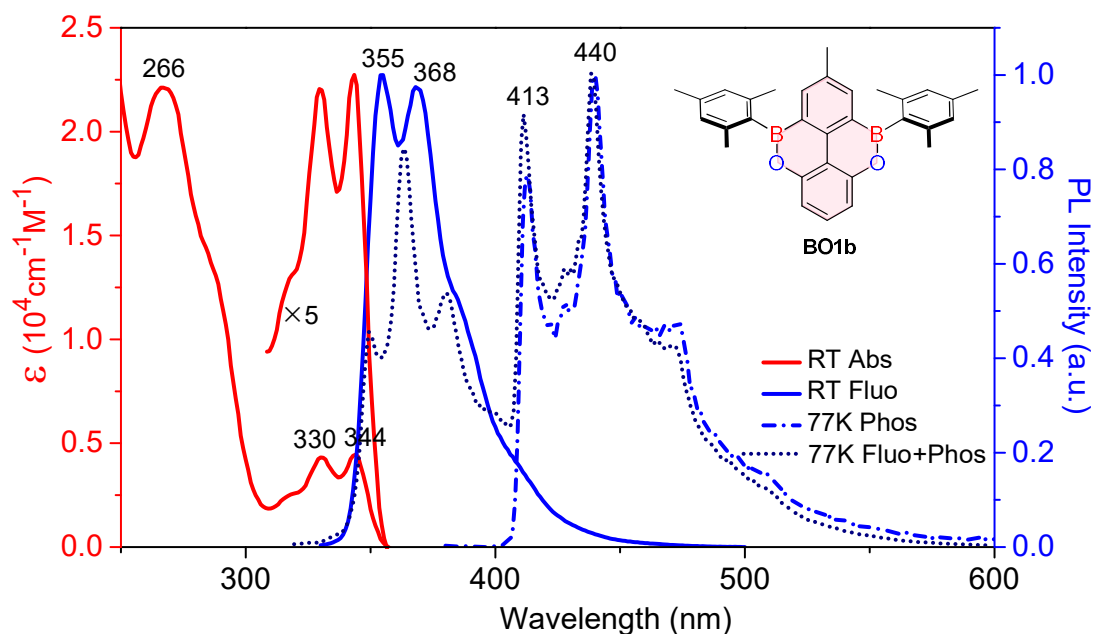


Fig. S22. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1b**. The chemical structure is shown in the inset.

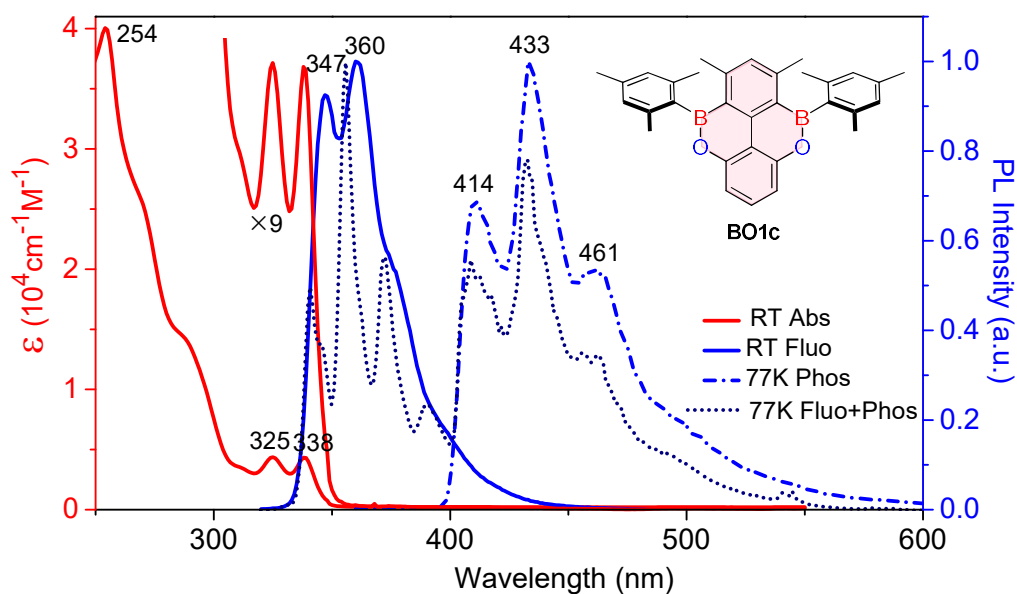


Fig. S23. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1c**. The chemical structure is shown in the inset.

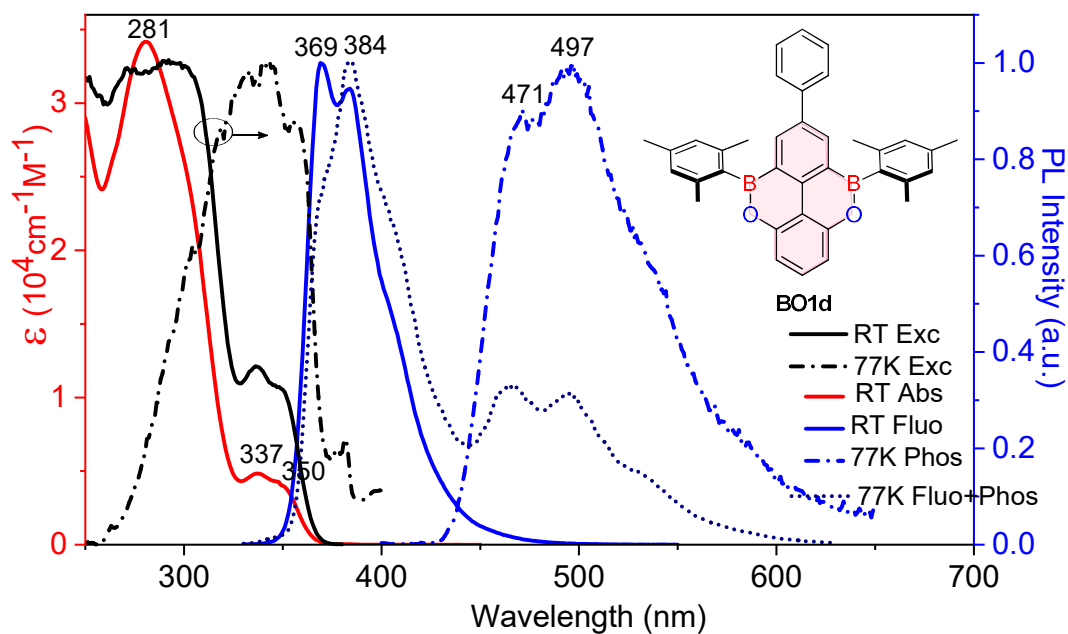


Fig. S24. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF and their corresponding excited spectra of **BO1d**. The chemical structure is shown in the inset.

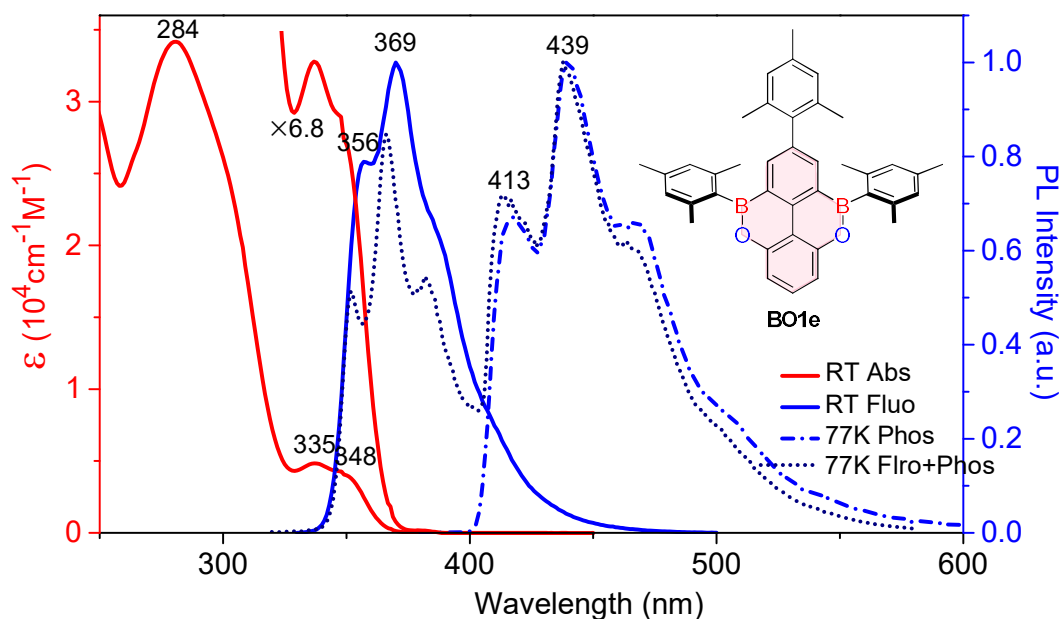


Fig. S25. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1e**. The chemical structure is shown in the inset.

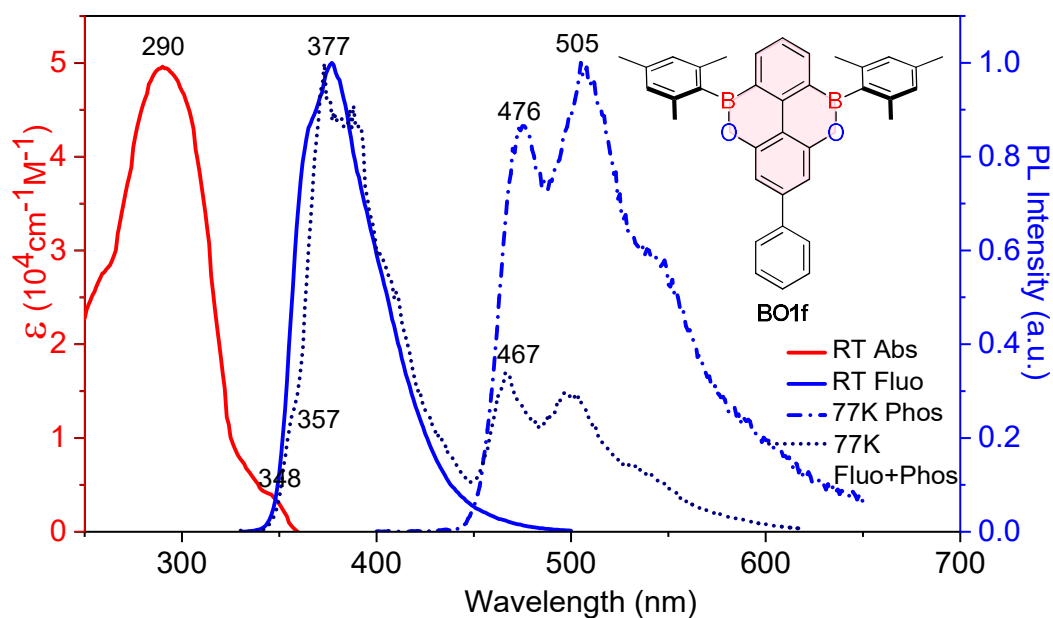


Fig. S26. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1f**. The chemical structure is shown in the inset.

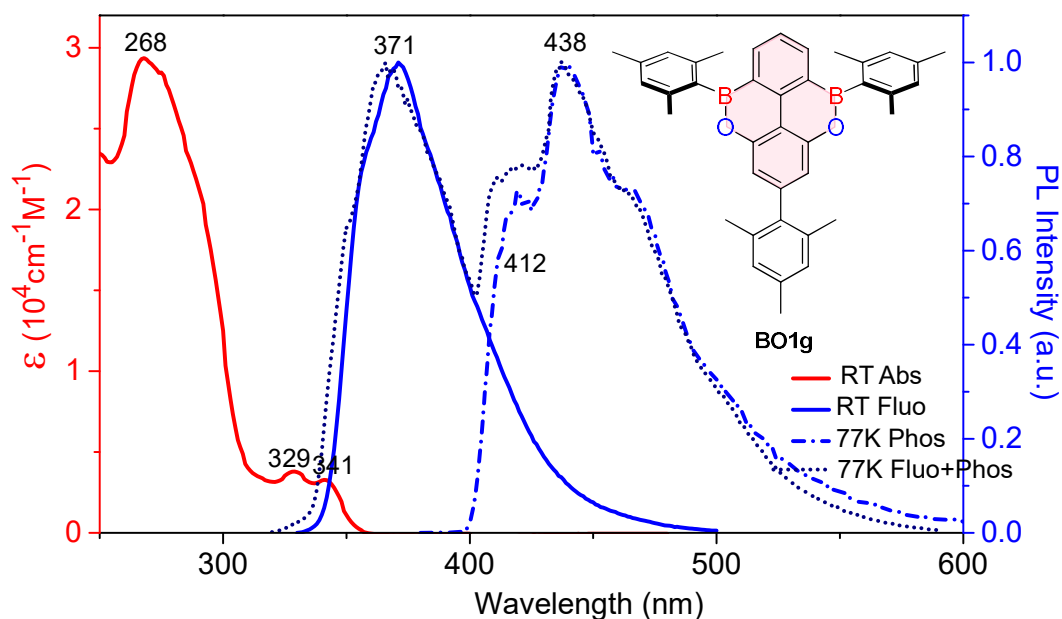


Fig. S27. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1g**. The chemical structure is shown in the inset.

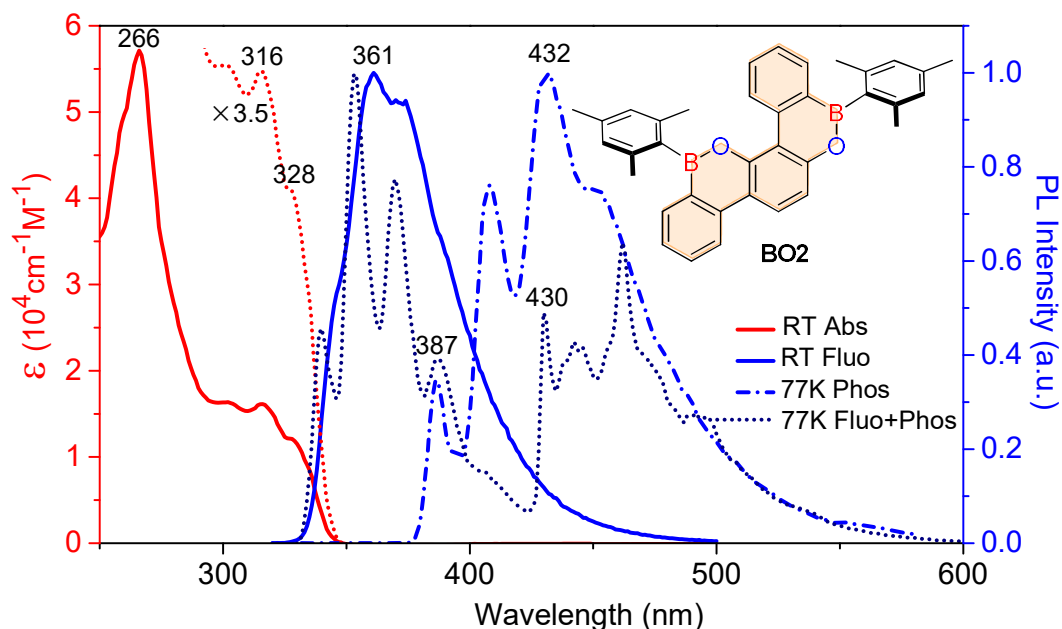


Fig. S28. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO2**. The chemical structure is shown in the inset.

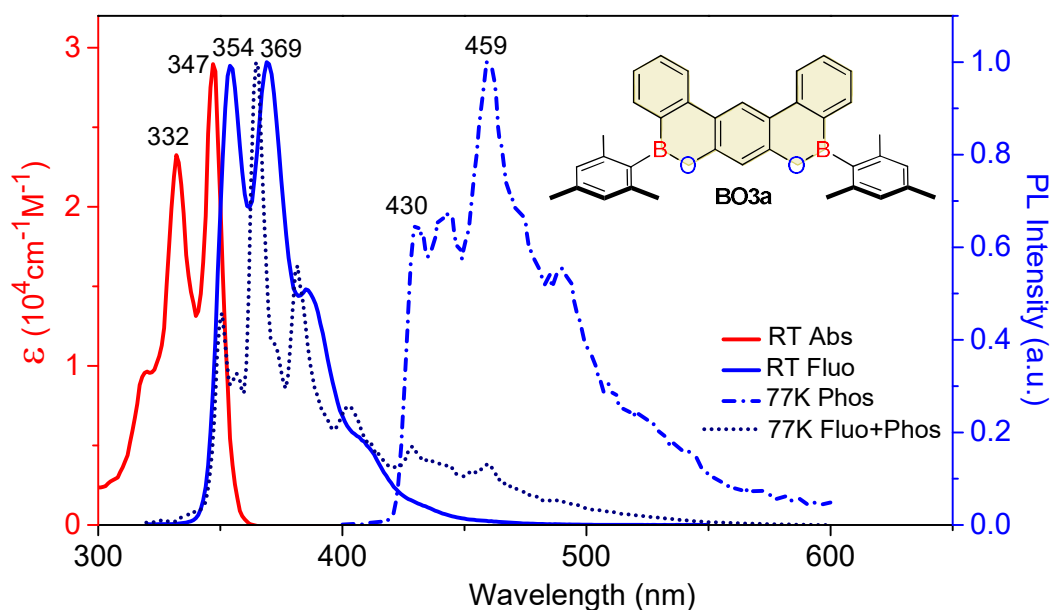


Fig. S29. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO3a**. The chemical structure is shown in the inset.

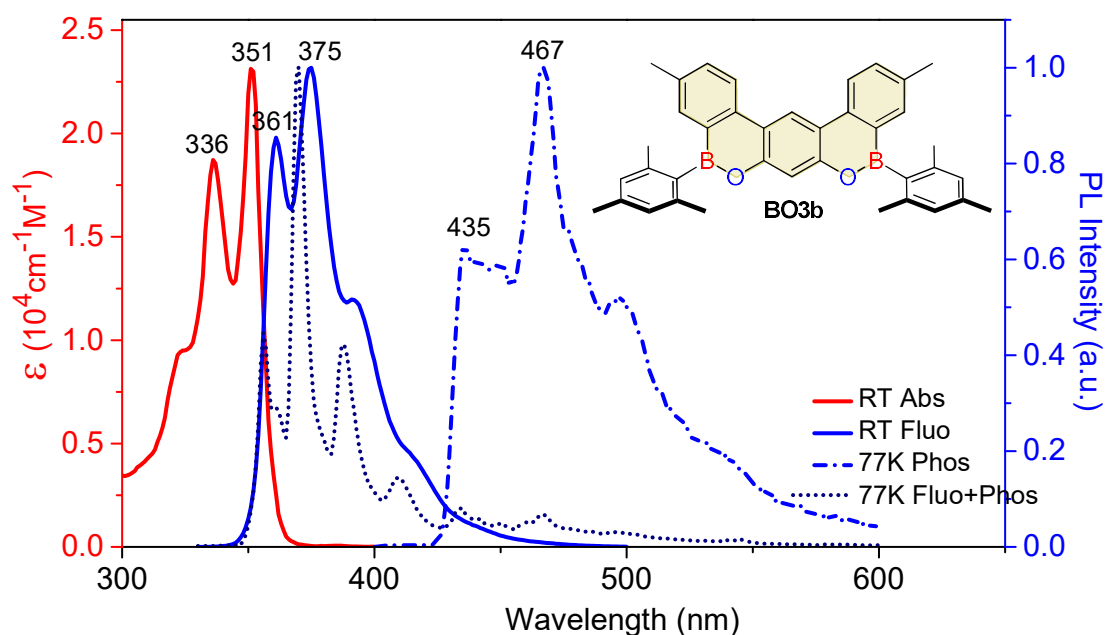


Fig. S30. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO3b**. The chemical structure is shown in the inset.

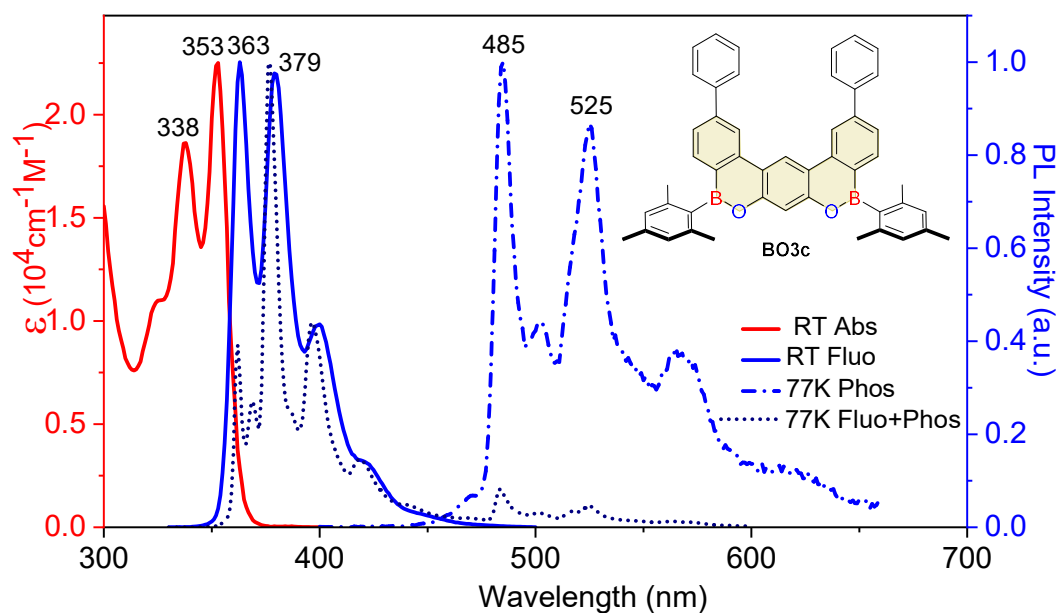


Fig. S31. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO3c**. The chemical structure is shown in the inset.

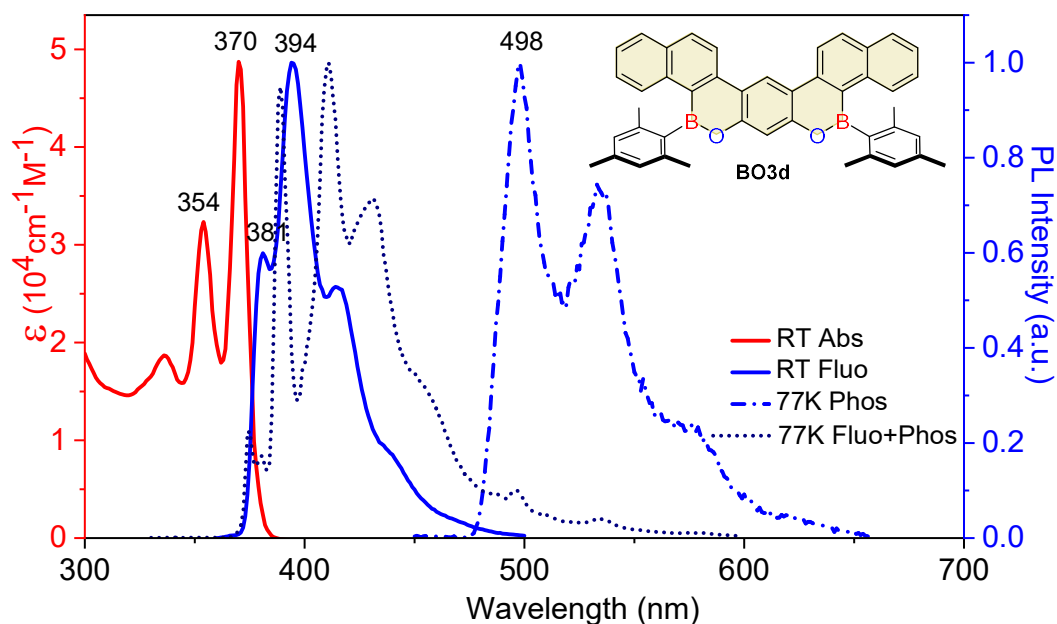


Fig. S32. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO3d**. The chemical structure is shown in the inset.

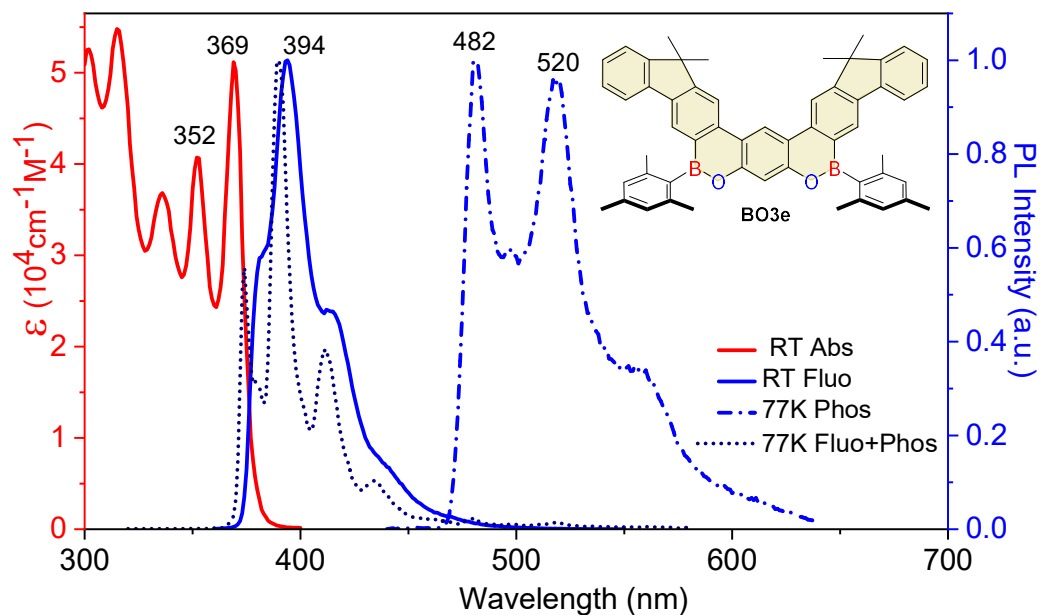


Fig. S33. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO3e**. The chemical structure is shown in the inset.

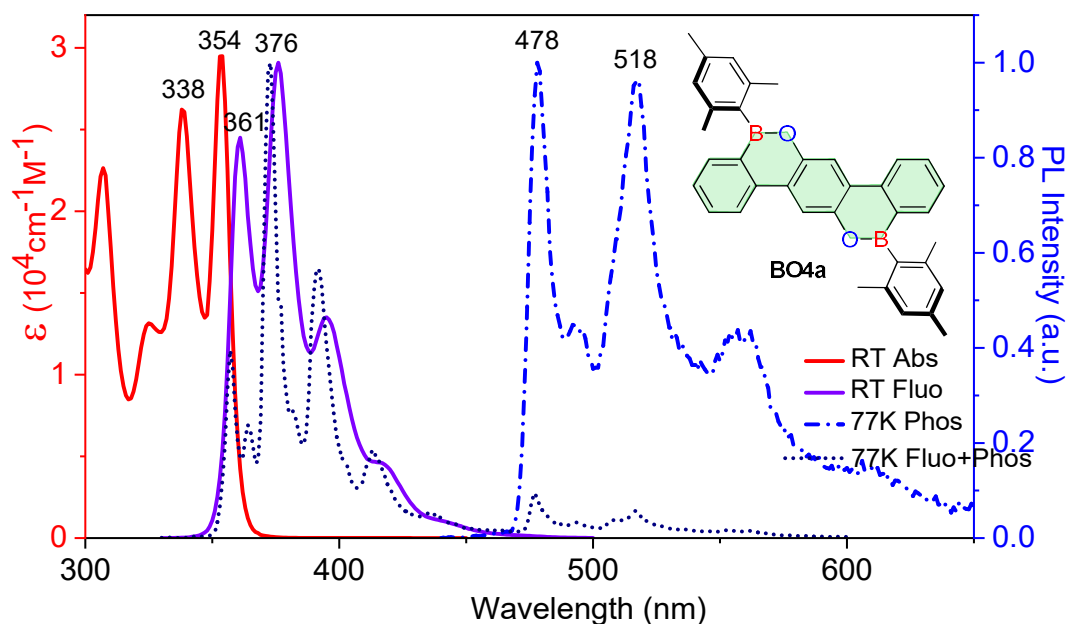


Fig. S34. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO4a**. The chemical structure is shown in the inset.

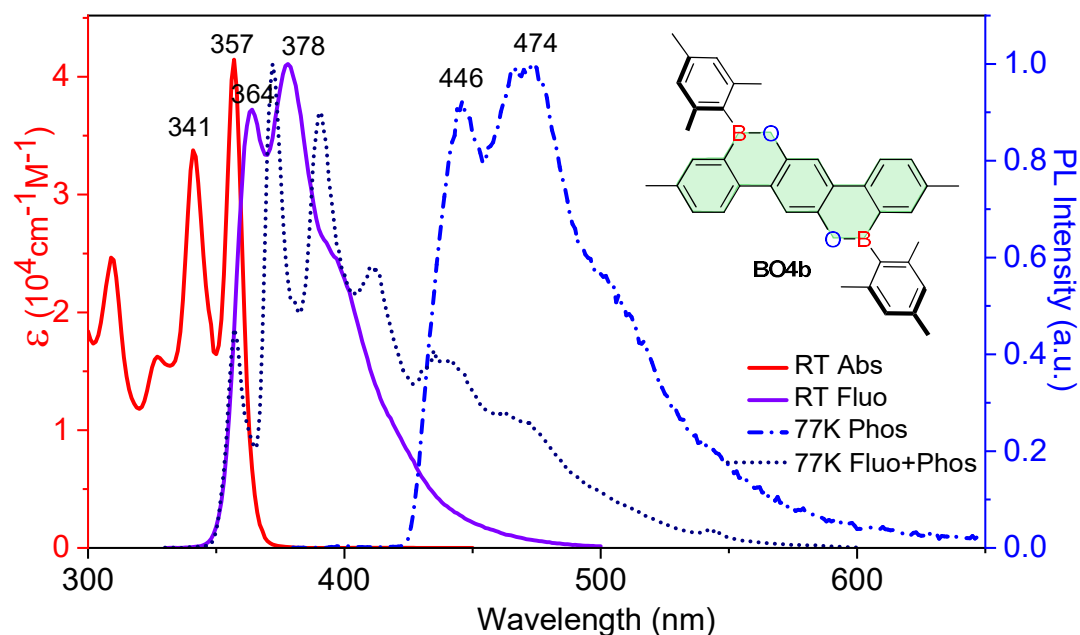


Fig. S35. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO4b**. The chemical structure is shown in the inset.

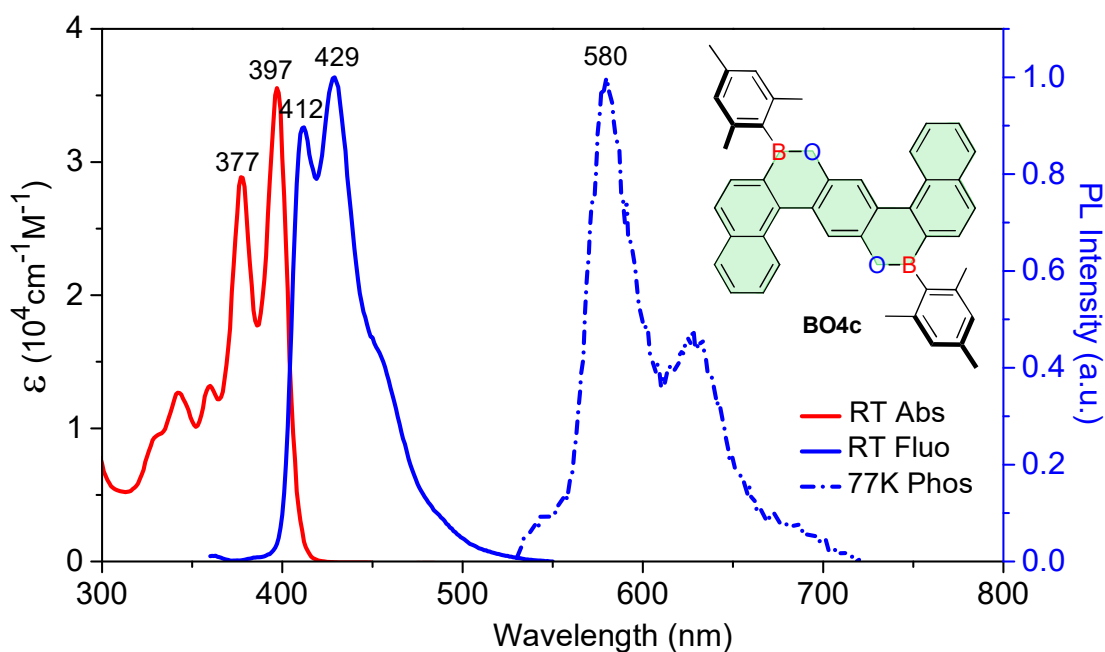


Fig. S36. Photophysical properties. Room-temperature absorption spectrum (red solid line) and luminescent spectrum in dichloromethane (blue solid line), and low-temperature (77 K) phosphorescent spectrum (blue dash-dotted line) in 2-MeTHF of **BO4c**. The chemical structure is shown in the inset.

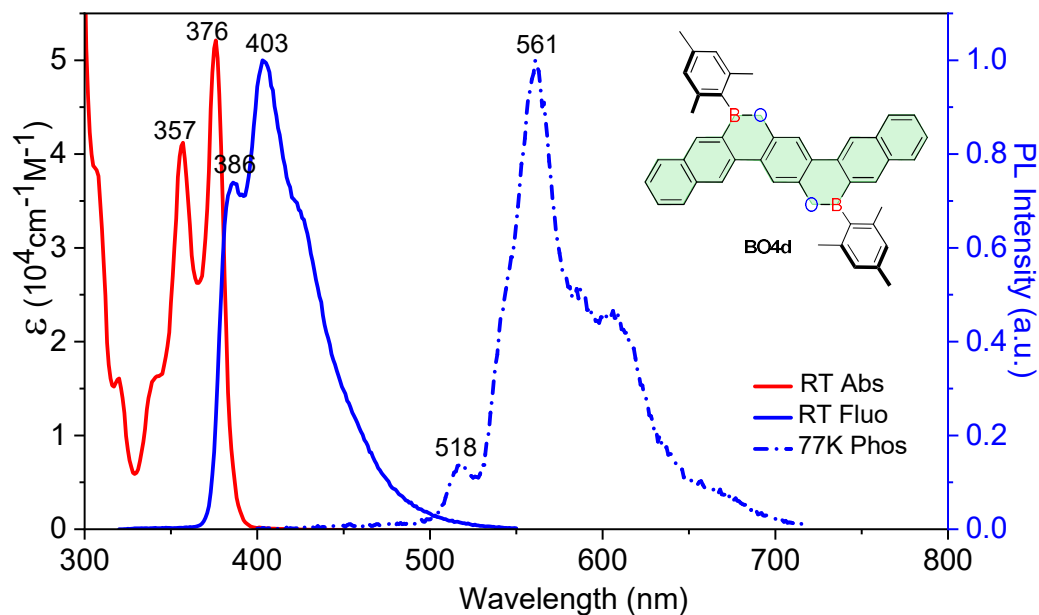


Fig. S37. Photophysical properties. Room-temperature absorption spectrum (red solid line) and luminescent spectrum in dichloromethane (blue solid line), and low-temperature (77 K) phosphorescent spectrum (blue dash-dotted line) in 2-MeTHF of **BO4d**. The chemical structure is shown in the inset.

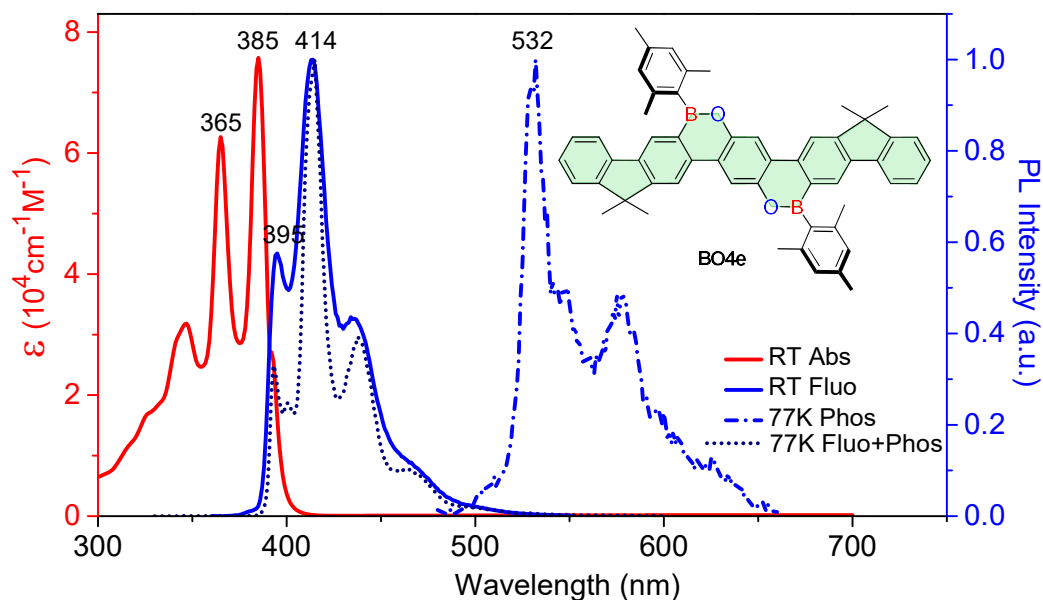


Fig. S38. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO4e**. The chemical structure is shown in the inset.

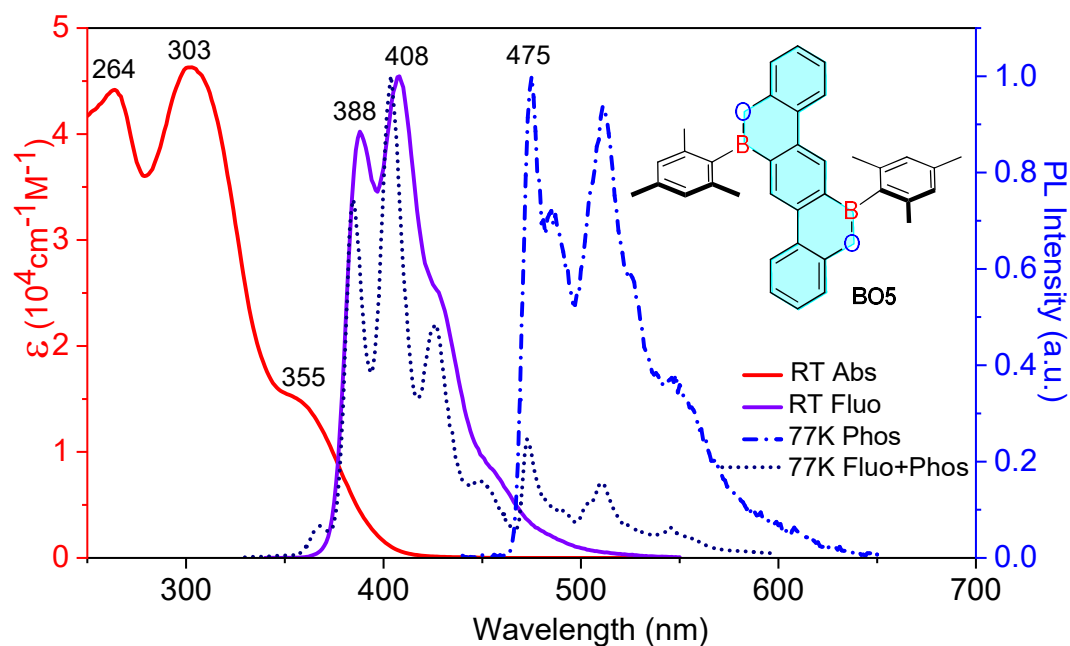


Fig. S39. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO5**. The chemical structure is shown in the inset.

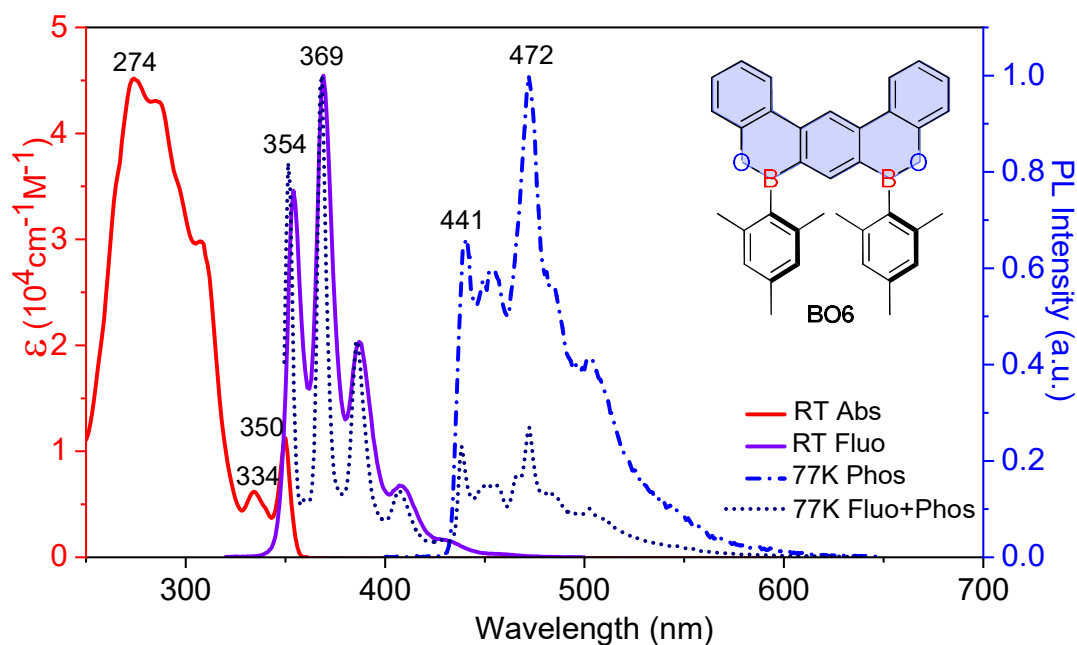


Fig. S40. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO6**. The chemical structure is shown in the inset.

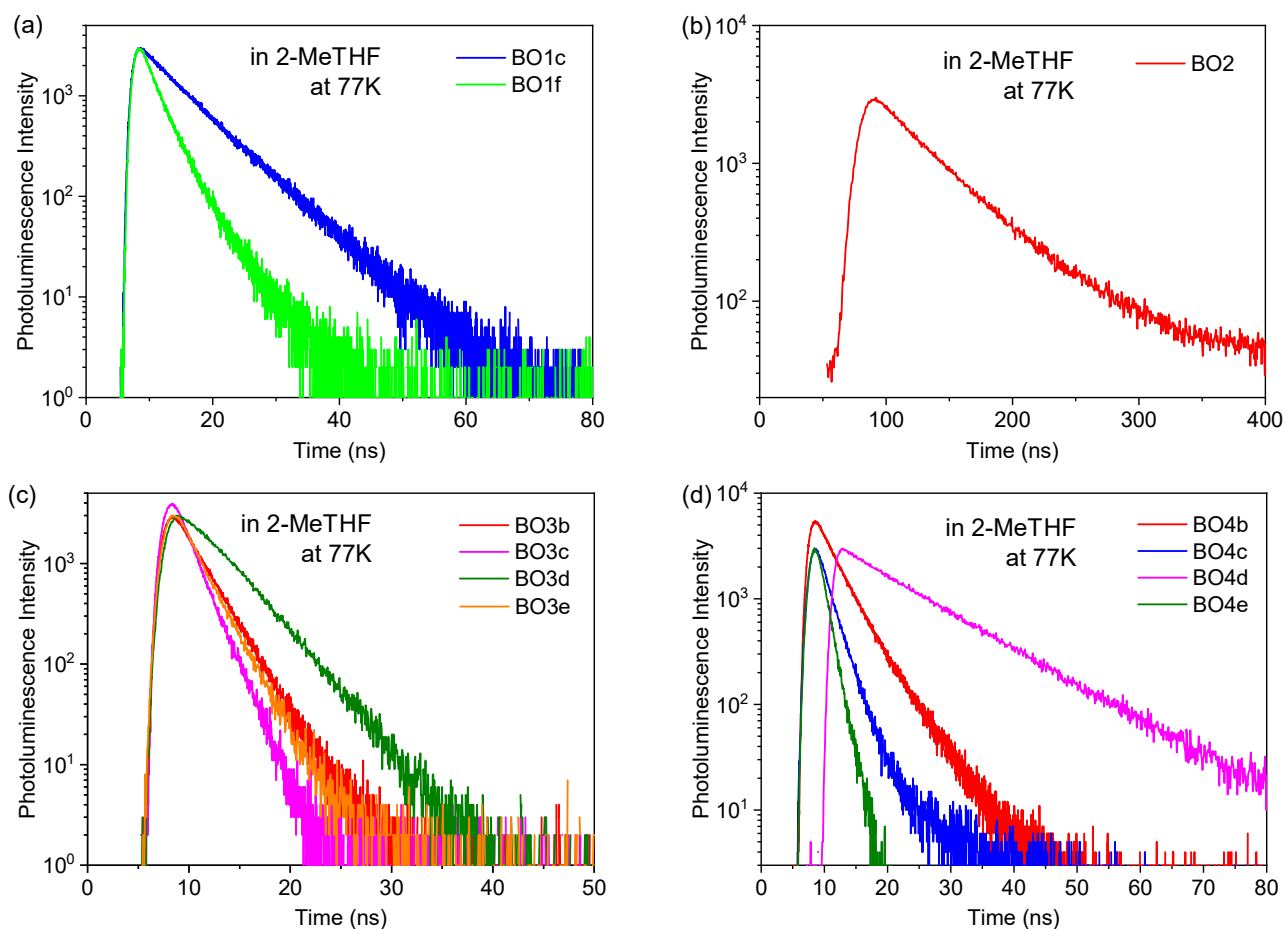


Fig. S41. Photophysical properties. Selected PL decay of (a) **BO1c**, **BO1f**, (b) **BO2**, (c) **BO3b**, **BO3c**, **BO3d**, **BO3e**, and (d) **BO4b**, **BO4c**, **BO4d**, **BO4e** in 2-MeTHF at 77 K excited at their corresponding first fluorescent peak.

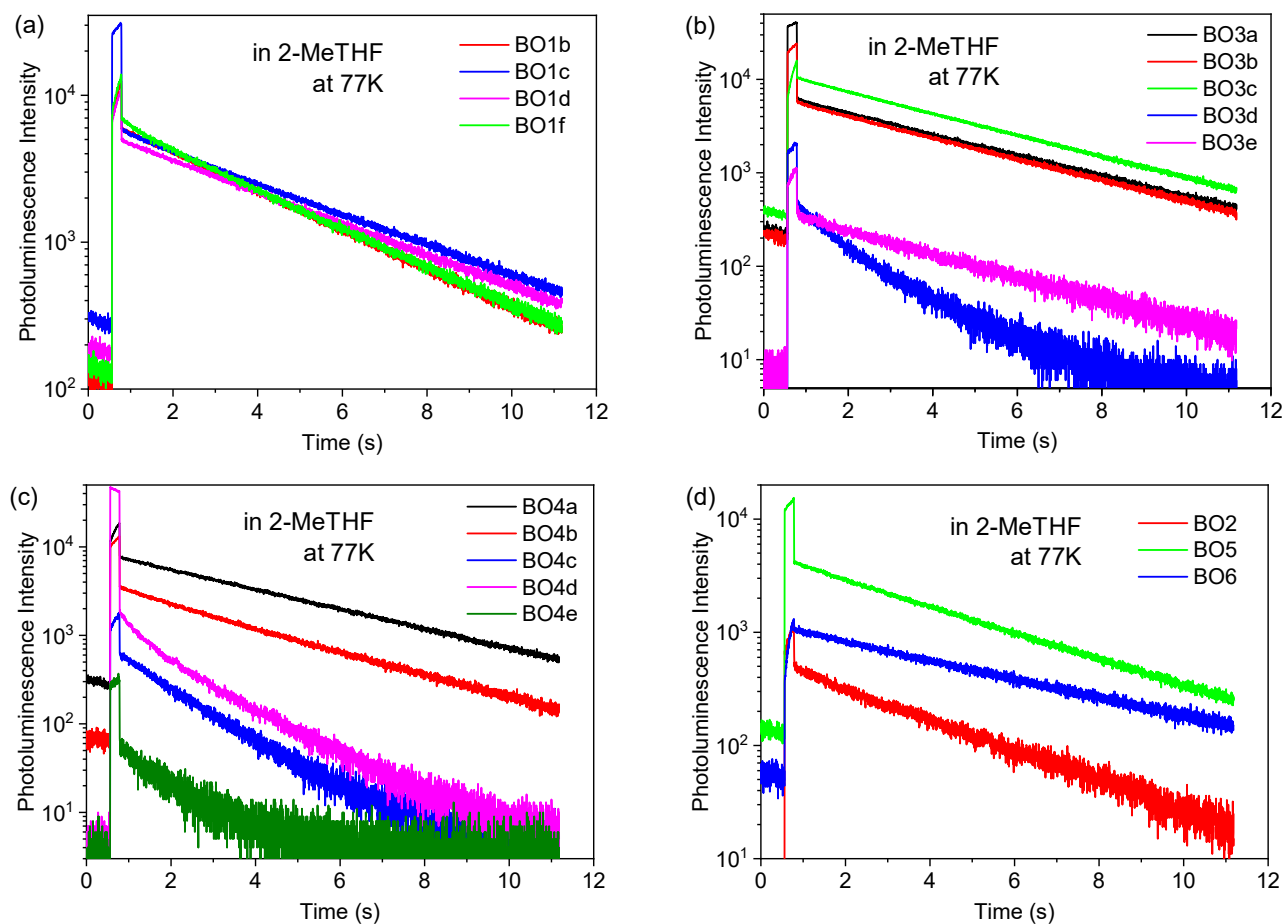


Fig. S42. Photophysical properties. Selected PL decay of (a) **BO1b**, **BO1c**, **BO1d**, **BO1f**, (b) **BO3a**, **BO3b**, **BO3c**, **BO3d**, **BO3e**, (c) **BO4a**, **BO4b**, **BO4c**, **BO4d**, **BO4e**, and (d) **BO2**, **BO5**, **BO6** in 2-MeTHF at 77 K excited at their corresponding first phosphorescent peak.

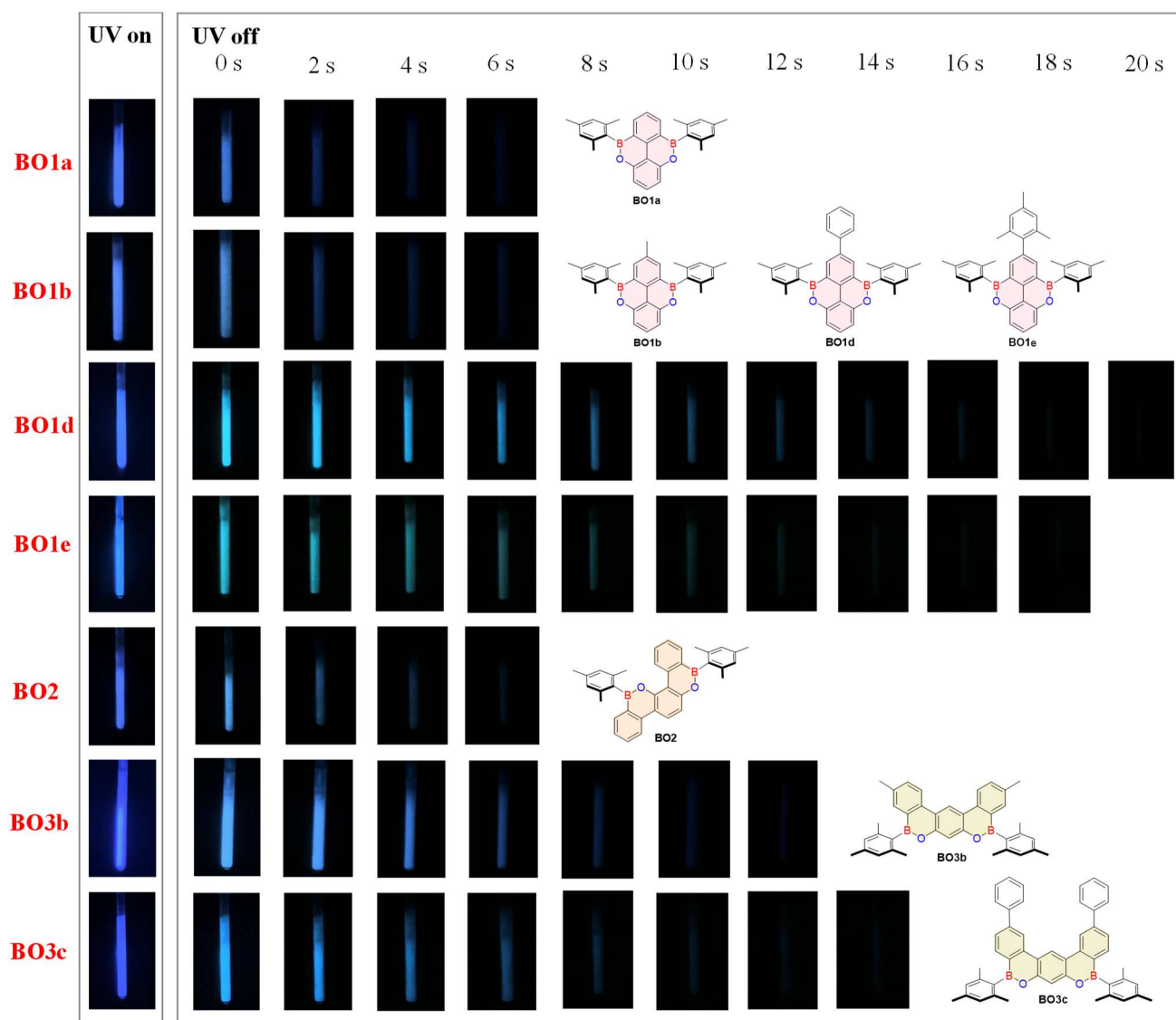


Fig. S43. Ultralong phosphorescence. Ultralong phosphorescent photographs of **BO1a**, **BO1b**, **BO1d**, **BO1e**, **BO2**, **BO3b** and **BO3c** at 77K in THF.

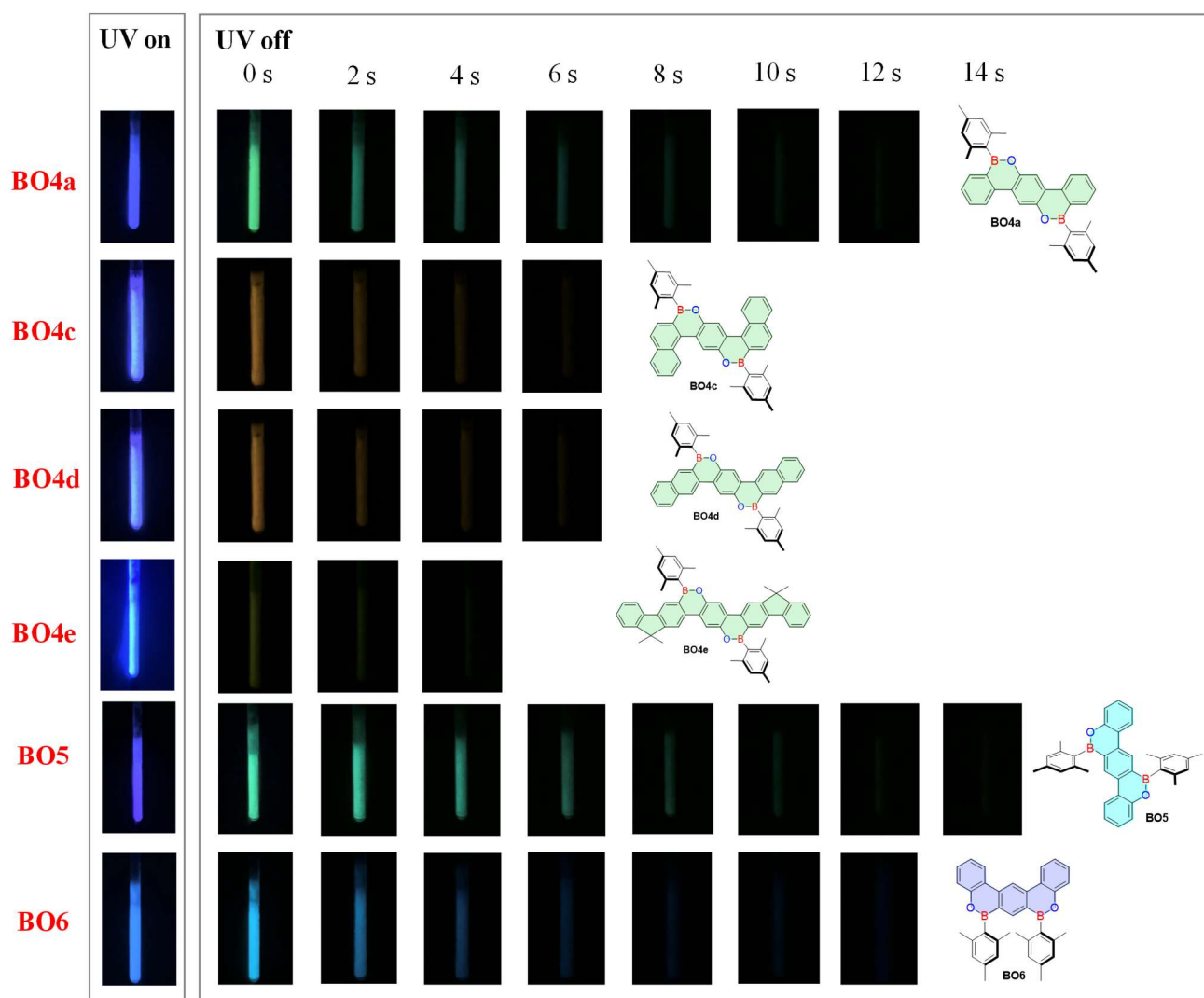


Fig. S44. Ultralong phosphorescence. Ultralong phosphorescent photographs of **BO4a**, **BO4c**, **BO4d**, **BO4e**, **BO5** and **BO6** at 77K in THF.

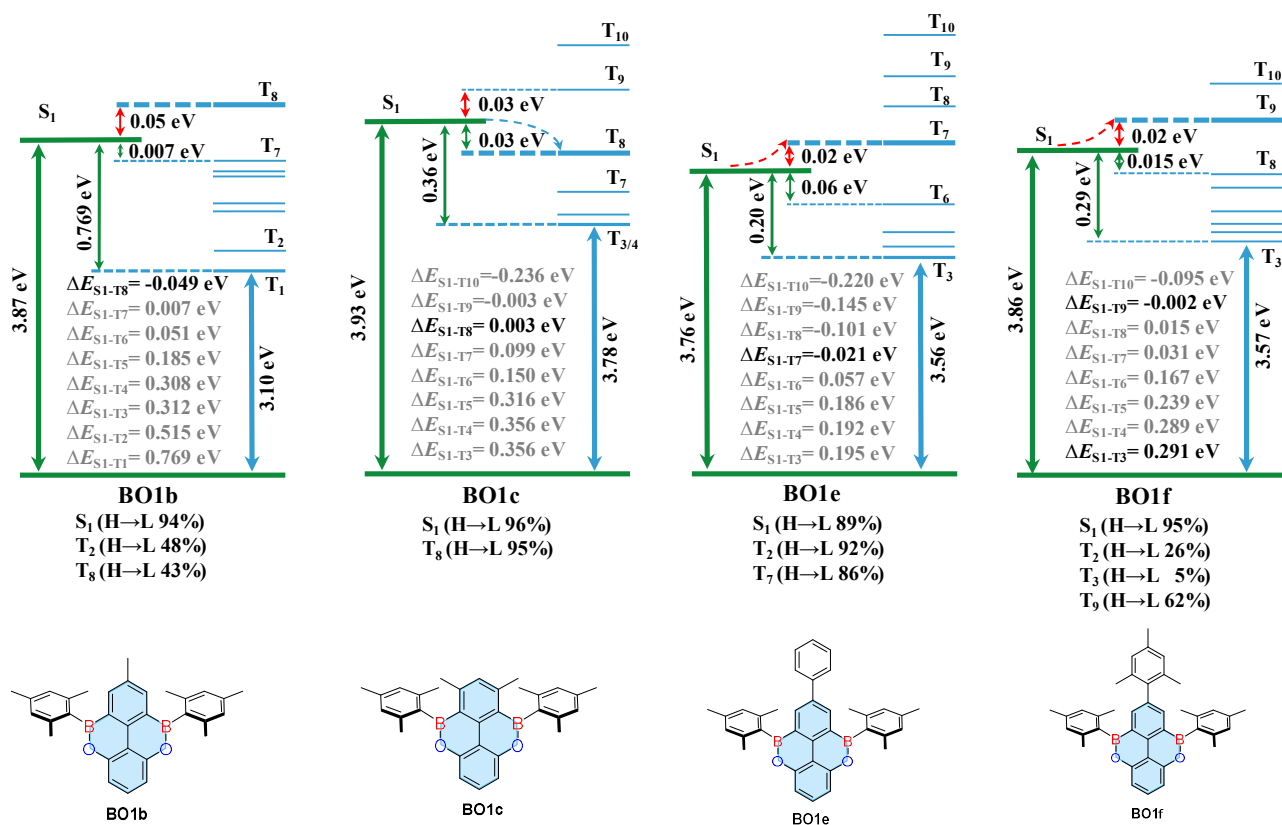


Fig. S45. Theoretical calculation. TD-DFT calculated singlet and triplet energy levels, main transition configurations of **BO1b**, **BO1c**, **BO1e** and **BO1f** at B3LYP/6-31G(d) level based on optimized S_0 geometry.

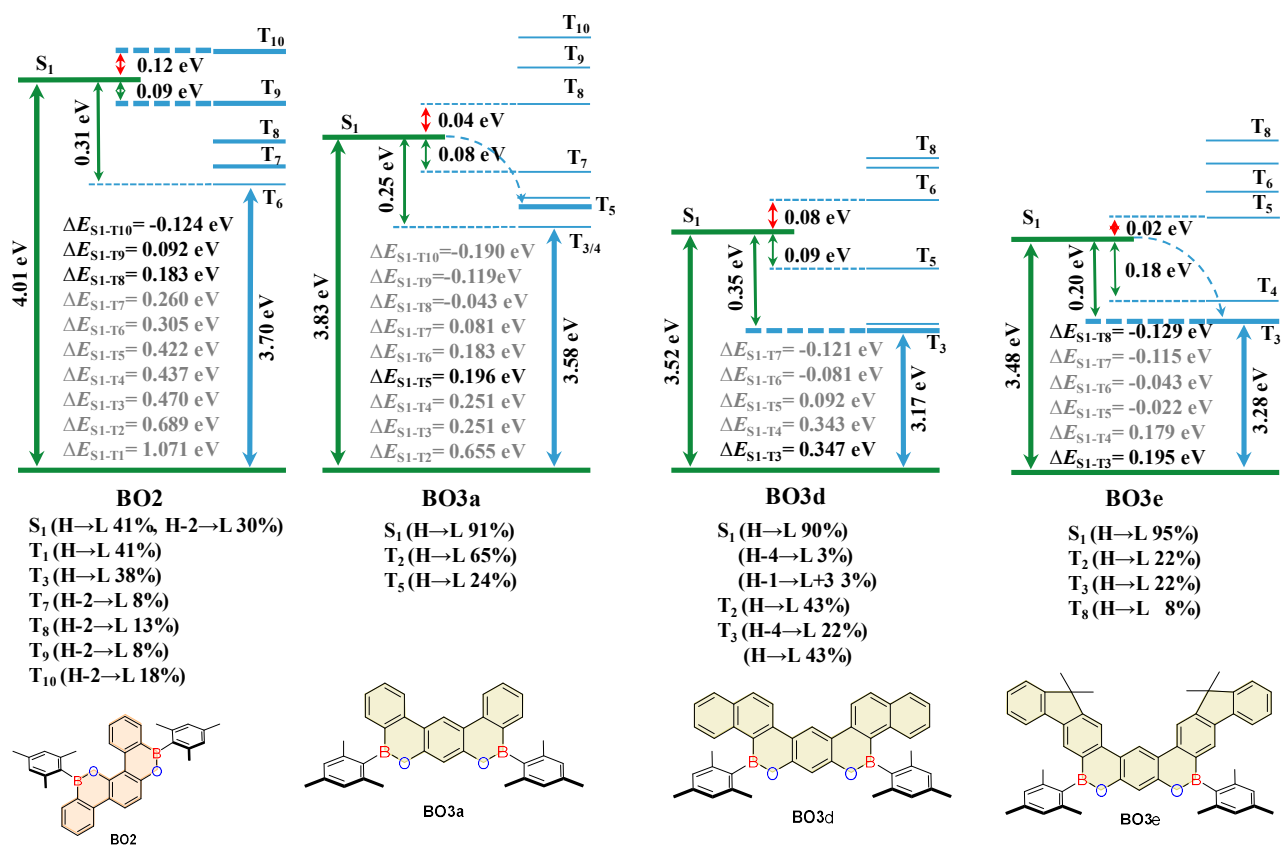


Fig. S46. Theoretical calculation. TD-DFT calculated singlet and triplet energy levels, main transition configurations of **BO2**, **BO3a**, **B3d** and **BO3e** at B3LYP/6-31G(d) level based on optimized S_0 geometry.

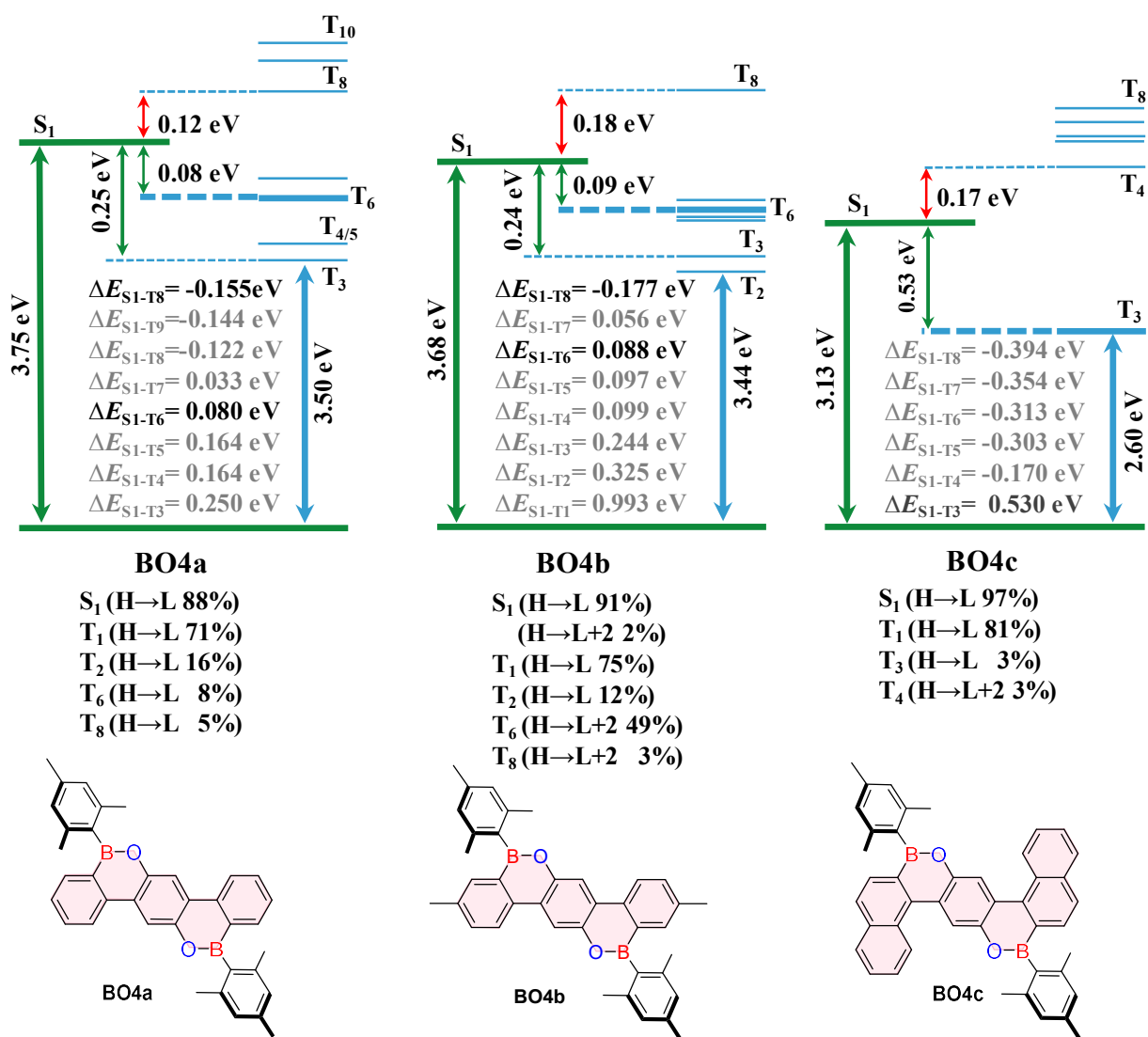


Fig. S47. Theoretical calculation. TD-DFT calculated singlet and triplet energy levels, main transition configurations of **BO4a**, **BO4b** and **BO4c** at B3LYP/6-31G(d) level based on optimized S_0 geometry.

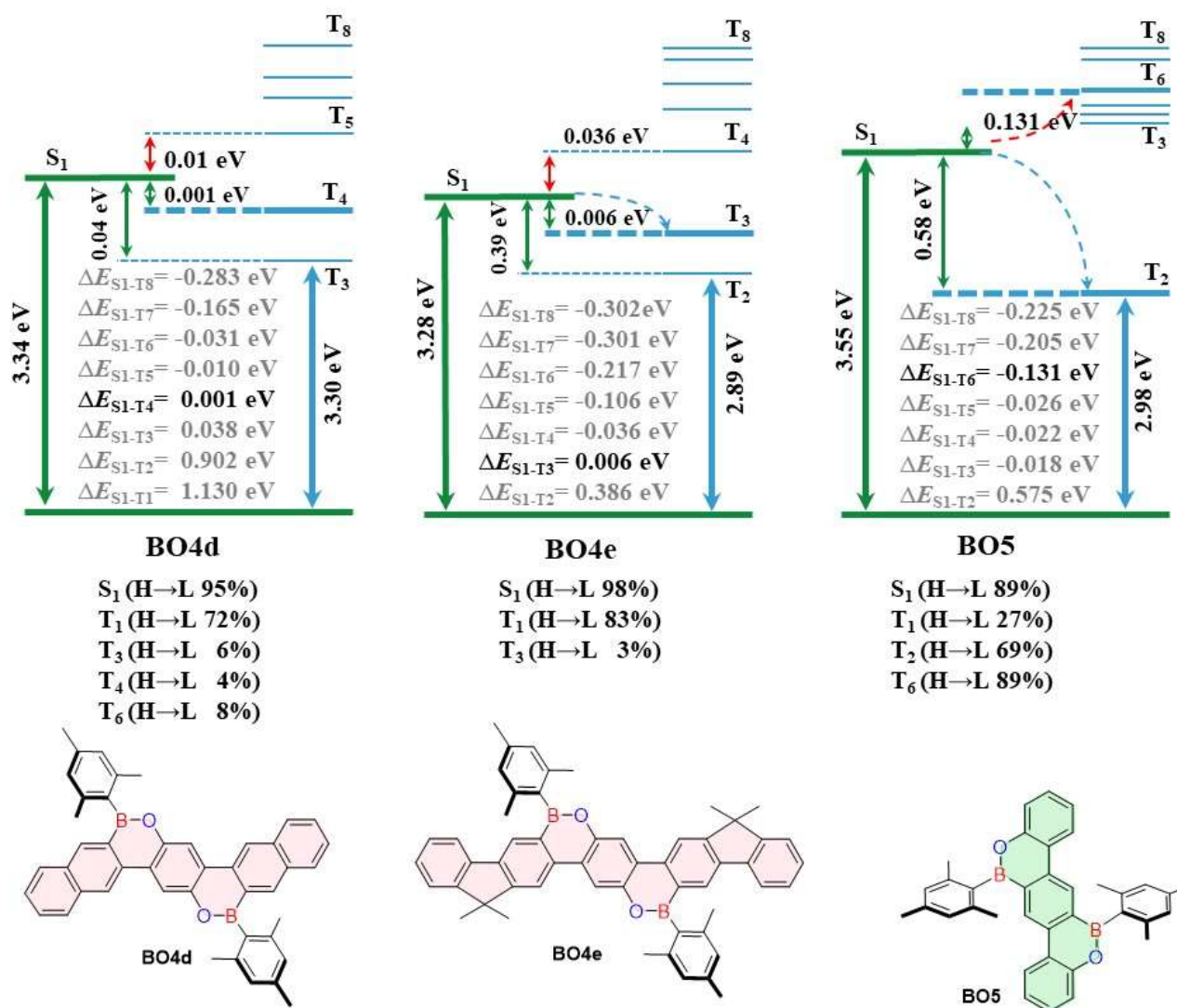


Fig. S48. Theoretical calculation. TD-DFT calculated singlet and triplet energy levels, main transition configurations of **BO4d**, **BO4e** and **BO5** at B3LYP/6-31G(d) level based on optimized S_0 geometry.

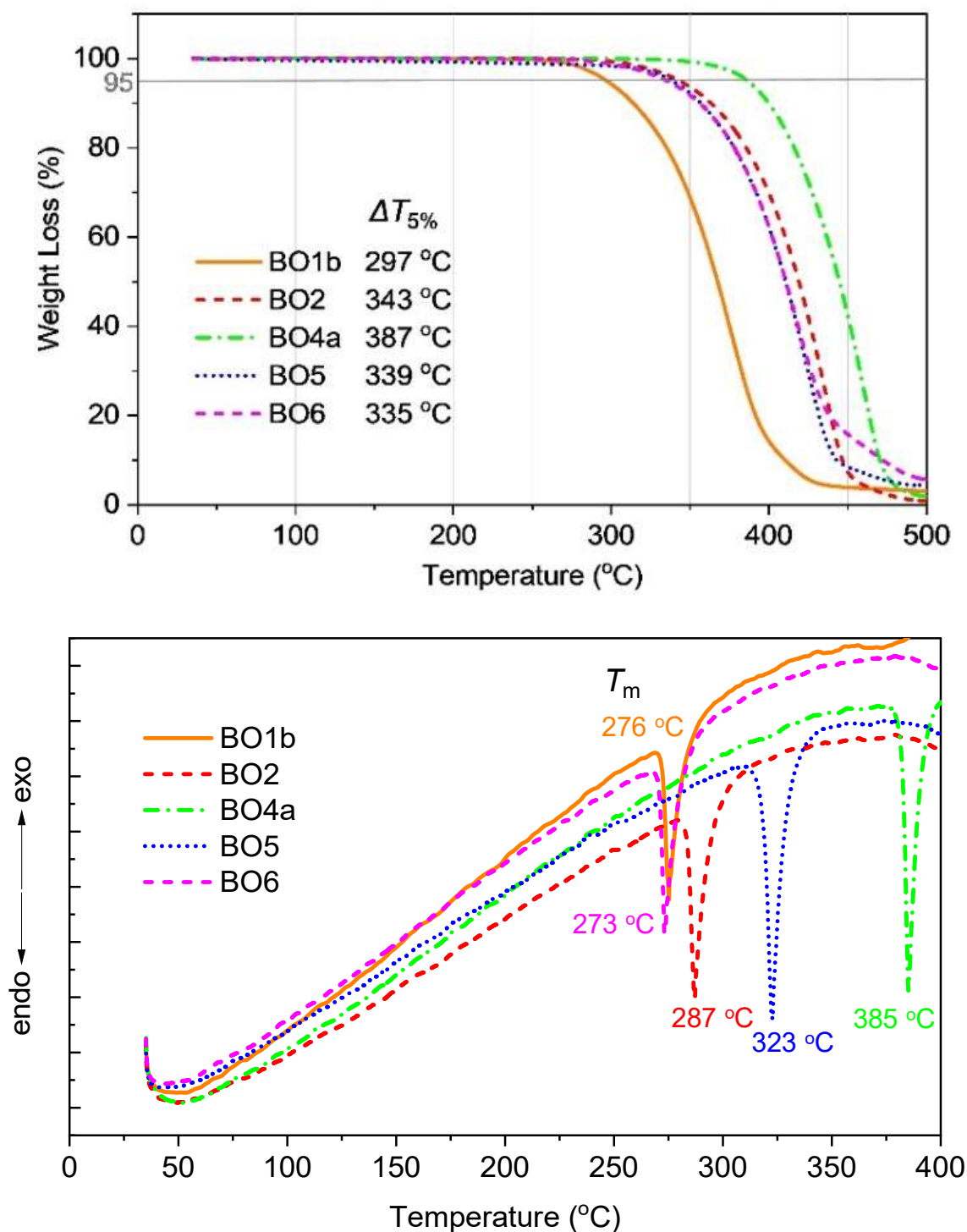


Fig. S49. Thermal properties. TGA (up) and DSC (down) curves of **BO1b**, **BO2**, **BO4a**, **BO5** and **BO6**. The strongly endothermic peaks at 276 °C for **BO1b**, 287 °C for **BO2**, 385 °C for **BO4a**, 323 °C for **BO5**, and 273 °C for **BO6** could be attributed to their melting processes, in good agreement with their corresponding melting temperatures (T_m) of 276.2–277.9, 287.1–288.2, >350, 320.1–322.5 and 271.8–272.9 °C, respectively.

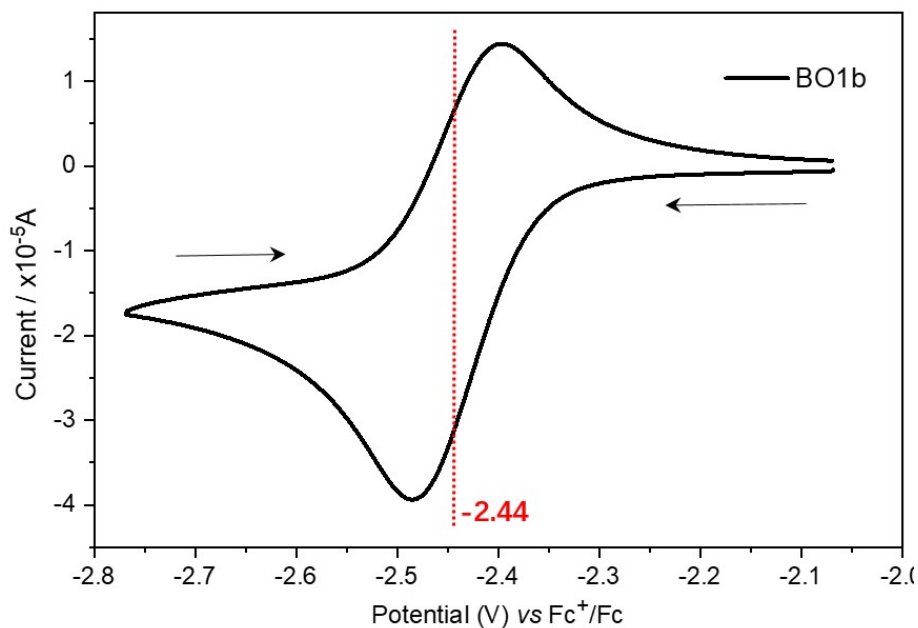


Fig. S50. Electrochemical properties. Cyclic voltammogram (CV) of **BO1b** in anhydrous *N,N*-dimethylformamide (DMF).

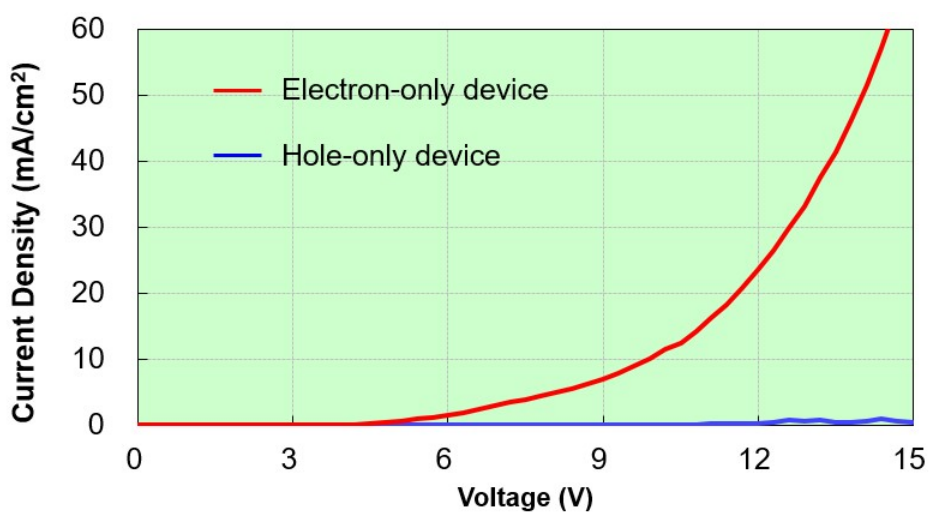


Fig. S51. Single carrier devices. Current density–voltage (J – V) characteristics of hole-only device with a structure of ITO/TAPC (10 nm)/**BO1b** (60 nm)/TAPC (10 nm)/Al and electron-only device with a structure of ITO/TmPyPB (10 nm)/**BO1b** (60 nm)/TmPyPB (10 nm)/LiF (1 nm)/Al.

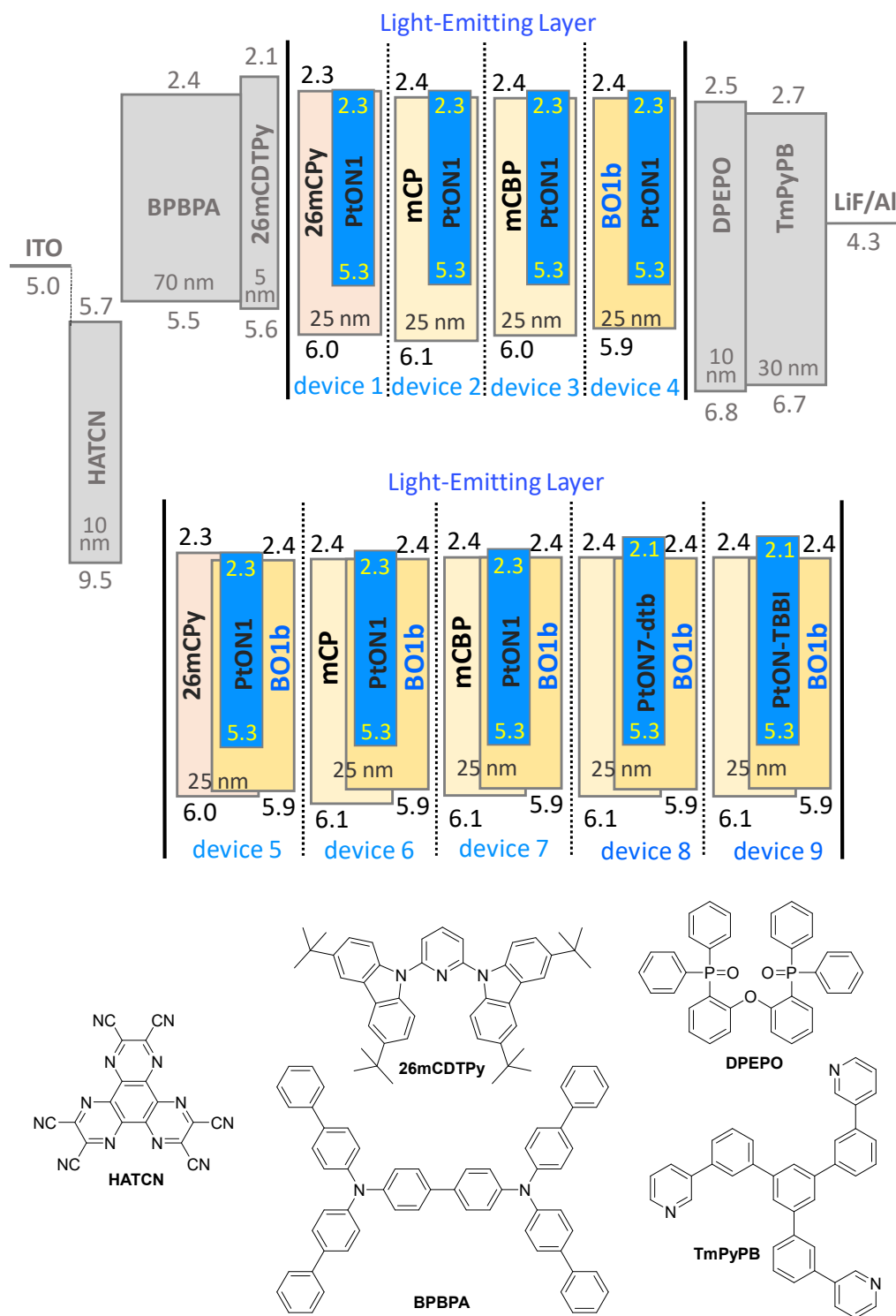


Fig. S52. Device and material structures. Energy level diagram of deep-blue OLEDs and chemical structures of materials used.

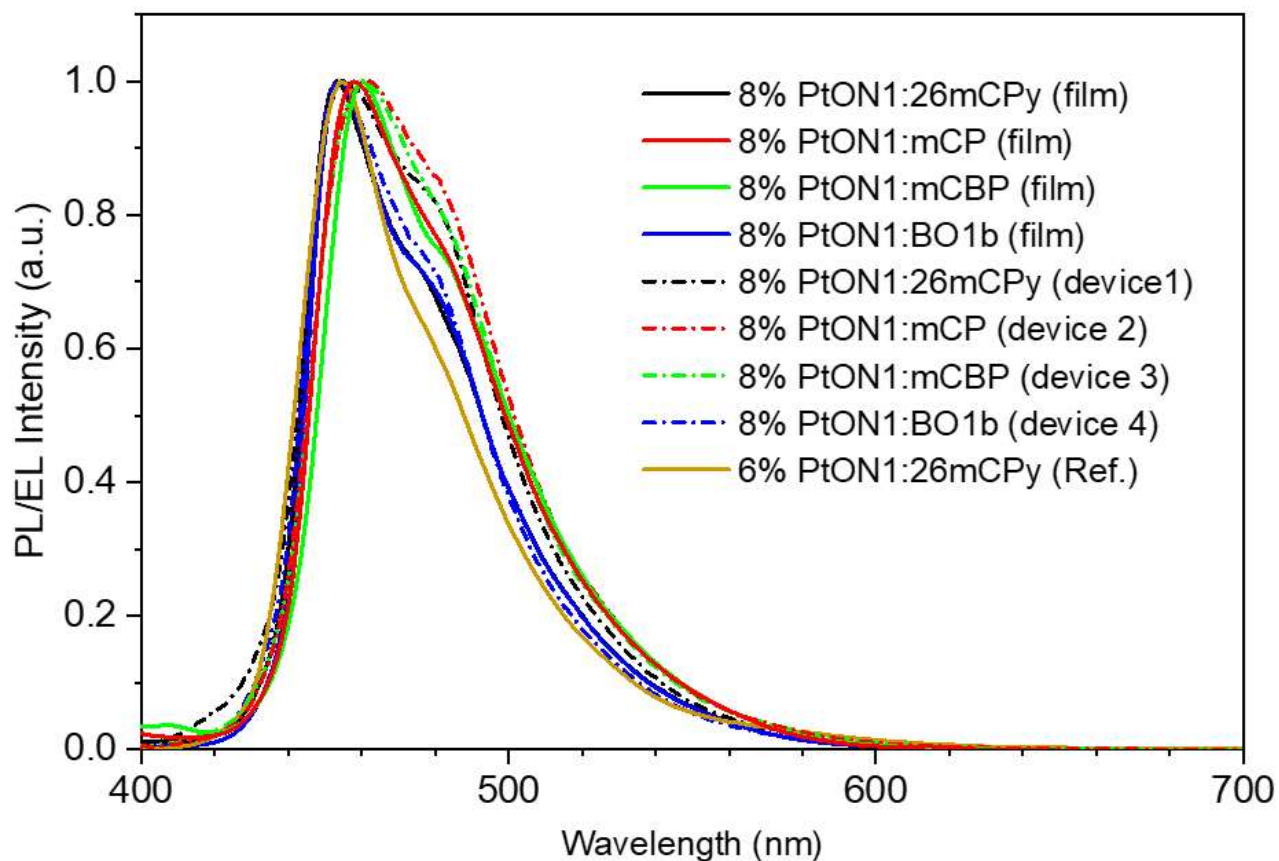
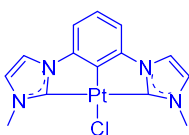


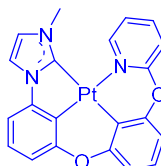
Fig. S53. PL and EL spectral comparison. The PL of PtON1-doped thin films versus the EL of PtON1-doped devices. The Ref. is the device with a structure of ITO/HATCN/NPD/TAPC/6%PtON1:26mCPy/DPPS/LiF/Al (X. C. Hang, T. Fleetham, E. Turner, J. Brooks, J. Li, *Angew. Chem. Int. Ed.* **2013**, 52, 6753–6756.)



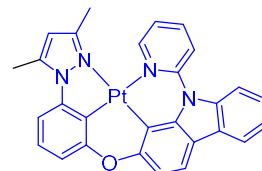
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Chem. Commun.
2011, 47, 9075.



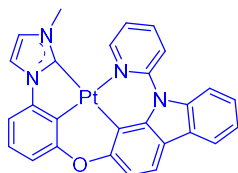
Pt-16 ^[2]
Org. Electron.
2012, 13, 1430.



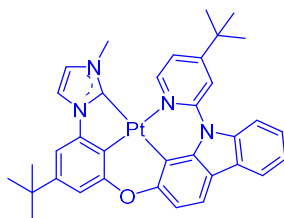
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Angew. Chem. Int. Ed.
2013, 52, 6753.



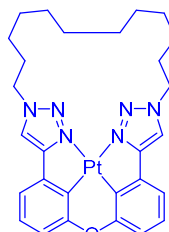
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2013, 52, 6753.



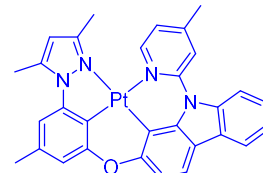
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2013, 52, 6753.



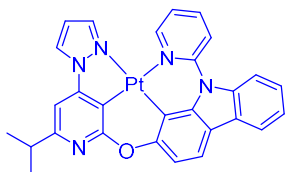
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Adv. Mater.
2014, 26, 7116.



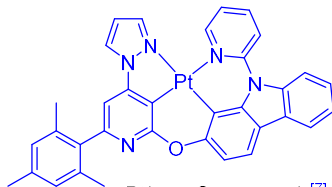
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Adv. Funct. Mater.
2017, 27, 1604318.



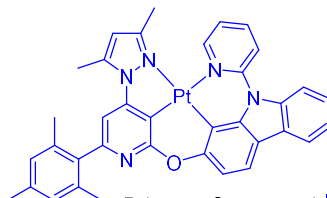
Pt(pzpyOczpy-4m) ^[6]
Mater. Chem. Front.
2019, 3, 2448.



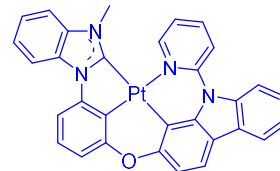
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Adv. Optical. Mater.
2020, 8, 2000406.



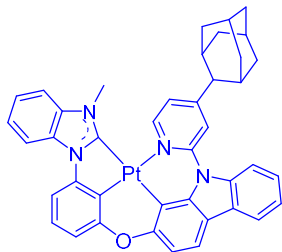
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Adv. Optical. Mater.
2020, 8, 2000406.



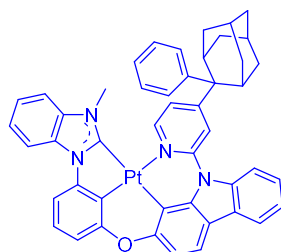
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ACS Appl. Mater. Interfaces
2021, 13, 52833.



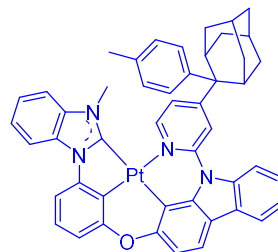
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Adv. Funct. Mater.
2021, 31, 2100967.



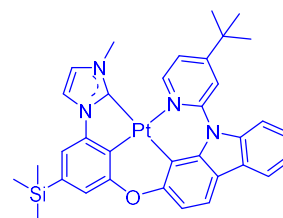
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Adv. Funct. Mater.
2021, 31, 2100967.



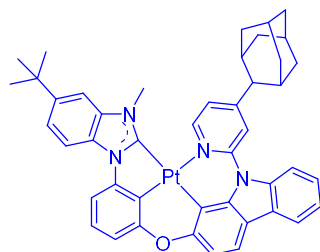
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2021, 31, 2100967.



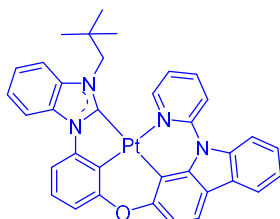
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Adv. Funct. Mater.
2021, 31, 2100967.



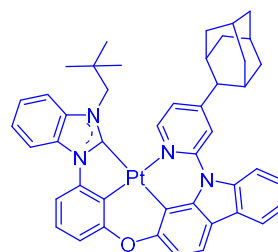
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ACS Appl. Mater. Interfaces
2022, 14, 34901.



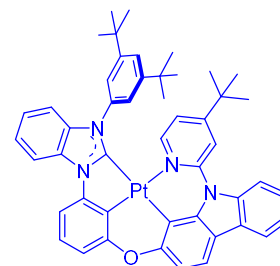
t-Pt-Ad ^[5]
Chem. Eng. J.
2022, 450, 137836.



Pt-NPT ^[5]
Chem. Eng. J.
2022, 450, 137836.



Pt-adNPt ^[5]
Chem. Eng. J.
2022, 450, 137836.



PtON-TBBI ^[6]
Nat. Photonics
2022, 16, 212.

Fig. S54. Deep-blue Pt(II) emitters. Chemical structures of dopants for Pt(II)-based deep-blue OLEDs discussed in this work.

Table S5. Performance data for Pt(II)-based deep-blue OLEDs with CIE_y < 0.20

emitter/host	CIE (x, y)	λ_{EL} (nm)	L_{max} (cd/m ²)	EQE(%) ^a max/100/1000	Reference/year
PtON1/ BO1b (device 4)	(0.138, 0.134)	453	8007	22.8/21.5/16.3	This work
PtON1/ BO1b /26mCPy (device 5)	(0.138, 0.130)	454	12982	24.8/24.4/20.9	This work
PtON1/ BO1b /mCP (device 6)	(0.138, 0.154)	460	13098	22.3/20.0/19.2	This work
PtON1/ BO1b /mCBP (device 7)	(0.138, 0.142)	456	15722	27.1/25.2/21.8	This work
PtON7-dtb/ BO1b /mCBP (device 8)	(0.138, 0.088)	453	5670	27.6/20.0/16.0	This work
PtON-TBBI/ BO1b /mCBP (device 9)	(0.134, 0.104)	458	9377	28.0/22.8/19.0	This work
Pt(tetra-NHC)/DP4	(0.16, 0.16)	460	1200	---/---/---	[1]/2011
Pt-16/26mCPy	(0.16, 0.15)	450	~3000	15.7/10.1/<5	[2]/2012
PtOO7/26mCPy	(0.15, 0.10)	448	1000	<9/4.1/0.5	[3]/2013
PtON1/26mCPy	(0.15, 0.13)	454	1000	25.2/23.3/16.8	[3]/2013
PtON7/26mCPy	(0.15, 0.14)	456	1000	23.7/20.4/15.4	[3]/2013
PtON7-dtb/TAPC:PO15	(0.148, 0.079)	452	1555	24.8/22.7/11.0	[4]/2014
Pt6/BCPO	(0.14, 0.14)	452	10676	9.7/9.5/7.6	[5]/2017
Pt(ppzOczpy-4m)/CzSi:CzAcSF	(0.159, 0.166)	450	~4000	19.5/<10/12.1	[6]/2019
Pt(pzpyOczpy- ⁱ Pr)/DPEPO	(0.14, 0.15)	454	1000	<20/17.2/11.2	[7]/2020
Pt(pzpyOczpy-mes)/DPEPO	(0.14, 0.15)	454	400	<20/15.0/6.6	[7]/2020
Pt(mpzpyOczpy-mes) /26mCPy:mCBP	(0.145, 0.195)	461	6518	---/12.1/---	[8]/2021
Pt-R/mCP	(0.138, 0.122)	~453	1645	22.0/---/---	[9]/2021
Pt-Ada/mCP	(0.145, 0.110)	~451	1078	21.2/---/---	[9]/2021
Pt-AdaPh/mCP	(0.137, 0.122)	~453	4528	23.5/---/---	[9]/2021
Pt-AdaTol/mCP	(0.140, 0.120)	~453	1593	22.0/---/---	[9]/2021
PtON7-TMS/mCBP	(0.142, 0.099)	452	2722	15.6/---/10.7	[10]/2022
t-Pt-Ad/mCP	(0.141, 0.092)	~453	3258	20.3/---/16.3	[11]/2022
Pt-NPT/mCP	(0.139, 0.118)	~451	3389	19.8/---/19.8	[11]/2022
Pt-adNPT/mCP	(0.143, 0.090)	~453	2512	11.2/---/15.7	[11]/2022
PtON-TBBI/SiCzCz:SiTrzCz2	(0.141, 0.197)	~455	~2000	25.4/24.6/23.4	[12]/2022

^a EQE @ Max/100/1000 cd m⁻².**Reference Pt(II)-based deep-blue OLEDs:**

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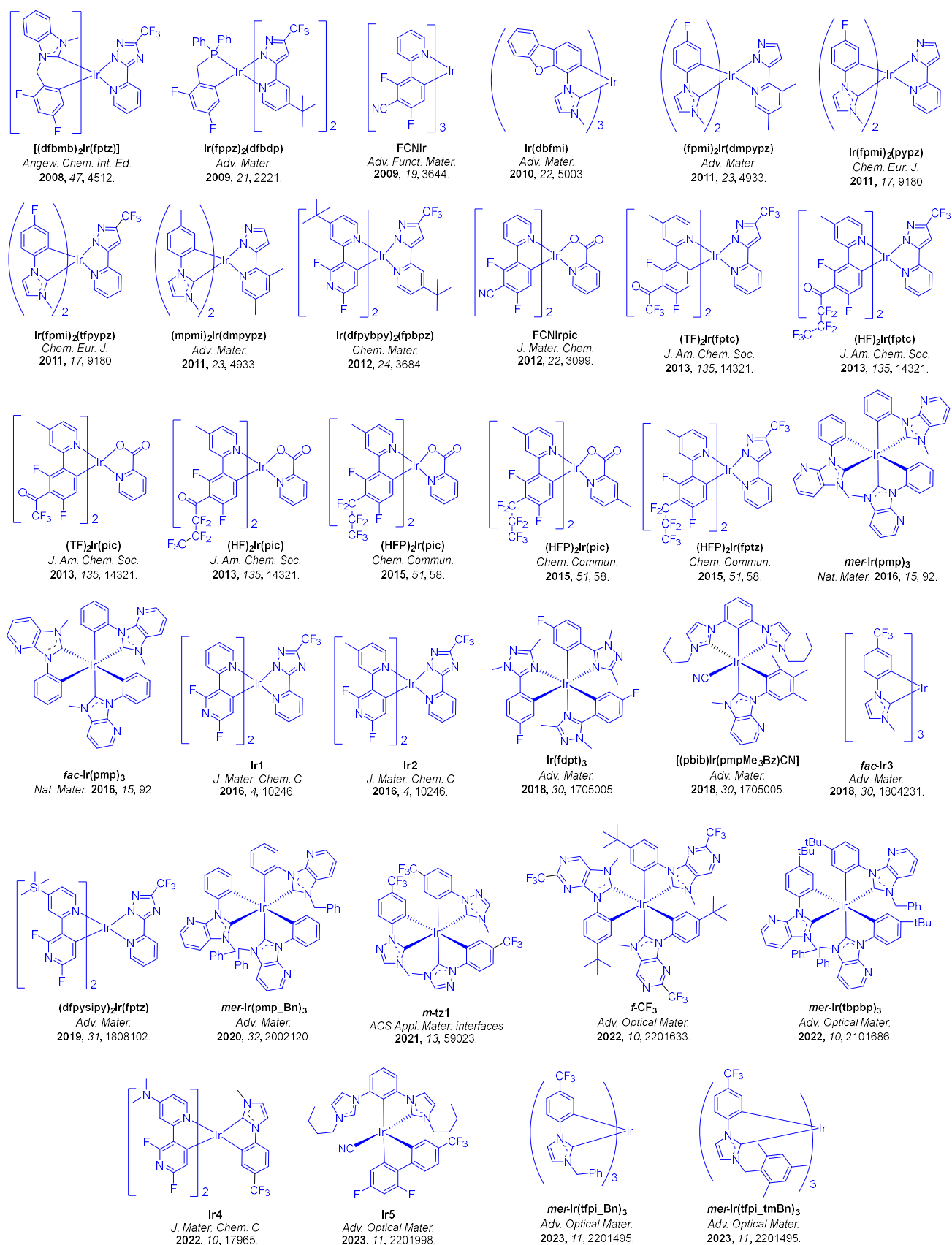


Fig. S55. Deep-blue Ir(II) emitters. Chemical structures of dopants for Ir(III)-based deep-blue OLEDs discussed in this work.

Table S6. Performance data for Ir(III)-based deep-blue OLEDs with CIE_y < 0.20

emitter/host	CIE (x, y)	λ_{EL} (nm)	L_{max} (cd/m ²)	EQE(%) max/100/1000	Reference/year
PtON1/ BO1b (device 4)	(0.138, 0.134)	453	8007	22.8/21.5/16.3	This work
PtON1/ BO1b /26mCPy (device 5)	(0.138, 0.130)	454	12982	24.8/24.4/20.9	This work
PtON1/ BO1b /mCP (device 6)	(0.138, 0.154)	460	13098	22.3/20.0/19.2	This work
PtON1/ BO1b /mCBP (device 7)	(0.138, 0.142)	456	15722	27.1/25.2/21.8	This work
PtON7-dtb/ BO1b /mCBP (device 8)	(0.138, 0.088)	453	5670	27.6/20.0/16.0	This work
PtON-TBBI/ BO1b /mCBP (device 9)	(0.134, 0.104)	458	9377	28.0/22.8/19.0	This work
Ir(dfmbm) ₂ (fptz)/UGH2	(0.16, 0.13)	434	<10000	6.0/~3/~1	[13]/2008
Ir(fppz) ₂ (dfbdp)/UGH2:CzSi	(0.15, 0.11)	---	1817	11.9/7.2/---	[14]/2009
FCNIr/PPO2	(0.14, 0.15)	452	<10000	18.4/13.5/~8	[15]/2009
FCNIr/PPO1	(0.14, 0.16)	452	<10000	17.1/12.2/<12	[15]/2009
Ir(dbfmi)/PPO2	(0.15, 0.19)	~450	<2500	18.6/13.3/6.2	[16]/2010
Ir(fpmi) ₂ (tfpypz)/UGH2:CzSi	(0.14, 0.10)	454	3446	7.6/~6/<6	[17]/2011
Ir(fpmi) ₂ (pypz)/UGH2	(0.14, 0.16)	466	5668	9.1/~9/<8	[17]/2011
Ir(fpmi) ₂ (pypz)/UGH2:CzSi	(0.14, 0.18)	470	8161	14.1/<12/<9	[17]/2011
(fpmi) ₂ Ir(dmpypz)/BCPO	(0.13, 0.16)	458	20649	17.1/16.5/15.1	[18]/2011
(mpmi) ₂ Ir(dmpypz)/BCPO	(0.13, 0.18)	464	23727	15.4/14.3/13.6	[18]/2011
FCNIrpic/mCPPO1	(0.14, 0.18)	~450	<5000	~25/25.1/24.0	[19]/2011
FCNIrpic/mCPPO1	(0.14, 0.17)	~460	<3500	22.0/~20/19.7	[20]/2011
FCNIrpic/DCPPO	(0.14, 0.17)	458	<8000	22.4/~20/18.4	[21]/2011
FCNIrpic/TSPC	(0.14, 0.18)	~450	<8000	22.4/18.4/---	[21]/2011
FCNIrpic/DFCzPO	(0.14, 0.18)	457	<5000	~21/~20/---	[22]/2011
FCNIrpic/mCPPO1	(0.14, 0.18)	458	<10000	24.7/~24/22.3	[23]/2012
Ir(dfpybpy) ₂ (fbbpz)/SimCP	(0.16, 0.19)	~420	<4000	4.9/---/---	[24]/2012
(TF) ₂ Ir(pic)/mCPPO1	(0.14, 0.16)	460	<3000	17.1/16.8/---	[25]/2013
(TF) ₂ Ir(fptc)/mCPPO1	(0.15, 0.12)	448	<2000	8.4/7.4/---	[25]/2013
(HF) ₂ Ir(pic)/mCPPO1	(0.14, 0.17)	460	<800	12.6/11.5/---	[25]/2013
(HF) ₂ Ir(fptc)/mCPPO1	(0.15, 0.13)	448	<400	8.4/7.10/---	[25]/2013
(dfpypy) ₂ Ir(pic)/CDBP	(0.16, 0.20)	~450	2373	<5/3.9/2.9	[26]/2013
(HFP) ₂ Ir(pic)/mCPPO1	(0.15, 0.16)	452	<1000	19.7/---/---	[27]/2015
(HFP) ₂ Ir(mpica)/mCPPO1	(0.15, 0.17)	452	<1000	21.4/---/---	[27]/2015
(HFP) ₂ Ir(fptz)/mCPPO1	(0.15, 0.15)	447	<1000	14.2/---/---	[27]/2015
fac-Ir(pmp) ₃ /TSPO1	(0.16, 0.09)	---	>7800	<15/---/---	[28]/2016
mer-Ir(pmp) ₃ /TSPO1	(0.16, 0.15)	---	~22000	<15/---/---	[28]/2016
Ir1/ <i>t</i> -BuCPO	(0.15, 0.13)	430	5080	11.2/10.8/8.3	[29]/2016
Ir2/ <i>t</i> -BuCPO	(0.14, 0.11)	440	4710	13.0/12.6/10.1	[29]/2016
fac-Ir(dbfmi) ₃ /TSPO1	(0.14, 0.11)	---	<2000	18.5/---/---	[30]/2017
mer-Ir(dbfmi) ₃ /TSPO1	(0.14, 0.14)	---	<2000	18.2/---/---	[30]/2017
fac-Ir3/DPEPO	(0.15, 0.05)	430	<500	13.4/12.5/---	[31]/2018
Ir(fdpt) ₃ (10 wt%)/DPEPO	(0.15, 0.11)	458	2727	22.5/16.5/11.1	[32]/2018
Ir(fdpt) ₃ (12 wt%)/DPEPO	(0.15, 0.11)	458	3195	19.4/17.8/12.6	[32]/2018
(dfpysipy) ₂ Ir(fptz)/mCBP:TSPO1	(0.15, 0.18)	---	870	19.5/17.5/----	[33]/2019

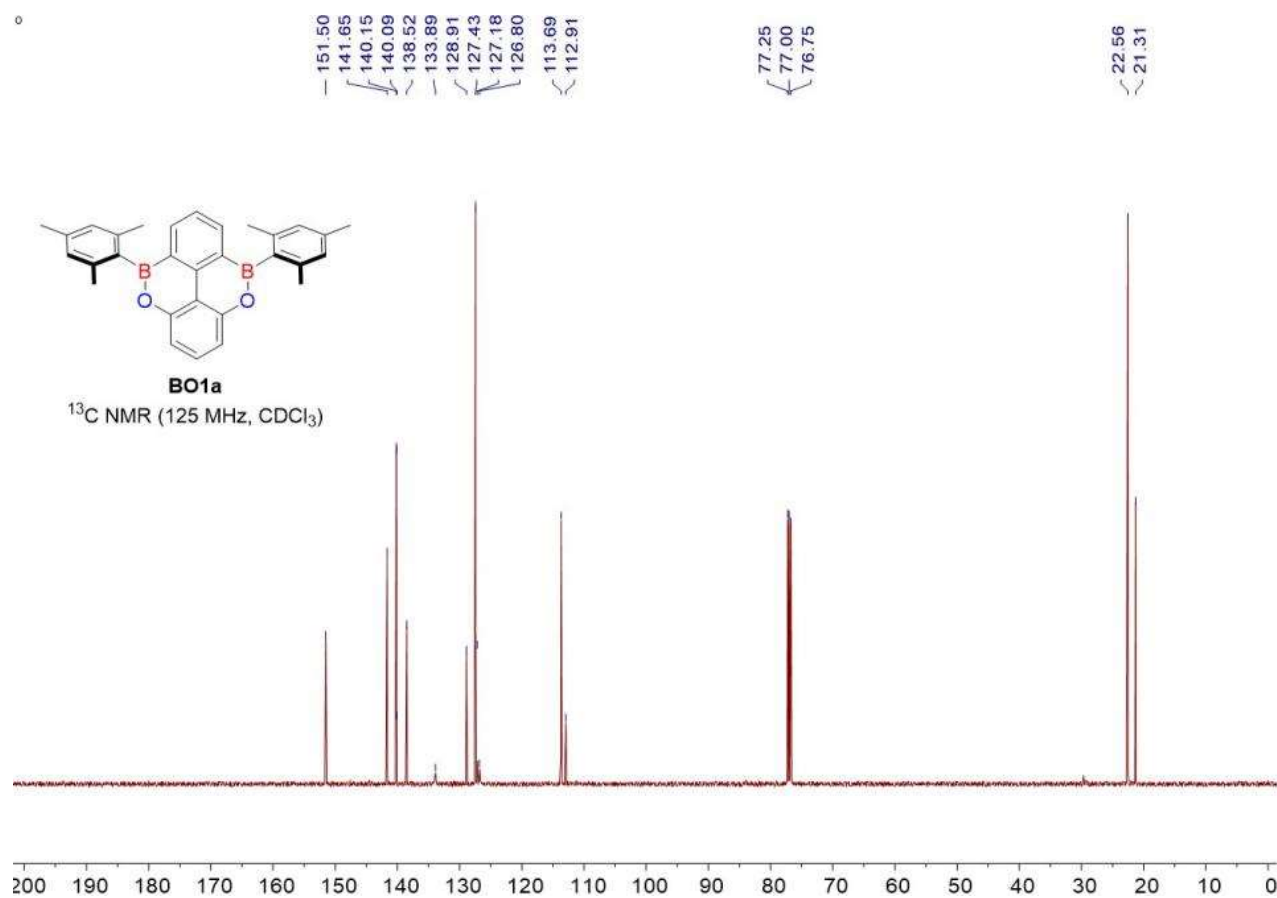
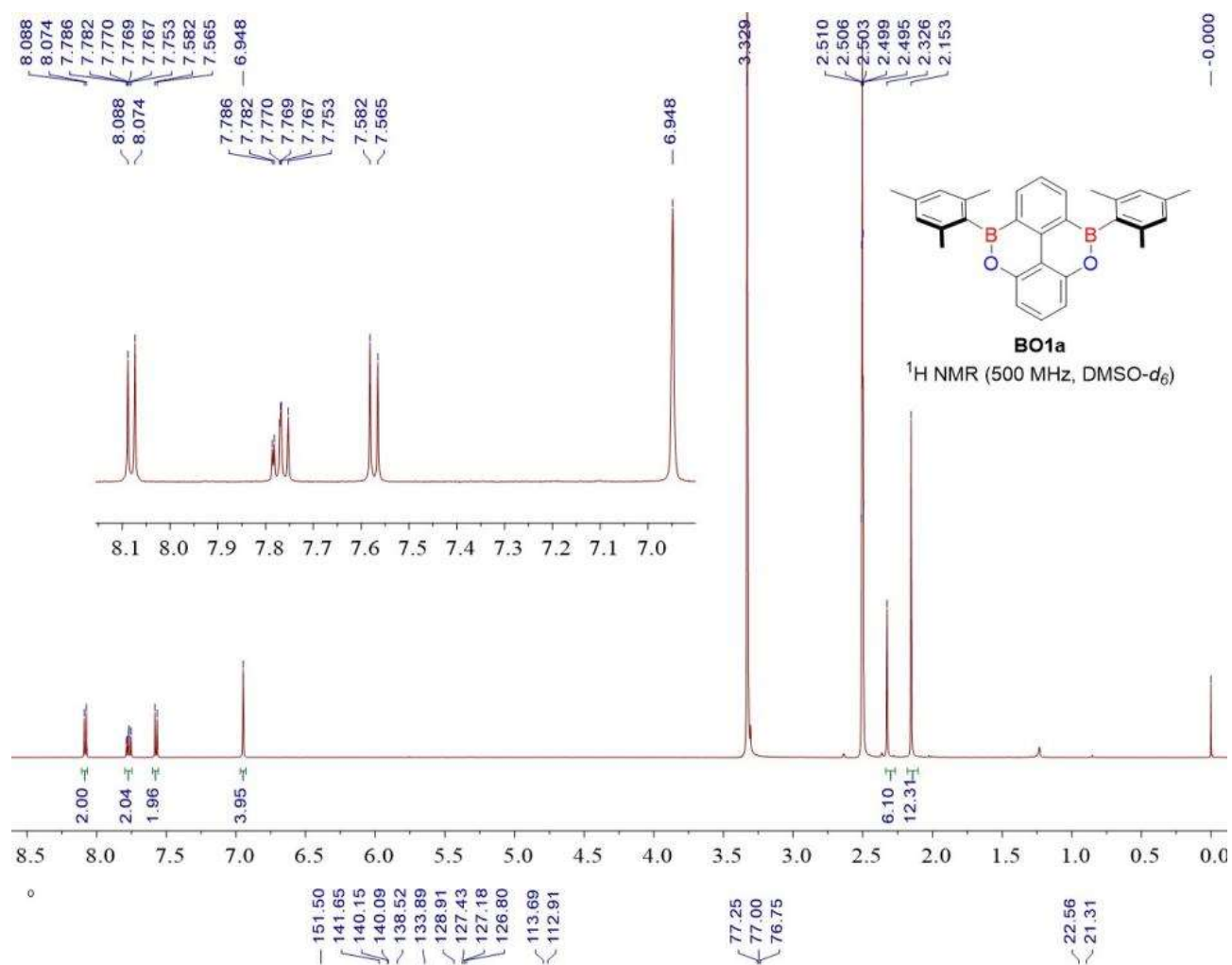
(dfpysipy) ₂ Ir(pic)/mCBP:TSPO1	(0.14, 0.19)	449	3000	29.0/28.0/23.2	[33]/2019
(dfpysipy) ₂ Ir(mpica)/mCBP:TSPO1	(0.14, 0.19)	450	2800	31.9/30.4/24.7	[33]/2019
mer-Ir(pmp_Bn) ₃ /TSPO1	(0.15, 0.09)	442	6453	24.8/16.6/13.1	[34]/2020
Ir(cb) ₃ //mCBP:SiCzTrz	(0.14, 0.19)	~470	<10000	20.3/20.2/18.6	[35]/2020
m-tzl/DPEPO:30%	(0.15, 0.06)	432	<1000	10.0/---/---	[36]/2021
Ir2/PPF	(0.16, 0.20)	465	4350	16.4/11.3/7.2	[37]/2022
[(pbib)Ir(pmpMe ₃ Bz)CN]/DPEPO	(0.17, 0.19)	469	1128	15.3/11.4/3.6	[38]/2022
f-CF ₃ /t-DABNA/mCBP ^b	(0.13, 0.14)	464	8188	23.8/16.4/10.4	[39]/2022
mer-Ir(tbpbp) ₃ /DPEPO	(0.16, 0.13)	449	2386	24.9/22.1/<10	[40]/2022
Ir/v-DABNA/mCBP ^b	(0.13, 0.19)	---	11100	15.8/<15.0/10.5	[41]/2023
mer-Ir(tfpi_Bn) ₃ /TSPO1	(0.16, 0.08)	424	632	12.2/10.8/<5	[42]/2023
mer-Ir(tfpi_tmBn) ₃ /TSPO1	(0.16, 0.08)	424	940	14.9/11.7/<5	[42]/2023

^a EQE @ Max/100/1000 cd m⁻². ^b Hyperfluorescent OLED.

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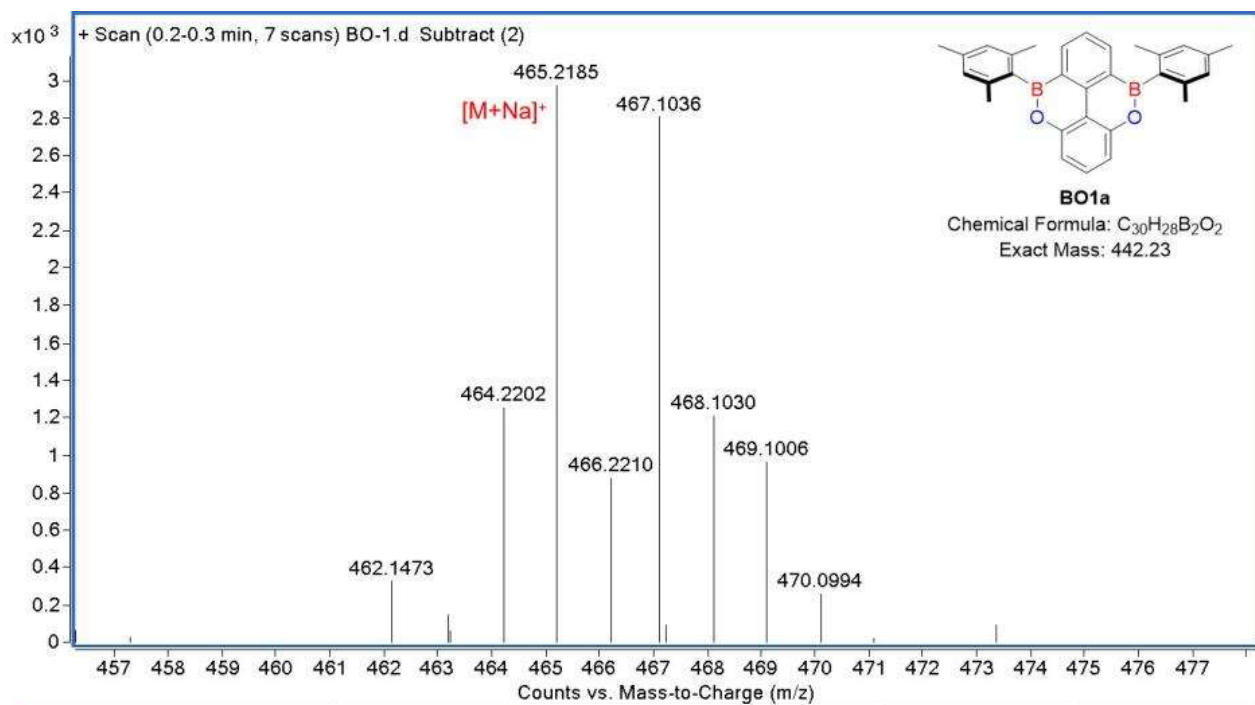
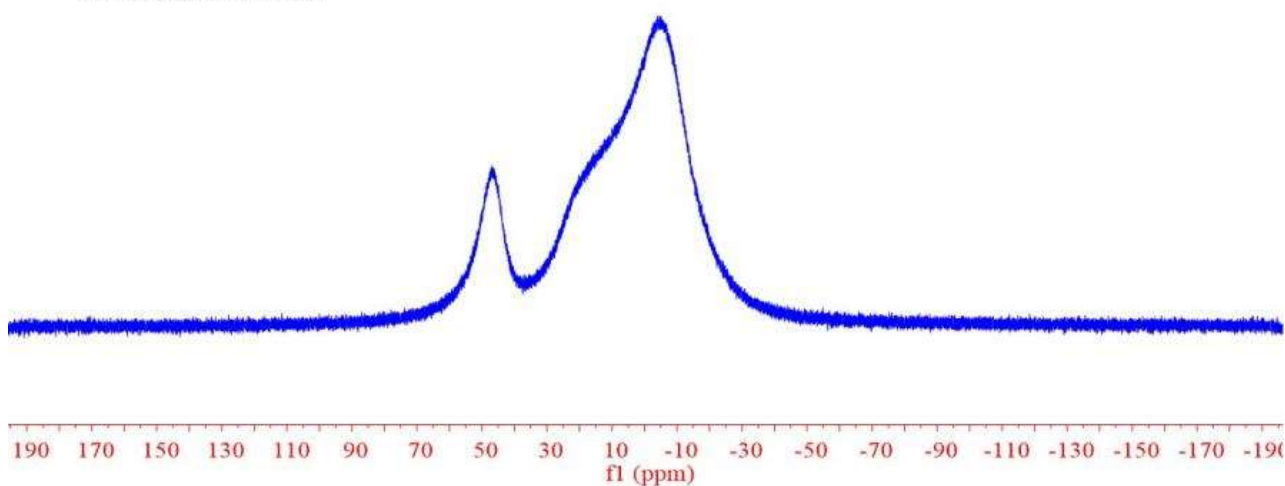


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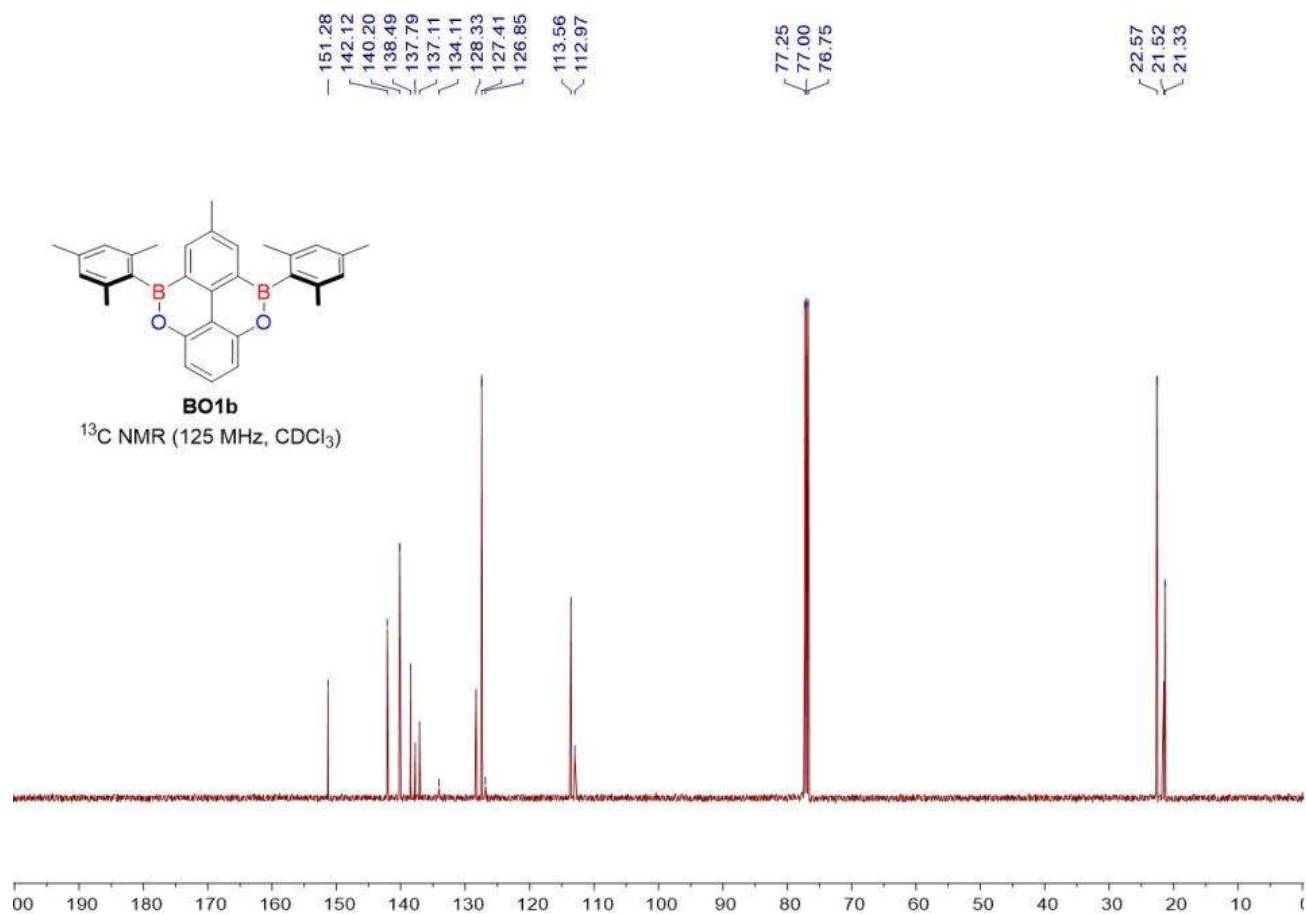
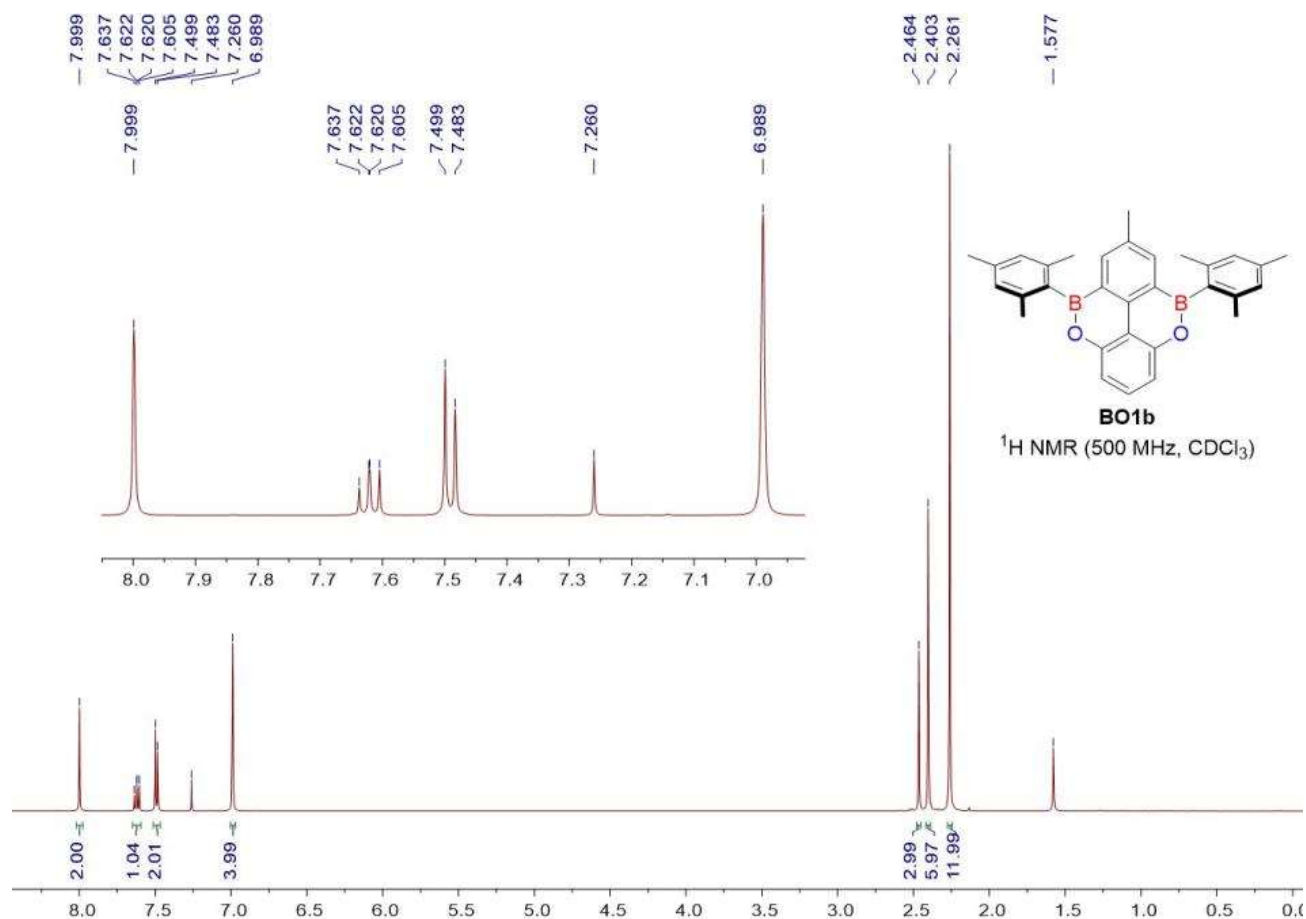


BO1a

^{11}B NMR (160 MHz, CDCl_3)



Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{30}\text{H}_{28}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{30}\text{H}_{28}[^{11}\text{B}]_2\text{NaO}_2$	465.2185	465.2168	-3.93

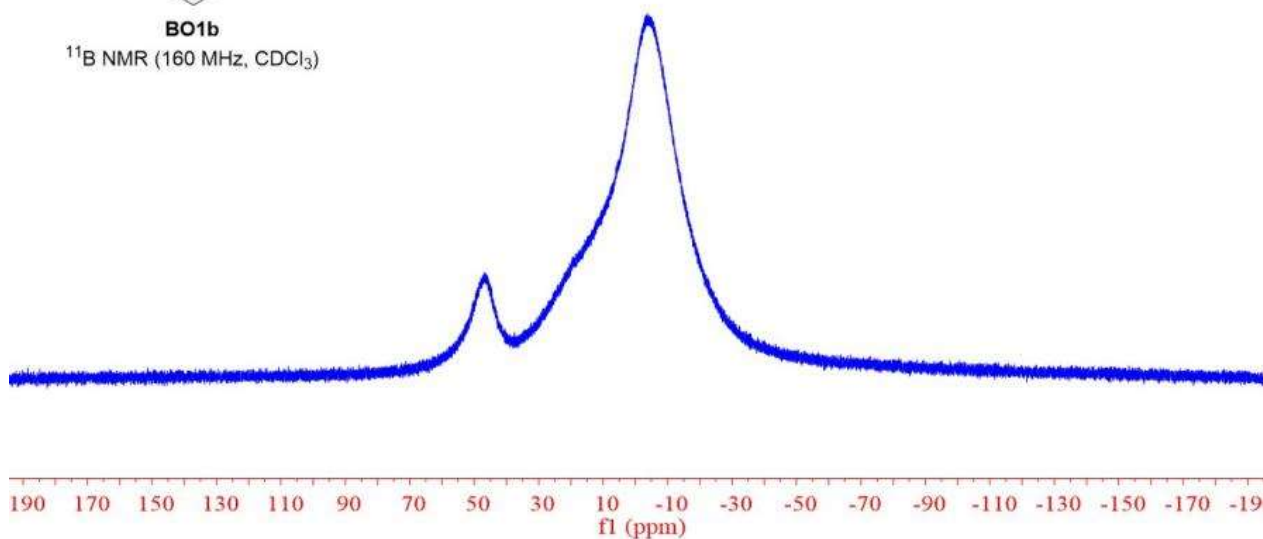


-49.59

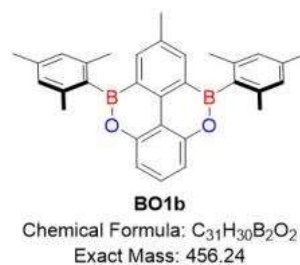
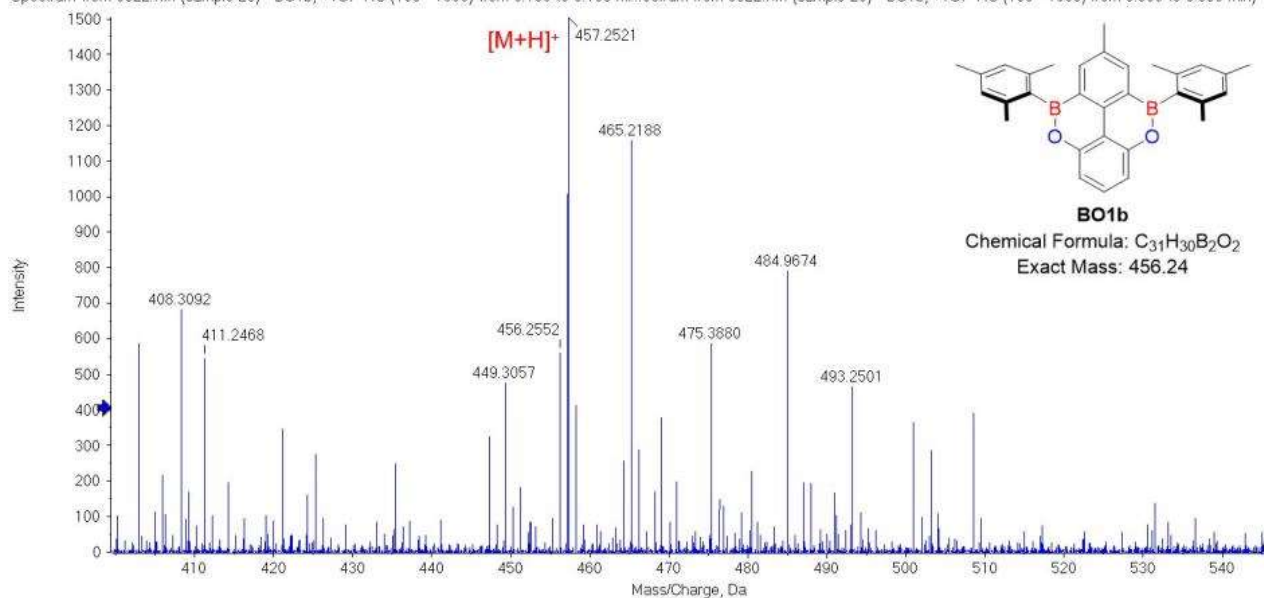


BO1b

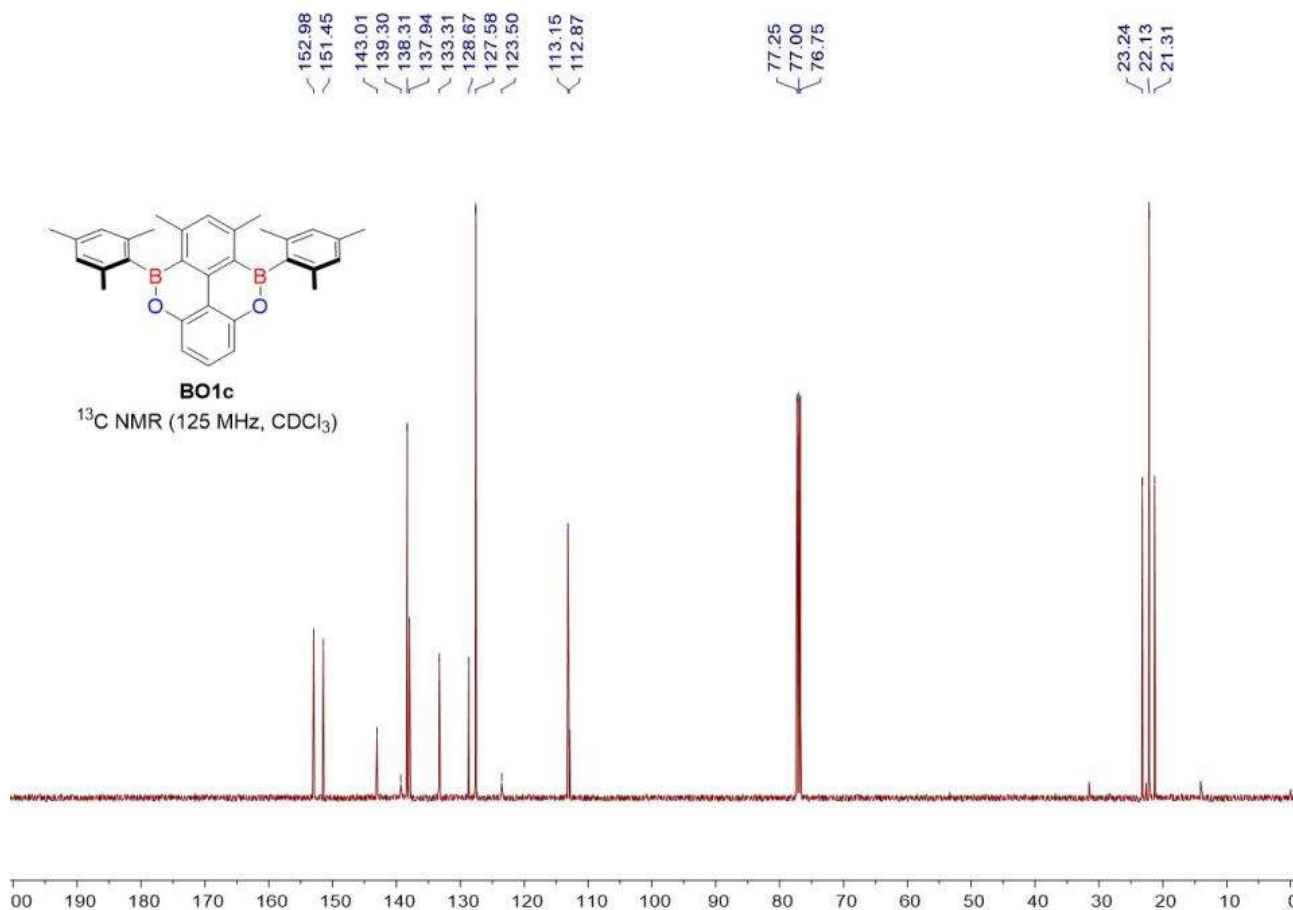
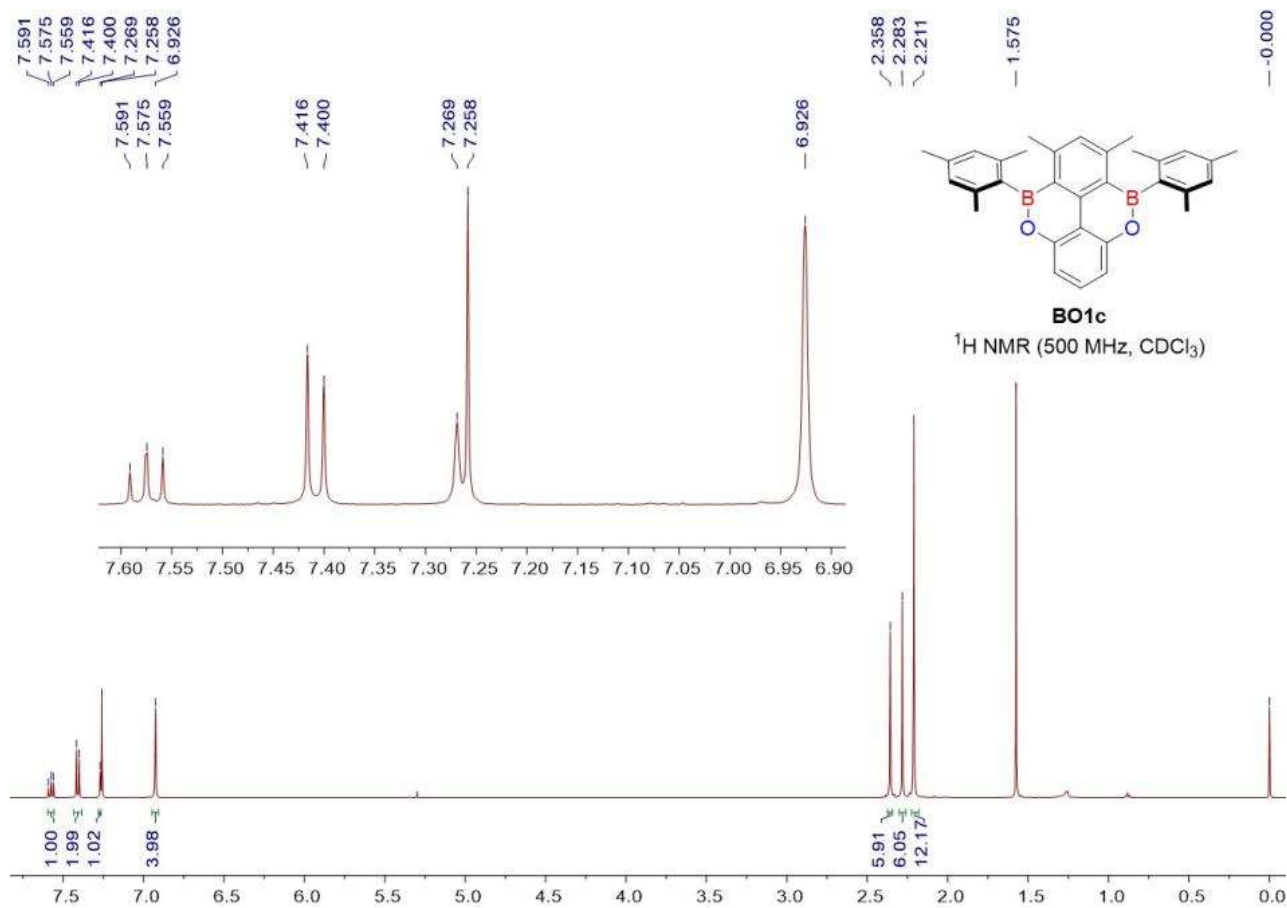
^{11}B NMR (160 MHz, CDCl_3)



Spectrum from 0922.wiff (sample 26) - BO1b, +TOF MS (100 - 1500) from 0.135 to 0.195 min.; spectrum from 0922.wiff (sample 26) - BO1b, +TOF MS (100 - 1500) from 0.660 to 0.809 min)



Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{31}\text{H}_{30}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{31}\text{H}_{31}[^{11}\text{B}]_2\text{O}_2$	457.2521	457.2505	-3.70

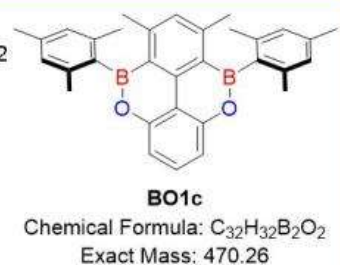
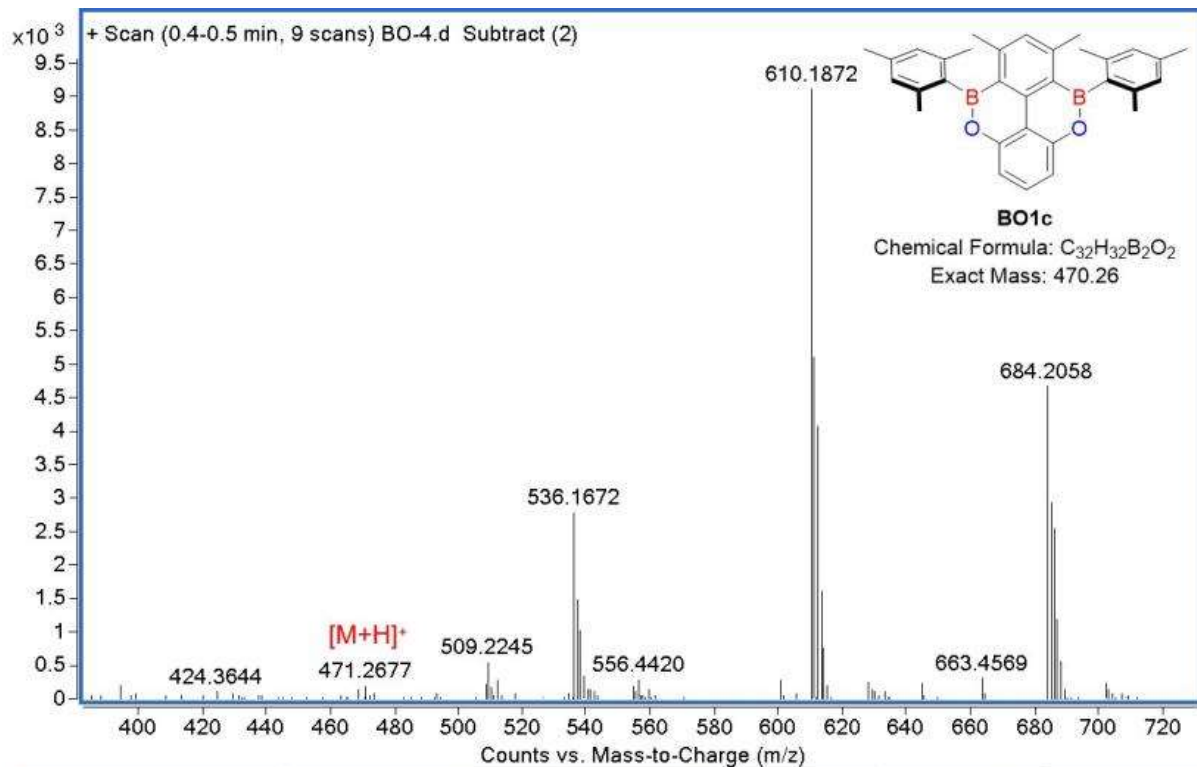
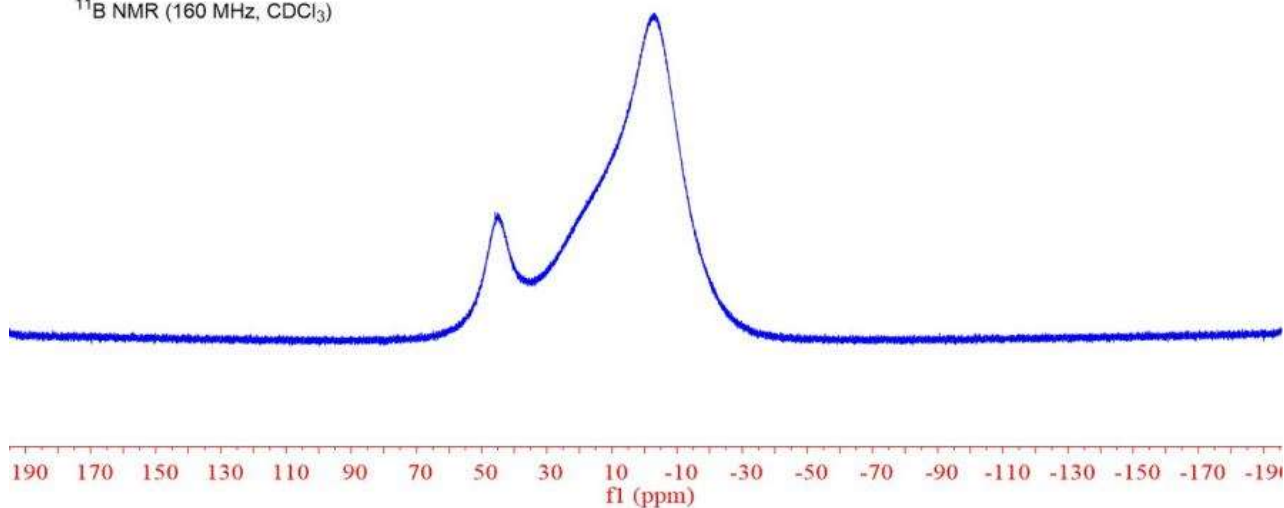


-45.80

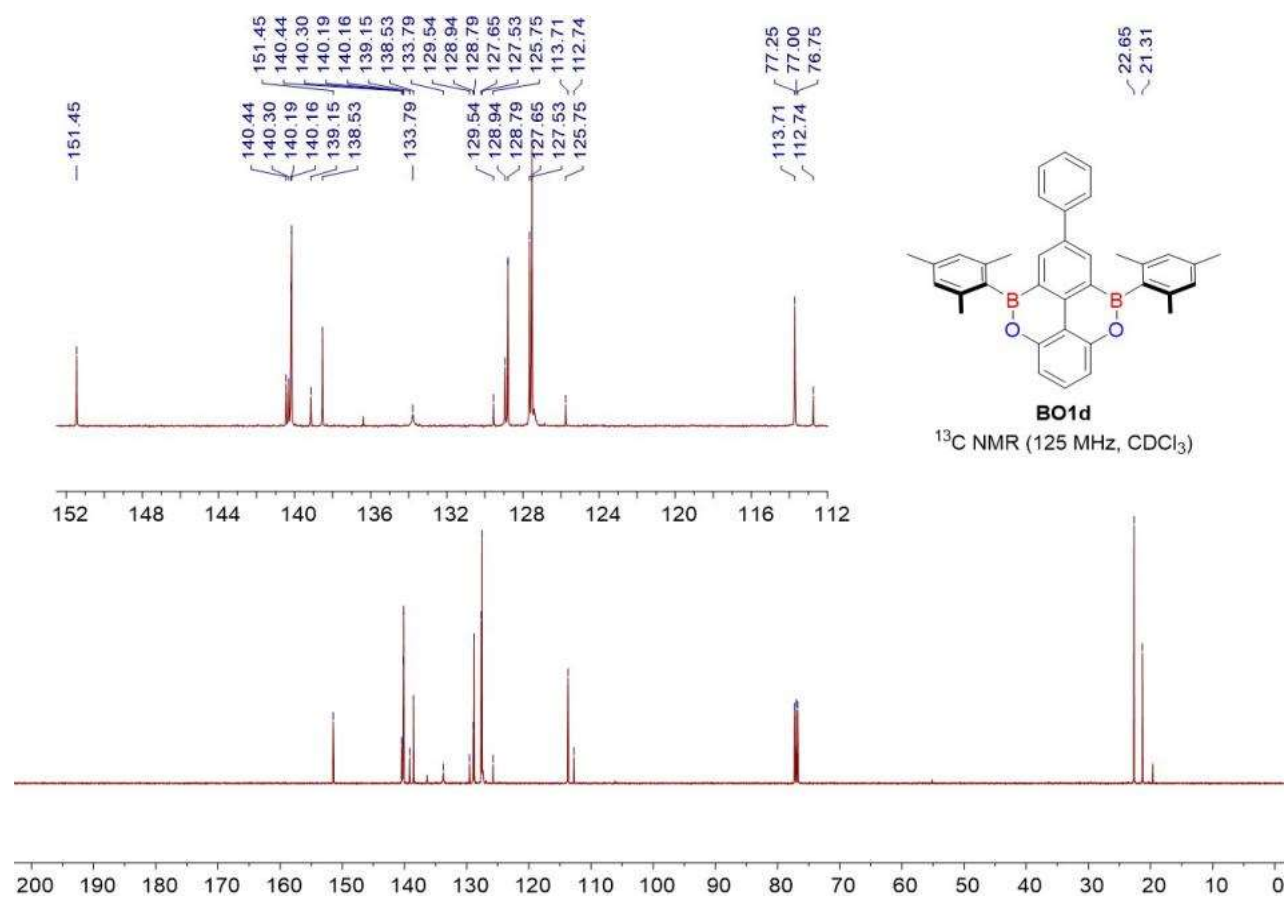
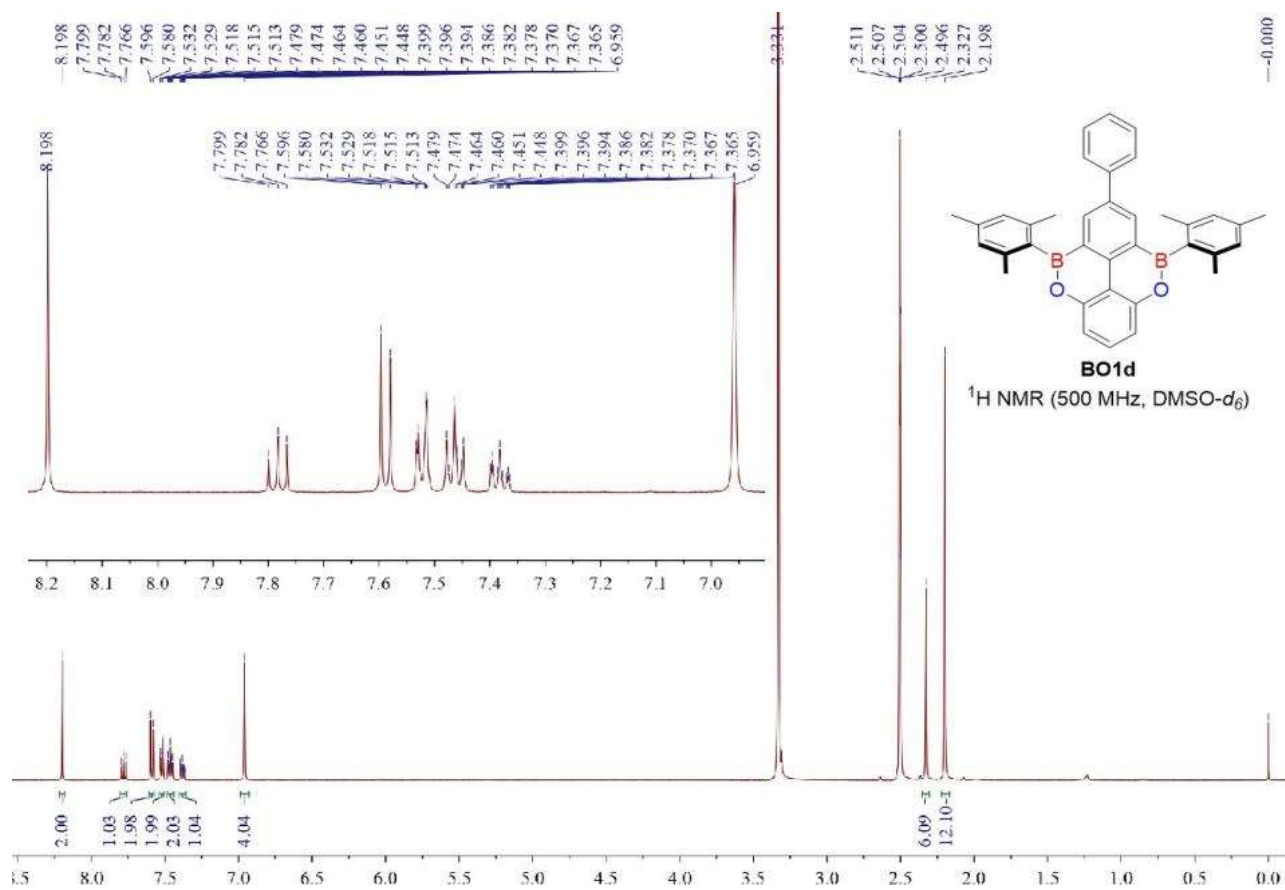


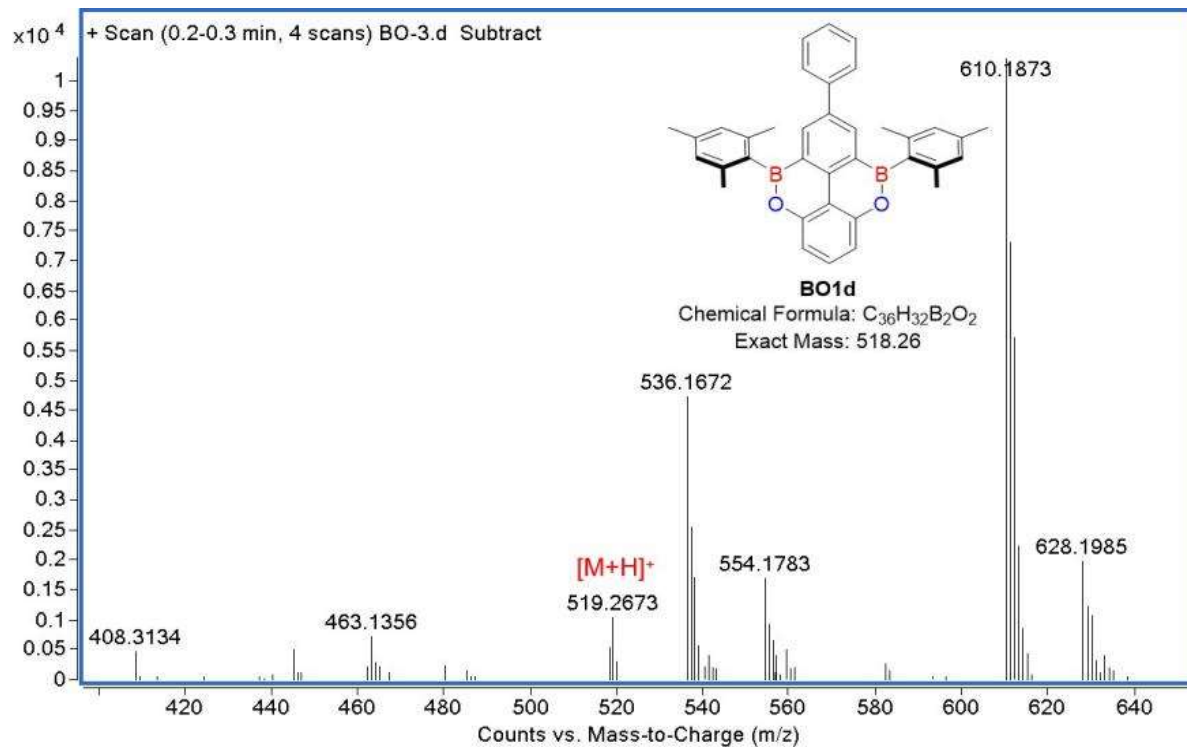
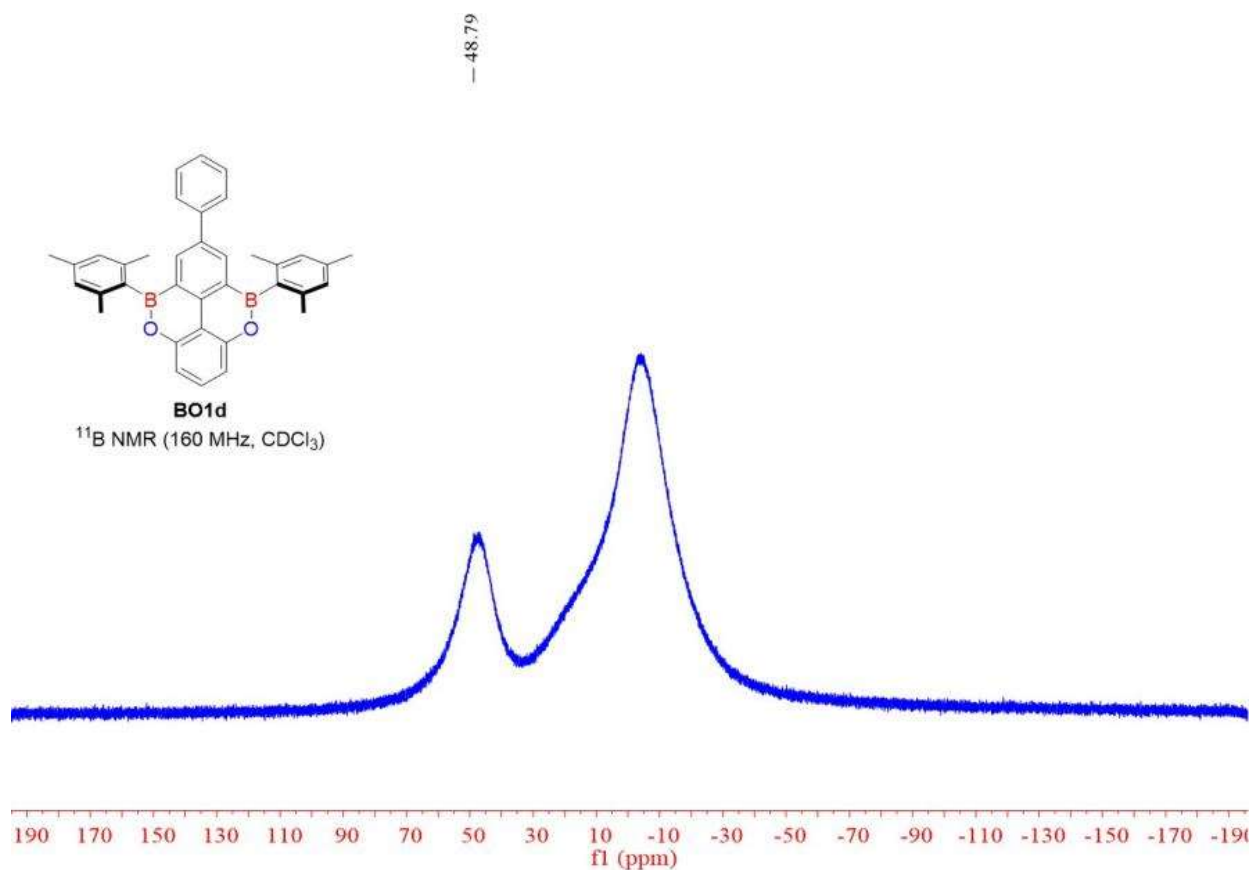
BO1c

^{11}B NMR (160 MHz, CDCl_3)

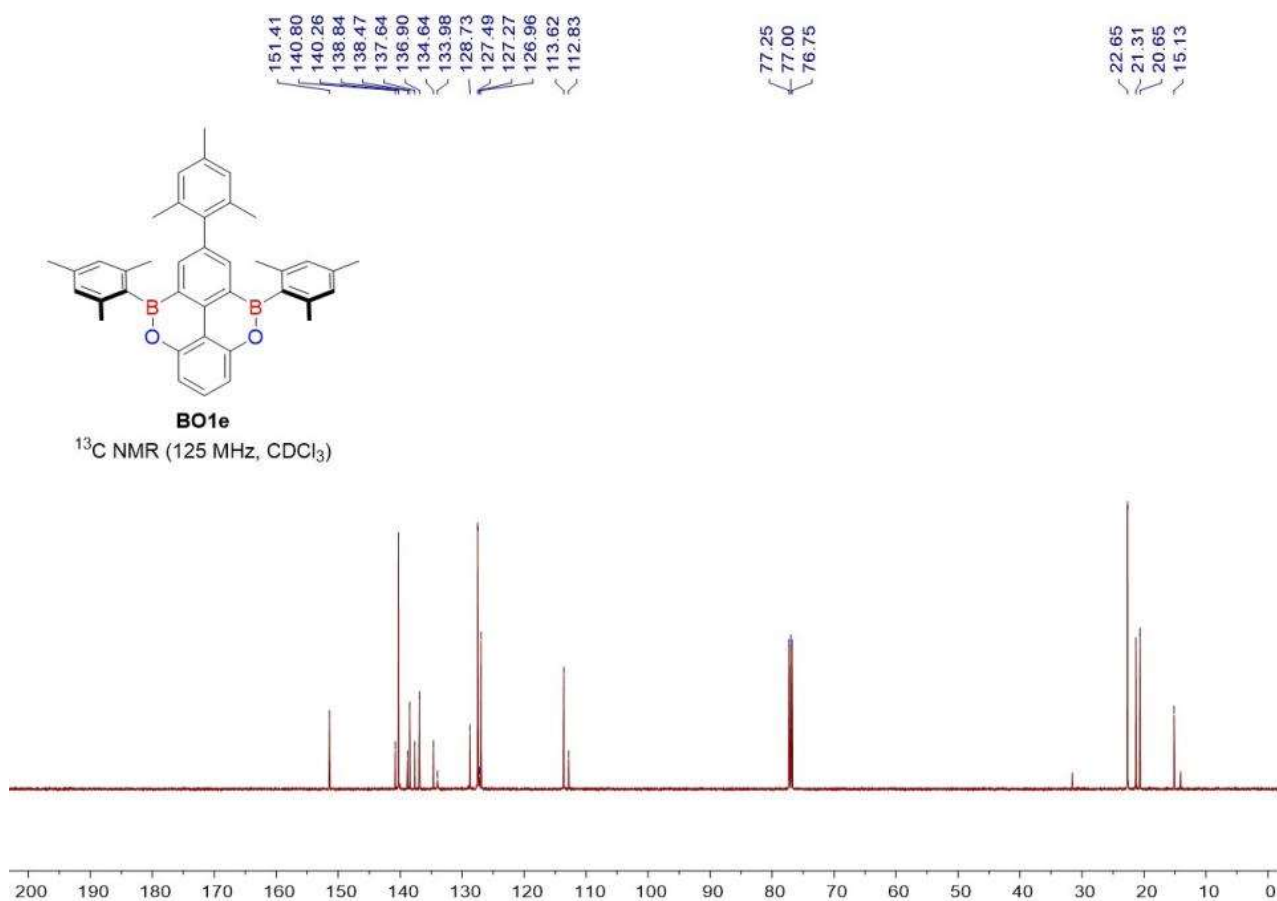
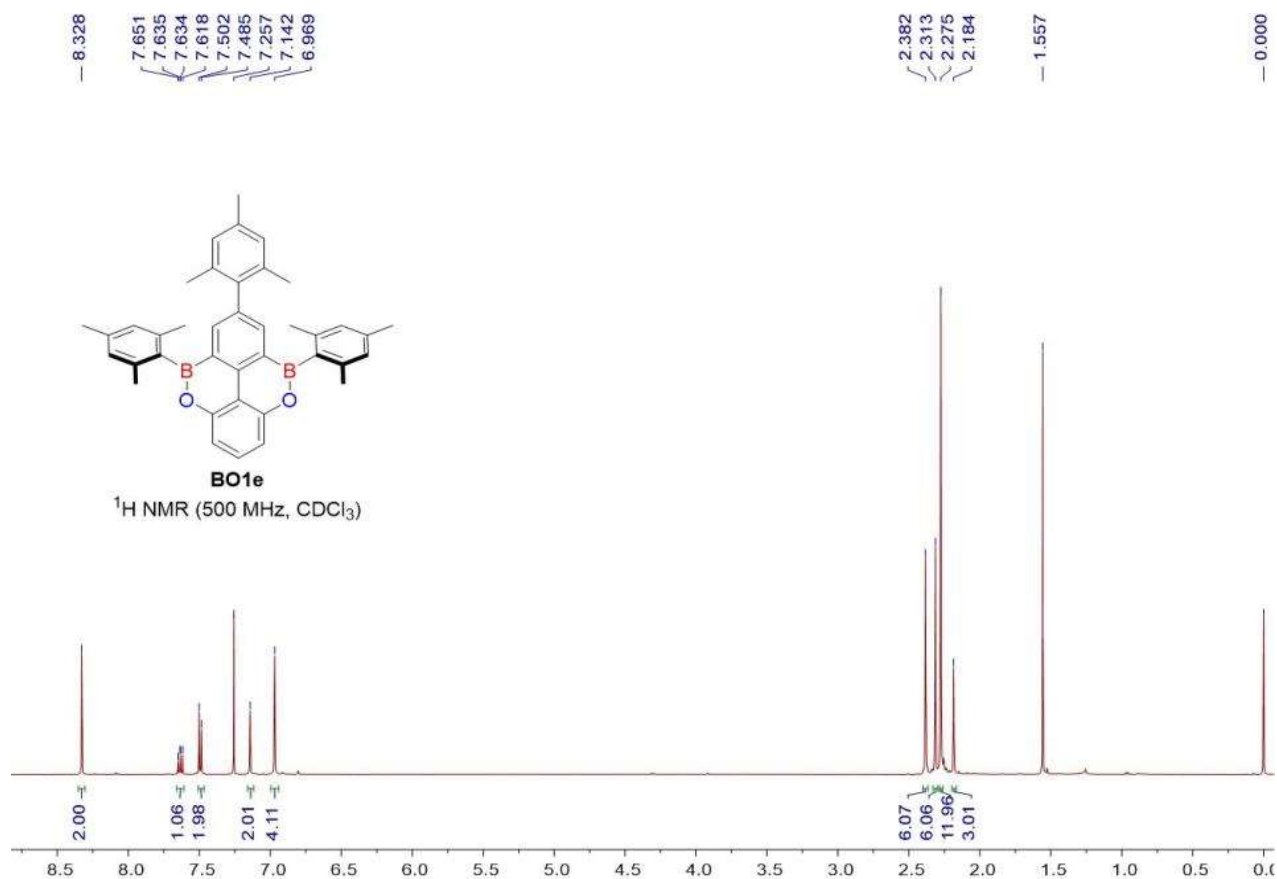


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$\text{C}_{32}\text{H}_{32}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{32}\text{H}_{33}[^{11}\text{B}]_2\text{O}_2$	471.2677	471.2661	-3.36	18

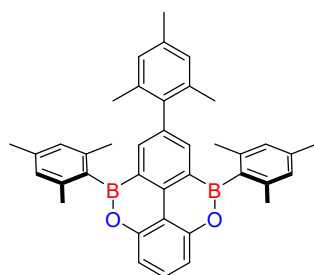




Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$\text{C}_{36}\text{H}_{32}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{36}\text{H}_{33}[^{11}\text{B}]_2\text{O}_2$	519.2673	519.2661	-2.28	22

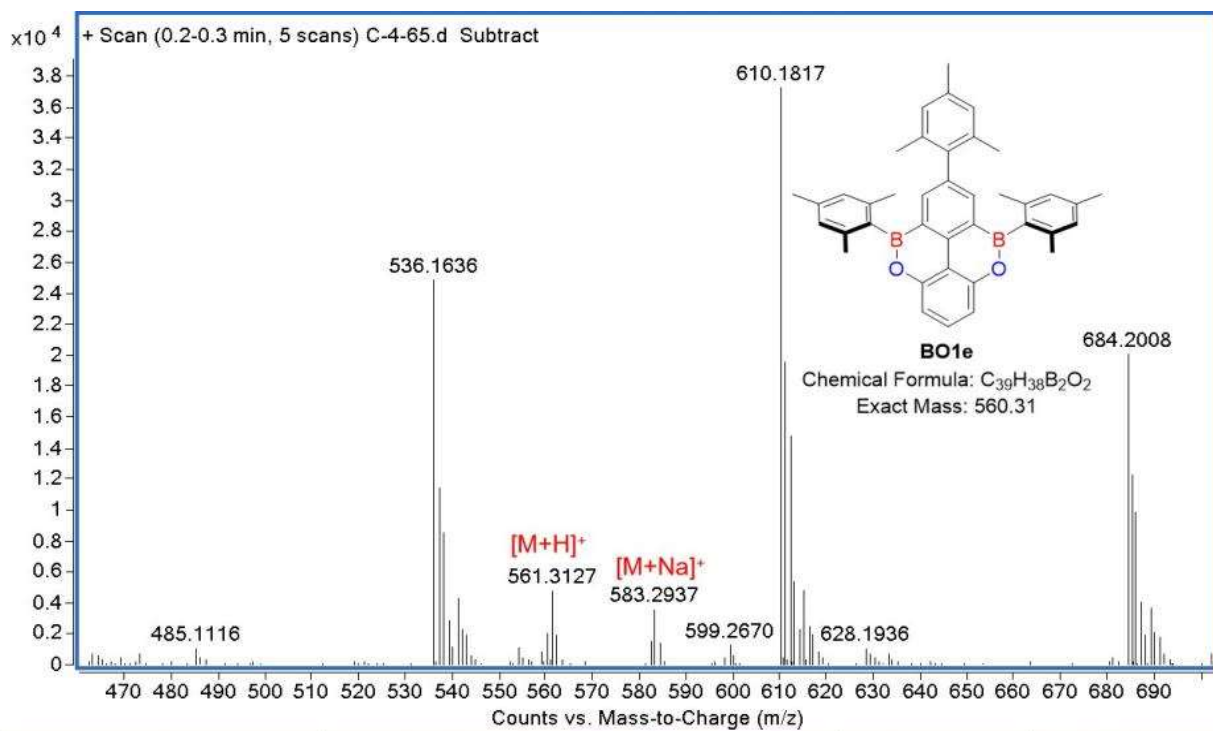
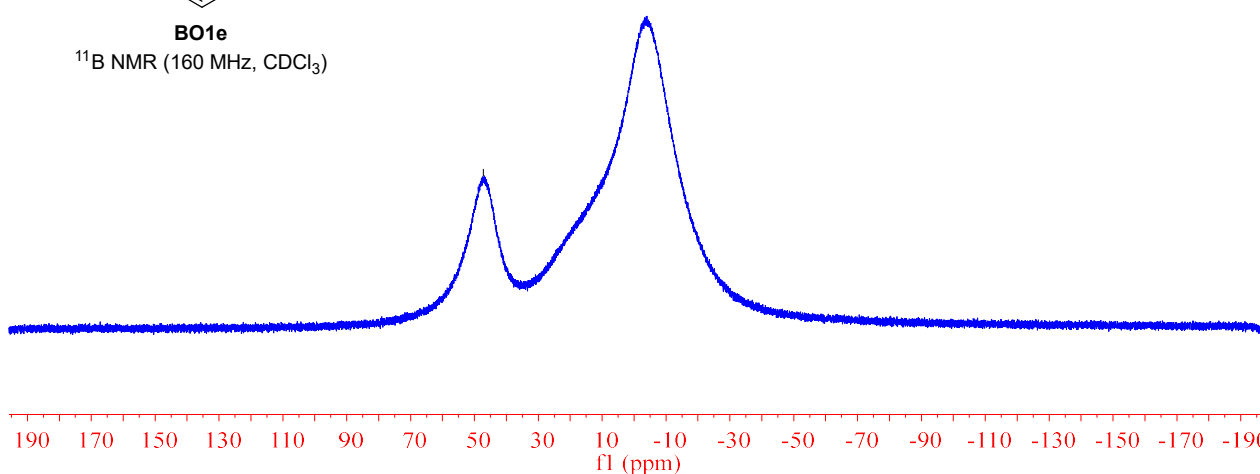


-47.17

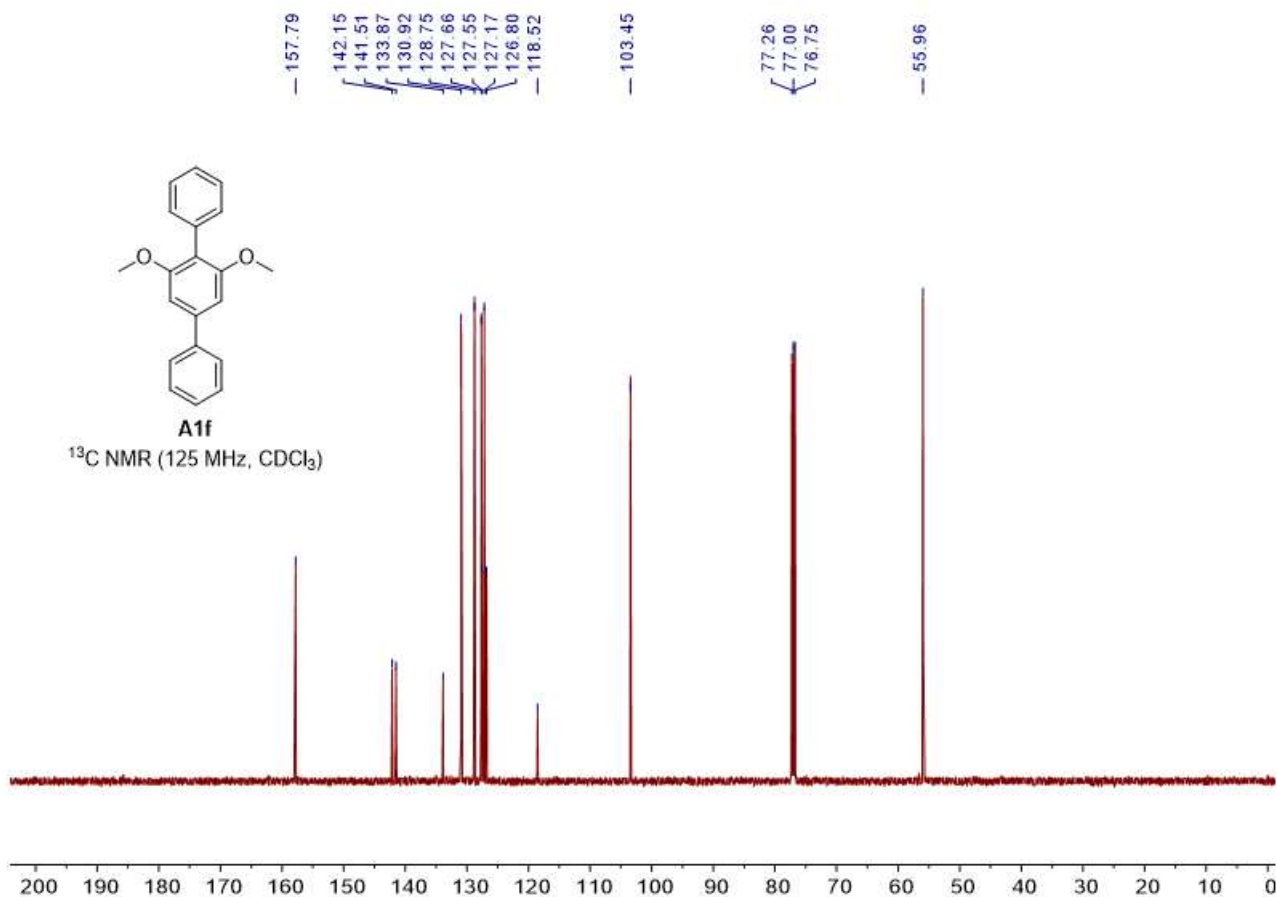
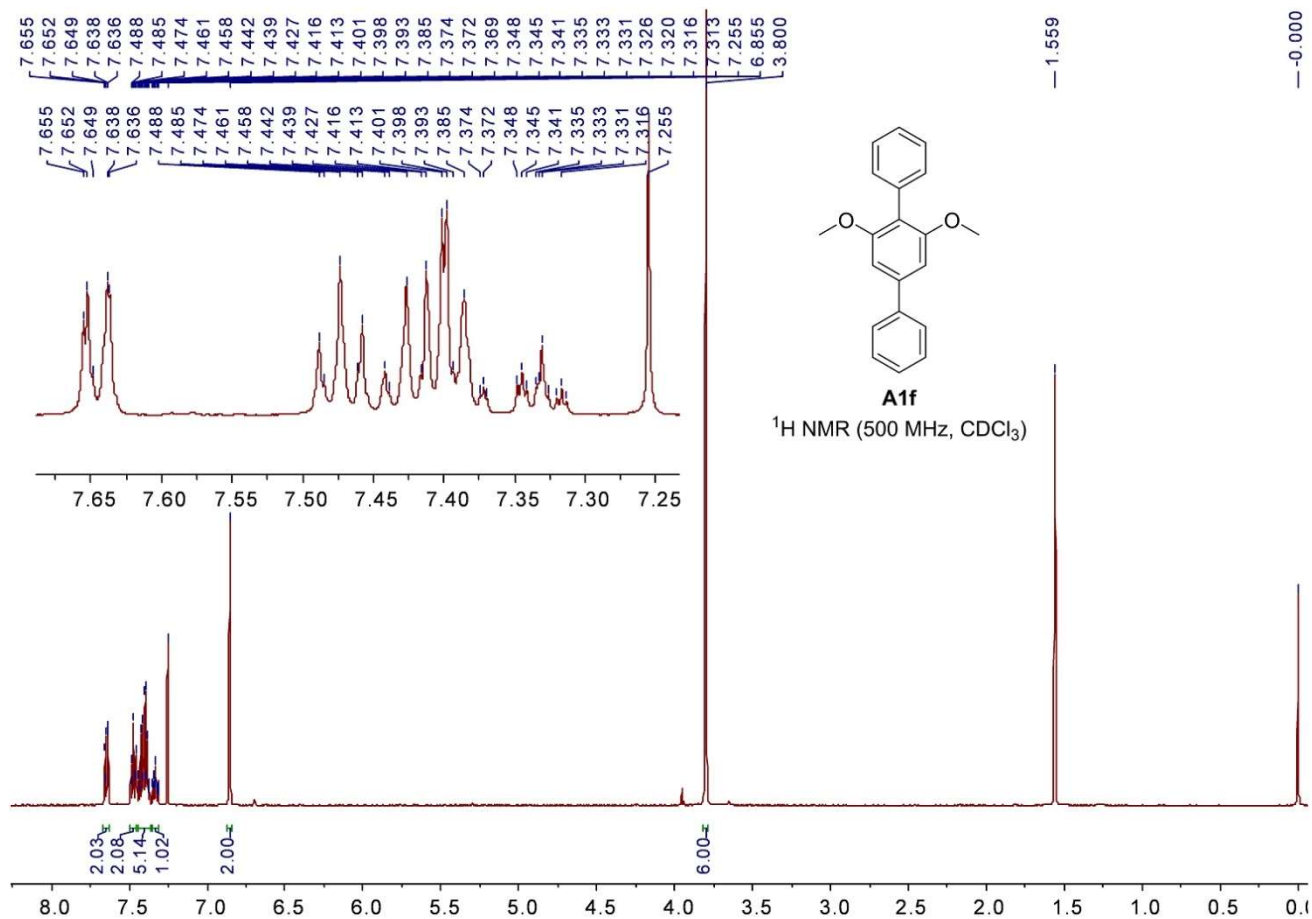


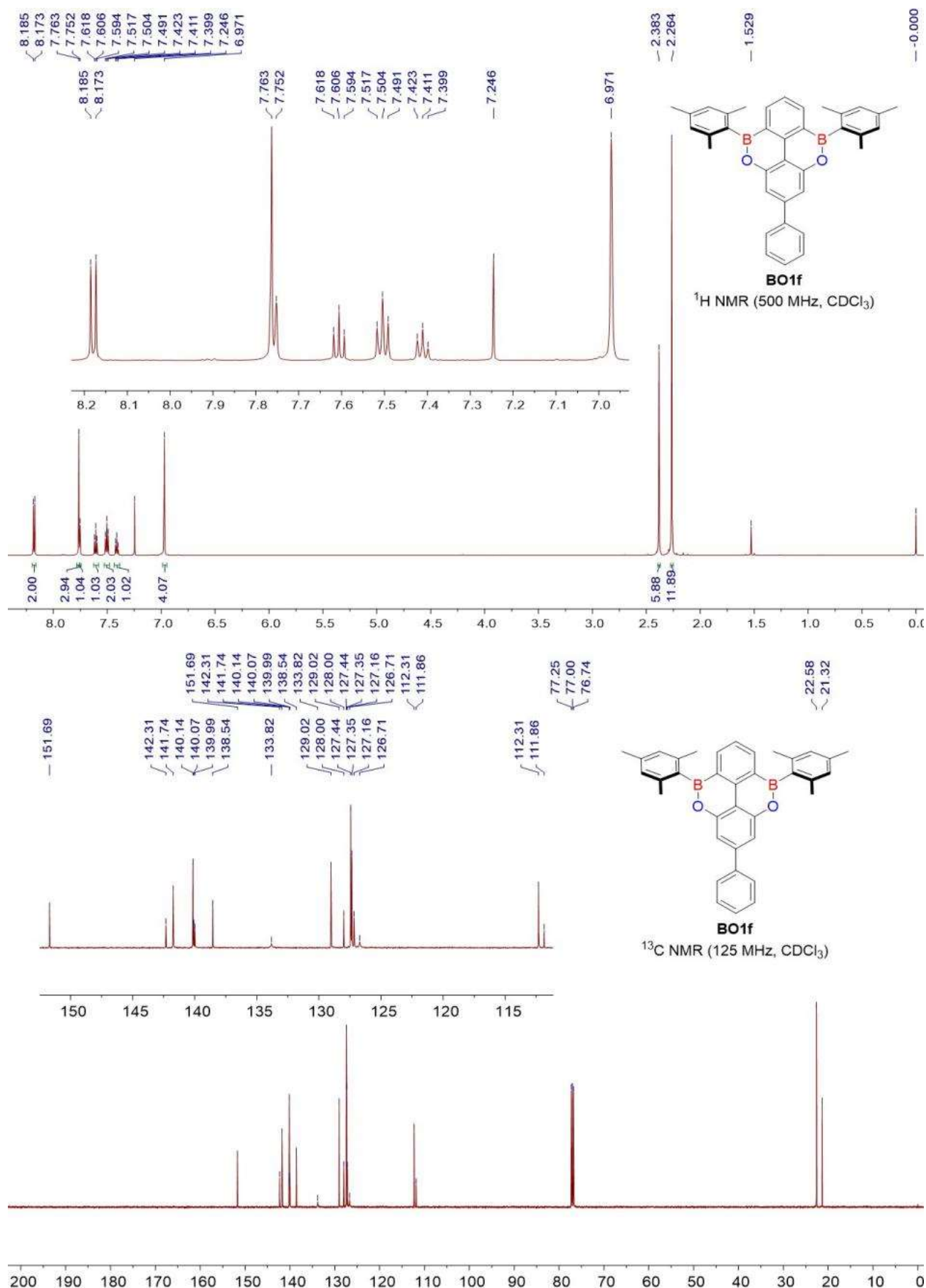
BO1e

^{11}B NMR (160 MHz, CDCl_3)

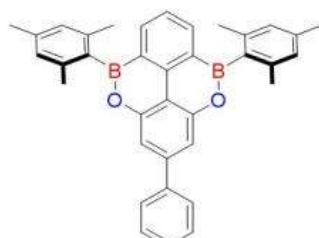


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{39}\text{H}_{38}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{39}\text{H}_{39}[^{11}\text{B}]_2\text{O}_2$	561.3127	561.3131	0.66



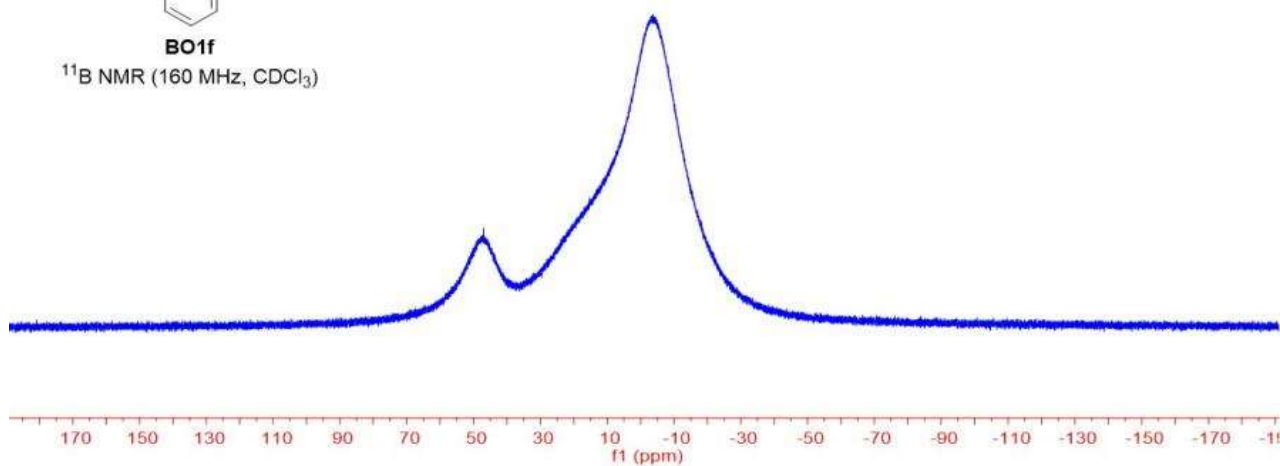


— 46.99

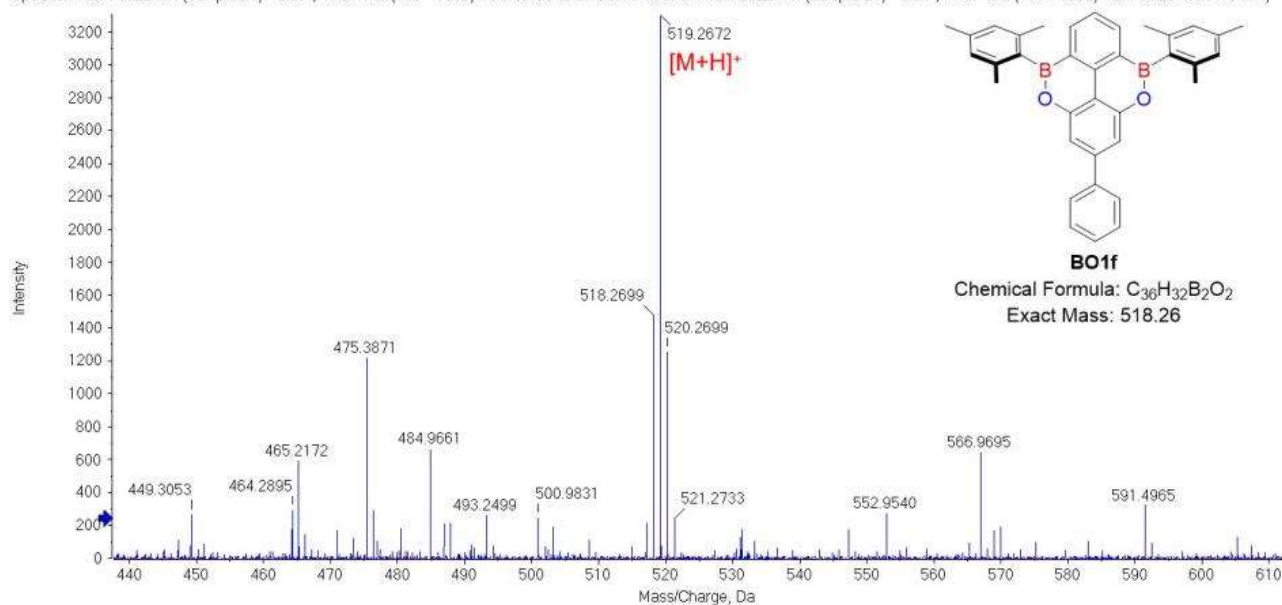


BO1f

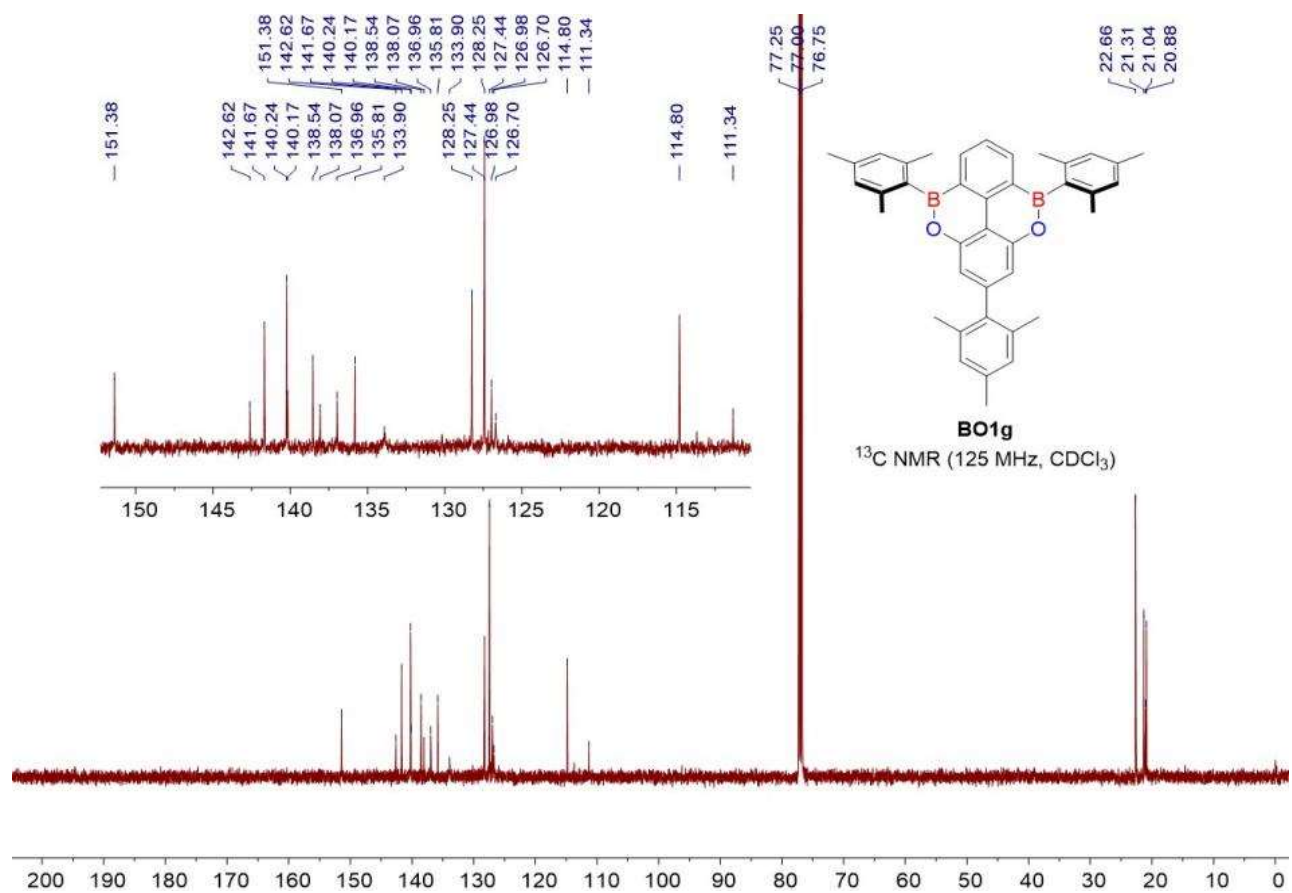
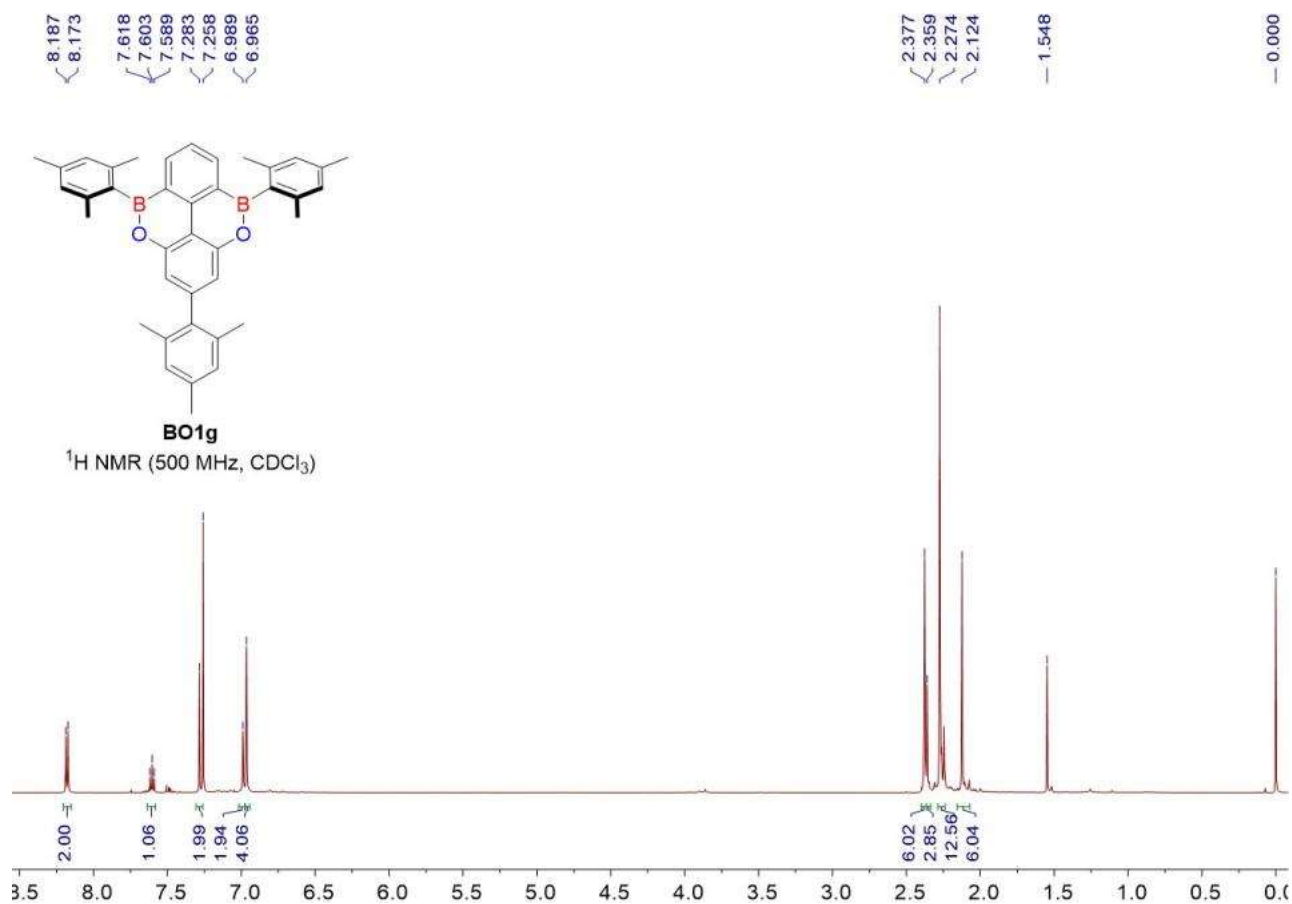
^{11}B NMR (160 MHz, CDCl_3)



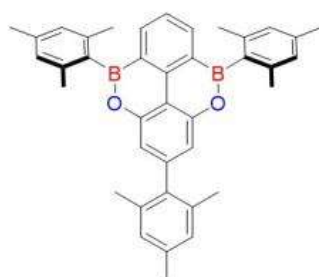
Spectrum from 0922.wiff (sample 27) - BO1f, +TOF MS (100 - 1500) from 0.135 to 0.195 min... Spectrum from 0922.wiff (sample 27) - BO1f, +TOF MS (100 - 1500) from 0.326 to 0.479 min



Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{36}\text{H}_{32}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{36}\text{H}_{33}[^{11}\text{B}]_2\text{O}_2$	519.2672	519.2661	-2.2

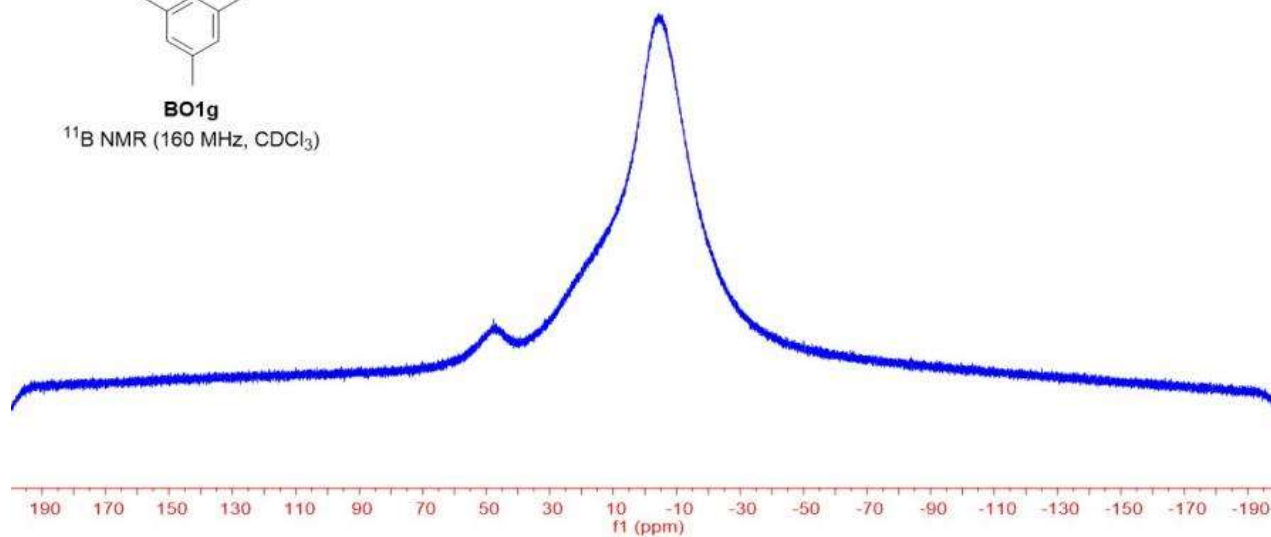


— 47.63

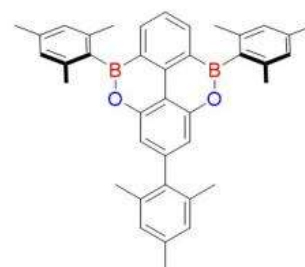
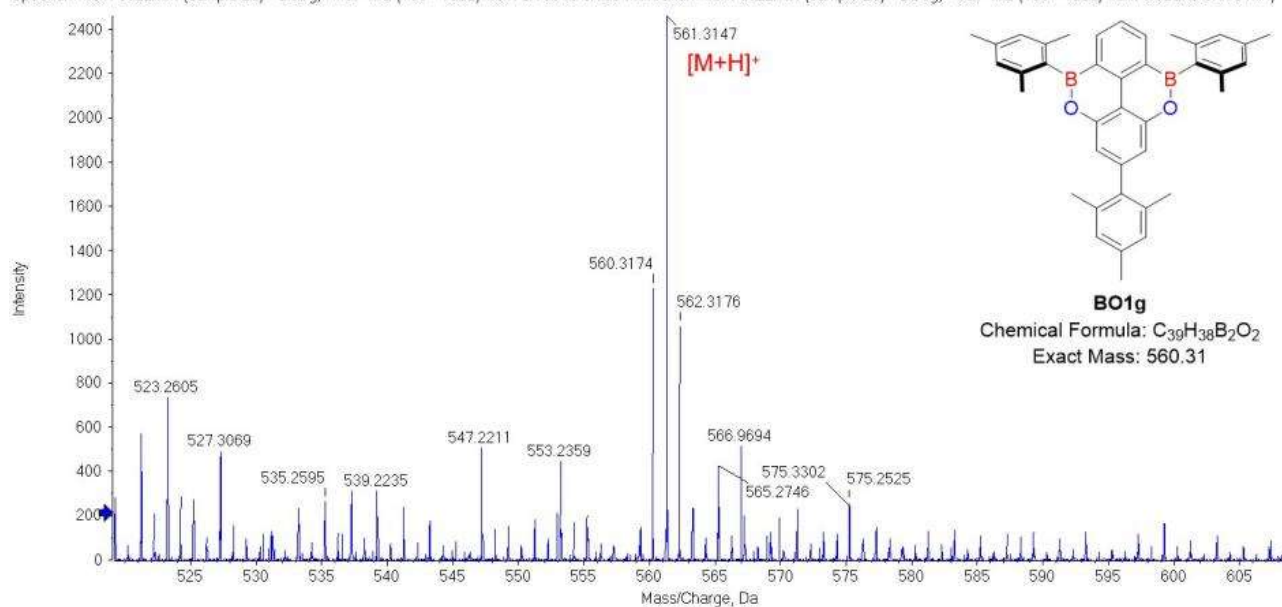


BO1g

^{11}B NMR (160 MHz, CDCl_3)



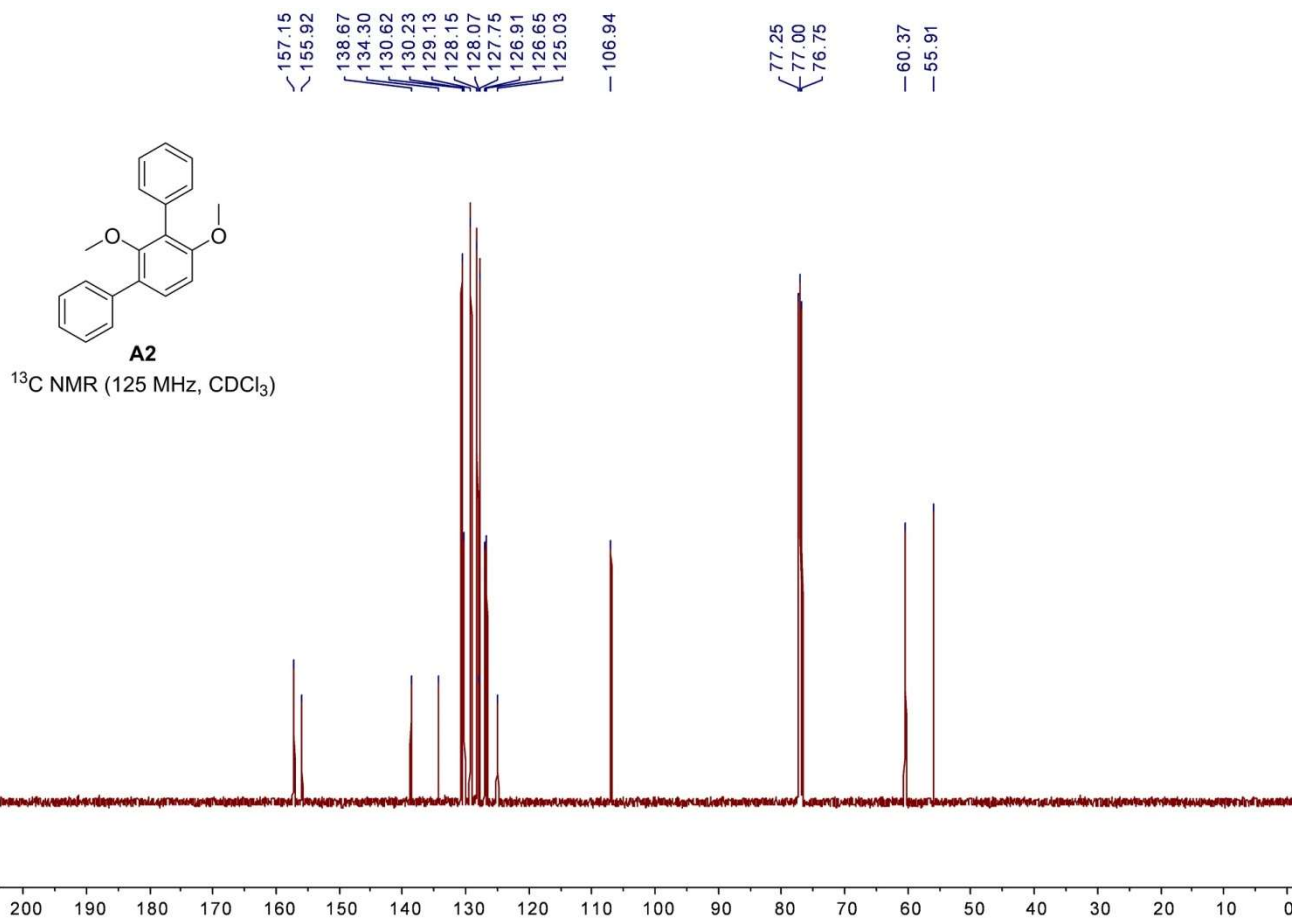
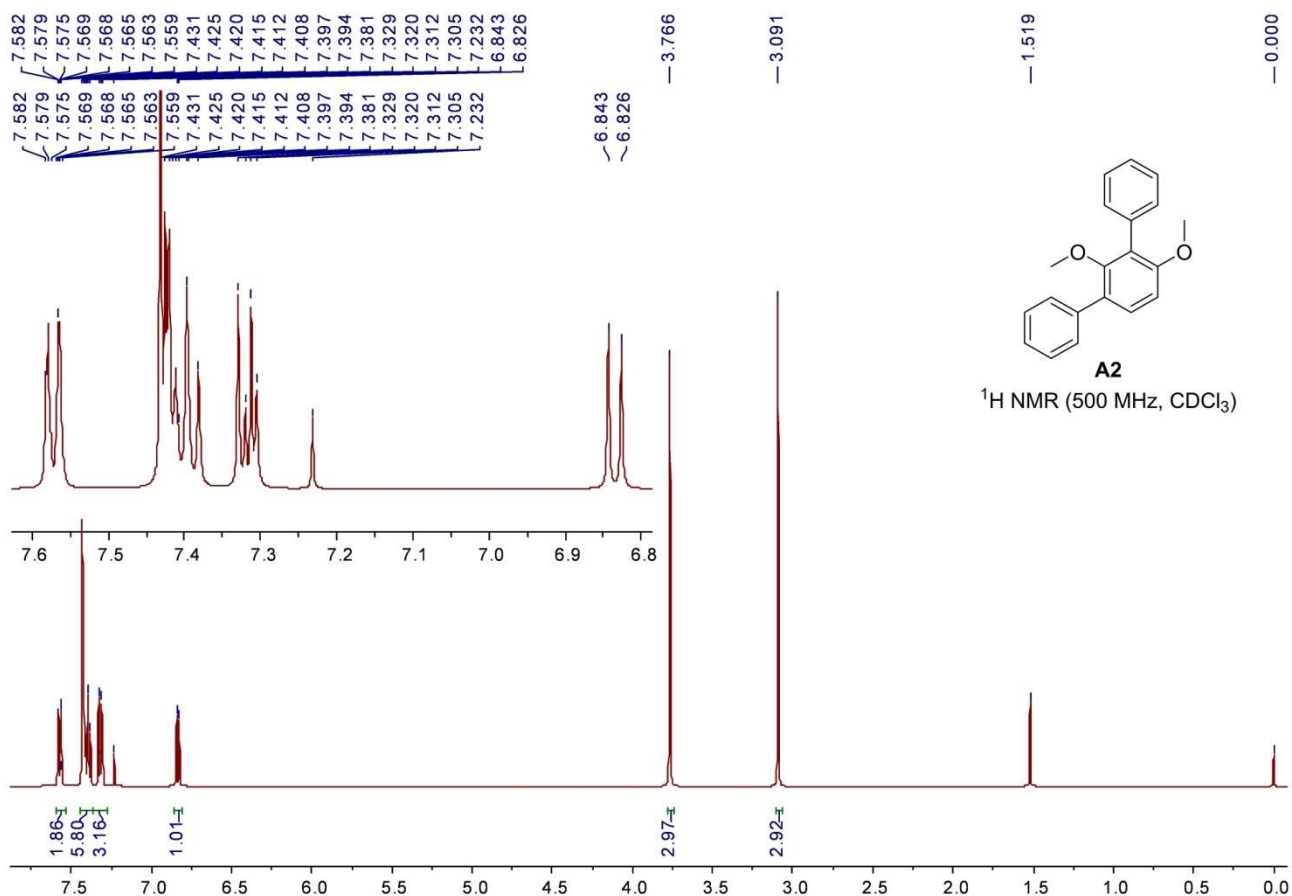
Spectrum from 0922.wiff (sample 28) - BO1g, +TOF MS (100 - 1500) from 0.135 to 0.195 min. Spectrum from 0922.wiff (sample 28) - BO1g, +TOF MS (100 - 1500) from 0.326 to 0.479 min

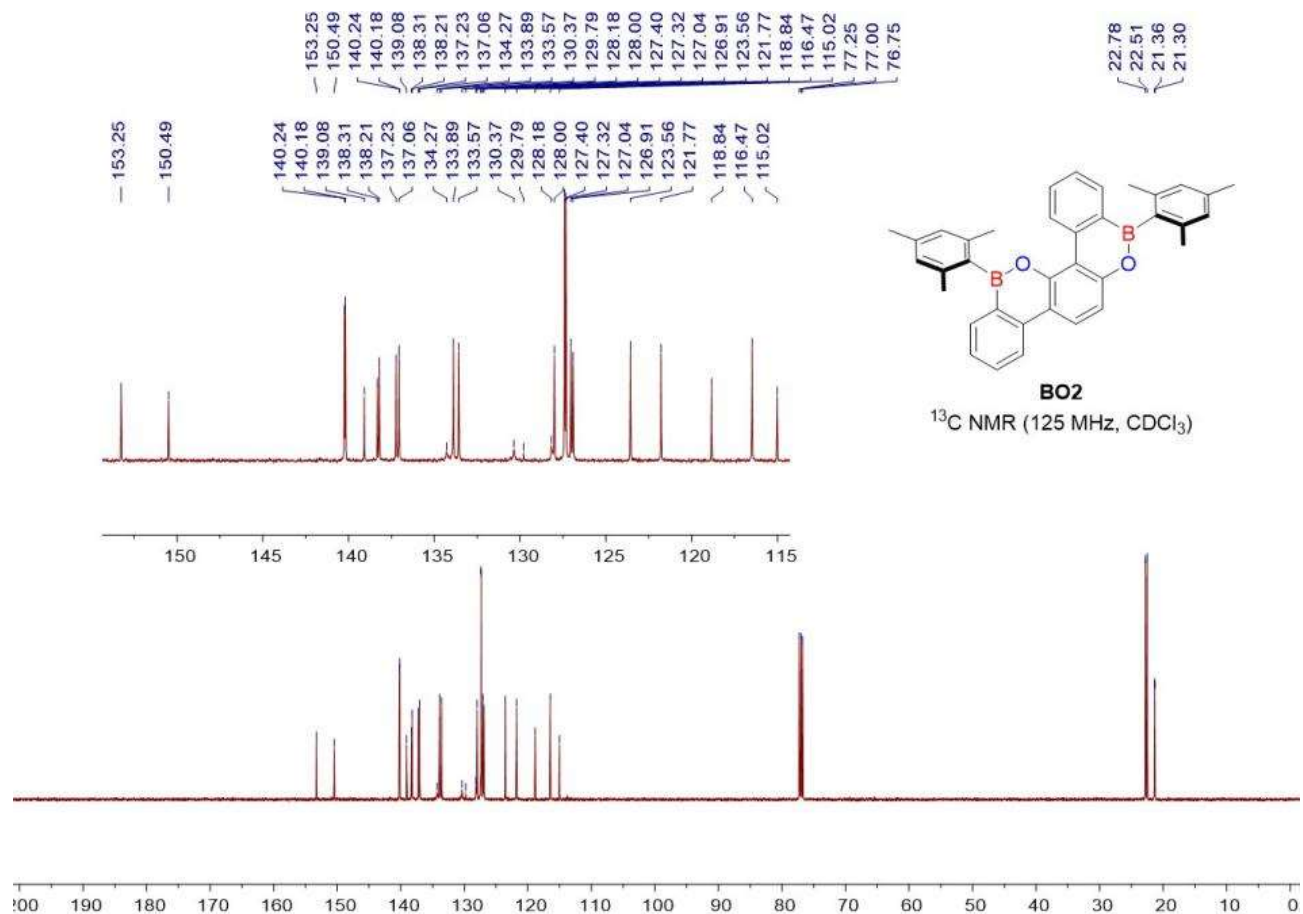
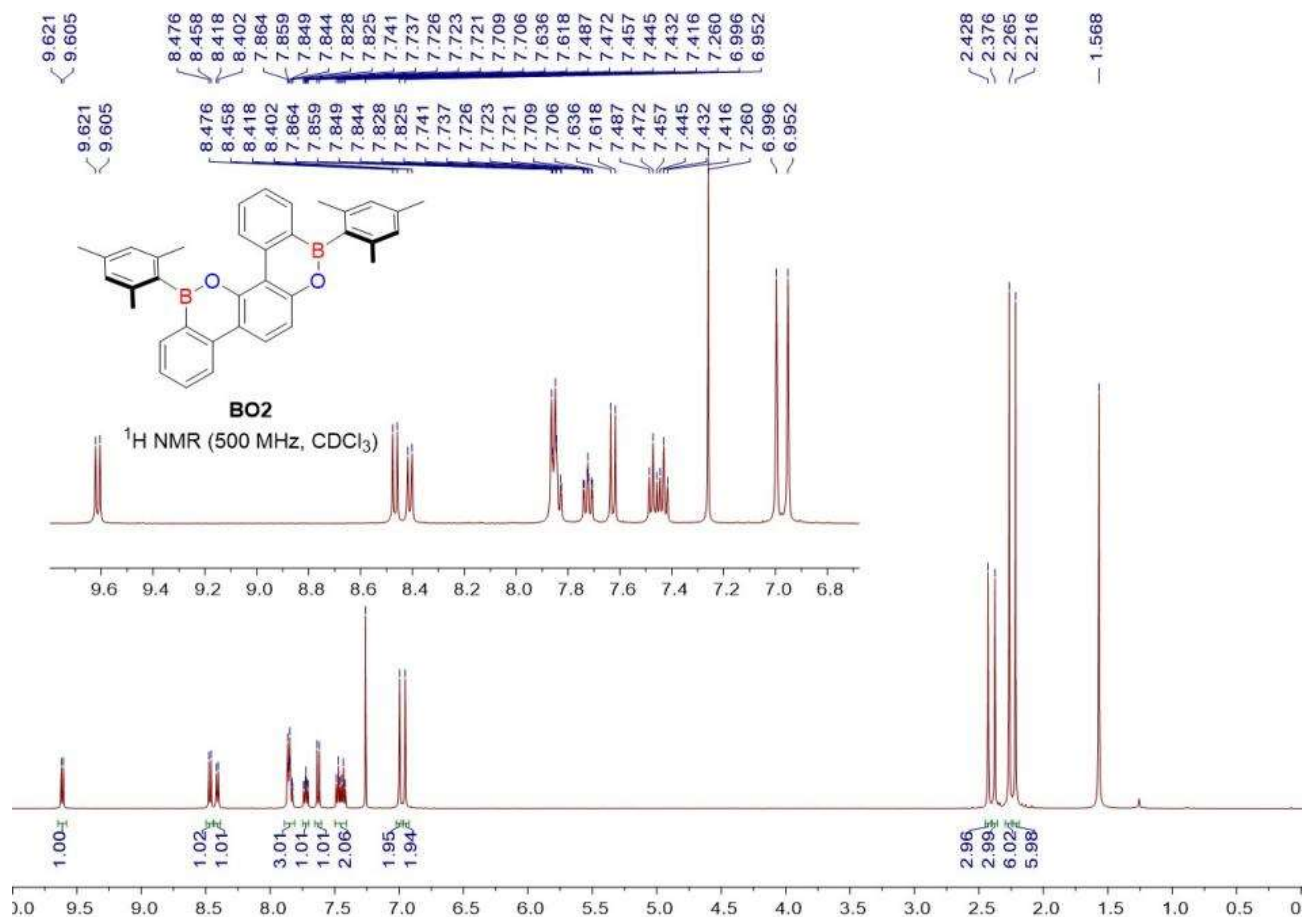


BO1g

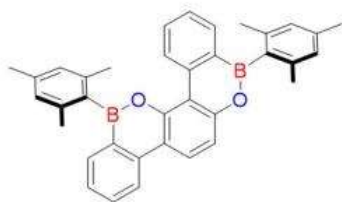
Chemical Formula: $\text{C}_{39}\text{H}_{38}\text{B}_2\text{O}_2$
Exact Mass: 560.31

Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{39}\text{H}_{38}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{39}\text{H}_{39}[^{11}\text{B}]_2\text{O}_2$	561.3147	561.3131	-2.9



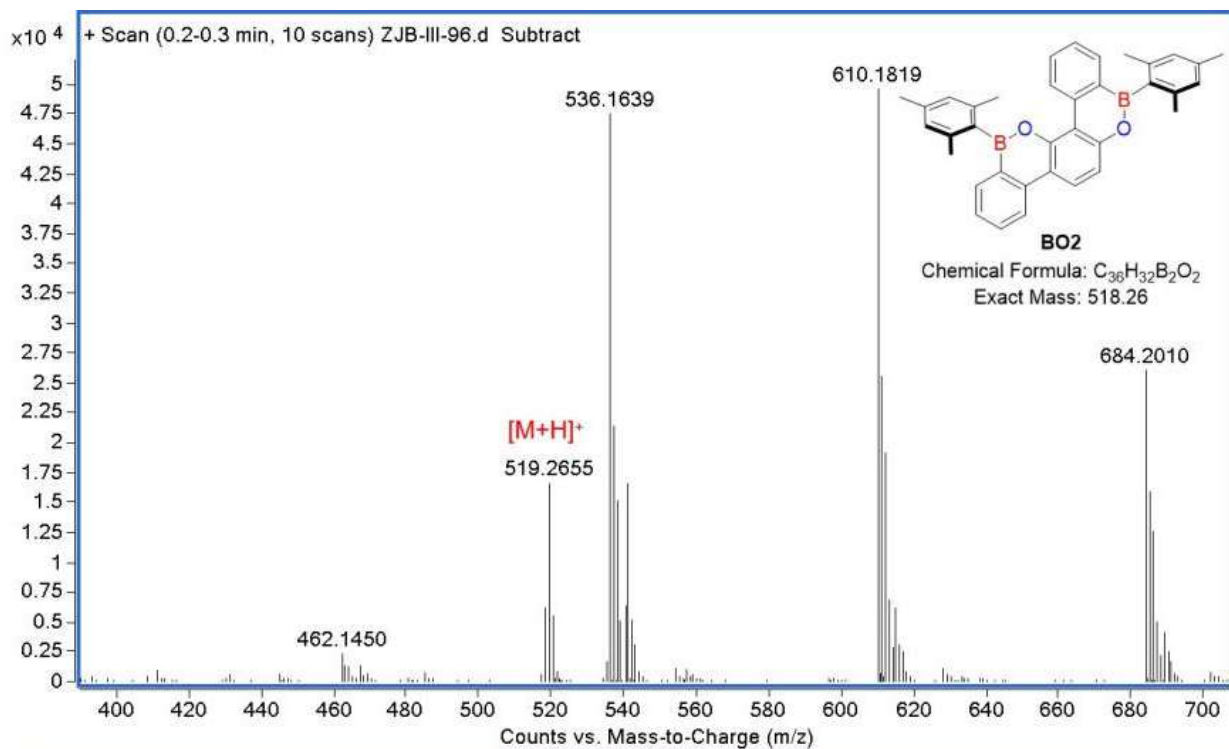
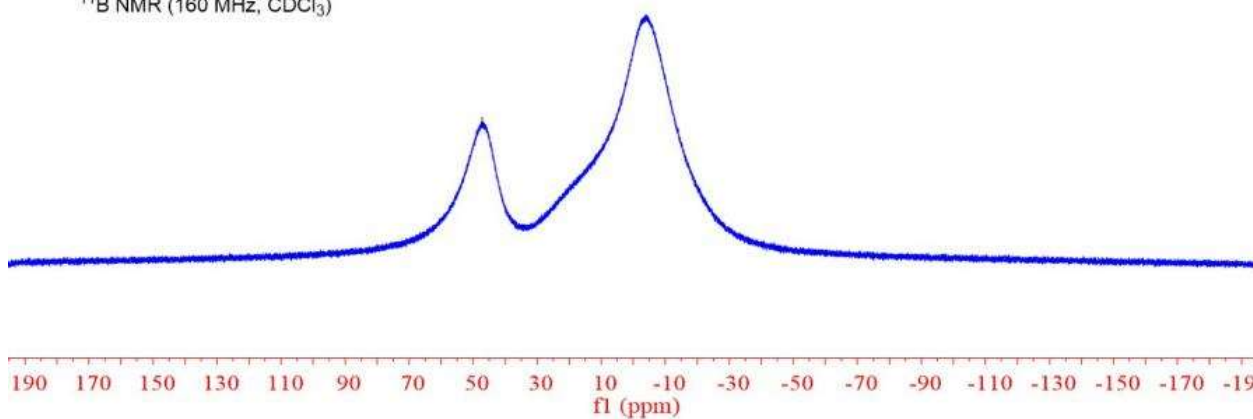


— 47.21

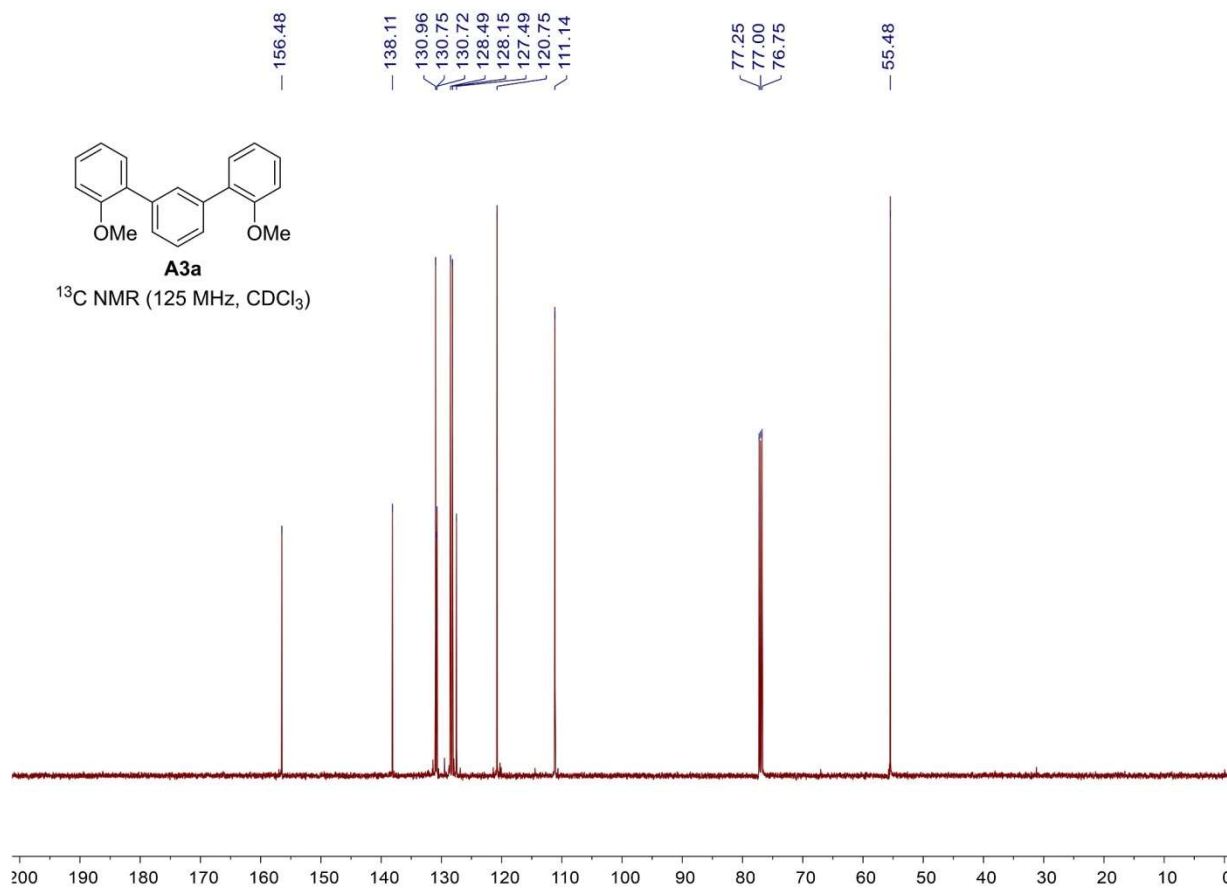
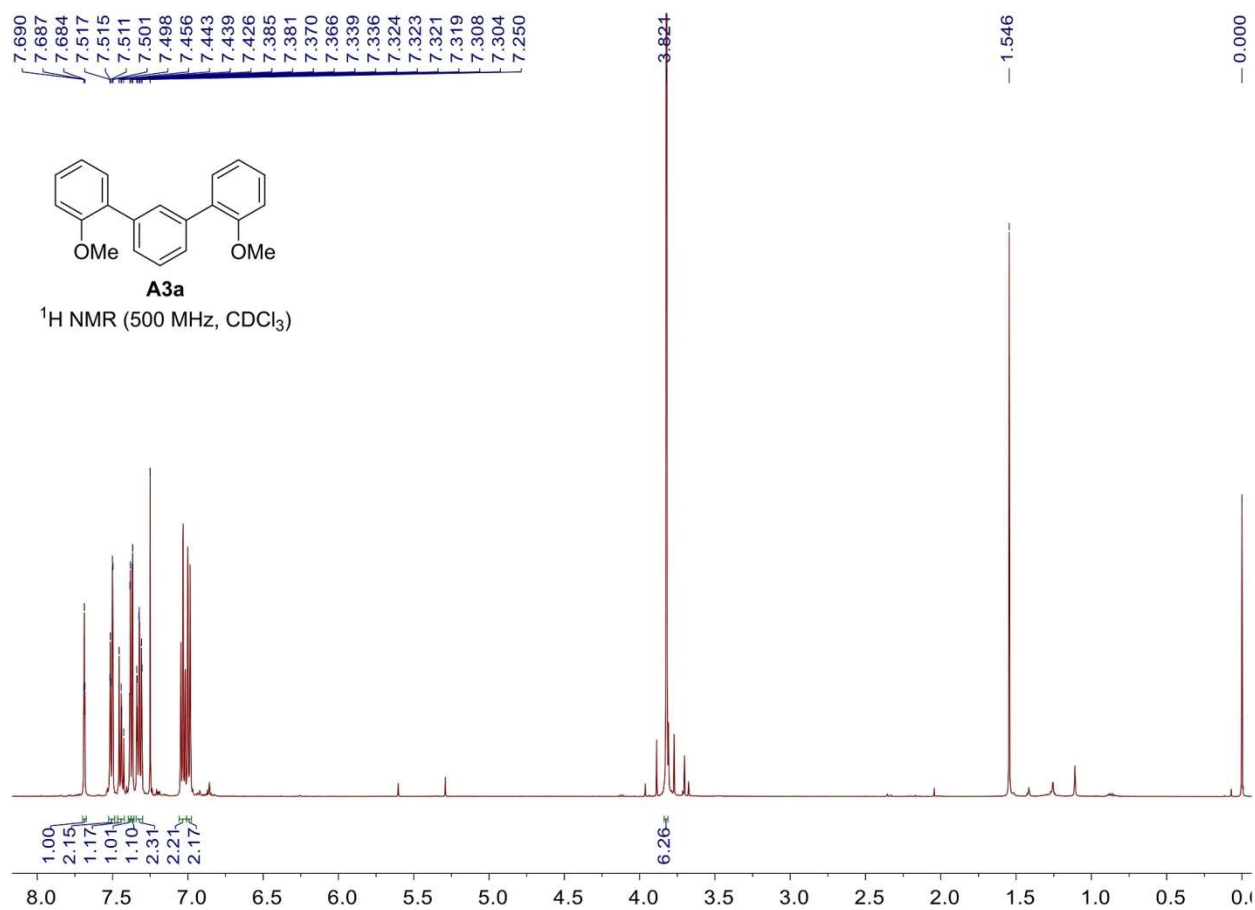


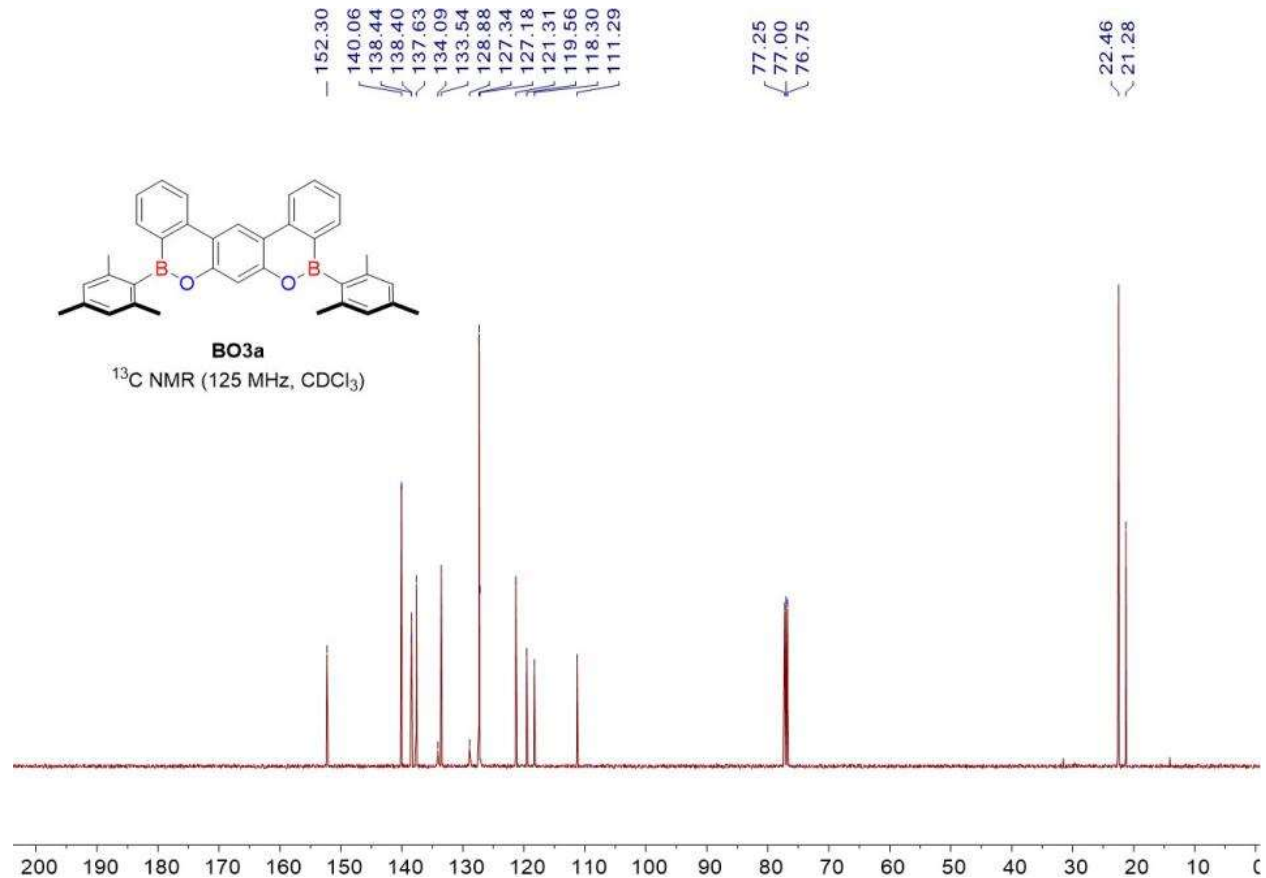
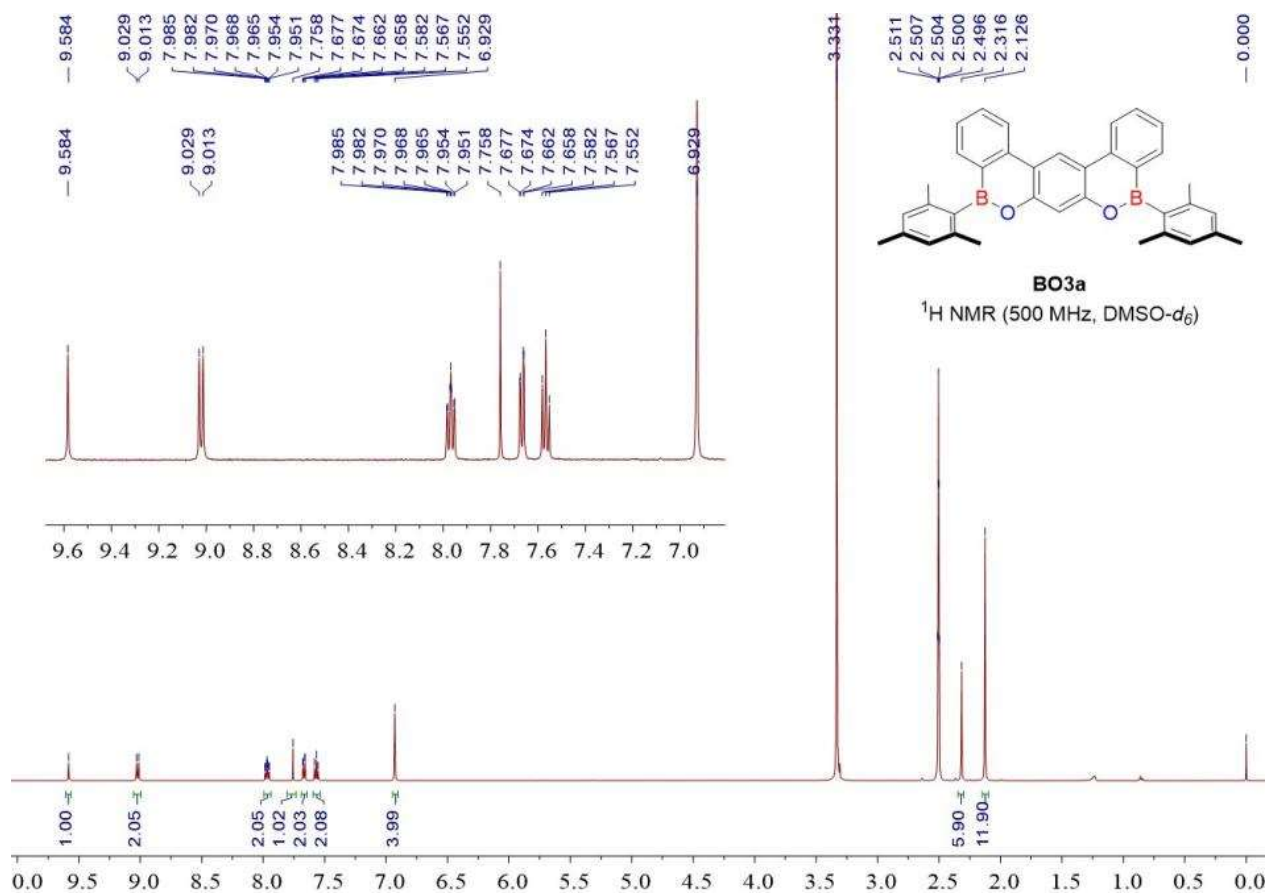
BO2

^{11}B NMR (160 MHz, CDCl_3)

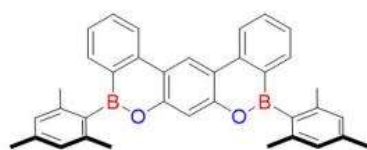


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{36}\text{H}_{32}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{36}\text{H}_{33}[^{11}\text{B}]_2\text{O}_2$	519.2655	519.2661	1.19



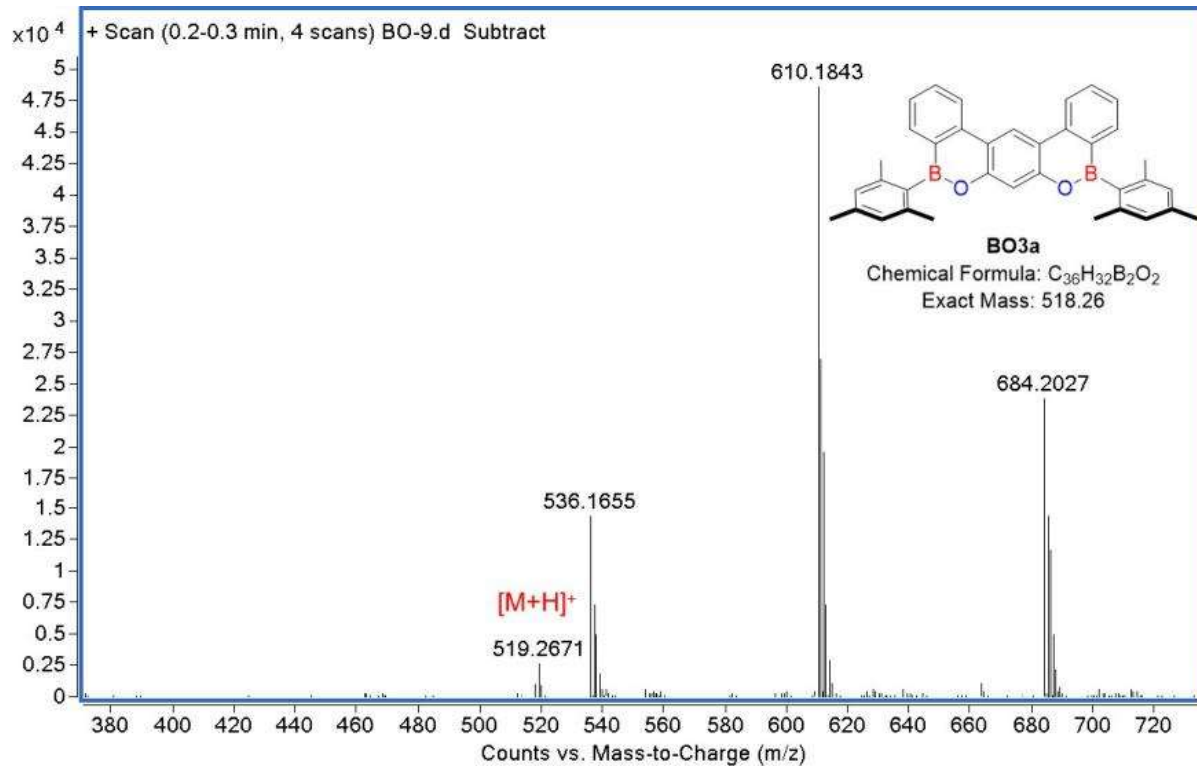
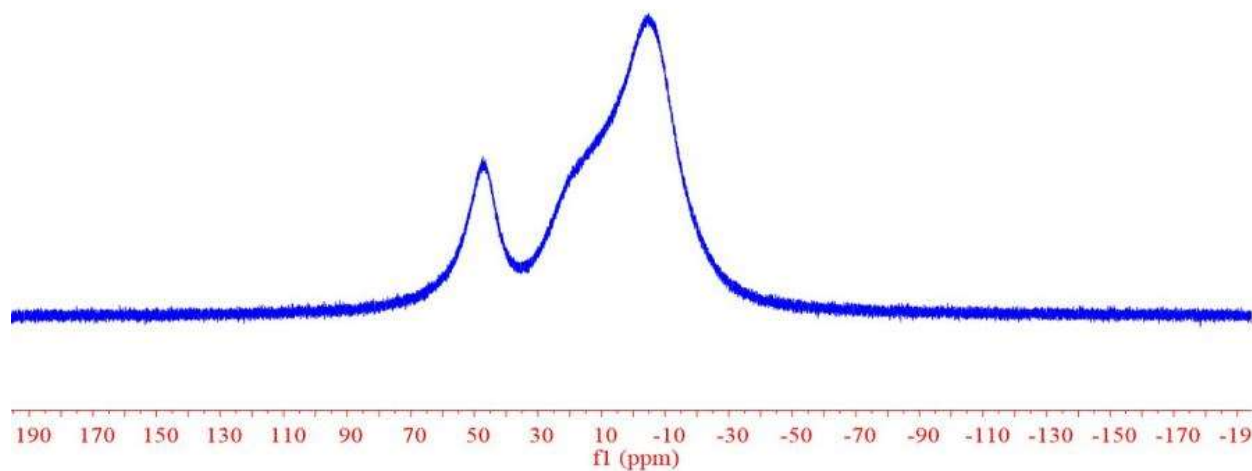


— 47.36

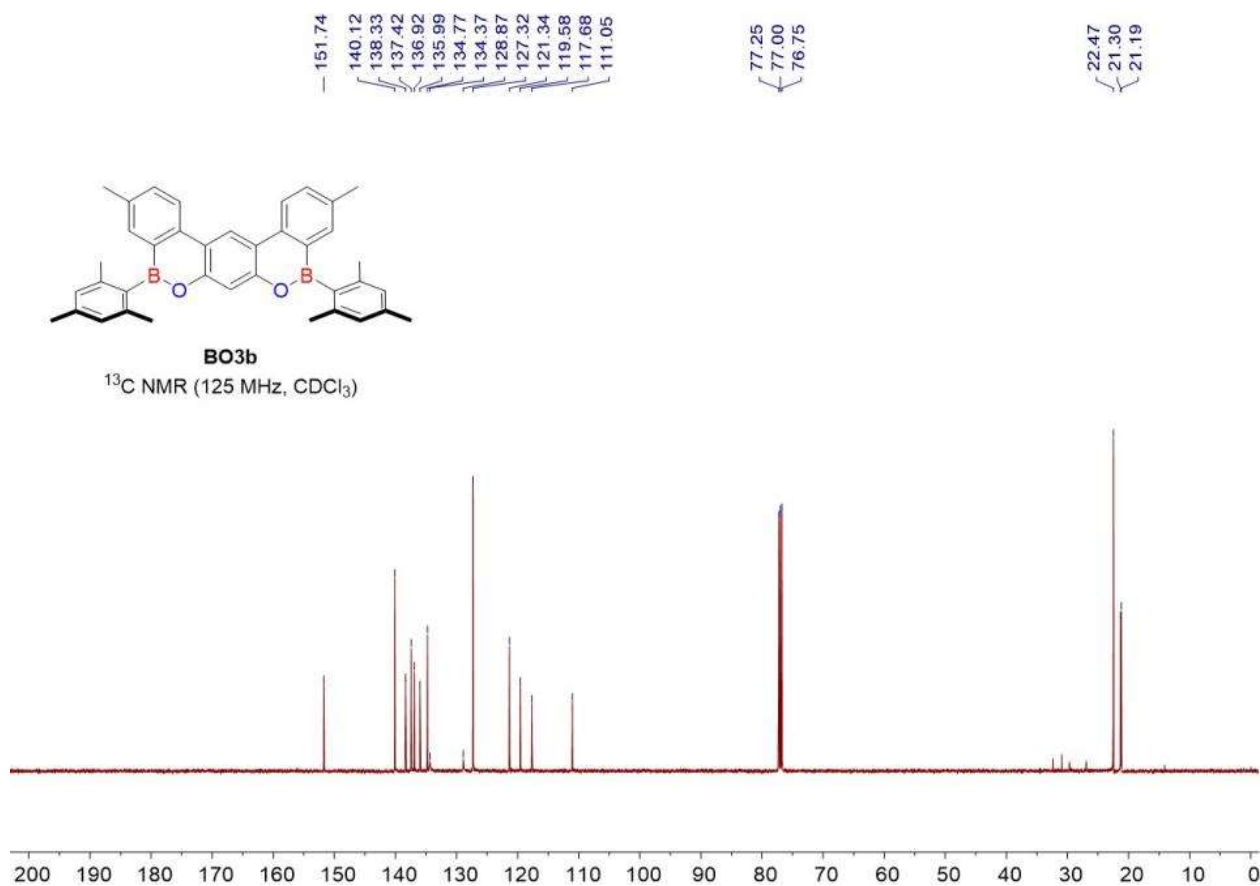
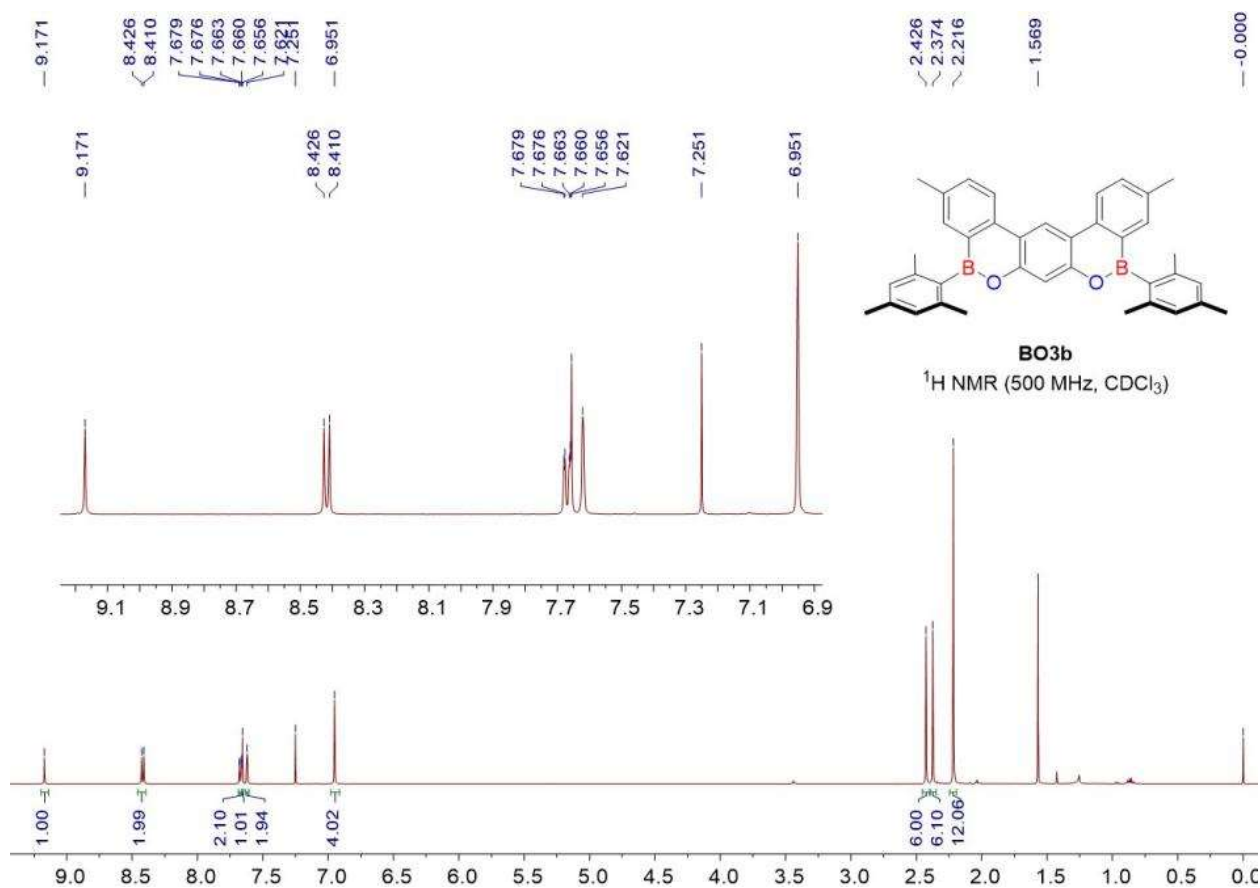


BO3a

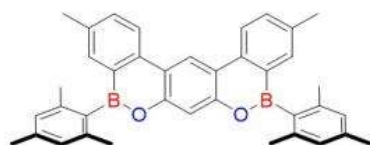
^{11}B NMR (160 MHz, CDCl_3)



Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$\text{C}_{36}\text{H}_{32}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{36}\text{H}_{33}[^{11}\text{B}]_2\text{O}_2$	519.2671	519.2661	-1.9	22

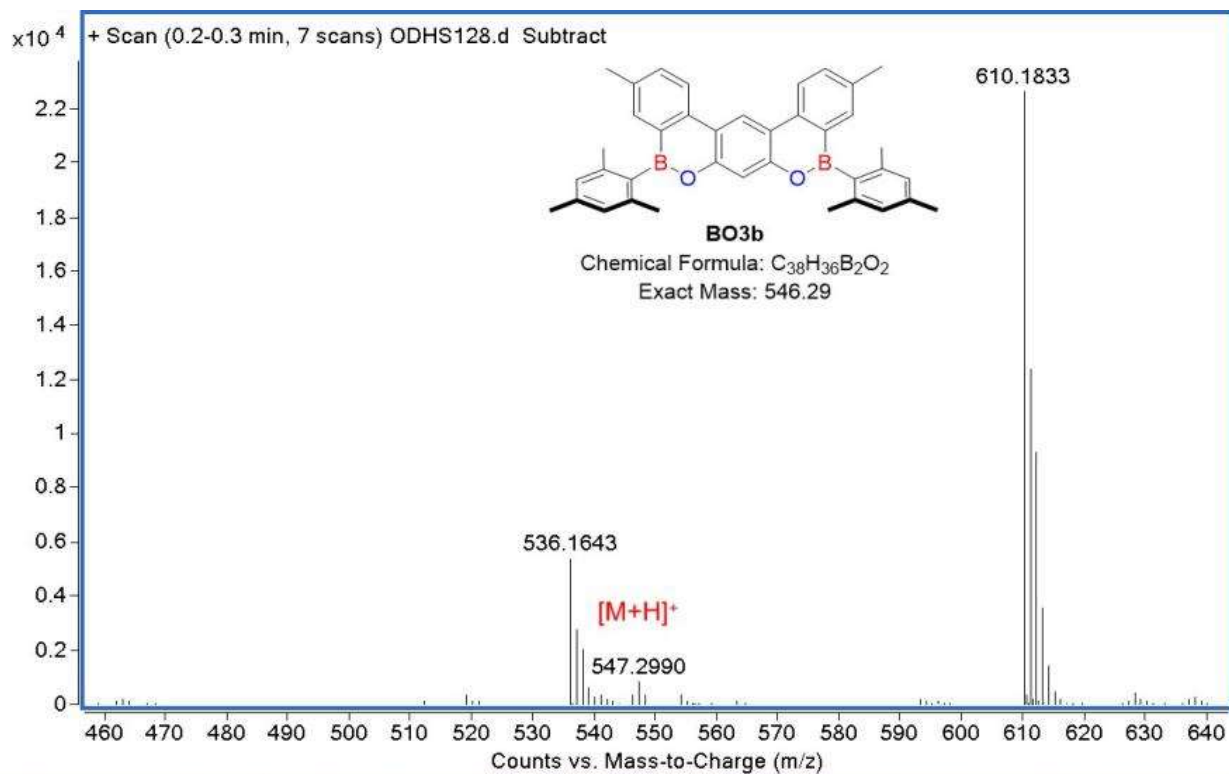
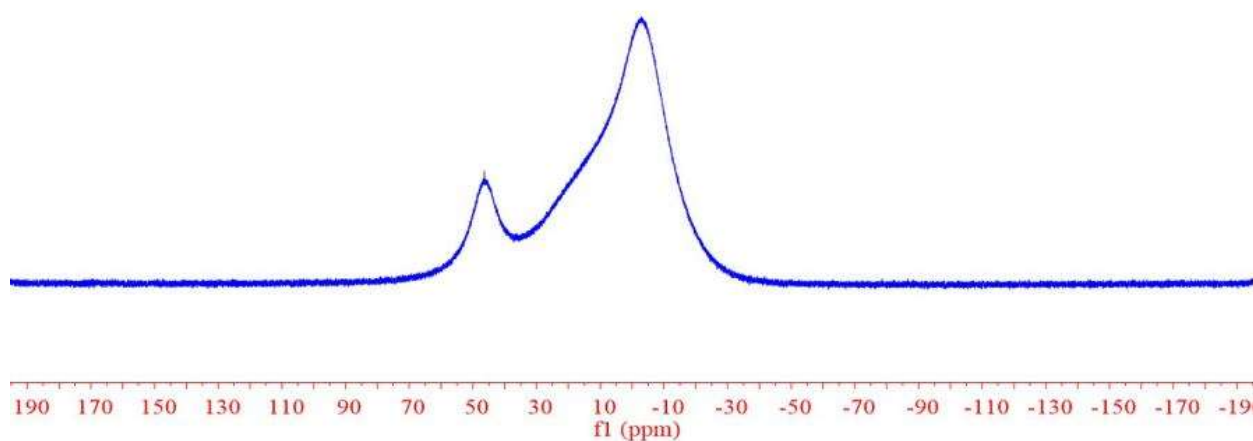


— 46.36

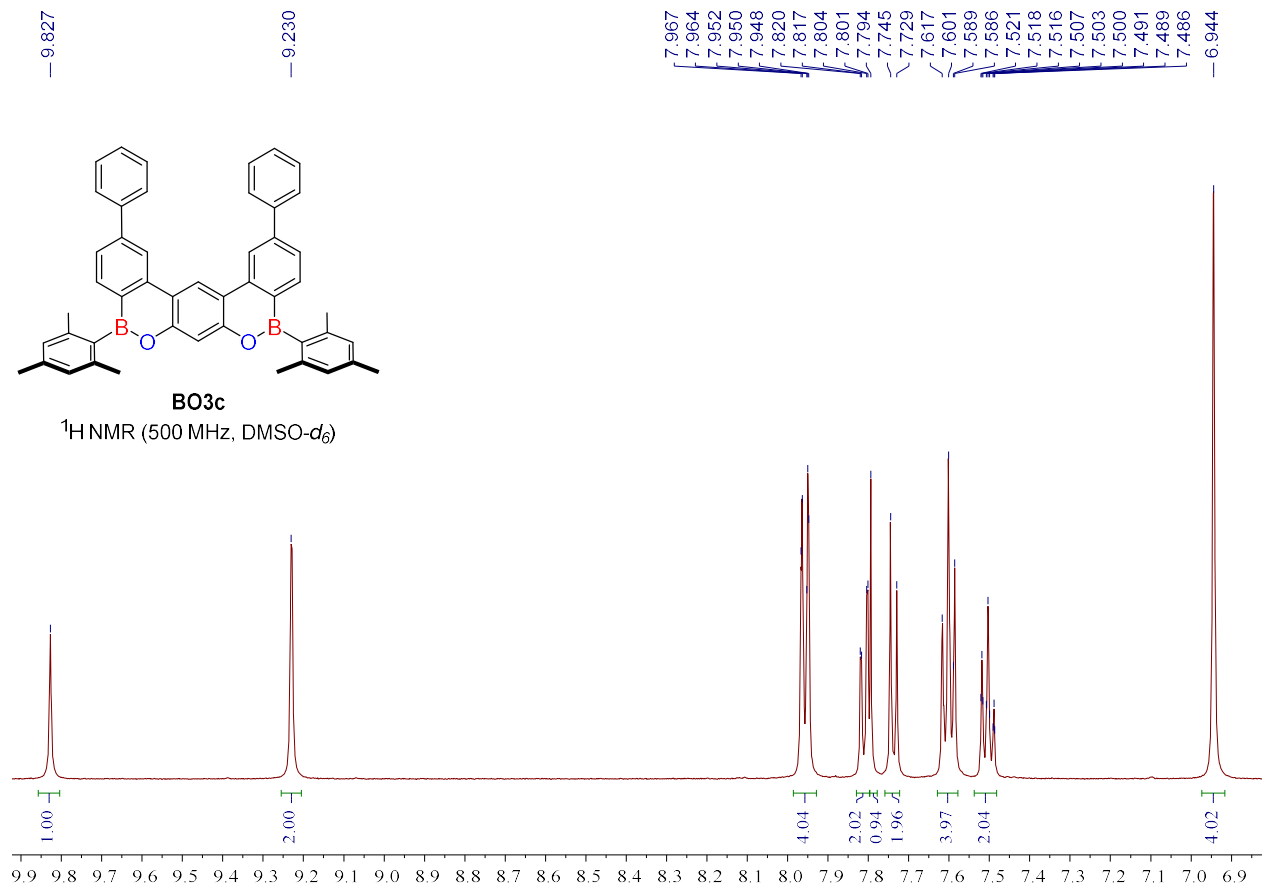
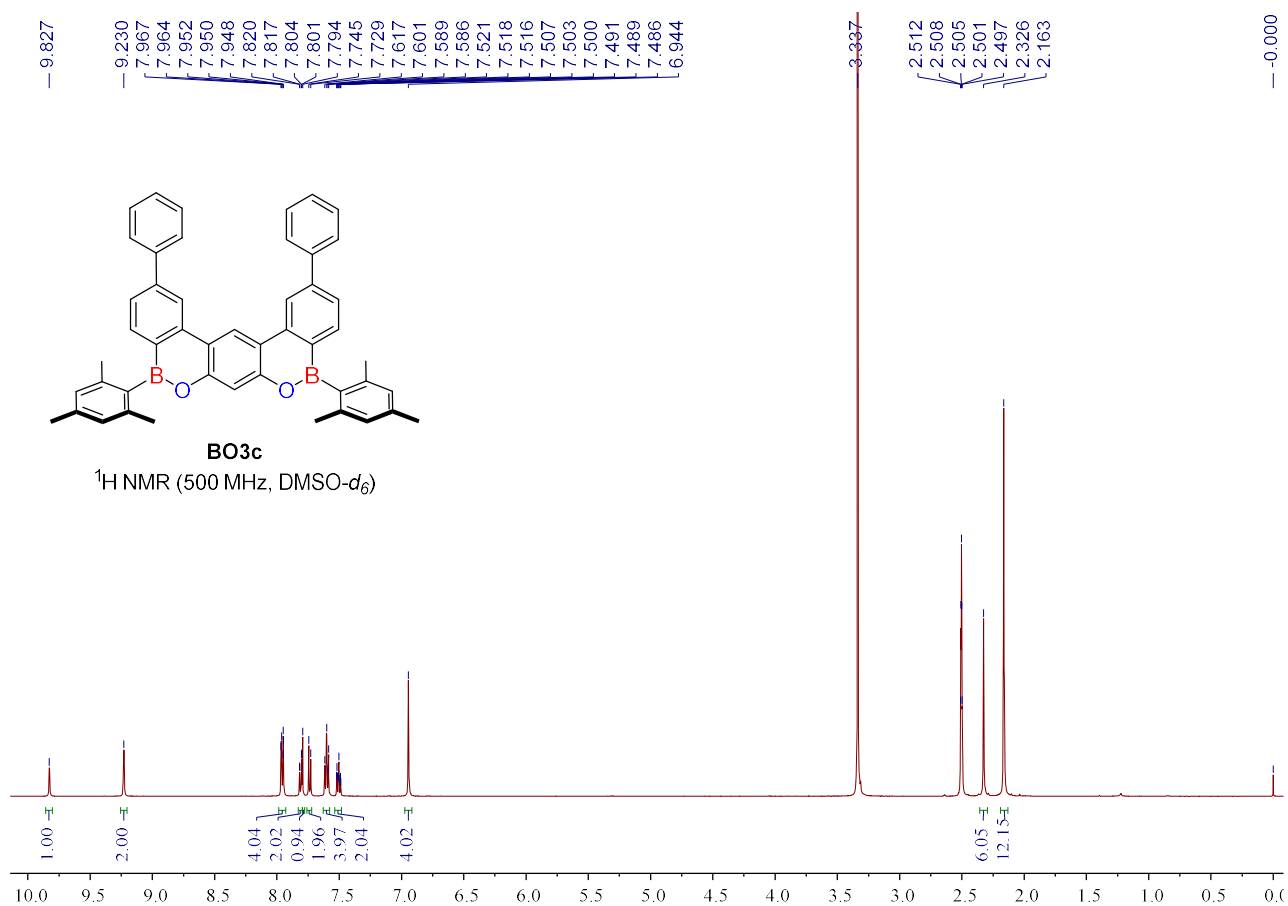


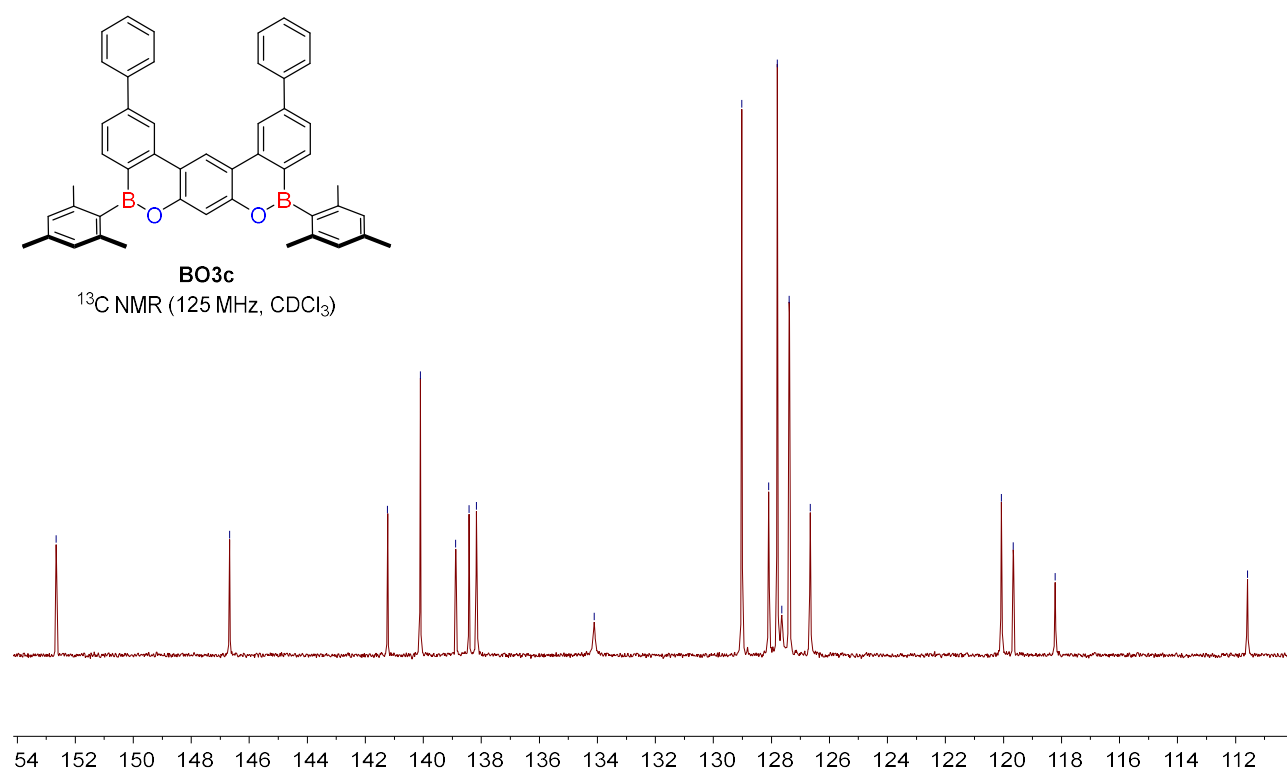
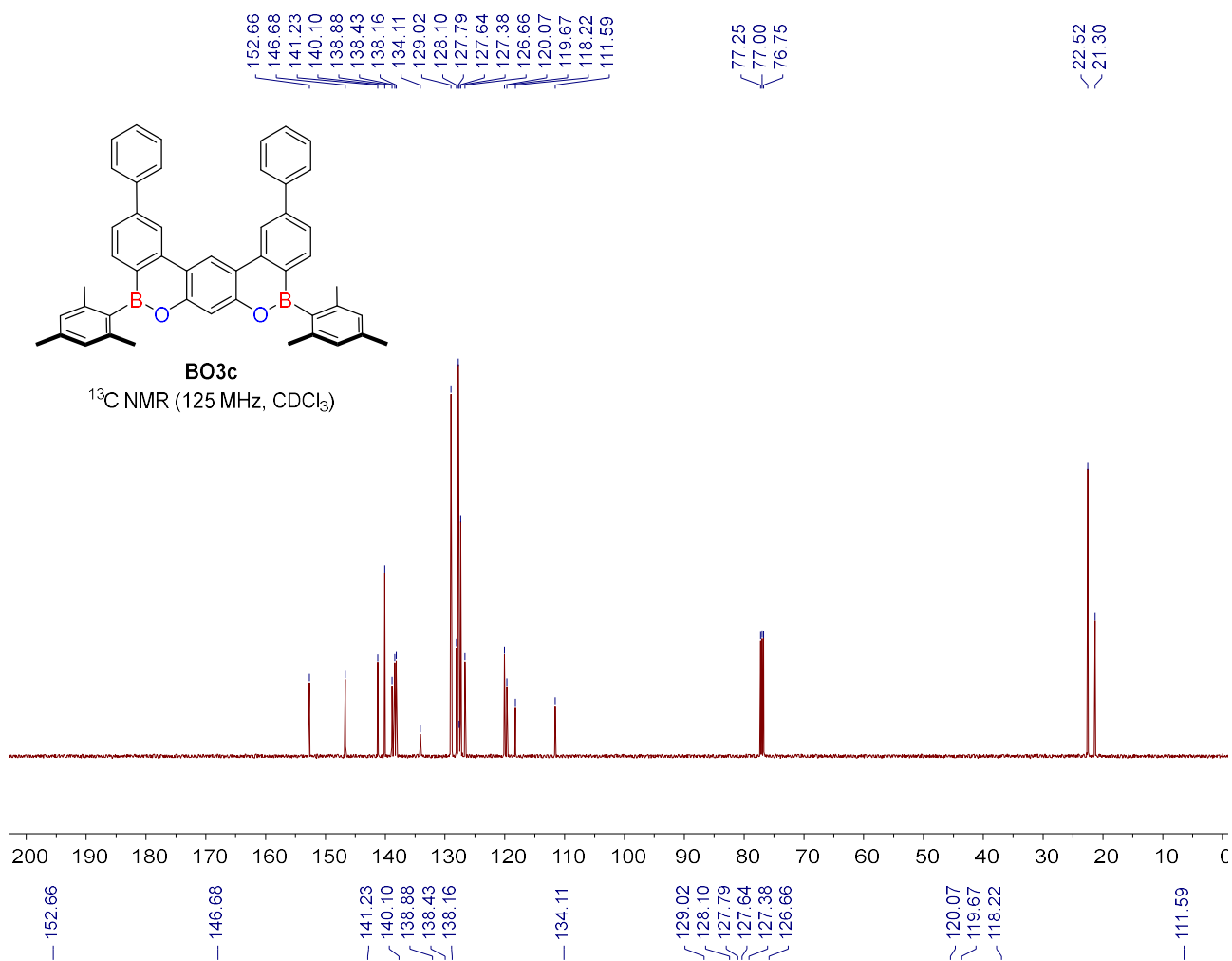
BO3b

^{11}B NMR (160 MHz, CDCl_3)

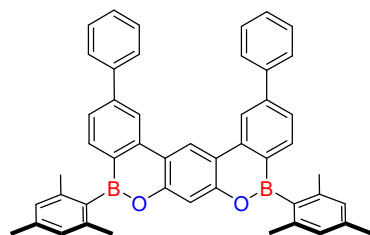


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$\text{C}_{38}\text{H}_{36}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{38}\text{H}_{37}[^{11}\text{B}]_2\text{O}_2$	547.299	547.2974	-2.9	22



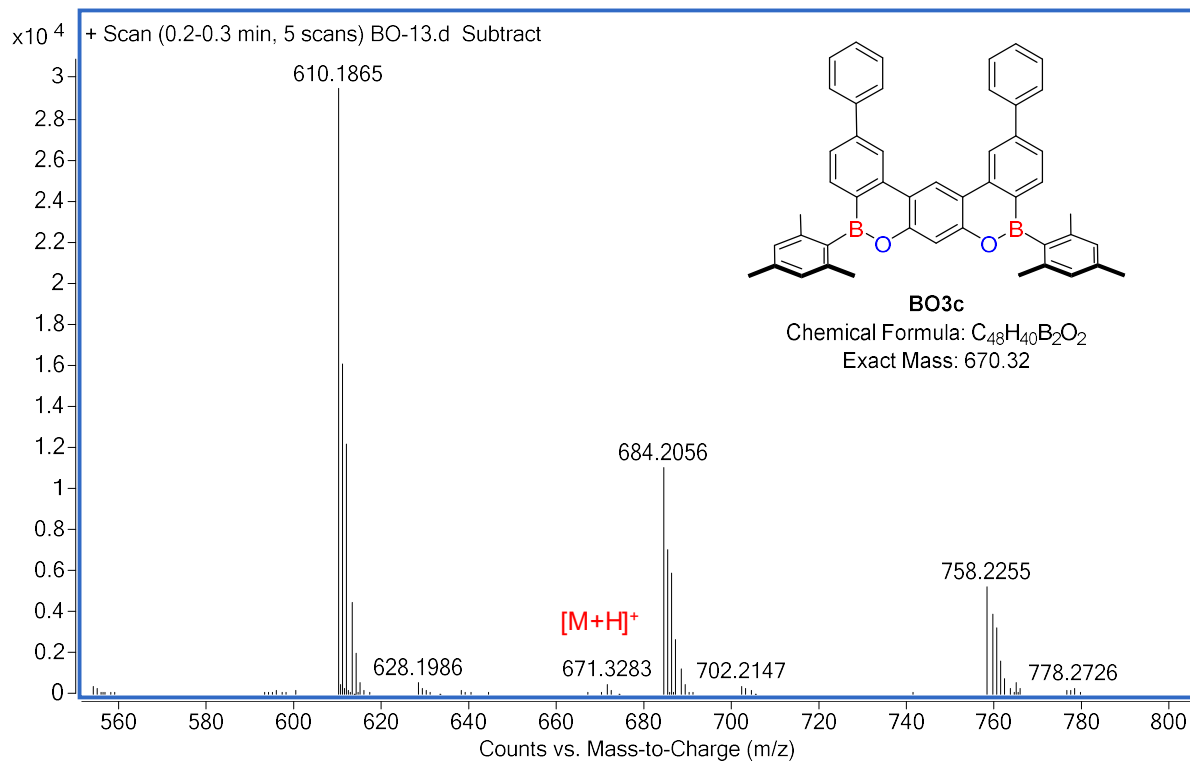
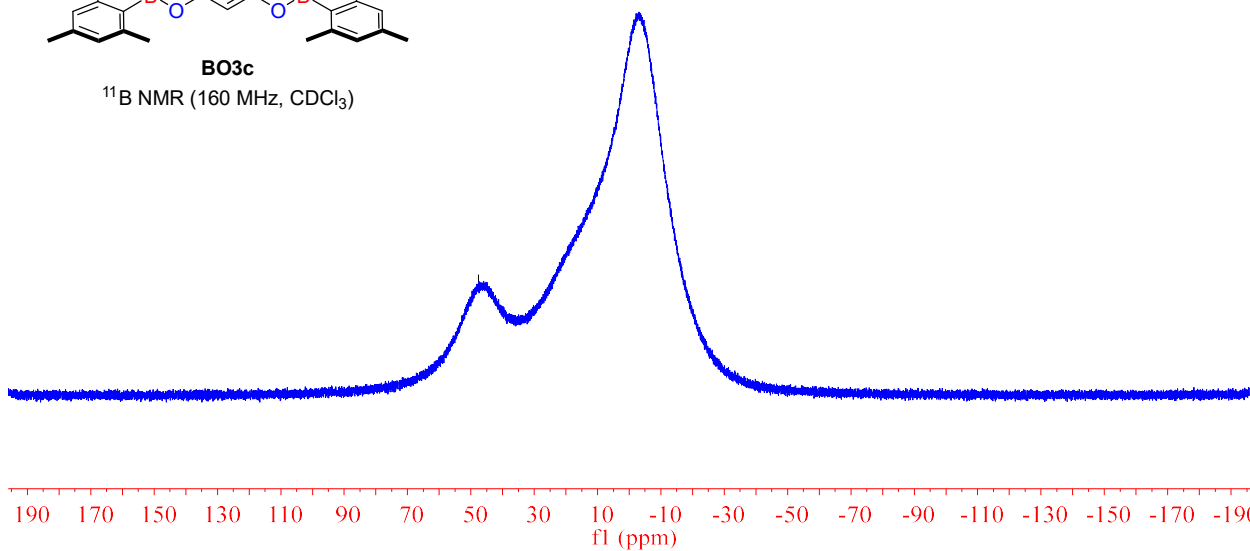


— 47.62

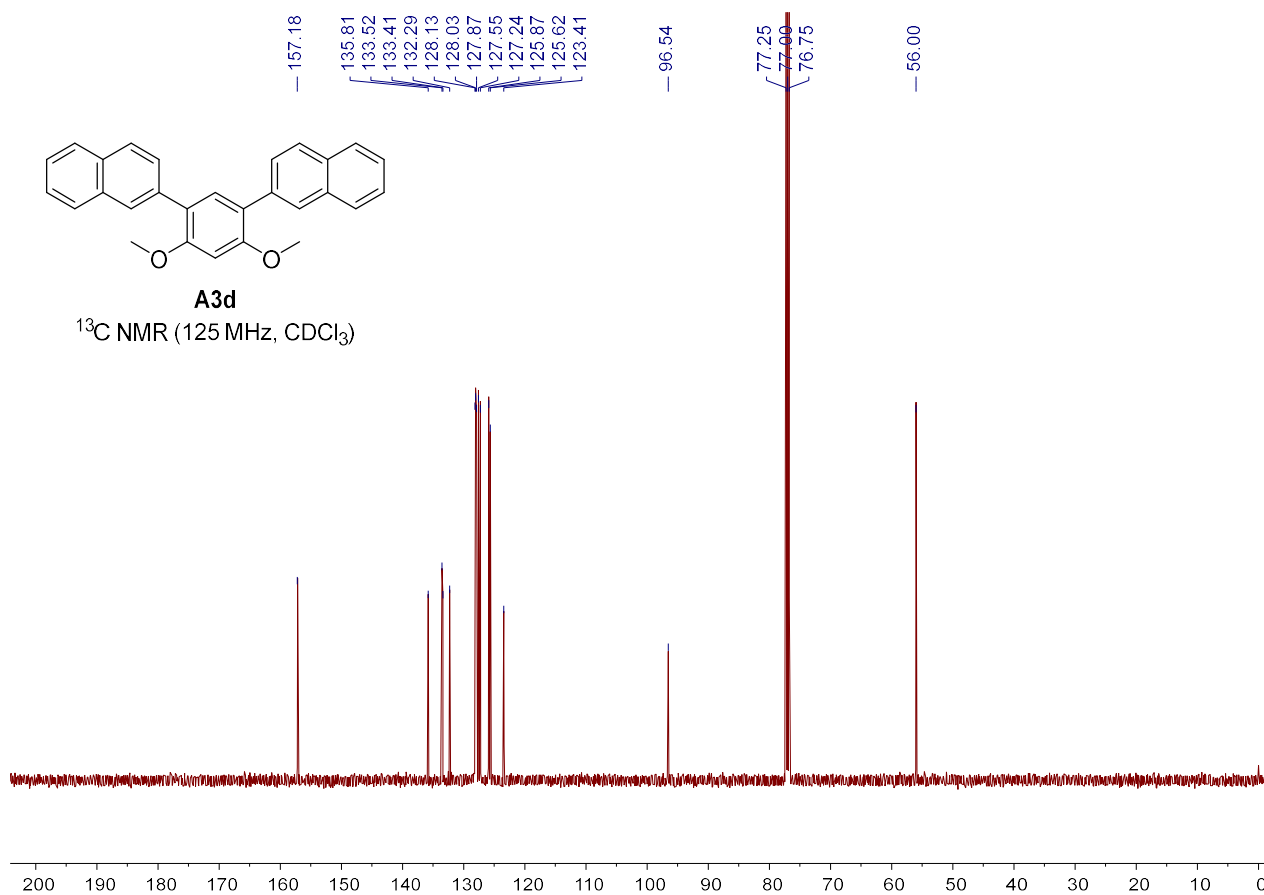
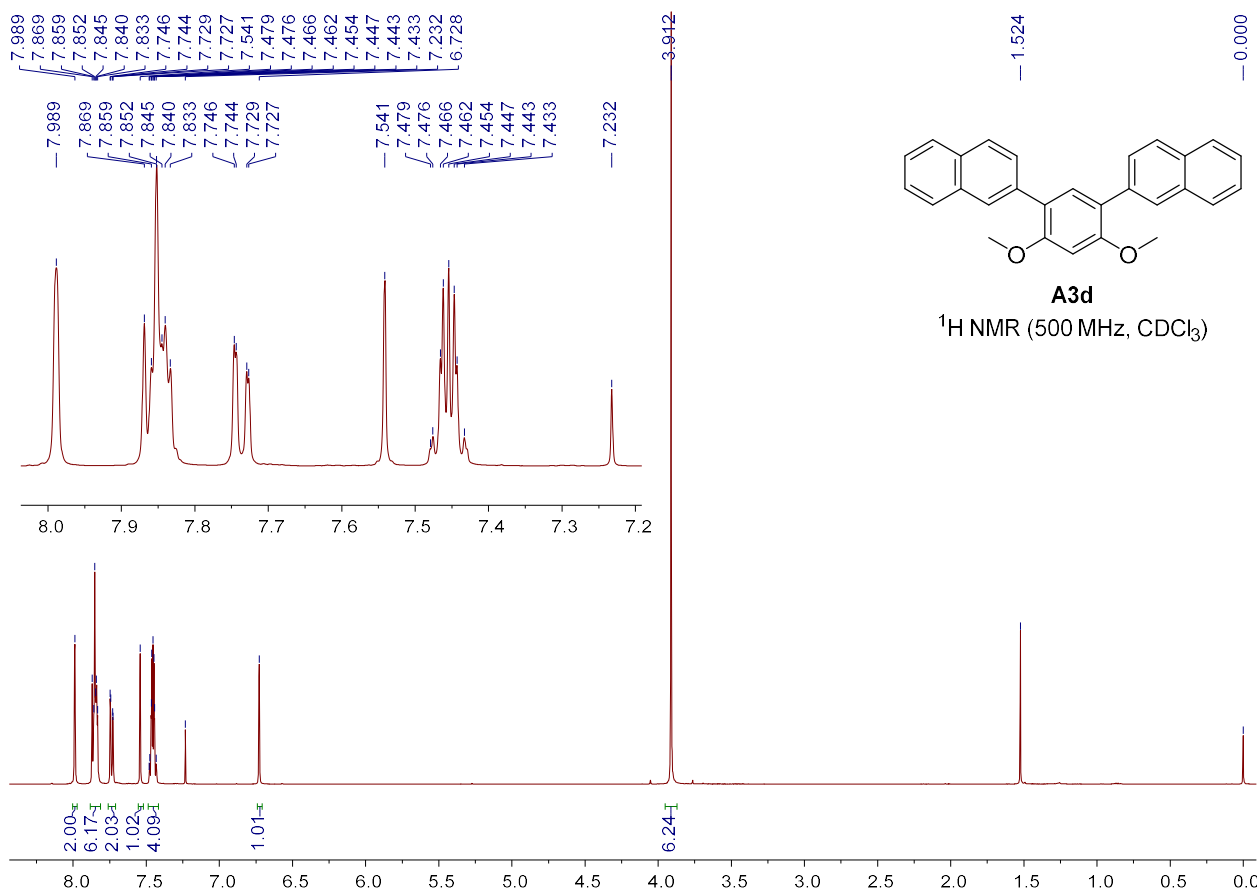


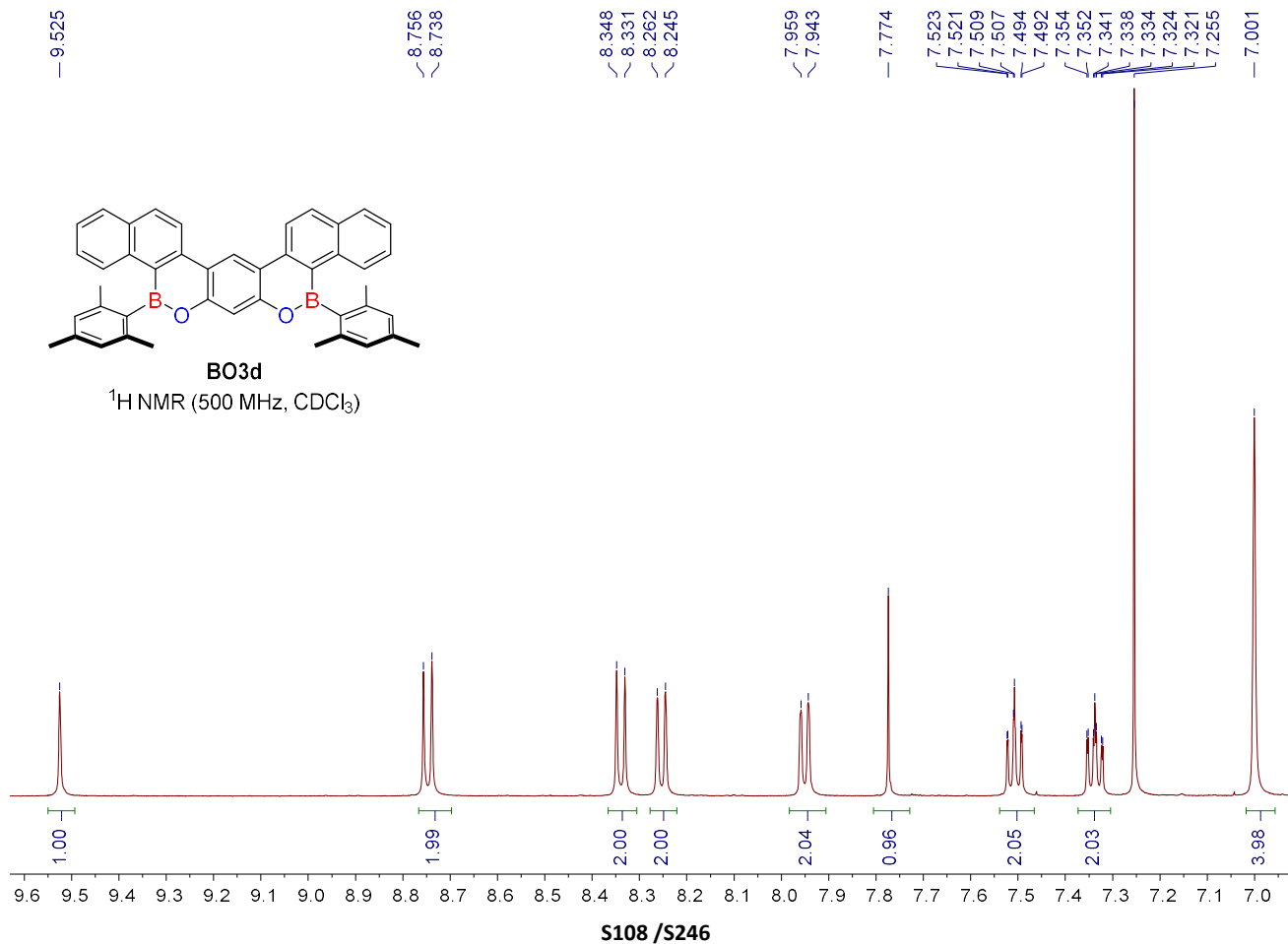
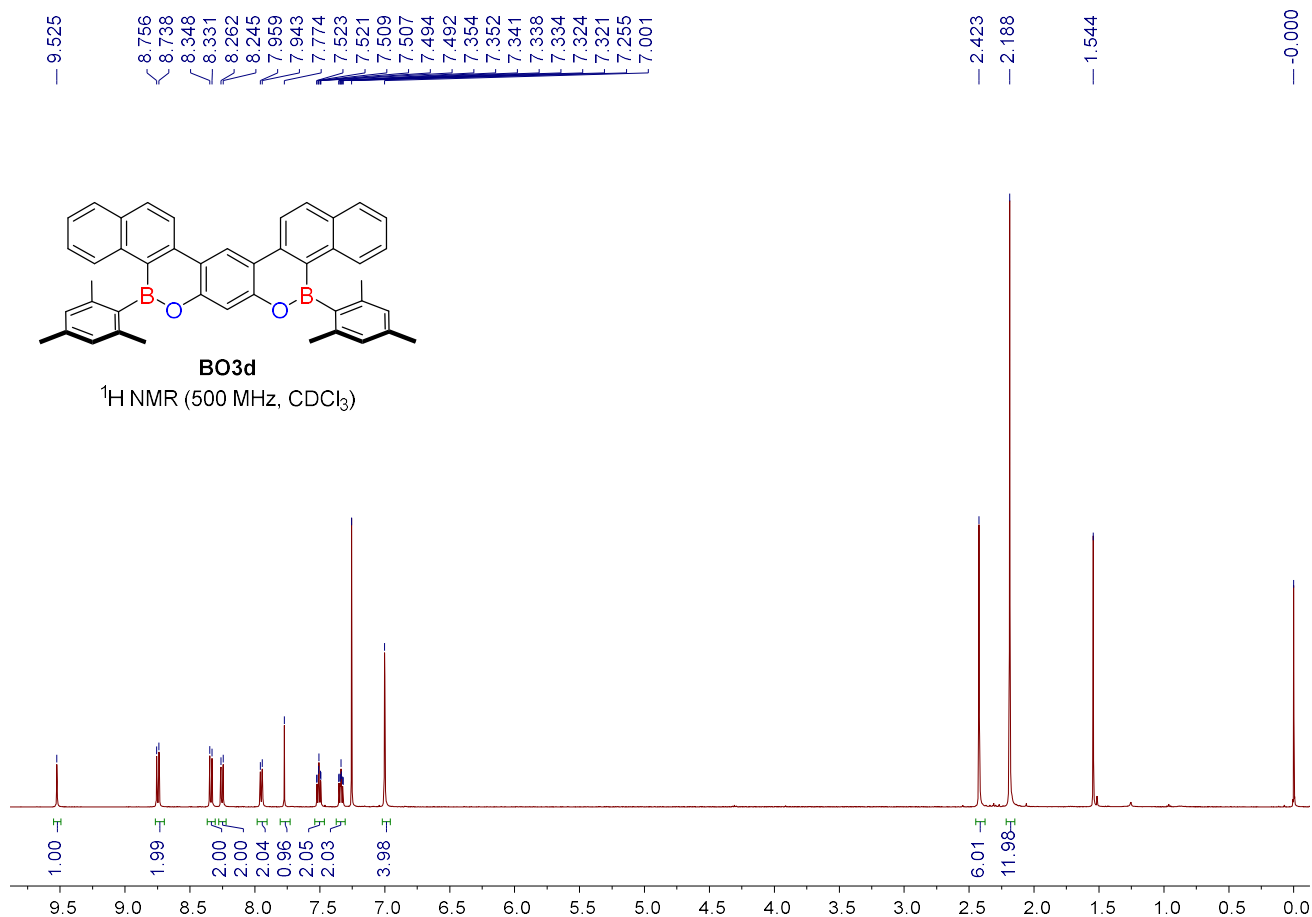
BO3c

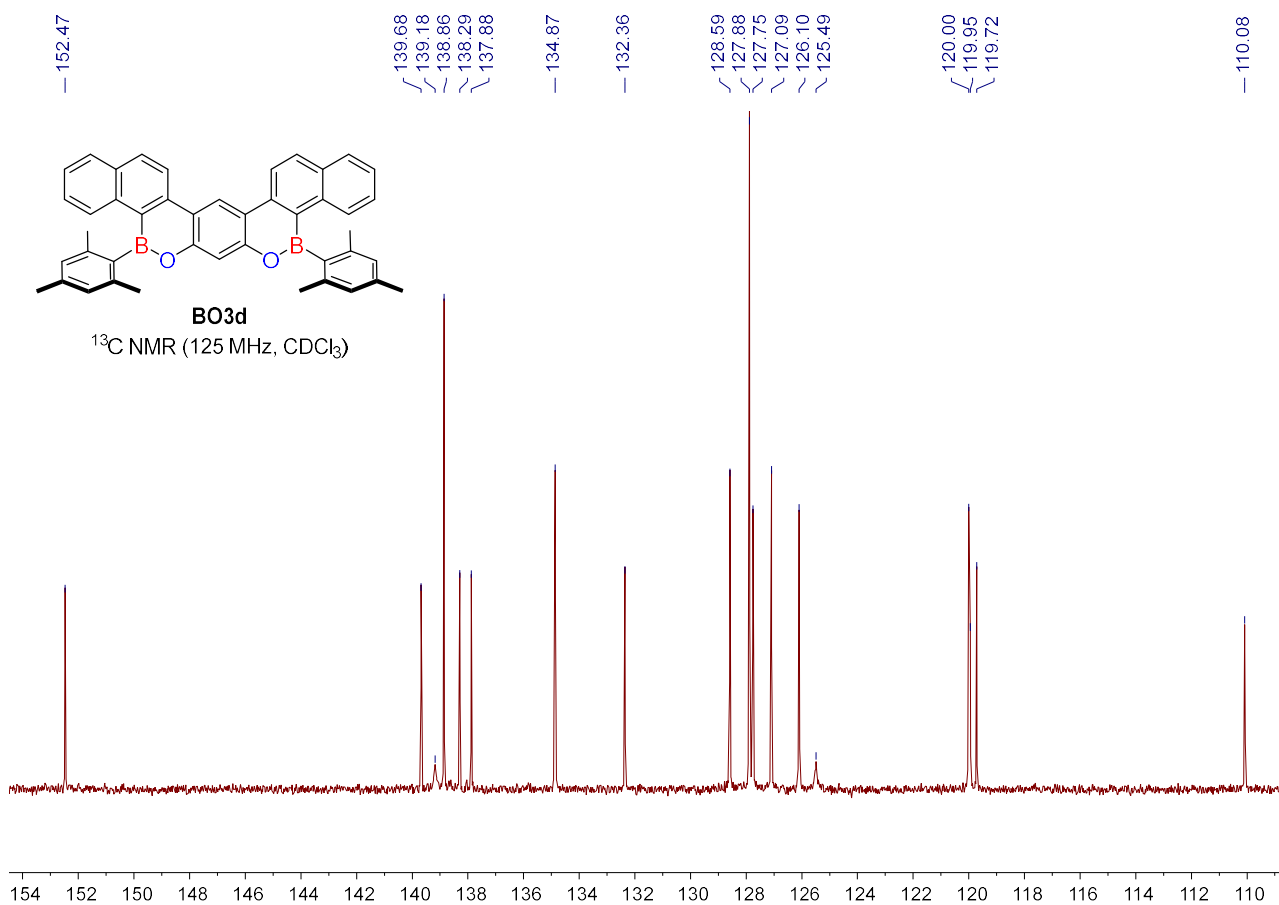
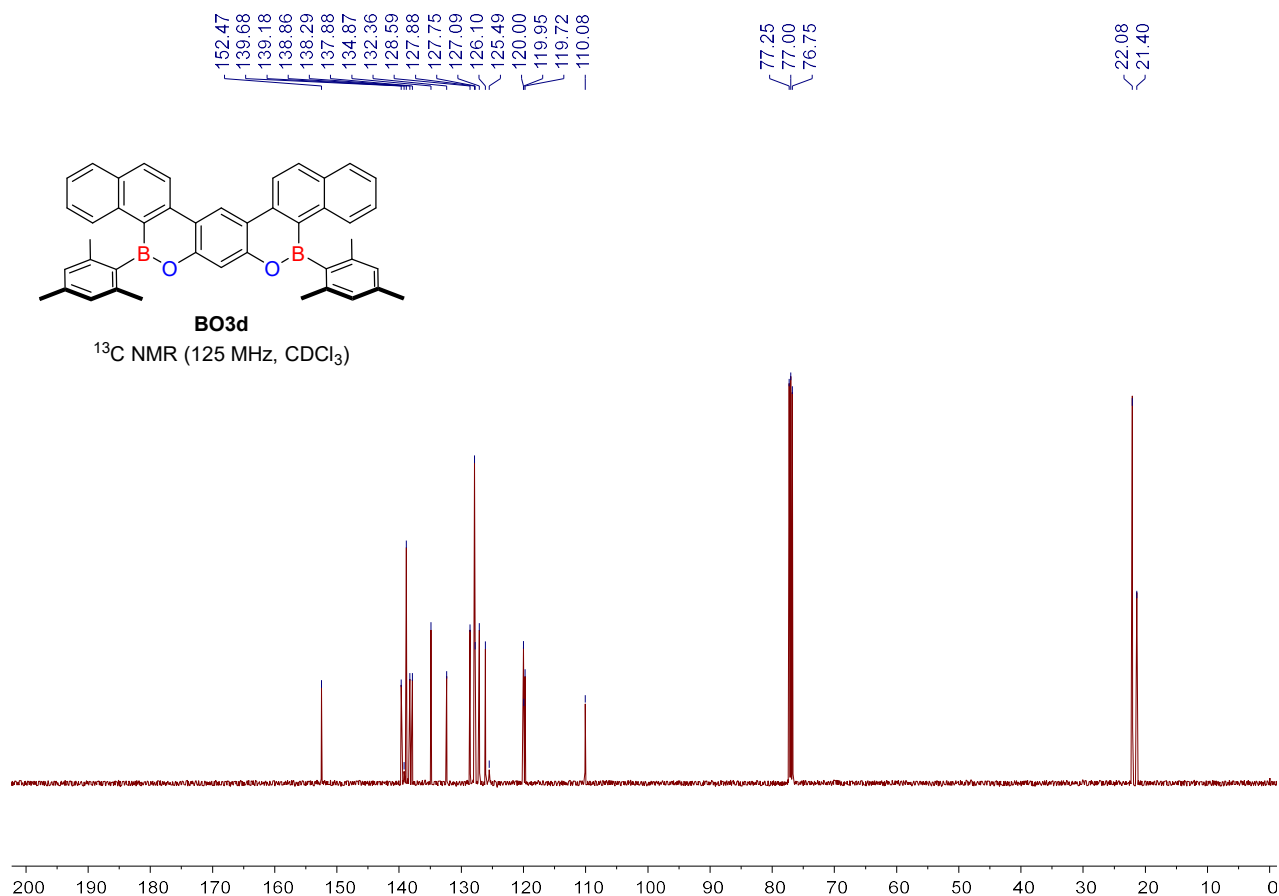
^{11}B NMR (160 MHz, CDCl_3)



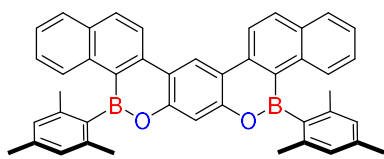
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$\text{C}_{48}\text{H}_{40}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{48}\text{H}_{41}[^{11}\text{B}]_2\text{O}_2$	671.3283	671.3287	0.62	30





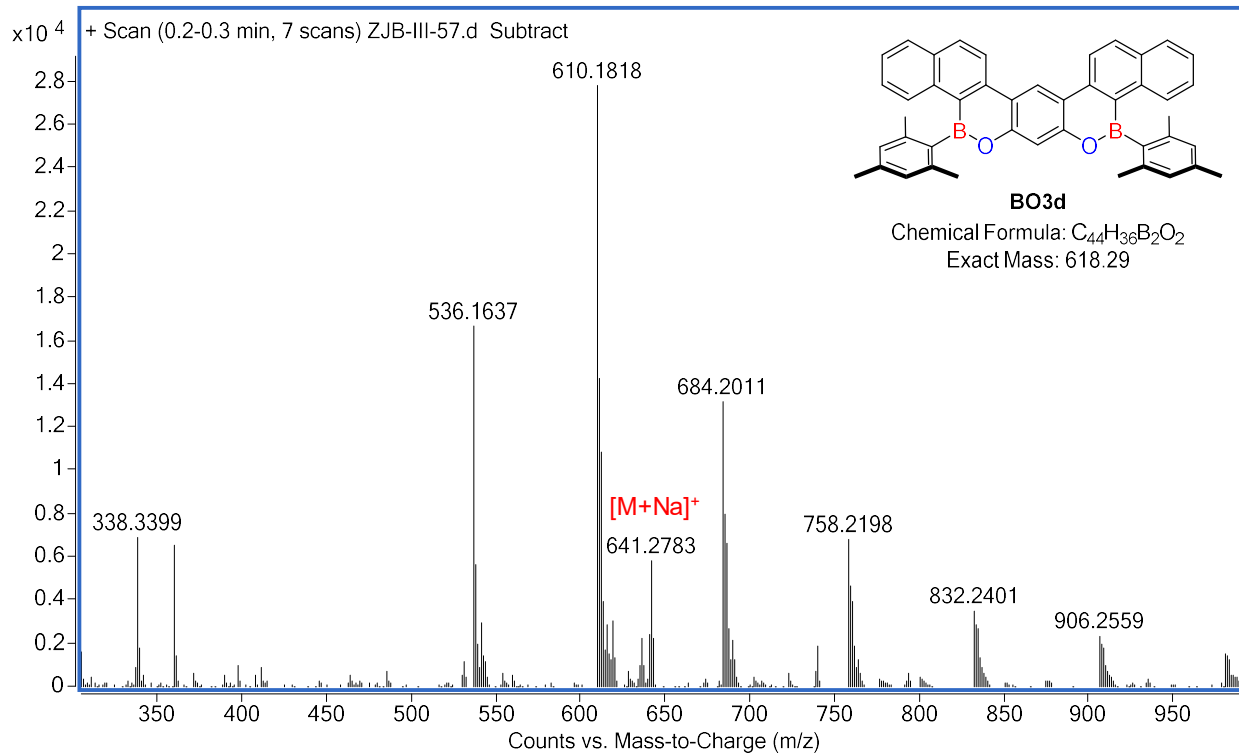
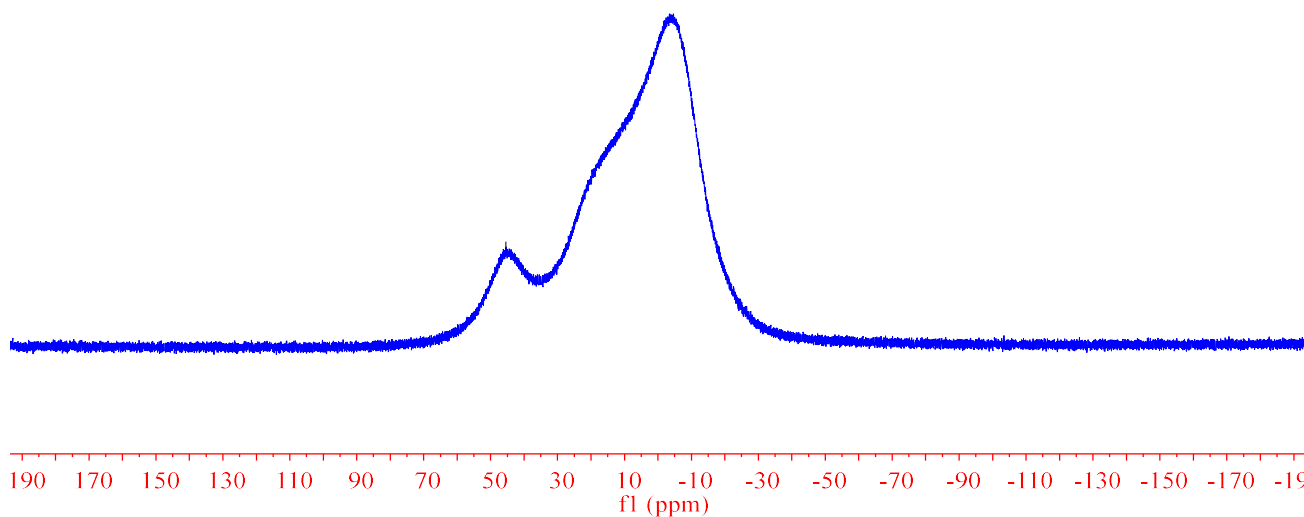


-45.48

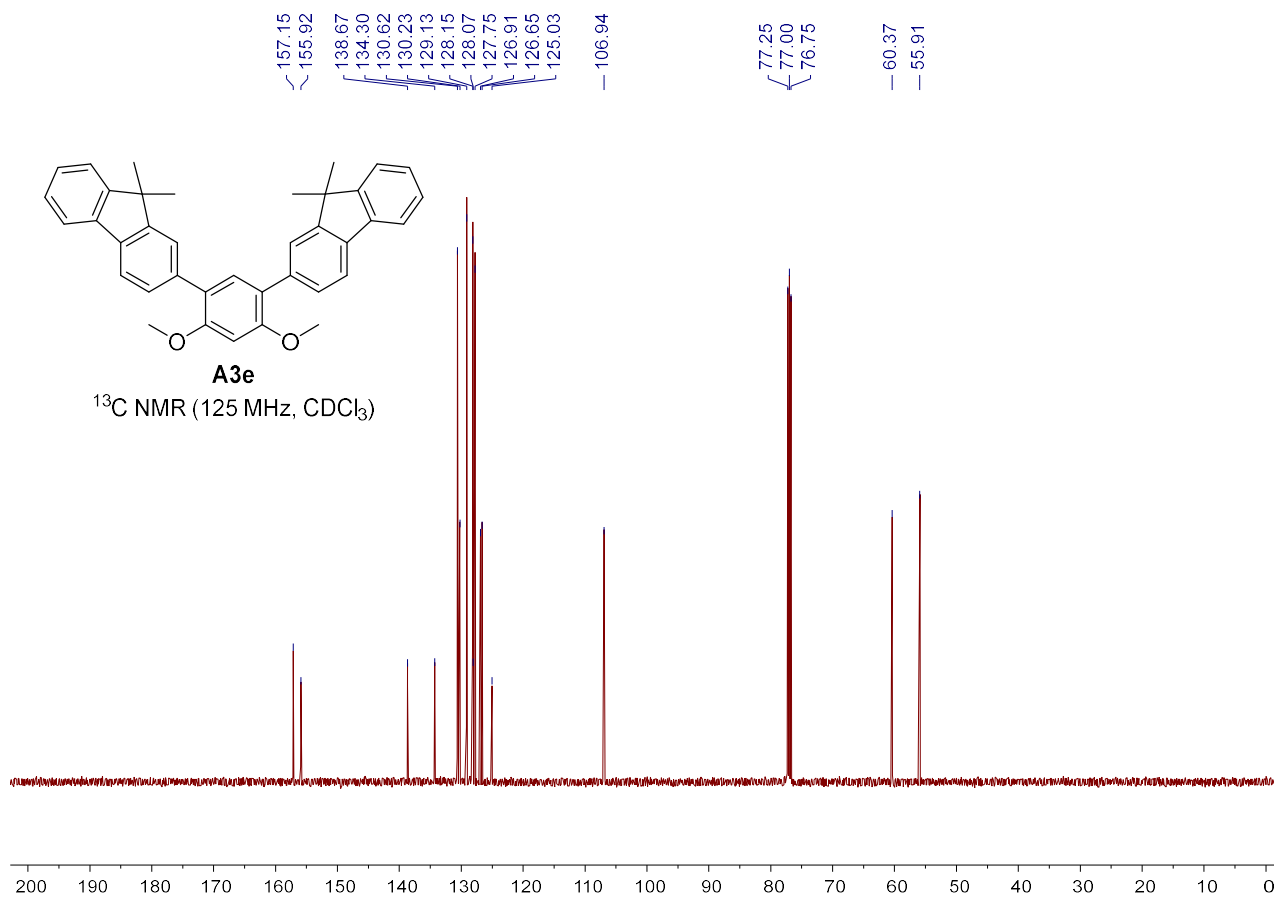
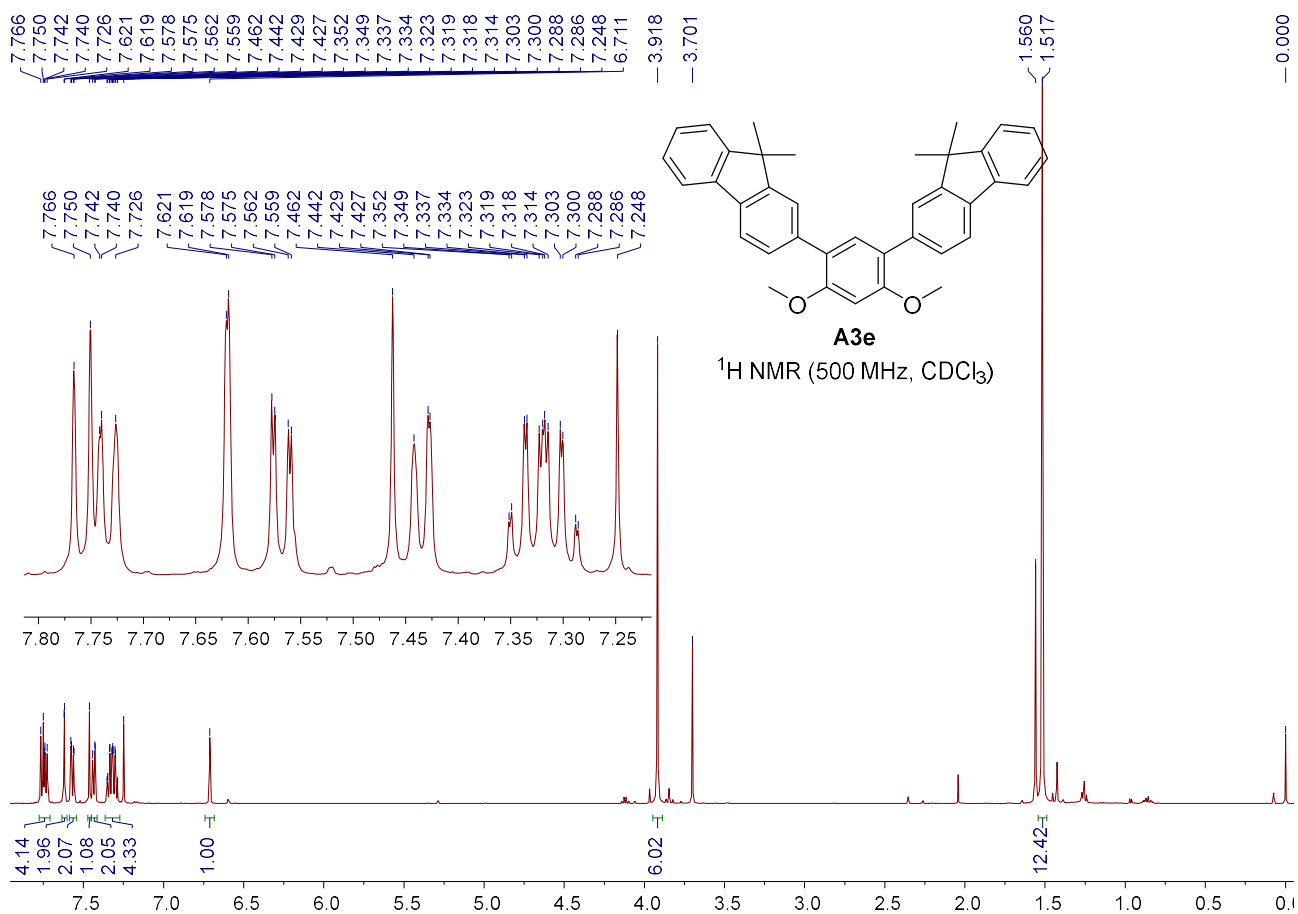


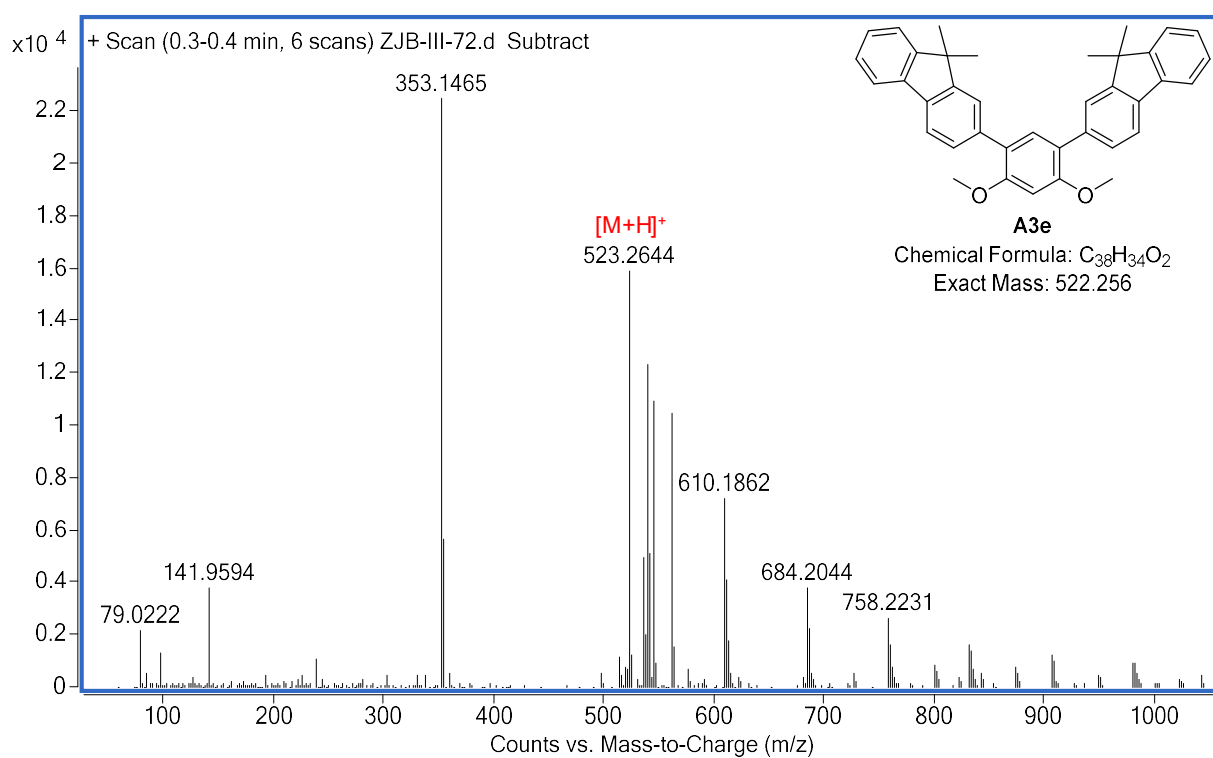
BO3d

^{11}B NMR (160 MHz, CDCl_3)

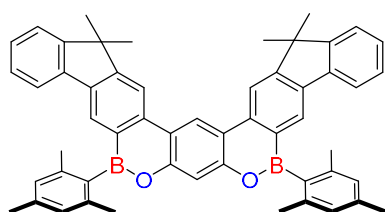


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{NaO}_2$	641.2783	641.2794	1.72



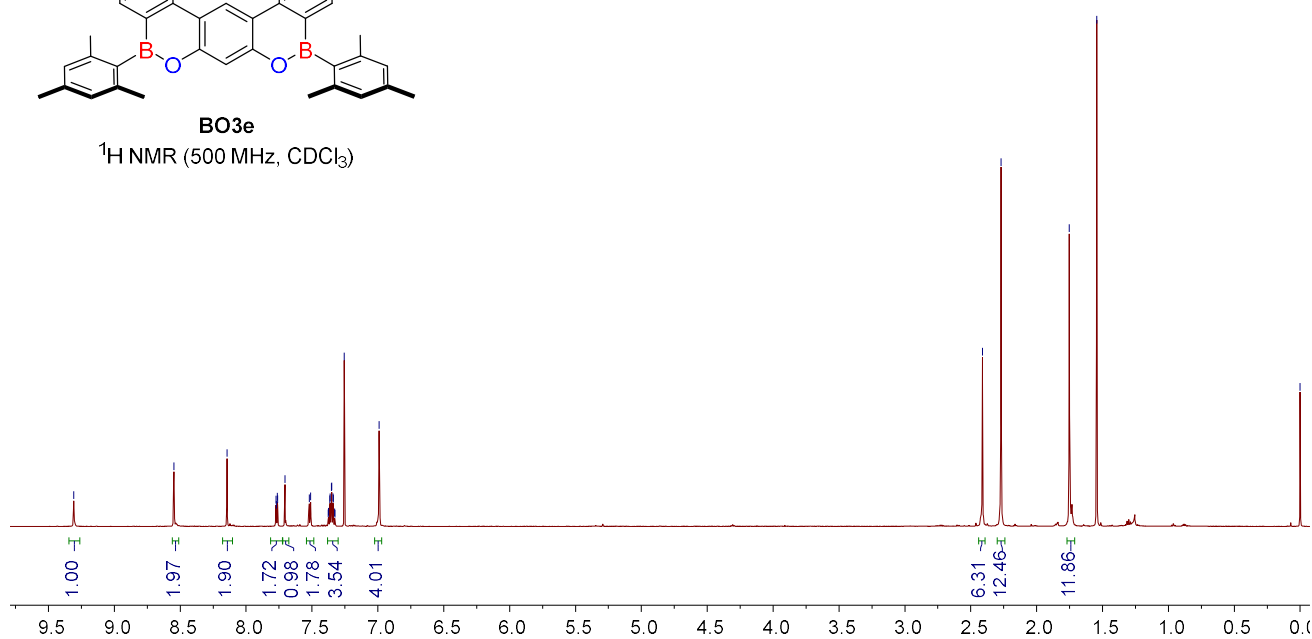


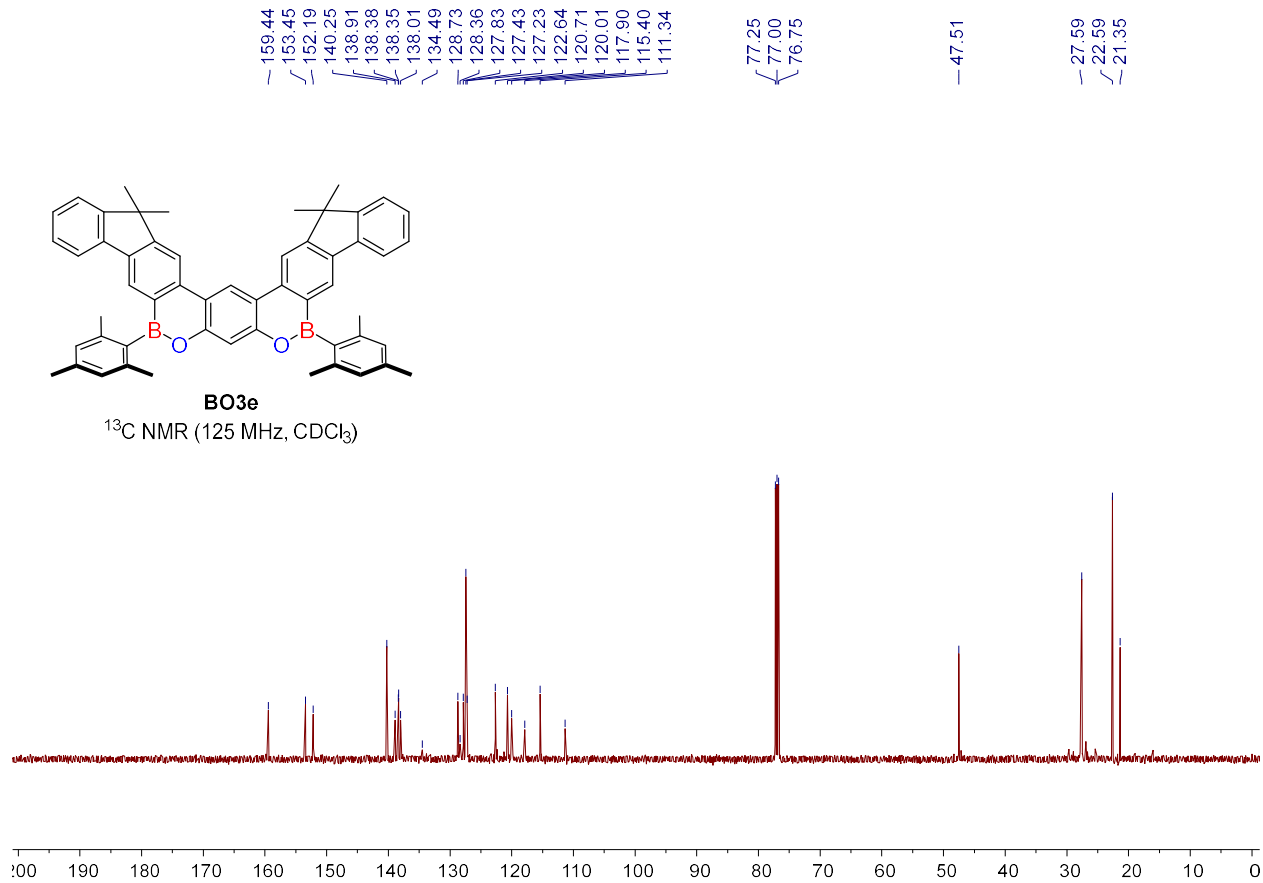
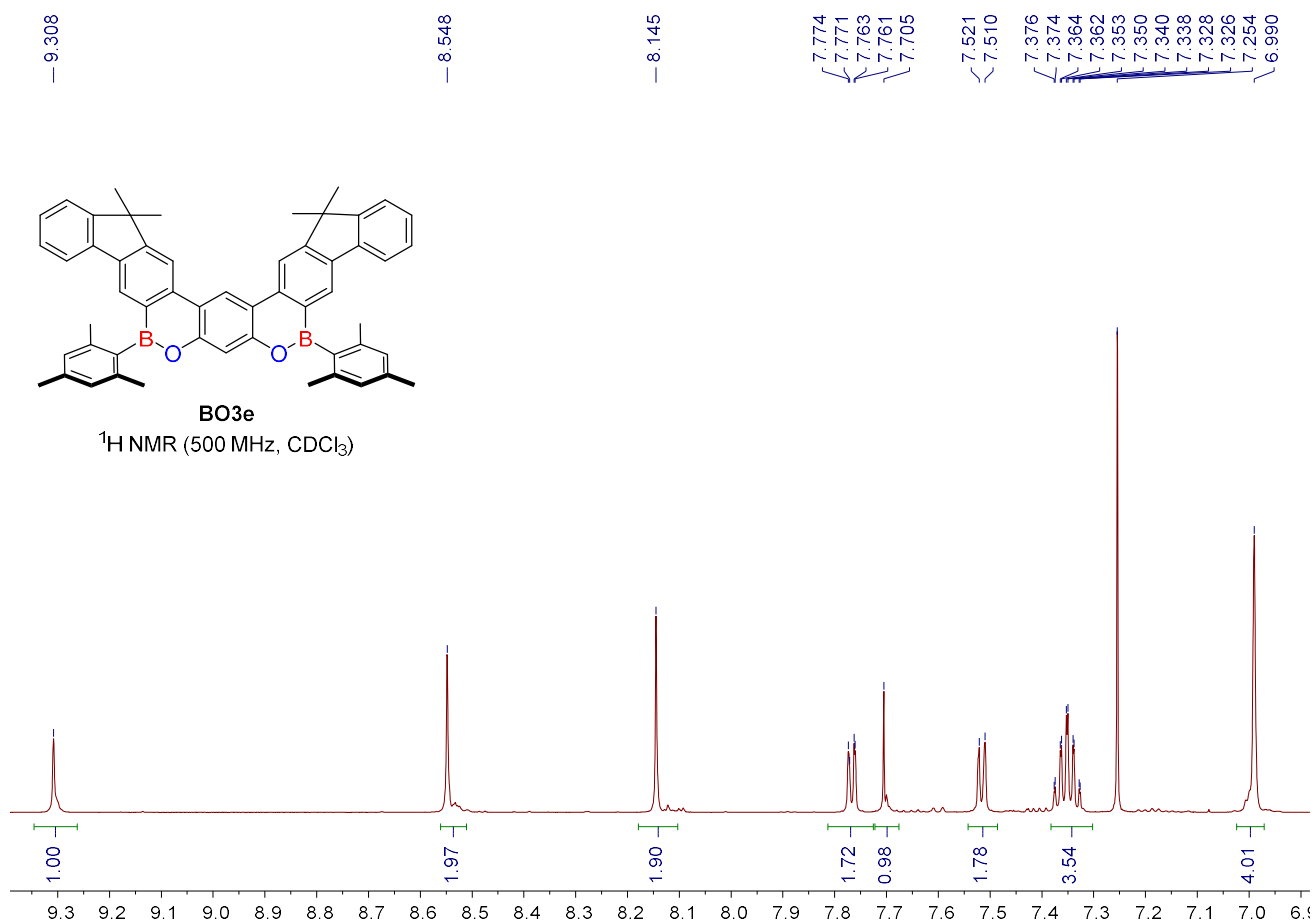
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$C_{38}H_{34}O_2$	$C_{38}H_{35}O_2$	523.2644	523.2632	-2.38	22

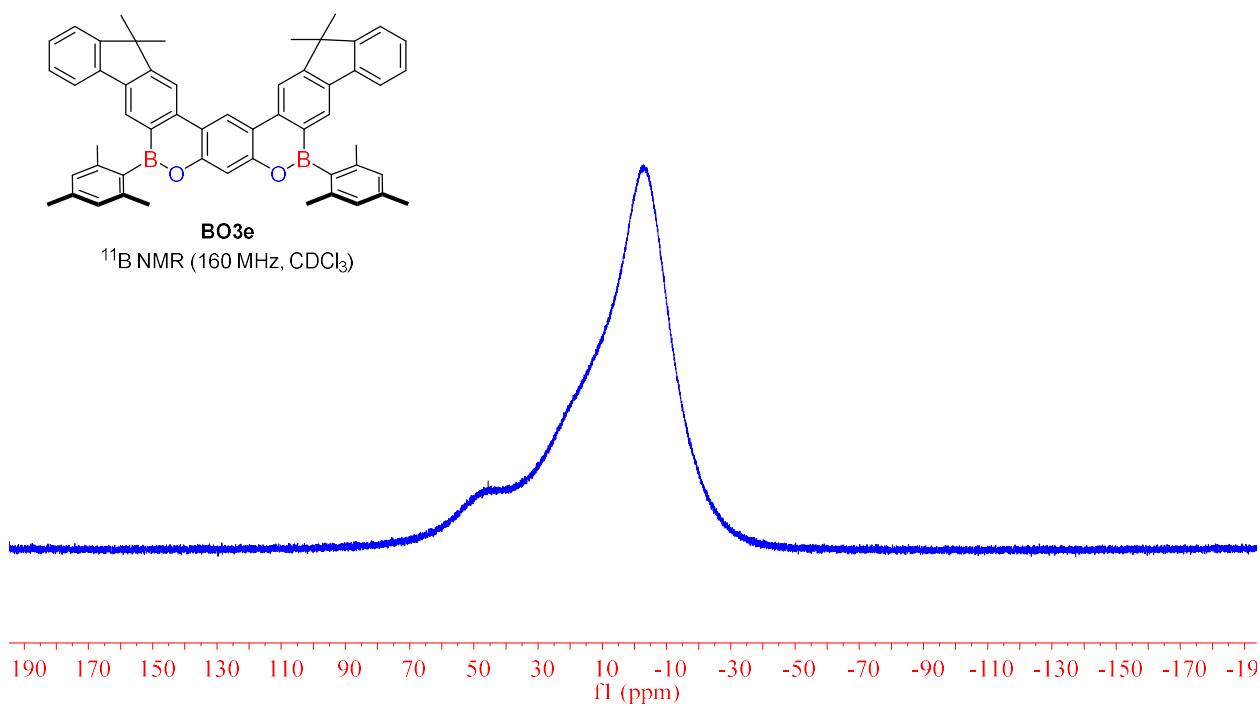
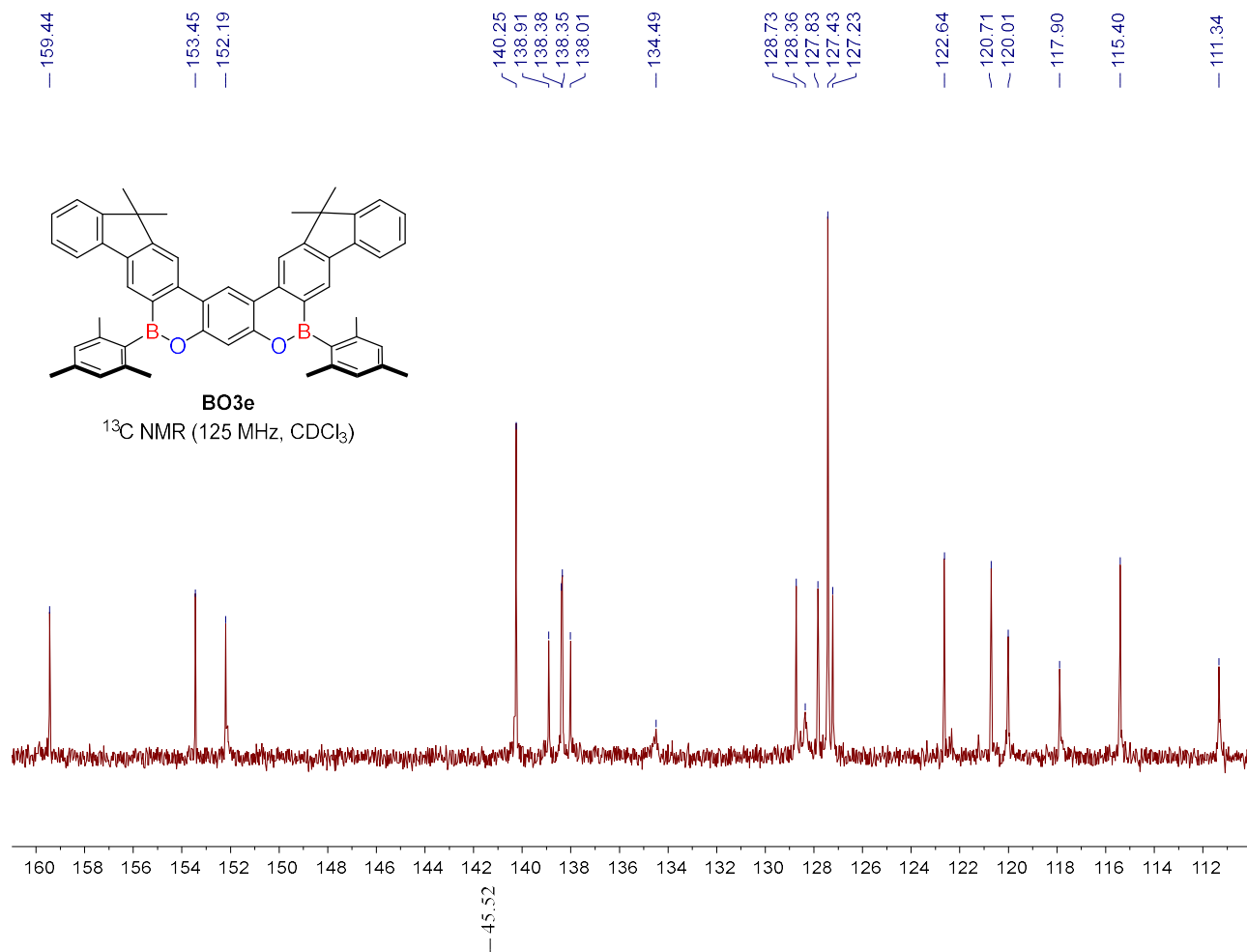


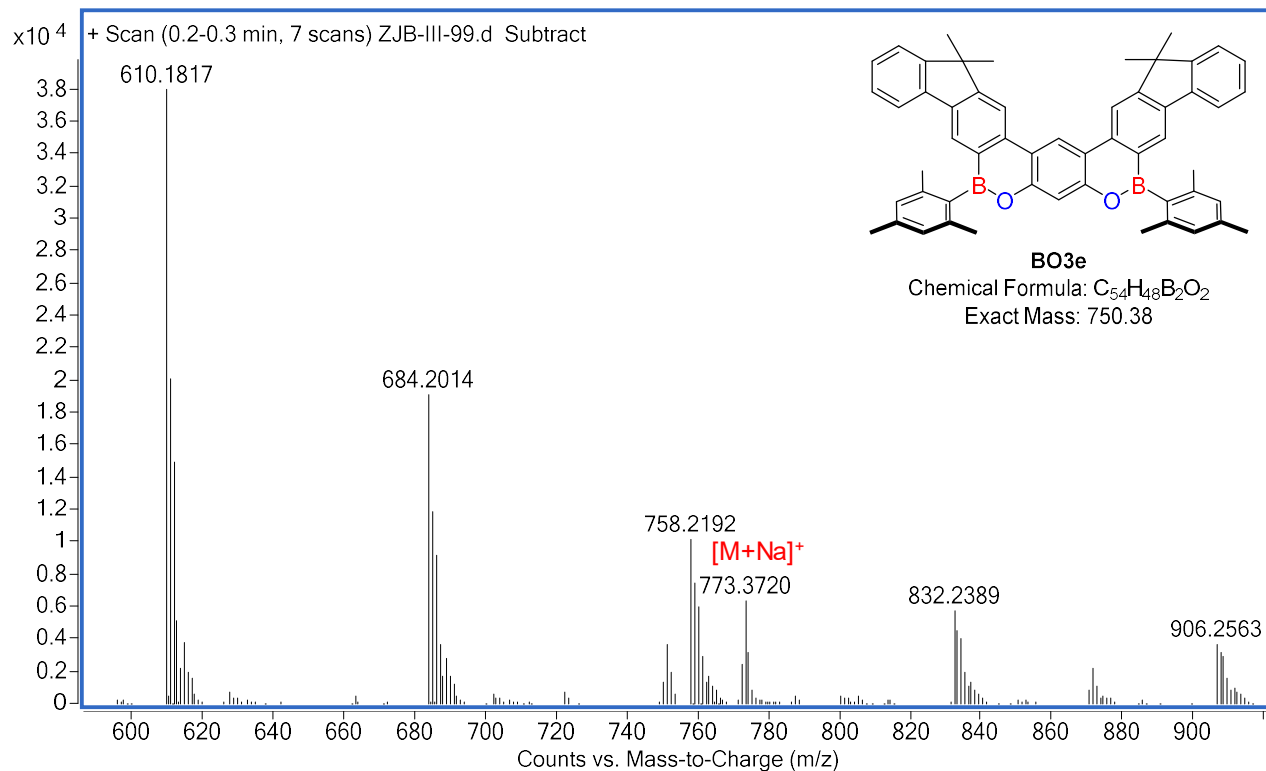
BO3e

1H NMR (500 MHz, $CDCl_3$)

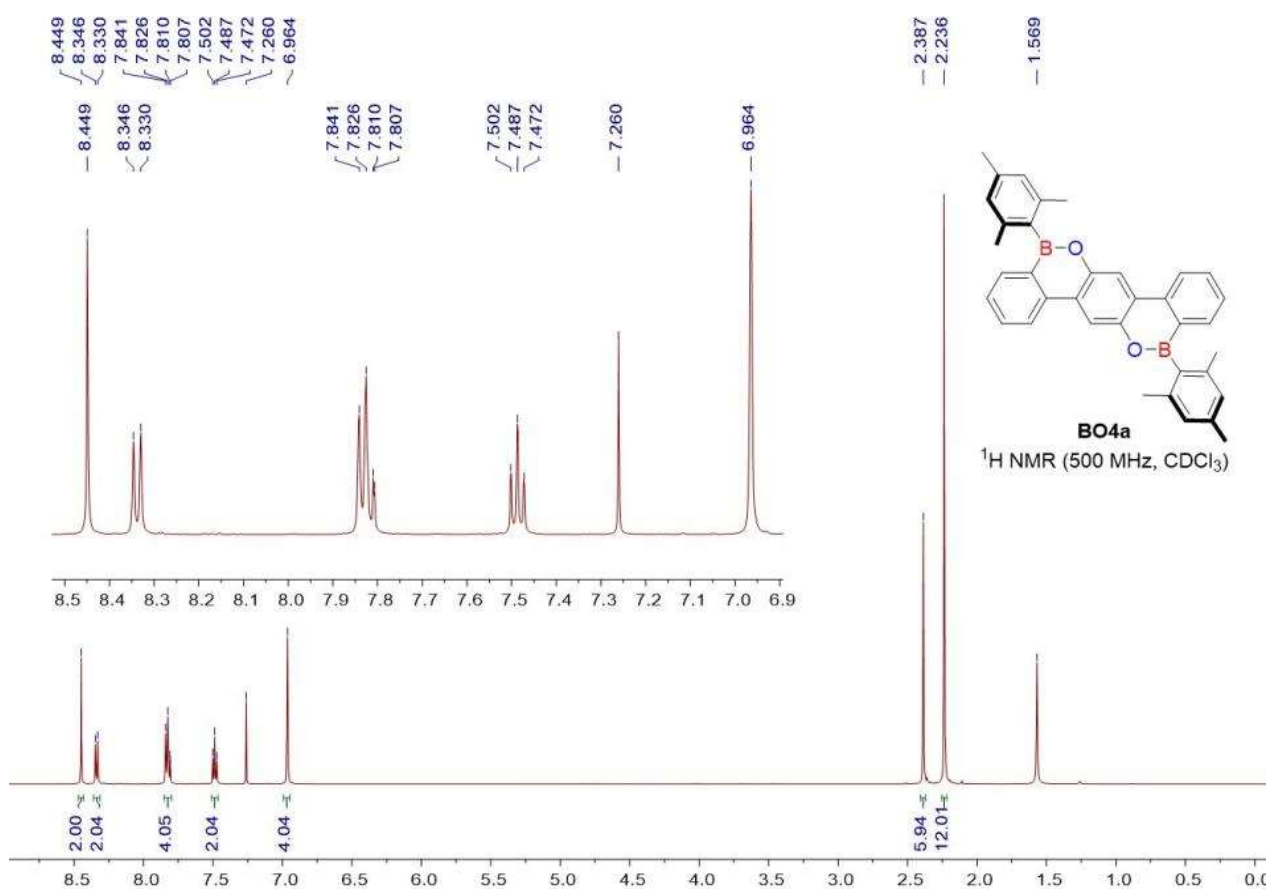


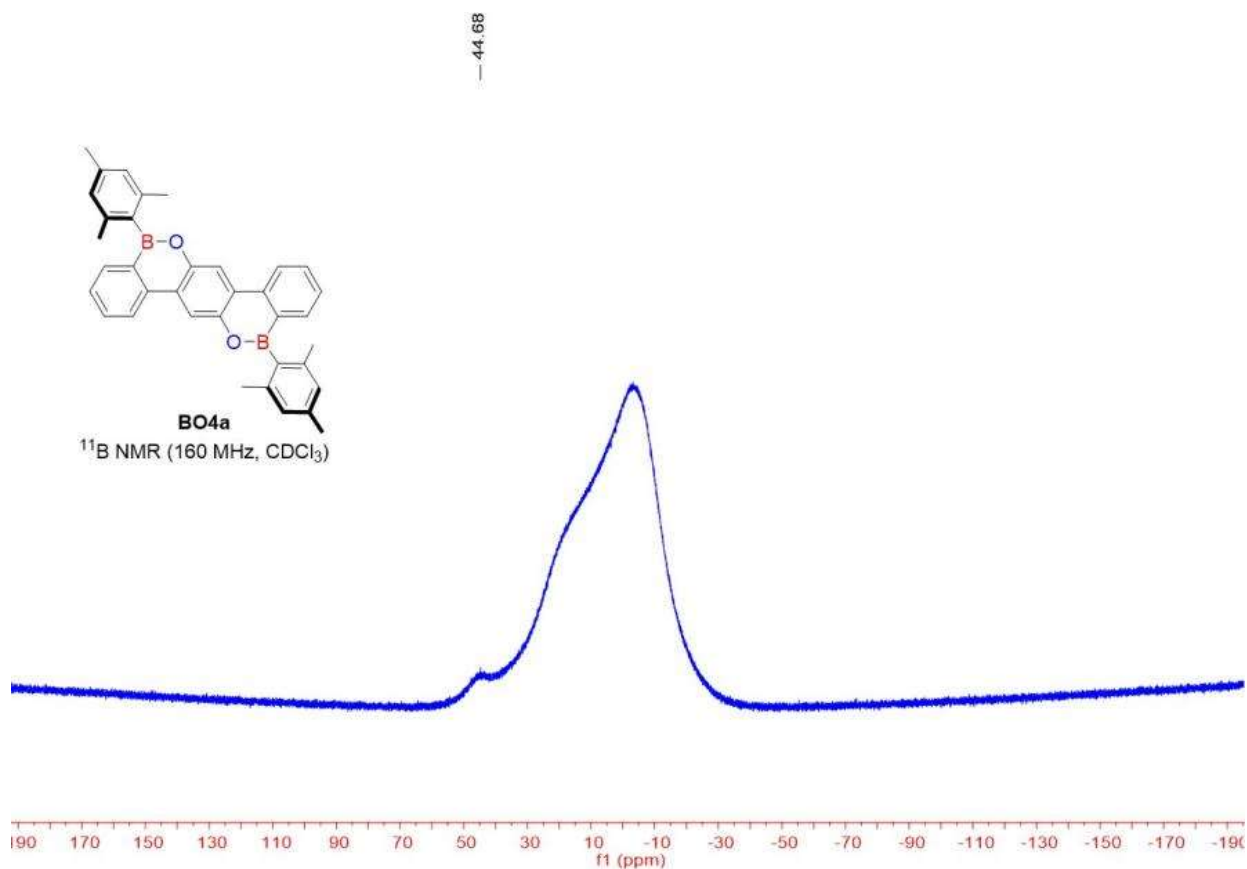
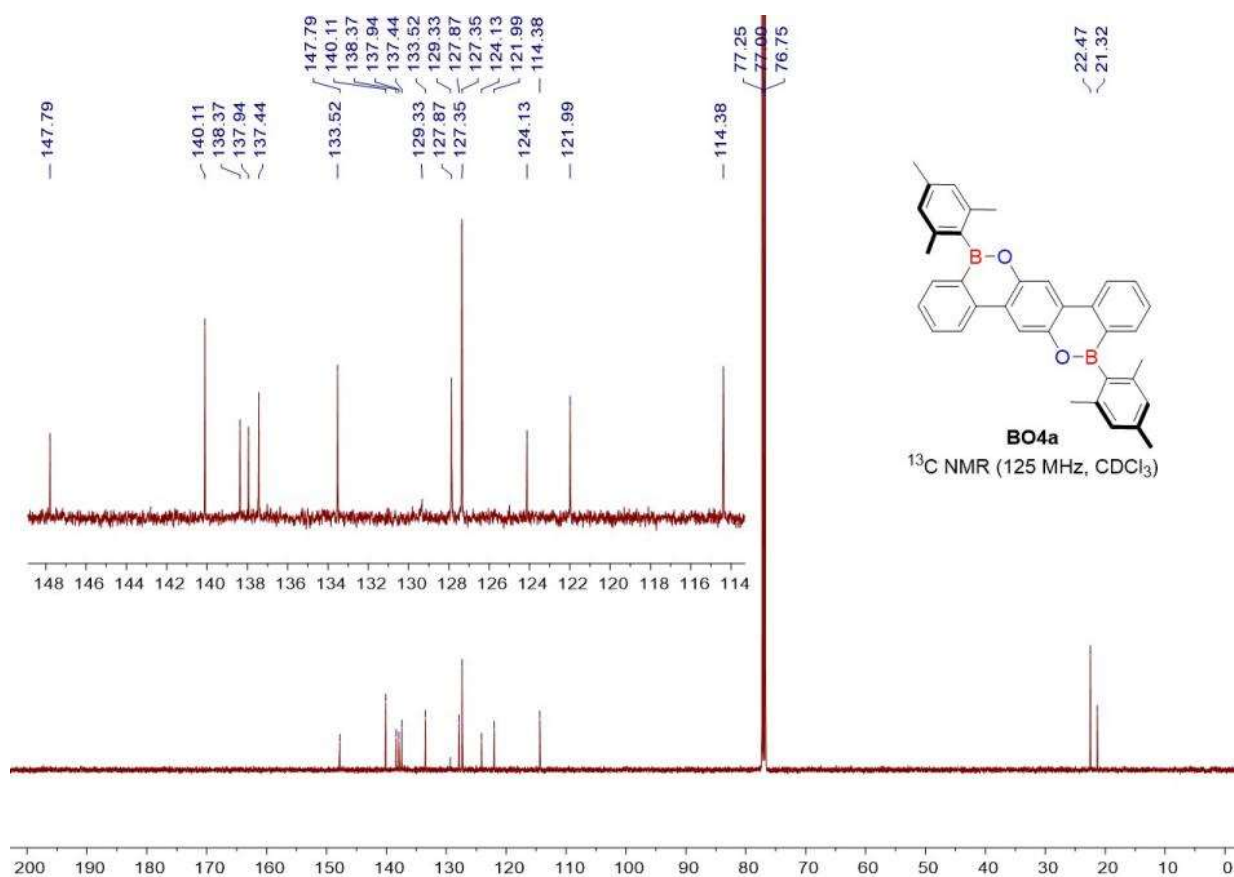




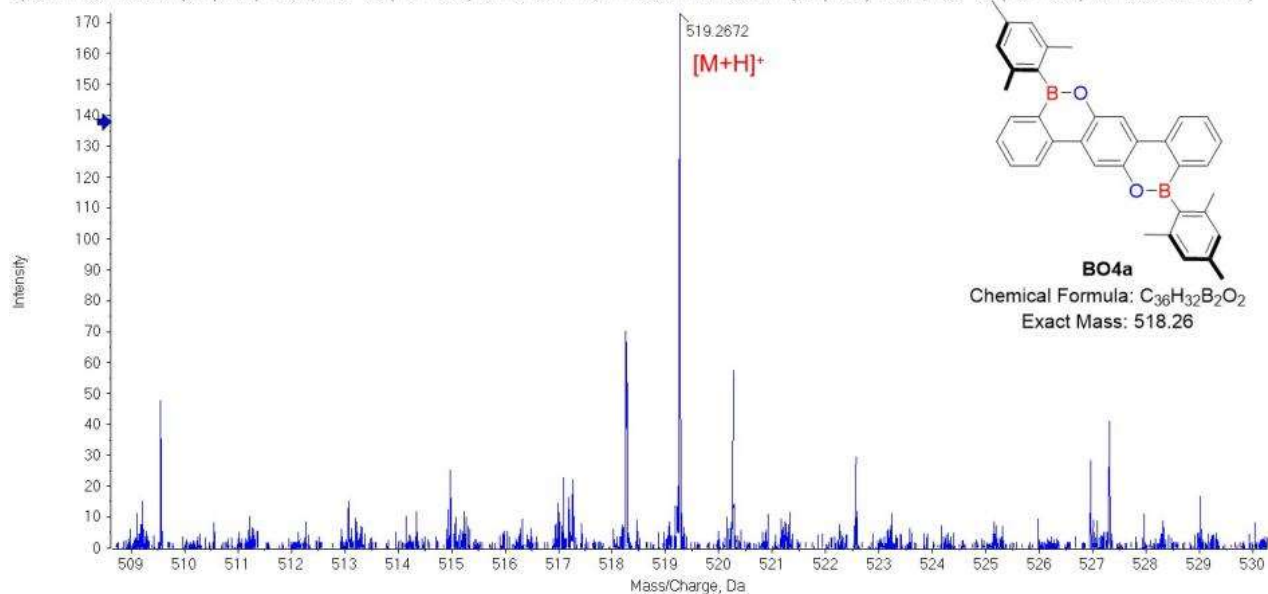


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$C_{54}H_{48}[^{11}B]_2O_2$	$C_{54}H_{48}[^{11}B]_2NaO_2$	773.3720	773.3733	1.68

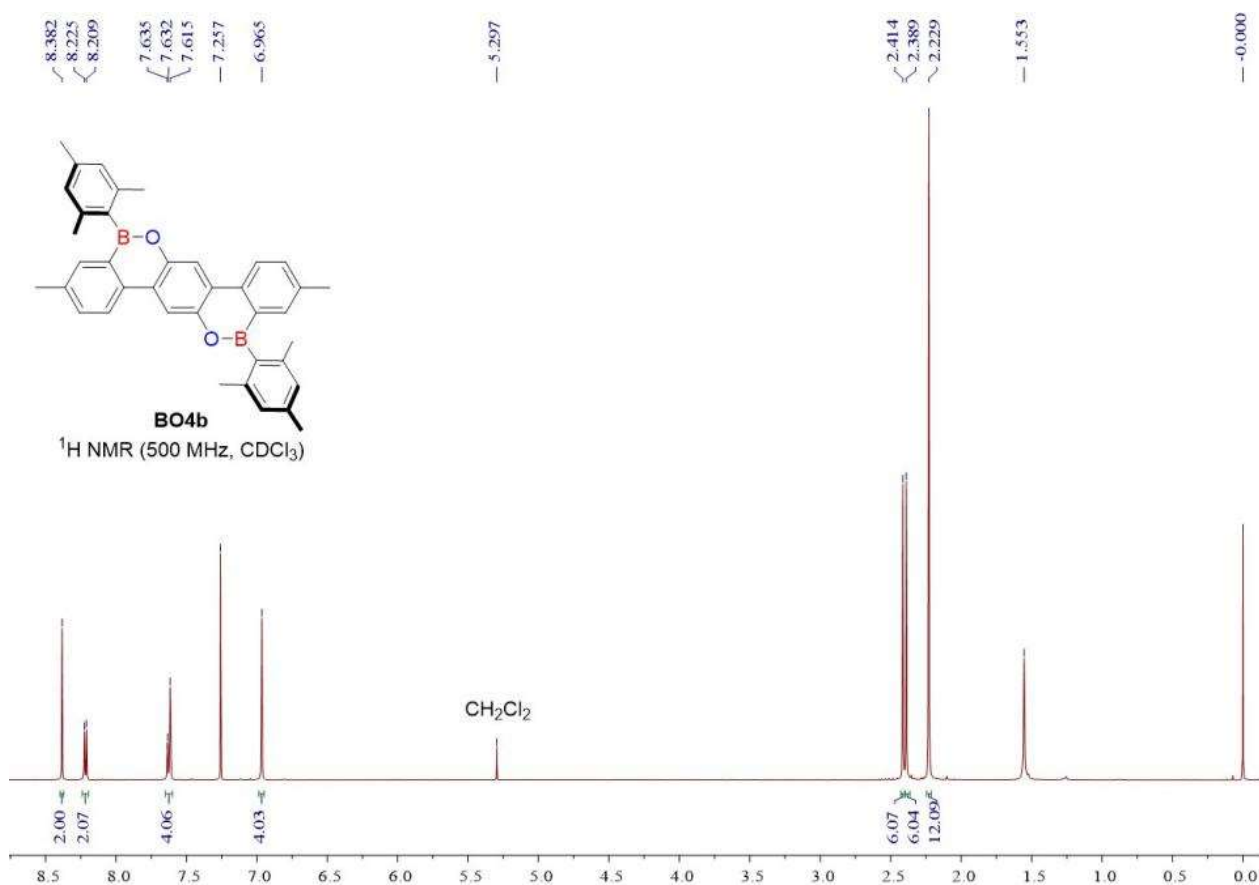


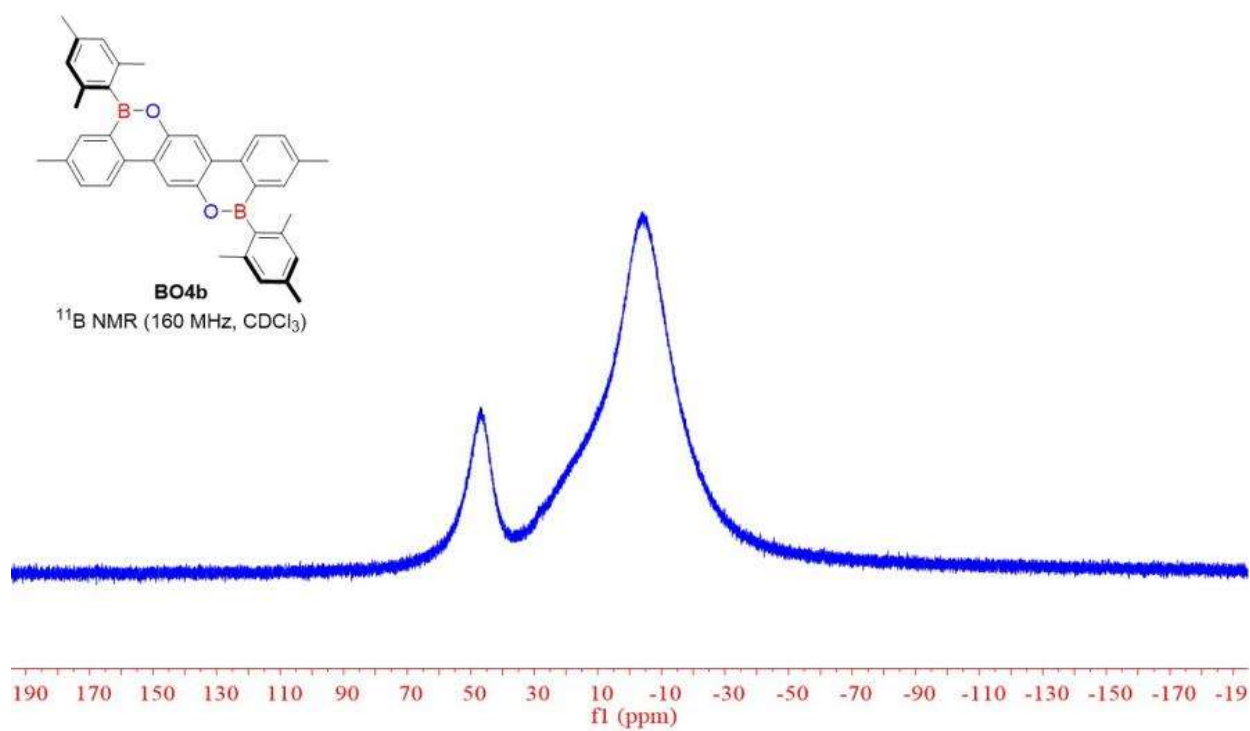
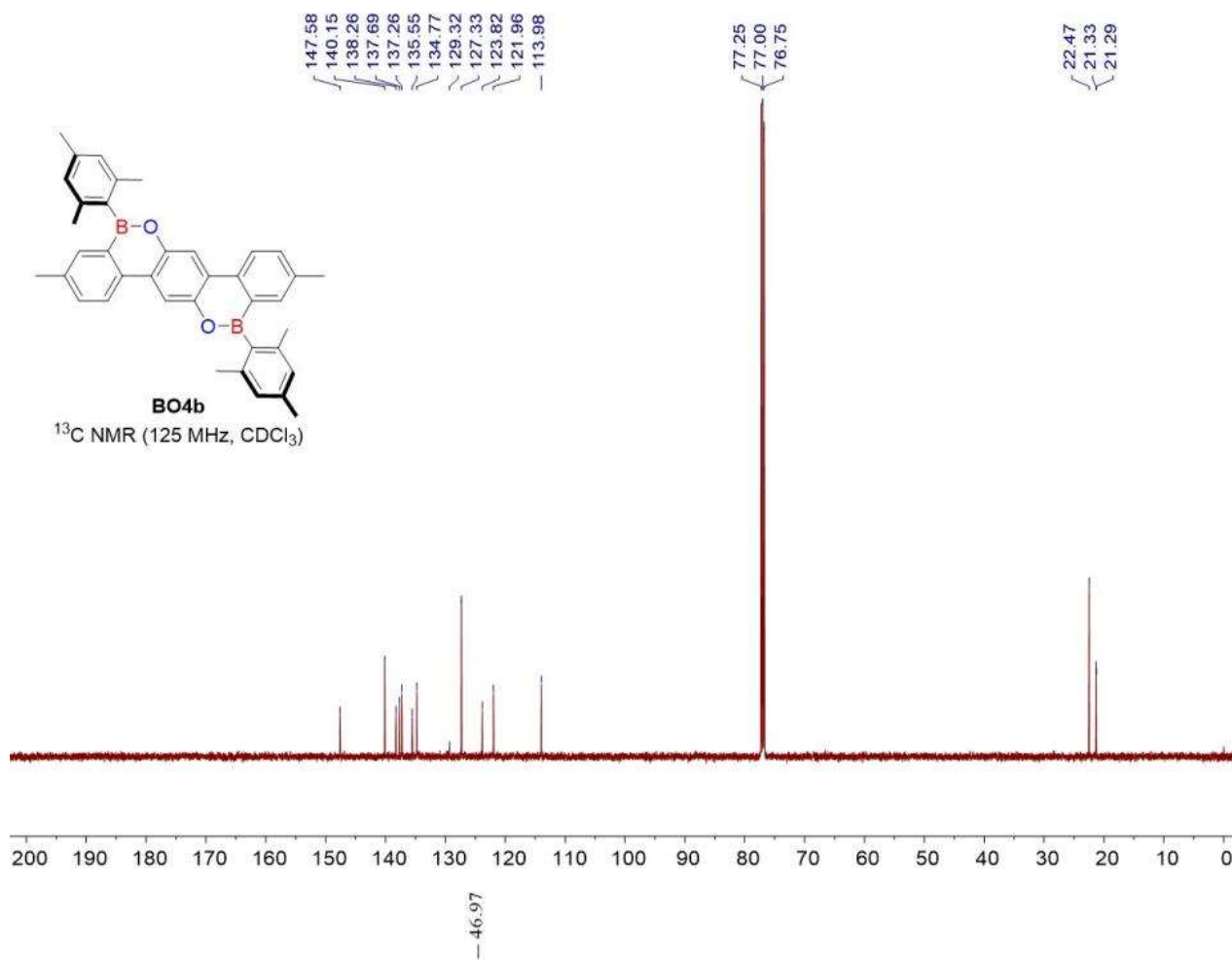


Spectrum from 0922.wiff (sample 29) - BO4a, +TOF MS (100 - 1500) from 0.135 to 0.195 min...pectrum from 0922.wiff (sample 29) - BO4a, +TOF MS (100 - 1500) from 0.325 to 0.479 min)

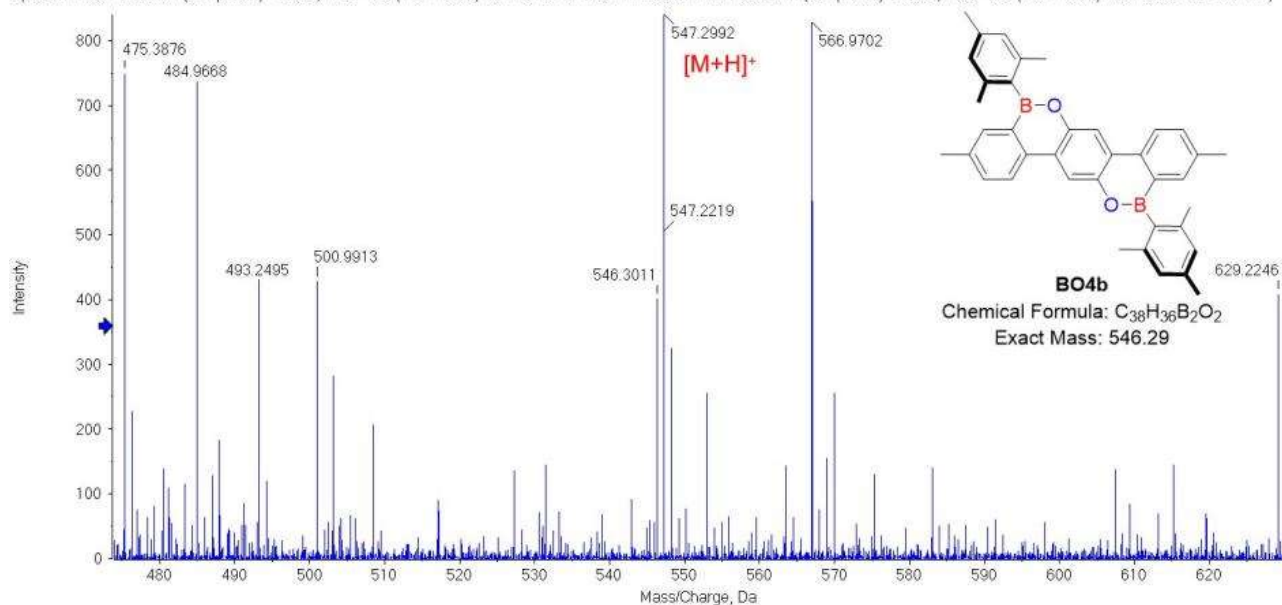


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$C_{36}H_{32}[^{11}B]_2O_2$	$C_{36}H_{33}[^{11}B]_2O_2$	519.2672	519.2661	-2.1

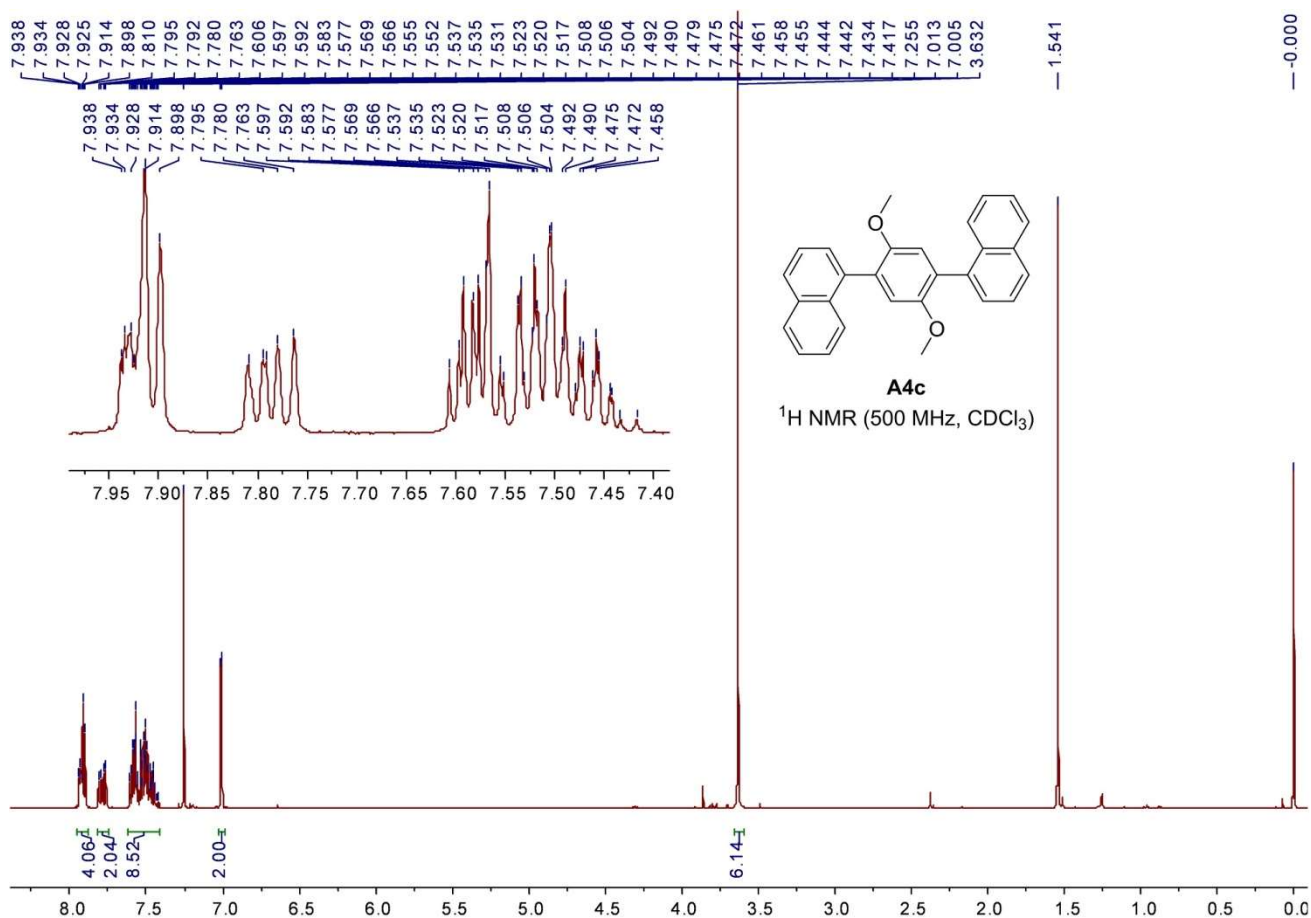


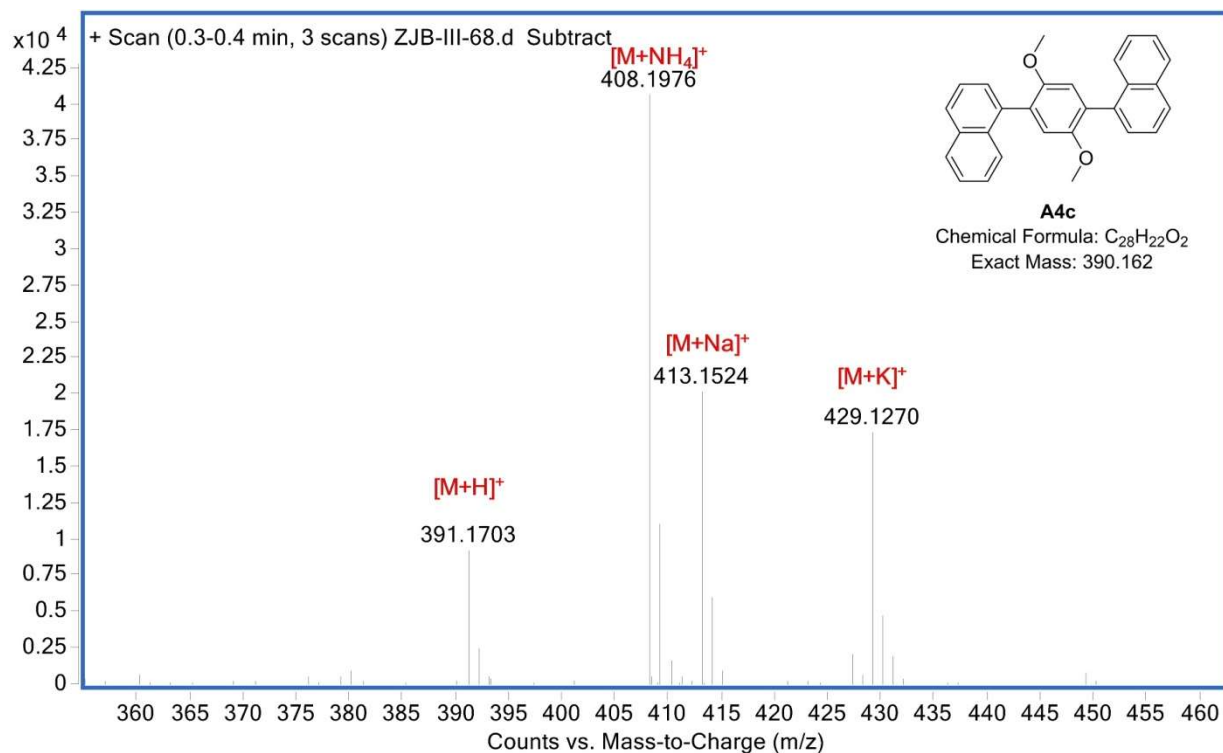
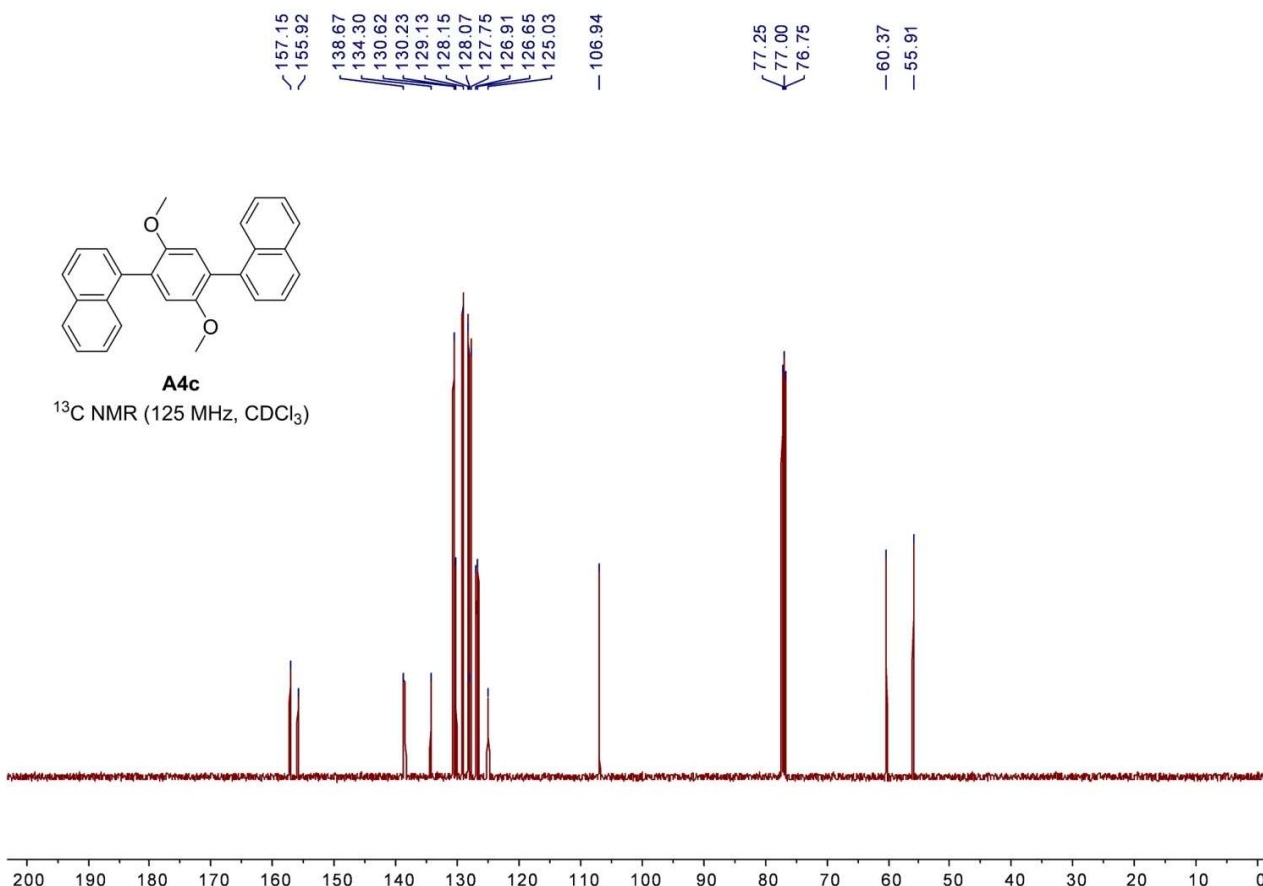


Spectrum from 0922.wiff (sample 30) - BO4b, +TOF MS (100 - 1500) from 0.130 to 0.191 min... Spectrum from 0922.wiff (sample 30) - BO4b, +TOF MS (100 - 1500) from 0.325 to 0.479 min)

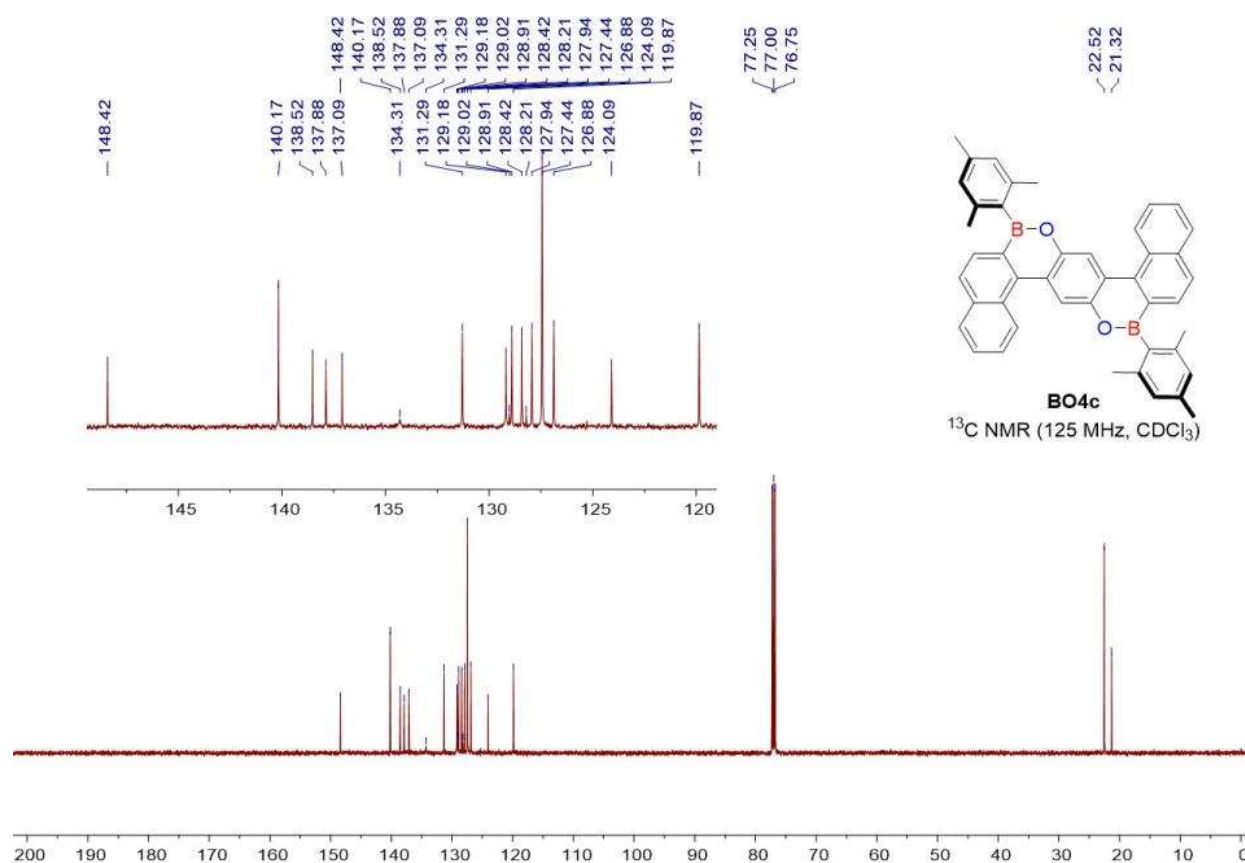
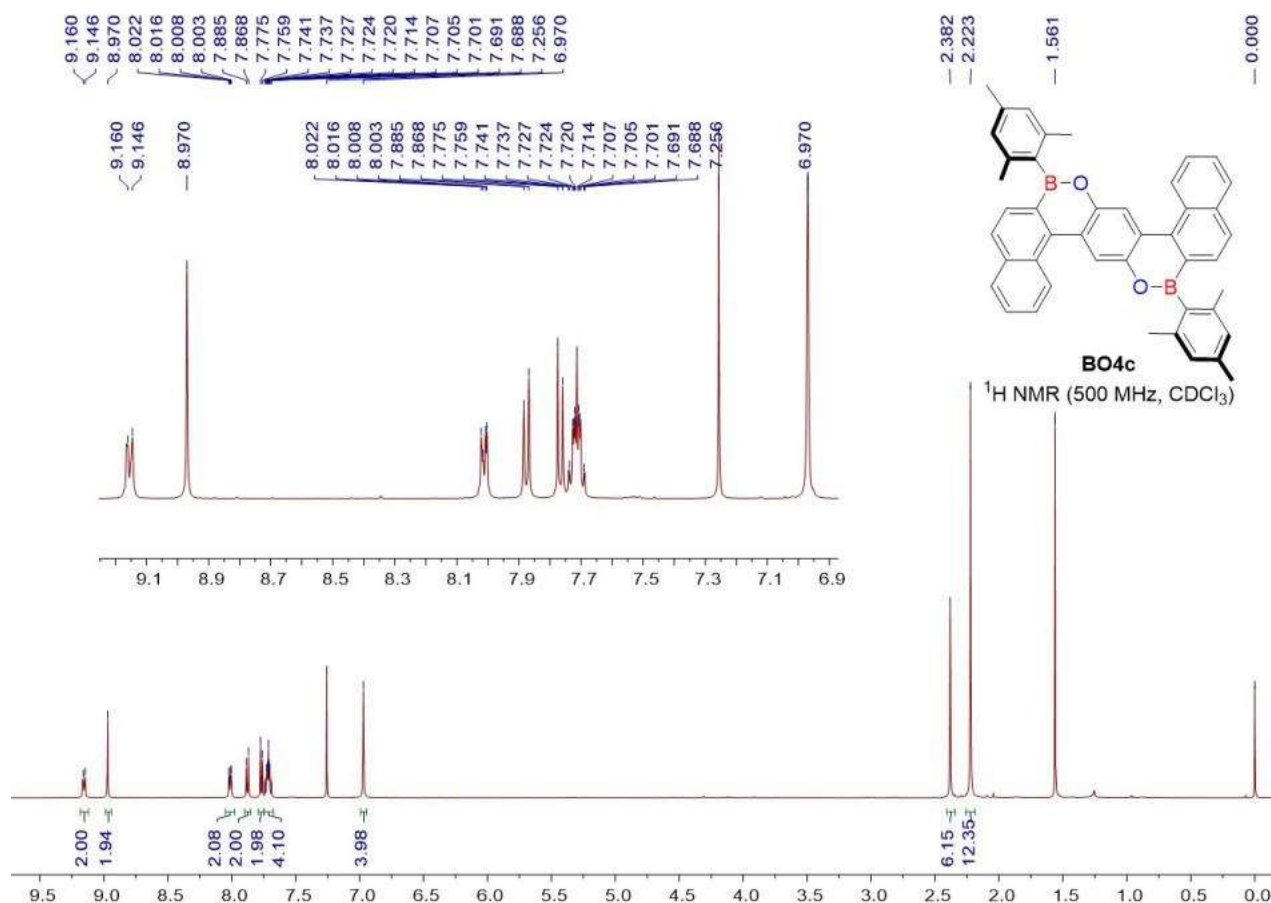


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
C ₃₈ H ₃₆ [¹¹ B] ₂ O ₂	C ₃₈ H ₃₇ [¹¹ B] ₂ O ₂	547.2992	547.2974	-3.3

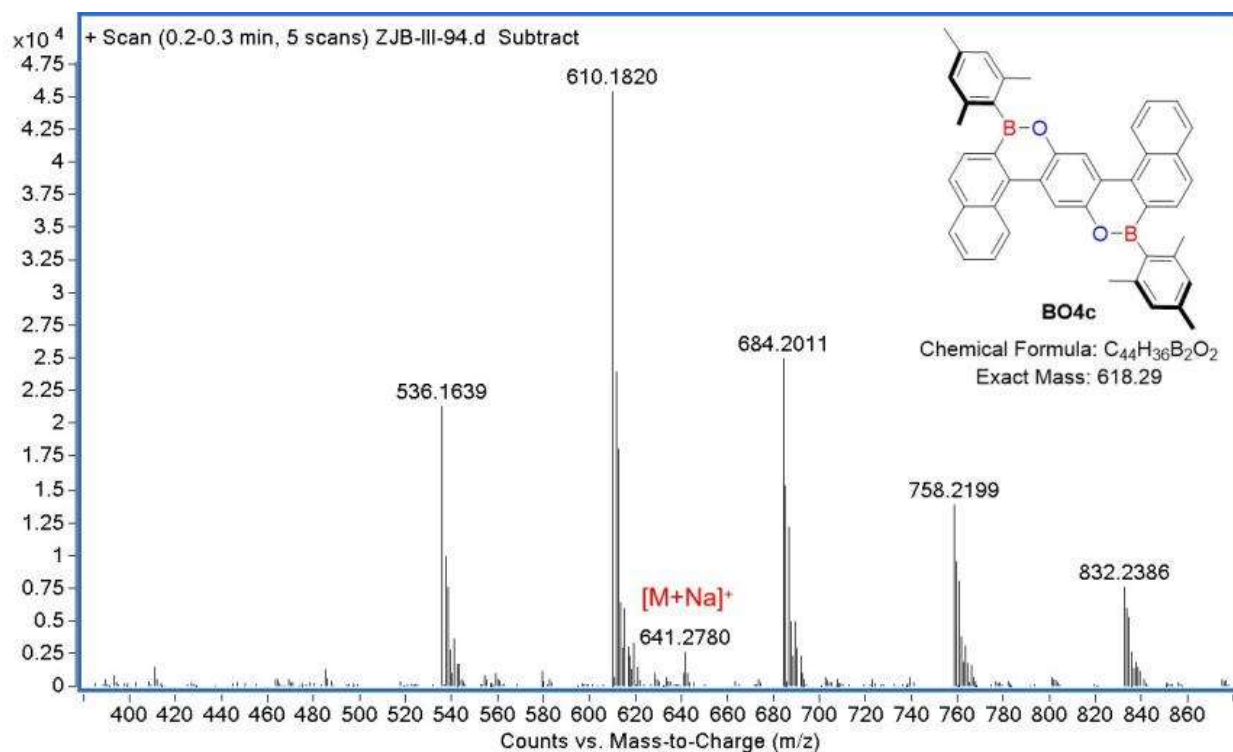
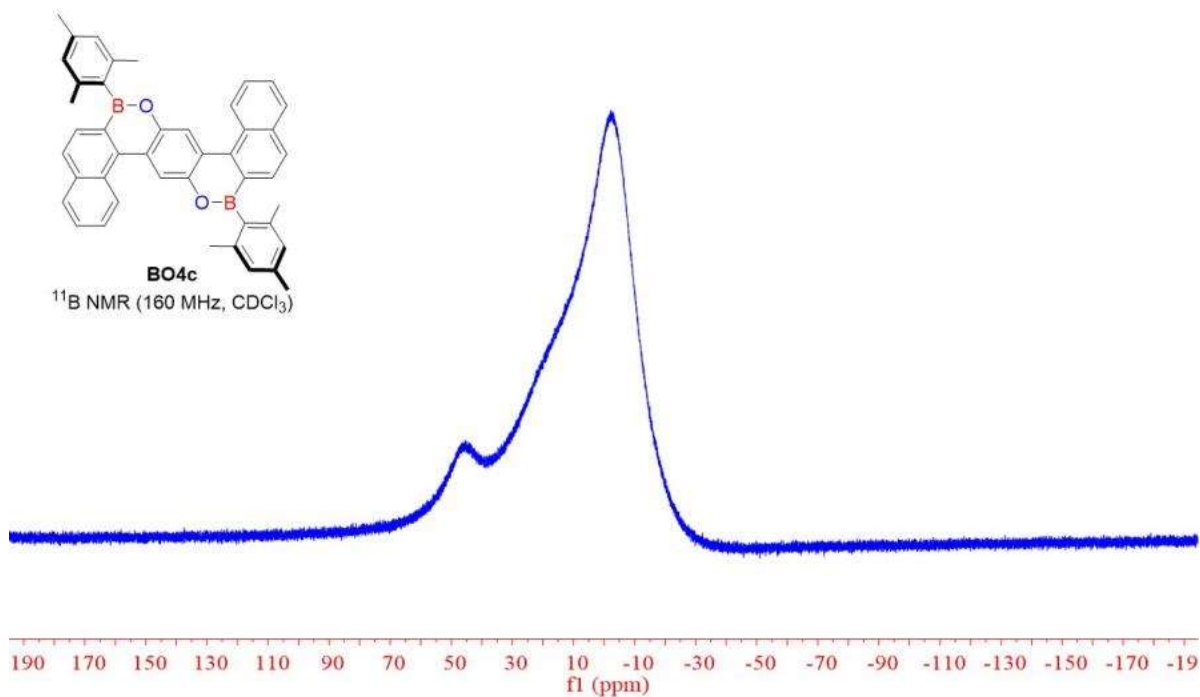




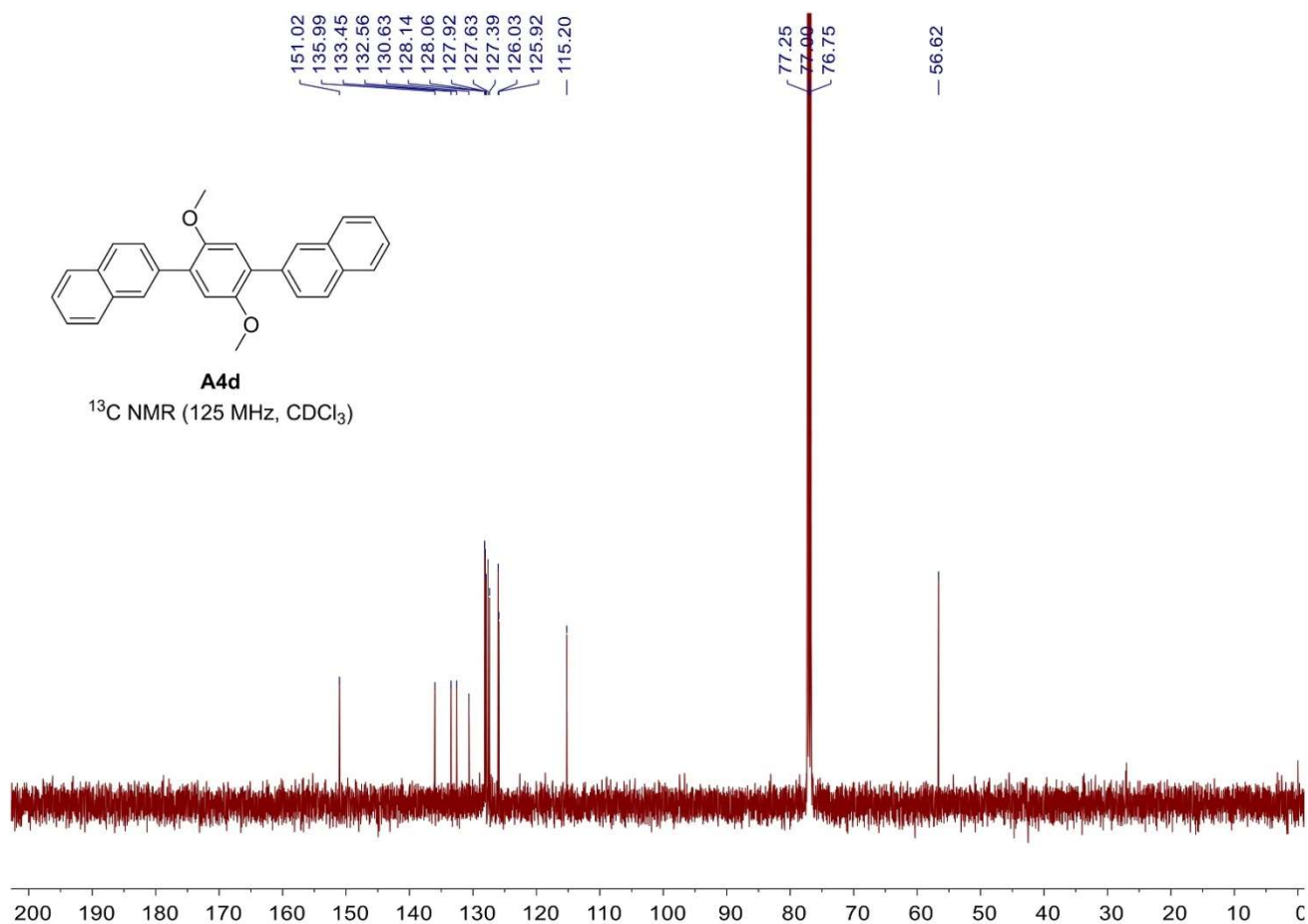
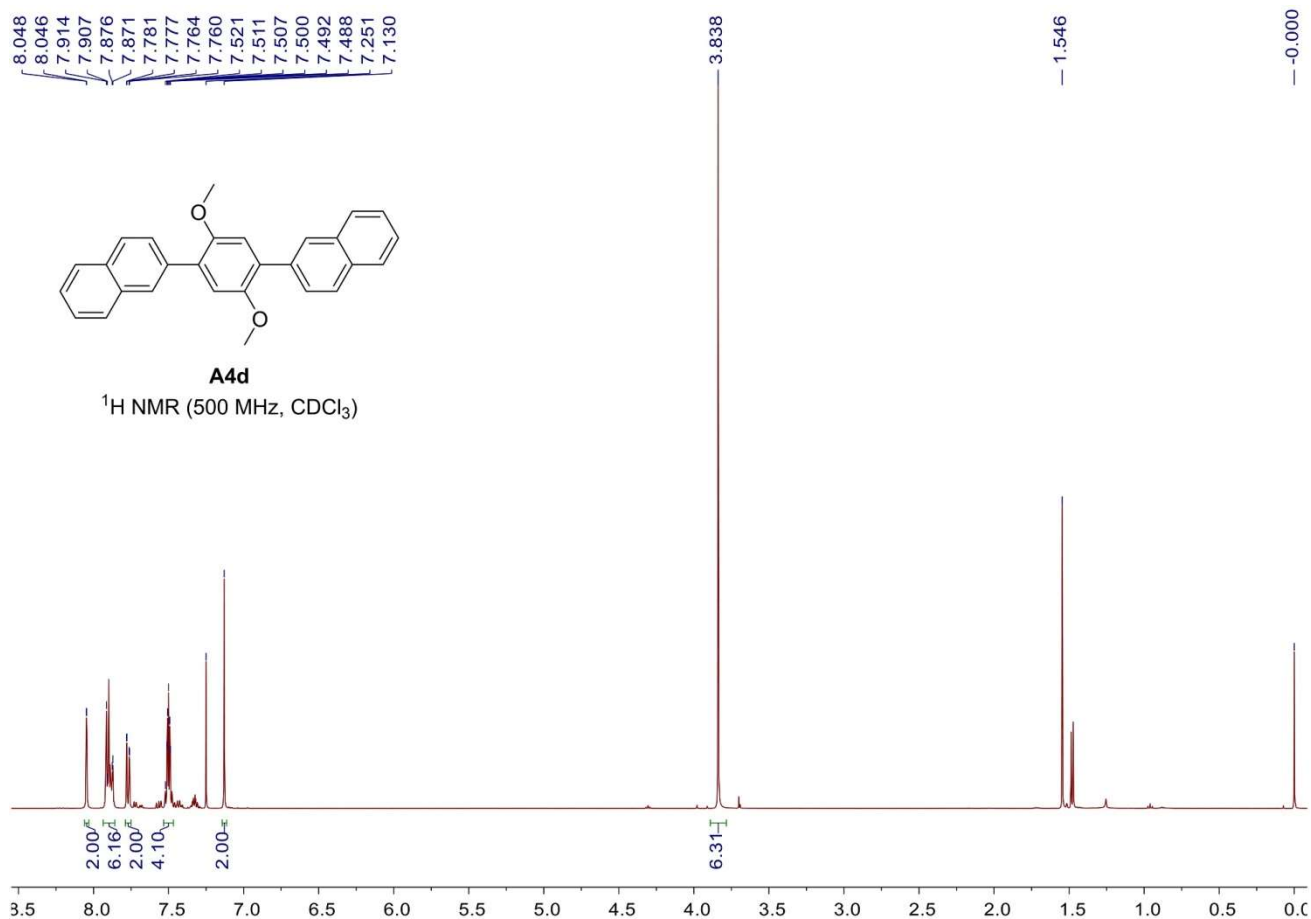
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
C ₂₈ H ₂₂ O ₂	C ₂₈ H ₂₆ NO ₂	408.1976	408.1958	-4.6	18

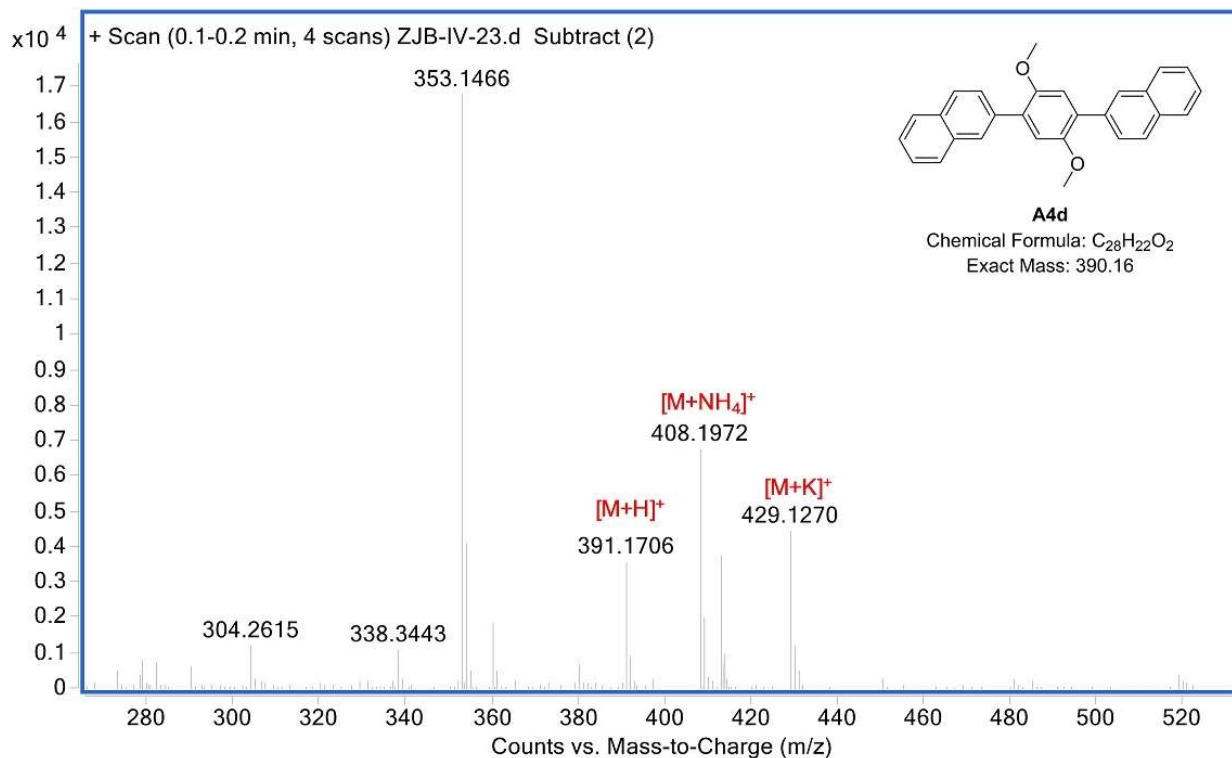


— 45.44

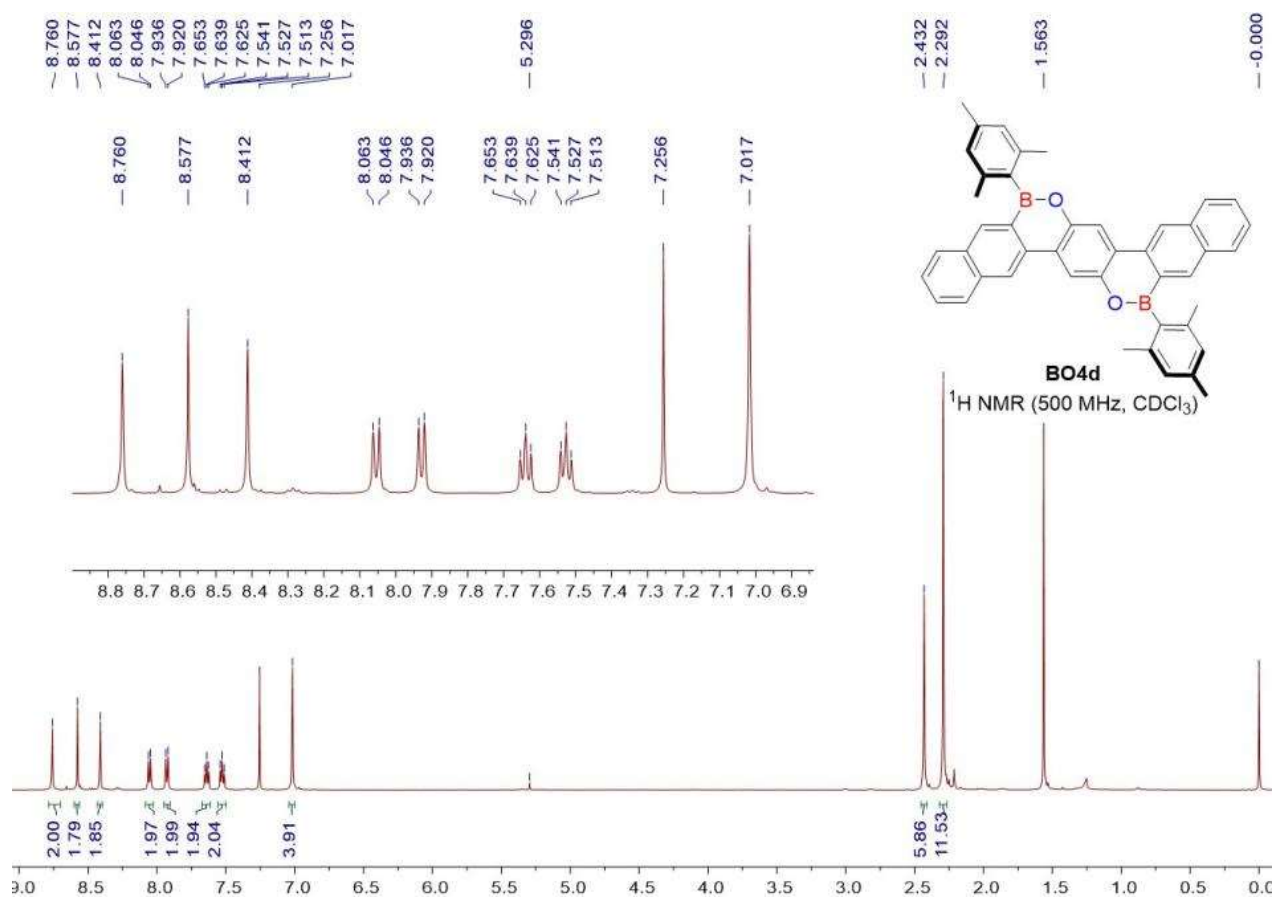


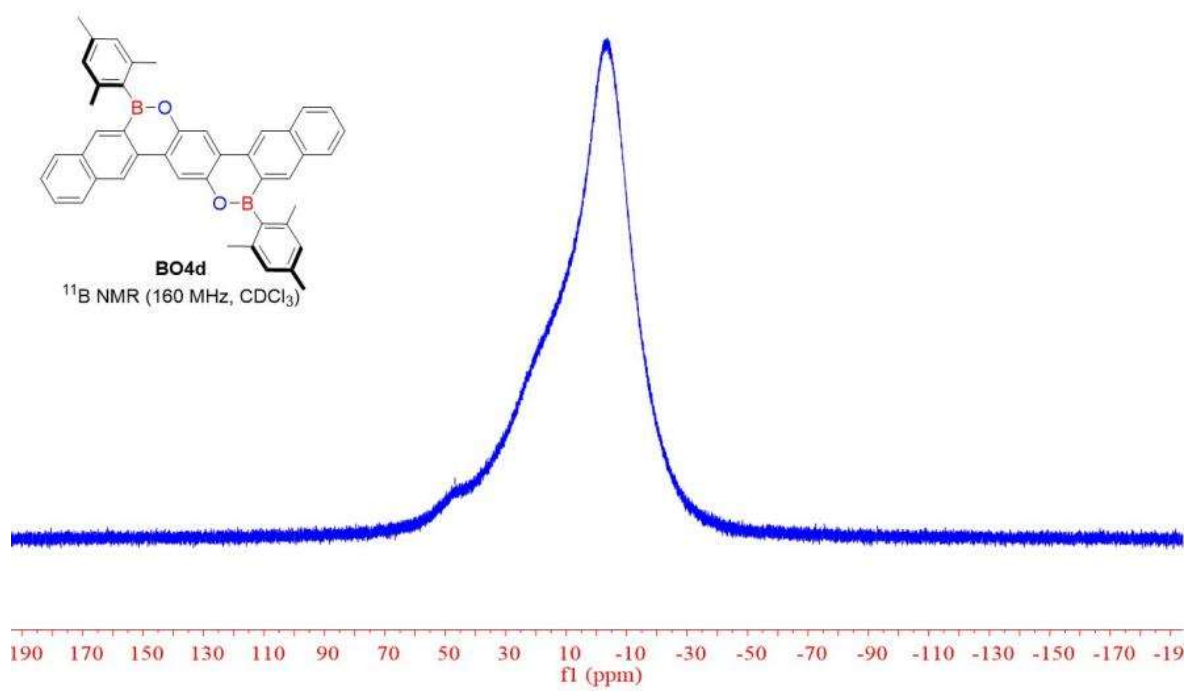
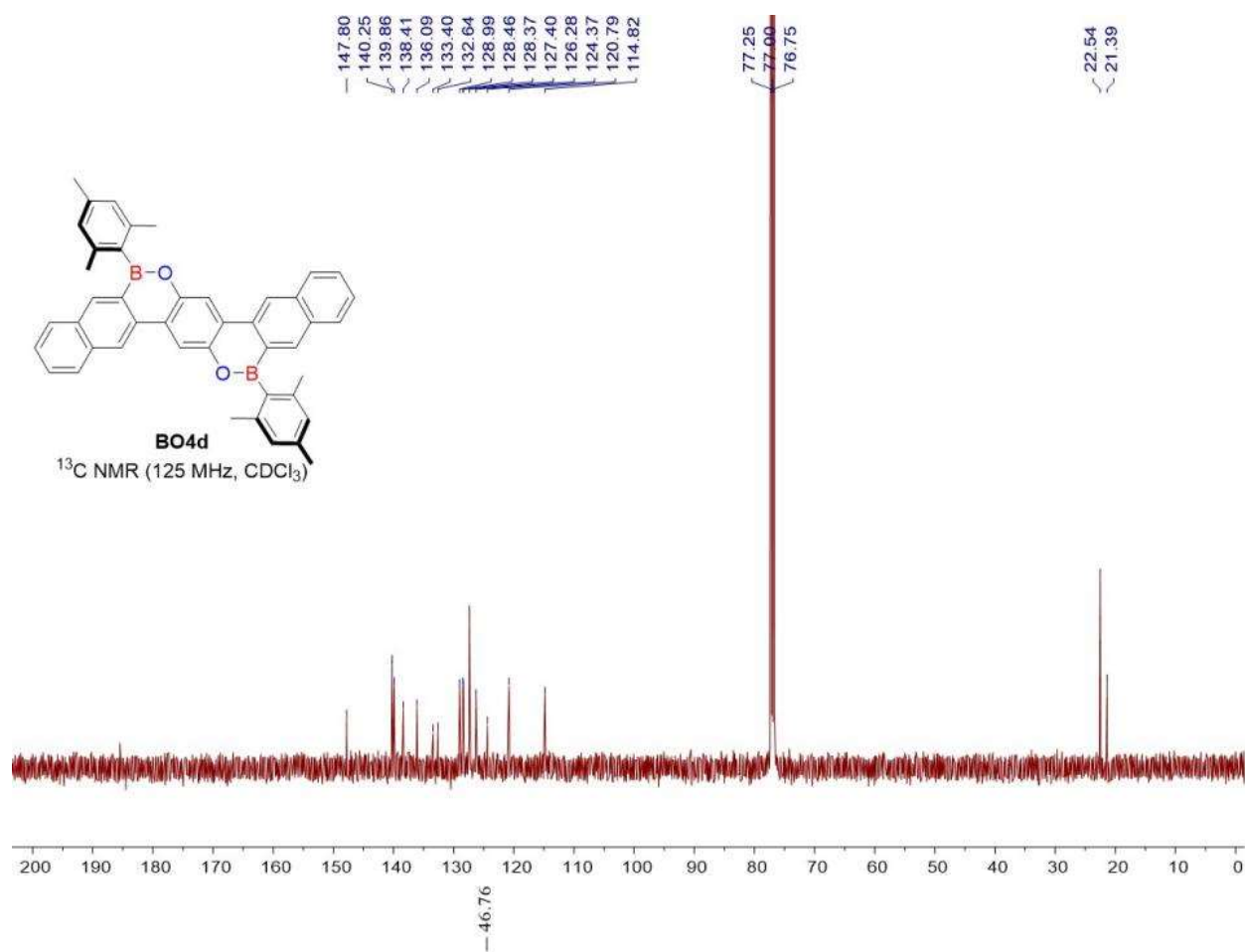
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{NaO}_2$	641.2780	641.2794	2.2

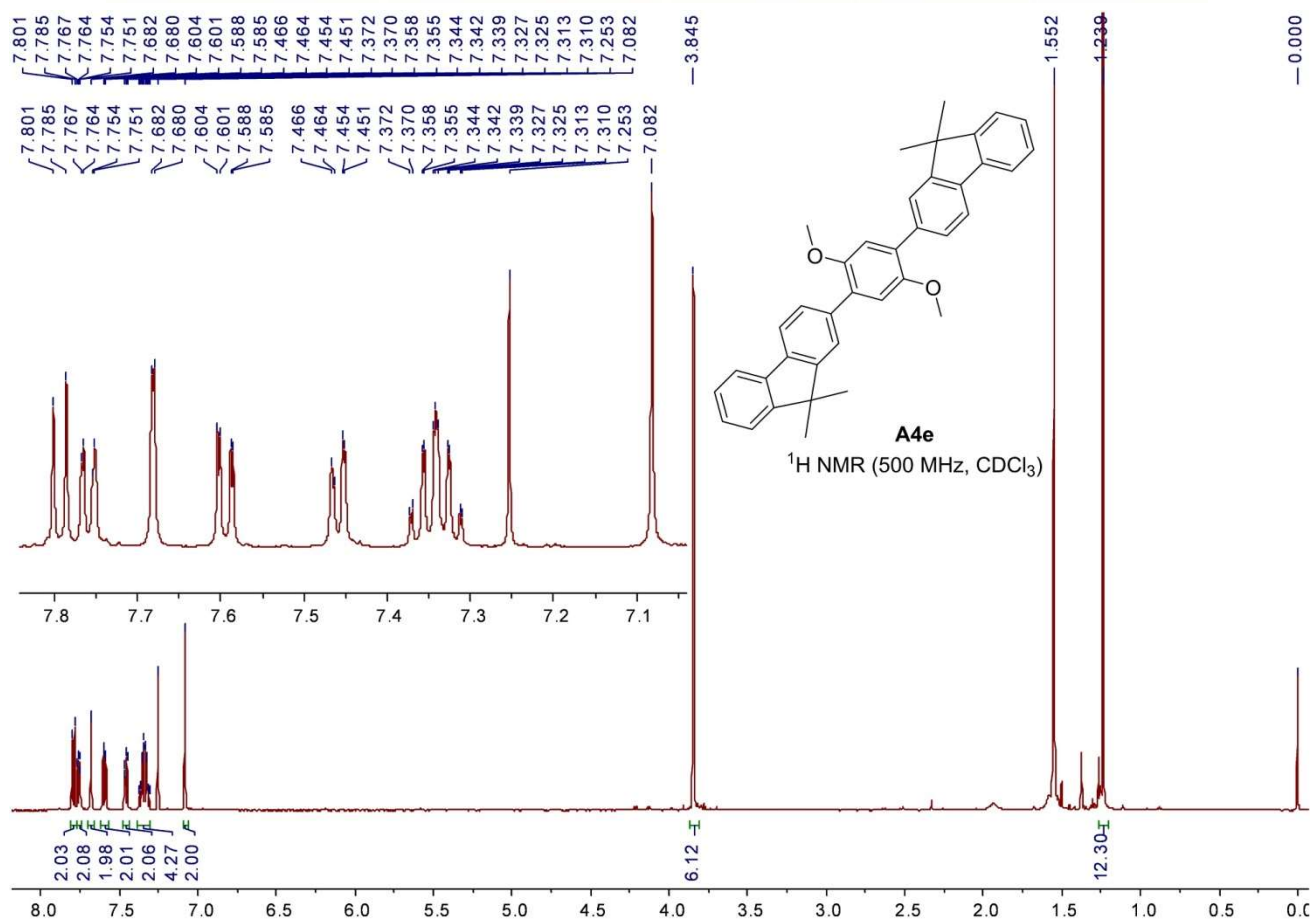
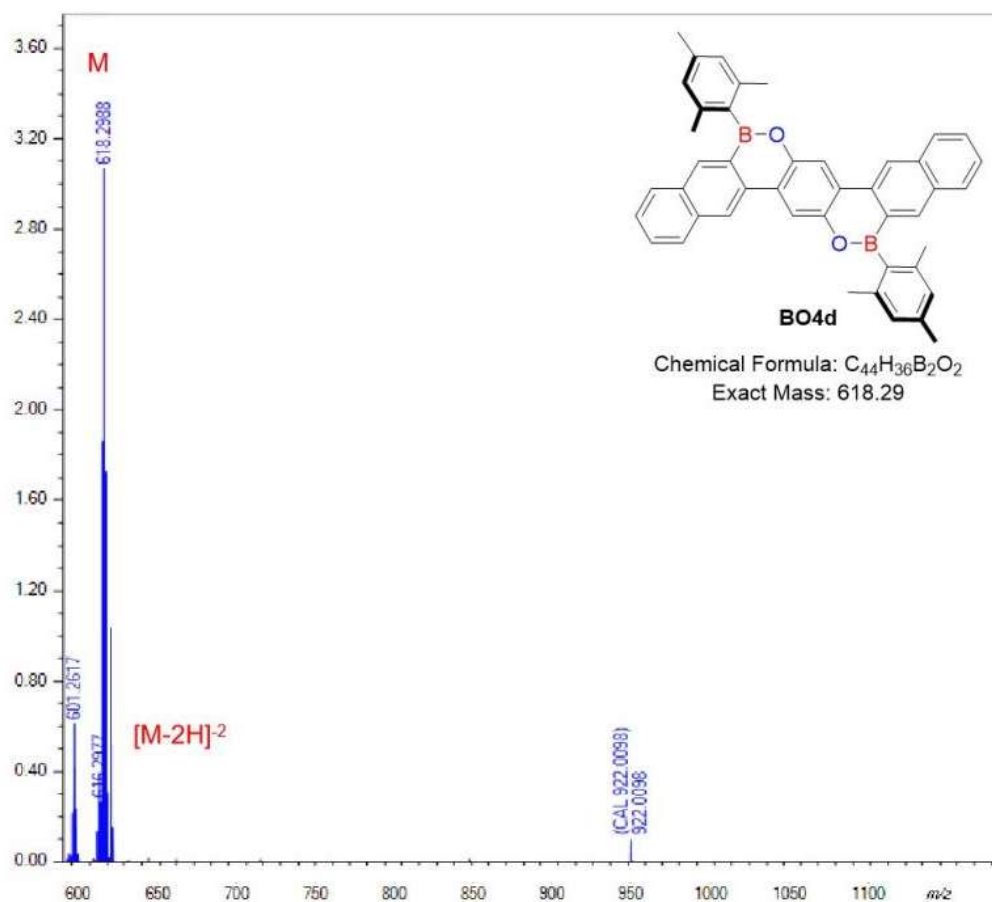


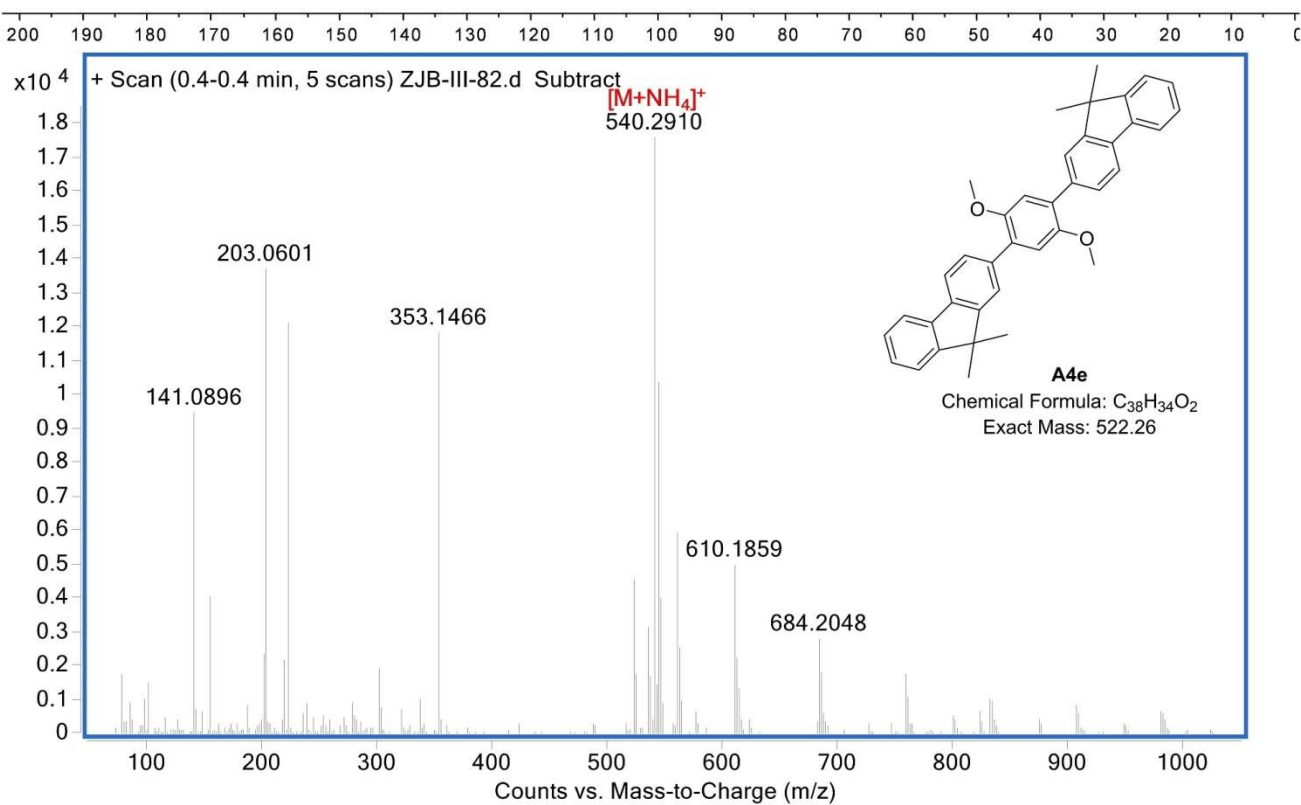
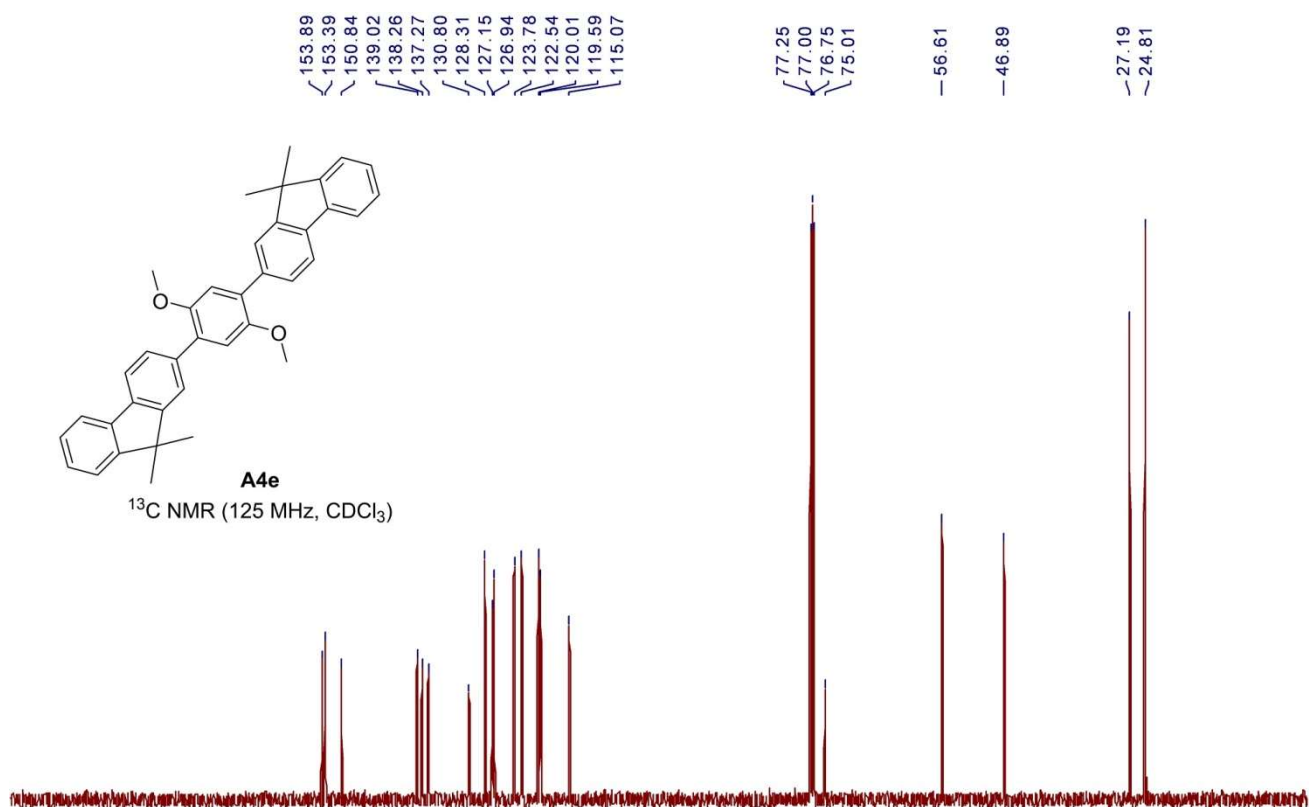


Formula(M)	Ion Formula	m/z	Calc m/z	Diff(ppm)	DBE
$C_{28}H_{22}O_2$	$C_{28}H_{26}NO_2$	408.1972	408.1958	-3.57	18

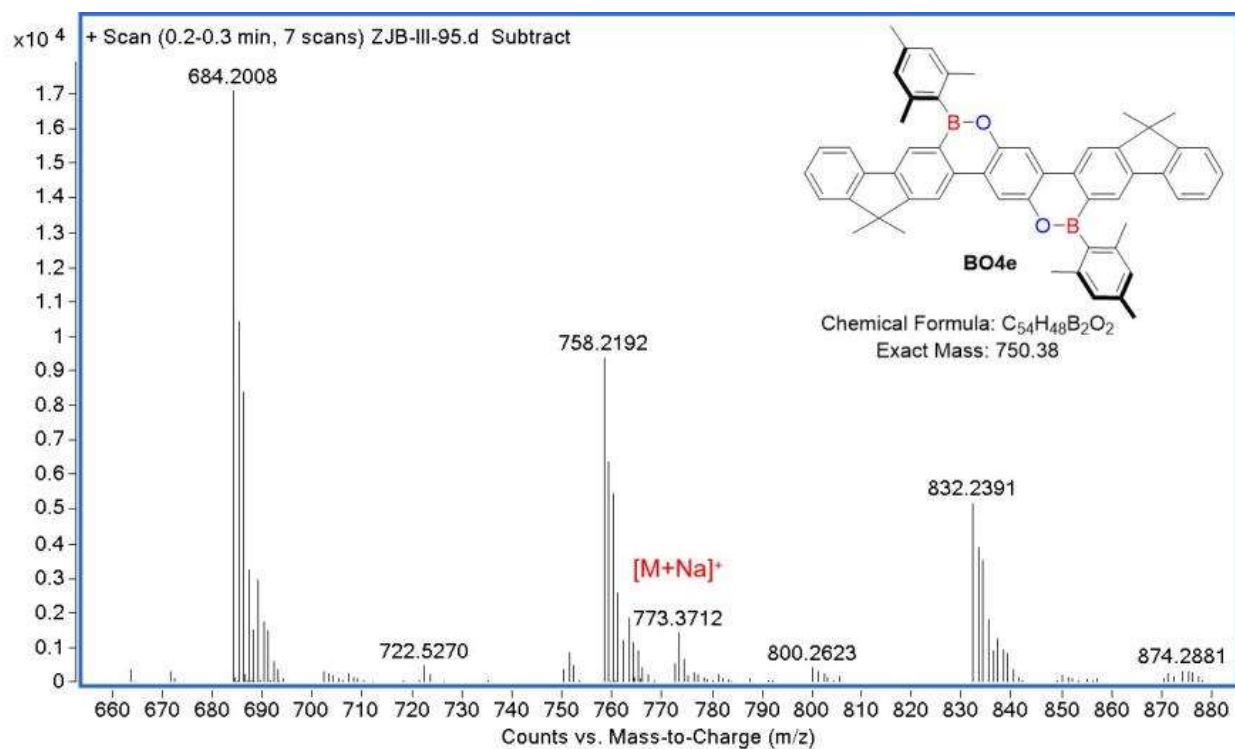
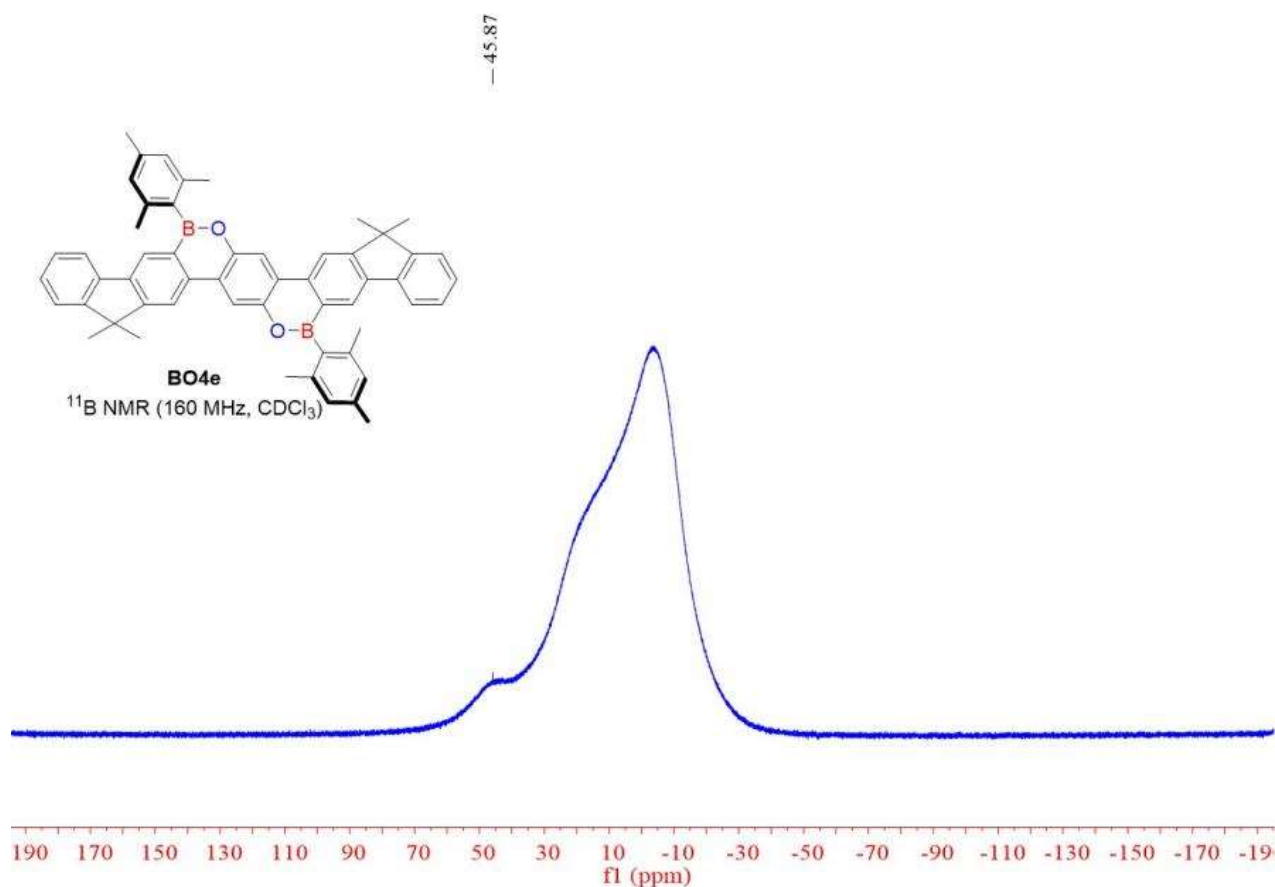




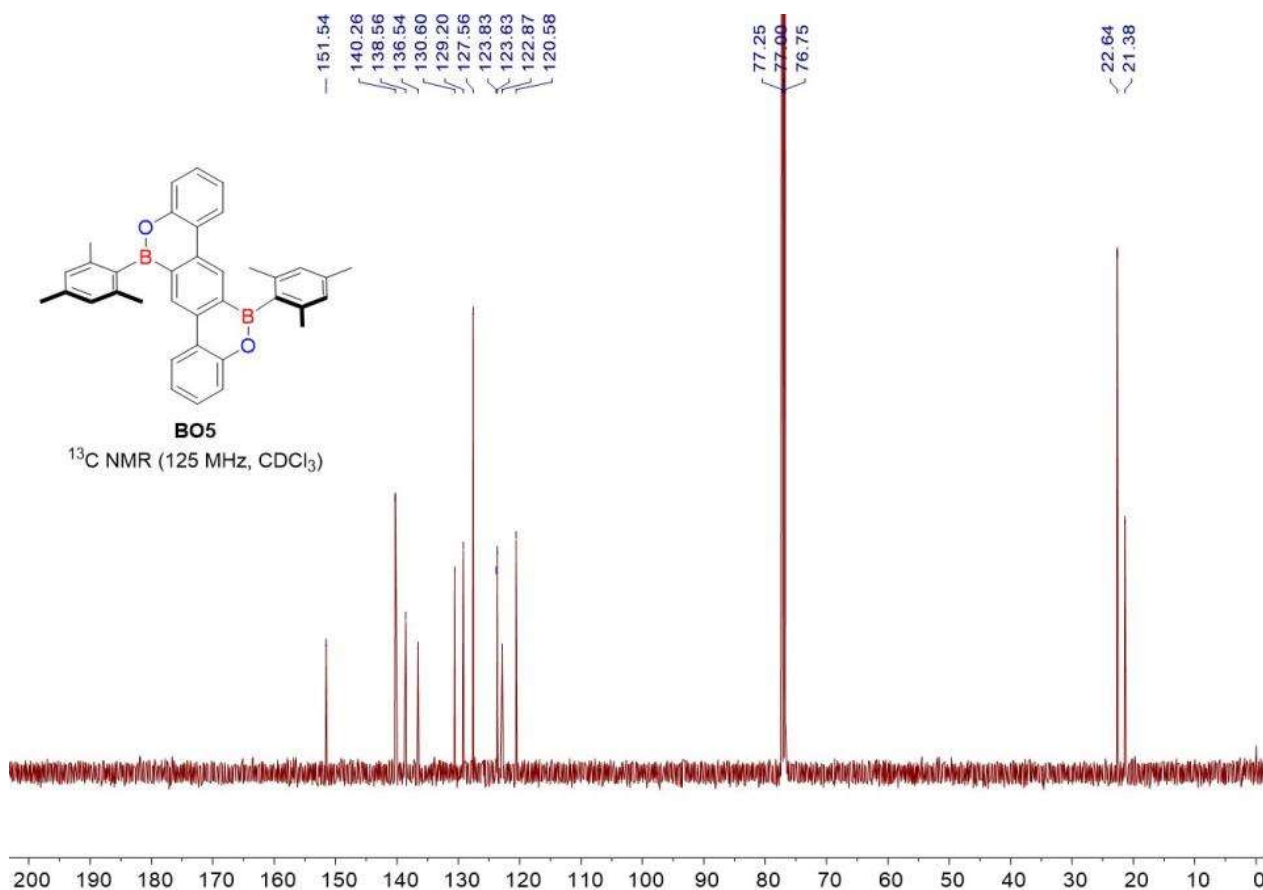
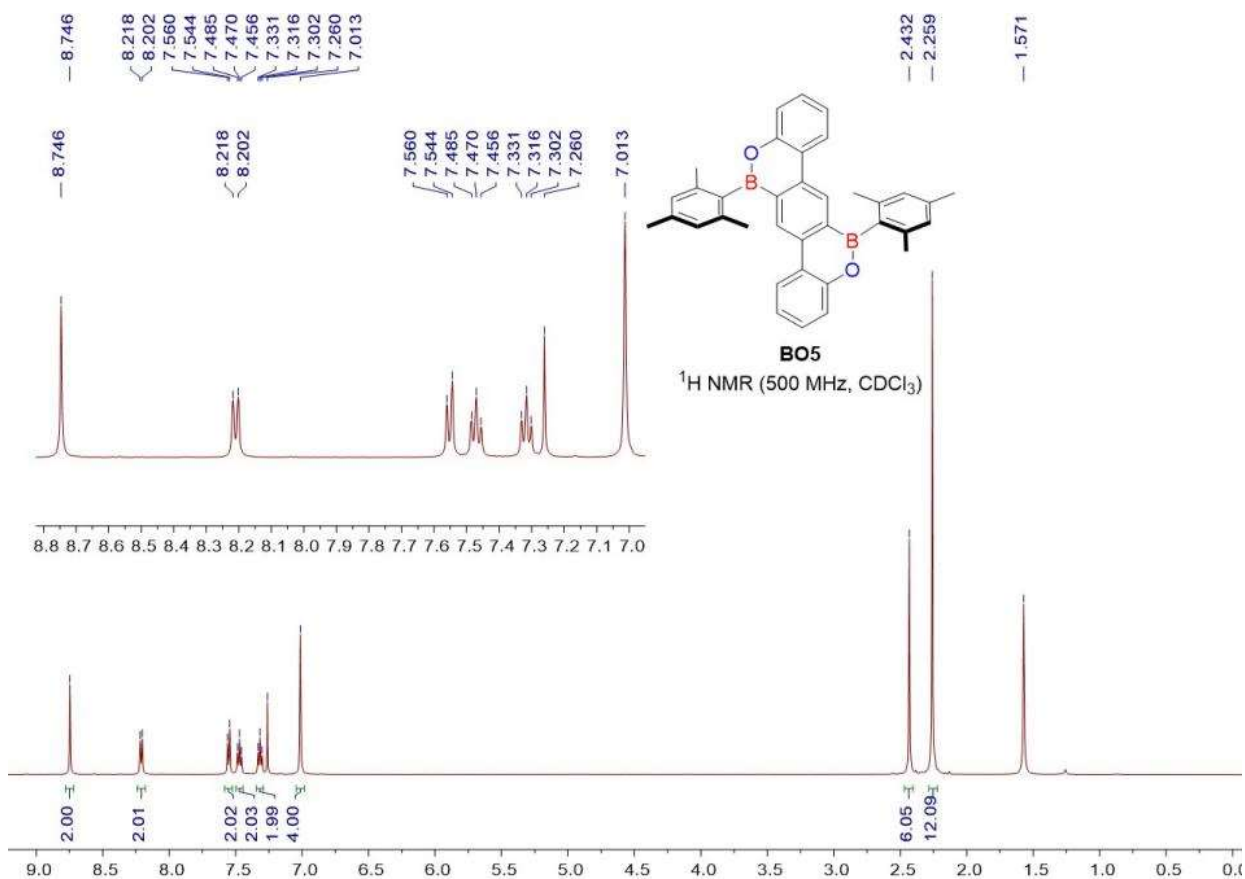


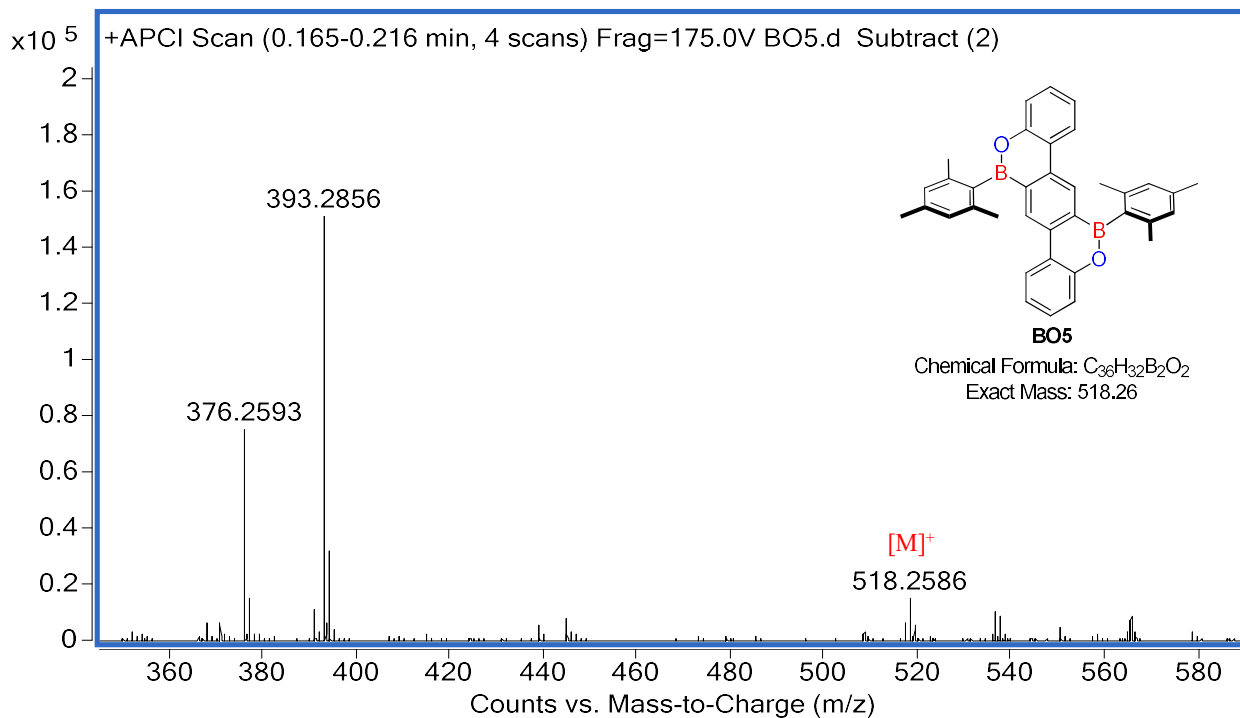
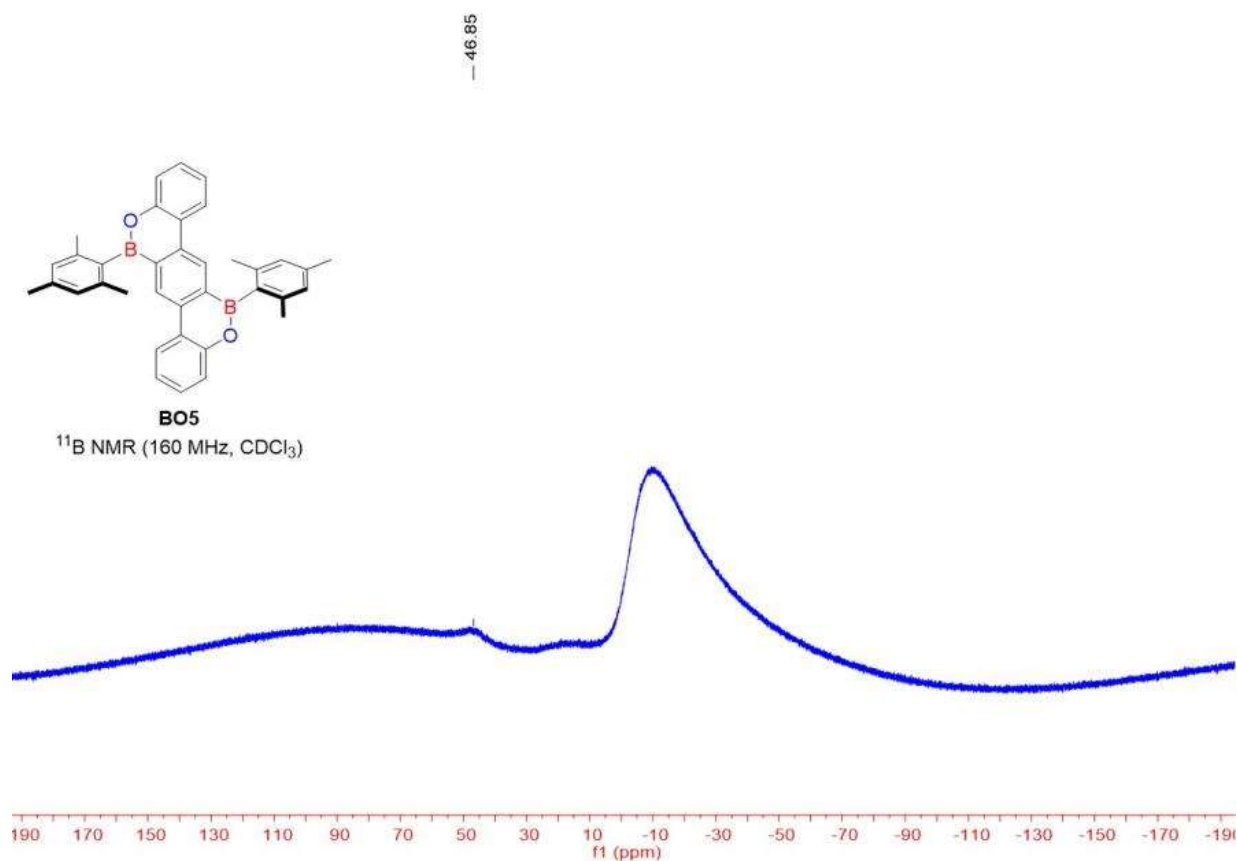


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
C ₃₈ H ₃₄ O ₂	C ₃₈ H ₃₈ NO ₂	540.2910	540.2897	-2.48	22

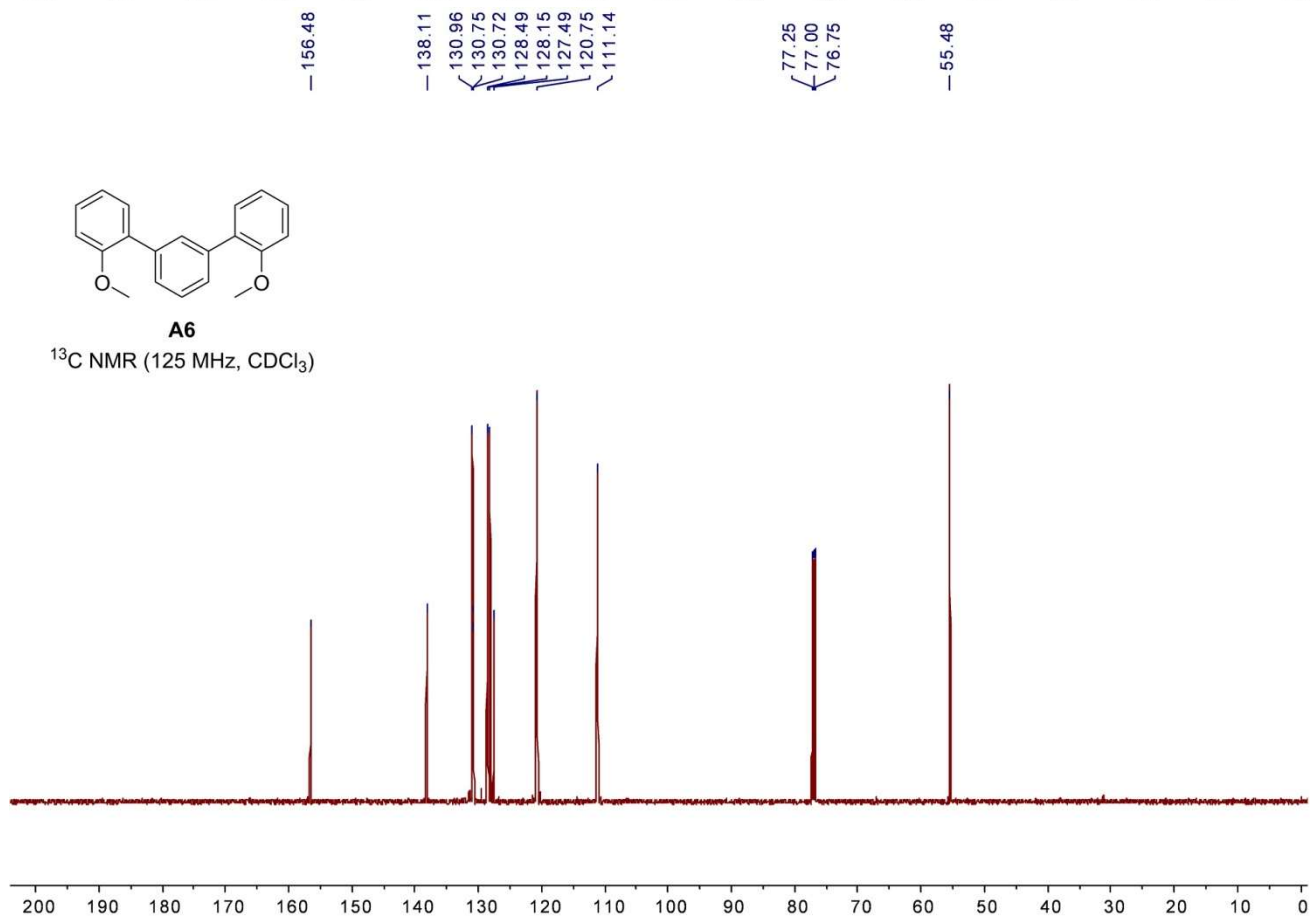
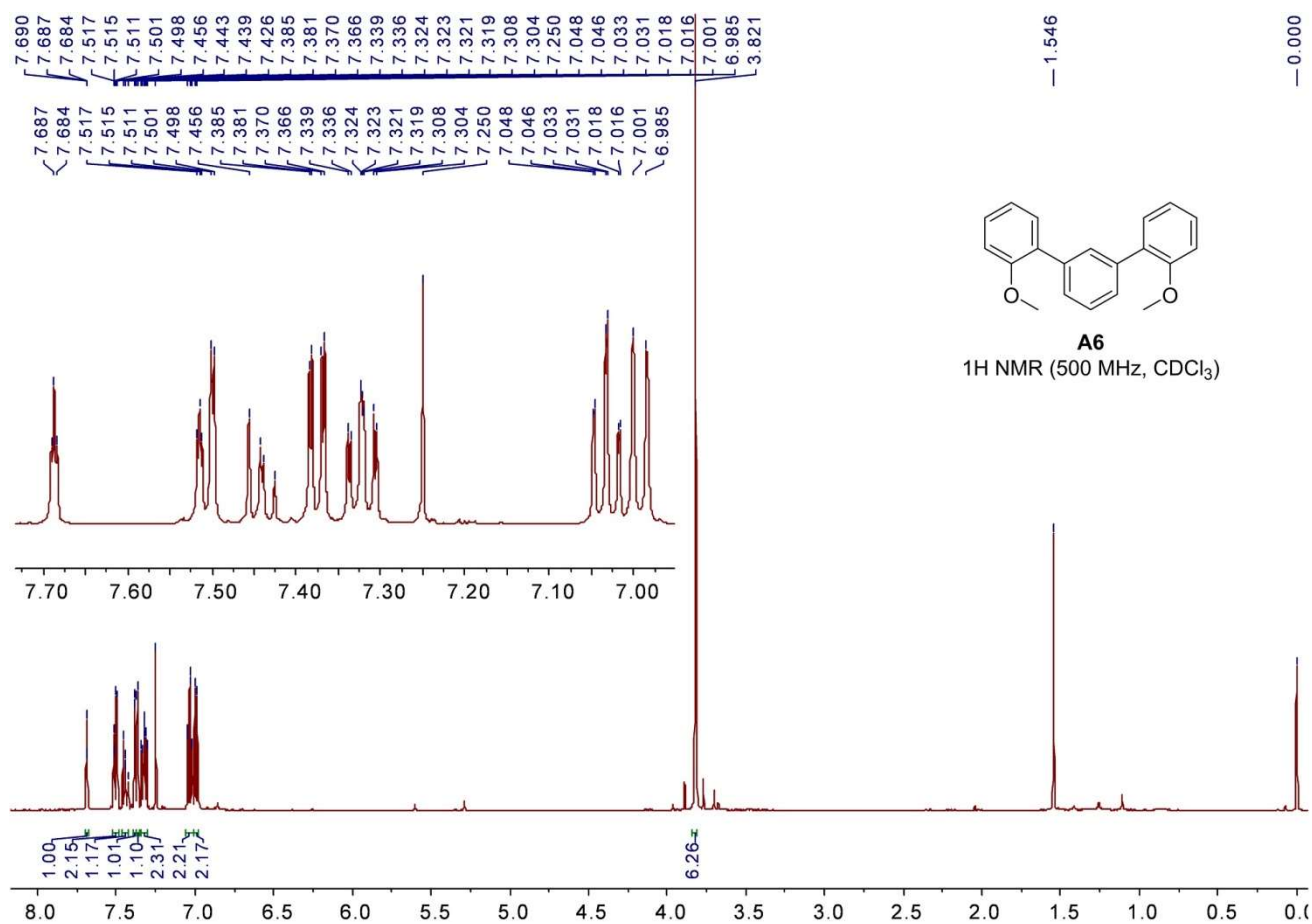


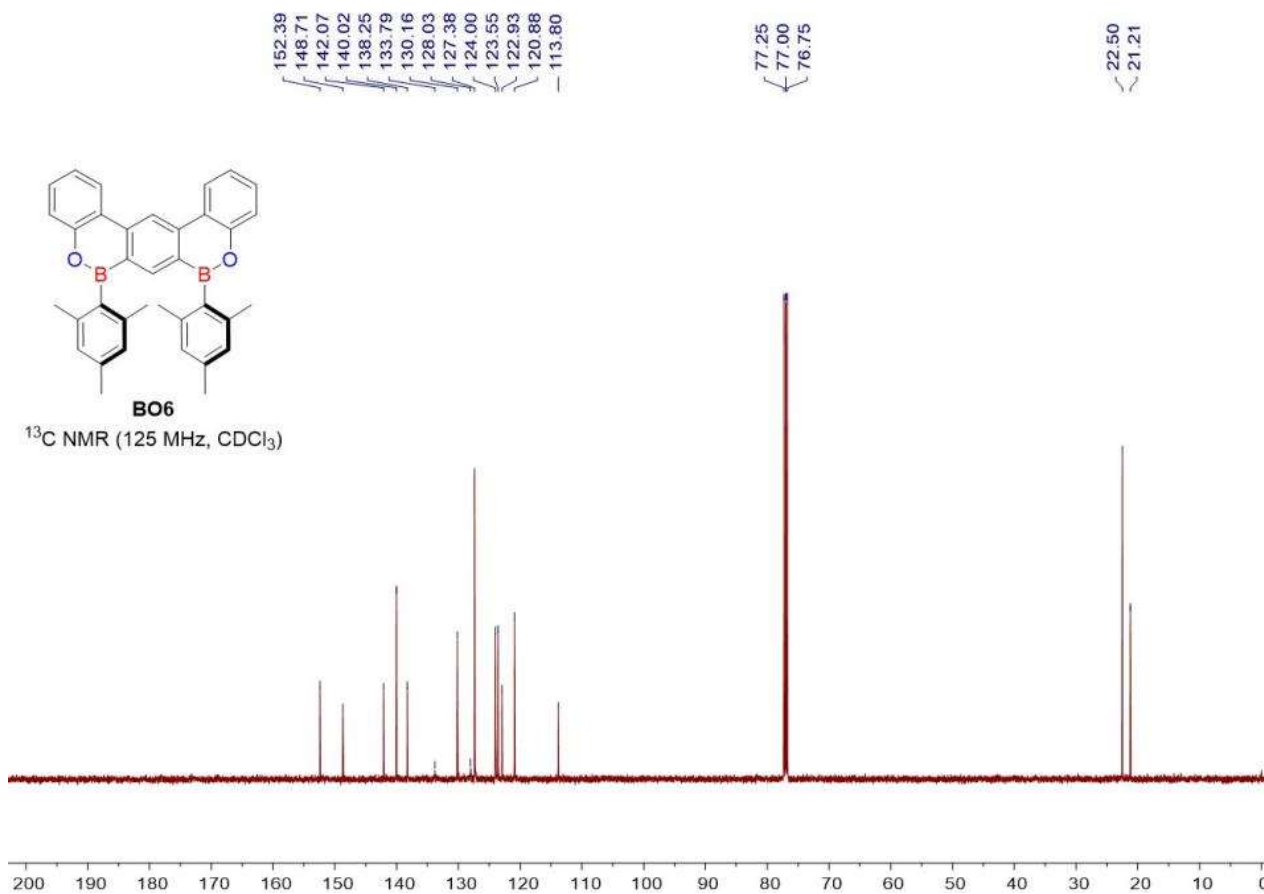
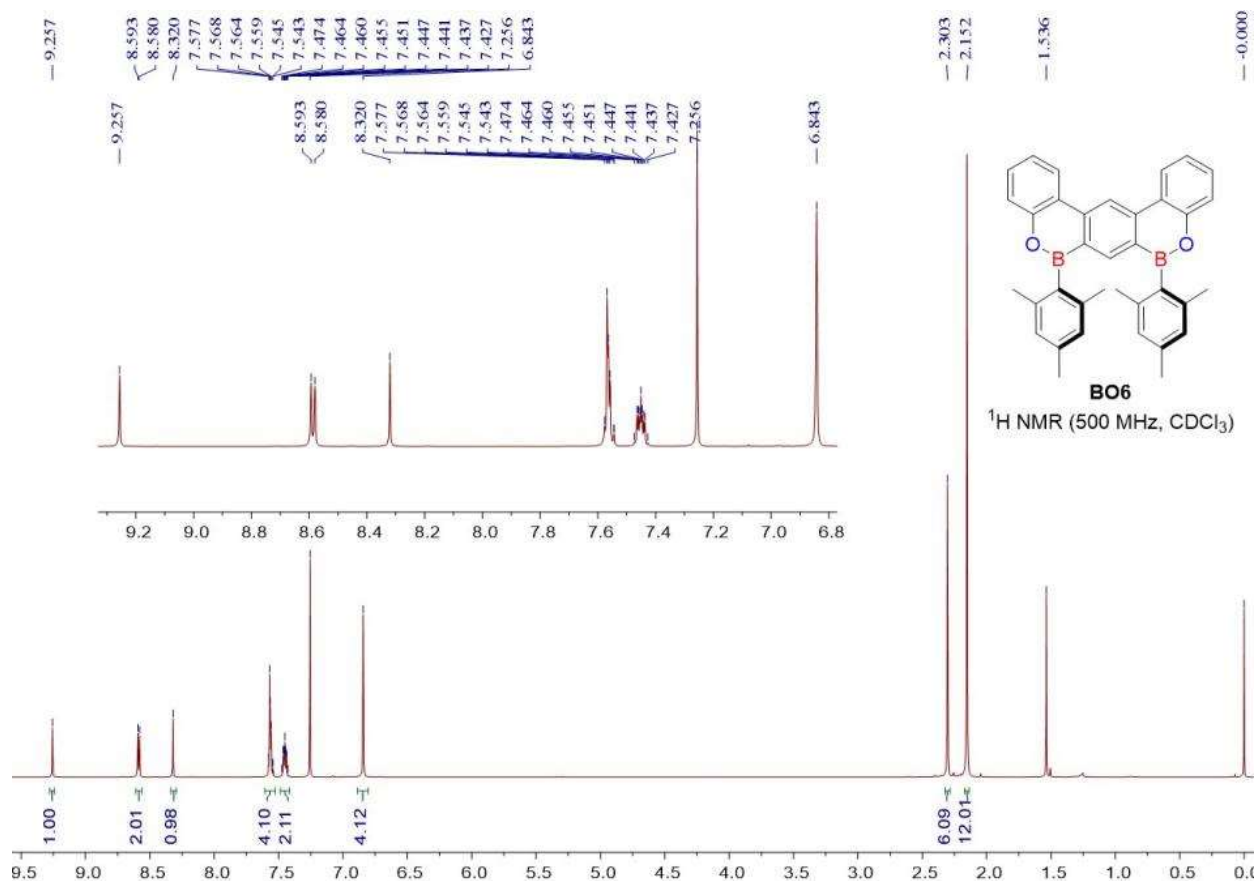
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{54}\text{H}_{48}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{54}\text{H}_{48}[^{11}\text{B}]_2\text{NaO}_2$	773.3712	773.3733	2.75



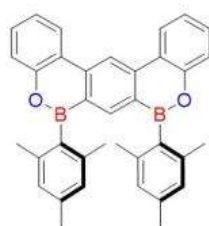


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{36}\text{H}_{32} [^{11}\text{B}]_2 \text{O}_2$	$\text{C}_{36}\text{H}_{32} [^{11}\text{B}]_2 \text{O}_2$	518.2586	518.2583	-0.59



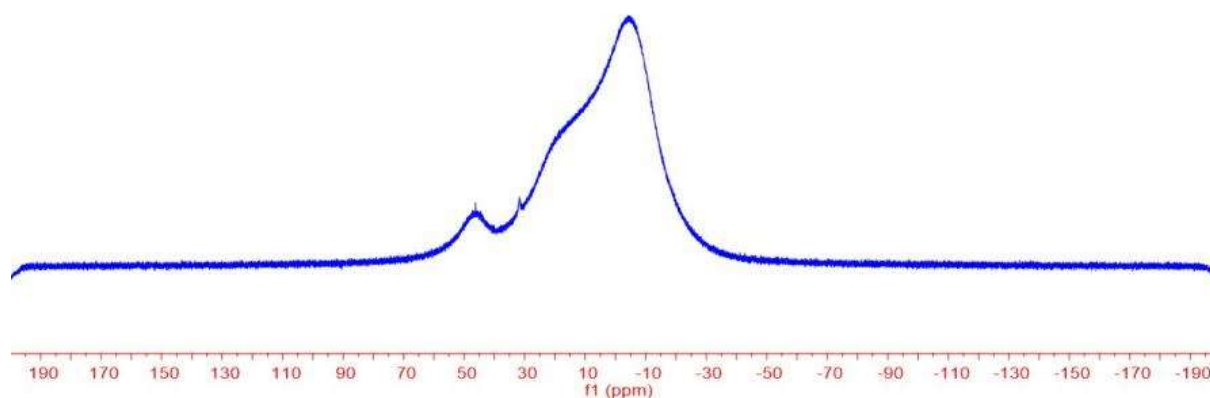


— 46.23

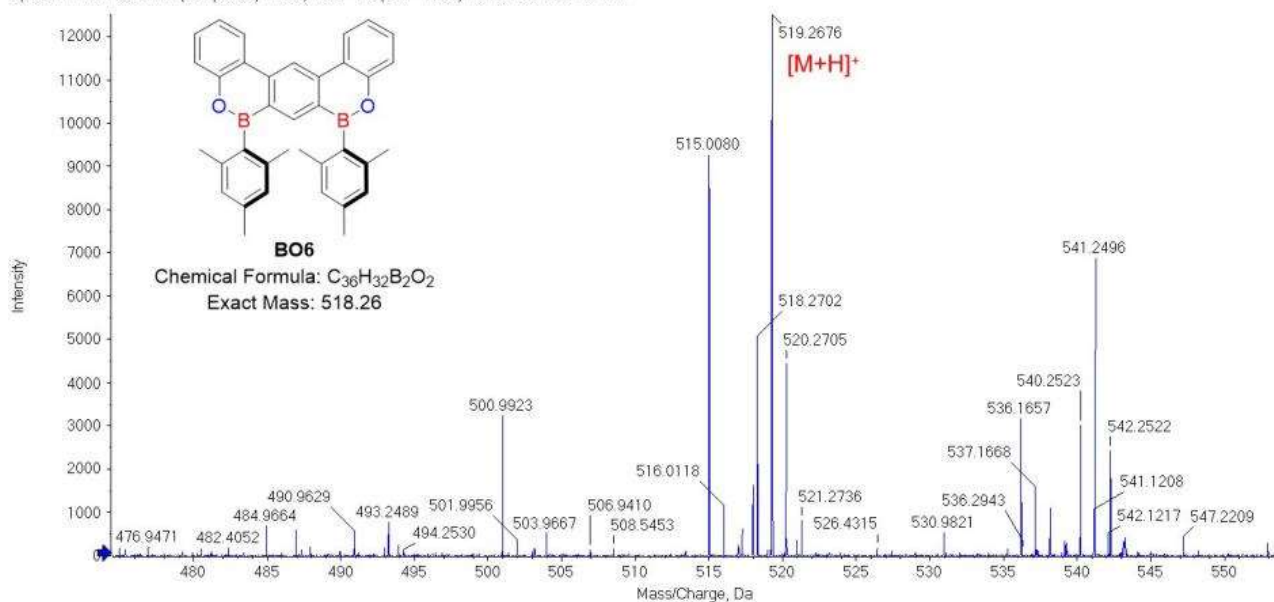


BO6

^{11}B NMR (160 MHz, CDCl_3)



Spectrum from 0922.wiff (sample 32) - BO6, +TOF MS (100 - 1500) from 0.130 to 0.191 min



Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{36}\text{H}_{32}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{36}\text{H}_{33}[^{11}\text{B}]_2\text{O}_2$	519.2676	519.2661	-3.0

Cartesian coordinates of the optimized structures

CC1a_S₀

C	-0.00000100	4.67049000	0.00006800
C	1.21031700	3.97921100	0.00005600
C	1.23396100	2.57501400	0.00002500
C	0.00000000	1.86011400	0.00000300
C	-1.23396200	2.57501400	0.00002000
C	-1.21031900	3.97921000	0.00005300
C	2.45931000	1.82867500	0.00002100
C	0.00000000	0.43415800	-0.00003900
C	1.24042400	-0.28156800	-0.00005700
C	2.48872500	0.46215400	-0.00001200
C	1.21096800	-1.68644100	-0.00012200
H	2.14782100	-2.23441000	-0.00014000
C	0.00000200	-2.37445300	-0.00016000
C	-1.21096500	-1.68644300	-0.00012600
C	-1.24042300	-0.28156900	-0.00006400
C	-2.48872400	0.46215200	-0.00002900
C	-2.45931000	1.82867300	0.00001000
H	-3.39604200	2.38194500	0.00004100
H	3.39604100	2.38194800	0.00004900
H	-0.00000200	5.75723000	0.00009300
H	2.15091700	4.52471800	0.00007300
H	-2.15092000	4.52471700	0.00006600
H	0.00000300	-3.46126100	-0.00021500
H	-2.14781700	-2.23441300	-0.00015100
C	-3.80509600	-0.25706800	-0.00001000
C	-4.42858200	-0.59044700	-1.22078900
C	-4.42848800	-0.59053700	1.22080700
C	-5.66534500	-1.24369100	-1.19762900
C	-5.66524200	-1.24377800	1.19769700
C	-6.30415700	-1.57550900	0.00004400
H	-6.14046300	-1.50077000	-2.14266700
H	-6.14029100	-1.50093600	2.14274800
C	3.80509700	-0.25706400	-0.00000500
C	4.42855900	-0.59046800	-1.22079100
C	4.42851000	-0.59051500	1.22080500
C	5.66532100	-1.24371000	-1.19764300
C	5.66526400	-1.24375900	1.19768300
C	6.30415700	-1.57550600	0.00002500
H	6.14042000	-1.50081000	-2.14268500
H	6.14032600	-1.50090400	2.14273100

C	7.65550800	-2.25208000	0.00004900
H	8.47033000	-1.51539900	0.00001700
H	7.78897600	-2.88170200	0.88638600
H	7.78897500	-2.88177200	-0.88624000
C	3.78114100	-0.25519000	2.54640100
H	3.66272800	0.82692000	2.67657500
H	2.77909500	-0.69235500	2.62806200
H	4.38251500	-0.63088200	3.38002600
C	3.78124300	-0.25511100	-2.54640500
H	2.77926000	-0.69240700	-2.62817500
H	3.66268900	0.82699200	-2.67649500
H	4.38272400	-0.63065500	-3.38001900
C	-7.65551000	-2.25207700	0.00008600
H	-7.78896900	-2.88169700	0.88642500
H	-8.47033000	-1.51539300	0.00006200
H	-7.78899000	-2.88177000	-0.88620100
C	-3.78108800	-0.25523700	2.54639400
H	-2.77908200	-0.69249300	2.62806500
H	-3.66257400	0.82686500	2.67653800
H	-4.38249500	-0.63085200	3.38003000
C	-3.78129400	-0.25506800	-2.54641200
H	-3.66274800	0.82703800	-2.67649000
H	-2.77931100	-0.69235700	-2.62820800
H	-4.38279000	-0.63060300	-3.38001900

BO1a_S₀

C	0.00001600	4.44592300	-0.00019000
C	-1.21505300	3.75947600	0.00595400
C	-1.20828000	2.36681300	0.00641400
C	-0.00000100	1.63909100	-0.00006900
C	1.20829000	2.36679700	-0.00661400
C	1.21507700	3.75946200	-0.00627500
C	-0.00000500	0.19266900	-0.00000500
C	-1.23966300	-0.49745800	0.01569800
C	-1.20813100	-1.90141400	0.01145300
H	-2.14855800	-2.44767700	0.01804600
C	-0.00002600	-2.60140000	0.00012800
C	1.20808700	-1.90143300	-0.01126800
C	1.23964300	-0.49747600	-0.01564700
H	0.00002200	5.53205600	-0.00023800
H	-2.16627100	4.28088100	0.01140100
H	2.16630100	4.28085600	-0.01176300
H	-0.00003200	-3.68808900	0.00018500
H	2.14850600	-2.44771100	-0.01781200

C	4.00432800	-0.24143500	-0.03117000
C	4.73194600	-0.34625000	1.17525700
C	4.60561800	-0.68306500	-1.22977200
C	6.02042300	-0.88782500	1.16679200
C	5.89836000	-1.21740600	-1.20397400
C	6.62447600	-1.32756300	-0.01525200
H	6.56599200	-0.96993300	2.10557200
H	6.34929300	-1.55568100	-2.13549800
C	-4.00433000	-0.24141800	0.03123000
C	-4.60561700	-0.68302600	1.22983000
C	-4.73194200	-0.34626700	-1.17520600
C	-5.89835300	-1.21738900	1.20404200
C	-6.02040800	-0.88785900	-1.16673200
C	-6.62446200	-1.32758000	0.01532200
H	-6.34927500	-1.55565500	2.13557400
H	-6.56597900	-0.97000200	-2.10550900
C	-8.03043300	-1.88150500	0.00896700
H	-8.77590700	-1.07689700	0.06811100
H	-8.23633500	-2.44425400	-0.90836000
H	-8.20345500	-2.54740300	0.86111800
C	-4.12589500	0.12484700	-2.48142600
H	-3.94695600	1.20715800	-2.47173300
H	-3.15950300	-0.35758900	-2.67779300
H	-4.78331100	-0.09595500	-3.32837400
C	-3.87316200	-0.56601000	2.55124300
H	-2.89488900	-1.06135200	2.52125800
H	-3.69172100	0.48369400	2.81639500
H	-4.44870200	-1.01606300	3.36645300
C	8.03045400	-1.88147000	-0.00889900
H	8.20350100	-2.54731400	-0.86108600
H	8.77591900	-1.07684900	-0.06797700
H	8.23634600	-2.44427200	0.90839900
C	3.87321300	-0.56599600	-2.55120600
H	2.89462000	-1.06068700	-2.52105800
H	3.69245700	0.48374700	-2.81668200
H	4.44845200	-1.01667000	-3.36628600
C	4.12583900	0.12476000	2.48148800
H	3.94580300	1.20688100	2.47144500
H	3.15999300	-0.35858500	2.67833100
H	4.78373500	-0.09507300	3.32831400
B	-2.54101600	0.33964100	0.02608200
B	2.54100500	0.33959700	-0.02609900
O	-2.41304400	1.71818200	0.01492900
O	2.41303800	1.71815200	-0.01505600

CC1b_S₀

C	1.21328000	4.12151000	-0.00131900
C	-1.23323900	2.71823900	0.00036200
C	0.00264100	4.81367400	-0.00197100
C	1.23591600	2.71670600	0.00041700
C	0.00089600	2.00337500	0.00202000
C	-1.20885600	4.12301700	-0.00137900
H	0.00331800	5.90130200	-0.00332100
H	2.15499400	4.66689700	-0.00243500
H	-2.14989100	4.66957100	-0.00254500
C	0.00002000	0.57788200	0.00539100
C	-0.00174900	-2.25595900	0.01153400
C	-1.23722100	-0.14053300	0.00537800
C	1.23635300	-0.14208200	0.00539600
C	1.20328500	-1.54652300	0.00727800
C	-1.20588000	-1.54500900	0.00732800
H	2.14443100	-2.09127600	0.00415500
H	-2.14772700	-2.08853000	0.00428300
C	2.48681500	0.59929700	0.00074600
C	2.46024400	1.96700900	-0.00034800
C	-2.48676100	0.60239600	0.00064400
C	-2.45850200	1.97007300	-0.00046700
C	-3.80219100	-0.11934900	-0.00234500
C	-6.30305100	-1.43631300	-0.00877200
C	-4.43331600	-0.44454400	1.21708900
C	-4.42127100	-0.45552100	-1.22501500
C	-5.66035200	-1.10566400	-1.20538300
C	-5.67217800	-1.09488400	1.19108900
H	-6.13562300	-1.35859400	-2.15259600
H	-6.15672100	-1.33945800	2.13579800
C	3.80176400	-0.12333600	-0.00215600
C	6.29822400	-1.44856700	-0.00833500
C	4.42971900	-0.45429600	1.21736800
C	4.41911100	-0.46288900	-1.22475700
C	5.65502300	-1.11906000	-1.20498300
C	5.66539300	-1.11068000	1.19150500
H	6.12594000	-1.38055400	-2.15203100
H	6.14443300	-1.36568900	2.13624700
C	-7.62518900	-2.16741500	-0.01198500
H	-8.21533000	-1.92540100	-0.90289400
H	-8.22406500	-1.91734800	0.87083000
H	-7.47744900	-3.25635400	-0.00630300
C	-3.79453200	-0.09623000	2.54300200

H	-3.67678700	0.98767800	2.66204300
H	-2.79185000	-0.53187400	2.63177100
H	-4.39976400	-0.46478200	3.37738200
C	-3.76951700	-0.11878000	-2.54759500
H	-4.36875300	-0.49078700	-3.38476000
H	-2.76779500	-0.55885000	-2.62449900
H	-3.64659000	0.96384300	-2.67283400
C	-0.00268200	-3.76699900	0.04697500
H	-0.89052800	-4.17831900	-0.44549900
H	-0.00262300	-4.13798700	1.08120300
H	0.88438000	-4.17944300	-0.44596300
C	3.78727200	-0.11260300	2.54323200
H	3.66972200	0.97080200	2.66697300
H	4.39027300	-0.48517400	3.37743800
H	2.78418900	-0.54821000	2.62740400
C	7.64783600	-2.12768400	-0.01176700
H	7.77682000	-2.75930100	-0.89775100
H	7.78337000	-2.75522000	0.87614900
H	8.46334700	-1.39111700	-0.01643200
C	3.76518800	-0.13039900	-2.54734600
H	2.76288200	-0.56963600	-2.62124200
H	4.36276100	-0.50561100	-3.38426700
H	3.64324800	0.95195100	-2.67586400
H	3.39953100	2.51805200	-0.00261500
H	-3.39710100	2.52229300	-0.00282400

BO1b_ S₀

C	0.00000300	4.59305200	0.00691700
C	-1.21529200	3.90659600	0.01235100
C	-1.20829000	2.51396200	0.01199900
C	0.00005600	1.78711900	0.00589200
C	1.20837400	2.51400900	-0.00071700
C	1.21532000	3.90664600	0.00037600
C	0.00008900	0.34174400	0.00685700
C	-1.23591100	-0.35205800	0.02064500
C	-1.20107200	-1.75476800	0.01597200
H	-2.14438900	-2.29831200	0.01749200
C	0.00021900	-2.47641600	0.00816500
C	1.20138300	-1.75471800	-0.00660900
C	1.23607600	-0.35198600	-0.01009200
H	-0.00001700	5.67919000	0.00743500
H	-2.16639200	4.42828800	0.01753500
H	2.16639400	4.42838100	-0.00512300
H	2.14466200	-2.29819300	-0.01854300

C	4.00159900	-0.09804500	-0.03298200
C	4.73135100	-0.20793500	1.17165700
C	4.60024700	-0.53634900	-1.23406900
C	6.01918700	-0.75101400	1.15905300
C	5.89236300	-1.07244900	-1.21255900
C	6.62055900	-1.18747100	-0.02557200
H	6.56642700	-0.83689000	2.09654700
H	6.34116700	-1.40810300	-2.14608200
C	-4.00160600	-0.09809300	0.02775300
C	-4.60775000	-0.53721400	1.22477500
C	-4.72400500	-0.20680000	-1.18142100
C	-5.89984300	-1.07296400	1.19490000
C	-6.01203500	-0.74958600	-1.17715800
C	-6.62076600	-1.18689900	0.00337700
H	-6.35445700	-1.40923300	2.12538800
H	-6.55355000	-0.83447300	-2.11806100
C	-8.02621800	-1.74214100	-0.00758000
H	-8.77278100	-0.93816100	0.04626400
H	-8.22769300	-2.30748400	-0.92431600
H	-8.20230800	-2.40600200	0.84555300
C	-4.11276200	0.26174200	-2.48613600
H	-3.93482700	1.34422800	-2.47817100
H	-3.14498200	-0.22012700	-2.67692500
H	-4.76627700	0.03833900	-3.33544700
C	-3.88089800	-0.41597900	2.54886300
H	-2.90079200	-0.90788500	2.52282200
H	-3.70392400	0.63469100	2.81317400
H	-4.45802400	-0.86686500	3.36253100
C	8.02599100	-1.74287400	-0.02369300
H	8.19684000	-2.40595300	-0.87849800
H	8.77226400	-0.93888900	-0.08134300
H	8.23300900	-2.30907500	0.89127800
C	3.86524600	-0.41390900	-2.55355800
H	2.88528200	-0.90580200	-2.52202600
H	3.68671300	0.63701200	-2.81581800
H	4.43734800	-0.86403000	-3.37119500
C	4.12807400	0.25953000	2.48045100
H	3.94951700	1.34191800	2.47421200
H	3.16172100	-0.22294900	2.67689100
H	4.78695700	0.03592500	3.32555600
B	-2.53830900	0.48397400	0.02743100
B	2.53837200	0.48409900	-0.02353500
O	-2.41222100	1.86282300	0.01855400
O	2.41231300	1.86292900	-0.01065100

C	0.00031800	-3.98735600	0.03751200
H	0.00814300	-4.36504600	1.06877300
H	-0.89009600	-4.39732700	-0.45066400
H	0.88296600	-4.39781900	-0.46413000

CC1c_ S₀

H	3.46143800	-0.07596400	0.00000000
C	2.37327600	-0.05626300	0.00000000
C	-0.39056200	-0.01337000	0.00000000
C	1.73595700	-0.04498800	-1.23962400
C	1.73595700	-0.04498800	1.23962400
C	0.31575900	-0.02145700	1.26611000
C	0.31575900	-0.02145700	-1.26611000
C	-1.82710700	0.00204600	0.00000000
C	-4.66434800	0.02793700	0.00000000
C	-2.56131600	0.00959400	1.22223600
C	-2.56131600	0.00959400	-1.22223600
C	-3.96650900	0.02217400	-1.20456600
C	-3.96650900	0.02217400	1.20456600
H	-4.50296600	0.02771100	-2.15124200
H	-4.50296600	0.02771100	2.15124200
H	-5.75187600	0.03754100	0.00000000
C	-0.46707300	-0.00631900	2.50040700
C	-0.46707300	-0.00631900	-2.50040700
C	-1.83310500	0.00679100	2.44710400
H	-2.39596600	0.01799300	3.37898200
C	-1.83310500	0.00679100	-2.44710400
H	-2.39596600	0.01799300	-3.37898200
C	2.64943000	-0.06263000	2.44890100
H	3.69108000	-0.09324900	2.11362200
H	2.48237000	-0.93094000	3.09246600
H	2.53088900	0.82162700	3.08177200
C	2.64943000	-0.06263000	-2.44890100
H	2.48237000	-0.93094000	-3.09246600
H	3.69108000	-0.09324900	-2.11362200
H	2.53088900	0.82162700	-3.08177200
C	0.10843300	0.00215100	-3.89134400
C	1.04588800	0.02356300	-6.55841100
C	0.30796400	-1.21205000	-4.58065100
C	0.35309900	1.22770700	-4.54522000
C	0.82422200	1.21591900	-5.86283800
C	0.77985100	-1.17945000	-5.89769400
H	1.02246700	2.16577500	-6.35845600
H	0.94347400	-2.12116100	-6.42070500

C	0.10843300	0.00215100	3.89134400
C	1.04588800	0.02356300	6.55841100
C	0.30796400	-1.21205000	4.58065100
C	0.35309900	1.22770700	4.54522000
C	0.82422200	1.21591900	5.86283800
C	0.77985100	-1.17945000	5.89769400
H	1.02246700	2.16577500	6.35845600
H	0.94347400	-2.12116100	6.42070500
C	0.12648000	2.54622200	3.83956600
H	0.70455000	2.61235600	2.90935200
H	0.41476600	3.38711600	4.47841400
H	-0.92615300	2.67596100	3.56041200
C	0.03422200	-2.54147200	3.91297100
H	0.60608900	-2.65291900	2.98315000
H	-1.02314500	-2.64398100	3.64062400
H	0.29686500	-3.37339600	4.57424700
C	1.52691100	0.03561500	7.99059700
H	2.11181000	-0.86079400	8.22487100
H	0.68284800	0.06565400	8.69364500
H	2.15117000	0.91219200	8.19677300
C	0.12648000	2.54622200	-3.83956600
H	0.70455000	2.61235600	-2.90935200
H	-0.92615300	2.67596100	-3.56041200
H	0.41476600	3.38711600	-4.47841400
C	0.03422200	-2.54147200	-3.91297100
H	0.29686500	-3.37339600	-4.57424700
H	-1.02314500	-2.64398100	-3.64062400
H	0.60608900	-2.65291900	-2.98315000
C	1.52691100	0.03561500	-7.99059700
H	2.11181000	-0.86079400	-8.22487100
H	2.15117000	0.91219200	-8.19677300
H	0.68284800	0.06565400	-8.69364500

BO1c_ S₀

C	0.00001100	-4.47302500	-0.00001500
C	1.21047600	-3.78182400	0.00068200
C	1.19999700	-2.38875100	0.00066300
C	0.00000400	-1.64848600	-0.00001400
C	-1.19998500	-2.38875800	-0.00069200
C	-1.21045600	-3.78183100	-0.00071100
C	0.00000000	-0.19372000	-0.00001300
C	1.25566400	0.48859300	0.00127100
C	1.23085300	1.90597100	0.00243900
C	-0.00001500	2.56668800	-0.00001300

C	-1.23087500	1.90595700	-0.00246400
C	-1.25566900	0.48858100	-0.00129600
H	0.00001500	-5.55916100	-0.00001500
H	2.16557000	-4.29606900	0.00116500
H	-2.16554800	-4.29608200	-0.00119400
C	-4.05775700	0.08073400	-0.00037700
C	-4.75007000	0.26908800	1.21542000
C	-4.75467500	0.25399300	-1.21437800
C	-6.09580400	0.64744600	1.19941300
C	-6.10162600	0.63235200	-1.19698500
C	-6.79184800	0.83536200	0.00094400
H	-6.61470500	0.79741000	2.14506200
H	-6.62491600	0.77008100	-2.14187500
C	4.05776000	0.08074400	0.00037100
C	4.75465800	0.25397600	1.21438700
C	4.75009600	0.26910900	-1.21541000
C	6.10161000	0.63233400	1.19702400
C	6.09583100	0.64746400	-1.19937400
C	6.79185400	0.83536200	-0.00089000
H	6.62488400	0.77004900	2.14192500
H	6.61474700	0.79744400	-2.14501100
C	8.25365100	1.21881400	-0.00459300
H	8.89650900	0.34018900	-0.15070900
H	8.48269900	1.92229500	-0.81307600
H	8.54859100	1.68381600	0.94203100
C	4.04628200	0.05610000	-2.54036000
H	3.75995400	-0.99481600	-2.67480200
H	3.12474000	0.64818900	-2.61371400
H	4.68749000	0.33462100	-3.38279000
C	4.05694700	0.02627800	2.54016000
H	3.13608900	0.61804900	2.62431000
H	3.77078500	-1.02591600	2.66428100
H	4.70209800	0.29531200	3.38266100
C	-8.25364500	1.21881400	0.00467900
H	-8.54860200	1.68383300	-0.94193200
H	-8.89650100	0.34018600	0.15079000
H	-8.48268000	1.92228000	0.81317800
C	-4.05698500	0.02631200	-2.54016500
H	-3.13613100	0.61808600	-2.62432200
H	-3.77082300	-1.02588000	-2.66430400
H	-4.70215100	0.29535400	-3.38265300
C	-4.04623700	0.05605200	2.54035500
H	-3.75990800	-0.99486700	2.67477400
H	-3.12469300	0.64813900	2.61370900

H	-4.68743300	0.33455600	3.38280000
B	2.54586900	-0.37581400	0.00100800
B	-2.54586800	-0.37582900	-0.00103700
O	2.40379700	-1.75172200	0.00105300
O	-2.40379000	-1.75173600	-0.00108300
H	-0.00002100	3.65436200	-0.00001400
C	-2.47850300	2.76155000	-0.00628100
H	-3.10641800	2.56683100	-0.88098700
H	-3.10691200	2.57401900	0.86966900
H	-2.21090600	3.82268300	-0.01041100
C	2.47846200	2.76159000	0.00625400
H	3.10637400	2.56689500	0.88096700
H	3.10688100	2.57406700	-0.86969000
H	2.21083900	3.82271700	0.01037300

CC1d_S₀

C	0.00000000	0.00000000	1.60467800
C	0.00000000	0.00000000	-1.23248100
C	-0.00834900	-1.20684000	0.89027900
C	0.00834900	1.20684000	0.89027900
C	0.00726900	1.23656600	-0.51282200
C	-0.00726900	-1.23656600	-0.51282200
C	0.00000000	0.00000000	-2.65742700
C	0.00000000	0.00000000	-5.46714800
C	0.01072500	1.23475300	-3.37125000
C	-0.01072500	-1.23475300	-3.37125000
C	-0.01050800	-1.21118500	-4.77590600
C	0.01050800	1.21118500	-4.77590600
H	-0.01862600	-2.15239700	-5.32202200
H	0.01862600	2.15239700	-5.32202200
H	0.00000000	0.00000000	-6.55475200
C	0.02109800	2.48724300	-1.25466600
C	-0.02109800	-2.48724300	-1.25466600
C	0.02170900	2.45955500	-2.62216900
H	0.03022700	3.39841000	-3.17381000
C	-0.02170900	-2.45955500	-2.62216900
H	-0.03022700	-3.39841000	-3.17381000
C	-0.03052000	-3.80207500	-0.53205800
C	-0.04734200	-6.29745800	0.79447400
C	-1.25577000	-4.40915000	-0.18358400
C	1.18638500	-4.43964800	-0.20979100
C	1.15519400	-5.67462200	0.44762200
C	-1.24106000	-5.64488800	0.47299600
H	2.09780800	-6.16124800	0.69606600

H	-2.18992800	-6.10777800	0.74185600
C	0.03052000	3.80207500	-0.53205800
C	0.04734200	6.29745800	0.79447400
C	-1.18638500	4.43964800	-0.20979100
C	1.25577000	4.40915000	-0.18358400
C	1.24106000	5.64488800	0.47299600
C	-1.15519400	5.67462200	0.44762200
H	2.18992800	6.10777800	0.74185600
H	-2.09780800	6.16124800	0.69606600
C	2.57538300	3.74438600	-0.50599000
H	2.64299400	2.74695400	-0.05475600
H	3.41463700	4.34127500	-0.13516100
H	2.70555800	3.60969700	-1.58659800
C	-2.51519800	3.80926100	-0.56281600
H	-2.60847900	2.80223700	-0.13824900
H	-2.63594600	3.70375600	-1.64786300
H	-3.34676000	4.41421600	-0.18754600
C	0.05691500	7.64633400	1.47488100
H	-0.83431200	7.78847200	2.09621500
H	0.07335900	8.46236400	0.73906400
H	0.93938900	7.76739200	2.11287000
C	2.51519800	-3.80926100	-0.56281600
H	2.60847900	-2.80223700	-0.13824900
H	2.63594600	-3.70375600	-1.64786300
H	3.34676000	-4.41421600	-0.18754600
C	-2.57538300	-3.74438600	-0.50599000
H	-3.41463700	-4.34127500	-0.13516100
H	-2.70555800	-3.60969700	-1.58659800
H	-2.64299400	-2.74695400	-0.05475600
C	-0.05691500	-7.64633400	1.47488100
H	-0.93938900	-7.76739200	2.11287000
H	0.83431200	-7.78847200	2.09621500
H	-0.07335900	-8.46236400	0.73906400
H	0.04265500	2.14846600	1.43033400
H	-0.04265500	-2.14846600	1.43033400
C	0.00000000	0.00000000	3.09134200
C	0.00000000	0.00000000	5.91248000
C	-0.71943000	0.96758200	3.81400200
C	0.71943000	-0.96758200	3.81400200
C	0.71920100	-0.96806700	5.20846500
C	-0.71920100	0.96806700	5.20846500
H	-1.30289900	1.71095400	3.27653600
H	1.30289900	-1.71095400	3.27653600
H	1.28950600	-1.72226700	5.74614100

H	-1.28950600	1.72226700	5.74614100
H	0.00000000	0.00000000	6.99993000

BO1d_S₀

C	0.00001600	5.26478500	-0.00007900
C	-1.21534800	4.57856600	0.01805600
C	-1.20851100	3.18602700	0.01830300
C	0.00001000	2.45924000	-0.00002700
C	1.20853500	3.18602200	-0.01838700
C	1.21537700	4.57856100	-0.01819000
C	0.00000800	1.01470300	-0.00000200
C	-1.23575200	0.32023800	0.02517500
C	-1.20358500	-1.08089900	0.02189200
C	0.00000400	-1.80680100	0.00001900
C	1.20359100	-1.08090600	-0.02186100
C	1.23576200	0.32023500	-0.02516000
H	0.00001800	6.35090700	-0.00009800
H	-2.16626400	5.10033600	0.03293000
H	2.16629500	5.10032600	-0.03308200
C	4.00301200	0.57754100	-0.06414900
C	4.74993800	0.51362200	1.13351400
C	4.58887600	0.10355900	-1.25826400
C	6.04160400	-0.02030200	1.12123500
C	5.88538400	-0.42176100	-1.23630200
C	6.63035800	-0.49167500	-0.05624900
H	6.60217400	-0.07099600	2.05339000
H	6.32434700	-0.78473700	-2.16421000
C	-4.00300300	0.57756100	0.06416000
C	-4.58889800	0.10367800	1.25830200
C	-4.74990600	0.51355200	-1.13351500
C	-5.88540600	-0.42164200	1.23635100
C	-6.04157100	-0.02037400	-1.12122200
C	-6.63035100	-0.49165400	0.05628600
H	-6.32439400	-0.78453700	2.16427900
H	-6.60211800	-0.07114300	-2.05338600
C	-8.03990300	-1.03640100	0.05588500
H	-8.77799500	-0.23186000	0.17680600
H	-8.27252000	-1.54834700	-0.88443600
H	-8.19625700	-1.74562800	0.87574100
C	-4.16197600	1.01964900	-2.43511900
H	-3.97545200	2.09990700	-2.39632500
H	-3.20227000	0.53730500	-2.66222700
H	-4.83480700	0.82810700	-3.27706800

C	-3.83834200	0.17977800	2.57253700
H	-2.85734600	-0.30673700	2.51212300
H	-3.66112900	1.22108700	2.87184300
H	-4.39942100	-0.30264000	3.37921500
C	8.03990900	-1.03642400	-0.05583600
H	8.19626200	-1.74567200	-0.87567400
H	8.77800200	-0.23188700	-0.17677700
H	8.27252700	-1.54834800	0.88449800
C	3.83825400	0.17949800	-2.57247100
H	2.85739900	-0.30730400	-2.51203700
H	3.66072800	1.22076500	-2.87173200
H	4.39944100	-0.30273300	-3.37918600
C	4.16205100	1.01985800	2.43508400
H	3.97579500	2.10016300	2.39627700
H	3.20221300	0.53775400	2.66213400
H	4.83478500	0.82815500	3.27707400
B	-2.53914000	1.15613000	0.05087600
B	2.53915200	1.15611700	-0.05088500
O	-2.41193500	2.53499400	0.03866900
O	2.41195500	2.53498300	-0.03873100
H	-2.14664400	-1.62068300	0.05966600
H	2.14665200	-1.62068700	-0.05963300
C	-0.00000700	-3.29227600	0.00001800
C	0.97911200	-4.01453400	0.70352800
C	-0.97914700	-4.01450900	-0.70349500
C	0.97964700	-5.40847900	0.70297100
H	1.73167200	-3.47881800	1.27542500
C	-0.97971600	-5.40845100	-0.70294200
H	-1.73169200	-3.47876800	-1.27538900
C	-0.00004200	-6.11203700	0.00001400
H	1.74266400	-5.94551200	1.26030100
H	-1.74274500	-5.94546700	-1.26027300
H	-0.00005700	-7.19865100	0.00001200

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C	-0.00096200	1.23888300	-0.00000400
C	0.00193000	-1.59394700	0.00000000
C	-1.20735500	0.52818600	-0.00002700
C	1.20688700	0.53066400	0.00001900
C	1.23895200	-0.87451000	0.00002000
C	-1.23656100	-0.87704800	-0.00002500
C	0.00337300	-3.01988400	0.00000700
C	0.00623000	-5.83032300	0.00002200
C	1.23851300	-3.73286000	0.00003200

C	-1.23031100	-3.73537500	-0.00001100
C	-1.20546900	-5.14015600	-0.00000300
C	1.21652100	-5.13769000	0.00003900
H	-2.14632100	-5.68695800	-0.00001600
H	2.15847900	-5.68258500	0.00005800
H	0.00733900	-6.91793600	0.00002800
C	2.48968100	-1.61578300	0.00004300
C	-2.48577900	-1.62086200	-0.00004300
C	2.46281900	-2.98339200	0.00004900
H	3.40202500	-3.53451700	0.00006600
C	-2.45614500	-2.98841200	-0.00003500
H	-3.39422900	-3.54144500	-0.00004800
C	-3.80256400	-0.90168500	-0.00006500
C	-6.30138300	0.41860500	-0.00010400
C	-4.42633400	-0.56881600	-1.22113100
C	-4.42640500	-0.56887900	1.22098100
C	-5.66318100	0.08536300	1.19814400
C	-5.66311200	0.08542200	-1.19833200
H	-6.13854000	0.34294000	2.14400300
H	-6.13841800	0.34304500	-2.14420500
C	3.80501500	-0.89395200	0.00005400
C	6.30131800	0.43109200	0.00007300
C	4.42820600	-0.55995300	-1.22099600
C	4.42815000	-0.55988400	1.22111400
C	5.66369100	0.09668900	1.19830500
C	5.66374500	0.09662200	-1.19816800
H	6.13851000	0.35522300	2.14417300
H	6.13860800	0.35510100	-2.14402900
C	3.78232400	-0.90068700	2.54554200
H	2.77327000	-0.47758800	2.62208700
H	4.37613400	-0.51571100	3.38065600
H	3.67740200	-1.98476100	2.67577300
C	3.78244200	-0.90083400	-2.54543500
H	2.77338600	-0.47775300	-2.62204900
H	3.67753900	-1.98491700	-2.67561400
H	4.37628500	-0.51589600	-3.38054200
C	7.64987100	1.11218800	0.00008400
H	7.78091200	1.74201700	-0.88682300
H	8.46649400	0.37682800	0.00012400
H	7.78087200	1.74206800	0.88696200
C	-3.77997200	-0.90848500	2.54541900
H	-2.77180200	-0.48330400	2.62206000
H	-3.67281500	-1.99235100	2.67553600
H	-4.37463000	-0.52482400	3.38053600

C	-3.77982200	-0.90835200	-2.54554800
H	-4.37448300	-0.52473800	-3.38068400
H	-3.67255800	-1.99220600	-2.67566800
H	-2.77169000	-0.48307400	-2.62214500
C	-7.65126100	1.09708000	-0.00012500
H	-7.78350300	1.72668700	-0.88701500
H	-7.78354700	1.72665500	0.88678000
H	-8.46645400	0.36013700	-0.00015800
H	2.14503700	1.07943900	0.00004100
H	-2.14661100	1.07506200	-0.00004700
C	-0.00301100	2.73915700	0.00000300
C	-0.00328400	5.56521000	0.00002100
C	-0.00121600	3.44613300	-1.22046000
C	-0.00190700	3.44611800	1.22047500
C	-0.00094700	4.84515100	1.19800000
C	-0.00028100	4.84516700	-1.19796600
H	0.00333800	5.38599700	2.14383700
H	0.00452500	5.38602500	-2.14379300
C	0.00400900	2.71684800	-2.54542300
H	0.00359000	3.42388000	-3.38112800
H	-0.87311000	2.06663900	-2.65112200
H	0.88542800	2.07185500	-2.64757300
C	0.00257000	2.71681500	2.54543200
H	-0.87476700	2.06683700	2.65075700
H	0.00197900	3.42383700	3.38114500
H	0.88377300	2.07158800	2.64794100
C	-0.03571400	7.07576600	0.00002400
H	-1.06853000	7.45115500	-0.00025300
H	0.45896700	7.48761400	-0.88670800
H	0.45848300	7.48759700	0.88703500

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C	-0.00822300	-5.65134300	-0.00398900
C	-1.22259200	-4.96340400	-0.01446700
C	-1.21386600	-3.57077600	-0.01346900
C	-0.00450100	-2.84550300	-0.00121600
C	1.20294000	-3.57400800	0.00964200
C	1.20796800	-4.96665500	0.00787200
C	-0.00259300	-1.39987900	-0.00000700
C	-1.23830600	-0.70522900	-0.02036100
C	-1.20342500	0.69792900	-0.01554900
C	0.00122800	1.41749400	0.00128000
C	1.20388600	0.69461000	0.01780000
C	1.23498400	-0.70863000	0.02130500

H	-0.00966700	-6.73747500	-0.00509200
H	-2.17432100	-5.48383900	-0.02442800
H	2.15831400	-5.48962800	0.01675700
C	4.00063500	-0.96755700	0.04825300
C	4.73231900	-0.86019000	-1.15538700
C	4.59875800	-0.53043700	1.25001500
C	6.02158400	-0.32068000	-1.14119100
C	5.89231400	0.00194800	1.23010500
C	6.62243500	0.11461700	0.04408000
H	6.57024400	-0.23636000	-2.07797100
H	6.34051400	0.33724000	2.16400300
C	-4.00471300	-0.95702200	-0.04719200
C	-4.60185100	-0.51565300	-1.24786000
C	-4.73613000	-0.85083400	1.15675200
C	-5.89418300	0.01971100	-1.22662100
C	-6.02411900	-0.30830600	1.14389000
C	-6.62398400	0.13127400	-0.04032600
H	-6.34163300	0.35825500	-2.15970000
H	-6.57255000	-0.22495800	2.08089400
C	-8.02933600	0.68675800	-0.03875200
H	-8.77561200	-0.11709700	-0.09826400
H	-8.23689800	1.25160300	0.87690600
H	-8.19923400	1.35127200	-0.89258500
C	-4.13442300	-1.32132500	2.46521400
H	-3.95556700	-2.40366400	2.45696300
H	-3.16835500	-0.83912300	2.66418500
H	-4.79434200	-1.09967100	3.30999800
C	-3.86492500	-0.63329500	-2.56665000
H	-2.88819200	-0.13472700	-2.53413200
H	-3.67896800	-1.68285600	-2.82921400
H	-4.43899000	-0.18641500	-3.38461600
C	8.02915600	0.66663500	0.04402900
H	8.19907500	1.33257300	0.89676600
H	8.77330500	-0.13894400	0.10684000
H	8.23991200	1.22894200	-0.87244300
C	3.86142700	-0.64948900	2.56844700
H	2.88571900	-0.14886000	2.53688500
H	3.67330100	-1.69925400	2.82863900
H	4.43628900	-0.20560200	3.38748300
C	4.12959700	-1.32622000	-2.46497600
H	3.94835400	-2.40818100	-2.45929500
H	3.16459100	-0.84144300	-2.66282300
H	4.79001400	-1.10403400	-3.30923300
B	-2.54210100	-1.53966300	-0.03687700

B	2.53655400	-1.54651200	0.03664500
O	-2.41691500	-2.91867800	-0.02631900
O	2.40774100	-2.92516300	0.02375400
H	-2.14316300	1.24618600	-0.02817100
H	2.14507700	1.24035300	0.03075400
C	0.00413300	2.91624200	0.00057000
C	0.12465400	3.62146300	-1.21499200
C	-0.11750200	3.62386500	1.21411800
C	0.12204400	5.01960700	-1.19368200
C	-0.11332300	5.02242300	1.18990600
C	0.00851000	5.74079100	-0.00205700
H	0.20999700	5.55895500	-2.13513300
H	-0.20879200	5.56388700	2.12930700
C	0.04285600	7.25160200	-0.00187800
H	1.07388000	7.62645700	0.05257500
H	-0.40259800	7.66305400	-0.91419500
H	-0.49841300	7.66535500	0.85564900
C	-0.25127500	2.89739100	2.53460700
H	-1.15991100	2.28442800	2.57223500
H	0.59162100	2.21846500	2.71078400
H	-0.29170000	3.60661300	3.36697400
C	0.24762600	2.89195500	-2.53484900
H	1.15193500	2.27279500	-2.57491800
H	-0.60049600	2.21844000	-2.70671400
H	0.28971400	3.59958500	-3.36848700

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C	0.00000000	0.00000000	-3.50164500
C	0.00000000	0.00000000	-0.69310600
C	0.00695500	1.21174300	-2.81335400
C	-0.00695500	-1.21174300	-2.81335400
C	-0.00727700	-1.24090900	-1.40791400
C	0.00727700	1.24090900	-1.40791400
C	0.00000000	0.00000000	0.73192000
C	0.00000000	0.00000000	3.56906100
C	-0.00214700	-1.23077300	1.45038200
C	0.00214700	1.23077300	1.45038200
C	0.00151300	1.20671400	2.85285100
C	-0.00151300	-1.20671400	2.85285100
H	0.03117100	2.15041000	3.39325200
H	-0.03117100	-2.15041000	3.39325200
C	-0.01563100	-2.48859600	-0.66210800
C	0.01563100	2.48859600	-0.66210800
C	-0.01339400	-2.45852900	0.70533600

H	-0.01949700	-3.39588500	1.25941700
C	0.01339400	2.45852900	0.70533600
H	0.01949700	3.39588500	1.25941700
C	0.02716300	3.80524900	-1.38163900
C	0.04940700	6.30398300	-2.70168700
C	-1.18845300	4.43976900	-1.71444900
C	1.25391400	4.41686800	-1.71657300
C	1.24193400	5.65414100	-2.37031200
C	-1.15452700	5.67661700	-2.36820600
H	2.19198600	6.12077200	-2.62844800
H	-2.09613600	6.16089100	-2.62479800
C	-0.02716300	-3.80524900	-1.38163900
C	-0.04940700	-6.30398300	-2.70168700
C	-1.25391400	-4.41686800	-1.71657300
C	1.18845300	-4.43976900	-1.71444900
C	1.15452700	-5.67661700	-2.36820600
C	-1.24193400	-5.65414100	-2.37031200
H	2.09613600	-6.16089100	-2.62479800
H	-2.19198600	-6.12077200	-2.62844800
C	2.51859600	-3.80335400	-1.37802000
H	2.60934300	-2.80400500	-1.82092700
H	3.34861400	-4.41425300	-1.74692900
H	2.64390800	-3.67902200	-0.29555700
C	-2.57243200	-3.75589700	-1.38180900
H	-2.64330400	-2.75437700	-1.82335200
H	-2.69739900	-3.63094000	-0.29937800
H	-3.41311600	-4.35046300	-1.75323600
C	-0.06149600	-7.65481700	-3.37818800
H	-0.94996600	-7.78056900	-4.00691700
H	-0.06804000	-8.46878500	-2.63994400
H	0.82389400	-7.79594200	-4.00802500
C	2.57243200	3.75589700	-1.38180900
H	2.64330400	2.75437700	-1.82335200
H	2.69739900	3.63094000	-0.29937800
H	3.41311600	4.35046300	-1.75323600
C	-2.51859600	3.80335400	-1.37802000
H	-3.34861400	4.41425300	-1.74692900
H	-2.64390800	3.67902200	-0.29555700
H	-2.60934300	2.80400500	-1.82092700
C	0.06149600	7.65481700	-3.37818800
H	-0.82389400	7.79594200	-4.00802500
H	0.94996600	7.78056900	-4.00691700
H	0.06804000	8.46878500	-2.63994400
H	-0.01222100	-2.15004100	-3.36085800

H	0.01222100	2.15004100	-3.36085800
H	0.00000000	0.00000000	-4.58931200
C	0.00000000	0.00000000	5.05543900
C	0.00000000	0.00000000	7.87616200
C	-0.75606300	0.93925900	5.77771200
C	0.75606300	-0.93925900	5.77771200
C	0.75604700	-0.93971800	7.17228500
C	-0.75604700	0.93971800	7.17228500
H	-1.36862800	1.65817600	5.23901400
H	1.36862800	-1.65817600	5.23901400
H	1.35540800	-1.67085100	7.71022200
H	-1.35540800	1.67085100	7.71022200
H	0.00000000	0.00000000	8.96357100

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C	-0.00008900	0.53373000	0.04588700
C	-0.00190500	3.36888000	0.09372800
C	1.20512000	1.26600700	0.05580900
C	-1.20622100	1.26443900	0.05720400
C	-1.21222600	2.65508800	0.08069500
C	1.20933900	2.65666600	0.08064200
H	-2.16815100	3.16862900	0.05906500
H	2.16462300	3.17041000	0.11924700
C	0.00075900	-0.91037300	0.01491100
C	0.00290200	-3.70259100	-0.08299800
C	-1.23945700	-1.60049900	-0.01022800
C	1.24195100	-1.59906000	0.00069200
C	1.21149300	-3.00256400	-0.05103900
C	-1.20672700	-3.00395600	-0.06270200
H	2.15320200	-3.54831100	-0.06895500
H	-2.14753700	-3.55084900	-0.09022500
H	0.00371800	-4.78924900	-0.12594400
C	-0.00298200	4.85397200	0.12026800
C	-0.00525000	7.67276300	0.17097000
C	0.95957400	5.58912800	-0.59299000
C	-0.96673300	5.56146000	0.85944000
C	-0.96761100	6.95554300	0.88481600
C	0.95826300	6.98322100	-0.56818200
H	1.69802100	5.06242000	-1.19226400
H	-1.70423400	5.01237300	1.43945200
H	-1.71735000	7.48241700	1.47063900
H	1.70721800	7.53203900	-1.13454600
H	-0.00609900	8.75995100	0.19053300
O	-2.41248500	0.61980700	0.03366900

O	2.41231000	0.62255800	0.05079900
B	2.54122800	-0.75797300	0.02878700
B	-2.53994900	-0.76079500	0.00495200
C	-4.00506400	-1.33575700	-0.03769900
C	-6.63150700	-2.40383900	-0.15737800
C	-4.72780400	-1.33464900	-1.25252700
C	-4.61468800	-1.87391300	1.11705800
C	-5.91072500	-2.39736900	1.04009100
C	-6.01930000	-1.86849000	-1.29569400
H	-6.36870400	-2.80969200	1.93893700
H	-6.56072300	-1.86883800	-2.24152100
C	4.00708700	-1.33252800	0.00862900
C	6.63465600	-2.40131700	-0.06610700
C	4.60458800	-1.85130800	1.17836400
C	4.74207400	-1.35159600	-1.19850200
C	6.03411600	-1.88543700	-1.21956600
C	5.90149700	-2.37529900	1.12359100
H	6.58529100	-1.90114400	-2.15962000
H	6.35023400	-2.77249800	2.03381900
C	3.86933200	-1.82032900	2.50264100
H	2.87230900	-2.27168300	2.42730400
H	3.72767800	-0.78975600	2.85524900
H	4.42270400	-2.35993500	3.27826800
C	4.13841300	-0.79887300	-2.47315400
H	3.18170600	-1.28324400	-2.71082300
H	4.80572200	-0.94766600	-3.32831000
H	3.93940000	0.27670000	-2.38579700
C	8.04365500	-2.94497600	-0.10153900
H	8.26142600	-3.43395100	-1.05792400
H	8.21326800	-3.67295000	0.69940200
H	8.78219000	-2.14135700	0.02641100
C	-8.03973100	-2.94743300	-0.21627500
H	-8.25160100	-3.40909000	-1.18739500
H	-8.77977300	-2.14842300	-0.06946100
H	-8.21316000	-3.69807200	0.56267700
C	-3.89559600	-1.86214700	2.45053500
H	-2.88982800	-2.29361300	2.37728200
H	-4.44870300	-2.42961500	3.20623800
H	-3.77696600	-0.83789800	2.82934100
C	-4.11178400	-0.76111900	-2.51203000
H	-3.15379600	-1.24305400	-2.74958100
H	-3.91193000	0.31240000	-2.40465500
H	-4.77167100	-0.89436800	-3.37544700

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C	-4.02489500	-0.03338600	0.00000600
C	-1.21607900	-0.01021700	0.00000200
C	-3.32656800	-1.23928900	0.00000300
C	-3.34655500	1.18387500	0.00000600
C	-1.94127300	1.22456300	0.00000400
C	-1.92078300	-1.25683700	0.00000100
C	0.20963500	0.00153600	0.00000100
C	3.04330700	0.02495800	-0.00000100
C	0.91667100	1.23897100	0.00000200
C	0.93705300	-1.22398500	-0.00000200
C	2.34119300	-1.18745700	-0.00000300
C	2.32118200	1.22561900	0.00000100
H	2.89541000	-2.12447900	-0.00000500
H	2.85992300	2.17162600	0.00000200
C	-1.20636500	2.47857100	0.00000400
C	-1.16518600	-2.49849600	-0.00000100
C	0.16143700	2.46005500	0.00000400
H	0.70766800	3.40204300	0.00000400
C	0.20213200	-2.45739400	-0.00000300
H	0.76381400	-3.39025300	-0.00000500
C	-1.87409000	-3.82094500	-0.00000300
C	-3.17457600	-6.33009400	-0.00000500
C	-2.20306500	-4.44672100	-1.22120000
C	-2.20305600	-4.44672800	1.22119400
C	-2.84715400	-5.68887700	1.19826900
C	-2.84716200	-5.68887100	-1.19827700
H	-3.10081600	-6.16633600	2.14414200
H	-3.10083100	-6.16632400	-2.14415100
C	-1.93709100	3.78911300	0.00000400
C	-3.27767900	6.27709000	0.00000300
C	-2.27618600	4.40945900	-1.22118800
C	-2.27618000	4.40946200	1.22119400
C	-2.94003300	5.64118400	1.19827100
C	-2.94003800	5.64117900	-1.19826500
H	-3.20128300	6.11452200	2.14415200
H	-3.20129100	6.11451700	-2.14414600
C	-1.93539800	3.76347200	2.54558700
H	-2.36936800	2.75936400	2.62628000
H	-2.31061500	4.36312300	3.38096700
H	-0.85195600	3.64781400	2.67077600
C	-1.93540700	3.76346400	-2.54557900
H	-2.36938100	2.75935700	-2.62626900
H	-0.85196500	3.64780200	-2.67076800

H	-2.31062200	4.36311400	-3.38096000
C	-3.96524000	7.62237900	0.00000000
H	-4.59562800	7.75062400	-0.88694800
H	-3.23369300	8.44239700	-0.00003900
H	-4.59557100	7.75065700	0.88698200
C	-1.87256200	-3.79538800	2.54557500
H	-2.32246100	-2.79832300	2.62624200
H	-0.79108900	-3.66247600	2.67069200
H	-2.23810900	-4.40094300	3.38098900
C	-1.87258000	-3.79537400	-2.54558100
H	-2.23812400	-4.40093000	-3.38099500
H	-0.79111000	-3.66245000	-2.67070000
H	-2.32249200	-2.79831400	-2.62624300
C	-3.84041900	-7.68627200	-0.00000500
H	-4.46860100	-7.82470800	-0.88698700
H	-4.46866300	-7.82467700	0.88693800
H	-3.09579200	-8.49443400	0.00003600
H	-3.90163100	2.11772200	0.00000800
H	-3.86627500	-2.18212000	0.00000300
H	-5.11253400	-0.04237200	0.00000800
C	4.54302900	0.03738400	-0.00000200
C	7.36821700	0.06630900	-0.00000300
C	5.24931400	0.04606100	-1.22086600
C	5.24931600	0.04602800	1.22086300
C	6.64831500	0.06146500	1.19822700
C	6.64831500	0.06149600	-1.19823000
H	7.18923200	0.07164200	2.14397200
H	7.18923000	0.07169700	-2.14397700
C	4.51858400	0.04307100	2.54522700
H	3.87735100	-0.84067100	2.65003900
H	3.86284200	0.91651800	2.64655300
H	5.22472400	0.05051000	3.38161700
C	4.51858300	0.04313800	-2.54523100
H	5.22472400	0.05057700	-3.38162000
H	3.86285900	0.91660100	-2.64654400
H	3.87733300	-0.84058900	-2.65005800
C	8.87903800	0.04980700	0.00000000
H	9.28567700	0.54839100	-0.88692900
H	9.26524500	-0.97900100	0.00007400
H	9.28567400	0.54851500	0.88686200

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C	-0.00510400	2.86438600	-0.00069700
C	-1.21437400	2.15426000	0.00497100

C	-1.20647700	0.76220800	0.00566200
C	0.00012400	0.03393400	-0.00052700
C	1.20402800	0.76666900	-0.00681200
C	1.20679500	2.15873900	-0.00630100
C	0.00280800	-1.41142600	-0.00030500
C	-1.23597200	-2.10299700	0.01567700
C	-1.20175200	-3.50687500	0.01159500
C	0.00791500	-4.20444200	0.00046100
C	1.21501000	-3.50244700	-0.01107100
C	1.24412400	-2.09844500	-0.01596700
H	-2.16679500	2.67425000	0.00995500
H	2.15729800	2.68224100	-0.01135400
C	4.00802200	-1.83314700	-0.03156900
C	4.73841900	-1.92822100	1.17400300
C	4.60855400	-2.28002200	-1.22863500
C	6.02867300	-2.46553700	1.16635300
C	5.90316200	-2.80979700	-1.20209300
C	6.63197900	-2.91030100	-0.01417700
H	6.57629500	-2.54011900	2.10456200
H	6.35351300	-3.15201500	-2.13246500
C	-4.00070000	-1.84822400	0.03171000
C	-4.60001800	-2.29365800	1.22989700
C	-4.72995600	-1.95037700	-1.17396400
C	-5.89234100	-2.82904200	1.20440700
C	-6.01791000	-2.49315700	-1.16525500
C	-6.61998500	-2.93663300	0.01640000
H	-6.34175100	-3.17012300	2.13564500
H	-6.56468300	-2.57317000	-2.10351600
C	-8.02550800	-3.49168400	0.01046300
H	-8.77154000	-2.68778000	0.07204400
H	-8.23197600	-4.05274100	-0.90777800
H	-8.19705400	-4.15944600	0.86145300
C	-4.12614500	-1.47516500	-2.47973300
H	-3.94834600	-0.39270800	-2.46721400
H	-3.15955300	-1.95617600	-2.67866800
H	-4.78451100	-1.69433500	-3.32636900
C	-3.86620300	-2.17932400	2.55079800
H	-2.88718200	-2.67299400	2.51833000
H	-3.68621200	-1.13006400	2.81873700
H	-4.44016200	-2.63257000	3.36535900
C	8.03993200	-3.45913500	-0.00737100
H	8.21290500	-4.13133600	-0.85457900
H	8.78226400	-2.65232100	-0.07531000
H	8.25053300	-4.01361200	0.91390800

C	3.87384400	-2.17278100	-2.54963200
H	2.89576200	-2.66809300	-2.51464400
H	3.69179500	-1.12499900	-2.82197400
H	4.44831200	-2.62838900	-3.36251600
C	4.13340600	-1.45131700	2.47860600
H	3.95202800	-0.36950000	2.46308900
H	3.16847400	-1.93496000	2.67921900
H	4.79275000	-1.66593600	3.32564400
B	-2.53777600	-1.26613500	0.02601700
B	2.54284100	-1.25678100	-0.02659600
O	-2.41124300	0.11295300	0.01418200
O	2.41115400	0.12184500	-0.01519300
H	-2.14100800	-4.05518200	0.01821600
H	2.15625300	-4.04734500	-0.01733000
H	0.00991500	-5.29113000	0.00079200
C	-0.00829400	4.36342500	-0.00073900
C	-0.00750200	5.06834500	1.22037500
C	-0.00738300	5.06833700	-1.22177000
C	-0.00745800	6.46670300	1.19702200
C	-0.00747000	6.46676000	-1.19836000
C	-0.01111000	7.18637100	-0.00069300
H	-0.00317700	7.00714000	2.14188100
H	-0.00333100	7.00723100	-2.14319100
C	-0.00224300	4.33904700	-2.54731900
H	0.88050200	3.69743600	-2.65358500
H	-0.87733200	3.68715700	-2.65405400
H	-0.00609800	5.04713100	-3.38162500
C	-0.00232900	4.33895600	2.54586800
H	-0.88078500	3.69206300	2.65546600
H	0.87706000	3.69229900	2.64917200
H	0.00040700	5.04699700	3.38021400
C	-0.04434700	8.69725300	-0.00051500
H	-1.07647300	9.07297300	0.00743900
H	0.45673600	9.10952000	0.88196800
H	0.44328500	9.10938000	-0.89050900

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C	-5.44156000	3.28017000	-0.02234400
C	-5.00334600	1.97163800	-0.00117900
C	-3.62112400	1.65977200	-0.02345100
C	-2.66391200	2.71919300	-0.05502900
C	-3.15016000	4.05032600	-0.07782800
C	-4.50332900	4.32824800	-0.06613100
C	-1.24322000	2.41079600	-0.06613400

C	-0.81649700	1.05997600	-0.20225700
C	0.59597900	0.75849900	-0.32734900
C	1.52257400	1.78021400	-0.00198400
C	1.06532500	3.10904400	0.20775600
C	-0.26164000	3.42499100	0.11495100
H	-6.50565500	3.49995600	-0.00989000
H	-5.71836400	1.15566400	0.03091000
H	-2.45342500	4.87931900	-0.13035000
H	-4.84154600	5.36058900	-0.09511800
H	1.79828000	3.88125000	0.42808100
H	-0.56534900	4.45591800	0.25405400
C	1.14373400	-0.51972400	-0.76512500
C	2.53711900	-0.79989800	-0.56387800
C	0.39041400	-1.48382000	-1.48541900
C	3.05324100	-2.06471900	-0.93957300
C	0.92890900	-2.69673900	-1.87251600
H	-0.62068900	-1.24748100	-1.79004000
C	2.26429200	-3.00897500	-1.56522000
H	0.31824400	-3.40073300	-2.43142700
H	2.68442200	-3.96868200	-1.85354000
H	4.10284100	-2.26849600	-0.75326300
C	-4.12042700	-0.84217600	0.18744100
C	-4.45641200	-1.29386500	1.48161800
C	-4.68034200	-1.47366600	-0.94255500
C	-5.33936300	-2.36930000	1.61997900
C	-5.56076100	-2.54564700	-0.75834600
C	-5.90567600	-3.00878700	0.51357300
H	-5.59048300	-2.71614300	2.62081300
H	-5.98735600	-3.03073000	-1.63447700
C	4.87351200	-0.04333700	0.19087800
C	5.82781800	0.21950900	-0.81387800
C	5.29091400	-0.54851000	1.44074100
C	7.18033800	-0.02171500	-0.54796800
C	6.65263600	-0.77470600	1.66369600
C	7.61565000	-0.51403200	0.68467800
H	7.91199300	0.17952700	-1.32835600
H	6.96819500	-1.16553600	2.62946300
C	-1.81538300	0.03585100	-0.08572200
C	-3.15649400	0.29490900	0.01617700
H	-1.49501300	-0.99468200	-0.00320700
C	3.41956000	0.22727400	-0.05707600
C	2.91310000	1.48070800	0.14022200
H	3.57674800	2.28487300	0.45043100
C	-4.34236300	-1.01481100	-2.34418700

H	-4.54656700	0.05340000	-2.48084700
H	-3.28044300	-1.16262000	-2.57513900
H	-4.92581600	-1.56809800	-3.08663900
C	-3.87211300	-0.63828200	2.71331600
H	-2.78119800	-0.74190700	2.74771500
H	-4.08647900	0.43654400	2.73745500
H	-4.28180400	-1.08527400	3.62439600
C	-6.88256500	-4.14816200	0.69055600
H	-7.90418000	-3.77700300	0.84903400
H	-6.90601200	-4.79690600	-0.19147000
H	-6.62602000	-4.76586700	1.55833700
C	4.28973600	-0.84787400	2.53440700
H	3.72293300	0.04650300	2.81824800
H	3.55498000	-1.59659900	2.21505600
H	4.79127900	-1.22878300	3.42939600
C	5.41355900	0.74925200	-2.16927200
H	4.66715200	0.10218700	-2.64438700
H	4.96318700	1.74606600	-2.09551100
H	6.27581400	0.81974400	-2.83958100
C	9.08462300	-0.73699900	0.96094400
H	9.53536100	0.13664800	1.45096600
H	9.24279800	-1.59522700	1.62332800
H	9.64409600	-0.91516500	0.03648100

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C	5.31203700	3.65090900	-0.17777000
C	4.95332500	2.31235800	-0.11912400
C	3.60114900	1.91783100	-0.07512800
C	2.58173900	2.90616700	-0.09923600
C	2.96344200	4.26311200	-0.15943600
C	4.30345000	4.62458000	-0.19615300
C	1.17004000	2.48784700	-0.06701400
C	0.83102300	1.11865200	-0.01706300
C	-0.51341400	0.63722400	0.00756800
C	-1.50856700	1.63864300	-0.02548600
C	-1.20184800	3.00384000	-0.07029700
C	0.11024900	3.41793800	-0.08999900
H	6.35748800	3.94476900	-0.21063400
H	5.72034200	1.54199600	-0.10738500
H	2.21753100	5.04998100	-0.17857200
H	4.56885500	5.67786700	-0.24207900
H	-2.02495100	3.70990800	-0.09107100
H	0.31957900	4.48032600	-0.12632400
C	-0.92877300	-0.78610800	0.06169500

C	-2.32766300	-1.07206700	0.05489300
C	-0.03683500	-1.88123000	0.12482400
C	-2.77149800	-2.40729200	0.10702700
C	-0.50929600	-3.18860700	0.17357700
H	1.02815000	-1.71967100	0.13955700
C	-1.87902600	-3.46785500	0.16401600
H	0.21027500	-4.00234500	0.22175700
H	-2.23502800	-4.49379700	0.20357200
H	-3.84207500	-2.59519600	0.10435300
B	3.17822200	0.44314000	-0.01050000
O	1.82148000	0.18174200	0.00846100
O	-2.84308500	1.35927800	-0.01880900
B	-3.34825600	0.07724600	0.00854600
C	4.13189700	-0.81078300	0.01628300
C	4.36537100	-1.54869000	-1.16577700
C	4.77351500	-1.21431700	1.20913400
C	5.22587800	-2.65087400	-1.14035700
C	5.62551700	-2.32310000	1.19979500
C	5.86436600	-3.05753800	0.03445500
H	5.40418700	-3.20400000	-2.06108600
H	6.11474400	-2.62149900	2.12570700
C	-4.91763800	-0.06586100	0.00725000
C	-5.64281900	0.02534000	1.21653700
C	-5.62307600	-0.29219800	-1.19382500
C	-7.03310500	-0.11601200	1.20716700
C	-7.01580400	-0.42703200	-1.16903200
C	-7.74081000	-0.34085900	0.02183500
H	-7.57807500	-0.05057100	2.14778100
H	-7.54674500	-0.60364000	-2.10303200
C	6.76737600	-4.26908300	0.05180600
H	7.59426100	-4.14362500	0.75960300
H	6.21813900	-5.17117300	0.35389800
H	7.19457700	-4.46545200	-0.93733000
C	3.69343000	-1.15658900	-2.46647000
H	2.60559300	-1.28821700	-2.41294600
H	3.87646400	-0.10368300	-2.71646700
H	4.05974400	-1.76263500	-3.30116800
C	4.53146100	-0.47262700	2.50821400
H	4.72420800	0.60204200	2.40723300
H	3.49131300	-0.58033800	2.84273400
H	5.17417300	-0.85329400	3.30842300
C	-4.88821500	-0.37569900	-2.51626900
H	-4.40993300	0.57944900	-2.76943700
H	-4.09589300	-1.13395700	-2.49388000

H	-5.56921800	-0.62962200	-3.33493600
C	-4.92359700	0.27584800	2.52628000
H	-4.15778800	-0.48623000	2.72006300
H	-4.41438300	1.24771000	2.52370600
H	-5.61970900	0.26796500	3.37110700
C	-9.24700700	-0.46400800	0.03049900
H	-9.72810600	0.52232600	0.07758200
H	-9.61383000	-0.96264500	-0.87283600
H	-9.59853100	-1.03401600	0.89814300

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C	1.22377600	0.08052300	-0.00004400
C	1.23125500	-1.35112900	-0.00000300
C	2.51907400	-2.04318600	0.00003600
C	3.72819200	-1.28249400	0.00001700
C	-0.00000100	0.75706400	-0.00006400
C	0.00000000	-2.01931600	0.00001400
C	-1.23125500	-1.35113000	-0.00001000
C	-1.22377800	0.08052200	-0.00005100
C	-3.72819200	-1.28249700	-0.00001800
C	-2.51907500	-2.04318800	0.00000700
H	-0.00000100	1.84526500	-0.00009400
H	0.00000000	-3.10107900	0.00005000
C	4.96858900	-1.96170700	0.00007900
C	2.62124200	-3.45227300	0.00010300
C	3.84772200	-4.09405800	0.00015100
C	5.03376000	-3.34337300	0.00014000
H	5.88152300	-1.37482800	0.00007300
H	1.72193900	-4.05845100	0.00012300
H	3.88818000	-5.17999100	0.00020400
H	5.99848800	-3.84336500	0.00018200
C	-4.96859000	-1.96171000	-0.00003400
C	-5.03376000	-3.34337700	-0.00000200
C	-3.84772100	-4.09406100	0.00003400
C	-2.62124100	-3.45227500	0.00003500
H	-5.88152300	-1.37483300	-0.00007200
H	-5.99848700	-3.84336900	-0.00001100
H	-3.88817800	-5.17999400	0.00005400
H	-1.72193700	-4.05845200	0.00005100
C	-4.93973200	0.98283700	-0.00003900
C	-5.53273600	1.36795400	-1.22082600
C	-5.53274100	1.36787000	1.22077500
C	-6.70240800	2.13482900	-1.19764300
C	-6.70241300	2.13474500	1.19764200

C	-7.30191000	2.53343700	0.00001100
H	-7.15745900	2.42598500	-2.14269500
H	-7.15746800	2.42583100	2.14271300
C	4.93973100	0.98283900	-0.00002500
C	5.53285600	1.36776500	-1.22081700
C	5.53262000	1.36806200	1.22078400
C	6.70252800	2.13463800	-1.19763900
C	6.70229500	2.13493300	1.19764600
C	7.30191200	2.53343400	0.00001400
H	7.15767400	2.42563900	-2.14269200
H	7.15725500	2.42617300	2.14271500
C	-4.92672800	0.96274200	-2.54641700
H	-3.92583800	1.38955800	-2.68097400
H	-4.81690000	-0.12523500	-2.62469100
H	-5.55103600	1.29993500	-3.37961300
C	-4.92674900	0.96253700	2.54633600
H	-4.81733600	-0.12547900	2.62468400
H	-3.92568000	1.38897000	2.68075100
H	-5.55084500	1.30003000	3.37957000
C	-8.54825700	3.38821300	0.00004200
H	-8.29822400	4.45781400	0.00024800
H	-9.16362500	3.20013800	-0.88636500
H	-9.16378800	3.19984000	0.88627400
C	8.54826000	3.38820700	0.00002700
H	8.29823000	4.45780900	-0.00029500
H	9.16354400	3.20020800	0.88650800
H	9.16387400	3.19975700	-0.88613000
C	4.92647800	0.96297000	2.54635100
H	3.92556200	1.38977300	2.68075400
H	4.81667100	-0.12500100	2.62472500
H	5.55068700	1.30026500	3.37958000
C	4.92699800	0.96230900	-2.54640200
H	4.81762200	-0.12571700	-2.62467200
H	3.92593000	1.38870300	-2.68094700
H	5.55116300	1.29975000	-3.37960400
C	-3.67771500	0.17197000	-0.00006900
C	-2.46718300	0.79860800	-0.00007600
C	3.67771400	0.17197200	-0.00004200
C	2.46718000	0.79861000	-0.00006000
H	-2.42691400	1.88571600	-0.00009300
H	2.42691100	1.88571800	-0.00008700

BO3a_S₀

C	1.20347900	0.15668400	0.00607000
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C	1.23611500	1.57222200	0.00897900
C	2.53316900	2.26872300	0.02392200
C	3.72148200	1.48939700	0.02301900
C	0.00002500	-0.53875800	-0.00009800
C	0.00001700	2.23253400	0.00017500
C	-1.23607700	1.57221800	-0.00875600
C	-1.20342900	0.15668000	-0.00612500
C	-3.72144400	1.48938300	-0.02263600
C	-2.53313600	2.26871600	-0.02348900
H	0.00002700	-1.62270500	-0.00020900
H	0.00001500	3.31480200	0.00030700
C	4.97012300	2.14120800	0.04706100
C	2.64208800	3.67283400	0.04442500
C	3.88729500	4.28859100	0.06405500
C	5.06292100	3.52639100	0.06629000
H	5.87286500	1.53550100	0.05212300
H	1.75469600	4.29721900	0.04671700
H	3.94507200	5.37410800	0.07980900
H	6.03251100	4.01631100	0.08463400
C	-4.97009500	2.14118800	-0.04629300
C	-5.06290200	3.52637700	-0.06516500
C	-3.88728200	4.28858300	-0.06298000
C	-2.64206600	3.67283000	-0.04368800
H	-5.87283300	1.53547600	-0.05132000
H	-6.03249900	4.01629600	-0.08319700
H	-3.94506800	5.37410200	-0.07849600
H	-1.75467800	4.29722100	-0.04600100
B	-3.61006800	-0.05128800	-0.00852700
O	-2.34122700	-0.59823700	-0.00836100
O	2.34127800	-0.59822200	0.00815300
B	3.61012700	-0.05126700	0.00845300
C	-4.81536000	-1.06496100	-0.01157000
C	-5.49594300	-1.38753200	1.18318500
C	-5.23516800	-1.66624200	-1.21842600
C	-6.56747200	-2.28572600	1.15280700
C	-6.31238000	-2.55767500	-1.21466100
C	-6.99141000	-2.88403700	-0.03724100
H	-7.08358100	-2.52466600	2.08134800
H	-6.62991500	-3.00797200	-2.15381400
C	4.81538700	-1.06497000	0.01122400
C	5.23419400	-1.66765400	1.21777000
C	5.49688800	-1.38625800	-1.18332300
C	6.31131700	-2.55915000	1.21387500
C	6.56830500	-2.28463300	-1.15308800

C	6.99124800	-2.88428700	0.03660600
H	6.62806800	-3.01051600	2.15278400
H	7.08506500	-2.52266400	-2.08149600
C	-5.06503300	-0.78381300	2.50460000
H	-4.04348900	-1.08656100	2.76881400
H	-5.07549400	0.31269100	2.47448300
H	-5.72304900	-1.10048800	3.32012600
C	-4.52543300	-1.35474500	-2.52026300
H	-4.49788800	-0.27551900	-2.71903000
H	-3.48548800	-1.70363300	-2.50175400
H	-5.02194600	-1.83475300	-3.36959700
C	-8.13274600	-3.87453300	-0.04572800
H	-7.77448800	-4.89685300	0.13666400
H	-8.86824700	-3.64647100	0.73350700
H	-8.65165400	-3.88085400	-1.01037600
C	8.13251600	-3.87486700	0.04500700
H	7.77380400	-4.89757200	-0.13426800
H	8.86644300	-3.64859200	-0.73621500
H	8.65339900	-3.87905200	1.00861900
C	5.06724700	-0.78093700	-2.50442700
H	4.04517400	-1.08156700	-2.76898600
H	5.07979400	0.31552900	-2.47364600
H	5.72478300	-1.09835700	-3.32004900
C	4.52344300	-1.35754800	2.51938500
H	4.49560800	-0.27852300	2.71920400
H	3.48356200	-1.70655100	2.49974900
H	5.01940000	-1.83833000	3.36860700

CC3b_S₀

C	-0.31396600	0.00003500	-1.22424100
C	1.11838800	-0.00011300	1.23144900
C	1.11838800	-0.00011300	-1.23144900
C	-0.99134900	0.00009000	0.00000000
C	-0.31396600	0.00003500	1.22424100
C	1.78772400	-0.00021400	0.00000000
H	-2.08052700	0.00018900	0.00000000
H	2.87078900	-0.00037300	0.00000000
C	1.80904200	-0.00009700	-2.51862000
C	3.11818700	0.00005300	-5.05671600
C	1.05318700	-0.00003000	-3.72819500
C	3.21864400	-0.00007700	-2.62697500
C	3.85564600	-0.00000700	-3.85378400
C	1.73406000	0.00004700	-4.96885400
H	3.82960200	-0.00006500	-1.72950600

H	4.94379500	-0.00000800	-3.89207000
H	1.14125200	0.00011900	-5.88019600
C	1.80904200	-0.00009700	2.51862000
C	3.11818700	0.00005300	5.05671600
C	3.21864400	-0.00007700	2.62697500
C	1.05318700	-0.00003000	3.72819500
C	1.73406000	0.00004700	4.96885400
C	3.85564600	-0.00000700	3.85378400
H	3.82960200	-0.00006500	1.72950600
H	1.14125200	0.00011900	5.88019600
H	4.94379500	-0.00000800	3.89207000
C	-0.40149700	0.00000500	3.67996700
C	-1.03041200	0.00008200	2.46910700
H	-2.11867800	0.00016800	2.43123600
C	-0.40149700	0.00000500	-3.67996700
C	-1.03041200	0.00008200	-2.46910700
H	-2.11867800	0.00016800	-2.43123600
C	-1.21088000	-0.00000400	4.94341800
C	-2.75899600	-0.00002100	7.30840700
C	-1.59515000	-1.22104500	5.53724500
C	-1.59521100	1.22102800	5.53722600
C	-2.36127200	1.19821800	6.70812900
C	-2.36125000	-1.19824700	6.70813100
H	-2.65236800	2.14415100	7.16374100
H	-2.65235700	-2.14418400	7.16372600
C	-1.21088000	-0.00000400	-4.94341800
C	-2.75899600	-0.00002100	-7.30840700
C	-1.59521100	1.22102800	-5.53722600
C	-1.59515000	-1.22104500	-5.53724500
C	-2.36125000	-1.19824700	-6.70813100
C	-2.36127200	1.19821800	-6.70812900
H	-2.65235700	-2.14418400	-7.16372600
H	-2.65236800	2.14415100	-7.16374100
C	3.82615900	0.00016600	6.38989700
H	4.47157200	0.88169800	6.49807500
H	4.47035600	-0.88215200	6.49894300
H	3.11427600	0.00105500	7.22132100
C	3.82615900	0.00016600	-6.38989700
H	4.47157200	0.88169800	-6.49807500
H	3.11427600	0.00105500	-7.22132100
H	4.47035600	-0.88215200	-6.49894300
C	-1.18920200	2.54523200	4.92983900
H	-0.10033900	2.62096800	4.82192200
H	-1.52761900	3.38042900	5.55130500

H	-1.61337400	2.67549200	3.92678200
C	-1.18913600	-2.54525200	4.92986700
H	-0.10022400	-2.62124500	4.82259600
H	-1.61272500	-2.67523800	3.92653200
H	-1.52812500	-3.38046500	5.55099900
C	-3.61270300	-0.00001400	8.55500100
H	-3.42392300	0.88670900	9.17030900
H	-3.42464800	-0.88722400	9.16982300
H	-4.68255500	0.00050200	8.30403900
C	-1.18913600	-2.54525200	-4.92986700
H	-0.10022400	-2.62124500	-4.82259600
H	-1.52812500	-3.38046500	-5.55099900
H	-1.61272500	-2.67523800	-3.92653200
C	-1.18920200	2.54523200	-4.92983900
H	-0.10033900	2.62096800	-4.82192200
H	-1.61337400	2.67549200	-3.92678200
H	-1.52761900	3.38042900	-5.55130500
C	-3.61270300	-0.00001400	-8.55500100
H	-3.42392300	0.88670900	-9.17030900
H	-4.68255500	0.00050200	-8.30403900
H	-3.42464800	-0.88722400	-9.16982300

BO3b_S₀

C	-1.20330400	-0.08192600	-0.00416700
C	-1.23591900	1.33357800	-0.00661900
C	-2.53290800	2.02771100	-0.01867800
C	-3.72147000	1.25279200	-0.01619300
C	0.00001000	-0.77768300	-0.00014600
C	0.00000600	1.99448800	-0.00000900
C	1.23593300	1.33358100	0.00653400
C	1.20332200	-0.08192200	0.00394400
C	3.72148600	1.25280100	0.01622600
C	2.53292100	2.02771500	0.01869600
H	0.00001100	-1.86166300	-0.00019600
H	0.00000200	3.07695800	0.00006600
C	-4.96965300	1.90582400	-0.03691700
C	-2.64926100	3.43161900	-0.03792400
C	-3.89464400	4.04178300	-0.05463100
C	-5.08632800	3.29253200	-0.05535800
H	-5.87043500	1.29555000	-0.04027500
H	-1.76538600	4.06134000	-0.04139900
H	-3.95027900	5.12871400	-0.06952400
C	4.96966200	1.90583900	0.03713500
C	5.08633100	3.29254500	0.05571700

C	3.89464300	4.04179200	0.05492200
C	2.64926600	3.43162400	0.03805300
H	5.87044800	1.29557200	0.04053200
H	3.95027200	5.12872300	0.06989300
H	1.76538800	4.06134000	0.04147400
B	3.61075400	-0.28770700	0.00279800
O	2.34240000	-0.83564700	0.00441900
O	-2.34238100	-0.83565700	-0.00469700
B	-3.61073000	-0.28771600	-0.00294100
C	4.81624200	-1.30197100	0.00429600
C	5.49228100	-1.62808700	-1.19197900
C	5.24076900	-1.90002000	1.21108900
C	6.56388100	-2.52636500	-1.16333700
C	6.31776200	-2.79174200	1.20576200
C	6.99225500	-3.12152400	0.02666200
H	7.07635400	-2.76798900	-2.09323300
H	6.63868100	-3.23963300	2.14495700
C	-4.81623500	-1.30196300	-0.00445300
C	-5.24123200	-1.89953100	-1.21131700
C	-5.49183000	-1.62851600	1.19195100
C	-6.31823700	-2.79123500	-1.20592900
C	-6.56346600	-2.52675800	1.16336600
C	-6.99229500	-3.12145300	-0.02669800
H	-6.63951200	-3.23876100	-2.14517600
H	-7.07560400	-2.76872100	2.09335800
C	5.05624200	-1.02780500	-2.51324300
H	4.03490300	-1.33402700	-2.77418800
H	5.06322700	0.06874600	-2.48429400
H	5.71311300	-1.34370400	-3.33005300
C	4.53590600	-1.58474900	2.51465100
H	4.50977000	-0.50496600	2.71044700
H	3.49559900	-1.93273600	2.50053700
H	5.03499200	-2.06302900	3.36350100
C	8.13334900	-4.11237700	0.03359100
H	7.77368300	-5.13578900	-0.13972000
H	8.86356000	-3.88950800	-0.75211500
H	8.65895400	-4.11275000	0.99467400
C	-8.13340500	-4.11229000	-0.03359800
H	-7.77355300	-5.13591900	0.13803200
H	-8.86274500	-3.89038400	0.75318400
H	-8.66006900	-4.11147500	-0.99410400
C	-5.05531000	-1.02868100	2.51325900
H	-4.03381900	-1.33485800	2.77365200
H	-5.06246300	0.06788300	2.48471300

H	-5.71179400	-1.34496700	3.33023000
C	-4.53680200	-1.58380800	-2.51500200
H	-4.51051000	-0.50394300	-2.71031600
H	-3.49655900	-1.93202100	-2.50143900
H	-5.03629700	-2.06160200	-3.36388500
C	6.43051000	3.98019900	0.07779900
H	7.24875000	3.25358500	0.07783000
H	6.56197000	4.63210700	-0.79515000
H	6.54361300	4.61131700	0.96839000
C	-6.43051300	3.98018200	-0.07719300
H	-7.24874700	3.25356200	-0.07749400
H	-6.56198300	4.63175900	0.79600400
H	-6.54361700	4.61163700	-0.96754300

CC3c_S₀

C	-1.22445300	-1.69573300	0.00465800
C	1.23158900	-0.26356200	0.00722400
C	-1.23159000	-0.26356000	0.00721200
C	-0.00000200	-2.37269100	0.00412900
C	1.22445100	-1.69573500	0.00466000
C	0.00000000	0.40513200	0.01012800
H	-0.00000200	-3.46177700	0.00317800
H	0.00000000	1.48794600	0.01671300
C	-2.52046100	0.42877900	0.00782300
C	-5.02529300	1.73219400	-0.00518900
C	-3.72724200	-0.33417300	0.00318100
C	-2.61997500	1.83603600	0.00493400
C	-3.84235200	2.50545900	0.00016600
C	-4.96358800	0.35246700	-0.00316700
H	-1.71562600	2.43494600	-0.02380500
H	-5.88105200	-0.22925300	0.00278200
C	2.52046000	0.42877700	0.00785900
C	5.02529400	1.73219000	-0.00509200
C	2.61997600	1.83603400	0.00501600
C	3.72724100	-0.33417600	0.00320200
C	4.96358800	0.35246200	-0.00311200
C	3.84235300	2.50545500	0.00027800
H	1.71562800	2.43494600	-0.02370400
H	5.88105100	-0.22925900	0.00283400
C	3.67927200	-1.78717100	0.00363200
C	2.46785300	-2.41503400	0.00394700
H	2.42808700	-3.50310600	0.00282600
C	-3.67927500	-1.78716800	0.00364600
C	-2.46785700	-2.41503200	0.00396000

H	-2.42809100	-3.50310400	0.00285900
C	4.94384500	-2.59467200	0.00172300
C	7.31251200	-4.13632500	-0.00168100
C	5.53530300	-2.97921100	-1.22038500
C	5.54123400	-2.97552300	1.22210300
C	6.71406600	-3.73851600	1.19744900
C	6.70823400	-3.74216500	-1.19908500
H	7.17277700	-4.02692100	2.14265800
H	7.16236100	-4.03345500	-2.14563000
C	-4.94384900	-2.59466700	0.00177000
C	-7.31251800	-4.13631800	-0.00156700
C	-5.54130100	-2.97536800	1.22216700
C	-5.53524400	-2.97935500	-1.22032000
C	-6.70817700	-3.74230500	-1.19898800
C	-6.71413300	-3.73836200	1.19754500
H	-7.16225700	-4.03370700	-2.14552100
H	-7.17289100	-4.02665400	2.14276600
H	-5.99178300	2.22932100	0.01654800
H	5.99178400	2.22931500	0.01666900
C	-3.90244000	3.98918200	-0.00151200
C	-4.01946600	6.80797300	-0.01036200
C	-4.87236100	4.66998800	-0.75798700
C	-2.99463300	4.75271200	0.75298600
C	-3.05148800	6.14599100	0.74788900
C	-4.92998200	6.06324500	-0.76301300
H	-5.56985600	4.10077200	-1.36768500
H	-2.25647900	4.24620800	1.37021000
H	-2.34397200	6.71583100	1.34610800
H	-5.68337900	6.56851200	-1.36319100
H	-4.06470700	7.89441000	-0.01364500
C	3.90244400	3.98917800	-0.00135100
C	4.01947800	6.80796900	-0.01010100
C	2.99464200	4.75268400	0.75317900
C	4.87236400	4.67000700	-0.75780500
C	4.92998900	6.06326400	-0.76278200
C	3.05150100	6.14596200	0.74813100
H	2.25649000	4.24615900	1.37038800
H	5.56985500	4.10081100	-1.36752500
H	5.68338500	6.56855100	-1.36294600
H	2.34399000	6.71578300	1.34637400
H	4.06472200	7.89440600	-0.01334500
C	-4.92353400	-2.57764600	-2.54388600
H	-4.81356300	-1.48919000	-2.62268400
H	-5.54337300	-2.91710300	-3.37979700

H	-3.92093000	-3.00396800	-2.67062700
C	-4.93618300	-2.56910700	2.54735700
H	-4.83093600	-1.48005700	2.62477600
H	-3.93238400	-2.99126700	2.67844600
H	-5.55786000	-2.90952000	3.38150000
C	-8.56153000	-4.98638600	-0.00325500
H	-9.17794800	-4.79505500	0.88210300
H	-8.31345000	-6.05689100	-0.00135300
H	-9.17403000	-4.79733300	-0.89182500
C	4.93604600	-2.56942900	2.54731300
H	4.83058800	-1.48040400	2.62477700
H	5.55779100	-2.90976000	3.38143800
H	3.93232900	-2.99179000	2.67839300
C	4.92366500	-2.57733200	-2.54393200
H	4.81391200	-1.48885000	-2.62268700
H	3.92097500	-3.00344600	-2.67068000
H	5.54343300	-2.91687700	-3.37986000
C	8.56152300	-4.98639600	-0.00340800
H	9.17792200	-4.79513300	0.88197900
H	9.17404400	-4.79727500	-0.89194900
H	8.31344200	-6.05690000	-0.00159200

BO3c_S₀

C	-1.20377500	-1.49931700	-0.00919900
C	-1.23606100	-0.08363900	-0.01235800
C	-2.53391400	0.61266900	-0.03143200
C	-3.72003200	-0.16860800	-0.02677900
C	-0.00003600	-2.19440200	-0.00023700
C	-0.00002400	0.57638600	0.00029100
C	1.23600700	-0.08365500	0.01263500
C	1.20371200	-1.49933200	0.00898300
C	3.71997600	-0.16865300	0.02747100
C	2.53386300	0.61264600	0.03183200
H	-0.00003500	-3.27834900	-0.00037500
H	-0.00002100	1.65856800	0.00066600
C	-4.96319600	0.49275400	-0.04593100
C	-2.63938400	2.01426800	-0.05205700
C	-3.87944500	2.66012100	-0.06957300
C	-5.05120100	1.87547000	-0.06521200
H	-5.87136500	-0.10475100	-0.05612900
H	-1.74709500	2.63025800	-0.02880400
H	-6.02174000	2.36120000	-0.10740000
C	4.96315000	0.49267200	0.04663100
C	5.05118000	1.87540100	0.06573100

C	3.87944200	2.66005200	0.06976100
C	2.63935300	2.01424200	0.05214700
H	5.87130900	-0.10484700	0.05698200
H	6.02172100	2.36112100	0.10795300
H	1.74709500	2.63025500	0.02843700
B	3.61035900	-1.70782300	0.01568000
O	2.34093400	-2.25497800	0.01417000
O	-2.34100800	-2.25494700	-0.01448200
B	-3.61043300	-1.70778700	-0.01523600
C	4.81620100	-2.72087700	0.02349800
C	5.50160200	-3.04378400	-1.16840500
C	5.23221200	-3.32083300	1.23237600
C	6.57402200	-3.94078900	-1.13332800
C	6.31039900	-4.21106700	1.23336600
C	6.99421900	-4.53761500	0.05877000
H	7.09377900	-4.18001700	-2.05977000
H	6.62493000	-4.66024300	2.17407100
C	-4.81626000	-2.72085400	-0.02314600
C	-5.23124700	-3.32174500	-1.23194700
C	-5.50263800	-3.04291900	1.16841100
C	-6.30941300	-4.21197700	-1.23319000
C	-6.57499100	-3.94002200	1.13308700
C	-6.99419300	-4.53770800	-0.05890800
H	-6.62317400	-4.66181800	-2.17383600
H	-7.09545800	-4.17865800	2.05928000
C	5.07469400	-2.44224000	-2.49212400
H	4.05522500	-2.74822400	-2.76057800
H	5.08150300	-1.34570000	-2.46272200
H	5.73724200	-2.75752100	-3.30453700
C	4.51732900	-3.00911400	2.53133000
H	4.48813200	-1.92978400	2.72922600
H	3.47774400	-3.35882100	2.50904300
H	5.01104300	-3.48816000	3.38284000
C	8.13672200	-5.52672000	0.07245900
H	7.78040700	-6.54971700	-0.10993600
H	8.87473100	-5.29868100	-0.70442200
H	8.65223300	-5.53120400	1.03894500
C	-8.13661600	-5.52689900	-0.07290000
H	-7.77990100	-6.55024800	0.10672500
H	-8.87342900	-5.30056900	0.70559800
H	-8.65363300	-5.52941600	-1.03860000
C	-5.07691800	-2.44045500	2.49210400
H	-4.05712600	-2.74498200	2.76097500
H	-5.08520200	-1.34393700	2.46244600

H	-5.73929500	-2.75643700	3.30438500
C	-4.51535000	-3.01094000	-2.53056100
H	-4.48575500	-1.93173000	-2.72906100
H	-3.47587100	-3.36087700	-2.50731700
H	-5.00858700	-3.49034900	-3.38214300
C	3.96004000	4.14324000	0.09294800
C	3.06096600	4.90516000	0.85832400
C	4.94092400	4.82154300	-0.65025100
C	3.13884600	6.29687400	0.87869800
H	2.31416300	4.39988600	1.46446800
C	5.01764800	6.21330300	-0.63197600
H	5.63130300	4.25313900	-1.26715100
C	4.11712800	6.95707100	0.13287300
H	2.43950500	6.86562300	1.48584300
H	5.77843300	6.71761900	-1.22193700
H	4.17819400	8.04185200	0.14879700
C	-3.96001600	4.14331200	-0.09312800
C	-4.94057000	4.82192300	0.65025500
C	-3.06116800	4.90495600	-0.85903100
C	-5.01720300	6.21366300	0.63159100
H	-5.63074000	4.25373800	1.26759100
C	-3.13895100	6.29668100	-0.87979200
H	-2.31459800	4.39947300	-1.46528700
C	-4.11691100	6.95716100	-0.13382200
H	-5.77773200	6.71823100	1.22166600
H	-2.43976000	6.86518200	-1.48734300
H	-4.17794000	8.04193800	-0.15002000

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C	-1.22039100	-0.45039800	-0.00865400
C	1.23404000	0.97875800	0.03444000
C	-1.23404100	0.97876900	0.03438600
C	0.00000200	-1.13234100	-0.02689900
C	1.22039600	-0.45040600	-0.00862300
C	0.00000400	1.64833900	0.04557800
H	-0.00000700	-2.22073000	-0.06140500
H	0.00002400	2.72873600	0.02837900
C	-2.52293800	1.66477700	0.04984000
C	-4.96490100	3.13117700	0.01151000
C	-3.74874000	0.94431500	-0.04853100
C	-2.55228400	3.08724400	0.18637900
C	-3.71812500	3.79063600	0.19118600
C	-4.99695500	1.70434700	-0.13178500
H	-1.62281100	3.62877100	0.31796200

C	2.52293700	1.66476400	0.04995800
C	4.96489200	3.13117500	0.01174100
C	2.55227900	3.08721700	0.18664400
C	3.74873900	0.94431800	-0.04847900
C	4.99694300	1.70436700	-0.13173300
C	3.71811800	3.79061100	0.19153500
H	1.62280000	3.62872300	0.31829600
C	3.68424500	-0.51657600	-0.04236400
C	2.46543800	-1.14339900	-0.02270400
H	2.44075500	-2.23153800	-0.00325400
C	-3.68423800	-0.51657600	-0.04239800
C	-2.46542800	-1.14339500	-0.02273500
H	-2.44074800	-2.23153400	-0.00326100
C	4.85732300	-1.45934700	0.01806000
C	6.94403300	-3.36114200	0.16651200
C	5.28640300	-2.13122800	-1.14665200
C	5.46323100	-1.74892700	1.25977600
C	6.49641800	-2.69067700	1.30896000
C	6.32591900	-3.06377100	-1.05164100
H	6.96379700	-2.90586000	2.26928900
H	6.66161400	-3.56936300	-1.95645400
C	-4.85730700	-1.45936100	0.01805800
C	-6.94400500	-3.36115200	0.16661800
C	-5.46315400	-1.74895800	1.25983900
C	-5.28644300	-2.13121400	-1.14661000
C	-6.32597800	-3.06377800	-1.05153800
C	-6.49630900	-2.69069100	1.30907700
H	-6.66173300	-3.56936100	-1.95632900
H	-6.96364500	-2.90587900	2.26943100
H	-3.70945800	4.87163100	0.31559600
H	3.70944800	4.87158800	0.31609100
C	-6.15982600	3.89082300	-0.04347300
H	-6.08878100	4.96978000	0.08065400
C	-7.37918900	3.28883700	-0.26158000
H	-8.28998800	3.88117500	-0.30618500
C	-7.42514900	1.89335900	-0.44315700
H	-8.37576300	1.40333300	-0.64090600
C	-6.27485200	1.12935900	-0.38084300
H	-6.36615700	0.06639500	-0.54066900
C	6.15981700	3.89082400	-0.04320700
H	6.08879600	4.96976500	0.08107300
C	7.37916200	3.28886100	-0.26147600
H	8.28995900	3.88120400	-0.30606000
C	7.42511100	1.89340600	-0.44326000

H	8.37571500	1.40342200	-0.64115600
C	6.27481800	1.12940400	-0.38097000
H	6.36609300	0.06646200	-0.54096500
C	-4.66450800	-1.83621000	-2.49359000
H	-4.65505300	-0.75989300	-2.70442100
H	-5.21784500	-2.33500000	-3.29575000
H	-3.62197400	-2.17359300	-2.54337700
C	-5.02455300	-1.04790500	2.52487700
H	-5.22399800	0.02981900	2.47353600
H	-3.94771100	-1.16317500	2.69568100
H	-5.55368000	-1.44655500	3.39619700
C	-8.04199400	-4.39532400	0.25195600
H	-8.75061000	-4.16205300	1.05443500
H	-7.63237200	-5.39345400	0.46058500
H	-8.60208800	-4.46446500	-0.68716100
C	5.02474900	-1.04787300	2.52485700
H	5.22474700	0.02976400	2.47374700
H	5.55351900	-1.44693200	3.39620700
H	3.94781900	-1.16262300	2.69544100
C	4.66434900	-1.83625200	-2.49358100
H	4.65488600	-0.75994600	-2.70446100
H	3.62180300	-2.17362200	-2.54323900
H	5.21759400	-2.33508600	-3.29577700
C	8.04196500	-4.39538800	0.25165200
H	8.74713000	-4.16565300	1.05815300
H	8.60602000	-4.46002100	-0.68543600
H	7.63175800	-5.39461400	0.45379300

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C	-1.20377500	-1.49931700	-0.00919900
C	-1.23606100	-0.08363900	-0.01235800
C	-2.53391400	0.61266900	-0.03143200
C	-3.72003200	-0.16860800	-0.02677900
C	-0.00003600	-2.19440200	-0.00023700
C	-0.00002400	0.57638600	0.00029100
C	1.23600700	-0.08365500	0.01263500
C	1.20371200	-1.49933200	0.00898300
C	3.71997600	-0.16865300	0.02747100
C	2.53386300	0.61264600	0.03183200
H	-0.00003500	-3.27834900	-0.00037500
H	-0.00002100	1.65856800	0.00066600
C	-4.96319600	0.49275400	-0.04593100
C	-2.63938400	2.01426800	-0.05205700
C	-3.87944500	2.66012100	-0.06957300

C	-5.05120100	1.87547000	-0.06521200
H	-5.87136500	-0.10475100	-0.05612900
H	-1.74709500	2.63025800	-0.02880400
H	-6.02174000	2.36120000	-0.10740000
C	4.96315000	0.49267200	0.04663100
C	5.05118000	1.87540100	0.06573100
C	3.87944200	2.66005200	0.06976100
C	2.63935300	2.01424200	0.05214700
H	5.87130900	-0.10484700	0.05698200
H	6.02172100	2.36112100	0.10795300
H	1.74709500	2.63025500	0.02843700
B	3.61035900	-1.70782300	0.01568000
O	2.34093400	-2.25497800	0.01417000
O	-2.34100800	-2.25494700	-0.01448200
B	-3.61043300	-1.70778700	-0.01523600
C	4.81620100	-2.72087700	0.02349800
C	5.50160200	-3.04378400	-1.16840500
C	5.23221200	-3.32083300	1.23237600
C	6.57402200	-3.94078900	-1.13332800
C	6.31039900	-4.21106700	1.23336600
C	6.99421900	-4.53761500	0.05877000
H	7.09377900	-4.18001700	-2.05977000
H	6.62493000	-4.66024300	2.17407100
C	-4.81626000	-2.72085400	-0.02314600
C	-5.23124700	-3.32174500	-1.23194700
C	-5.50263800	-3.04291900	1.16841100
C	-6.30941300	-4.21197700	-1.23319000
C	-6.57499100	-3.94002200	1.13308700
C	-6.99419300	-4.53770800	-0.05890800
H	-6.62317400	-4.66181800	-2.17383600
H	-7.09545800	-4.17865800	2.05928000
C	5.07469400	-2.44224000	-2.49212400
H	4.05522500	-2.74822400	-2.76057800
H	5.08150300	-1.34570000	-2.46272200
H	5.73724200	-2.75752100	-3.30453700
C	4.51732900	-3.00911400	2.53133000
H	4.48813200	-1.92978400	2.72922600
H	3.47774400	-3.35882100	2.50904300
H	5.01104300	-3.48816000	3.38284000
C	8.13672200	-5.52672000	0.07245900
H	7.78040700	-6.54971700	-0.10993600
H	8.87473100	-5.29868100	-0.70442200
H	8.65223300	-5.53120400	1.03894500
C	-8.13661600	-5.52689900	-0.07290000

H	-7.77990100	-6.55024800	0.10672500
H	-8.87342900	-5.30056900	0.70559800
H	-8.65363300	-5.52941600	-1.03860000
C	-5.07691800	-2.44045500	2.49210400
H	-4.05712600	-2.74498200	2.76097500
H	-5.08520200	-1.34393700	2.46244600
H	-5.73929500	-2.75643700	3.30438500
C	-4.51535000	-3.01094000	-2.53056100
H	-4.48575500	-1.93173000	-2.72906100
H	-3.47587100	-3.36087700	-2.50731700
H	-5.00858700	-3.49034900	-3.38214300
C	3.96004000	4.14324000	0.09294800
C	3.06096600	4.90516000	0.85832400
C	4.94092400	4.82154300	-0.65025100
C	3.13884600	6.29687400	0.87869800
H	2.31416300	4.39988600	1.46446800
C	5.01764800	6.21330300	-0.63197600
H	5.63130300	4.25313900	-1.26715100
C	4.11712800	6.95707100	0.13287300
H	2.43950500	6.86562300	1.48584300
H	5.77843300	6.71761900	-1.22193700
H	4.17819400	8.04185200	0.14879700
C	-3.96001600	4.14331200	-0.09312800
C	-4.94057000	4.82192300	0.65025500
C	-3.06116800	4.90495600	-0.85903100
C	-5.01720300	6.21366300	0.63159100
H	-5.63074000	4.25373800	1.26759100
C	-3.13895100	6.29668100	-0.87979200
H	-2.31459800	4.39947300	-1.46528700
C	-4.11691100	6.95716100	-0.13382200
H	-5.77773200	6.71823100	1.22166600
H	-2.43976000	6.86518200	-1.48734300
H	-4.17794000	8.04193800	-0.15002000

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C	-0.00010000	-1.22450400	1.85808100
C	0.00000000	1.23310100	0.42530500
C	0.00000000	-1.23310100	0.42530500
C	0.00000000	0.00000000	2.53435400
C	0.00010000	1.22450400	1.85808100
C	0.00000000	0.00000000	-0.24233200
H	0.00000000	0.00000000	3.62350500
H	0.00000000	0.00000000	-1.32497300
C	0.00007700	-2.51914700	-0.26869000

C	0.00014400	-5.03144600	-1.55682400
C	-0.00022600	-3.73147000	0.49382800
C	0.00049000	-2.61075500	-1.68375700
C	0.00051100	-3.83587800	-2.31596700
C	-0.00019800	-4.97904400	-0.17375400
H	0.00084900	-1.70493000	-2.28333700
H	-0.00043300	-5.88978300	0.41887800
C	-0.00007700	2.51914700	-0.26869000
C	-0.00014400	5.03144600	-1.55682400
C	-0.00049000	2.61075500	-1.68375700
C	0.00022600	3.73147000	0.49382800
C	0.00019800	4.97904400	-0.17375400
C	-0.00051100	3.83587800	-2.31596700
H	-0.00084900	1.70493000	-2.28333700
H	0.00043300	5.88978300	0.41887800
C	0.00048600	3.67807200	1.94871900
C	0.00035200	2.46731600	2.57673200
H	0.00049500	2.42813300	3.66486000
C	-0.00048600	-3.67807200	1.94871900
C	-0.00035200	-2.46731600	2.57673200
H	-0.00049500	-2.42813300	3.66486000
C	0.00084400	4.94046800	2.75998400
C	0.00157100	7.30332500	4.31121000
C	1.22218600	5.53345000	3.14486800
C	-1.22010100	5.53380600	3.14541800
C	-1.19685700	6.70374100	3.91303000
C	1.19966900	6.70335100	3.91247100
H	-2.14263900	7.15904900	4.20502500
H	2.14573400	7.15837800	4.20400900
C	-0.00084400	-4.94046800	2.75998400
C	-0.00157100	-7.30332500	4.31121000
C	-1.22218600	-5.53345000	3.14486800
C	1.22010100	-5.53380600	3.14541800
C	1.19685700	-6.70374100	3.91303000
C	-1.19966900	-6.70335100	3.91247100
H	2.14263900	-7.15904900	4.20502500
H	-2.14573400	-7.15837800	4.20400900
C	-2.54459300	4.92716400	2.73924300
H	-2.62171800	4.82243300	1.65016500
H	-3.37953100	5.54748800	3.08028700
H	-2.67402200	3.92291600	3.16080800
C	2.54627900	4.92627000	2.73819900
H	2.62246600	4.82028000	1.64919000
H	2.67598200	3.92249400	3.16083200

H	3.38155900	5.54690000	3.07784900
C	0.00206400	8.54879900	5.16653400
H	-0.88706400	9.16202200	4.98247700
H	0.88690100	9.16613400	4.97550100
H	0.00694800	8.29634000	6.23601500
C	2.54459300	-4.92716400	2.73924300
H	2.62171800	-4.82243300	1.65016500
H	3.37953100	-5.54748800	3.08028700
H	2.67402200	-3.92291600	3.16080800
C	-2.54627900	-4.92627000	2.73819900
H	-2.62246600	-4.82028000	1.64919000
H	-2.67598200	-3.92249400	3.16083200
H	-3.38155900	-5.54690000	3.07784900
C	-0.00206400	-8.54879900	5.16653400
H	-0.88690100	-9.16613400	4.97550100
H	-0.00694800	-8.29634000	6.23601500
H	0.88706400	-9.16202200	4.98247700
C	-0.00026000	6.16971500	-2.48305600
C	-0.00061400	7.93122800	-4.63727600
C	-0.00069900	5.67294100	-3.80221800
C	0.00000000	7.54600200	-2.23961300
C	-0.00018100	8.42263100	-3.32678700
C	-0.00087400	6.55230600	-4.88069000
H	0.00033400	7.93084900	-1.22214200
H	0.00001700	9.49647200	-3.15430200
H	-0.00120600	6.18097800	-5.90390300
H	-0.00074600	8.62650900	-5.47363200
C	0.00026000	-6.16971500	-2.48305600
C	0.00061400	-7.93122800	-4.63727600
C	0.00000000	-7.54600200	-2.23961300
C	0.00069900	-5.67294100	-3.80221800
C	0.00087400	-6.55230600	-4.88069000
C	0.00018100	-8.42263100	-3.32678700
H	-0.00033400	-7.93084900	-1.22214200
H	0.00120600	-6.18097800	-5.90390300
H	-0.00001700	-9.49647200	-3.15430200
H	0.00074600	-8.62650900	-5.47363200
C	-0.00090000	4.14320700	-3.81420800
C	0.00090000	-4.14320700	-3.81420800
C	-1.26422600	-3.58713800	-4.50563300
H	-1.28473800	-3.87301300	-5.56420600
H	-1.28617400	-2.49187700	-4.45379200
H	-2.17394800	-3.96949100	-4.03096600
C	1.26656500	-3.58747600	-4.50492200

H	1.28762300	-3.87342500	-5.56346300
H	2.17591700	-3.97001900	-4.02970000
H	1.28874700	-2.49221700	-4.45314200
C	-1.26656500	3.58747600	-4.50492200
H	-2.17591700	3.97001900	-4.02970000
H	-1.28874700	2.49221700	-4.45314200
H	-1.28762300	3.87342500	-5.56346300
C	1.26422600	3.58713800	-4.50563300
H	1.28473800	3.87301300	-5.56420600
H	1.28617400	2.49187700	-4.45379200
H	2.17394800	3.96949100	-4.03096600

BO3e_S₀

C	-1.20366800	-1.67021300	0.00103800
C	-1.23759100	-0.25404500	0.00040500
C	-2.53352700	0.44322700	-0.00117100
C	-3.72328300	-0.33936400	0.00353500
C	0.00000400	-2.36472400	-0.00008400
C	0.00000500	0.40517200	-0.00005300
C	1.23760100	-0.25404200	-0.00052800
C	1.20367800	-1.67021200	-0.00119200
C	3.72329300	-0.33936800	-0.00362100
C	2.53353700	0.44322600	0.00108000
H	0.00000900	-3.44868800	-0.00009600
H	-0.00000300	1.48725300	-0.00003200
C	-4.97934000	0.29894600	-0.00274000
C	-2.63466600	1.85237300	-0.00978400
C	-3.87787100	2.45794000	-0.01375700
C	-5.06178000	1.68454400	-0.01062000
H	-5.87795700	-0.31337900	-0.00213900
H	-1.74199000	2.47046200	-0.01398800
C	4.97934600	0.29894500	0.00271600
C	5.06178000	1.68454500	0.01064300
C	3.87787600	2.45794000	0.01376900
C	2.63467300	1.85237300	0.00973100
H	5.87797200	-0.31336600	0.00213100
H	1.74198700	2.47044600	0.01391400
B	3.60814400	-1.87882500	-0.00880400
O	2.34024300	-2.42662500	-0.00355700
O	-2.34023600	-2.42662700	0.00338700
B	-3.60813000	-1.87882400	0.00865700
C	4.81402400	-2.89310300	-0.00910600
C	5.43462100	-3.27797500	-1.21723500
C	5.29457900	-3.43077200	1.20529700

C	6.50811400	-4.17464600	-1.19378000
C	6.37041500	-4.32339100	1.19438600
C	6.99063000	-4.71150100	0.00282500
H	6.97873700	-4.46100700	-2.13299600
H	6.73413600	-4.72538100	2.13879900
C	-4.81402400	-2.89308700	0.00899100
C	-5.29490600	-3.43044100	-1.20540400
C	-5.43431100	-3.27825200	1.21720100
C	-6.37075400	-4.32306600	-1.19442200
C	-6.50780600	-4.17489900	1.19381700
C	-6.99064000	-4.71147300	-0.00280300
H	-6.73473500	-4.72481800	-2.13883500
H	-6.97819300	-4.46147100	2.13308900
C	4.93710700	-2.74115600	-2.54395300
H	3.91666200	-3.08529100	-2.75674200
H	4.91362800	-1.64440100	-2.55560200
H	5.57450100	-3.06938500	-3.37125400
C	4.64886800	-3.05088600	2.52220400
H	4.63648100	-1.96318600	2.66876400
H	3.60709000	-3.39218200	2.56975800
H	5.18173200	-3.49327700	3.36998000
C	8.13232300	-5.70171700	0.00808900
H	7.76307900	-6.73608600	-0.01367800
H	8.78106800	-5.57073700	-0.86465100
H	8.74913500	-5.59874900	0.90774600
C	-8.13230500	-5.70172200	-0.00793200
H	-7.76307000	-6.73603800	0.01645600
H	-8.78241400	-5.56908200	0.86354900
H	-8.74770900	-5.60050900	-0.90874200
C	-4.93644200	-2.74173200	2.54390600
H	-3.91601900	-3.08609000	2.75644300
H	-4.91275700	-1.64498200	2.55571500
H	-5.57373800	-3.06996600	3.37128000
C	-4.64954600	-3.05025100	-2.52239600
H	-4.63703300	-1.96251000	-2.66863100
H	-3.60783400	-3.39169600	-2.57038000
H	-5.18273600	-3.49230700	-3.37014200
C	6.21318800	2.59325000	0.01795900
C	5.73595500	3.91904600	0.02497700
C	7.58479300	2.32957700	0.01863200
C	6.62987400	4.98420200	0.03240700
C	8.47680200	3.40369100	0.02623500
H	7.95507500	1.30763400	0.01342000
C	8.00479300	4.72075700	0.03301100

H	6.27417400	6.01204700	0.03772000
H	9.54703800	3.21508400	0.02690200
H	8.71132700	5.54645700	0.03882000
C	-6.21318900	2.59324600	-0.01786900
C	-5.73595700	3.91903600	-0.02486500
C	-7.58480000	2.32956400	-0.01850400
C	-6.62989100	4.98420100	-0.03222600
C	-8.47681000	3.40366600	-0.02604300
H	-7.95505400	1.30761000	-0.01331100
C	-8.00480000	4.72074100	-0.03279200
H	-6.27419900	6.01204700	-0.03751800
H	-9.54704900	3.21507800	-0.02667900
H	-8.71134800	5.54643000	-0.03855000
C	4.20708900	3.95148300	0.02298500
C	-4.20708900	3.95147600	-0.02291800
C	-3.65700000	4.64116400	-1.29176600
H	-3.95944400	5.69435000	-1.31893700
H	-2.56147400	4.60565400	-1.31020500
H	-4.03038200	4.15529500	-2.19873900
C	-3.66040700	4.65565400	1.23944400
H	-2.56497500	4.61925000	1.26177200
H	-3.96187600	5.70939600	1.25323000
H	-4.03712200	4.18088100	2.15090500
C	3.66044700	4.65569600	-1.23937200
H	2.56501500	4.61928000	-1.26174300
H	3.96190100	5.70944300	-1.25311400
H	4.03720100	4.18095900	-2.15083500
C	3.65696700	4.64112900	1.29184000
H	3.95941100	5.69431300	1.31905900
H	2.56143900	4.60562200	1.31024700
H	4.03032100	4.15522700	2.19880600

CC4a_S₀

C	-1.41210100	3.51561200	-0.00027900
C	-4.18961600	3.05398500	-0.00073200
C	-1.90955200	2.17683900	-0.00040400
C	-2.33175100	4.59077600	-0.00036600
C	-3.69783500	4.36948900	-0.00058800
C	-3.30940600	1.98489800	-0.00064300
H	-1.94416900	5.60564200	-0.00025300
H	-4.38634600	5.21120200	-0.00065800
H	-3.71450900	0.97773600	-0.00078300
H	-5.26164300	2.87127900	-0.00091700
C	-0.96942000	1.05810000	-0.00030000

C	0.96942000	-1.05810000	-0.00030000
C	0.43498400	1.33829400	-0.00021300
C	-1.36025900	-0.28472500	-0.00023700
C	-0.43498400	-1.33829400	-0.00021300
C	1.36025900	0.28472500	-0.00023700
H	-2.41407000	-0.54886300	-0.00017500
H	2.41407000	0.54886300	-0.00017500
C	1.90955200	-2.17683900	-0.00040400
C	3.69783500	-4.36948900	-0.00058800
C	3.30940600	-1.98489800	-0.00064300
C	1.41210100	-3.51561200	-0.00027900
C	2.33175100	-4.59077600	-0.00036600
C	4.18961600	-3.05398500	-0.00073200
H	3.71450900	-0.97773600	-0.00078300
H	1.94416900	-5.60564200	-0.00025300
H	5.26164300	-2.87127900	-0.00091700
H	4.38634600	-5.21120200	-0.00065800
C	0.02230800	3.76187300	-0.00005700
C	0.88283900	2.70304300	-0.00006000
H	1.95606500	2.88725200	0.00007900
C	-0.88283900	-2.70304300	-0.00006000
H	-1.95606500	-2.88725200	0.00007900
C	-0.02230800	-3.76187300	-0.00005700
C	0.56152100	5.16224000	0.00023300
C	1.63161300	7.77800300	0.00077700
C	0.82861600	5.81726800	-1.22088600
C	0.82732700	5.81718500	1.22148900
C	1.35901200	7.11145200	1.19889100
C	1.36025900	7.11137100	-1.19776600
H	1.56670500	7.61041100	2.14487100
H	1.56899400	7.61028800	-2.14356300
C	-0.56152100	-5.16224000	0.00023300
C	-1.63161300	-7.77800300	0.00077700
C	-0.82732700	-5.81718500	1.22148900
C	-0.82861600	-5.81726800	-1.22088600
C	-1.36025900	-7.11137100	-1.19776600
C	-1.35901200	-7.11145200	1.19889100
H	-1.56899400	-7.61028800	-2.14356300
H	-1.56670500	-7.61041100	2.14487100
C	0.55644300	5.13922100	-2.54512900
H	-0.48923700	4.81804400	-2.62438600
H	1.17111300	4.23959400	-2.67126200
H	0.76845600	5.81386100	-3.38070000
C	0.55380900	5.13925800	2.54551800

H	-0.49205600	4.81847000	2.62392800
H	0.76536300	5.81383600	3.38125700
H	1.16805400	4.23941800	2.67218100
C	2.17640600	9.18725500	0.00064400
H	1.36453500	9.92761000	-0.01801600
H	2.80494700	9.37419000	-0.87721500
H	2.77549200	9.38571200	0.89625800
C	-0.55644300	-5.13922100	-2.54512900
H	-1.17111300	-4.23959400	-2.67126200
H	-0.76845600	-5.81386100	-3.38070000
H	0.48923700	-4.81804400	-2.62438600
C	-0.55380900	-5.13925800	2.54551800
H	-1.16805400	-4.23941800	2.67218100
H	0.49205600	-4.81847000	2.62392800
H	-0.76536300	-5.81383600	3.38125700
C	-2.17640600	-9.18725500	0.00064400
H	-2.77549200	-9.38571200	0.89625800
H	-1.36453500	-9.92761000	-0.01801600
H	-2.80494700	-9.37419000	-0.87721500

BO4a_S₀

C	3.91402400	4.17890000	-0.00136400
C	4.27916500	2.83886700	0.00579300
C	3.31171300	1.81555300	0.01192900
C	1.93513500	2.16745800	0.00650600
C	1.57769900	3.52959300	-0.00149900
C	2.55428400	4.51759400	-0.00449800
C	0.93574600	1.08977100	0.00665000
C	1.35768200	-0.26076100	0.00632000
C	0.44888600	-1.31131800	0.00634500
H	0.85962000	-2.31412100	0.00739100
C	-0.93574300	-1.08975900	0.00668600
C	-1.35767800	0.26077300	0.00632000
C	-0.44888300	1.31133000	0.00631000
H	4.67112900	4.95821200	-0.00562300
H	5.33029800	2.56156700	0.00617500
H	0.53399200	3.82630900	-0.00571500
H	2.25586600	5.56290800	-0.01056200
H	-0.85961700	2.31413300	0.00732700
C	-1.93513200	-2.16744700	0.00658000
C	-1.57769500	-3.52958200	-0.00141000
C	-2.55428100	-4.51758300	-0.00436800
C	-3.91402000	-4.17888800	-0.00120700
C	-4.27916100	-2.83885500	0.00593200

C	-3.31171000	-1.81554100	0.01202300
H	-0.53398900	-3.82629800	-0.00564900
H	-2.25586300	-5.56289700	-0.01042100
H	-4.67112600	-4.95820000	-0.00543200
H	-5.33029400	-2.56155500	0.00633300
B	3.70459300	0.31988900	0.01540200
O	2.68367300	-0.60686700	0.00769900
B	-3.70458900	-0.31987800	0.01546200
O	-2.68367000	0.60687900	0.00770200
C	5.17637100	-0.24254900	0.01028900
C	5.91367800	-0.36000200	1.20840200
C	5.78405000	-0.63069100	-1.20440000
C	7.22320600	-0.85130500	1.17477100
C	7.09499300	-1.11562900	-1.20387400
C	7.83256800	-1.23712300	-0.02207400
H	7.78102000	-0.93400700	2.10622700
H	7.55294600	-1.40401100	-2.14880400
C	-5.17636900	0.24255500	0.01036800
C	-5.78414500	0.63052500	-1.20432800
C	-5.91358400	0.36016900	1.20852200
C	-7.09508900	1.11546200	-1.20376600
C	-7.22311500	0.85146700	1.17492600
C	-7.83257200	1.23711700	-0.02192400
H	-7.55311200	1.40372300	-2.14869900
H	-7.78085000	0.93430800	2.10641600
C	-5.29396600	-0.02231100	2.53739000
H	-4.89100600	-1.04237000	2.52087400
H	-4.46251600	0.64552100	2.79815000
H	-6.02664700	0.03296100	3.34894800
C	-5.02432700	0.52593300	-2.51096500
H	-4.15603300	1.19653800	-2.52377100
H	-4.64579600	-0.49055200	-2.67935600
H	-5.65917000	0.78787700	-3.36347100
C	-9.23824400	1.79164700	-0.03713000
H	-9.23466900	2.88903400	0.01251600
H	-9.77057300	1.51246400	-0.95320500
H	-9.82126000	1.43040100	0.81683200
C	5.02412800	-0.52629200	-2.51099200
H	4.15599200	-1.19710400	-2.52373500
H	4.64534500	0.49010000	-2.67937700
H	5.65898000	-0.78810100	-3.36353300
C	5.29415100	0.02259900	2.53727700
H	4.89066700	1.04244400	2.52052400
H	4.46309700	-0.64557800	2.79842300

H	6.02702900	-0.03204900	3.34870000
C	9.23823800	-1.79165800	-0.03730700
H	9.23467200	-2.88902400	0.01281600
H	9.77039300	-1.51287000	-0.95360300
H	9.82141600	-1.43004700	0.81638900

CC4b_S₀

C	-4.45243900	3.63111600	-0.00149700
C	-4.62719100	2.25565300	-0.00155000
C	-3.53740200	1.35381300	-0.00102800
C	-2.20818800	1.87003300	-0.00060500
C	-2.04794500	3.27367700	-0.00056600
C	-3.13282300	4.12959300	-0.00096400
C	-1.07375000	0.95169200	-0.00025000
C	-1.33011700	-0.45737400	-0.00030600
C	-0.26186400	-1.36455300	0.00001500
H	-0.50804200	-2.42183600	-0.00003200
C	1.07378900	-0.95179100	0.00039400
C	1.33015500	0.45727500	0.00042400
C	0.26190100	1.36445300	0.00010800
H	-5.63364500	1.84715100	-0.00204700
H	-1.05114600	3.70179900	-0.00020400
H	-2.96628200	5.20469300	-0.00089300
H	0.50808100	2.42173500	0.00012600
C	2.20822600	-1.87013000	0.00079500
C	2.04798700	-3.27377400	0.00087400
C	3.13286700	-4.12968700	0.00133600
C	4.45248400	-3.63120900	0.00183000
C	4.62723300	-2.25574700	0.00177100
C	3.53744100	-1.35390800	0.00117000
H	1.05118900	-3.70189800	0.00056300
H	2.96632800	-5.20478800	0.00135200
H	5.63368400	-1.84723800	0.00225500
C	-5.14896700	-0.65040600	-0.00093000
C	-5.79923400	-0.92864100	-1.22095100
C	-5.80093200	-0.92475400	1.22034100
C	-7.08438300	-1.48184900	-1.19756500
C	-7.08516700	-1.47742500	1.19780000
C	-7.74413900	-1.76862100	-0.00019600
H	-7.58171000	-1.69299300	-2.14253100
H	-7.58342800	-1.68517100	2.14318100
C	5.14899200	0.65034400	0.00085200
C	5.79923700	0.92886000	1.22076500
C	5.80090500	0.92458200	-1.22052500

C	7.08434300	1.48227100	1.19724900
C	7.08502700	1.47741400	-1.19811500
C	7.74401700	1.76890400	-0.00014900
H	7.58163700	1.69368100	2.14216800
H	7.58323500	1.68509800	-2.14354200
C	-9.11888000	-2.39620500	0.00288800
H	-9.05962300	-3.48567600	0.12955200
H	-9.73505700	-2.01022300	0.82267200
H	-9.64849600	-2.20663400	-0.93671200
C	-5.13018500	-0.63932700	-2.54658800
H	-4.82488500	0.41068300	-2.62355300
H	-4.22305800	-1.24027700	-2.68094200
H	-5.80512800	-0.85757100	-3.38007200
C	-5.13221000	-0.63098300	2.54514000
H	-4.22375500	-1.22968400	2.68049700
H	-4.82907600	0.41984600	2.61958700
H	-5.80649600	-0.84872700	3.37928100
C	-5.62961500	4.57677600	-0.00195800
H	-5.61664300	5.23057700	-0.88335700
H	-6.57917800	4.03297100	-0.00268000
H	-5.61771000	5.23008700	0.87982400
C	5.62966000	-4.57686900	0.00239300
H	5.61775900	-5.23026900	-0.87932400
H	6.57922200	-4.03306300	0.00306600
H	5.61668300	-5.23058000	0.88385700
C	5.13210700	0.63060300	-2.54523600
H	4.82870800	-0.42016300	-2.61940500
H	4.22379900	1.22950200	-2.68074100
H	5.80643600	0.84797000	-3.37944100
C	5.13025800	0.63979900	2.54649800
H	4.22347100	1.24122300	2.68105800
H	4.82442200	-0.41005000	2.62345000
H	5.80545500	0.85764900	3.37988000
C	9.11877100	2.39645100	-0.00356300
H	9.05994800	3.48493800	-0.13852300
H	9.64546500	2.21374000	0.93901800
H	9.73752400	2.00444000	-0.81856700
C	3.75981300	0.08401000	0.00095300
C	2.68689800	0.92623900	0.00067700
C	-2.68686200	-0.92633700	-0.00062000
C	-3.75977500	-0.08410900	-0.00091600
H	-2.85285700	-2.00156100	-0.00051400
H	2.85289200	2.00146200	0.00051700

BO4b_S₀

C	-4.23179800	-3.89026500	-0.00006600
C	-4.47505100	-2.51936100	0.00829000
C	-3.43613000	-1.56852000	0.01650400
C	-2.08998400	-2.01644300	0.01146100
C	-1.84052400	-3.40302300	0.00246500
C	-2.88830400	-4.31133200	-0.00207600
C	-1.01346100	-1.01803100	0.01206200
C	-1.33446100	0.36009900	0.01146500
C	-0.35115800	1.34107200	0.01164100
H	-0.68701800	2.37155100	0.01262000
C	1.01346900	1.01805600	0.01200500
C	1.33447000	-0.36007500	0.01149900
C	0.35116700	-1.34104700	0.01172900
H	-5.50260000	-2.16147100	0.00720100
H	-0.82327900	-3.78106400	-0.00126600
H	-2.66503000	-5.37652100	-0.00894200
H	0.68702600	-2.37152600	0.01277100
C	2.08999300	2.01646500	0.01134800
C	1.84053100	3.40304700	0.00220600
C	2.88830800	4.31135500	-0.00239100
C	4.23180700	3.89028900	-0.00028300
C	4.47505900	2.51938800	0.00817900
C	3.43613700	1.56854400	0.01645600
H	0.82328400	3.78108200	-0.00162200
H	2.66503800	5.37654400	-0.00939200
H	5.50260600	2.16149300	0.00712300
B	-3.71838100	-0.04814000	0.02001000
O	-2.63184600	0.80122600	0.01218400
B	3.71839200	0.04816500	0.02006100
O	2.63185300	-0.80119900	0.01226100
C	-5.14195900	0.62797900	0.01128900
C	-5.88445600	0.77969600	1.20268300
C	-5.69753600	1.09412200	-1.20078300
C	-7.14705700	1.38094600	1.16461300
C	-6.96304700	1.68833000	-1.20493900
C	-7.70422600	1.84531700	-0.02996600
H	-7.70854800	1.49084500	2.09109500
H	-7.38092600	2.03673100	-2.14819300
C	5.14196000	-0.62796900	0.01135600
C	5.69738900	-1.09439100	-1.20069900
C	5.88459300	-0.77944600	1.20267700
C	6.96287600	-1.68860900	-1.20488600
C	7.14720300	-1.38071400	1.16457300

C	7.70421300	-1.84534600	-0.02995900
H	7.38064000	-2.03720600	-2.14812100
H	7.70881500	-1.49039800	2.09100500
C	-9.05562900	2.52137000	-0.04719900
H	-8.95969600	3.60752100	0.08661700
H	-9.57475100	2.35809600	-0.99802400
H	-9.69963700	2.15221700	0.75840800
C	-5.31911200	0.31595500	2.52986700
H	-5.02219000	-0.73947200	2.49956900
H	-4.42604500	0.89087900	2.80755600
H	-6.04981300	0.43398200	3.33655500
C	-4.93211300	0.95495800	-2.50100800
H	-3.99815500	1.52991100	-2.47912300
H	-4.65989800	-0.08954900	-2.70095200
H	-5.52262800	1.31109200	-3.35122700
C	-5.35592200	-4.89826900	-0.00861900
H	-5.31018900	-5.55718600	0.86775100
H	-6.33257600	-4.40472100	-0.00496500
H	-5.30970700	-5.54262900	-0.89572200
C	5.35592600	4.89829800	-0.00871400
H	5.31103900	5.55614400	0.86851400
H	6.33258000	4.40474100	-0.00655800
H	5.30886100	5.54374200	-0.89497400
C	5.31939000	-0.31556700	2.52987200
H	5.02127900	0.73950600	2.49914000
H	4.42710000	-0.89134100	2.80831200
H	6.05060700	-0.43235300	3.33627400
C	4.93181800	-0.95546200	-2.50086100
H	3.99783300	-1.53036200	-2.47874500
H	4.65963400	0.08901800	-2.70099300
H	5.52221700	-1.31180300	-3.35107500
C	9.05561400	-2.52139900	-0.04729800
H	8.95949000	-3.60788400	0.08363700
H	9.57586400	-2.35576900	-0.99710800
H	9.69868200	-2.15428100	0.75997700

CC4c_S₀

C	-1.22419300	3.54665700	-0.02225000
C	-4.00383700	3.39669700	-0.57807000
C	-1.77574600	2.29693600	-0.40404000
C	-2.08419000	4.67339700	0.16913400
C	-3.42977300	4.58568500	-0.04187900
C	-3.16773900	2.25733500	-0.82004300
H	-1.64192200	5.60514900	0.50886100

H	-4.07608700	5.44083000	0.14591700
C	-0.91370600	1.12091000	-0.35241700
C	0.91370600	-1.12091000	-0.35241700
C	0.50725900	1.30581900	-0.23378900
C	-1.37212700	-0.20215000	-0.26753900
C	-0.50725900	-1.30581900	-0.23378900
C	1.37212700	0.20215000	-0.26753900
H	-2.43141300	-0.39906500	-0.14522900
H	2.43141300	0.39906500	-0.14522900
C	1.77574600	-2.29693600	-0.40404000
C	3.42977300	-4.58568500	-0.04187900
C	3.16773900	-2.25733500	-0.82004300
C	1.22419300	-3.54665700	-0.02225000
C	2.08419000	-4.67339700	0.16913400
C	4.00383700	-3.39669700	-0.57807000
H	1.64192200	-5.60514900	0.50886100
H	4.07608700	-5.44083000	0.14591700
C	0.20672100	3.69908900	0.17168700
C	1.02521400	2.61859100	0.00252900
H	2.10279900	2.73824700	0.10109900
C	-1.02521400	-2.61859100	0.00252900
H	-2.10279900	-2.73824700	0.10109900
C	-0.20672100	-3.69908900	0.17168700
C	0.80085400	5.03240500	0.52151200
C	1.97572400	7.51512900	1.18778200
C	1.19331900	5.92535100	-0.49856100
C	0.99383300	5.38319000	1.87452400
C	1.57799000	6.61718000	2.18234000
C	1.77574600	7.14785200	-0.14639200
H	1.72770100	6.88089400	3.22873300
H	2.08225000	7.83083800	-0.93801400
C	-0.80085400	-5.03240500	0.52151200
C	-1.97572400	-7.51512900	1.18778200
C	-0.99383300	-5.38319000	1.87452400
C	-1.19331900	-5.92535100	-0.49856100
C	-1.77574600	-7.14785200	-0.14639200
C	-1.57799000	-6.61718000	2.18234000
H	-2.08225000	-7.83083800	-0.93801400
H	-1.72770100	-6.88089400	3.22873300
C	0.99696900	5.57863200	-1.95752000
H	-0.05841500	5.38450900	-2.18513300
H	1.54920000	4.67287400	-2.23575800
H	1.33735500	6.39500800	-2.60239900
C	0.58350500	4.44623600	2.98855500

H	-0.47901200	4.18192400	2.92107700
H	0.75734400	4.90320500	3.96793300
H	1.14324500	3.50382800	2.94960300
C	2.57777100	8.85462000	1.54281800
H	1.80558000	9.63410200	1.60365700
H	3.30562700	9.17891800	0.79057200
H	3.08386800	8.82227800	2.51389000
C	-0.99696900	-5.57863200	-1.95752000
H	-1.54920000	-4.67287400	-2.23575800
H	-1.33735500	-6.39500800	-2.60239900
H	0.05841500	-5.38450900	-2.18513300
C	-0.58350500	-4.44623600	2.98855500
H	-1.14324500	-3.50382800	2.94960300
H	0.47901200	-4.18192400	2.92107700
H	-0.75734400	-4.90320500	3.96793300
C	-2.57777100	-8.85462000	1.54281800
H	-3.08386800	-8.82227800	2.51389000
H	-1.80558000	-9.63410200	1.60365700
H	-3.30562700	-9.17891800	0.79057200
C	-5.37673300	3.35624100	-0.92864900
H	-5.99146000	4.22693600	-0.70813500
C	-5.91926600	2.26013100	-1.56425400
H	-6.97198400	2.24490900	-1.83596900
C	-3.74821700	1.17918300	-1.54471900
H	-3.12170300	0.35890700	-1.87218200
C	-5.08232000	1.17753000	-1.90380500
H	-5.48304600	0.34003300	-2.47024100
C	3.74821700	-1.17918300	-1.54471900
H	3.12170300	-0.35890700	-1.87218200
C	5.08232000	-1.17753000	-1.90380500
H	5.48304600	-0.34003300	-2.47024100
C	5.91926600	-2.26013100	-1.56425400
H	6.97198400	-2.24490900	-1.83596900
C	5.37673300	-3.35624100	-0.92864900
H	5.99146000	-4.22693600	-0.70813500

BO4c_S₀

C	-1.01076800	-1.04457800	-0.02899000
C	-1.32525300	0.32010500	0.19527400
C	-0.35175200	1.30960300	0.26045300
H	-0.69611600	2.30094100	0.51774700
C	1.00989600	1.04248900	0.03523100
C	1.32468000	-0.32224900	-0.18677600
C	0.35118800	-1.31131700	-0.25415600

H	0.69635900	-2.30249500	-0.51022900
B	-3.69038400	-0.05817700	0.04308800
O	-2.61536100	0.75251100	0.33493400
B	3.68740400	0.05234600	-0.00497600
O	2.61571600	-0.75570200	-0.31644800
C	-5.11582100	0.61309500	0.08160500
C	-5.97531000	0.45313700	1.19054500
C	-5.55519700	1.39111500	-1.01285000
C	-7.23636400	1.05869400	1.18677200
C	-6.82353000	1.97875000	-0.98685300
C	-7.68025500	1.82730000	0.10737600
H	-7.88806000	0.92721800	2.04906500
H	-7.15131100	2.56876000	-1.84137200
C	5.11351200	-0.61733400	-0.03363000
C	5.77112800	-0.85379000	-1.26200100
C	5.75791700	-0.99048800	1.16576400
C	7.03947000	-1.44034300	-1.27103300
C	7.02751600	-1.57773300	1.12142900
C	7.68580900	-1.81299100	-0.08786000
H	7.53735800	-1.60908800	-2.22469300
H	7.51262500	-1.85941400	2.05460600
C	-9.03483000	2.49676300	0.13356300
H	-8.96893100	3.51446800	0.54187900
H	-9.46149800	2.57948400	-0.87209000
H	-9.74403800	1.94294800	0.75821400
C	-5.54453000	-0.35899900	2.39528000
H	-5.34347400	-1.40452400	2.13078000
H	-4.62518000	0.04034300	2.84197900
H	-6.31638600	-0.35576500	3.17153700
C	-4.66281600	1.59349900	-2.22078900
H	-3.74607600	2.13428800	-1.95533900
H	-4.35322100	0.63716600	-2.66222400
H	-5.17346000	2.16663700	-3.00122100
C	5.07932900	-0.78606700	2.50543000
H	4.75236800	0.25144500	2.64534000
H	4.18632500	-1.41748000	2.60223600
H	5.74986900	-1.03793000	3.33337300
C	5.11337000	-0.47374400	-2.57276200
H	4.19000300	-1.04247100	-2.73674500
H	4.84267300	0.58978500	-2.59608900
H	5.77799100	-0.66449800	-3.42142300
C	9.04525300	-2.47204300	-0.12181600
H	8.96298600	-3.54474300	-0.34335600
H	9.68565900	-2.03275700	-0.89511200

H	9.56133200	-2.37663000	0.83933500
C	-1.59697200	-6.30635600	0.00066200
C	-2.78140500	-5.74414200	-0.41783500
C	-2.97169000	-4.33766200	-0.40849400
C	-1.88681400	-3.47519000	-0.02908000
C	-0.70786500	-4.10009300	0.46631800
C	-0.56528300	-5.47215500	0.48117300
H	-5.05077400	-4.45478900	-1.00616600
H	-1.46892200	-7.38530400	-0.00197000
H	-3.60850600	-6.37388100	-0.73676400
C	-4.24654000	-3.78427700	-0.71276600
C	-2.09281400	-2.04199600	-0.08997000
H	0.07707500	-3.49512500	0.89949500
H	0.34382700	-5.91190100	0.88193000
C	-3.40370200	-1.54921100	-0.24542000
C	-4.46584200	-2.44129800	-0.56570800
H	-5.46015900	-2.02798600	-0.71118500
C	3.40186000	1.54900600	0.25791700
C	2.09210600	2.04026000	0.08899500
C	1.88664100	3.47174800	-0.00088600
C	2.97313800	4.34142400	0.35683000
C	4.24941800	3.79403000	0.66509300
C	4.46702200	2.44791100	0.54762700
H	-0.08177300	3.47336500	-0.91976800
C	0.70558300	4.08695200	-0.50350100
C	2.78337100	5.74795400	0.33809100
H	5.05679000	4.47067900	0.93482300
H	5.46358900	2.03884600	0.68929800
C	1.59726500	6.30189100	-0.08639300
C	0.56314100	5.45837800	-0.54516300
H	3.61205600	6.38374400	0.64046500
H	1.46939900	7.38070300	-0.10499600
H	-0.34790100	5.89035600	-0.94998900

CC4d_S₀

C	-1.21060900	-0.76838900	-0.00010000
C	-1.24159900	0.65927400	-0.00002200
C	-0.04323200	1.38561100	0.00003800
H	-0.11985900	2.46843900	0.00009400
C	1.21061000	0.76839100	0.00003400
C	1.24160000	-0.65927100	0.00000200
C	0.04323300	-1.38560900	-0.00006900
H	0.11985900	-2.46843600	-0.00008700
C	-4.98349000	1.47147900	0.00001200

C	-5.58549200	1.84204700	1.22096000
C	-5.58551700	1.84223800	-1.22086700
C	-6.77350700	2.58025500	1.19779500
C	-6.77353300	2.58043600	-1.19756300
C	-7.38247100	2.96434100	0.00015300
H	-7.23534800	2.86038400	2.14288200
H	-7.23540300	2.86069900	-2.14259500
C	4.98349100	-1.47147800	0.00008700
C	5.58546200	-1.84216700	-1.22083900
C	5.58554500	-1.84211800	1.22098700
C	6.77347800	-2.58037100	-1.19763200
C	6.77355600	-2.58032900	1.19772600
C	7.38246700	-2.96434700	0.00003300
H	7.23530400	-2.86058200	-2.14270100
H	7.23543900	-2.86051300	2.14277600
C	-8.64865900	3.78940500	0.00022600
H	-8.42381400	4.86458200	0.00030100
H	-9.25956000	3.58697000	-0.88611800
H	-9.25954100	3.58684300	0.88655400
C	-4.96920000	1.45277300	2.54655600
H	-4.82644200	0.36854500	2.62237800
H	-3.98208600	1.90991600	2.68341200
H	-5.60455300	1.76904700	3.37959400
C	-4.96927100	1.45314300	-2.54653800
H	-3.98225300	1.91047100	-2.68346800
H	-4.82632600	0.36894500	-2.62242900
H	-5.60475800	1.76934900	-3.37950100
C	4.96931600	-1.45292100	2.54663500
H	4.82654700	-0.36869900	2.62251900
H	3.98221500	-1.91008500	2.68352000
H	5.60471700	-1.76922900	3.37962300
C	4.96915400	-1.45299700	-2.54646000
H	3.98212000	-1.91030000	-2.68335800
H	4.82622400	-0.36879300	-2.62229000
H	5.60459000	-1.76917300	-3.37947200
C	8.64865200	-3.78941700	0.00000600
H	8.42380200	-4.86459200	0.00018600
H	9.25944200	-3.58704500	-0.88642800
H	9.25964600	-3.58679600	0.88624500
C	-6.22159200	-4.96680900	-0.00041900
C	-6.21215500	-3.59327300	-0.00033000
C	-4.98230000	-2.87320000	-0.00027900
C	-3.74894700	-3.60712900	-0.00032200
C	-3.79675900	-5.03145500	-0.00041300

C	-4.99995300	-5.69416100	-0.00046000
H	-5.86022100	-0.90865200	-0.00015700
H	-7.16513800	-5.50583400	-0.00045600
H	-7.14412600	-3.03292900	-0.00029700
C	-4.92866500	-1.46709400	-0.00018600
C	-2.53412400	-2.89452100	-0.00026900
H	-2.86095600	-5.58572700	-0.00044300
H	-5.02401200	-6.78054800	-0.00052900
C	-2.47895700	-1.50377400	-0.00017800
C	-3.72299200	-0.76756100	-0.00014200
C	2.47895900	1.50377600	0.00007100
C	2.53412500	2.89452300	0.00007800
C	3.74894900	3.60713100	0.00013300
C	4.98230200	2.87320200	0.00018600
C	4.92866600	1.46709600	0.00018000
C	3.72299300	0.76756400	0.00011600
H	2.86095900	5.58573000	0.00010500
C	3.79676200	5.03145800	0.00014200
C	6.21215700	3.59327400	0.00024600
H	5.86022300	0.90865400	0.00022300
C	6.22159400	4.96681100	0.00025100
C	4.99995600	5.69416300	0.00019900
H	7.14412800	3.03293000	0.00028700
H	7.16514100	5.50583500	0.00029800
H	5.02401500	6.78055000	0.00020700
H	1.61694300	3.47530500	0.00004100
H	-1.61694100	-3.47530200	-0.00030200
C	-3.70276900	0.69101300	-0.00005800
C	-2.50852400	1.34378700	0.00000500
C	2.50852400	-1.34378500	0.00005000
C	3.70277000	-0.69101100	0.00011700
H	-2.49600300	2.43166200	0.00009000
H	2.49600300	-2.43165900	0.00003000

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C	-1.16995400	-0.83477600	-0.00610300
C	-1.25665500	0.57647500	-0.00240100
C	-0.12271600	1.37828400	-0.00413900
H	-0.28180700	2.45034900	-0.00135400
C	1.16998600	0.83482400	-0.00605600
C	1.25668400	-0.57642700	-0.00245200
C	0.12274500	-1.37823500	-0.00423500
H	0.28183800	-2.45030100	-0.00154300
B	-3.67590600	0.58743900	0.01854400

O	-2.46128100	1.23696500	0.00618700
B	3.67593700	-0.58739500	0.01850700
O	2.46130900	-1.23691800	0.00605900
C	-4.96774600	1.48928700	0.03542000
C	-5.63715300	1.77287600	1.24559300
C	-5.48152300	2.02104600	-1.16819800
C	-6.79193200	2.56268300	1.23380500
C	-6.63877500	2.80478200	-1.14561200
C	-7.30942100	3.09003100	0.04780800
H	-7.29964400	2.77113400	2.17421300
H	-7.02782400	3.20113800	-2.08230400
C	4.96774600	-1.48929000	0.03539900
C	5.48176000	-2.02067400	-1.16828000
C	5.63685100	-1.77333300	1.24563100
C	6.63896200	-2.80449200	-1.14569100
C	6.79158300	-2.56320300	1.23384400
C	7.30931400	-3.09018300	0.04778500
H	7.02819500	-3.20057400	-2.08242200
H	7.29905900	-2.77200600	2.17430100
C	-8.54277400	3.96344200	0.05581500
H	-8.27705400	5.02867300	0.09282100
H	-9.14686500	3.81353000	-0.84592400
H	-9.17510300	3.75634900	0.92576300
C	-5.10684000	1.24531200	2.56340800
H	-4.98420000	0.15545800	2.54641000
H	-4.12390300	1.67373900	2.79869500
H	-5.77972400	1.49183600	3.39096700
C	-4.78561000	1.74974600	-2.48641400
H	-3.77811100	2.18374300	-2.50293100
H	-4.67351700	0.67369300	-2.67184100
H	-5.34410700	2.17387800	-3.32695500
C	5.10632800	-1.24605400	2.56347700
H	4.98484100	-0.15605500	2.54707400
H	4.12281700	-1.67359200	2.79795000
H	5.77850200	-1.49376800	3.39125800
C	4.78613000	-1.74891700	-2.48655300
H	3.77861400	-2.18286700	-2.50341600
H	4.67411600	-0.67280100	-2.67165600
H	5.34477500	-2.17280300	-3.32711900
C	8.54260100	-3.96368600	0.05579100
H	8.27680200	-5.02889600	0.09283000
H	9.14668900	-3.81383700	-0.84595900
H	9.17496000	-3.75662400	0.92572700
C	-5.99085700	-5.25346400	-0.07153500

C	-6.03474000	-3.87919700	-0.04883600
C	-4.83601200	-3.11394000	-0.03576100
C	-3.57249500	-3.79386500	-0.04701000
C	-3.56395300	-5.21724200	-0.07079900
C	-4.74163200	-5.92737300	-0.08253200
H	-5.78909500	-1.17791600	-0.00622000
H	-6.91161500	-5.83010700	-0.08123300
H	-6.98768200	-3.35548100	-0.04036000
C	-4.83487600	-1.70077500	-0.01262900
C	-2.37913700	-3.03558100	-0.03608500
H	-2.60787000	-5.73524600	-0.07948500
H	-4.72039000	-7.01372800	-0.10049300
C	-2.39638600	-1.64802600	-0.01258800
C	-3.66097500	-0.96033000	0.00099700
C	2.39642200	1.64807500	-0.01250000
C	2.37917700	3.03563000	-0.03594700
C	3.57253700	3.79391200	-0.04683700
C	4.83605200	3.11398200	-0.03561400
C	4.83491100	1.70081500	-0.01254600
C	3.66100700	0.96037300	0.00105100
H	2.60791900	5.73529700	-0.07923600
C	3.56400100	5.21728900	-0.07056900
C	6.03478300	3.87923600	-0.04865300
H	5.78912800	1.17795700	-0.00616700
C	5.99090400	5.25350500	-0.07129400
C	4.74168200	5.92741700	-0.08226800
H	6.98772400	3.35551700	-0.04019700
H	6.91166400	5.83014500	-0.08096400
H	4.72044300	7.01377300	-0.10018400
H	1.43955100	3.58011400	-0.04862100
H	-1.43951000	-3.58006200	-0.04876100

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C	-0.81810400	3.70201500	-0.00011300
C	-3.63016600	3.68606400	0.00160200
C	-1.52938600	2.45945200	0.00058000
C	-1.53792500	4.92020900	-0.00005900
C	-2.92217000	4.91285000	0.00074000
C	-2.94663800	2.48864500	0.00154500
H	-0.98461600	5.85541800	-0.00058600
C	-0.78378400	1.20422700	0.00037500
C	0.78378400	-1.20422700	0.00037500
C	0.64826100	1.24909000	0.00016400
C	-1.38780100	-0.05827200	0.00020400

C	-0.64826100	-1.24909000	0.00016400
C	1.38780100	0.05827200	0.00020400
H	-2.47049000	-0.14812400	-0.00009600
H	2.47049000	0.14812400	-0.00009600
C	1.52938600	-2.45945200	0.00058000
C	2.92217000	-4.91285000	0.00074000
C	2.94663800	-2.48864500	0.00154500
C	0.81810400	-3.70201500	-0.00011300
C	1.53792500	-4.92020900	-0.00005900
C	3.63016600	-3.68606400	0.00160200
H	0.98461600	-5.85541800	-0.00058600
C	0.63766000	3.70660000	-0.00067000
C	1.31388000	2.52155300	-0.00036000
H	2.40285600	2.52789800	-0.00061500
C	-1.31388000	-2.52155300	-0.00036000
H	-2.40285600	-2.52789800	-0.00061500
C	-0.63766000	-3.70660000	-0.00067000
C	1.39792900	5.00050300	-0.00147900
C	2.86000600	7.41961300	-0.00316900
C	1.76352500	5.60523900	-1.22301500
C	1.76360500	5.60680900	1.21910000
C	2.48894000	6.80339000	1.19548200
C	2.48880800	6.80173700	-1.20107300
H	2.77184300	7.26472900	2.14109700
H	2.77165900	7.26180400	-2.14734100
C	-1.39792900	-5.00050300	-0.00147900
C	-2.86000600	-7.41961300	-0.00316900
C	-1.76360500	-5.60680900	1.21910000
C	-1.76352500	-5.60523900	-1.22301500
C	-2.48880800	-6.80173700	-1.20107300
C	-2.48894000	-6.80339000	1.19548200
H	-2.77165900	-7.26180400	-2.14734100
H	-2.77184300	-7.26472900	2.14109700
C	1.38780100	4.97714400	-2.54643000
H	0.30387800	4.83033800	-2.62744300
H	1.84801600	3.98909100	-2.66858600
H	1.70854400	5.60608000	-3.38298700
C	1.38780100	4.98065800	2.54340800
H	0.30367300	4.83575800	2.62532400
H	1.71014200	5.60989700	3.37912000
H	1.84641900	3.99195300	2.66619300
C	3.61543500	8.72811600	-0.00446500
H	2.92722500	9.58475400	-0.01893000
H	4.26157800	8.81712800	-0.88489400

H	4.24161100	8.83048800	0.88875100
C	-1.38780100	-4.97714400	-2.54643000
H	-1.84801600	-3.98909100	-2.66858600
H	-1.70854400	-5.60608000	-3.38298700
H	-0.30387800	-4.83033800	-2.62744300
C	-1.38780100	-4.98065800	2.54340800
H	-1.84641900	-3.99195300	2.66619300
H	-0.30367300	-4.83575800	2.62532400
H	-1.71014200	-5.60989700	3.37912000
C	-3.61543500	-8.72811600	-0.00446500
H	-4.24161100	-8.83048800	0.88875100
H	-2.92722500	-9.58475400	-0.01893000
H	-4.26157800	-8.81712800	-0.88489400
H	-3.50472100	1.55650400	0.00240200
H	3.50472100	-1.55650400	0.00240200
C	-3.89599500	6.01064300	0.00102600
C	-6.12330000	7.67925400	0.00196100
C	-5.19296300	5.45839100	0.00213800
C	-3.71146000	7.39605500	0.00036700
C	-4.83484800	8.22576200	0.00084000
C	-6.30776600	6.29117200	0.00261100
H	-2.71135400	7.82410700	-0.00050100
H	-4.70797200	9.30595900	0.00033800
H	-7.31421800	5.87659600	0.00346100
H	-6.98843800	8.33837000	0.00232500
C	3.89599500	-6.01064300	0.00102600
C	6.12330000	-7.67925400	0.00196100
C	5.19296300	-5.45839100	0.00213800
C	3.71146000	-7.39605500	0.00036700
C	4.83484800	-8.22576200	0.00084000
C	6.30776600	-6.29117200	0.00261100
H	2.71135400	-7.82410700	-0.00050100
H	4.70797200	-9.30595900	0.00033800
H	7.31421800	-5.87659600	0.00346100
H	6.98843800	-8.33837000	0.00232500
C	-5.14013400	3.92943400	0.00260900
C	-5.80512600	3.34436900	1.26869200
H	-5.34550500	3.74679700	2.17751000
H	-5.70643000	2.25236200	1.29022100
H	-6.87483700	3.58494500	1.29100000
C	-5.80688900	3.34357600	-1.26219400
H	-6.87666400	3.58400400	-1.28311600
H	-5.70807800	2.25157100	-1.28324400
H	-5.34862600	3.74554600	-2.17190100

C	5.14013400	-3.92943400	0.00260900
C	5.80688900	-3.34357600	-1.26219400
H	5.70807800	-2.25157100	-1.28324400
H	5.34862600	-3.74554600	-2.17190100
H	6.87666400	-3.58400400	-1.28311600
C	5.80512600	-3.34436900	1.26869200
H	5.70643000	-2.25236200	1.29022100
H	6.87483700	-3.58494500	1.29100000
H	5.34550500	-3.74679700	2.17751000

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C	5.58046300	1.24109900	0.01997400
C	5.13988700	-0.07589900	0.00699500
C	3.76125600	-0.36455000	-0.00485300
C	2.81958600	0.70366200	0.00197000
C	3.28230800	2.03834600	0.01558500
C	4.64019900	2.29794300	0.02334700
C	1.38888900	0.37434100	-0.00073400
C	0.97535000	-0.97945000	-0.00342300
C	-0.36681100	-1.33562200	-0.00236500
H	-0.58989900	-2.39605100	-0.00499100
C	-1.38884600	-0.37431100	0.00074600
C	-0.97530100	0.97948100	0.00342200
C	0.36685200	1.33565700	0.00236500
H	5.84828800	-0.90098400	0.00721100
H	2.57820800	2.86487600	0.02091900
H	0.58994400	2.39608300	0.00497000
C	-2.81954600	-0.70362900	-0.00194600
C	-3.28226700	-2.03831700	-0.01541100
C	-4.64015700	-2.29791000	-0.02315800
C	-5.58042000	-1.24106500	-0.01990000
C	-5.13984300	0.07593500	-0.00706100
C	-3.76121200	0.36458300	0.00475200
H	-2.57816400	-2.86484400	-0.02062900
B	3.24081700	-1.82012700	-0.01609100
O	1.87541300	-2.01232500	-0.00883200
B	-3.24076400	1.82016000	0.01592200
O	-1.87537300	2.01236500	0.00881200
C	4.13774700	-3.11626100	-0.01811700
C	4.40402800	-3.79766000	1.19022900
C	4.69243000	-3.61523300	-1.21686700
C	5.20937900	-4.94041700	1.18339100
C	5.49253200	-4.76251900	-1.18958500
C	5.76195200	-5.44238700	0.00125200

H	5.41178000	-5.45090400	2.12373200
H	5.91487800	-5.13501500	-2.12158000
C	-4.13775100	3.11626100	0.01785400
C	-4.40476100	3.79714400	-1.19062100
C	-4.69177900	3.61568400	1.21671100
C	-5.21015700	4.93986700	-1.18378900
C	-5.49195900	4.76291800	1.18942100
C	-5.76208800	5.44228700	-0.00153600
H	-5.41309200	5.44997800	-2.12422000
H	-5.91378500	5.13578000	2.12150500
C	6.92916200	1.81728500	0.03300800
C	8.18426600	1.20425000	0.03551200
C	6.81506500	3.22189400	0.04371300
C	9.32592200	2.00780200	0.04865300
H	8.27466600	0.12105100	0.02749300
C	7.95634400	4.01623100	0.05666900
C	9.21452800	3.40251400	0.05911000
H	10.30966400	1.54602500	0.05082300
H	7.88150400	5.10124700	0.06485300
H	10.11233400	4.01477800	0.06923300
C	-6.92911900	-1.81724500	-0.03286800
C	-8.18421400	-1.20420900	-0.03544000
C	-6.81502500	-3.22186300	-0.04341800
C	-9.32588100	-2.00776100	-0.04849100
C	-7.95630200	-4.01619100	-0.05628300
C	-9.21449200	-3.40246700	-0.05879000
H	-10.30961500	-1.54596600	-0.05071000
H	-7.88148200	-5.10120800	-0.06434300
H	-10.11229000	-4.01474400	-0.06884300
C	6.60417200	-6.69719200	0.00807800
H	5.98138700	-7.59630000	-0.09476100
H	7.32104300	-6.70374600	-0.82012300
H	7.16567000	-6.79923000	0.94329000
C	3.82311200	-3.29936900	2.49797700
H	4.10559800	-2.25725300	2.69587800
H	2.72676800	-3.33711600	2.48908400
H	4.17003700	-3.90206100	3.34342800
C	4.41410900	-2.93110600	-2.53999000
H	3.34921400	-2.98423600	-2.80132200
H	4.68350500	-1.86821600	-2.51374200
H	4.97654800	-3.39739800	-3.35529200
C	-4.41273200	2.93202100	2.53992100
H	-4.68279200	1.86927600	2.51438600
H	-3.34758600	2.98462900	2.80032200

H	-4.97421400	3.39901200	3.35548200
C	-3.82459500	3.29830700	-2.49849200
H	-2.72822300	3.33530100	-2.48995600
H	-4.10786600	2.25635900	-2.69617100
H	-4.17137500	3.90112900	-3.34391000
C	-6.60436500	6.69705300	-0.00841700
H	-5.98144700	7.59630100	0.09237300
H	-7.16738600	6.79801700	-0.94283400
H	-7.31989200	6.70451200	0.82093400
C	5.34803900	3.65326800	0.03864700
C	5.00714100	4.47919200	-1.22227200
H	3.94041000	4.73024400	-1.24575100
H	5.57362800	5.41747200	-1.23216000
H	5.24877600	3.92487200	-2.13469800
C	4.99238800	4.45854500	1.30879200
H	3.92567600	4.71038100	1.32347100
H	5.22240400	3.88888300	2.21473200
H	5.55959200	5.39584400	1.34097800
H	-8.27461800	-0.12100900	-0.02754100
H	-5.84824200	0.90102300	-0.00734600
C	-5.34800100	-3.65323700	-0.03832200
C	-5.00708700	-4.47906200	1.22265100
H	-5.57357500	-5.41734000	1.23262200
H	-3.94035700	-4.73011700	1.24613600
H	-5.24870700	-3.92467000	2.13503700
C	-4.99237100	-4.45860400	-1.30842000
H	-3.92565700	-4.71043000	-1.32310400
H	-5.55956900	-5.39591000	-1.34052700
H	-5.22241300	-3.88900600	-2.21439200

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C	-0.20047600	5.71816300	-0.00002300
C	-1.35566100	4.95873500	-0.00017000
C	-1.29891500	3.54714200	-0.00010900
C	-0.03520600	2.89253900	0.00005000
C	1.12822700	3.69376000	0.00027800
C	1.05042600	5.07648700	0.00023300
C	-0.00391000	1.43227000	-0.00002300
C	-1.23523100	0.69564500	0.00004500
C	-1.19111900	-0.70539900	0.00001900
H	-2.13918100	-1.22941500	0.00017900
C	0.00391700	-1.43228500	-0.00010500
C	1.23523800	-0.69566000	-0.00009600
C	1.19112600	0.70538300	-0.00012600

H	-0.25777500	6.80323700	-0.00008200
H	-2.33048000	5.44108900	-0.00031100
H	2.10803500	3.22835300	0.00056600
H	1.96313800	5.66619500	0.00042100
H	2.13918900	1.22939900	-0.00024100
C	0.03521500	-2.89255500	-0.00022900
C	1.29892400	-3.54715600	0.00005200
H	-2.10802600	-3.22837200	-0.00111500
C	-1.12821700	-3.69377800	-0.00067200
C	1.35567200	-4.95874900	0.00004500
C	0.20048900	-5.71817900	-0.00028600
C	-1.05041400	-5.07650500	-0.00068700
H	2.33049200	-5.44110100	0.00028600
H	0.25778900	-6.80325300	-0.00027500
H	-1.96312500	-5.66621400	-0.00104700
C	-3.80408000	0.65308200	0.00013000
C	-4.42012900	0.30568000	-1.22074700
C	-4.41954200	0.30481500	1.22104500
C	-5.64124900	-0.37650200	-1.19751400
C	-5.64068700	-0.37736300	1.19787800
C	-6.27183700	-0.72378200	0.00021400
H	-6.11048200	-0.64409300	-2.14257700
H	-6.10952100	-0.64558800	2.14295500
C	3.80408500	-0.65309200	0.00004900
C	4.41987000	-0.30534700	-1.22088100
C	4.41979700	-0.30514300	1.22091100
C	5.64098200	0.37683800	-1.19770700
C	5.64092700	0.37707100	1.19768600
C	6.27181900	0.72381300	-0.00000800
H	6.11005500	0.64465400	-2.14278500
H	6.10991000	0.64509200	2.14274600
C	3.78081900	-0.65570800	2.54659400
H	2.76814700	-0.24374900	2.62805900
H	3.68964000	-1.74036900	2.67717500
H	4.37244300	-0.26456100	3.38005700
C	3.78087500	-0.65599900	-2.54652400
H	3.68805300	-1.74060800	-2.67628800
H	2.76885300	-0.24254200	-2.62867800
H	4.37337700	-0.26636200	-3.38006700
C	7.60663900	1.43246300	-0.00012000
H	7.72634000	2.06280800	0.88767000
H	8.43872900	0.71538900	-0.00317200
H	7.72382000	2.06731000	-0.88505300
C	-7.60667000	-1.43240800	0.00023800

H	-8.43874800	-0.71531600	-0.00177900
H	-7.72433800	-2.06653100	-0.88514800
H	-7.72590700	-2.06347500	0.88757800
C	-3.78024400	0.65490200	2.54669200
H	-2.76818500	0.24145600	2.62841800
H	-3.68744600	1.73945900	2.67691500
H	-4.37252900	0.26486800	3.38020300
C	-3.78145800	0.65681500	-2.54642600
H	-3.69026400	1.74153000	-2.67654800
H	-2.76882000	0.24485200	-2.62831800
H	-4.37329600	0.26606200	-3.37992100
C	-2.50589300	2.76701700	-0.00010600
C	-2.50515600	1.40342400	0.00009800
C	2.50516300	-1.40343700	0.00006300
C	2.50590200	-2.76703000	0.00023100
H	-3.45449800	3.29974200	-0.00023600
H	3.45450700	-3.29975300	0.00046200

BO5_S0

C	0.85072600	-5.66203700	0.12341400
C	1.91341800	-4.76832900	0.10688900
C	1.66602400	-3.39340100	0.08025000
C	0.35376600	-2.87380700	0.06828900
C	-0.70099600	-3.80992500	0.08641000
C	-0.46324000	-5.17739800	0.11346600
C	0.14987100	-1.41796100	0.03582300
C	1.29085900	-0.56563900	0.02683700
C	1.11944600	0.82356700	-0.00986400
H	2.01512400	1.43691100	-0.01790900
C	-0.14986100	1.41795100	-0.03606600
C	-1.29085700	0.56562600	-0.02698800
C	-1.11944300	-0.82357400	0.00973400
H	1.04188500	-6.73116000	0.14452200
H	2.94555100	-5.10408700	0.11495200
H	-1.72719800	-3.45836100	0.07971600
H	-1.30065800	-5.86901100	0.12707100
H	-2.01511500	-1.43692400	0.01790300
C	-0.35375800	2.87379300	-0.06872700
C	-1.66601000	3.39339600	-0.08054300
H	1.72721200	3.45832800	-0.08074700
C	0.70101000	3.80990000	-0.08722100
C	-1.91340400	4.76832200	-0.10733600
C	-0.85070700	5.66201800	-0.12418800
C	0.46325700	5.17736900	-0.11443300

H	-2.94553600	5.10408100	-0.11526800
H	-1.04185500	6.73114000	-0.14541700
H	1.30067700	5.86897500	-0.12832400
O	2.77088400	-2.58141500	0.06807700
B	2.70196800	-1.20639000	0.04927400
B	-2.70196600	1.20639300	-0.04929800
O	-2.77087400	2.58141600	-0.06811600
C	4.06853700	-0.42317500	0.03783000
C	4.76354500	-0.22090600	-1.17553500
C	4.61995800	0.08846300	1.23230400
C	5.97229900	0.48080500	-1.17662900
C	5.83330600	0.78450000	1.19680800
C	6.52731700	0.99009500	0.00173700
H	6.49390300	0.63460100	-2.12006700
H	6.24691000	1.17383100	2.12566800
C	-4.06854100	0.42319200	-0.03757700
C	-4.62016100	-0.08859300	-1.23195200
C	-4.76332400	0.22100700	1.17587700
C	-5.83338600	-0.78474100	-1.19619000
C	-5.97206200	-0.48081900	1.17723500
C	-6.52721900	-0.99025800	-0.00094800
H	-6.24704100	-1.17431000	-2.12493500
H	-6.49346300	-0.63462300	2.12077800
C	-4.20835800	0.76075000	2.47829400
H	-3.19617100	0.38391400	2.67481100
H	-4.14492700	1.85583900	2.46277700
H	-4.83723100	0.47613300	3.32786100
C	-3.91995000	0.12478700	-2.55876300
H	-3.86578400	1.19062900	-2.81570200
H	-2.88996000	-0.25248200	-2.54123000
H	-4.44601700	-0.38348900	-3.37314600
C	-7.85120700	-1.71862400	0.01733500
H	-7.96442400	-2.32388000	0.92375300
H	-8.69372100	-1.01424100	-0.00708700
H	-7.95664200	-2.38139500	-0.84811200
C	7.85128800	1.71850100	-0.01651100
H	8.69382900	1.01388900	-0.00228700
H	7.96030000	2.33156800	-0.91822300
H	7.96082700	2.37380600	0.85406900
C	3.91932400	-0.12466000	2.55894200
H	2.89043500	0.25567000	2.54200500
H	3.86204800	-1.19065000	2.81453800
H	4.44695200	0.38106300	3.37390100
C	4.20865900	-0.76039900	-2.47808700

H	4.14422800	-1.85542200	-2.46242800
H	3.19689000	-0.38266800	-2.67506900
H	4.83813200	-0.47647300	-3.32744100

CC6_S₀

C	-0.84024100	1.22976000	0.00015200
C	-2.27554600	1.23348500	0.00017900
C	-2.99474200	2.50582300	0.00037700
C	-2.24173500	3.71357200	0.00055200
C	-0.16909000	0.00000300	-0.00001200
C	-2.93756400	0.00005900	-0.00000100
C	-2.27559800	-1.23339600	-0.00018600
C	-0.84029400	-1.22973000	-0.00017300
C	-2.24188800	-3.71348400	-0.00055900
C	-2.99484700	-2.50570600	-0.00037400
H	0.91554000	-0.00002100	-0.00001900
H	-4.01932000	0.00008200	0.00000200
C	-2.91165700	4.95746500	0.00077600
C	-4.40407000	2.60533800	0.00041500
C	-5.04184900	3.83463300	0.00062700
C	-4.29234600	5.02381200	0.00081500
H	-2.31762600	5.86851500	0.00091500
H	-5.01309700	1.70779000	0.00027000
H	-6.12767700	3.87700900	0.00064900
H	-4.79548100	5.98684700	0.00099300
C	-2.91186000	-4.95735100	-0.00078700
C	-4.29255100	-5.02364400	-0.00081100
C	-5.04200800	-3.83443500	-0.00060400
C	-4.40418000	-2.60516600	-0.00039200
H	-2.31786400	-5.86842500	-0.00093600
H	-4.79572500	-5.98665800	-0.00098900
H	-6.12783700	-3.87676900	-0.00061200
H	-5.01317100	-1.70759400	-0.00023100
C	1.38984900	-2.51233100	-0.00009500
C	2.09654700	-2.53679400	-1.22072500
C	2.09607500	-2.53810500	1.22075000
C	3.49376400	-2.59408100	-1.19732900
C	3.49332600	-2.59535900	1.19781200
C	4.21231200	-2.62857800	0.00037100
H	4.03427800	-2.61000700	-2.14208800
H	4.03349000	-2.61230500	2.14275000
C	1.38995900	2.51228200	0.00008000
C	2.09664900	2.53665000	1.22072000
C	2.09619500	2.53809400	-1.22075500

C	3.49386400	2.59389800	1.19734000
C	3.49345100	2.59529800	-1.19780000
C	4.21242600	2.62844900	-0.00035500
H	4.03437000	2.60975200	2.14210600
H	4.03362600	2.61226100	-2.14273200
C	1.36751300	-2.50485900	2.54607300
H	0.72151600	-3.38116400	2.67537900
H	2.07596000	-2.48270900	3.37992300
H	0.72085100	-1.62335000	2.62857300
C	1.36845000	-2.50204700	-2.54626000
H	2.07718100	-2.47994500	-3.37987000
H	0.72171800	-3.37768800	-2.67633900
H	0.72260200	-1.61990000	-2.62837200
C	5.72058100	-2.72344500	0.00055700
H	6.15200900	-2.24902900	0.88859000
H	6.05484100	-3.76987700	-0.00298600
H	6.15265100	-2.24290500	-0.88388200
C	1.36853400	2.50181600	2.54624300
H	2.07725300	2.47963600	3.37985900
H	0.72180000	3.37744200	2.67638100
H	0.72268500	1.61965800	2.62827500
C	1.36765200	2.50492000	-2.54609200
H	0.72188900	3.38138200	-2.67549900
H	2.07611500	2.48251200	-3.37992300
H	0.72076700	1.62357100	-2.62853000
C	5.72070000	2.72324200	-0.00051000
H	6.15277200	2.24202900	0.88356500
H	6.15207800	2.24945900	-0.88890200
H	6.05501100	3.76965400	0.00380700
C	-0.10985000	-2.48666900	-0.00031200
C	-0.80626500	-3.65895000	-0.00051200
C	-0.80611400	3.65898000	0.00049600
C	-0.10974400	2.48667400	0.00028300
H	-0.26312700	-4.60160800	-0.00054600
H	-0.26294000	4.60161800	0.00057700

BO6_S₀

C	-0.95280200	1.17594300	0.01210900
C	-2.37531800	1.08456600	0.01111500
C	-3.15566000	2.33358200	0.01743300
C	-2.48309100	3.57552600	0.02316800
C	-0.21041900	-0.01212800	0.00243200
C	-2.98288600	-0.17822400	0.00287500
C	-2.22894700	-1.35935400	-0.00451700

C	-0.80576400	-1.28021100	-0.00520500
C	-2.03769000	-3.84539400	-0.02058900
C	-2.85413400	-2.69291300	-0.01224200
H	0.87538600	0.05274600	0.00062100
H	-4.06348200	-0.24294900	0.00231000
C	-3.18018200	4.78757700	0.02856300
C	-4.56558600	2.37517600	0.01723900
C	-5.26398500	3.57440600	0.02254200
C	-4.56817900	4.78986700	0.02826600
H	-2.60528200	5.70810900	0.03312500
H	-5.12827300	1.44786600	0.01262600
H	-6.35008100	3.56589100	0.02221200
H	-5.10857100	5.73221000	0.03259300
C	-2.58449200	-5.13224400	-0.02835400
C	-3.96219200	-5.30092500	-0.02768700
C	-4.79856100	-4.17756900	-0.01919300
C	-4.24887600	-2.90328700	-0.01164600
H	-1.90328300	-5.97713800	-0.03469800
H	-4.38569600	-6.30125000	-0.03370600
H	-5.87785700	-4.29917800	-0.01843800
H	-4.91854000	-2.05004800	-0.00495600
B	0.02435100	-2.58217600	-0.01448500
O	-0.67111300	-3.77498700	-0.02172000
O	-1.11798100	3.66914600	0.02438400
B	-0.28453300	2.56825400	0.02080900
C	1.59640500	-2.67808700	-0.01551100
C	2.31293600	-2.71065100	-1.23148800
C	2.31306100	-2.73185800	1.19962400
C	3.70869800	-2.79202800	-1.21500900
C	3.70883100	-2.81282000	1.18157700
C	4.42681900	-2.84658300	-0.01714100
H	4.24903700	-2.81182600	-2.16015200
H	4.24928600	-2.84918000	2.12617500
C	1.26465900	2.85137800	0.01847200
C	1.99435400	2.88377500	1.22681600
C	1.94826200	3.07435200	-1.19657800
C	3.37085700	3.12849100	1.20211500
C	3.32548400	3.31557500	-1.18674600
C	4.05631300	3.34897100	0.00417400
H	3.92207300	3.14579900	2.14099700
H	3.84104700	3.47853300	-2.13185800
C	1.58081400	-2.70698300	2.52580200
H	0.91484900	-3.57270600	2.63284900
H	2.28022400	-2.72148700	3.36778100

H	0.95789400	-1.80904800	2.62765300
C	1.58041100	-2.66269700	-2.55686200
H	2.27971800	-2.65961000	-3.39903600
H	0.91671900	-3.52805400	-2.68007200
H	0.95527900	-1.76459900	-2.64152400
C	5.93356600	-2.96336500	-0.01824000
H	6.37212900	-2.50181100	0.87317000
H	6.25280800	-4.01448900	-0.02964000
H	6.37237800	-2.48253500	-0.89928900
C	1.29707700	2.66519300	2.55410200
H	2.01098600	2.66594200	3.38396300
H	0.55775500	3.45177800	2.75334300
H	0.76069900	1.70832200	2.57814800
C	1.19972900	3.05632400	-2.51372800
H	0.45116900	3.85733400	-2.56024600
H	1.88012200	3.18862000	-3.36099200
H	0.66514200	2.10924700	-2.66245900
C	5.53961700	3.63825200	-0.00083800
H	6.04768200	3.14176000	0.83309500
H	6.01032000	3.30356400	-0.93161800
H	5.73725100	4.71474500	0.09398500

BO1a_T₁

C	-0.02920400	4.41066600	-0.16656200
C	-1.24207300	3.73388100	-0.12697300
C	-1.23938500	2.34018300	-0.06803100
C	-0.01377300	1.58691300	-0.04672400
C	1.21708500	2.33204000	-0.09068600
C	1.20140900	3.70929200	-0.14982200
C	-0.03192200	0.18011600	0.00620500
C	-1.26642600	-0.52523100	0.05865700
C	-1.24025400	-1.91931100	0.10847100
H	-2.16506400	-2.48774500	0.13068700
C	0.04517800	-2.62997900	0.14064400
C	1.23542800	-1.95658800	0.09755300
C	1.28464900	-0.52685400	-0.00124700
H	-0.01914800	5.49643700	-0.21051500
H	-2.19420000	4.25493500	-0.13925600
H	2.14857000	4.23869800	-0.18304700
H	0.03781800	-3.71606900	0.20859800
H	2.17303700	-2.50632000	0.14054900
C	4.03222900	-0.25194700	-0.05897800
C	4.88055500	-0.00033500	1.04834600
C	4.53978200	-1.01565900	-1.13832900

C	6.17668500	-0.52186800	1.06903500
C	5.84638900	-1.51466100	-1.08747000
C	6.68184200	-1.28228900	0.00846700
H	6.80964400	-0.33340800	1.93604000
H	6.22406800	-2.09504800	-1.92893300
C	-4.03341700	-0.24220000	0.06864300
C	-4.59836600	-0.77540800	1.24904700
C	-4.81169700	-0.22795400	-1.11232600
C	-5.90367500	-1.28072300	1.22886000
C	-6.10994200	-0.74598700	-1.09869500
C	-6.67739800	-1.27597300	0.06503800
H	-6.32690800	-1.68754800	2.14699600
H	-6.69260400	-0.73841300	-2.01962400
C	-8.09344700	-1.80188200	0.06810800
H	-8.81712800	-0.99151400	0.23318000
H	-8.34897800	-2.27261400	-0.88807900
H	-8.24549400	-2.54054100	0.86274100
C	-4.24680700	0.33591400	-2.39995800
H	-4.02634600	1.40626500	-2.30358000
H	-3.30870100	-0.16100000	-2.68142900
H	-4.94886300	0.21150100	-3.23085100
C	-3.82387800	-0.77629500	2.55116300
H	-2.83386200	-1.23316500	2.43553400
H	-3.66504500	0.24580900	2.92101800
H	-4.35961700	-1.32719400	3.33127000
C	8.09736500	-1.80781600	0.03566700
H	8.21322900	-2.68335400	-0.61254200
H	8.80978600	-1.04703900	-0.31300000
H	8.40055900	-2.09176700	1.04997700
C	3.70887200	-1.26975000	-2.38018300
H	2.79393900	-1.83270300	-2.15919500
H	3.39622400	-0.32915700	-2.85150400
H	4.27763600	-1.83851300	-3.12341300
C	4.39478400	0.81693300	2.22748000
H	4.17399800	1.84897600	1.93105600
H	3.47043100	0.40350300	2.65215000
H	5.14373600	0.84457100	3.02572500
B	-2.56292200	0.31402900	0.04387000
B	2.56192400	0.30466900	-0.06578000
O	-2.42967300	1.70196500	-0.03074000
O	2.42976600	1.70872800	-0.07968400

BO1b_T1

C	0.02372800	4.55536600	0.08173500
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C	1.23778000	3.87945700	0.05689200
C	1.23586900	2.48421300	0.02583300
C	0.01359100	1.73422200	0.01876000
C	-1.21674600	2.47547700	0.04740200
C	-1.20373800	3.85630600	0.07809100
C	0.03287400	0.32204600	-0.00818400
C	1.26402800	-0.38103500	-0.04666900
C	1.23489300	-1.77997500	-0.07122100
H	2.15950300	-2.35074800	-0.07688800
C	-0.05286500	-2.50982700	-0.09434100
C	-1.23632500	-1.80987200	-0.06198500
C	-1.27974900	-0.38492400	0.00881300
H	0.01403600	5.64199900	0.10428800
H	2.18923300	4.40182100	0.05957100
H	-2.15178600	4.38463300	0.09996000
H	-2.17783000	-2.35556300	-0.09511900
C	-4.02871900	-0.10971100	0.06715400
C	-4.87160000	0.09858500	-1.05209500
C	-4.54179000	-0.82769400	1.17391200
C	-6.17034400	-0.41786000	-1.05625600
C	-5.85042900	-1.32336800	1.13938500
C	-6.68199300	-1.13189400	0.03260800
H	-6.79981900	-0.26135900	-1.93216200
H	-6.23246100	-1.86853500	2.00228700
C	4.03057300	-0.09977100	-0.05610700
C	4.59475600	-0.66657000	-1.22126900
C	4.81102100	-0.05094200	1.12247700
C	5.90066200	-1.16977900	-1.18877300
C	6.10995200	-0.56787400	1.12181500
C	6.67633200	-1.13053900	-0.02687300
H	6.32306800	-1.60212200	-2.09561000
H	6.69419800	-0.53286800	2.04114900
C	8.09311800	-1.65450900	-0.01722600
H	8.81532000	-0.84960500	-0.21278600
H	8.35284000	-2.09190000	0.95356400
H	8.24325900	-2.41985100	-0.78663300
C	4.24883000	0.55058500	2.39422000
H	4.03714400	1.61975800	2.26959200
H	3.30599800	0.06936400	2.68673300
H	4.94870200	0.44205600	3.22922500
C	3.81768700	-0.70795500	-2.52125300
H	2.83640500	-1.18045400	-2.39343500
H	3.63856400	0.30307100	-2.91145500
H	4.36187400	-1.26481600	-3.29127400

C	-8.10016300	-1.65149400	0.02323400
H	-8.21752500	-2.51083700	0.69264200
H	-8.80818400	-0.87977100	0.35648900
H	-8.40843600	-1.95853000	-0.98276100
C	-3.71130900	-1.04169500	2.42375300
H	-2.81389500	-1.64051200	2.22575400
H	-3.36942100	-0.08815500	2.84605100
H	-4.29090200	-1.55690200	3.19716000
C	-4.37790100	0.86754800	-2.26020100
H	-4.16711900	1.91315100	-2.00622000
H	-3.44596900	0.44271100	-2.65609800
H	-5.11785400	0.85647600	-3.06728600
B	2.55922800	0.45693200	-0.04537200
B	-2.55698700	0.44633700	0.05800700
O	2.42683400	1.84662700	0.00206200
O	-2.42754700	1.85131100	0.04910900
C	-0.00501000	-4.00221100	-0.16381200
H	0.54357300	-4.32749600	-1.06085900
H	0.55239900	-4.41015900	0.69291900
H	-1.00250600	-4.45054600	-0.18024400

BO1c_T1

C	0.00006200	4.54062100	0.00002400
C	-1.21171100	3.85163900	0.04527900
C	-1.20485400	2.45364800	0.04151000
C	0.00001100	1.72333500	-0.00005300
C	1.20490900	2.45359900	-0.04153800
C	1.21182100	3.85157100	-0.04524800
C	-0.00004100	0.26981500	-0.00011600
C	-1.23741700	-0.41522000	0.14712100
C	-1.16649300	-1.90430500	0.37020300
C	-0.00001100	-2.56754200	-0.00062900
C	1.16644400	-1.90428700	-0.37104800
C	1.23739700	-0.41527400	-0.14745400
H	0.00009000	5.62758200	0.00003800
H	-2.16590300	4.36864700	0.07315300
H	2.16603400	4.36854400	-0.07307600
C	4.02230900	-0.08025500	0.02927500
C	4.46057000	-0.83553300	1.14346100
C	4.96331200	0.24935200	-0.97563700
C	5.79474500	-1.25222900	1.22625100
C	6.28549200	-0.19108600	-0.86534000
C	6.72474700	-0.94140100	0.23107900
H	6.11524000	-1.83245600	2.09113900

H	6.99247200	0.05468500	-1.65761000
C	-4.02232100	-0.08013500	-0.02916800
C	-4.96306400	0.24915400	0.97608400
C	-4.46086000	-0.83509300	-1.14346600
C	-6.28525800	-0.19132000	0.86602000
C	-5.79502900	-1.25183800	-1.22601100
C	-6.72477200	-0.94134900	-0.23048500
H	-6.99204000	0.05420100	1.65854400
H	-6.11572900	-1.83184000	-2.09097600
C	-8.16631500	-1.37748100	-0.34373600
H	-8.79353100	-0.57208500	-0.75061800
H	-8.27349900	-2.24166500	-1.00827400
H	-8.58211600	-1.64605700	0.63427400
C	-3.51144000	-1.18318200	-2.27139500
H	-3.13279700	-0.28205000	-2.77099800
H	-2.63509300	-1.73968200	-1.91312500
H	-4.00725000	-1.79777100	-3.03016500
C	-4.55842900	1.06241400	2.18868900
H	-3.68516400	0.63065500	2.69516300
H	-4.28674900	2.08670700	1.90792900
H	-5.37307000	1.11514600	2.91833500
C	8.16628100	-1.37750300	0.34455800
H	8.58192800	-1.64705900	-0.63325300
H	8.79360100	-0.57173700	0.75054100
H	8.27351000	-2.24104800	1.00991400
C	4.55896000	1.06289000	-2.18815300
H	3.68574600	0.63130100	-2.69485700
H	4.28732600	2.08715300	-1.90724300
H	5.37373500	1.11568400	-2.91764600
C	3.51085600	-1.18407900	2.27100500
H	3.13165100	-0.28315000	2.77054400
H	2.63487300	-1.74091200	1.91235900
H	4.00663400	-1.79853100	3.02990400
B	-2.53074000	0.41843800	0.06575900
B	2.53075800	0.41834900	-0.06584900
O	-2.39639800	1.81173100	0.04954800
O	2.39645200	1.81163300	-0.04953900
H	-0.00010100	-3.65866100	-0.00094000
C	2.30530700	-2.63043800	-1.01510900
H	2.58071400	-2.15689700	-1.97077200
H	3.22107800	-2.61626700	-0.40931200
H	2.03777200	-3.67296000	-1.21687200
C	-2.30527500	-2.63069200	1.01411100
H	-2.58089800	-2.15726800	1.96975800

H	-3.22100300	-2.61664500	0.40821600
H	-2.03759600	-3.67319000	1.21580400

BO1d_T₁

C	-0.00000800	5.22814100	-0.00001400
C	-1.22105700	4.54895800	0.01128500
C	-1.22967800	3.15620500	0.01171100
C	-0.00000400	2.41497400	0.00000900
C	1.22966800	3.15621000	-0.01170500
C	1.22104200	4.54896300	-0.01130200
C	-0.00000100	0.99037100	0.00001500
C	-1.26403200	0.30008900	0.01898700
C	-1.23198400	-1.12077300	-0.01678600
C	0.00000400	-1.83357700	0.00001400
C	1.23198900	-1.12076800	0.01682000
C	1.26403200	0.30009300	-0.01895200
H	-0.00001100	6.31580300	-0.00002300
H	-2.16927200	5.07642900	0.02157600
H	2.16925600	5.07643700	-0.02160100
C	4.01845800	0.57337100	-0.08423000
C	4.86260000	0.75643300	1.03820400
C	4.53245700	-0.11743100	-1.20781400
C	6.16364100	0.24481200	1.02888800
C	5.84238000	-0.61059100	-1.18627000
C	6.67570600	-0.44203600	-0.07675200
H	6.79391700	0.38338200	1.90732700
H	6.22416200	-1.13539500	-2.06194700
C	-4.01846000	0.57335900	0.08424000
C	-4.53249700	-0.11741900	1.20782100
C	-4.86256700	0.75640300	-1.03822300
C	-5.84242100	-0.61057700	1.18624500
C	-6.16361000	0.24478600	-1.02893800
C	-6.67571200	-0.44204100	0.07669800
H	-6.22423000	-1.13536400	2.06192000
H	-6.79385800	0.38334200	-1.90740000
C	-8.09566400	-0.95726000	0.08249900
H	-8.79751600	-0.18550900	0.42866400
H	-8.41746800	-1.25871500	-0.92093200
H	-8.20753100	-1.81946400	0.74941400
C	-4.36834700	1.49621400	-2.26422700
H	-4.17802800	2.55301400	-2.04065400
H	-3.42476400	1.07609500	-2.63658800
H	-5.09944900	1.44963300	-3.07825900
C	-3.69835600	-0.30848600	2.45861100

H	-2.80316200	-0.91275100	2.26648000
H	-3.35196200	0.65262000	2.85958700
H	-4.27590400	-0.80675200	3.24458600
C	8.09565700	-0.95725900	-0.08258800
H	8.20750700	-1.81946100	-0.74950600
H	8.79750300	-0.18550800	-0.42876800
H	8.41748400	-1.25871500	0.92083600
C	3.69826800	-0.30853100	-2.45856600
H	2.80311400	-0.91284300	-2.26639700
H	3.35180700	0.65255900	-2.85952200
H	4.27580500	-0.80676400	-3.24457100
C	4.36841800	1.49626500	2.26421100
H	4.17809100	2.55306000	2.04062400
H	3.42484700	1.07615100	2.63660700
H	5.09954400	1.44970000	3.07822000
B	-2.54366400	1.12275200	0.05907300
B	2.54366100	1.12276100	-0.05902700
O	-2.41956900	2.53474700	0.02890000
O	2.41956100	2.53475500	-0.02888500
H	-2.17029700	-1.66340200	0.00363100
H	2.17030300	-1.66339500	-0.00359300
C	0.00000900	-3.29731800	0.00001600
C	1.09482500	-4.02783600	0.52181700
C	-1.09480100	-4.02784500	-0.52178700
C	1.08893900	-5.41740900	0.52937100
H	1.93361200	-3.49340200	0.95599100
C	-1.08890200	-5.41741900	-0.52934200
H	-1.93359200	-3.49341800	-0.95596200
C	0.00002100	-6.11907200	0.00001500
H	1.93296300	-5.95824500	0.94990000
H	-1.93292100	-5.95826200	-0.94987200
H	0.00002600	-7.20644400	0.00001400

BO1e_T₁

C	-0.01602400	-5.63727200	0.05500100
C	-1.23269200	-4.95678700	0.00886400
C	-1.23367900	-3.56652000	-0.00686600
C	-0.01414200	-2.81138600	0.02334600
C	1.21687300	-3.55381500	0.06887800
C	1.20907800	-4.93312600	0.08534900
C	-0.02903200	-1.40756300	0.01121200
C	-1.26704100	-0.69301900	-0.04094900
C	-1.24817500	0.68841800	-0.03770400
C	0.03475200	1.44269900	-0.01815100

C	1.22931000	0.70835200	-0.01500300
C	1.27238600	-0.68939400	0.04244100
H	-0.00640500	-6.72369600	0.06699200
H	-2.18273200	-5.48178800	-0.01708100
H	2.15855100	-5.45850700	0.12268400
C	4.02489600	-0.95382900	0.14473000
C	4.85419800	-1.08196300	-0.99438500
C	4.54495100	-0.30764800	1.29059600
C	6.15136900	-0.55969600	-0.97870400
C	5.85047400	0.19666800	1.27529600
C	6.67125400	0.08290400	0.14932400
H	6.77223900	-0.65657700	-1.86922400
H	6.23812100	0.68767600	2.16779100
C	-4.03236000	-0.97381800	-0.13683000
C	-4.58144800	-0.45757200	-1.33120300
C	-4.81840000	-0.95596200	1.03822500
C	-5.88122300	0.06248800	-1.33167600
C	-6.11129400	-0.42530900	1.00438700
C	-6.66407100	0.08754800	-0.17422900
H	-6.29220300	0.45742100	-2.26054300
H	-6.70153400	-0.40972700	1.92046200
C	-8.07492900	0.62709000	-0.19869700
H	-8.80599600	-0.18037500	-0.34424600
H	-8.33022700	1.12701400	0.74272000
H	-8.21618000	1.34465800	-1.01437600
C	-4.26657000	-1.50338100	2.33849200
H	-4.05611300	-2.57735300	2.26094300
H	-3.32437400	-1.01152000	2.61548300
H	-4.97117500	-1.35813800	3.16391800
C	-3.79209600	-0.48922300	-2.62380300
H	-2.78909400	-0.06432000	-2.49693300
H	-3.66217600	-1.51832200	-2.98549600
H	-4.29881700	0.07472600	-3.41397000
C	8.08689400	0.60996900	0.16204200
H	8.18458600	1.48292700	0.81732600
H	8.79093400	-0.15043400	0.52813300
H	8.41652500	0.89935300	-0.84212900
C	3.72067100	-0.17742500	2.55609400
H	2.80965000	0.41123000	2.39451500
H	3.40183000	-1.15965400	2.92839300
H	4.29478400	0.30767900	3.35264000
C	4.34805600	-1.77714700	-2.24151000
H	4.14061400	-2.83646000	-2.04780900
H	3.41126100	-1.33043500	-2.60042500

H	5.07857600	-1.71793900	-3.05511400
B	-2.56540000	-1.54168000	-0.09091400
B	2.55493700	-1.51884100	0.11262800
O	-2.43342100	-2.92293900	-0.05774800
O	2.43003900	-2.91777700	0.10272100
H	-2.17499600	1.24402700	-0.13372300
H	2.17217300	1.25005700	0.00768000
C	0.02691800	2.90825800	-0.02052500
C	0.79661300	3.64804800	-0.96898100
C	-0.76831900	3.62543400	0.92788400
C	0.73624700	5.04277300	-0.95712300
C	-0.77415500	5.01771100	0.90311000
C	-0.03563700	5.75344400	-0.03304500
H	1.30097500	5.59446800	-1.70752400
H	-1.36263300	5.55065300	1.64904000
C	-0.05244900	7.26127400	-0.02148300
H	0.63616300	7.65719600	0.73822600
H	0.25531600	7.67385800	-0.98801400
H	-1.04968400	7.64959500	0.21544800
C	-1.53159900	2.92426400	2.03083700
H	-2.45901900	2.46134800	1.67260000
H	-0.93609900	2.12750500	2.48926700
H	-1.80412000	3.63817400	2.81475800
C	1.62964900	2.98615800	-2.04617400
H	2.63040400	2.71552600	-1.68511500
H	1.16681100	2.06812000	-2.42025100
H	1.76790000	3.67048500	-2.88979100

BO1f_T1

C	0.00000000	0.51683800	-0.05156300
C	-0.00001000	3.41648800	-0.10153100
C	-1.23069900	1.28287400	-0.06122300
C	1.23069300	1.28288300	-0.06121000
C	1.23860100	2.64100600	-0.08576900
C	-1.23861500	2.64099800	-0.08576000
H	2.20554400	3.12858400	-0.09217600
H	-2.20556100	3.12856900	-0.09213200
C	0.00000500	-0.88797100	-0.02482900
C	0.00000800	-3.69167200	0.08388600
C	1.25249200	-1.59488500	-0.00401400
C	-1.25247900	-1.59488900	-0.00398600
C	-1.21574000	-2.98888500	0.05429000
C	1.21575300	-2.98888000	0.05428600
H	-2.15471300	-3.53921600	0.07958600

H	2.15472400	-3.53921400	0.07959700
H	0.00001100	-4.77775000	0.13126700
C	-0.00001300	4.82899600	-0.12691000
C	-0.00002200	7.69327800	-0.17711500
C	-1.22399300	5.59861200	-0.14061100
C	1.22396200	5.59861700	-0.14067600
C	1.21331400	6.97689000	-0.16481500
C	-1.21335400	6.97688400	-0.16474000
H	-2.18030400	5.08812300	-0.13216100
H	2.18027700	5.08813500	-0.13224500
H	2.15760800	7.51686000	-0.17453500
H	-2.15765200	7.51685000	-0.17438200
H	-0.00002500	8.77950000	-0.19604000
O	2.43651400	0.62367100	-0.04491800
O	-2.43651500	0.62365500	-0.04496800
B	-2.55576900	-0.75593500	-0.02313500
B	2.55577900	-0.75591500	-0.02315300
C	4.01760100	-1.33845400	0.01329200
C	6.63984800	-2.41750600	0.12517100
C	4.74835600	-1.33011700	1.22355100
C	4.61759600	-1.88824400	-1.14098700
C	5.91172700	-2.41717400	-1.06772200
C	6.03729300	-1.86991100	1.26300300
H	6.36217200	-2.83865300	-1.96613300
H	6.58438700	-1.86577400	2.20555500
C	-4.01758900	-1.33848100	0.01329800
C	-6.63986900	-2.41745200	0.12507500
C	-4.61771100	-1.88778200	-1.14107100
C	-4.74822800	-1.33057700	1.22369600
C	-6.03713300	-1.87030100	1.26309900
C	-5.91192100	-2.41667900	-1.06785400
H	-6.58412600	-1.86647600	2.20572000
H	-6.36250700	-2.83775800	-1.96637500
C	-3.89316000	-1.87837600	-2.47152000
H	-2.87262800	-2.27038200	-2.38457000
H	-3.81095400	-0.85845400	-2.87129900
H	-4.42169300	-2.48123000	-3.21740100
C	-4.14178700	-0.74572100	2.48262500
H	-3.18564900	-1.22585700	2.73113000
H	-4.80792400	-0.87158000	3.34233000
H	-3.94084600	0.32661700	2.36673800
C	-8.04559200	-2.96780900	0.18021100
H	-8.25516700	-3.43764500	1.14796200
H	-8.21575600	-3.71340300	-0.60421800

H	-8.78926500	-2.17103600	0.03979500
C	8.04561900	-2.96776800	0.18000400
H	8.25973400	-3.42616700	1.15218800
H	8.78888600	-2.17305800	0.02629300
H	8.21172300	-3.72266500	-0.59640500
C	3.89284400	-1.87932000	-2.47133200
H	2.87265900	-2.27220900	-2.38428300
H	4.42179200	-2.48164300	-3.21734400
H	3.80969500	-0.85942900	-2.87099100
C	4.14216200	-0.74475800	2.48236900
H	3.18575200	-1.22432800	2.73090700
H	3.94181300	0.32767400	2.36632100
H	4.80819200	-0.87085800	3.34212100

BO1g_T₁

C	-0.01195000	2.88514700	0.00362500
C	-1.24277000	2.12011700	0.02892700
C	-1.24019200	0.76106900	0.00989200
C	0.00127700	-0.00942700	0.00205800
C	1.23562100	0.77259900	-0.00465200
C	1.22577400	2.13168000	-0.02213100
C	0.00772800	-1.39487700	0.00089200
C	-1.25293400	-2.11878200	0.01086800
C	-1.20580300	-3.50627500	0.00088400
C	0.02072000	-4.20690100	-0.00168000
C	1.24072800	-3.49491700	-0.00303800
C	1.27503500	-2.10704200	-0.01048500
H	-2.20005700	2.62762200	-0.00739400
H	2.17847500	2.64761100	0.01484900
C	4.03809700	-1.83432000	0.03175400
C	4.76741600	-1.83570900	1.24375600
C	4.64440700	-2.36551000	-1.12764300
C	6.05880800	-2.36839200	1.27958600
C	5.94193200	-2.88798000	-1.05772900
C	6.66706300	-2.89927800	0.13625500
H	6.60375200	-2.37278100	2.22345400
H	6.39698800	-3.29522500	-1.96037000
C	-4.01821500	-1.87198800	-0.03250600
C	-4.62037000	-2.41124800	1.12523200
C	-4.74630000	-1.87844400	-1.24533600
C	-5.91255600	-2.94668300	1.05298800
C	-6.03213300	-2.42406500	-1.28351400
C	-6.63616700	-2.96331400	-0.14176700
H	-6.36444000	-3.36005400	1.95442600

H	-6.57603700	-2.43218800	-2.22796600
C	-8.03779400	-3.52382900	-0.19884300
H	-8.78818400	-2.72219300	-0.15714400
H	-8.21094000	-4.07784800	-1.12890000
H	-8.23418900	-4.19934400	0.64073600
C	-4.13805500	-1.30433500	-2.50823600
H	-3.93466000	-0.23183100	-2.39960900
H	-3.18278300	-1.78868200	-2.75189600
H	-4.80397400	-1.43554000	-3.36734300
C	-3.90532800	-2.38015300	2.46051400
H	-2.86744200	-2.72331700	2.37717600
H	-3.87363300	-1.36056900	2.86868000
H	-4.41100800	-3.01221700	3.19817700
C	8.07472300	-3.44476600	0.19021200
H	8.27212000	-4.12874100	-0.64229900
H	8.81643900	-2.63604000	0.13261400
H	8.26026200	-3.98508200	1.12585200
C	3.92760100	-2.33924900	-2.46208200
H	2.89393700	-2.69489600	-2.37862600
H	3.88337900	-1.31900400	-2.86741800
H	4.43994000	-2.96326700	-3.20199000
C	4.15481700	-1.27010100	2.50839200
H	3.94160100	-0.19923100	2.40243000
H	3.20416800	-1.76367800	2.75160700
H	4.82250200	-1.39719100	3.36674700
B	-2.55848300	-1.28387700	0.00025700
B	2.57279200	-1.26010800	0.00125900
O	-2.44622900	0.09817100	-0.01575800
O	2.44769900	0.12083400	0.02006300
H	-2.13957500	-4.06623200	-0.00301100
H	2.17961500	-4.04627700	-0.00028200
H	0.02576200	-5.29372500	-0.00266500
C	-0.02018200	4.34123500	0.00383300
C	-0.85918200	5.07521100	0.90827500
C	0.81183800	5.08616900	-0.89832200
C	-0.84228100	6.46800100	0.88673600
C	0.77568900	6.47829100	-0.87760800
C	-0.04089700	7.19979900	0.00210000
H	-1.46078100	7.00603400	1.60440600
H	1.39298500	7.02422400	-1.59039500
C	1.67363200	4.42422100	-1.95299400
H	2.65300400	4.11709600	-1.56315000
H	1.19991000	3.52937100	-2.36771000
H	1.86307200	5.12279600	-2.77465700

C	-1.70295100	4.40177400	1.97024200
H	-2.68124800	4.08117800	1.58864300
H	-1.21366600	3.51357700	2.38113000
H	-1.89517700	5.09799900	2.79328100
C	-0.07665300	8.70669800	-0.02309500
H	-0.81177400	9.07371900	-0.75379600
H	-0.35800100	9.11768700	0.95273500
H	0.89520500	9.12757600	-0.30449800

BO2_T1

C	5.32241100	3.63559600	-0.30827800
C	4.96732900	2.29646000	-0.24369400
C	3.61864800	1.89833600	-0.14199300
C	2.59491000	2.89262700	-0.11699100
C	2.97772300	4.25486000	-0.18495500
C	4.31347000	4.61364400	-0.27568200
C	1.19568200	2.48610600	-0.02690500
C	0.86703300	1.14078600	0.04299100
C	-0.51789700	0.64413600	0.15117900
C	-1.55262900	1.70627200	-0.03255600
C	-1.22773500	3.03109200	-0.08879400
C	0.11669000	3.45542200	-0.04175400
H	6.36629100	3.92982000	-0.38514400
H	5.73525100	1.52600700	-0.27273700
H	2.23054900	5.04109500	-0.16767800
H	4.58073200	5.66712000	-0.32585200
H	-2.03481600	3.75175100	-0.18383100
H	0.33459500	4.51495300	-0.06313300
C	-0.91311000	-0.67424300	0.43165900
C	-2.34169100	-0.99519700	0.39818600
C	-0.01319500	-1.76088400	0.77918700
C	-2.76805600	-2.28444000	0.68193600
C	-0.49062300	-3.02451600	1.05564500
H	1.04883600	-1.57761100	0.83387000
C	-1.86791900	-3.31716100	1.01211800
H	0.21769000	-3.80711600	1.31940500
H	-2.23011200	-4.31739100	1.23333400
H	-3.83493600	-2.49675200	0.64684000
B	3.19608900	0.42968700	-0.06990300
O	1.82943900	0.18695100	0.00329900
O	-2.88143200	1.39011900	-0.13993000
B	-3.36243700	0.10950500	0.04437200
C	4.13232900	-0.83762400	-0.08469200
C	4.25465600	-1.61358000	-1.26086300

C	4.86960500	-1.21766600	1.06001300
C	5.10161800	-2.72605700	-1.27817600
C	5.70492900	-2.33982500	1.00959100
C	5.83568000	-3.10843600	-0.15052100
H	5.19350400	-3.30752300	-2.19536400
H	6.26789400	-2.62050500	1.89948200
C	-4.91921800	-0.08213400	-0.08951300
C	-5.76800300	0.32499300	0.96610800
C	-5.49458400	-0.65847600	-1.24292200
C	-7.14922000	0.14068400	0.85950700
C	-6.88297600	-0.82399600	-1.31922900
C	-7.72870200	-0.43136300	-0.27871000
H	-7.78988600	0.44844000	1.68575800
H	-7.31357300	-1.27106500	-2.21491900
C	6.72219600	-4.33139200	-0.17857800
H	7.53373000	-4.25533800	0.55347400
H	6.15257400	-5.24048400	0.05981600
H	7.16885500	-4.48072700	-1.16813400
C	3.47734700	-1.24735100	-2.50850000
H	2.39619300	-1.34352700	-2.34766900
H	3.66441400	-0.20835200	-2.81060600
H	3.74896900	-1.89209200	-3.35077400
C	4.75092700	-0.44032800	2.35556300
H	4.97819500	0.62336700	2.21633400
H	3.73323900	-0.49680500	2.76479900
H	5.43319300	-0.83201600	3.11721800
C	-4.63144700	-1.06823200	-2.41848900
H	-4.22227300	-0.18948100	-2.93548800
H	-3.77793100	-1.68025100	-2.10352200
H	-5.20513200	-1.64287000	-3.15321100
C	-5.18936200	0.95402300	2.21666200
H	-4.44159100	0.30171800	2.68741200
H	-4.68825100	1.90307700	1.98883300
H	-5.96799900	1.15513700	2.95969300
C	-9.22664900	-0.59520100	-0.38584400
H	-9.70826000	0.34499800	-0.68842500
H	-9.49510100	-1.35361000	-1.12921400
H	-9.66817900	-0.88807900	0.57388700

BO3a_T1

C	1.20862400	-0.19715700	-0.02437700
C	1.24791700	-1.64896900	-0.03198800
C	2.52643100	-2.30168400	-0.08103000
C	3.73501700	-1.50831200	-0.08080500

C	0.00001100	0.49741000	0.00006400
C	-0.00000300	-2.31837800	-0.00000400
C	-1.24791700	-1.64896100	0.03202300
C	-1.20861500	-0.19714200	0.02446900
C	-3.73501300	-1.50828200	0.08083800
C	-2.52642400	-2.30166400	0.08107500
H	0.00001700	1.58022900	0.00008400
H	-0.00001300	-3.39794100	-0.00004800
C	4.97188900	-2.17263000	-0.16074000
C	2.64468800	-3.72155900	-0.14505700
C	3.87887900	-4.33452000	-0.21114500
C	5.06062400	-3.55881600	-0.22142700
H	5.88025900	-1.57542600	-0.18221900
H	1.75457200	-4.34117400	-0.15105900
H	3.94188700	-5.41805700	-0.26171600
H	6.03013600	-4.04529100	-0.28172800
C	-4.97188100	-2.17261000	0.16079200
C	-5.06061000	-3.55879400	0.22149800
C	-3.87886200	-4.33450300	0.21123100
C	-2.64467600	-3.72153900	0.14513300
H	-5.88025500	-1.57541300	0.18228200
H	-6.03012100	-4.04526800	0.28181300
H	-3.94186900	-5.41803900	0.26183200
H	-1.75455300	-4.34114500	0.15117300
B	-3.63166300	0.01210300	0.03643200
O	-2.32009100	0.54432000	0.04047600
O	2.32011200	0.54430200	-0.04036100
B	3.63166600	0.01208100	-0.03639700
C	-4.79643200	1.06452800	0.02361200
C	-5.64082700	1.22005100	-1.10106600
C	-5.02003100	1.88582700	1.15565300
C	-6.67410800	2.16301900	-1.07192700
C	-6.06687500	2.81082100	1.15293700
C	-6.90644300	2.96819900	0.04582100
H	-7.31128100	2.27528800	-1.94762000
H	-6.23318900	3.42421300	2.03712200
C	4.79644500	1.06450100	-0.02362600
C	5.02013400	1.88561700	-1.15577800
C	5.64074100	1.22020700	1.10110000
C	6.06696100	2.81063000	-1.15311500
C	6.67401200	2.16318400	1.07190200
C	6.90642700	2.96819700	-0.04595000
H	6.23334600	3.42388000	-2.03738500
H	7.31111900	2.27558500	1.94762600

C	-5.43090100	0.40434100	-2.36196200
H	-4.40687800	0.50626600	-2.74214800
H	-5.60143700	-0.66561900	-2.19595300
H	-6.11102800	0.72891400	-3.15614100
C	-4.14144700	1.76741500	2.38431500
H	-4.08993500	0.73321400	2.74804100
H	-3.11300300	2.08328600	2.17267600
H	-4.51960400	2.38842100	3.20269100
C	-8.01139500	3.99856000	0.04929600
H	-7.63226300	4.99022300	-0.23291100
H	-8.80390000	3.73959900	-0.66083100
H	-8.46457000	4.09813900	1.04198400
C	8.01137300	3.99856500	-0.04949700
H	7.63218300	4.99029900	0.23238600
H	8.80375500	3.73979300	0.66083600
H	8.46472200	4.09789100	-1.04213100
C	5.43064100	0.40475000	2.36212800
H	4.40689700	0.50772100	2.74280000
H	5.60002500	-0.66538200	2.19608500
H	6.11145700	0.72869600	3.15597100
C	4.14165900	1.76698600	-2.38449700
H	4.09021000	0.73272500	-2.74806500
H	3.11318700	2.08285900	-2.17299500
H	4.51986400	2.38787400	-3.20293900

BO3b_T₁

C	1.21023100	-0.04738200	0.01843400
C	1.24721000	1.40435900	0.02674900
C	2.52543300	2.05807500	0.07120600
C	3.73520100	1.26836200	0.06477100
C	-0.00000100	-0.74060400	0.00000400
C	-0.00000600	2.07243200	0.00000500
C	-1.24721600	1.40436000	-0.02673700
C	-1.21023500	-0.04737600	-0.01842400
C	-3.73520700	1.26836700	-0.06477100
C	-2.52544500	2.05807800	-0.07119700
H	-0.00000100	-1.82450900	0.00000200
H	-0.00000700	3.15351900	0.00000200
C	4.97237800	1.93543900	0.14174700
C	2.64906300	3.47703900	0.13754300
C	3.88193700	4.08727600	0.19990600
C	5.08252600	3.32328800	0.20592000
H	5.88027100	1.33395700	0.15991100
H	1.76001100	4.10040300	0.14810500

H	3.94276500	5.17283100	0.25240800
C	-4.97238800	1.93544000	-0.14175200
C	-5.08253900	3.32328700	-0.20592400
C	-3.88195300	4.08727200	-0.19989800
C	-2.64907600	3.47703700	-0.13753100
H	-5.88027800	1.33395400	-0.15992300
H	-3.94278000	5.17282800	-0.25239600
H	-1.76002400	4.10040300	-0.14808300
B	-3.63331400	-0.25163200	-0.01723100
O	-2.32041700	-0.78940300	-0.02831200
O	2.32041400	-0.78941000	0.02831600
B	3.63331100	-0.25163500	0.01722900
C	-4.79969000	-1.30353200	0.00273300
C	-5.65049400	-1.44601100	1.12486900
C	-5.01942000	-2.13671300	-1.12192900
C	-6.68651700	-2.38711000	1.10007000
C	-6.06873700	-3.05981300	-1.11531000
C	-6.91549400	-3.20316200	-0.01111000
H	-7.32854600	-2.48933400	1.97471800
H	-6.23140700	-3.68294400	-1.99455700
C	4.79969000	-1.30353200	-0.00273700
C	5.01942700	-2.13671100	1.12192500
C	5.65049800	-1.44600500	-1.12487300
C	6.06875300	-3.05980200	1.11530800
C	6.68652800	-2.38709600	-1.10007300
C	6.91551000	-3.20314500	0.01110900
H	6.23143200	-3.68292600	1.99455800
H	7.32855900	-2.48931400	-1.97471900
C	-5.44430200	-0.61928000	2.37887100
H	-4.41762200	-0.70981700	2.75578700
H	-5.62323300	0.44837100	2.20363700
H	-6.11995400	-0.94296600	3.17768500
C	-4.13391700	-2.03193700	-2.34638600
H	-4.09026700	-1.00268700	-2.72643200
H	-3.10358900	-2.33199000	-2.11966700
H	-4.49978600	-2.67103800	-3.15675500
C	-8.02215800	-4.23112200	-0.00946100
H	-7.64720200	-5.21780500	0.29661000
H	-8.82328300	-3.95750400	0.68589700
H	-8.46201700	-4.34887000	-1.00650400
C	8.02218500	-4.23109400	0.00946200
H	7.64724500	-5.21777600	-0.29663200
H	8.82331900	-3.95745700	-0.68587900
H	8.46203000	-4.34885300	1.00650900

C	5.44429900	-0.61927800	-2.37887700
H	4.41763800	-0.70988000	-2.75583000
H	5.62315400	0.44838300	-2.20363100
H	6.12000000	-0.94291700	-3.17766900
C	4.13393400	-2.03193200	2.34638900
H	4.09028200	-1.00268000	2.72642900
H	3.10360500	-2.33199100	2.11967800
H	4.49981100	-2.67102700	3.15675900
C	-6.41817400	4.01254500	-0.28648900
H	-7.24336300	3.29373800	-0.28169900
H	-6.56227000	4.70051200	0.55803700
H	-6.49971600	4.61627100	-1.20092800
C	6.41816000	4.01254700	0.28646700
H	7.24334800	3.29373800	0.28175100
H	6.56227800	4.70044900	-0.55811000
H	6.49967900	4.61634600	1.20086000

BO3c_T₁

C	-1.21047700	-1.47854200	-0.02001700
C	-1.24618400	-0.02485500	-0.02467900
C	-2.52653700	0.63485200	-0.06524900
C	-3.73239200	-0.16178200	-0.05484100
C	-0.00005000	-2.17016500	0.00005700
C	-0.00000100	0.64005200	0.00012100
C	1.24615200	-0.02488200	0.02485600
C	1.21040600	-1.47856300	0.02015900
C	3.73236400	-0.16188300	0.05499000
C	2.52654600	0.63479000	0.06538600
H	-0.00006100	-3.25411900	0.00003900
H	0.00000700	1.72085500	0.00018100
C	-4.96438000	0.51694100	-0.12180900
C	-2.63652300	2.04901800	-0.12055500
C	-3.86426300	2.70003900	-0.17442700
C	-5.04444300	1.90012800	-0.17631700
H	-5.88010200	-0.07038800	-0.14851800
H	-1.73860500	2.65789600	-0.09725800
H	-6.01482300	2.38300400	-0.25657200
C	4.96437700	0.51679600	0.12200000
C	5.04449000	1.89997800	0.17649300
C	3.86434500	2.69992800	0.17452400
C	2.63658000	2.04894800	0.12064100
H	5.88007600	-0.07056500	0.14876400
H	6.01488300	2.38282100	0.25677900
H	1.73868800	2.65786200	0.09727300

B	3.63306200	-1.68001000	0.01596600
O	2.31835000	-2.22044500	0.03484800
O	-2.31845000	-2.22039600	-0.03474300
B	-3.63313800	-1.67991600	-0.01586200
C	4.79889900	-2.73060500	-0.00392300
C	5.65598600	-2.86591600	-1.12254400
C	5.01300300	-3.57003000	1.11768700
C	6.69238300	-3.80635700	-1.09696800
C	6.06366100	-4.49125500	1.11186800
C	6.91655200	-4.62766900	0.01138800
H	7.33885500	-3.90390100	-1.96878700
H	6.22275600	-5.11848600	1.98877000
C	-4.79901700	-2.73047100	0.00391600
C	-5.01322800	-3.56962300	-1.11787000
C	-5.65599600	-2.86604600	1.12259000
C	-6.06388500	-4.49085500	-1.11217100
C	-6.69240900	-3.80646400	1.09687800
C	-6.91667800	-4.62752000	-0.01165100
H	-6.22305800	-5.11787700	-1.98920800
H	-7.33881800	-3.90419400	1.96872200
C	5.45661600	-2.03383200	-2.37420400
H	4.42786700	-2.10936200	-2.74844400
H	5.65129900	-0.96906800	-2.19823000
H	6.12548400	-2.36521400	-3.17547600
C	4.12181000	-3.47280700	2.33862500
H	4.07686800	-2.44622400	2.72558600
H	3.09254000	-3.77152500	2.10546700
H	4.48408500	-4.11715600	3.14634300
C	8.02460000	-5.65390900	0.01057500
H	7.65140000	-6.64040900	-0.29814600
H	8.82694100	-5.37790300	-0.68232700
H	8.46199100	-5.77286700	1.00851800
C	-8.02474000	-5.65374600	-0.01098200
H	-7.65152300	-6.64032900	0.29745600
H	-8.82700800	-5.37790100	0.68206900
H	-8.46223200	-5.77244900	-1.00891100
C	-5.45637100	-2.03437700	2.37448300
H	-4.42807300	-2.11170900	2.74962600
H	-5.64906800	-0.96927500	2.19842900
H	-6.12648400	-2.36471200	3.17514600
C	-4.12212800	-3.47211100	-2.33885400
H	-4.07727500	-2.44544700	-2.72561100
H	-3.09282200	-3.77081600	-2.10583100
H	-4.48442200	-4.11631900	-3.14667500

C	3.94921300	4.17787400	0.22645900
C	2.99553900	4.93899800	0.92804700
C	4.99038200	4.86368000	-0.42663400
C	3.07480600	6.32989600	0.96731900
H	2.20325900	4.43199100	1.47343200
C	5.06994000	6.25482300	-0.38623000
H	5.72691900	4.30171200	-0.99571800
C	4.11244500	6.99566800	0.31017800
H	2.33053900	6.89499600	1.52393300
H	5.87877500	6.76222400	-0.90725500
H	4.17607400	8.08058900	0.34368700
C	-3.94908100	4.17798500	-0.22642800
C	-4.99020500	4.86385900	0.42666800
C	-2.99540800	4.93904300	-0.92808900
C	-5.06971400	6.25500300	0.38620100
H	-5.72674100	4.30194500	0.99580400
C	-3.07462700	6.32994200	-0.96742500
H	-2.20316700	4.43198300	-1.47348300
C	-4.11221900	6.99578200	-0.31027700
H	-5.87851300	6.76245600	0.90723000
H	-2.33036300	6.89498900	-1.52409600
H	-4.17581200	8.08070300	-0.34383700

BO3d_T1

C	-1.19037100	-0.24024600	0.12321500
C	-1.22165900	1.18347100	0.14034600
C	0.00776400	-0.92791400	0.09978900
C	0.02039100	1.84602800	0.09535600
C	1.26022500	1.18450600	0.07663500
C	1.21783600	-0.22420200	0.08104900
H	0.01555800	-2.01183400	0.10277000
H	0.00357000	2.92639800	0.04946300
B	3.63244000	-0.42668500	0.02408200
O	2.35115200	-0.96151300	0.05765300
O	-2.32973800	-0.99115600	0.15801200
B	-3.61447800	-0.45632200	0.06285000
C	4.73123400	-1.56353700	0.00558600
C	5.17716100	-2.10985200	-1.21723000
C	5.23188800	-2.09700100	1.21363800
C	6.11253600	-3.14987300	-1.21509100
C	6.16606000	-3.13662700	1.18093800
C	6.61888200	-3.68019600	-0.02524900
H	6.45349000	-3.55627400	-2.16597400
H	6.54940500	-3.53266100	2.12008400

C	-4.74848000	-1.55244300	0.10522600
C	-4.90639800	-2.45429800	-0.97364300
C	-5.59166500	-1.69006700	1.23269500
C	-5.89934400	-3.43720000	-0.92229000
C	-6.56497900	-2.69404000	1.25608600
C	-6.73801900	-3.57793700	0.18749100
H	-6.01921900	-4.11271100	-1.76783700
H	-7.20487800	-2.78890500	2.13187400
C	4.65511400	-1.57179000	-2.53331800
H	3.57361700	-1.73073800	-2.63056600
H	4.83108600	-0.49233600	-2.62643000
H	5.13906000	-2.06113900	-3.38463300
C	4.76852700	-1.54457500	2.54560000
H	4.95219100	-0.46501900	2.62073800
H	3.69163000	-1.69836100	2.69030400
H	5.28668800	-2.02783700	3.38007400
C	7.60555700	-4.82475400	-0.03961300
H	7.09530100	-5.79225100	0.06181000
H	8.17282300	-4.85397100	-0.97609600
H	8.32054800	-4.74991600	0.78735900
C	-7.77951100	-4.67118600	0.24150500
H	-7.35736500	-5.60336500	0.64098500
H	-8.61990500	-4.39375800	0.88690800
H	-8.17644200	-4.89790200	-0.75417100
C	-5.44661300	-0.77529000	2.43160500
H	-4.44225200	-0.83939200	2.86863800
H	-5.61415300	0.27441200	2.16390900
H	-6.16383600	-1.03753600	3.21606500
C	-4.01644500	-2.36420800	-2.19702600
H	-4.00262100	-1.35108000	-2.61928800
H	-2.97909300	-2.62047800	-1.95273900
H	-4.35487700	-3.04579100	-2.98394800
C	7.47218800	1.90586200	-0.08617600
C	6.29279200	1.18937600	-0.05383600
C	5.02623300	1.83640200	-0.02187500
C	5.03586700	3.26980400	-0.02493900
C	6.26037800	3.98268300	-0.05851900
C	7.46490100	3.31656600	-0.08882100
H	8.41879000	1.37229500	-0.11001700
H	6.33669300	0.10922100	-0.05273700
C	3.79665000	3.96333100	0.00842800
H	6.22780800	5.06990500	-0.05971800
H	8.40044400	3.86856500	-0.11455100
C	2.60748200	3.29246500	0.04114200

H	3.80811600	5.05119500	0.00872300
H	1.68964700	3.86732800	0.07069200
C	-4.96222900	1.80367200	-0.29823400
C	-5.01828800	3.22192300	-0.04271700
C	-3.82730200	3.90011700	0.39860500
C	-2.60376100	3.23553400	0.47138700
H	-6.10848600	0.12814300	-1.02495700
C	-6.13226400	1.18353000	-0.78518400
C	-6.21811700	3.90557400	-0.22439500
H	-3.88538300	4.96228400	0.61847700
H	-1.72310500	3.80724500	0.74889400
C	-7.38564800	3.24653900	-0.68875000
C	-7.33690000	1.89819000	-0.97232600
H	-6.25727300	4.96898600	-0.00049900
H	-8.30424700	3.81130400	-0.82088400
H	-8.21430400	1.37495200	-1.34073100
C	2.56193600	1.86587000	0.04148100
C	3.76397100	1.12014300	0.01250400
C	-2.49273400	1.87760000	0.19696200
C	-3.74153800	1.07595400	-0.04170200

BO3e_T₁

C	-1.20777700	1.62409000	-0.00493600
C	-1.25019500	0.18124200	-0.00238900
C	-2.52672800	-0.47298500	0.00504100
C	-3.73630000	0.32542300	-0.01202100
C	0.00000200	2.31765800	0.00005900
C	0.00000200	-0.48602600	0.00006000
C	1.25019900	0.18123700	0.00251600
C	1.20778000	1.62408400	0.00505800
C	3.73630700	0.32541400	0.01212300
C	2.52673700	-0.47299200	-0.00492800
H	0.00000200	3.40073900	0.00005700
H	0.00000100	-1.56595700	0.00004900
C	-4.98174000	-0.30993300	0.02039400
C	-2.64643200	-1.90203900	0.03995300
C	-3.88004900	-2.49610100	0.06267700
C	-5.07329400	-1.70453600	0.05506600
H	-5.88190300	0.30071300	0.02181200
H	-1.75391800	-2.51956200	0.05326100
C	4.98174900	-0.30994100	-0.02034400
C	5.07330500	-1.70454100	-0.05504000
C	3.88006300	-2.49610400	-0.06262800
C	2.64644400	-1.90204200	-0.03986500

H	5.88191200	0.30070400	-0.02177500
H	1.75393100	-2.51956600	-0.05316200
B	3.62120800	1.85060600	0.03655800
O	2.32164900	2.37930000	0.01304700
O	-2.32164400	2.37930900	-0.01292400
B	-3.62120400	1.85061500	-0.03640400
C	4.79371000	2.89868500	0.05386700
C	5.55276000	3.13642700	1.22249400
C	5.10512200	3.62878500	-1.11700100
C	6.59214900	4.07290200	1.19961900
C	6.15355000	4.55279900	-1.10625300
C	6.90955600	4.79290100	0.04508600
H	7.16565900	4.24762000	2.10852500
H	6.38719500	5.09864600	-2.01904500
C	-4.79371000	2.89868800	-0.05382600
C	-5.10514000	3.62889300	1.11696100
C	-5.55276500	3.13629600	-1.22248500
C	-6.15359200	4.55289200	1.10611100
C	-6.59216700	4.07274900	-1.19971500
C	-6.90959000	4.79286500	-0.04525100
H	-6.38725600	5.09882400	2.01884500
H	-7.16568000	4.24735500	-2.10864200
C	5.24166800	2.41196100	2.51733200
H	4.21354400	2.60632700	2.84864800
H	5.34162300	1.32517000	2.41522300
H	5.91211400	2.73446800	3.32051200
C	4.31575900	3.41399700	-2.39217400
H	4.31495400	2.35883900	-2.69469100
H	3.26770300	3.71201300	-2.26850100
H	4.73267700	3.99594800	-3.22036600
C	8.01715700	5.82078900	0.04742800
H	7.62880000	6.82459700	0.26728100
H	8.77443100	5.59322900	0.80538600
H	8.51708800	5.87491700	-0.92602400
C	-8.01720100	5.82074200	-0.04774100
H	-7.62910000	6.82425000	-0.26941500
H	-8.77532700	5.59216000	-0.80454500
H	-8.51603300	5.87618200	0.92619400
C	-5.24166000	2.41167400	-2.51723100
H	-4.21353600	2.60600900	-2.84856800
H	-5.34160200	1.32489400	-2.41498300
H	-5.91210700	2.73406900	-3.32045500
C	-4.31579200	3.41424600	2.39216700
H	-4.31497300	2.35911800	2.69478900

H	-3.26774000	3.71226900	2.26848000
H	-4.73273300	3.99627200	3.22029500
C	6.21968200	-2.58961600	-0.08904400
C	5.75900500	-3.92897500	-0.11559100
C	7.59532500	-2.31069600	-0.09718500
C	6.66671300	-4.97889300	-0.14866100
C	8.49649800	-3.37186400	-0.13100800
H	7.95322000	-1.28471800	-0.07765800
C	8.03979700	-4.69723900	-0.15632900
H	6.32525200	-6.01127200	-0.16853500
H	9.56461600	-3.17186000	-0.13781100
H	8.75684200	-5.51322100	-0.18223600
C	-6.21966800	-2.58961000	0.08902600
C	-5.75899100	-3.92897000	0.11556500
C	-7.59531200	-2.31069000	0.09713400
C	-6.66669900	-4.97888800	0.14859400
C	-8.49648500	-3.37185700	0.13091600
H	-7.95320700	-1.28471200	0.07761200
C	-8.03978500	-4.69723400	0.15622800
H	-6.32523900	-6.01126700	0.16846100
H	-9.56460300	-3.17185400	0.13769100
H	-8.75683000	-5.51321600	0.18210200
C	4.23059900	-3.98495500	-0.10185100
C	-4.23058400	-3.98495400	0.10186700
C	-3.68250200	-4.66238600	1.37835800
H	-4.00244900	-5.70980000	1.42820300
H	-2.58650500	-4.64433800	1.38617900
H	-4.03868000	-4.15308400	2.27936700
C	-3.70651800	-4.72199400	-1.15150100
H	-2.61100800	-4.69978300	-1.18345900
H	-4.02215300	-5.77192800	-1.14352200
H	-4.08398000	-4.25859200	-2.06848200
C	3.70656800	-4.72201400	1.15152100
H	2.61105900	-4.69980400	1.18350900
H	4.02220400	-5.77194700	1.14351700
H	4.08405500	-4.25862500	2.06849900
C	3.68248100	-4.66236800	-1.37833600
H	4.00242300	-5.70978200	-1.42820400
H	2.58648300	-4.64431700	-1.38612700
H	4.03863500	-4.15305500	-2.27934800

BO4a_T₁

C	3.88557600	4.18028500	-0.02569200
C	4.26403300	2.83132400	-0.00937900

C	3.32003100	1.80379000	0.01128100
C	1.91139000	2.13891100	0.00674200
C	1.54732500	3.52773800	-0.00782000
C	2.51561500	4.51190900	-0.02303300
C	0.95638700	1.09959200	0.01054500
C	1.37549600	-0.29494800	0.01122600
C	0.48364300	-1.32214200	0.01082100
H	0.88512000	-2.32839300	0.01214300
C	-0.95638600	-1.09958900	0.01063400
C	-1.37549500	0.29495100	0.01121800
C	-0.48364200	1.32214600	0.01073000
H	4.63819400	4.96416200	-0.04046200
H	5.32016900	2.56848000	-0.01273300
H	0.50154300	3.81716000	-0.00910500
H	2.21511800	5.55744400	-0.03486800
H	-0.88511900	2.32839700	0.01198000
C	-1.91138900	-2.13890800	0.00692700
C	-1.54732500	-3.52773600	-0.00752100
C	-2.51561500	-4.51190800	-0.02263100
C	-3.88557700	-4.18028400	-0.02529000
C	-4.26403300	-2.83132100	-0.00908700
C	-3.32003000	-1.80378600	0.01145900
H	-0.50154300	-3.81715900	-0.00880000
H	-2.21511900	-5.55744400	-0.03438000
H	-4.63819500	-4.96416300	-0.03997600
H	-5.32016900	-2.56847700	-0.01244300
B	3.72203800	0.31329500	0.02333500
O	2.70549200	-0.62604500	0.01333600
B	-3.72203700	-0.31329100	0.02337800
O	-2.70549100	0.62604800	0.01331300
C	5.19613100	-0.24117900	0.02018700
C	5.96248600	-0.28956300	1.20517000
C	5.77816200	-0.69088600	-1.18715800
C	7.27632100	-0.77183700	1.16549700
C	7.09339700	-1.16410900	-1.19273000
C	7.86108500	-1.21486100	-0.02388300
H	7.85682700	-0.80157800	2.08732400
H	7.53188000	-1.49868200	-2.13277900
C	-5.19613000	0.24118200	0.02025700
C	-5.77820400	0.69083900	-1.18708500
C	-5.96244300	0.28960900	1.20526600
C	-7.09343900	1.16406300	-1.19262800
C	-7.27628000	0.77188100	1.16562100
C	-7.86108500	1.21486100	-0.02375500

H	-7.53195500	1.49860000	-2.13267300
H	-7.85675400	0.80165500	2.08746800
C	-5.36847700	-0.14430800	2.52965800
H	-4.89679300	-1.13202200	2.46098600
H	-4.59312300	0.55748100	2.86589500
H	-6.13185400	-0.19047200	3.31343000
C	-4.98675000	0.65798700	-2.47818800
H	-4.10345400	1.30644100	-2.42058900
H	-4.62631500	-0.35462400	-2.70411100
H	-5.59266900	0.99110500	-3.32714500
C	-9.27135500	1.75600400	-0.04538600
H	-9.27689800	2.85316000	0.01645200
H	-9.79202700	1.48308500	-0.97056200
H	-9.85863700	1.37913100	0.79906900
C	4.98666100	-0.65809000	-2.47823400
H	4.10338400	-1.30656600	-2.42058600
H	4.62619000	0.35450400	-2.70417300
H	5.59255700	-0.99121600	-3.32720300
C	5.36856500	0.14439200	2.52957200
H	4.89686600	1.13209600	2.46088600
H	4.59323400	-0.55739700	2.86586300
H	6.13197300	0.19059000	3.31331200
C	9.27135400	-1.75600200	-0.04554400
H	9.27690000	-2.85315900	0.01630600
H	9.79200200	-1.48309400	-0.97073700
H	9.85865800	-1.37912000	0.79889100

BO4b_T₁

C	-4.19568200	-3.90025400	0.00422600
C	-4.45428400	-2.52068400	0.01085200
C	-3.44119000	-1.56147500	0.02065600
C	-2.05981100	-1.99324000	0.01714500
C	-1.80362400	-3.40614600	0.01194600
C	-2.83872300	-4.31277100	0.00628000
C	-1.03252200	-1.02830400	0.01460300
C	-1.34906400	0.39015300	0.01217800
C	-0.38717000	1.35196300	0.01212300
H	-0.71535400	2.38354000	0.01092800
C	1.03252400	1.02831200	0.01454900
C	1.34906500	-0.39014500	0.01218000
C	0.38717200	-1.35195500	0.01217400
H	-5.48823100	-2.18062600	0.00778600
H	-0.78374000	-3.77451000	0.01165600
H	-2.61196700	-5.37716900	0.00190000

H	0.71535500	-2.38353300	0.01101600
C	2.05981300	1.99324800	0.01703700
C	1.80362500	3.40615300	0.01177000
C	2.83872400	4.31277800	0.00604700
C	4.19568300	3.90026100	0.00400000
C	4.45428600	2.52069200	0.01068600
C	3.44119300	1.56148200	0.02055200
H	0.78374200	3.77451700	0.01146600
H	2.61196800	5.37717500	0.00161000
H	5.48823200	2.18063300	0.00761400
B	-3.73574200	-0.04734900	0.02113300
O	-2.65383900	0.81355800	0.01052900
B	3.73574500	0.04735600	0.02108600
O	2.65384000	-0.81355000	0.01053300
C	-5.16381200	0.61786700	0.01042200
C	-5.90988700	0.76584600	1.20009000
C	-5.71940000	1.08065100	-1.20318400
C	-7.17668000	1.35822600	1.15848300
C	-6.98884400	1.66601300	-1.21071400
C	-7.73411300	1.81818000	-0.03756200
H	-7.74115000	1.46467900	2.08356700
H	-7.40689700	2.01089200	-2.15519400
C	5.16381200	-0.61786400	0.01040400
C	5.71934400	-1.08080800	-1.20318100
C	5.90993900	-0.76569800	1.20004400
C	6.98877500	-1.66616900	-1.21070300
C	7.17674100	-1.35808900	1.15844500
C	7.73411000	-1.81818900	-0.03756000
H	7.40677900	-2.01116900	-2.15516200
H	7.74125400	-1.46442900	2.08351300
C	-9.09028500	2.48448100	-0.05857500
H	-9.00220000	3.57174700	0.07154200
H	-9.60723100	2.31429100	-1.00938900
H	-9.73251100	2.11353400	0.74762600
C	-5.34286400	0.31250700	2.53011400
H	-5.00300100	-0.72943600	2.49431600
H	-4.47693700	0.92060300	2.82315100
H	-6.08708900	0.39477500	3.32889800
C	-4.94962900	0.94577100	-2.50120200
H	-4.02000800	1.52760400	-2.47707000
H	-4.66904300	-0.09702900	-2.69836300
H	-5.54038500	1.29640500	-3.35354900
C	-5.30659600	-4.91647000	-0.00571500
H	-5.25480900	-5.57762400	0.86994200

H	-6.28918100	-4.43485800	-0.00355300
H	-5.25201500	-5.56324200	-0.89190300
C	5.30659700	4.91647700	-0.00595600
H	5.25507200	5.57735600	0.86992700
H	6.28918100	4.43486200	-0.00422300
H	5.25175500	5.56352800	-0.89192100
C	5.34298500	-0.31223200	2.53005500
H	5.00293100	0.72964200	2.49412100
H	4.47720100	-0.92043600	2.82329100
H	6.08731300	-0.39423700	3.32876900
C	4.94950900	-0.94607400	-2.50117700
H	4.01984600	-1.52783300	-2.47690200
H	4.66899000	0.09671700	-2.69848300
H	5.54019200	-1.29688200	-3.35350200
C	9.09028100	-2.48449000	-0.05861800
H	9.00203900	-3.57201400	0.06921700
H	9.60813400	-2.31243100	-1.00861000
H	9.73175300	-2.11516300	0.74891700

BO4c_T₁

C	-1.01647600	-1.06641800	-0.08735100
C	-1.34099900	0.33068500	0.12184600
C	-0.38071100	1.30392700	0.19519400
H	-0.72214800	2.29634900	0.45278700
C	1.01463500	1.04123700	0.01035900
C	1.34273500	-0.34315600	-0.15692800
C	0.38577500	-1.32826700	-0.24123800
H	0.73430100	-2.32592800	-0.46810500
B	-3.72157300	-0.07182200	0.07452900
O	-2.63624000	0.74991600	0.31287100
B	3.70583200	0.07454900	-0.00003500
O	2.64080800	-0.76225100	-0.26098200
C	-5.14981100	0.58430400	0.16224000
C	-6.01896500	0.31387700	1.24269500
C	-5.58512400	1.46344100	-0.85663800
C	-7.28450900	0.90950600	1.28422800
C	-6.85893200	2.03402200	-0.78850400
C	-7.72481800	1.77273700	0.27810900
H	-7.94270000	0.69436200	2.12436300
H	-7.18471300	2.69873400	-1.58717600
C	5.13723900	-0.58463800	0.00999800
C	6.03218200	-0.42463800	-1.07100600
C	5.54604800	-1.35535600	1.12185800
C	7.29643700	-1.02161500	-1.02272400

C	6.81870600	-1.93383600	1.14062800
C	7.70991800	-1.78190000	0.07445400
H	7.97494700	-0.89014900	-1.86413700
H	7.12248200	-2.51673200	2.00878400
C	-9.08578500	2.42544400	0.35015800
H	-9.01818200	3.44441200	0.75479700
H	-9.54720400	2.50323200	-0.64078200
H	-9.76658600	1.86282600	0.99764600
C	-5.58962700	-0.59064600	2.38016200
H	-5.27524600	-1.57691000	2.02019200
H	-4.73980700	-0.16554800	2.92989200
H	-6.40323700	-0.73871900	3.09750900
C	-4.68558000	1.79087300	-2.03146300
H	-3.79102800	2.33676600	-1.70872200
H	-4.33859300	0.88385900	-2.54306400
H	-5.20680900	2.40809700	-2.77015800
C	4.61791700	-1.55798800	2.30257800
H	4.28979400	-0.60150700	2.73000500
H	3.71276900	-2.10427400	2.01090100
H	5.10781200	-2.12487900	3.10072300
C	5.63539600	0.37287000	-2.29713100
H	4.75185700	-0.05609600	-2.78688800
H	5.38816600	1.41127800	-2.04571500
H	6.44380900	0.39214300	-3.03505400
C	9.06901100	-2.44227800	0.09567500
H	9.02606000	-3.45659700	-0.32401800
H	9.79842000	-1.87837400	-0.49590300
H	9.45653500	-2.53134100	1.11648600
C	-1.48780700	-6.30987700	-0.30458500
C	-2.64045200	-5.70903500	-0.81582200
C	-2.84715300	-4.32014800	-0.71413800
C	-1.82453500	-3.49174600	-0.13941800
C	-0.71914500	-4.13166000	0.43329400
C	-0.54206800	-5.52338200	0.34360600
H	-4.86730000	-4.37897500	-1.51380300
H	-1.34770000	-7.38347500	-0.39221000
H	-3.41092600	-6.31752100	-1.28321400
C	-4.09890400	-3.73751400	-1.09084000
C	-2.03672400	-2.03515100	-0.13508500
H	0.00828400	-3.55201400	0.98890000
H	0.33978800	-5.97684200	0.78722400
C	-3.42106100	-1.54212300	-0.27243700
C	-4.38442400	-2.39552800	-0.78357900
H	-5.39004900	-2.01584500	-0.94808000

C	3.39491500	1.56690200	0.23178200
C	2.06029900	2.03388100	0.05332500
C	1.83639800	3.47227200	-0.03378800
C	2.89390600	4.35470800	0.37162400
C	4.17066700	3.82417100	0.71456800
C	4.42104500	2.48007400	0.57418100
H	-0.08940500	3.44376000	-1.02880100
C	0.67075800	4.06835700	-0.57838500
C	2.68190400	5.75634400	0.35769100
H	4.95586600	4.50976300	1.02351800
H	5.42125300	2.09120200	0.74593600
C	1.50204400	6.29615400	-0.10968200
C	0.50346700	5.44171000	-0.61388500
H	3.48739400	6.40349300	0.69649000
H	1.35792700	7.37298100	-0.12357600
H	-0.40039300	5.85992300	-1.04808900

BO4d_T₁

C	-1.18612200	-0.84315600	-0.00004400
C	-1.25707900	0.60805700	0.00480600
C	-0.14434000	1.39556100	0.00271700
H	-0.29710600	2.46743400	0.00667600
C	1.18613100	0.84316100	0.00009900
C	1.25708700	-0.60805500	0.00488100
C	0.14434800	-1.39555600	0.00265700
H	0.29711300	-2.46742900	0.00658700
B	-3.67890600	0.59017100	0.02039700
O	-2.46809700	1.24990100	0.01327700
B	3.67891100	-0.59016500	0.02075500
O	2.46810400	-1.24989700	0.01343400
C	-4.97667700	1.48189700	0.03721700
C	-5.65054800	1.75757400	1.24668000
C	-5.49147700	2.01245500	-1.16649600
C	-6.81140300	2.53837100	1.23391000
C	-6.65482200	2.78700700	-1.14472700
C	-7.33024700	3.06435700	0.04790800
H	-7.32290800	2.74058600	2.17360800
H	-7.04501700	3.18215200	-2.08143400
C	4.97668300	-1.48189300	0.03740600
C	5.49148200	-2.01222400	-1.16640700
C	5.65054700	-1.75781300	1.24682000
C	6.65482500	-2.78678600	-1.14478600
C	6.81139400	-2.53861600	1.23390000
C	7.33024200	-3.06437200	0.04779500

H	7.04502100	-3.18175100	-2.08156900
H	7.32289000	-2.74102300	2.17356100
C	-8.57047500	3.92794100	0.05502000
H	-8.31316700	4.99511900	0.09491300
H	-9.17132700	3.77523600	-0.84840500
H	-9.20308200	3.71402000	0.92310500
C	-5.11819300	1.23203800	2.56440100
H	-4.97204300	0.14532100	2.54004900
H	-4.14640500	1.68002800	2.80962800
H	-5.80174700	1.45817200	3.38902300
C	-4.79045100	1.74863400	-2.48348500
H	-3.78708100	2.19226300	-2.49782600
H	-4.66808700	0.67373600	-2.66908500
H	-5.35119000	2.16795400	-3.32492300
C	5.11818500	-1.23254900	2.56464700
H	4.97208600	-0.14582200	2.54053800
H	4.14636900	-1.68054900	2.80974900
H	5.80170900	-1.45890400	3.38923300
C	4.79046100	-1.74814300	-2.48334600
H	3.78708800	-2.19176400	-2.49777600
H	4.66810300	-0.67320800	-2.66873900
H	5.35119900	-2.16730200	-3.32486400
C	8.57046000	-3.92797100	0.05475200
H	8.31314500	-4.99514400	0.09472900
H	9.17117600	-3.77530800	-0.84877000
H	9.20320200	-3.71402700	0.92273400
C	-5.94870000	-5.28422700	-0.08411500
C	-5.98931200	-3.89365100	-0.06264400
C	-4.80555800	-3.13671700	-0.04393000
C	-3.53565300	-3.81019800	-0.04723800
C	-3.52562700	-5.23258900	-0.06942600
C	-4.70812600	-5.95058200	-0.08734100
H	-5.76830200	-1.19263400	-0.01817800
H	-6.87208700	-5.85594200	-0.09841100
H	-6.94483200	-3.37433400	-0.06002400
C	-4.80776700	-1.70402000	-0.02064600
C	-2.34805400	-3.05120000	-0.03022700
H	-2.56927900	-5.74991700	-0.07216700
H	-4.68027700	-7.03680900	-0.10414300
C	-2.36473900	-1.62729400	-0.00913900
C	-3.65188800	-0.95749400	-0.00133900
C	2.36474200	1.62729500	-0.00888900
C	2.34805300	3.05120900	-0.02996600
C	3.53565000	3.81020900	-0.04691300

C	4.80555700	3.13672900	-0.04355100
C	4.80776700	1.70402900	-0.02027700
C	3.65189200	0.95749900	-0.00101800
H	2.56927500	5.74992500	-0.07187700
C	3.52562400	5.23259900	-0.06909400
C	5.98930700	3.89366300	-0.06220800
H	5.76830300	1.19264600	-0.01776100
C	5.94869600	5.28424300	-0.08367400
C	4.70812400	5.95059400	-0.08695200
H	6.94482900	3.37434800	-0.05954800
H	6.87208300	5.85595700	-0.09792600
H	4.68027300	7.03682100	-0.10375000
H	1.40554000	3.58829400	-0.03631600
H	-1.40554300	-3.58828900	-0.03652700

BO4e_T₁

C	5.55465100	-1.27259200	-0.01606500
C	5.11812200	0.06295100	-0.00535400
C	3.76059100	0.36619200	0.00612300
C	2.78001100	-0.70577900	0.00137200
C	3.25146800	-2.06762400	-0.00806400
C	4.59535100	-2.33057400	-0.01623000
C	1.40777000	-0.37761000	0.00189100
C	0.97391600	1.00469600	0.00379700
C	-0.34272800	1.35800700	0.00195800
H	-0.56894900	2.41669300	0.00352700
C	-1.40775300	0.37759900	-0.00176000
C	-0.97390000	-1.00470800	-0.00365500
C	0.34274400	-1.35801800	-0.00181600
H	5.83937700	0.87716600	-0.00633800
H	2.54040900	-2.88724500	-0.01011300
H	0.56896400	-2.41670400	-0.00337800
C	-2.77999600	0.70577000	-0.00127500
C	-3.25145400	2.06761400	0.00811400
C	-4.59533900	2.33056300	0.01621100
C	-5.55463900	1.27257900	0.01601800
C	-5.11810700	-0.06296400	0.00536100
C	-3.76057400	-0.36620200	-0.00603400
H	-2.54039700	2.88723700	0.01017500
B	3.25302700	1.82477100	0.01487800
O	1.88809300	2.02842300	0.00813500
B	-3.25301000	-1.82478000	-0.01473100
O	-1.88807700	-2.02843700	-0.00798000
C	4.16184200	3.11217300	0.01617800

C	4.46311700	3.77101800	-1.19637000
C	4.69115900	3.62644300	1.21982500
C	5.27843100	4.90666900	-1.18873100
C	5.50269700	4.76565000	1.19313000
C	5.80704900	5.42317100	-0.00184800
H	5.50786000	5.39979400	-2.13213800
H	5.90609000	5.14971100	2.12883900
C	-4.16184000	-3.11217400	-0.01605200
C	-4.46349900	-3.77081400	1.19651600
C	-4.69079800	-3.62662600	-1.21977100
C	-5.27881800	-4.90645500	1.18881300
C	-5.50236100	-4.76582300	-1.19314000
C	-5.80708400	-5.42314300	0.00184900
H	-5.50853100	-5.39942900	2.13223100
H	-5.90547200	-5.15003200	-2.12890800
C	6.88434700	-1.84699800	-0.02772900
C	8.14791000	-1.23669900	-0.03224900
C	6.76983900	-3.25864200	-0.03476500
C	9.28410400	-2.04308400	-0.04360800
H	8.24107900	-0.15392700	-0.02709500
C	7.90850700	-4.05216200	-0.04598700
C	9.16969600	-3.43977600	-0.05040800
H	10.26958200	-1.58503100	-0.04728800
H	7.83275600	-5.13706600	-0.05135200
H	10.06632100	-4.05350600	-0.05922300
C	-6.88433700	1.84698400	0.02759900
C	-8.14790000	1.23668500	0.03206500
C	-6.76983000	3.25862900	0.03461200
C	-9.28409600	2.04306800	0.04334900
C	-7.90850000	4.05214900	0.04576000
C	-9.16968900	3.43976100	0.05012800
H	-10.26957300	1.58501500	0.04698600
H	-7.83275000	5.13705200	0.05110800
H	-10.06631500	4.05349100	0.05888400
C	6.66075100	6.67021000	-0.00886100
H	6.04381000	7.57641000	0.06196700
H	7.35606700	6.68524000	0.83742600
H	7.24709600	6.75075000	-0.93084900
C	3.90801000	3.25583500	-2.50865500
H	4.18681900	2.20851500	-2.68255100
H	2.81196900	3.30167400	-2.52457300
H	4.27790300	3.84210600	-3.35592100
C	4.37253400	2.96718100	2.54636100
H	3.30444100	3.04922900	2.78631100

H	4.61636900	1.89789000	2.53803400
H	4.93075000	3.43068900	3.36616100
C	-4.37180400	-2.96753600	-2.54630400
H	-4.61599300	-1.89832000	-2.53829500
H	-3.30358200	-3.04928300	-2.78577300
H	-4.92952000	-3.43138300	-3.36625200
C	-3.90878600	-3.25540800	2.50888000
H	-2.81273900	-3.30101800	2.52504400
H	-4.18785200	-2.20813000	2.68262400
H	-4.27874300	-3.84168400	3.35611500
C	-6.66080200	-6.67017200	0.00882900
H	-6.04377700	-7.57643300	-0.06046100
H	-7.24830200	-6.74994900	0.93015200
H	-7.35505900	-6.68589300	-0.83831100
C	5.30226100	-3.68801800	-0.02814800
C	4.96193200	-4.51040400	1.23495900
H	3.89477700	-4.75923300	1.25925300
H	5.52741500	-5.44937100	1.24759100
H	5.20404000	-3.95359200	2.14574100
C	4.94647400	-4.49632100	-1.29607400
H	3.87924600	-4.74567400	-1.30980300
H	5.17678000	-3.92902600	-2.20342900
H	5.51236000	-5.43460500	-1.32632500
H	-8.24106800	0.15391200	0.02692700
H	-5.83936000	-0.87718200	0.00632400
C	-5.30225200	3.68800600	0.02806300
C	-4.96185900	4.51036400	-1.23504500
H	-5.52734400	5.44933000	-1.24772800
H	-3.89470200	4.75919500	-1.25928800
H	-5.20391800	3.95353000	-2.14582700
C	-4.94653100	4.49633700	1.29598900
H	-3.87930400	4.74569100	1.30976800
H	-5.51241900	5.43462200	1.32619000
H	-5.17688400	3.92906300	2.20334500

BO5_T1

C	-0.83267300	5.64603100	0.09441400
C	-1.90775000	4.74691900	0.08308900
C	-1.67878800	3.38228200	0.06365000
C	-0.34558400	2.83611900	0.05424200
C	0.72277100	3.79316300	0.06677900
C	0.48303900	5.15362400	0.08623400
C	-0.15282600	1.43401400	0.03229500
C	-1.32665800	0.55014700	0.02263600

C	-1.15417800	-0.80746000	-0.01112900
H	-2.04366600	-1.43004300	-0.02084500
C	0.15283600	-1.43402600	-0.03219500
C	1.32666700	-0.55015900	-0.02249900
C	1.15418800	0.80744800	0.01124900
H	-1.02100400	6.71510200	0.10957900
H	-2.93627700	5.09354500	0.08928500
H	1.74761200	3.44021800	0.06142900
H	1.32062000	5.84546200	0.09542800
H	2.04367700	1.43002900	0.02095200
C	0.34559500	-2.83613100	-0.05422200
C	1.67879900	-3.38229200	-0.06368600
H	-1.74760000	-3.44023100	-0.06141400
C	-0.72275900	-3.79317400	-0.06679800
C	1.90776300	-4.74692800	-0.08320700
C	0.83268600	-5.64604000	-0.09456500
C	-0.48302600	-5.15363500	-0.08633400
H	2.93629100	-5.09355200	-0.08944000
H	1.02101900	-6.71511000	-0.10979400
H	-1.32060700	-5.84547300	-0.09555400
O	-2.79138800	2.57618900	0.05432800
B	-2.72928400	1.19494900	0.04049400
B	2.72929200	-1.19495900	-0.04039800
O	2.79140100	-2.57619800	-0.05434000
C	-4.10077500	0.42116100	0.03114200
C	-4.78020200	0.19122700	-1.18624800
C	-4.67427100	-0.05182800	1.23117600
C	-5.99424800	-0.50125900	-1.18584500
C	-5.89179000	-0.74069400	1.19674700
C	-6.56982300	-0.97441800	-0.00226300
H	-6.50339300	-0.67697500	-2.13226700
H	-6.32142800	-1.10185100	2.12971500
C	4.10077900	-0.42116200	-0.03104500
C	4.67440800	0.05149500	-1.23117000
C	4.78004200	-0.19085700	1.18633700
C	5.89189700	0.74037200	-1.19681400
C	5.99410700	0.50164500	1.18586100
C	6.56981300	0.97443700	0.00222300
H	6.32161700	1.10129100	-2.12984000
H	6.50314300	0.67764500	2.13228600
C	4.20239300	-0.69108200	2.49453000
H	3.19169300	-0.29898300	2.66637100
H	4.12730400	-1.78560200	2.50541200
H	4.82306400	-0.39196300	3.34514700

C	3.99499900	-0.19860500	-2.56224500
H	3.97386800	-1.26924300	-2.80417100
H	2.95471700	0.14863800	-2.55905700
H	4.51556300	0.31275800	-3.37826500
C	7.89842800	1.69437000	0.01984500
H	8.00248500	2.32406600	0.91058400
H	8.73632100	0.98411200	0.02766300
H	8.02118200	2.33188700	-0.86214500
C	-7.89837600	-1.69446400	-0.02006700
H	-8.73627400	-0.98428700	-0.03249700
H	-8.00045600	-2.32756700	-0.90863800
H	-8.02302300	-2.32863900	0.86405300
C	-3.99481100	0.19796000	2.56228700
H	-2.95442800	-0.14896400	2.55888200
H	-3.97398600	1.26851200	2.80462600
H	-4.51515700	-0.31386400	3.37815600
C	-4.20267600	0.69182500	-2.49435300
H	-4.12763900	1.78634900	-2.50495100
H	-3.19196900	0.29981600	-2.66636800
H	-4.82339400	0.39289100	-3.34500100

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C	-1.24789600	-0.85338900	0.06293900
C	-1.25111700	-2.30549500	0.04882900
C	-2.49992900	-3.01334700	0.07763000
C	-3.72834400	-2.25811900	0.11415900
C	-0.00042100	-0.20559200	0.00008300
C	-0.00449700	-2.98438400	-0.00017100
C	1.24411500	-2.30914500	-0.04893800
C	1.24521300	-0.85700800	-0.06289400
C	3.72147900	-2.26901700	-0.11445700
C	2.49081000	-3.02066600	-0.07771100
H	0.00119800	0.88470300	0.00020400
H	-0.00609400	-4.06923500	-0.00048300
C	-4.97138800	-2.89299600	0.13902300
C	-2.63325600	-4.43246800	0.06989300
C	-3.86992000	-5.04813300	0.09547100
C	-5.05282900	-4.28209500	0.12999700
H	-5.85867700	-2.26727100	0.16685000
H	-1.74347800	-5.05337400	0.04272600
H	-3.92938300	-6.13370200	0.08876400
H	-6.02243100	-4.77190200	0.14996600
C	4.96263800	-2.90763500	-0.13936500
C	5.03994500	-4.29694800	-0.13010500

C	3.85476100	-5.05950300	-0.09525800
C	2.61994200	-4.44019200	-0.06964200
H	5.85178400	-2.28456100	-0.16739600
H	6.00808200	-4.78964500	-0.15011300
H	3.91104300	-6.14523900	-0.08829900
H	1.72833300	-5.05844500	-0.04207800
B	2.56752100	-0.12137500	-0.11985100
O	3.73775400	-0.91590900	-0.12828200
O	-3.74058900	-0.90487600	0.12782200
B	-2.56816900	-0.11388800	0.11968700
C	2.80563400	1.43492700	-0.14256700
C	2.51968000	2.20840600	-1.29025200
C	3.31757500	2.08713000	1.00410900
C	2.73971300	3.59116400	-1.27190200
C	3.51884800	3.47022000	0.99110700
C	3.23759600	4.24280800	-0.14076300
H	2.51680400	4.17367200	-2.16546600
H	3.90400700	3.95802900	1.88652500
C	-2.80147900	1.44314900	0.14257100
C	-2.51384900	2.21546400	1.29057400
C	-3.31063800	2.09722300	-1.00431800
C	-2.72949700	3.59894300	1.27237500
C	-3.50756900	3.48091100	-0.99114400
C	-3.22457100	4.25239200	0.14108000
H	-2.50533500	4.18053600	2.16621800
H	-3.89064300	3.97011100	-1.88670100
C	3.64708300	1.29906300	2.25502300
H	4.46450400	0.58993600	2.07450500
H	3.94906400	1.95986600	3.07429600
H	2.78583800	0.71150600	2.59991800
C	1.98969100	1.56520300	-2.55635500
H	1.94942600	2.28803900	-3.37806600
H	2.62193100	0.72856700	-2.87992700
H	0.97820100	1.16357000	-2.41817000
C	3.49234100	5.73181800	-0.14598100
H	3.25679500	6.18221100	0.82529400
H	4.54761900	5.95426200	-0.35736800
H	2.89263800	6.23870500	-0.90978500
C	-1.98674000	1.57036100	2.55691800
H	-1.94469600	2.29293900	3.37876500
H	-2.62186200	0.73570400	2.87995700
H	-0.97645600	1.16551400	2.41930700
C	-3.64171400	1.31046400	-2.25564400
H	-4.46078800	0.60311400	-2.07565900

H	-3.94200300	1.97232900	-3.07468300
H	-2.78172500	0.72111500	-2.60062800
C	-3.47445700	5.74222500	0.14627900
H	-2.87759400	6.24637600	0.91409100
H	-3.23166000	6.19278700	-0.82315300
H	-4.53023900	5.96794900	0.35153500