

Supplementary Information

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

Guijie Li^{1*}, Kewei Xu¹, Jianbing Zheng¹, Xiaoli Fang¹, Yun-Fang Yang¹, Weiwei Lou¹, Qingshan Chu¹, Jianxin Dai¹, Qidong Chen¹, Yuning Yang¹, Yuanbin She^{1*}

¹College of Chemical Engineering, State Key Laboratory Breeding Base of Green-Chemical Synthesis Technology, Zhejiang University of Technology, Hangzhou, Zhejiang 310014, P. R. China

E-mail: guijieli@zjut.edu.cn; sheyb@zjut.edu.cn

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Supplementary 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 ultiplicities: 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 Mo-K α 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. The spin-orbit coupling (SOC) matrix elements between S_1 and T_n states of **BO1a** and **BO1d** and **BO6** were evaluated using PySOC at the B3LYP/6-31G(d,p) level [Gao. X., Bai, D., Fazzi, D., Niehaus, T., Barbatti, M., Thiel, W. *J. Chem. Theory Comput.* **13**, 515–524 (2017)].

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, and the relationship with k_r and Φ_{PL} . [Turro, N. J., Ramamurthy, V., Scaiano, J. C. Modern Molecular Photochemistry of Organic Molecules; University Science Books; pp195–200, (2009).]

$$\Phi_{\text{PL}} = k_r / (k_r + k_{nr}) \quad (\text{S1})$$

$$k_r = \nu^2 f \quad (\text{S2})$$

Where the Φ_{PL} is photoluminescence efficiency, k_r is radiative rate, k_{nr} is non-radiative rate, ν is the wavenumber corresponding to the maximum wavelength of absorption, f is oscillator strength. From the **Equation S1** and **Equation S2**, we can see that the f plays an critical role in the increase of Φ_{PL} .

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:

$$f \equiv 4.3 \times 10^{-9} \int \varepsilon d\bar{\nu} \quad (\text{S3})$$

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 $\Delta\bar{\nu}_{1/2}$ (in cm^{-1}) is the full-width half-maximum (FWHM) of the absorption band.

With the experiment data extracted from the UV-Vis spectrum and **Equation S3**, the approximate of f can be obtained as **Equation S4**:

$$f \sim 4.3 \times 10^{-9} \varepsilon_{\max} \Delta\bar{\nu}_{1/2} \quad (\text{S4})$$

Therefore, the f of **BO4a**, **BO4b** and **BO4e** can be calculated as:

$$f(\text{BO4a}) = (4.3 \times 10^{-9}) \times (2.95 \times 10^4) \times [(1/(348.5 \times 10^{-7}) - (1/(357.5 \times 10^{-7}))] = 0.092.$$

$$f(\text{BO4b}) = (4.3 \times 10^{-9}) \times (4.15 \times 10^4) \times [(1/(352.5 \times 10^{-7}) - (1/(361.0 \times 10^{-7}))] = 0.12.$$

$$f(\text{BO4e}) = (4.3 \times 10^{-9}) \times (7.57 \times 10^4) \times [(1/(379.0 \times 10^{-7}) - (1/(390.0 \times 10^{-7}))] = 0.24.$$

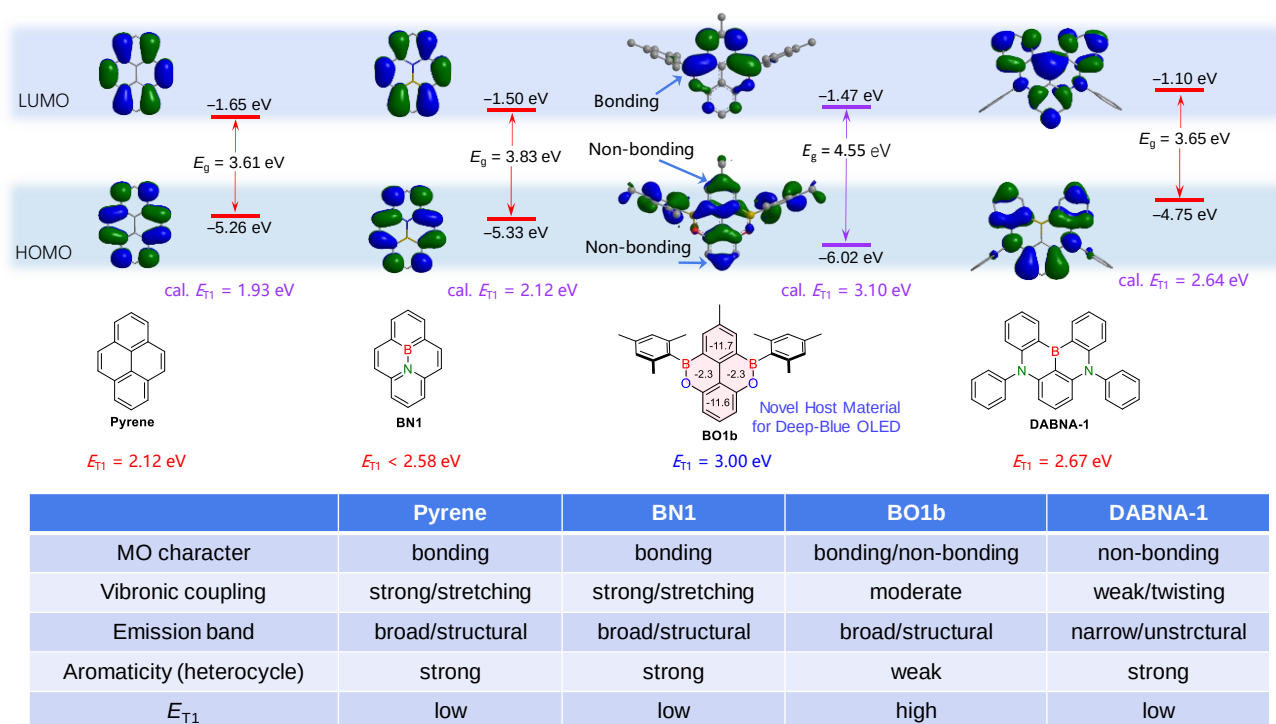
Moreover, the increase of the f from **BO4a**, **BO4b** and **BO4e** can be explained by the relationship between the classical concept of oscillator strength and the quantum mechanical transition dipole moment (**Equation S5**).

$$\text{Oscillator strength } f \propto \mu_i^2 = (e\mathbf{r})^2 \text{ Transition dipole moment} \quad (\text{S5})$$

Where μ_i is the induced transition dipole moment (or dipole strength) corresponding to electronic transition (absorption or emission). The dipole strength of a transition may be set equal to $e\mathbf{r}$, which can be viewed as the average size of the transition dipole, where $\mathbf{r}$ is the dipole length. By combining the classical oscillator strength with the quantization of oscillation of electrons, we have the expression relating f and μ_i , which is given by **Equation S6**,

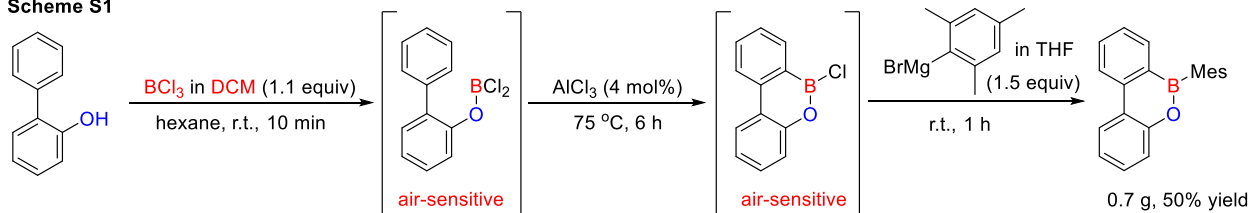
$$f = \left(\frac{8\pi m_e \bar{\nu}}{3he^2} \right) \mu_i^2 \cong 10^{-5} \bar{\nu} |e\mathbf{r}_i|^2 \quad (\text{S6})$$

The f is a function of the μ_i , where m_e is the mass of electron, $\bar{\nu}$ is the energy of the transition (in cm^{-1}), h is Planck's constant. The μ_i and $\mathbf{r}$ should be much larger for the delocalized ICT transition in **BO4e** than those in **BO4a** and **BO4b**, this is because **BO4e** with two fluorenyl units possesses longer linear conjugation system compared to **BO4a** and **BO4b**.

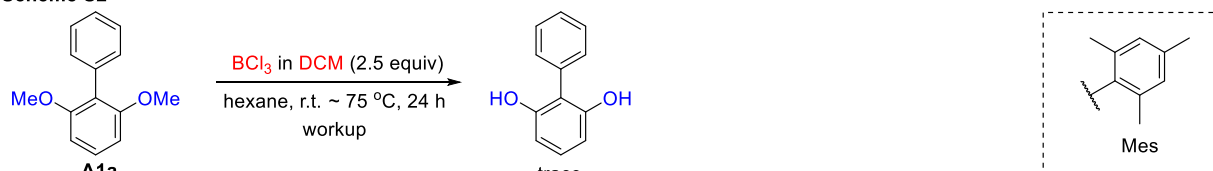


Supplementary Fig. 1. Theoretical calculation, chemical structures and photophysical properties of Pyrene, BN1, BO1b and DABNA-1. Comparison of calculated frontier orbital distributions, energy levels/gaps, calculated and experimental E_{T1} , MO character, aromaticity.

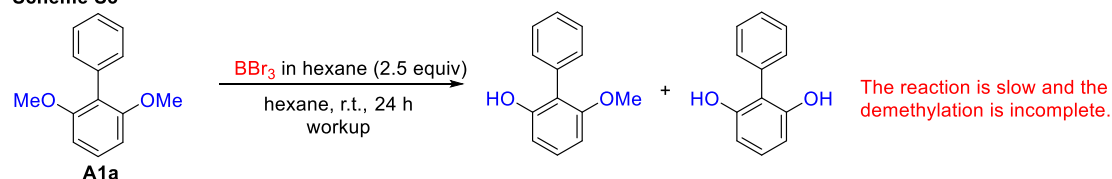
Scheme S1



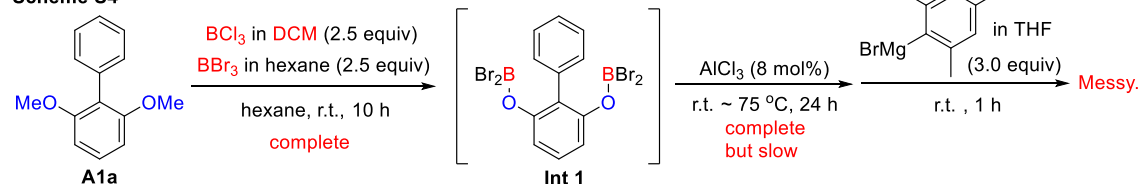
Scheme S2



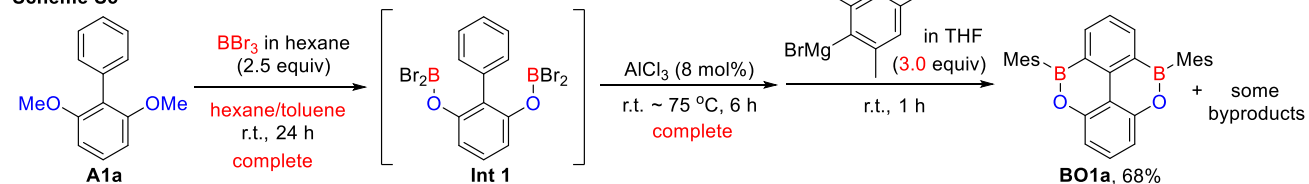
Scheme S3



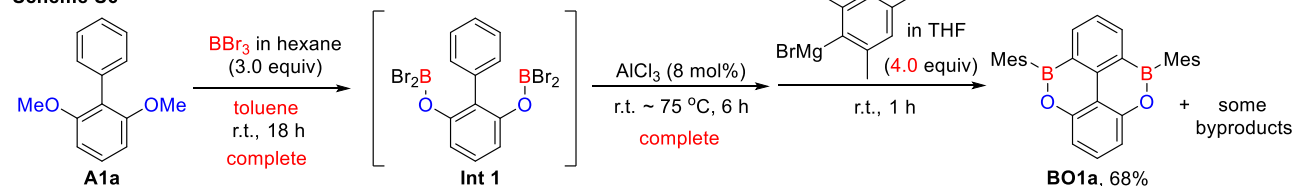
Scheme S4



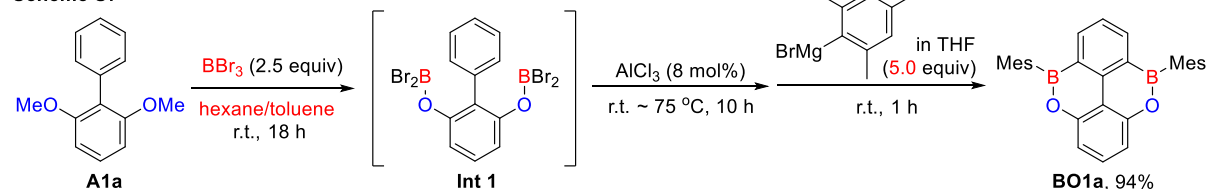
Scheme S5



Scheme S6



Scheme S7



Supplementary Fig. 2. Reaction condition optimization. Template reactions and selected optimization of reaction conditions

Supplementary Discussion

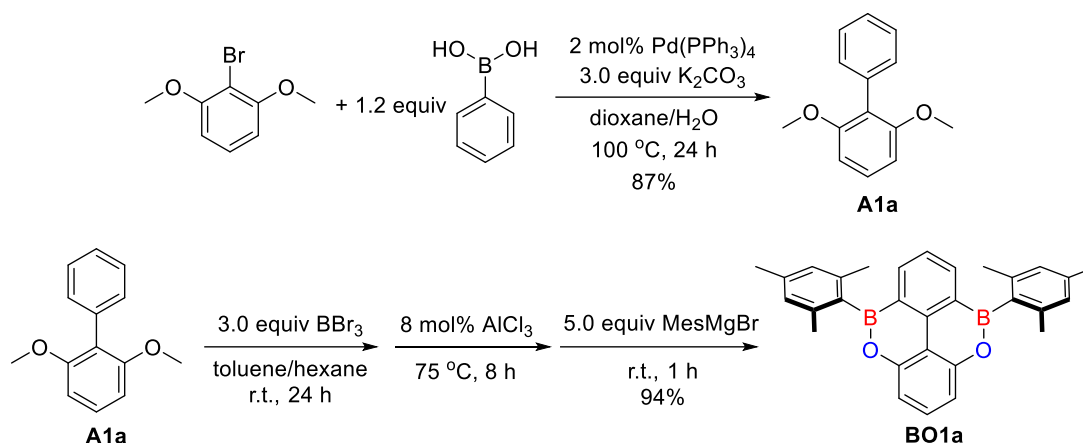
Reaction Condition Optimization. We initiated our examination by carrying out template reactions (see Supporting Information [Figure S1](#), [Scheme S1](#)). To our delight, [1,1'-Biphenyl]-2-ol smoothly transformed into 9,10-boroxarophenanthrene in hexane with 50% isolated yield using BCl₃-dichloromethane 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 $\text{Pd(PPh}_3)_4$ 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 AlCl_3 is highly hygroscopic and should be weighed quickly!), the flask was placed in oil bath (75 °C) and stirred for 8–10 hours, 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 1–10 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.

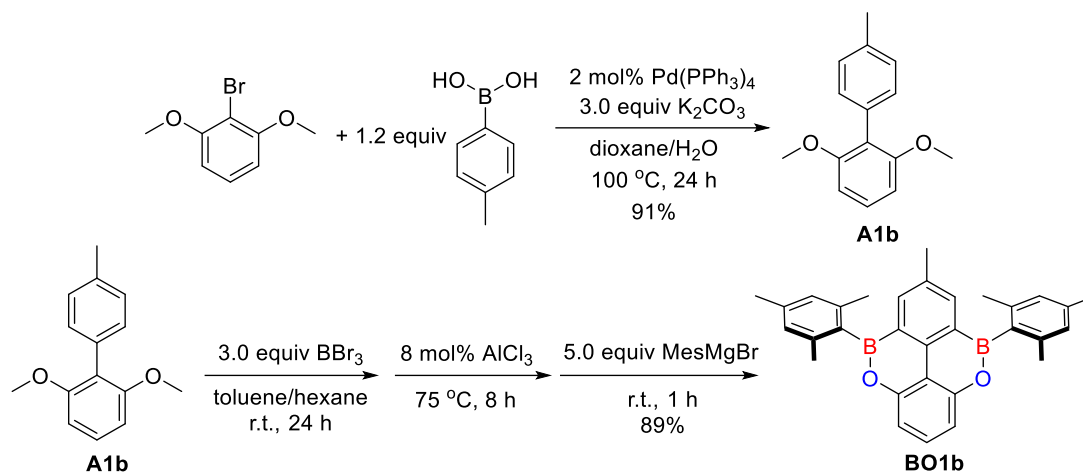
Synthesis of **BO1a**:



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.* **133**, 4243–4245 (2011).

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.

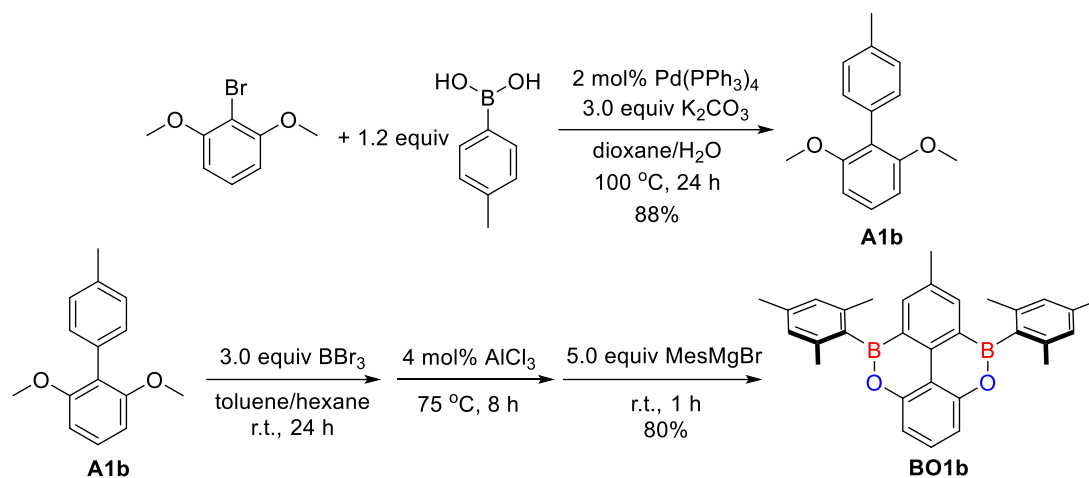
Synthesis of **BO1b**:



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 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.* **47**, 677–679 (2011).

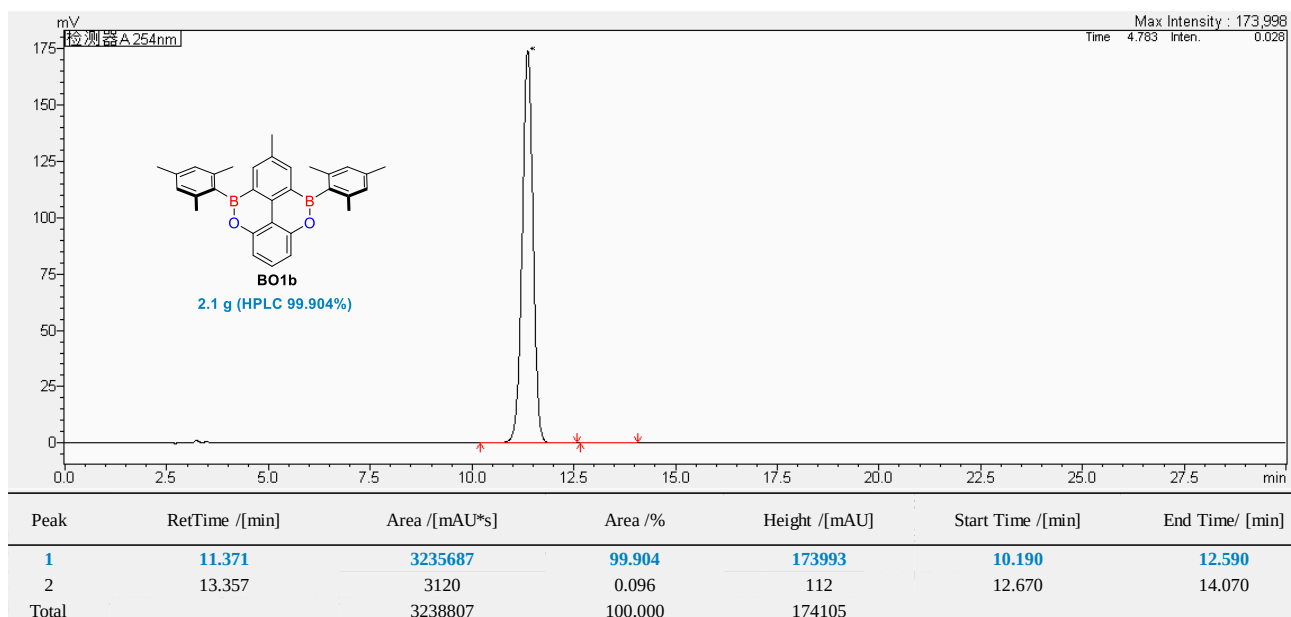
Synthesis of **BO1b:** Following the general procedure, BBr₃ (1.16 mL, d = 2.6 g/mL, 12.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A1b** (913 mg, 4.00 mmol, 1.0 equiv) in toluene (40 mL) and *n*-hexane (40 mL) and stirred at room temperature for 24 hours, added AlCl₃ (42 mg, 0.32 mmol, 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.

Large scale synthesis of **BO1b**:

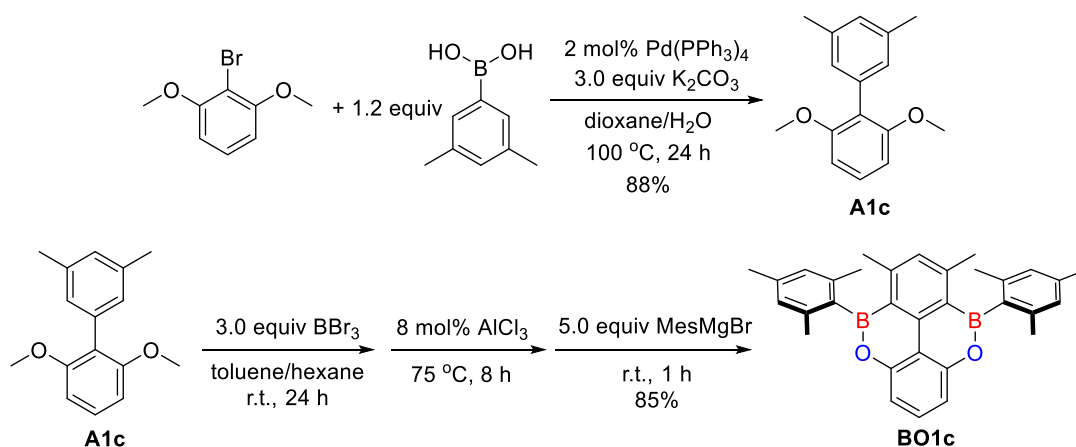


Synthesis of **A1b:** Following the general procedure, the reaction of 2-bromo-1,3-dimethoxybenzene (13.02 g, 60.00 mmol, 1.0 equiv), 4-methylphenylboronic acid (9.79 g, 72.00 mmol, 1.2 equiv), $\text{Pd(PPh}_3)_4$ (1.39 mg, 1.20 mmol, 0.02 equiv) and K_2CO_3 (24.89 g, 180.00 mmol, 3.0 equiv), in 40 mL H_2O) in dioxane (160 mL) at $100\text{ }^\circ\text{C}$ for 24 hours afforded **A1b** (eluent: petroleum ether/ethyl acetate = 20:1–10:1) as a white solid 12.00 g in 88% yield. The structure was confirmed by ^1H NMR, which was in agreement with the above result.

Synthesis of **BO1b:** Following the general procedure, BBr_3 (7.60 mL, $d = 2.6\text{ g/mL}$, 78.84 mmol, 3.0 equiv) was added dropwise to a mixture of **A1b** (6.00 g, 26.28 mmol, 1.0 equiv) in toluene (150 mL) and *n*-hexane (150 mL) and stirred at room temperature for 24 hours, added AlCl_3 (140 mg, 1.05 mmol, 0.04 equiv) and stirred at $75\text{ }^\circ\text{C}$ for 8 hours, cooled down to room temperature, added MesMgBr (131.40 mL, 1.0 M in THF, 131.40 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 9.56 g in 80% yield. The structure was confirmed by ^1H NMR, which was in agreement with the above result. The obtained **BO1b** was further purified by recrystallization in toluene/methanol; and then 2.5 g **BO1b** was sublimated in a seven zone thermal gradient sublimator at $40/100/130/150/250/250/270\text{ }^\circ\text{C}$, 1.6×10^{-6} Torr to obtain white solid 2.1 g in 84% yield; purity, 99.90% by HPLC, HPLC analysis condition: column: Masiall® C18-BIO, $5\mu\text{m}$, $250 \times 4.6\text{ mm}$; mobile phase: methanol/tetrahydrofuran = 95/5(v/v); flow rate: 1.0 mL/min; Abs. detector: 254 nm.



Synthesis of **BO1c**:

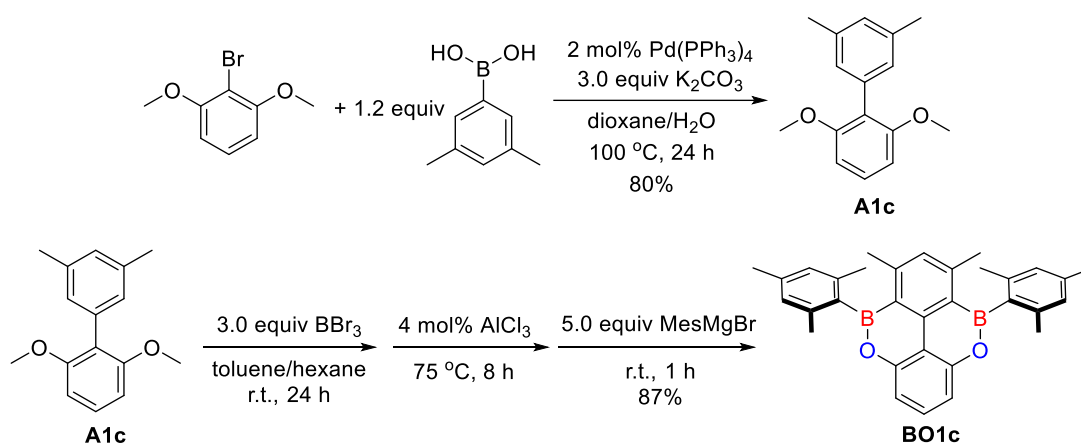


Synthesis of **A1c:** Following the general procedure, the reaction of 2-bromo-1,3-dimethoxybenzene (2.17 g, 10.00 mmol, 1.0 equiv), 3,5-dimethylphenylboronic acid (1.80 g, 12.00 mmol, 1.2 equiv), Pd(PPh₃)₄ (213 mg, 0.20 mmol, 0.02 equiv) and K₂CO₃ (4.15 g, 30.00 mmol, 3.0 equiv, in 15 mL H₂O) in dioxane (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

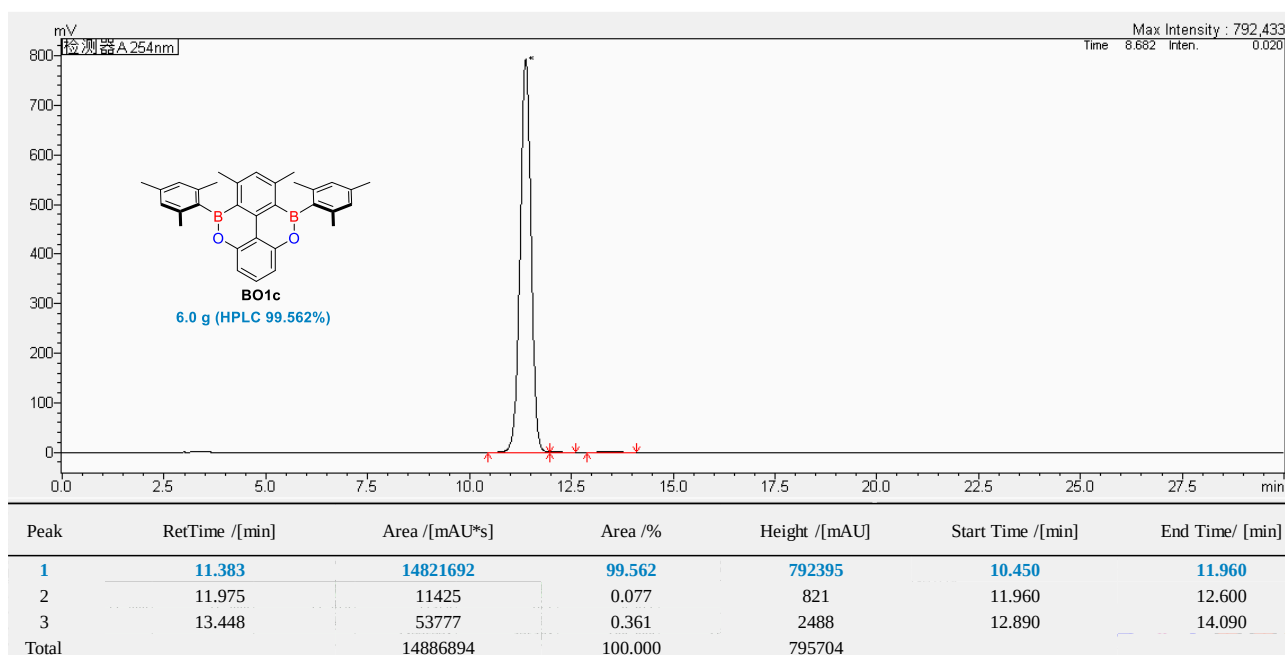
BO1c (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.62 g in 85% yield. m.p.: 209.8–210.0 °C. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.21 (s, 12H), 2.28 (s, 6H), 2.36 (s, 6H), 6.93 (s, 4H), 7.27 (s, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.57 (t, *J* = 8.0 Hz, 1H). ¹³C NMR (125 MHz, CDCl₃): 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.

Large scale synthesis of **BO1c**:

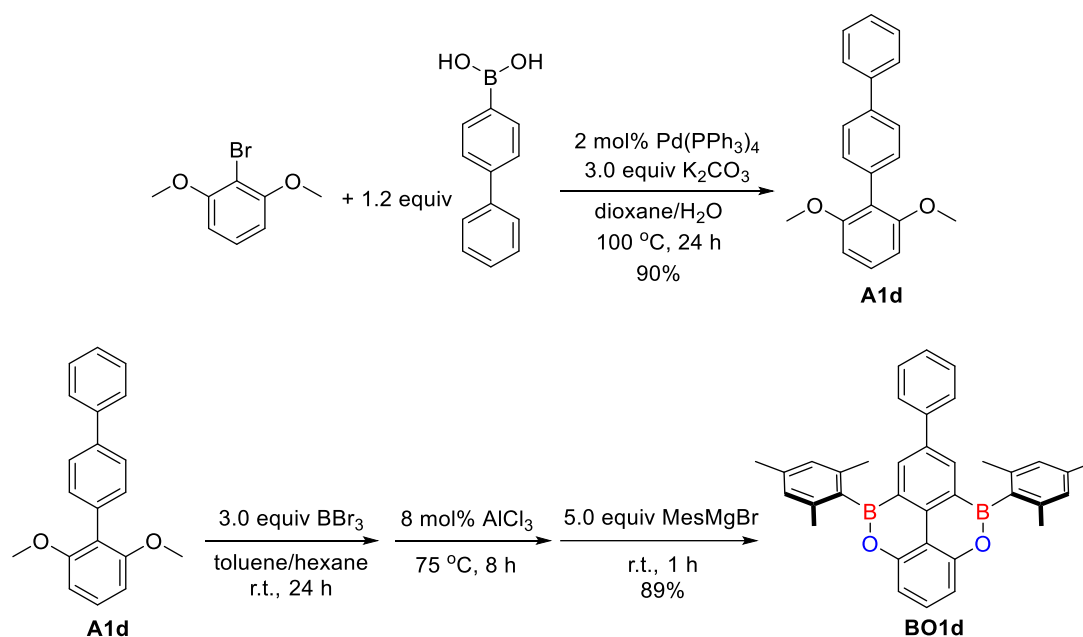


Synthesis of A1c: Following the general procedure, the reaction of 2-bromo-1,3-dimethoxybenzene (10.85 g, 50.00 mmol, 1.0 equiv), 3,5-dimethylphenylboronic acid (9.00 g, 60.00 mmol, 1.2 equiv), Pd(PPh₃)₄ (1.16 g, 1.00 mmol, 0.02 equiv) and K₂CO₃ (20.73 g, 150.00 mmol, 3.0 equiv, in 20 mL H₂O) in dioxane (80 mL) at 100 °C for 24 hours afforded **A1c** (eluent: petroleum ether/ethyl acetate = 10:1–5:1) as a white solid 9.69 g in 80% yield. The structure was confirmed by ¹H NMR, which was in agreement with the above result.

Synthesis of BO1c: Following the general procedure, BBr₃ (11.57 mL, d = 2.6 g/mL, 120.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A1c** (9.69 g, 40.00 mmol, 1.0 equiv) in toluene (200 mL) and *n*-hexane (200 mL) and stirred at room temperature for 24 hours, added AlCl₃ (213 mg, 1.60 mmol, 0.04 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (200 mL, 1.0 M in THF, 200 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 16.30 g in 87% yield. The structure was confirmed by ¹H NMR, which was in agreement with the above result. The obtained **BO1c** was further purified by recrystallization in toluene/methanol; and then 6.4 g **BO1c** was sublimated in a seven zone thermal gradient sublimator at 40/100/130/150/250/250/270 °C, 5.0×10⁻⁵ Torr to obtain white solid 6.0 g in 94% yield; purity, 99.56% by HPLC, HPLC analysis condition: column: Masiall® C18-BIO, 5μm, 250 × 4.6 mm; mobile phase: methanol/tetrahydrofuran = 95/5(v/v); flow rate: 1.0 mL/min; Abs. detector: 254 nm.



Synthesis of **BO1d**:

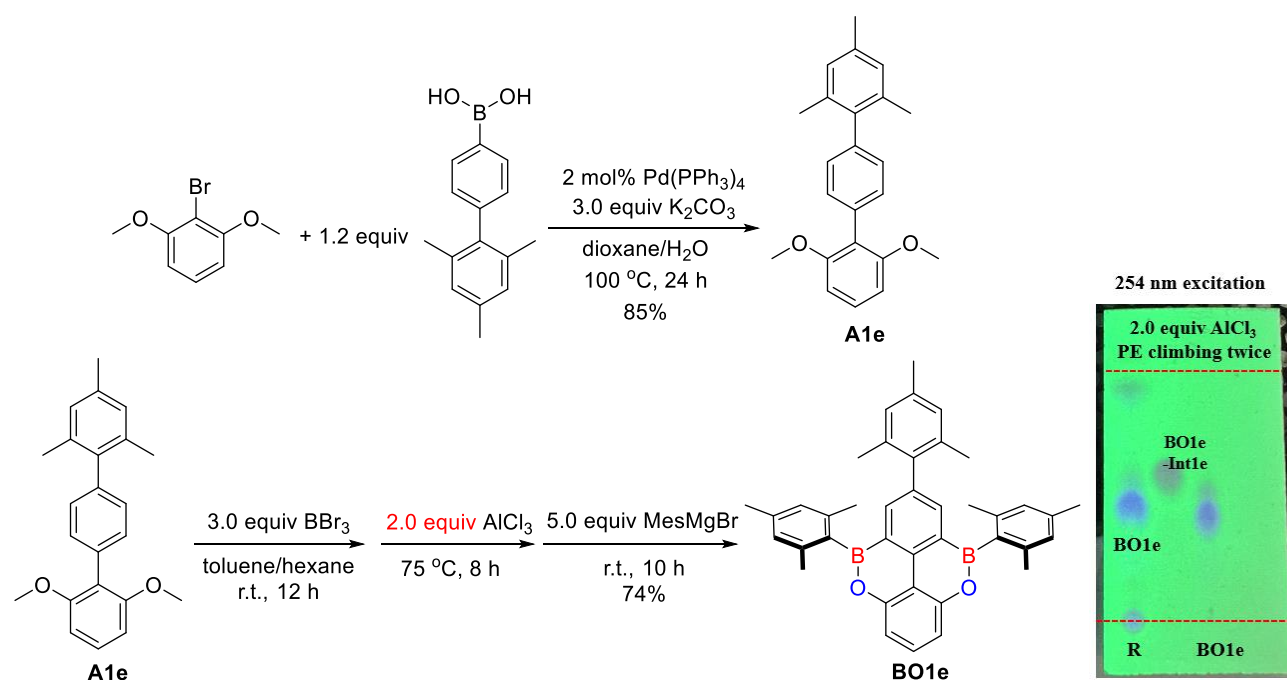


Synthesis of **A1d**: Following the general procedure, the reaction of 2-bromo-1,3-dimethoxybenzene (2.17 g, 10.00 mmol, 1.0 equiv), [1,1'-biphenyl]-4-ylboronic acid (2.38 g, 12.00 mmol, 1.2 equiv), Pd(PPh₃)₄ (213 mg, 0.20 mmol, 0.02 equiv) and K₂CO₃ (4.15 g, 30.00 mmol, 3.0 equiv), in 15 mL H₂O) in 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. m.p.: 205.7–206.2 °C. 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 ^{13}C NMR is agreement with the previous reoprt (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.* **52**, 5055–5059 (2011).

Synthesis of BO1d: Following the general procedure, BBr_3 (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 AlCl_3 (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, $\text{DMSO}-d_6$): 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). ^{13}C NMR (125 MHz, CDCl_3): 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. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 48.79. HRMS (ESI): calcd for $\text{C}_{36}\text{H}_{33}[^{11}\text{B}]_2\text{O}_2^+ [\text{M}+\text{H}]^+$ 519.2661, found 519.2673.

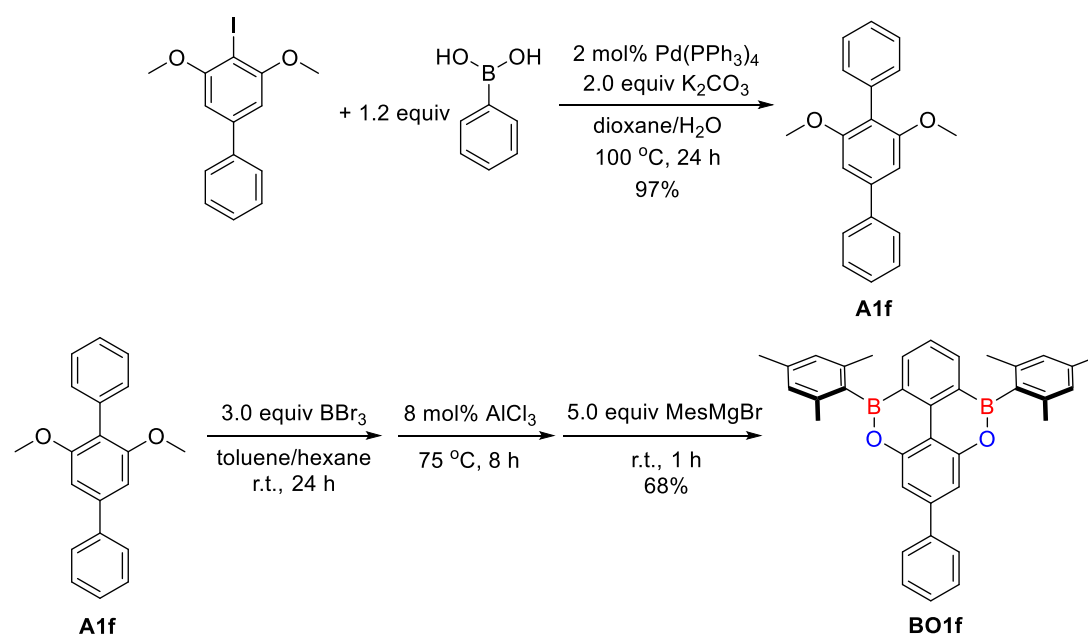
Synthesis of BO1e:



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), $\text{Pd}(\text{PPh}_3)_4$ (213 mg, 0.20 mmol, 0.02 equiv) and K_2CO_3 (4.15 g, 30.00 mmol, 3.0 equiv, in 15 mL H_2O) 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. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 2.10 (s, 6H), 2.34 (s, 3H), 3.76 (s, 6H), 6.68 (d, $J = 8.5$ Hz, 2H), 6.96 (s, 2H), 7.16 (dt, $J = 8.5$,

1.5 Hz, 2H), 7.28 (t, $J = 8.5$ Hz, 1H), 7.38 (dt, $J = 8.0, 2.0$ Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 20.91, 21.00, 55.98, 104.49, 119.66, 127.99, 128.53, 130.79, 132.16, 136.24, 136.32, 139.06, 139.20, 157.80. Synthesis of **BO1e**: 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 **A1e** (332 mg, 1.00 mmol, 1.0 equiv) in toluene (5 mL) and *n*-hexane (5 mL) and stirred at room temperature for 12 hours, added AlCl_3 (267 mg, 2.00 mmol, 2.00 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (5.0 mL, 1.0 M in THF, 5.00 mmol, 5.0 equiv) and stirred at room temperature for another 10 hour to afford **BO1e** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 417 mg in 74% yield. ^1H NMR (500 MHz, CDCl_3): 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). ^{13}C NMR (125 MHz, CDCl_3): 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, 140.80, 151.41. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 47.17. HRMS (ESI): calcd for $\text{C}_{39}\text{H}_{39}[^{11}\text{B}]_2\text{O}_2^+ [\text{M}+\text{H}]^+$ 561.3131, found 561.3127.

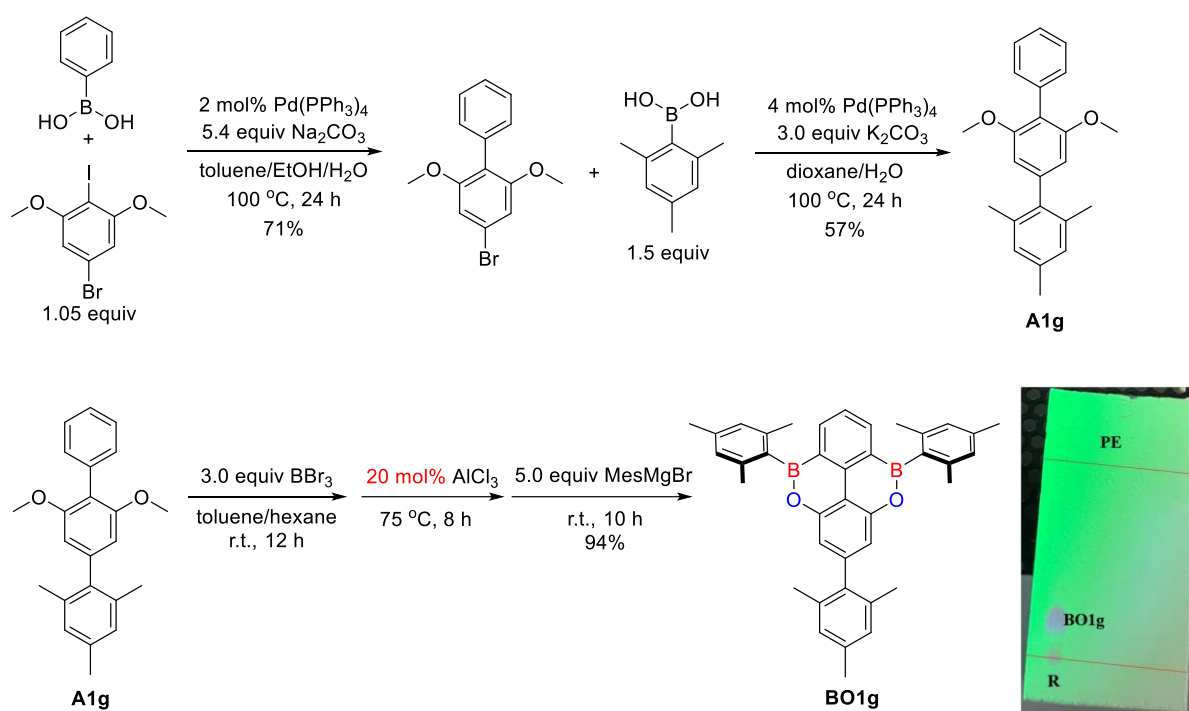
Synthesis of **BO1f**:



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), $\text{Pd}(\text{PPh}_3)_4$ (46 mg, 0.04 mmol, 0.02 equiv) and K_2CO_3 (552 mg, 4.00 mmol, 2.0 equiv, in 5 mL H_2O) 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, CDCl_3): 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). ^{13}C NMR (125 MHz, CDCl_3): 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, BBr_3 (0.29 mL, $d = 2.6 \text{ g/mL}$, 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 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, 5.00 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, CDCl_3): δ (ppm) 2.26 (s, 12H), 2.38 (s, 6H), 6.97 (s, 4H), 7.41 (t, $J = 6.0 \text{ Hz}$, 1H), 7.50 (t, $J = 6.5 \text{ Hz}$, 2H), 7.61 (t, $J = 6.0 \text{ Hz}$, 1H), 7.75 (s, 1H), 7.76 (s, 3H), 8.18 (d, $J = 6.0 \text{ Hz}$, 2H). ^{13}C NMR (125 MHz, CDCl_3): 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. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 46.99. 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 **BO1g**:



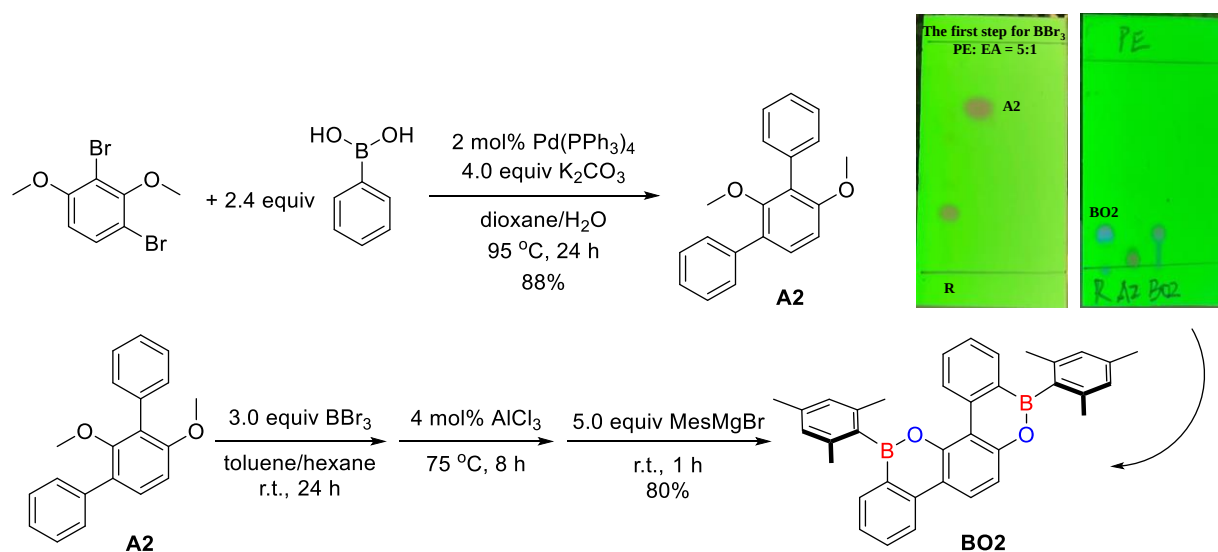
Synthesis of 4-bromo-2,6-dimethoxy-1,1'-biphenyl: Following the general procedure, the reaction of 5-bromo-2-iodo-1,3-dimethoxybenzene (3.6 g, 10.5 mmol, 1.05 equiv), phenylboronic acid (1.21 g, 11.70 mmol, 1.0 equiv), $\text{Pd}(\text{PPh}_3)_4$ (270 mg, 0.23 mmol, 0.02 equiv) and Na_2CO_3 (6.70 g, 63.18 mmol, 5.4 equiv, in 10 mL H_2O) in dioxane (40 mL) and EtOH (10 mL) at 100°C for 24 hours afforded 4-bromo-2,6-dimethoxy-1,1'-biphenyl (eluent: petroleum ether/dichloromethane = 50:1–30:1) as a white solid 2.08 g in 71% yield, which was used directly for the next step. The 5-bromo-2-iodo-1,3-dimethoxybenzene was synthesized according the previous report (Wang, G., Chen, M., Wang, J., Jiang, Z., Liu, D., Lou, D., Zhao, H., Li, K., Li, S., Wu, T., Jiang, Z., Sun, X., Wang, P. Reinforced

topological nanoassemblies: 2D hexagon-fused wheel to 3D prismatic metallo-lamellar structure with molecular weight of 119 K daltons. *J. Am. Chem. Soc.* **1421**, 7690–7698 (2020).

Synthesis of A1g: Following the general procedure, the reaction of 4-bromo-2,6-dimethoxy-1,1'-biphenyl (1.99 g, 7.00 mmol, 1.0 equiv), phenylboronic acid (1.64 g, 10.50 mmol, 1.5 equiv), Pd(PPh₃)₄ (324 mg, 0.28 mmol, 0.04 equiv) and K₂CO₃ (2.90 g, 21.00 mmol, 2.0 equiv, in 5 mL H₂O) in dioxane (20 mL) at 100 °C for 24 hours afforded **A1g** (eluent: petroleum ether/dichloromethane = 40:1–10:1) as a white solid 1.27 g in 57% 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). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 20.64, 20.99, 55.93, 105.29, 117.52, 126.66, 127.61, 128.05, 131.07, 134.17, 136.02, 136.76, 139.28, 141.68, 157.51.

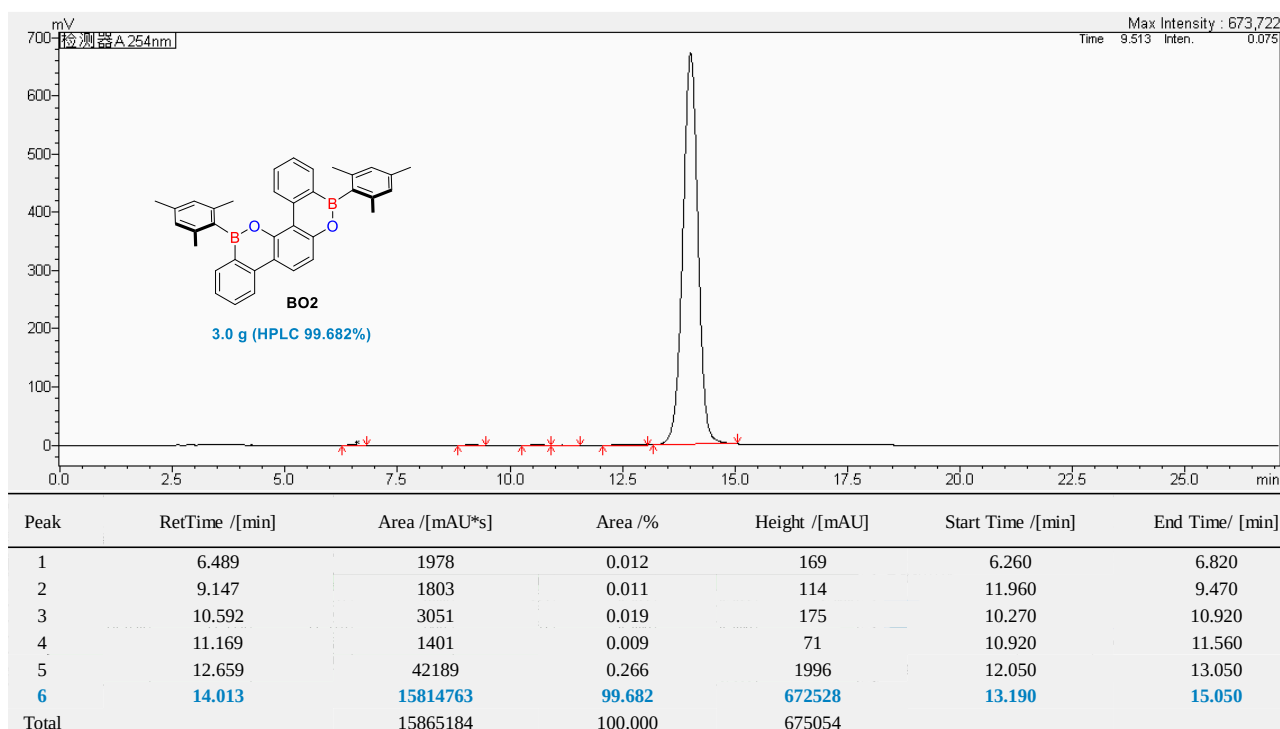
Synthesis of BO1g: Following the general procedure, BBr₃ (0.63 mL, d = 2.6 g/mL, 6.51 mmol, 3.0 equiv) was added dropwise to a mixture of **A1g** (720 mg, 1.00 mmol, 1.0 equiv) in toluene (20 mL) and *n*-hexane (20 mL) and stirred at room temperature for 24 hours, added AlCl₃ (57 mg, 0.43 mmol, 0.20 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (10.85 mL, 1.0 M in THF, 10.85 mmol, 5.0 equiv) and stirred at room temperature for another 10 hour to afford **BO1g** (eluent: petroleum ether ~ petroleum ether/dichloromethane = 10:1) as a white solid 1.15 g in 96% yield. m.p.: 151.8–152.4 °C. 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.

Large scale synthesis of **BO2**:

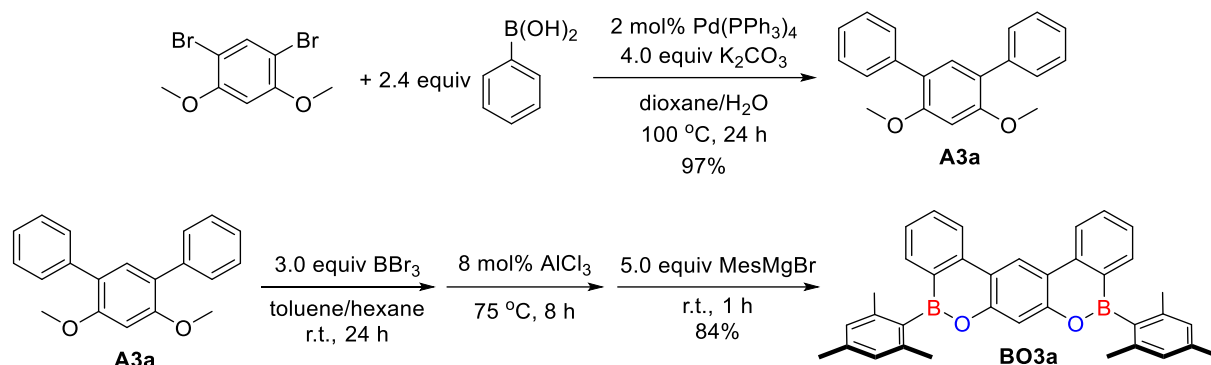


Synthesis of **A2**: Following the general procedure, the reaction of 1,3-dibromo-2,4-dimethoxybenzene (7.37 g, 24.90 mmol, 1.0 equiv), boronic acid (7.29 g, 59.76 mmol, 2.4 equiv), Pd(PPh₃)₄ (578 mg, 0.50 mmol, 0.02 equiv) and K₂CO₃ (13.76 g, 99.60 mmol, 4.0 equiv, in 20 mL H₂O) in dioxane (80 mL) at 100 °C for 24 hours afforded **A2** (eluent: petroleum ether/ethyl acetate = 20:1–10:1) as a white solid 6.36 mg in 88% 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 (4.68 mL, d = 2.6 g/mL, 48.57 mmol, 3.0 equiv) was added dropwise to a mixture of **A2** (4.72 g, 16.19 mmol, 1.0 equiv) in toluene (50 mL) and *n*-hexane (50 mL) and stirred at room temperature for 24 hours, added AlCl₃ (87 mg, 0.65 mmol, 0.04 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (80.95 mL, 1.0 M in THF, 80.95 mmol, 5.0 equiv) and stirred at room temperature for another 1 hour to afford **BO2** (eluent: eluent: petroleum ether ~ petroleum ether/dichloromethane = 5:1~ toluene) as a white solid 6.71 g in 80% yield. (Note: **BO2** has a very poor solubility, and toluene was used to dissolve all the product in the column chromatography.) 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. The obtained **BO2** was further purified by recrystallization in toluene/methanol; and then 3.4 g **BO2** was sublimated in a seven zone thermal gradient sublimator at 40/100/130/150/250/250/280 °C, 5.0×10⁻⁵ Torr to obtain white solid 3.0 g in 88% yield; purity, 99.68% by HPLC, HPLC analysis condition: column: Masiall® C18-BIO, 5μm, 250 × 4.6 mm; mobile phase: methanol/tetrahydrofuran = 95/5(v/v); flow rate: 1.0 mL/min; Abs. detector: 254 nm.



Synthesis of **BO3a**:

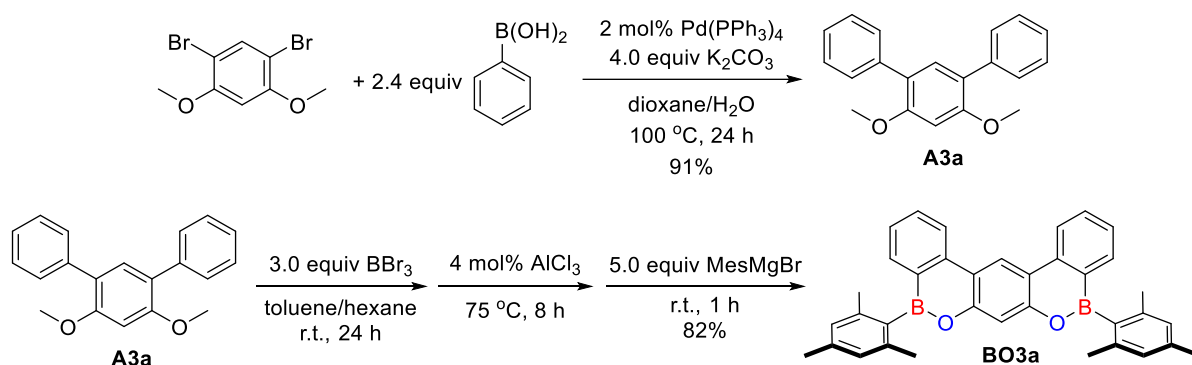


Synthesis of **A3a**: Following the general procedure, the reaction of 1,5-dibromo-2,4-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), boronic acid (1.17 g, 9.60 mmol, 2.4 equiv), $\text{Pd(PPh}_3)_4$ (92 mg, 0.08 mmol, 0.02 equiv) and K_2CO_3 (2.21 g, 16.00 mmol, 4.0 equiv, in 10 mL H_2O) in dioxane (40 mL) at 100 °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, $J = 7.5$ Hz, 4H), 7.55 (d, $J = 7.5$ 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.* **50**, 458–462 (2011).

Synthesis of **BO3a**: Following the general procedure, BBr_3 (0.87 mL, $d = 2.6$ 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 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 **BO3a** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.30 g in 84% yield. m.p.: 235.5–236.2 °C. ¹H NMR (500 MHz, DMSO-*d*₆): δ (ppm) 2.13 (s, 12H), 2.32 (s, 6H), 6.93 (s, 4H), 7.57 (t, *J* = 7.5 Hz, 2H), 7.67 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.76 (s, 1H), 7.97 (td, *J* = 7.5, 1.5 Hz, 2H), 9.02 (d, *J* = 8.0 Hz, 2H), 9.58 (s, 1H). ¹³C NMR (125 MHz, CDCl₃): 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. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 47.36. HRMS (ESI): calcd for C₃₆H₃₃[¹¹B]₂O₂⁺ [M+H]⁺ 519.2661, found 519.2671.

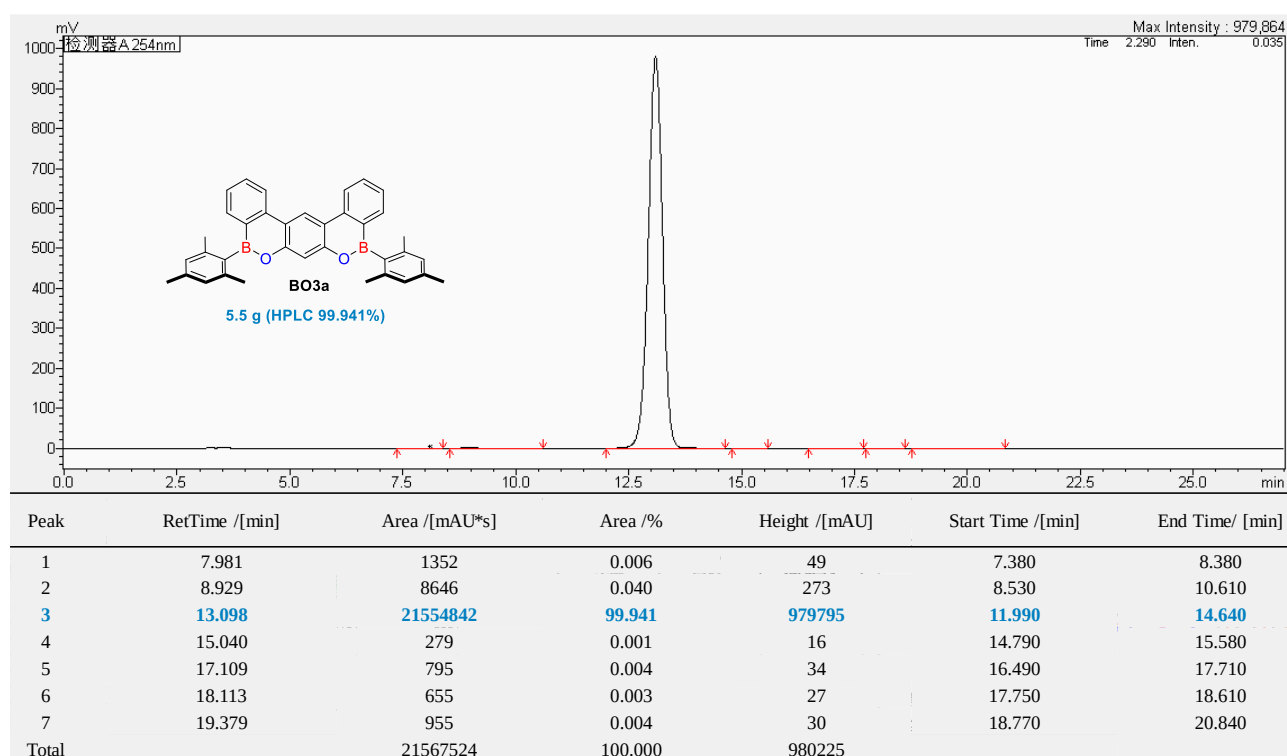
Large scale synthesis of **BO3a**:



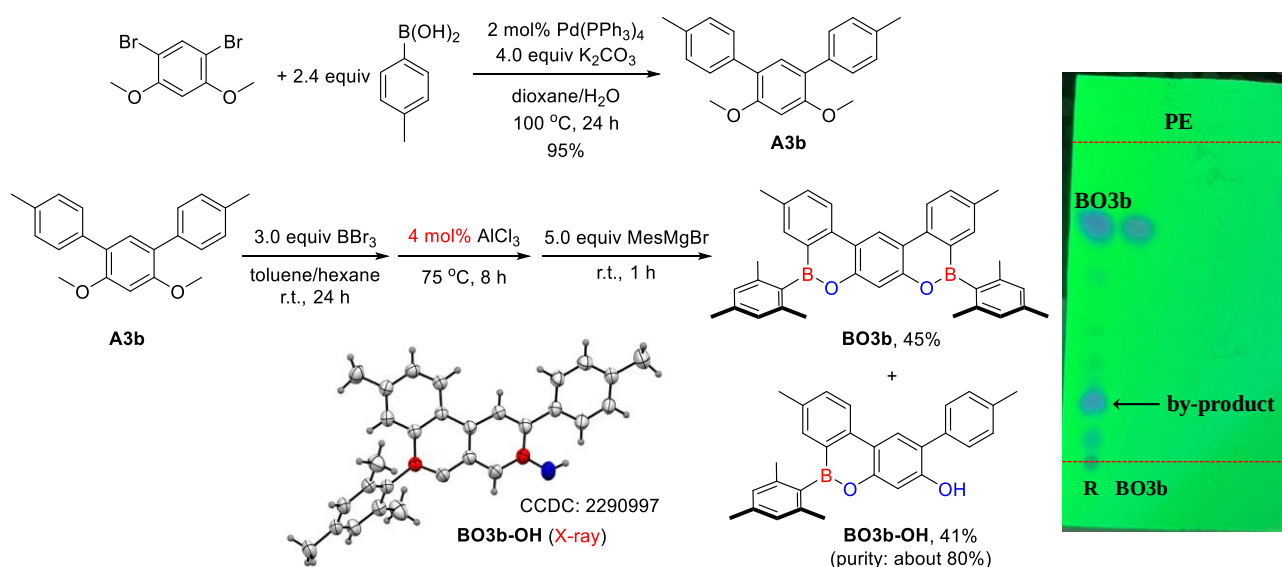
Synthesis of A3a: Following the general procedure, the reaction of 1,5-dibromo-2,4-dimethoxybenzene (8.88 g, 30.00 mmol, 1.0 equiv), boronic acid (8.78 g, 72 mmol, 2.4 equiv), Pd(PPh₃)₄ (693 mg, 0.60 mmol, 0.02 equiv) and K₂CO₃ (16.58 g, 120.00 mmol, 4.0 equiv, in 20 mL H₂O) in dioxane (80 mL) at 100 °C for 24 hours afforded **A3a** (eluent: petroleum ether/ethyl acetate = 20:1–10:1) as a white solid 7.93 g in 91% yield. The structure was confirmed by ¹H NMR, which was in agreement with the above result.

Synthesis of BO3a: Following the general procedure, BBr₃ (7.47 mL, d = 2.6 g/mL, 77.49 mmol, 3.0 equiv) was added dropwise to a mixture of **A3a** (7.50 g, 25.83 mmol, 1.0 equiv) in toluene (100 mL) and *n*-hexane (100 mL) and stirred at room temperature for 24 hours, added AlCl₃ (137 mg, 1.03 mmol, 0.04 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (129.15 mL, 1.0 M in THF, 129.15 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 10.98 g in 82% yield. The structure was confirmed by ^1H NMR, which was in agreement with the above result. The obtained **BO3a** was further purified by recrystallization in toluene/methanol; and then 6.1 g **BO3a** was sublimated in a seven zone thermal gradient sublimator at 40/100/130/150/250/250/280 °C, 5.6×10^{-5} Torr to obtain white solid 5.5 g in 90% yield; purity, 99.94% by HPLC, HPLC analysis condition: column: Masiall® C18-BIO, 5 μm , 250 $\times$ 4.6 mm; mobile phase: methanol/tetrahydrofuran = 95/5(v/v); flow rate: 1.0 mL/min; Abs. detector: 254 nm.



Synthesis of **BO3b**:

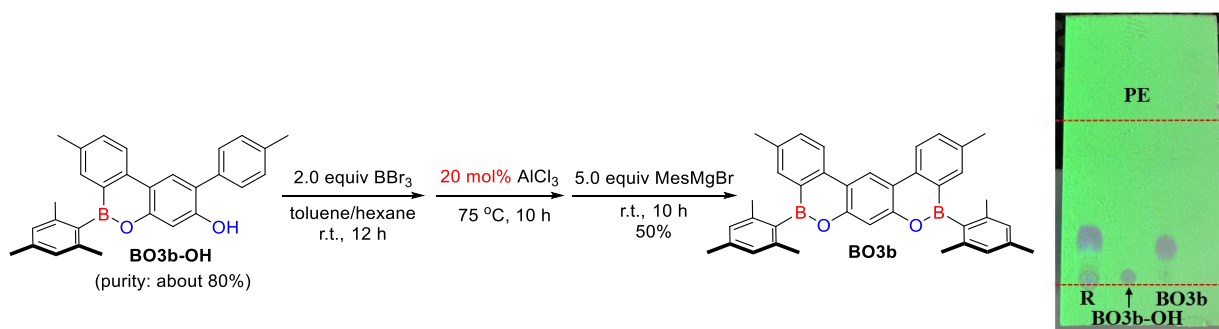


Synthesis of **A3b**: Following the general procedure, the reaction of 1,5-dibromo-2,4-

dimethoxybenzene (4.44 g, 15.00 mmol, 1.0 equiv), 4-methylboronic acid (4.89 g, 36.00 mmol, 2.4 equiv), Pd(PPh₃)₄ (347 mg, 0.30 mmol, 0.02 equiv) and K₂CO₃ (8.29 g, 60.00 mmol, 4.0 equiv, in 15 mL H₂O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A3b** (eluent: petroleum ether/ethyl acetate = 20:1–10:1) as a white solid 4.52 g in 95% yield. ¹H NMR (500 MHz, CDCl₃): 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). ¹³C NMR (125 MHz, CDCl₃): 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, BBr₃ (4.10 mL, *d* = 2.6 g/mL, 42.60 mmol, 3.0 equiv) was added dropwise to a mixture of **A3b** (4.52 g, 14.20 mmol, 1.0 equiv) in toluene (50 mL) and *n*-hexane (50 mL) and stirred at room temperature for 24 hours, added AlCl₃ (76 mg, 0.57 mmol, 0.04 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (71 mL, 1.0 M in THF, 71 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 3.52 g in 45% yield; and a by-product **BO3b-OH** as a white solid 3.22 g in 41% yield, which was not very pure, the purity was about 80% on the basis of ¹H NMR spectrum. **BO3b**: m.p.: 243.2–244.0 °C. ¹H NMR (500 MHz, CDCl₃): 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). ¹³C NMR (125 MHz, CDCl₃): 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. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 46.36. HRMS (ESI): calcd for C₃₈H₃₇[¹¹B]₂O₂⁺ [M+H]⁺ 547.2974, found 547.2990. **BO3b-OH**: ¹H NMR (500 MHz, DMSO-*d*₆) δ 2.09 (s, 6H), 2.31 (s, 3H), 2.32 (s, 3H), 2.37 (s, 3H), 6.90 (s, 2H), 7.07 (s, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.37 (s, 1H), 7.54–7.57 (m, 2H), 7.61 (dd, *J* = 8.0, 2.0 Hz, 1H), 8.22 (s, 1H), 8.33 (d, *J* = 8.5 Hz, 1H), 10.17 (s, 1H). HRMS (ESI): calcd for C₂₉H₂₈¹¹BO₂⁺ [M+H]⁺ 419.2177, found 419.2172.

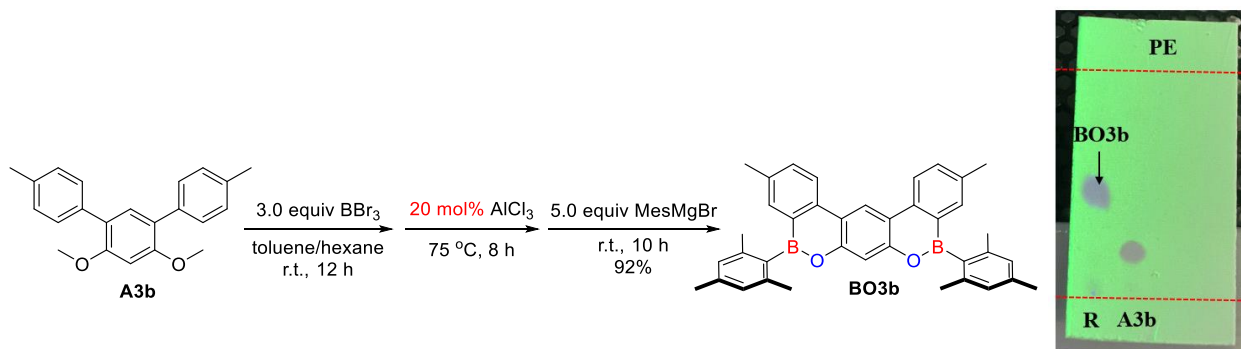
Synthesis of BO3b from BO3b-OH:



Synthesis of BO3b: Following the general procedure, BBr₃ (0.19 mL, *d* = 2.6 g/mL, 2.0 mmol, 2.0 equiv) was added dropwise to a mixture of **BO3b-OH** (418 mg, 1.0 mmol, 1.0 equiv) in toluene (5 mL) and *n*-hexane (5 mL) and the mixture was stirred at room temperature for 12 hours, then AlCl₃ (26 mg, 0.20 mmol, 0.2 equiv) was added and the mixture was stirred at 75 °C for 10 hours, cooled down to room temperature; then MesMgBr (5 mL, 1.0 M in THF, 5.00 mmol, 5.0 equiv) was added

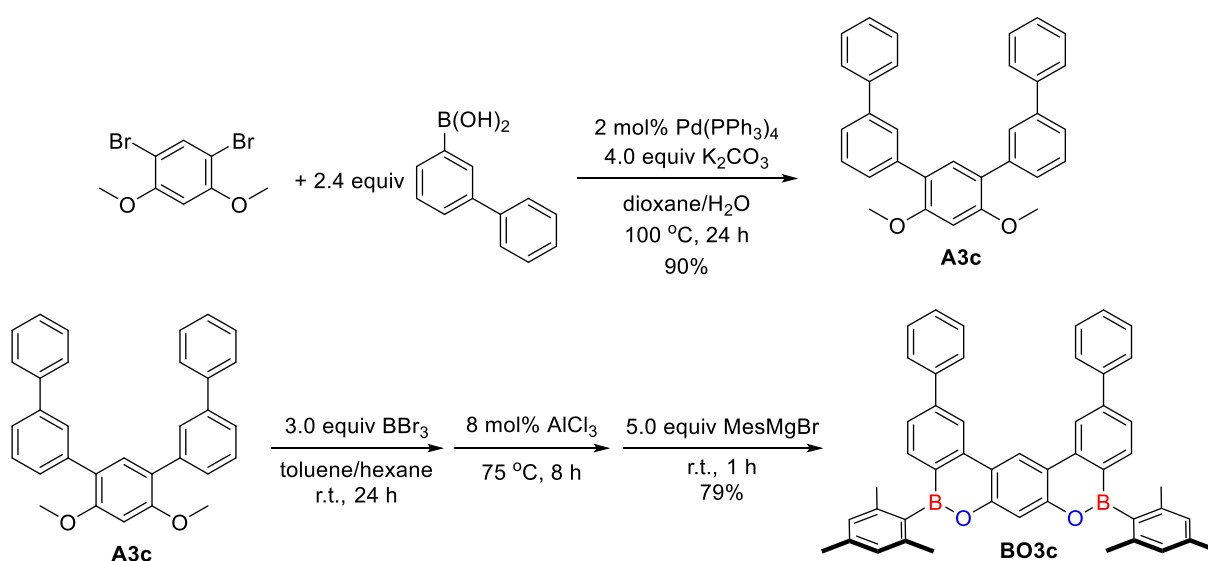
and the mixture was stirred at room temperature for another 10 hour to afford **BO3b** (eluent: petroleum ether ~ petroleum ether/dichloromethane = 100:1–10:1) as a white solid 273 mg in 50% yield. The structure was confirmed by ^1H NMR, which was in agreement with the above result.

Improved synthesis of **BO3b**:



Synthesis of **BO3b:** Following the general procedure, BBr_3 (0.91 mL, $d = 2.6 \text{ g/mL}$, 9.42 mmol, 3.0 equiv) was added dropwise to a mixture of **A3b** (1.00 g, 3.14 mmol, 1.0 equiv) in toluene (10 mL) and *n*-hexane (10 mL) and the mixture was stirred at room temperature for 12 hours; then AlCl_3 (84 mg, 0.63 mmol, 0.20 equiv) was added and the mixture was stirred at 75 °C for 8 hours, cooled down to room temperature; MesMgBr (15.7 mL, 1.0 M in THF, 15.70 mmol, 5.0 equiv) was added and the mixture was stirred at room temperature for another 10 hour to afford **BO3b** (eluent: petroleum ether ~ petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.59 g in 92% yield. The structure was confirmed by ^1H NMR, which was in agreement with the above result.

Synthesis of **BO3c**:

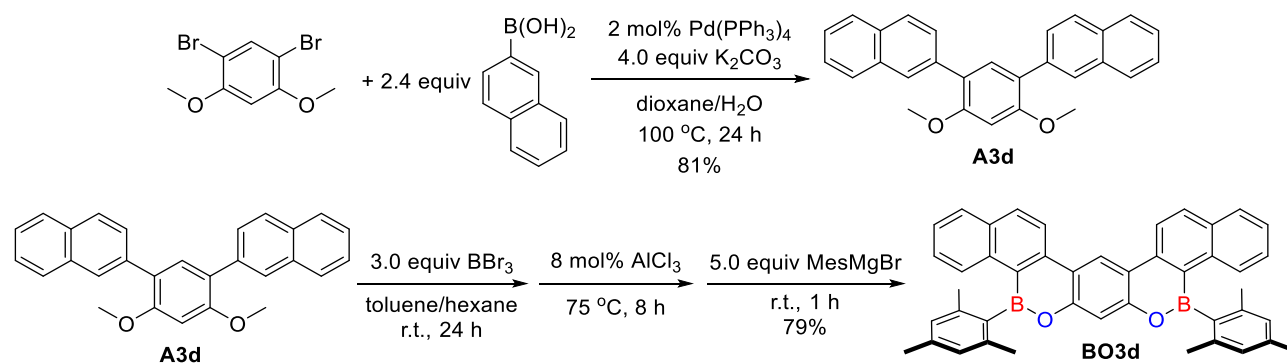


Synthesis of **A3c:** Following the general procedure, the reaction of 1,5-dibromo-2,4-

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. m.p.: 220.9–221.2 °C. 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 BO3d:

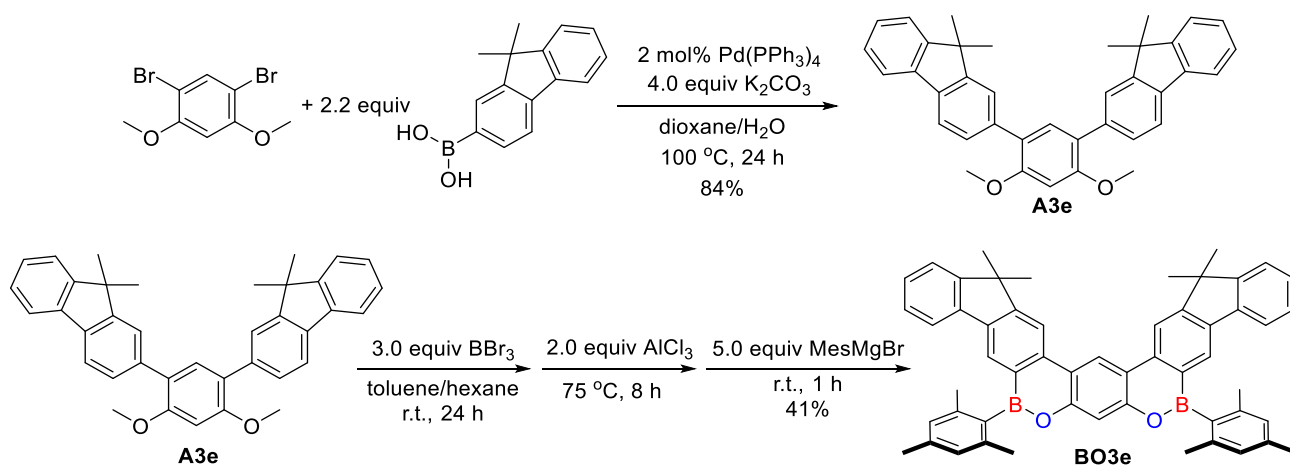


Synthesis of A3d: Following the general procedure, the reaction of 1,5-dibromo-2,4-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), naphthalen-2-ylboronic acid (1.65 g, 9.60 mmol, 2.4 equiv), Pd(PPh₃)₄ (92 mg, 0.08 mmol, 0.02 equiv) and K₂CO₃ (2.21 g, 16.00 mmol, 4.0 equiv, in 20 mL H₂O) in dioxane (60 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, CDCl_3): 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). ^{13}C NMR (125 MHz, CDCl_3): 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, BBr_3 (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 AlCl_3 (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, CDCl_3): 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). ^{13}C NMR (125 MHz, CDCl_3): 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. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 45.48. HRMS (ESI): calcd for $\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{NaO}_2^+ [\text{M}+\text{Na}]^+$ 641.2794, found 641.2783.

Synthesis of **BO3e**:

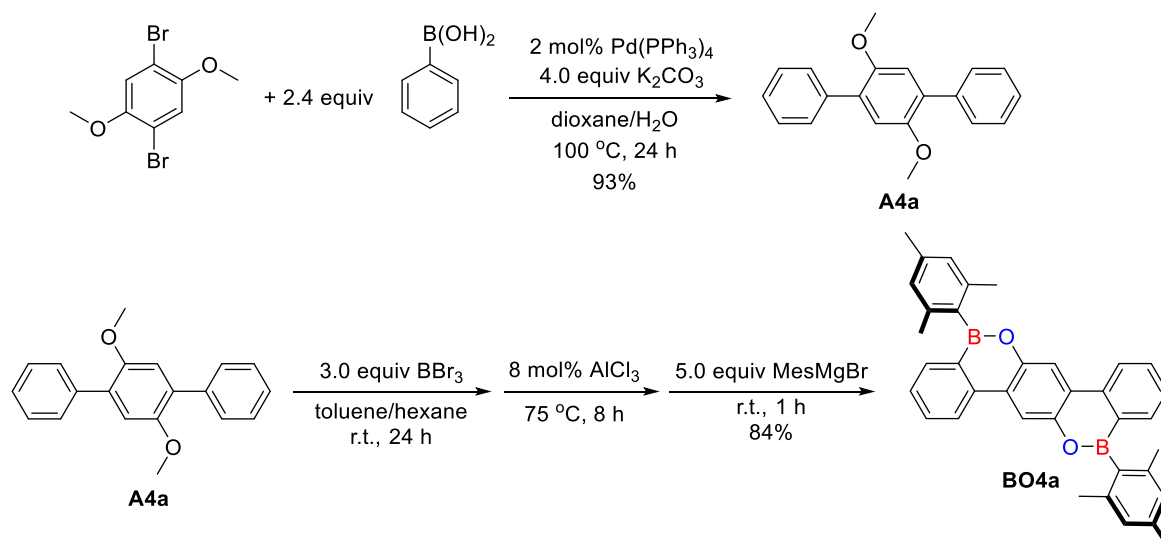


Synthesis of **A3e:** Following the general procedure, the reaction of 1,5-dibromo-2,4-dimethoxybenzene (1.26 g, 4.26 mmol, 1.0 equiv), (9,9-dimethyl-9H-fluoren-2-yl) boronic acid (2.23 g, 9.37 mmol, 2.2 equiv), $\text{Pd}(\text{PPh}_3)_4$ (100 mg, 0.087 mmol, 0.02 equiv) and K_2CO_3 (2.35 g, 17.03 mmol, 4.0 equiv, in 20 mL H_2O) 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, CDCl_3): 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). ^{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 $\text{C}_{38}\text{H}_{35}\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 523.2632, found 523.2644.

Synthesis of **BO3e:** 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 **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 AlCl_3 (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, CDCl_3): 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). ^{13}C NMR (125 MHz, CDCl_3): 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. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 45.52. HRMS (ESI): calcd for $\text{C}_{54}\text{H}_{48}[^{11}\text{B}]_2\text{NaO}_2^+$ $[\text{M}+\text{Na}]^+$ 773.3733, found 773.3720.

Synthesis of **BO4a**:

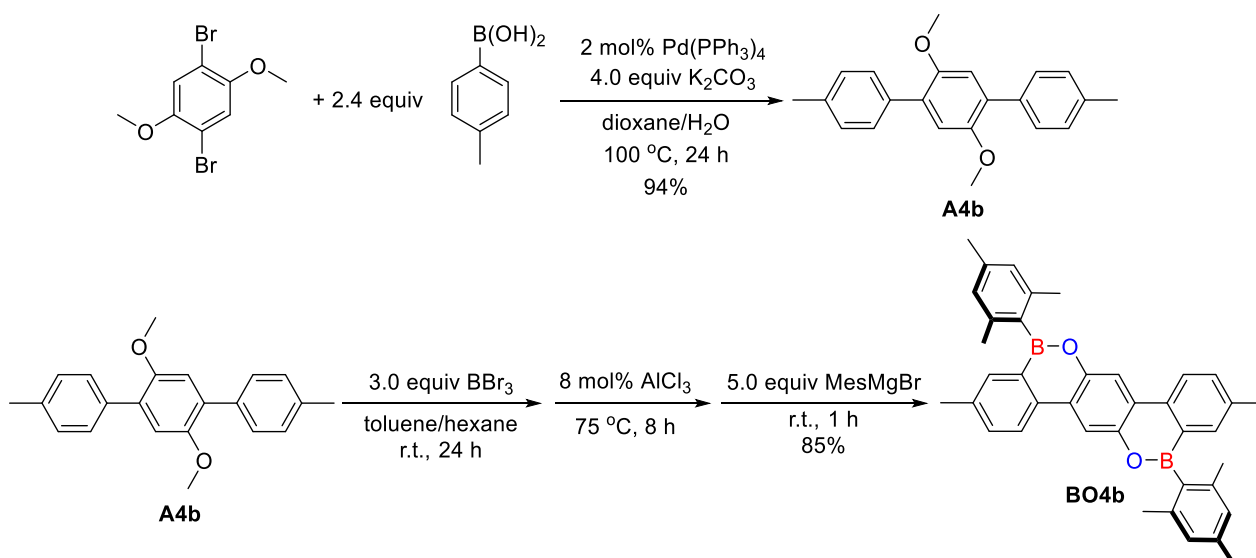


Synthesis of **A4a:** Following the general procedure, the reaction of 1,4-dibromo-2,5-dimethoxybenzene (2.37 g, 8.00 mmol, 1.0 equiv), boronic acid (2.34 g, 19.20 mmol, 2.4 equiv), $\text{Pd}(\text{PPh}_3)_4$ (185 mg, 0.16 mmol, 0.02 equiv) and K_2CO_3 (4.42 g, 32.00 mmol, 4.0 equiv, in 20 mL H_2O)

in dioxane (80 mL) at 100 °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, DMSO-*d*₆): δ (ppm) 3.76 (s, 6H), 7.03 (s, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 4H), 7.56 (d, *J* = 8.0, 4H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 56.35, 114.73, 127.07, 128.05, 129.41, 130.36, 138.28, 150.59. The ¹³C NMR is in agreement with the previous report (Bolligera, J. L., Frech, C. M. Polyaromatic the 1,3-diaminobenzene-derived aminophosphine palladium pincer complex {C₆H₃ACHTUNG TRENUNG[NHP(piperidiny)]₂Pd(Cl)}—a highly active Suzuki–Miyaura catalyst with excellent functional group tolerance. *Adv. Synth. Catal.* **352**, 1075–1080 (2010).

Synthesis of BO4a: 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 **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 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 **BO4a** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.74 g in 84% yield. m.p.: >350 °C. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.24 (s, 12H), 2.39 (s, 6H), 6.96 (s, 4H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.81–7.84 (m, 4H), 8.34 (d, *J* = 8.0 Hz, 2H), 8.45 (s, 2H). ¹³C NMR (125 MHz, CDCl₃): 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. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 44.68. HRMS (ESI): calcd for C₃₆H₃₃[¹¹B]₂O₂⁺ [M+H]⁺ 519.2661, found 519.2672.

Synthesis of **BO4b**:

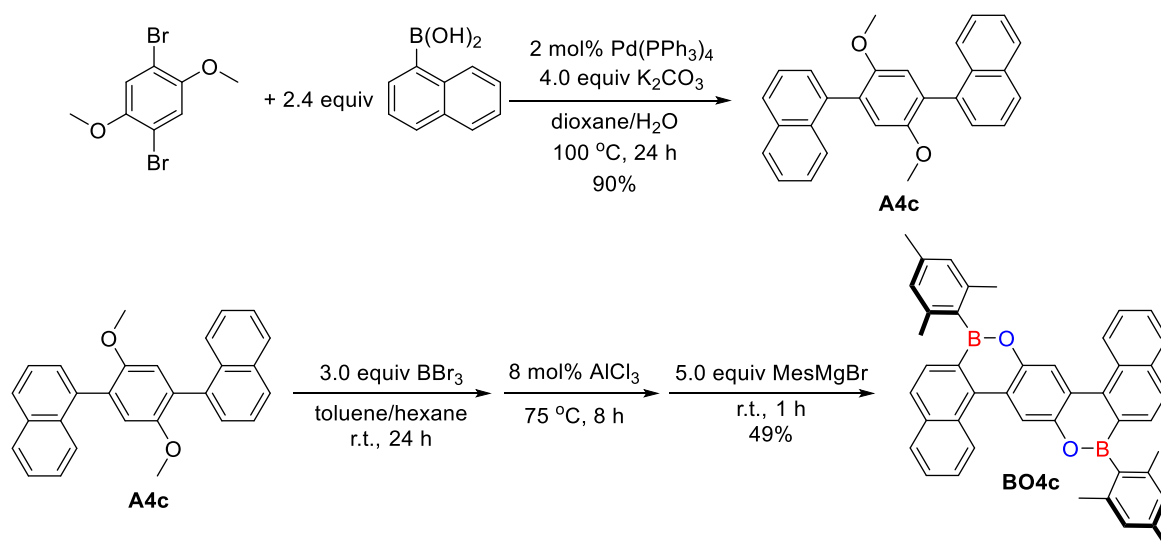


Synthesis of A4b: Following the general procedure, the reaction of 1,4-dibromo-2,5-dimethoxybenzene (2.37 g, 8.00 mmol, 1.0 equiv), 4-methylboronic acid (2.61 g, 19.20 mmol, 2.4

equiv), Pd(PPh₃)₄ (185 mg, 0.16 mmol, 0.02 equiv) and K₂CO₃ (4.42 g, 32.00 mmol, 4.0 equiv, in 20 mL H₂O) in dioxane (80 mL) at 100 °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, DMSO-*d*₆): δ (ppm) 2.35 (s, 6H), 3.74 (s, 6H), 6.98 (s, 2H), 7.23 (d, *J* = 8.0 Hz, 4H), 7.45 (d, *J* = 8.0 Hz, 4H). ¹³C NMR (125 MHz, CDCl₃): 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, BBr₃ (1.16 mL, *d* = 2.6 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 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 **BO4b** (eluent: petroleum ether/dichloromethane = 100:1–10:1) as a white solid 1.86 g in 85% yield. ¹H NMR (500 MHz, CDCl₃): 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 Hz, 2H), 8.38 (s, 2H). ¹³C NMR (125 MHz, CDCl₃): 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. ¹¹B NMR (160 MHz, CDCl₃): δ (ppm) 46.97. HRMS (ESI): calcd for C₃₈H₃₇[¹¹B]₂O₂⁺ [M+H]⁺ 547.2974, found 547.2992.

Synthesis of **BO4c**:

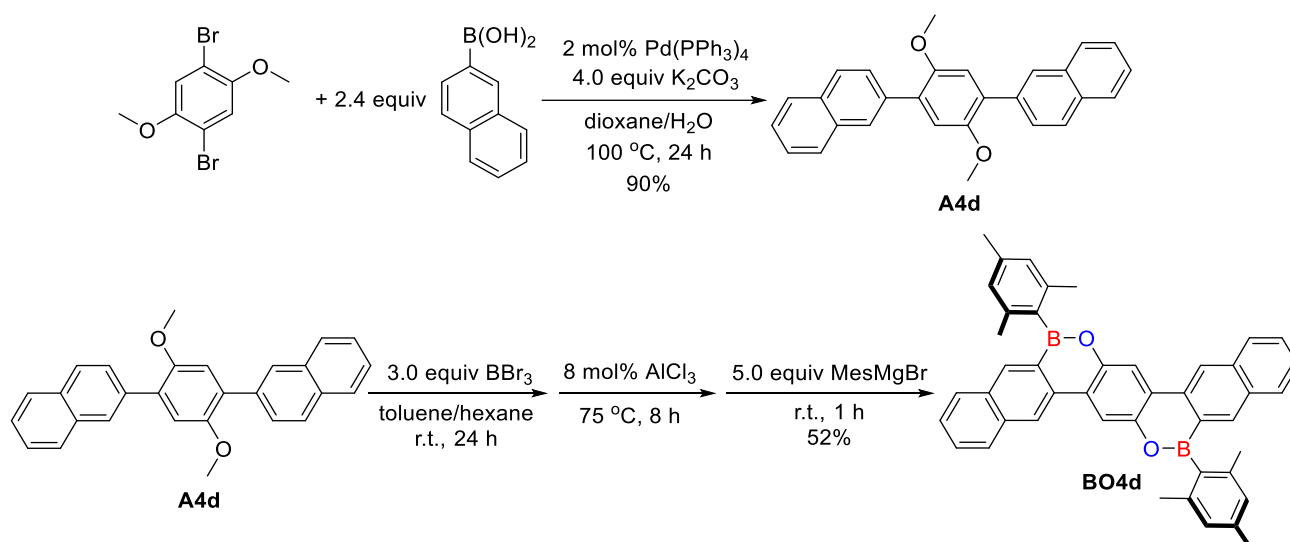


Synthesis of **A4c**: Following the general procedure, the reaction of 1,4-dibromo-2,5-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), naphthalen-1-ylboronic acid (1.66 g, 9.60 mmol, 2.4 equiv), Pd(PPh₃)₄ (92 mg, 0.08 mmol, 0.02 equiv) and K₂CO₃ (2.21 g, 16.00 mmol, 4.0 equiv, in 20 mL H₂O) in dioxane (60 mL) at 100 °C for 24 hours afforded **A4c** (eluent: petroleum ether/ethyl acetate = 10:1–3:1) as a white solid 1.41 g in 90% yield. ¹H NMR (500 MHz, CDCl₃): 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 BO4d:

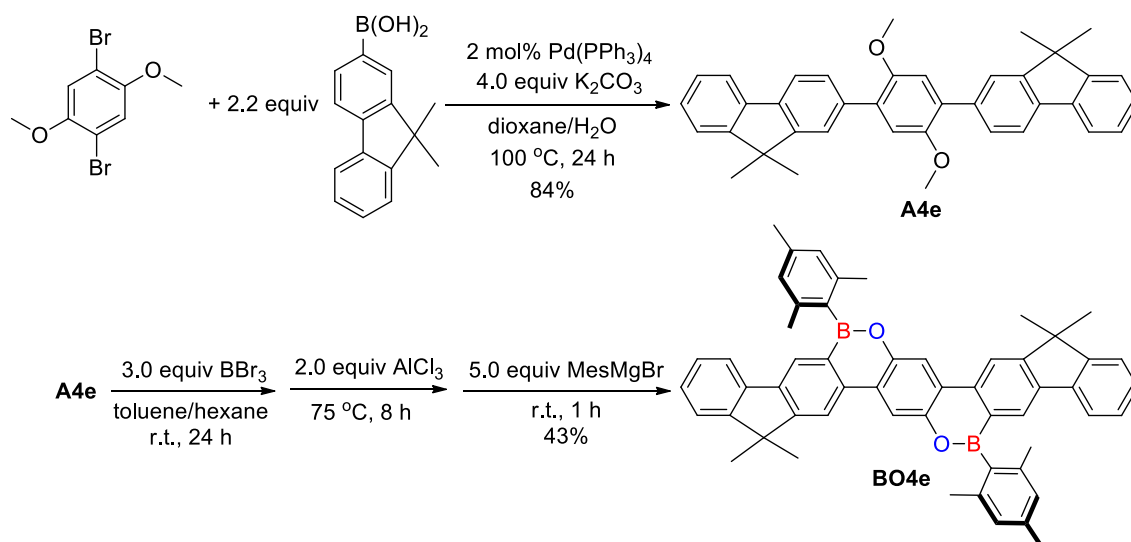


Synthesis of A4d: Following the general procedure, the reaction of 1,4-dibromo-2,5-dimethoxybenzene (1.18 g, 4.00 mmol, 1.0 equiv), naphthalen-2-ylboronic acid (1.65 g, 9.60 mmol, 2.4 equiv), $\text{Pd}(\text{PPh}_3)_4$ (92 mg, 0.08 mmol, 0.02 equiv) and K_2CO_3 (2.21 g, 16.00 mmol, 4.0 equiv, in 20 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 $\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{O}_2^- [\text{M}]^-$ 618.2907, found 618.2988.

Synthesis of BO4e:

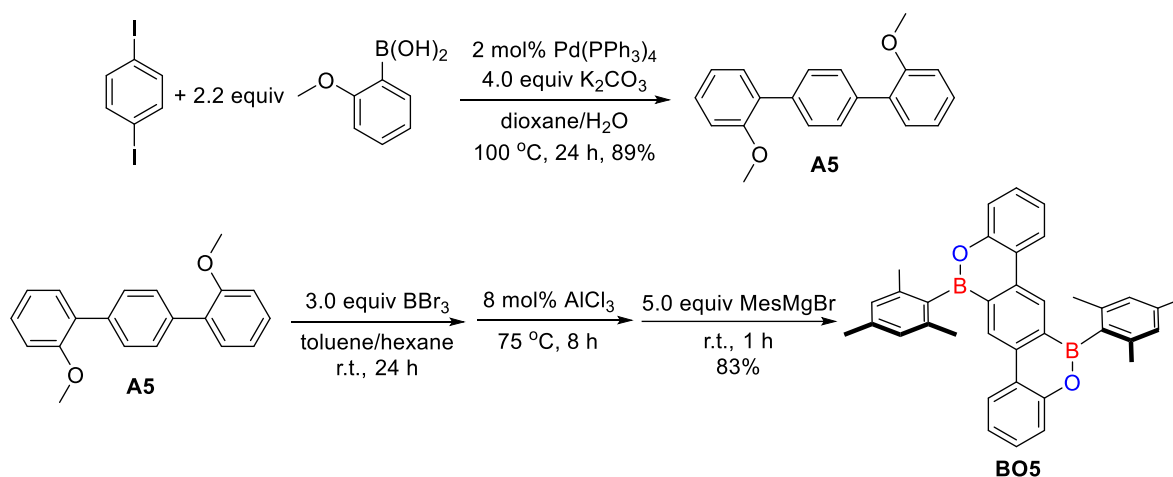


Synthesis of A4e: Following the general procedure, the reaction of 1,4-dibromo-2,5-dimethoxybenzene (1.26 g, 4.26 mmol, 1.0 equiv), (9,9-dimethyl-9H-fluoren-2-yl) boronic acid (2.23 g, 9.37 mmol, 2.2 equiv), $\text{Pd}(\text{PPh}_3)_4$ (98 mg, 0.085 mmol, 0.02 equiv) and K_2CO_3 (2.36 g, 17.04 mmol, 4.0 equiv, in 20 mL H_2O) 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, CDCl_3): 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). ^{13}C NMR (125 MHz, CDCl_3): 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 $\text{C}_{38}\text{H}_{38}\text{NO}_2^+ [\text{M}+\text{NH}_4]^+$ 540.2897, found 540.2910.

Synthesis of **BO4e:** 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 **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 AlCl_3 (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, CDCl_3): 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). ^{13}C NMR (125 MHz, CDCl_3): 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. ^{11}B NMR (160 MHz, CDCl_3): δ (ppm) 45.87. HRMS (ESI): calcd for $\text{C}_{54}\text{H}_{48}[\text{B}]_2\text{NaO}_2 [\text{M}+\text{Na}]^+$ 773.3733, found 773.3712.

Synthesis of **BO5**:

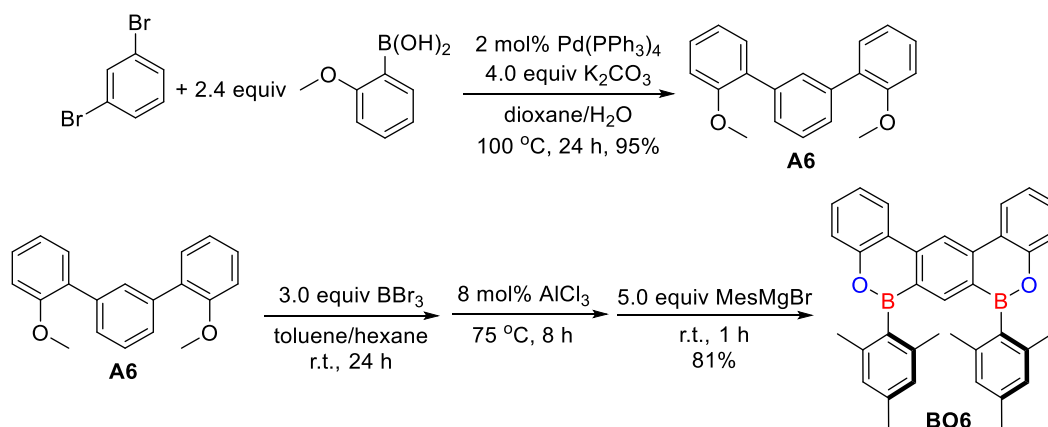


Synthesis of **A5:** Following the general procedure, the reaction of 1,4-diiodobenzene (6.60 g, 20.00 mmol, 1.0 equiv), 2-methoxyphenylboronic acid (6.69 g, 44.00 mmol, 2.2 equiv), $\text{Pd}(\text{PPh}_3)_4$ (462 mg, 0.40 mmol, 0.02 equiv) and K_2CO_3 (11.06 g, 80.00 mmol, 4.0 equiv, in 30 mL H_2O) in dioxane (120 mL) at 100 °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, $d = 2.6$ 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 °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.: 320.1–322.5 °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, 110.57, 122.86, 123.63, 123.83, 127.56, 129.20, 130.60, 133.15, 136.53, 138.56, 140.26, 151.53. ^{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.

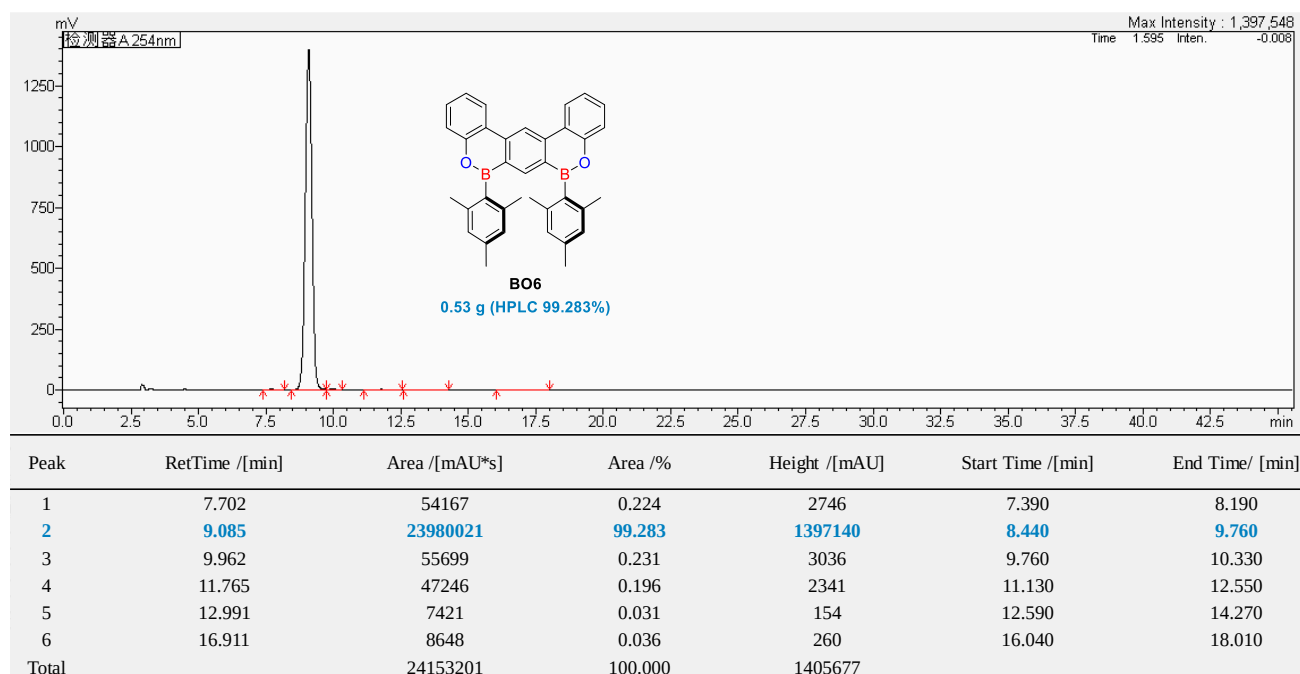
Synthesis of BO6:



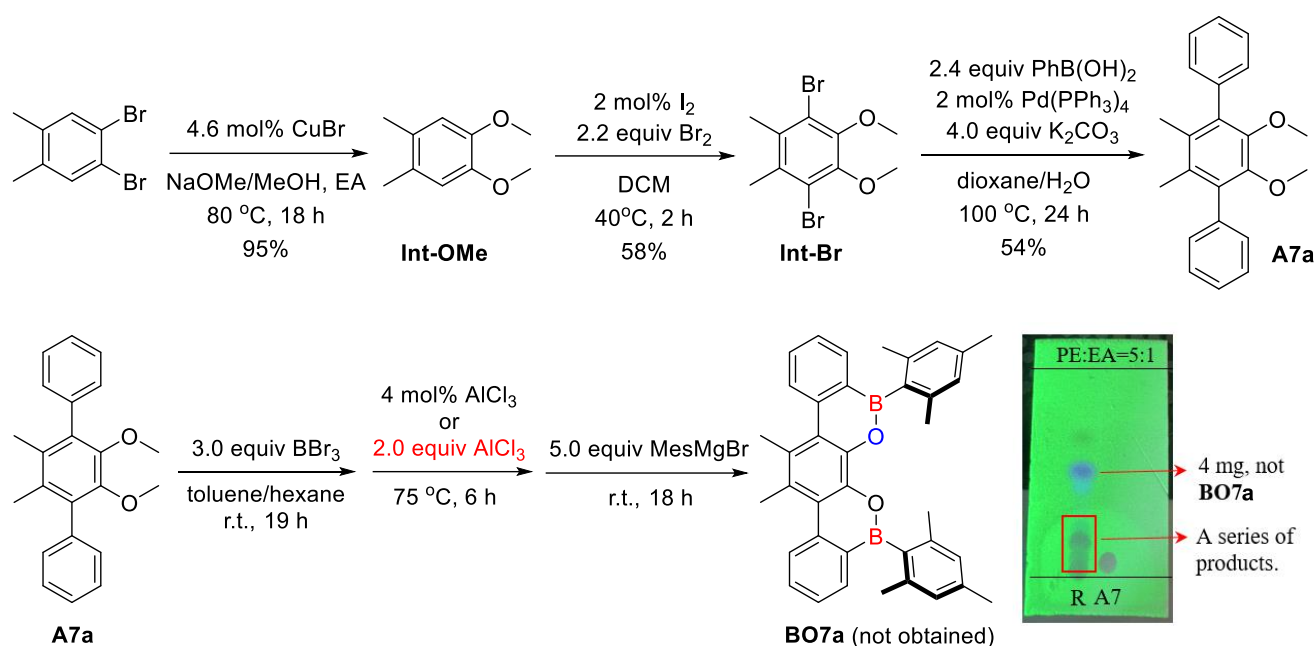
Synthesis of A6: Following the general procedure, the reaction of 1,3-dibromobenzene (1.18 g, 5.00 mmol, 1.0 equiv), 2-methoxyphenylboronic acid (1.82 g, 12.00 mmol, 2.4 equiv), $\text{Pd}(\text{PPh}_3)_4$ (116 mg, 0.10 mmol, 0.02 equiv) and K_2CO_3 (2.76 g, 20.00 mmol, 4.0 equiv, in 20 mL H_2O) in dioxane (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, CDCl_3): 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). ^{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 and ^{13}C 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.* 5600–5602 (2009).

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. The obtained **BO6** was further purified by recrystallization in toluene/methanol; and then 0.60 g **BO6** was sublimated in a seven zone thermal gradient sublimator at 130/150/160/200/240/240/260 °C, 5.0×10⁻⁵ Torr to obtain white solid 0.53 g in 88% yield; purity, 99.28% by HPLC, HPLC analysis condition: column: Masiall® C18-BIO, 5 μ m, 250 × 4.6 mm; mobile phase: methanol/tetrahydrofuran = 95/5(v/v); flow rate: 1.0 mL/min; Abs. detector: 254 nm.



Attempt for the synthesis of **BO7a**:



Synthesis of **Int-OMe**: 1,2-Dibromo-4,5-dimethylbenzene (10.0 g, 37.9 mmol, 1.0 equiv), CuBr (250 mg, 1.74 mmol, 4.6 mol%), NaOMe/MeOH (30 wt%, 300 mL), and ethyl acetate (3 mL) were added sequentially to a dry three-neck round-bottom flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. The deep-blue solution was then heated at 80 °C for 18 hours. The solution was cooled to room temperature, poured into H₂O (300 mL), and extracted with dichloromethane. The combined organic layers were dried with Na₂SO₄ and concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether–petroleum ether/acetic ether =10:1) to obtain the desired product as a white solid 6.0 g in 95% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.00 (s, 6H), 3.84 (s, 6H), 6.67 (s, 2H).

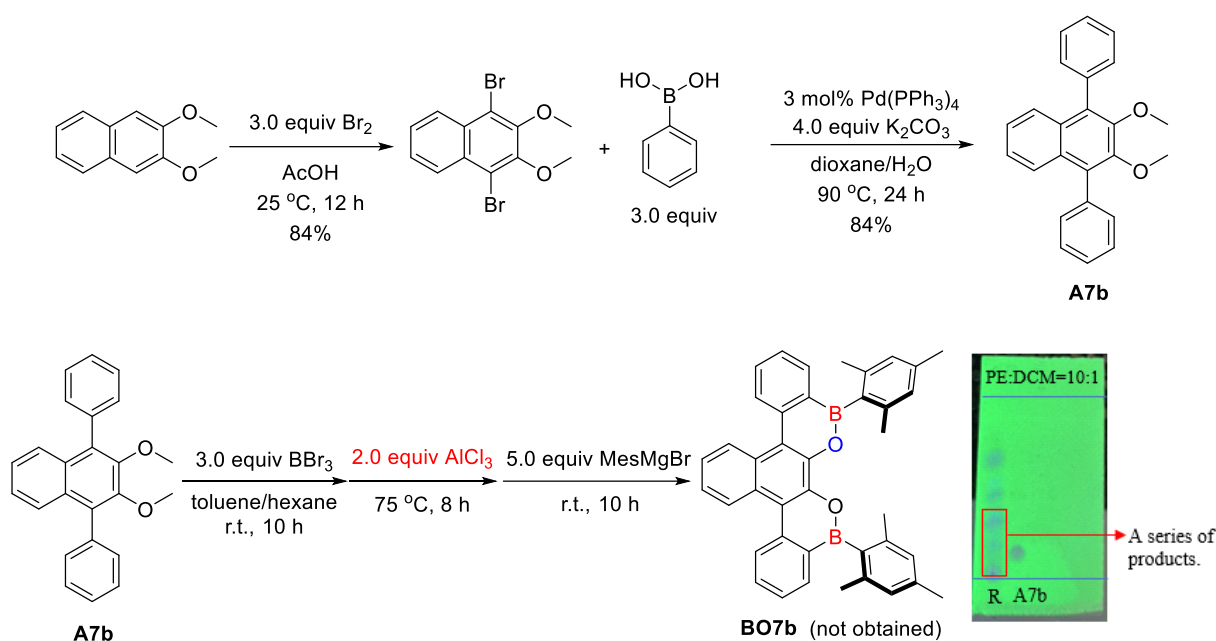
Synthesis of **Int-Br**: **Int-OMe** (4.90 g, 29.48 mmol, 1.0 equiv) was dissolved in 30 mL of dichloromethane. To this stirred solution was added I₂ (150 mg, 0.59 mmol, 0.02 equiv) followed by a slow dropwise addition of a solution of Br₂ (10.37 g, 64.86 mmol, 2.2 equiv) in 30 mL of dichloromethane. After the addition was completed, the resulting solution was heated to 40 °C for 2 hours. Upon cooling, 5M aq. NaOH (30 mL) was added to the reaction mixture. The filtrate was washed with water (30 mL), dried over anhydrous sodium sulfate, and concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether) to obtain the desired product as a white solid 5.54 g in 58% yield. ¹H NMR (500 MHz, CDCl₃): δ (ppm) 2.44 (s, 6H), 3.87 (s, 6H).

Synthesis of **A7a**: Following the general procedure, the reaction of **Int-Br** (5.00 g, 15.43 mmol, 1.0 equiv), phenylboronic acid (4.52 g, 37.03 mmol, 2.4 equiv), Pd(PPh₃)₄ (358 mg, 0.31 mmol, 0.02 equiv) and K₂CO₃ (8.53 g, 61.72 mmol, 4.0 equiv, in 10 mL H₂O) in dioxane (40 mL) at 100 °C for 24

hours afforded **A7a** (eluent: petroleum ether– petroleum ether/acetic ether =100:1) as a white solid 2.65 g in 54% yield. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 2.00 (s, 6H), 3.59 (s, 6H), 7.28–7.30(m, 4H), 7.35–7.38 (m, 2H), 7.44–7.46(m, 4H). ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) 17.55, 60.58, 126.76, 128.01, 129.79, 130.95, 136.20, 138.19, 148.40.

Synthesis of **BO7a**: Following the general procedure, BBr_3 (0.29 mL, $d = 2.6 \text{ g/mL}$, 3.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A7a** (318 mg, 1.00 mmol, 1.0 equiv) in toluene (5 mL) and *n*-hexane (5 mL) and stirred at room temperature for 19 hours, added AlCl_3 (5 mg, 0.04 mmol, 0.04 equiv) and stirred at 75 °C for 6 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 18 hours; TLC showed that the reaction was messy, no desired **BO7a** was isolated. We also tried to used more AlCl_3 (267 mg, 2.00 mmol, 2.0 equiv), but the products shown by TLC were similar.

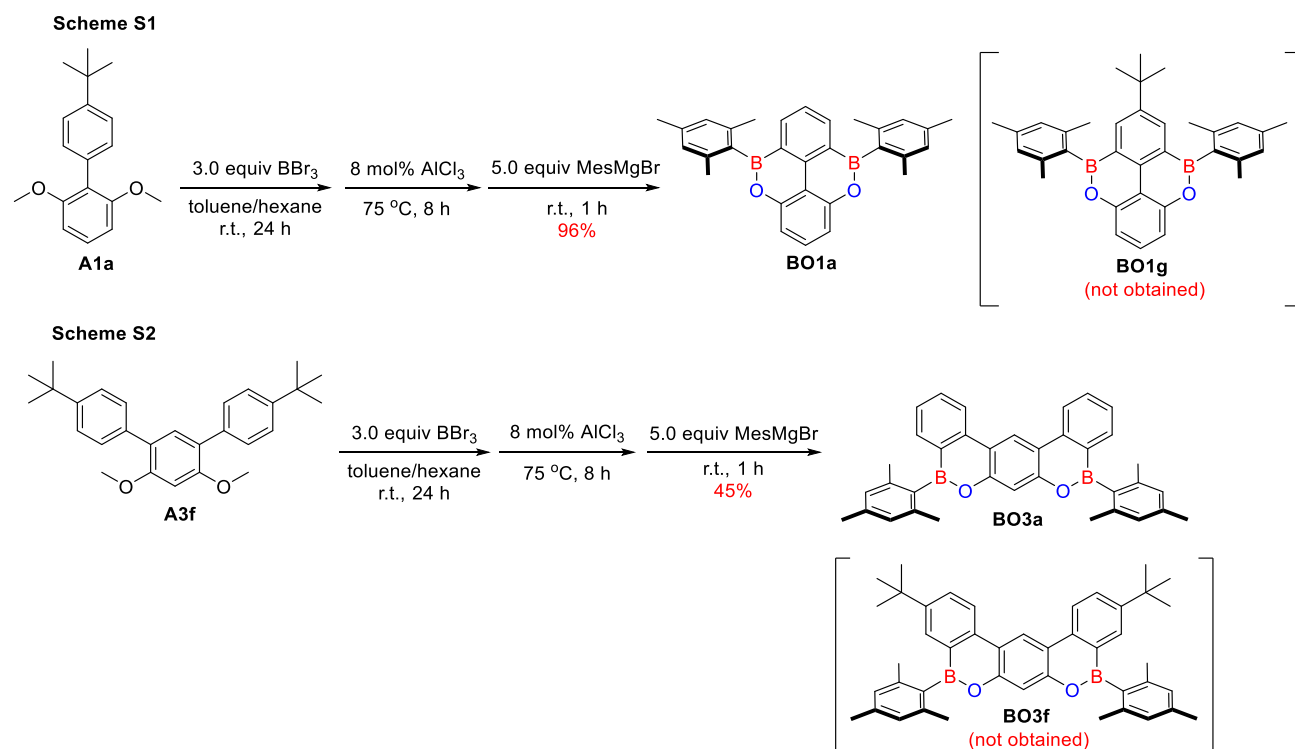
Attempt for the synthesis of **BO7b**:



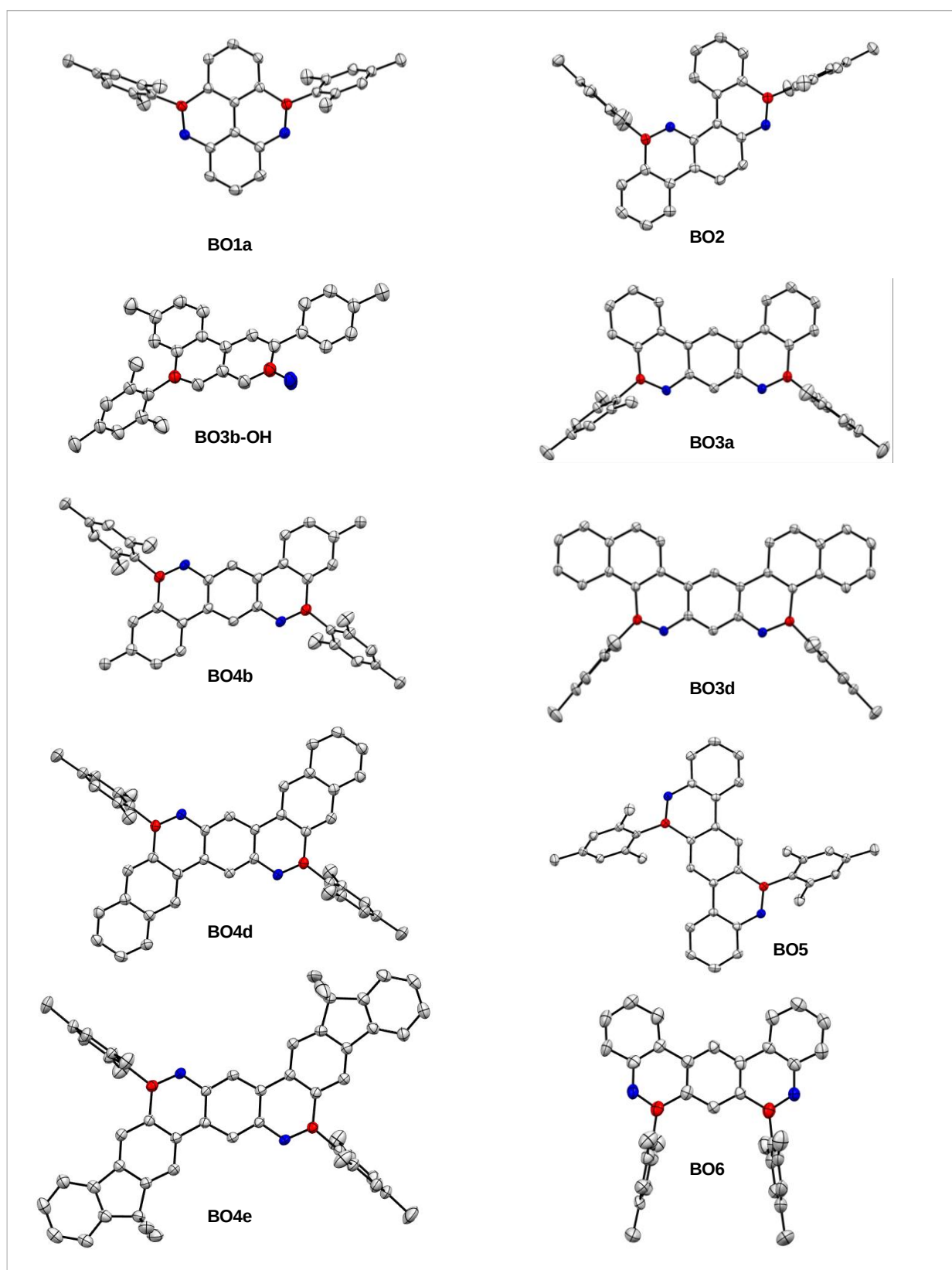
Synthesis of 1,4-dibromo-2,3-dimethoxynaphthalene: 2,3-dimethoxynaphthalene (8.17 g, 43.40 mmol, 1.0 equiv, in 500 mL AcOH) was added sequentially to a dry one-neck round-bottom flask and cooled to 0°C. To this stirred solution was added Br_2 (20.81 g, 130.20 mmol, 3.0 equiv), and the reaction was stirred at room temperature for 12 hours. The solution was poured into 5M aq. NaOH (150 mL) and extracted with acetic ether, and dried over anhydrous sodium sulfate, and concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether/dichloromethane = 50:1–30:1) to obtain the desired product as a white solid 12.60 g in 84% yield. ^1H NMR (500 MHz, CDCl_3): δ (ppm) 4.00 (s, 6H), 7.55–7.59 (m, 2H), 8.22–8.26 (m, 2H).

Synthesis of **A7b**: Following the general procedure, the reaction of 2,3-dimethoxynaphthalene (4.00 g, 11.60 mmol, 1.0 equiv), phenylboronic acid (4.24 g, 34.80 mmol, 3.0 equiv), Pd(PPh₃)₄ (402 mg, 0.35 mmol, 0.03 equiv) and K₂CO₃ (6.41 g, 46.40 mmol, 4.0 equiv, in 10 mL H₂O) in dioxane (40 mL) at 90 °C for 24 hours afforded **A7b** (eluent: petroleum ether– petroleum ether/ dichloromethane =20:1) as a white solid 3.3 g (impurity) in 84% yield. (1.5 g of crude product was further purified by sublimation to obtain **A7b** as a white solid 620 mg) ¹H NMR (500 MHz, CDCl₃): δ (ppm) 3.72 (s, 6H), 7.25–7.29 (m, 2H), 7.44–7.48 (m, 6H), 7.51–7.55 (m, 6H). ¹³C NMR (125 MHz, CDCl₃): δ (ppm) 61.07, 124.95, 125.92, 127.34, 128.21, 130.51, 130.59, 132.16, 136.17, 149.41.

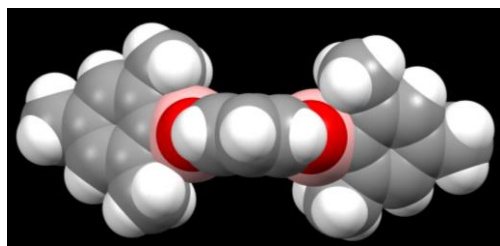
Synthesis of **BO7b**: Following the general procedure, BBr₃ (0.29 mL, d = 2.6 g/mL, 3.00 mmol, 3.0 equiv) was added dropwise to a mixture of **A7b** (340 mg, 1.00 mmol, 1.0 equiv) in toluene (5 mL) and *n*-hexane (5 mL) and stirred at room temperature for 10 hours, added AlCl₃ (267 mg, 2.00 mmol, 2.0 equiv) and stirred at 75 °C for 8 hours, cooled down to room temperature, added MesMgBr (5 mL, 1.0 M in THF, 5.00 mmol, 5.0 equiv) and stirred at room temperature for another 10 hours; TLC showed that the reaction was messy, no desired **BO7b** was isolated.



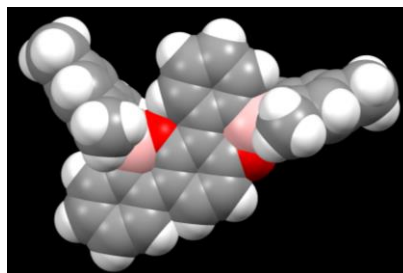
Supplementary Fig. 3. AlCl₃ induced de-*tert*-butylation reactions. The observed de-*tert*-butylation reactions catalyzed by AlCl₃



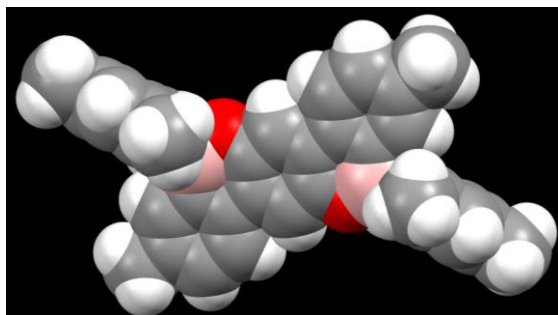
Supplementary Fig. 4. Single crystal diffraction structures of BO-PAHs. ORTEP drawing of X-ray single crystal diffraction structures of **BO1a**, **BO2**, **BO3a**, **BO3b-OH**, **BO3d**, **BO4b**, **BO4d**, **BO4e**, **BO5** and **BO6**. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 35% or 50% probability level.



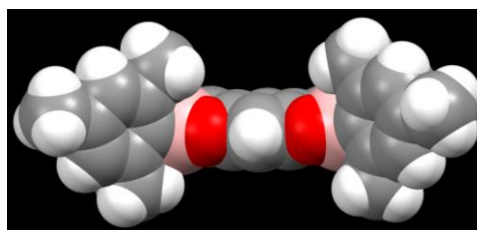
BO1a (top view)



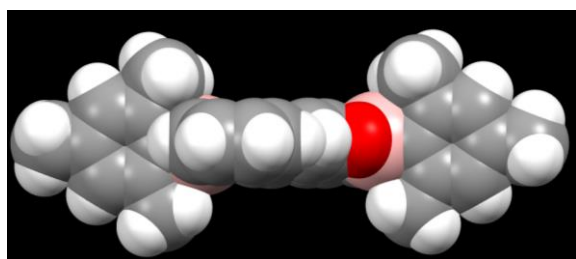
BO2 (front view)



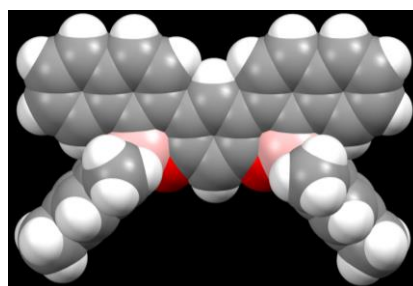
BO4b (front view)



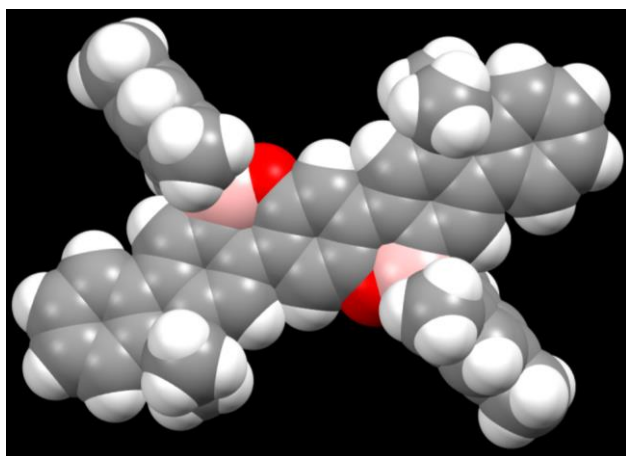
BO3a (bottom view)



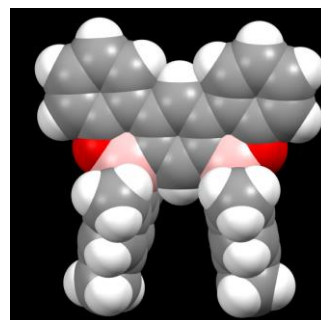
BO4d (top view)



BO3d (front view)



BO4e (front view)



BO6 (front view)

Supplementary Fig. 5. Spacefill drawing of X-ray single crystal diffraction structures of **BO1a**, **BO2**, **BO3a**, **BO3d**, **BO4b**, **BO4d**, **BO4e** and **BO6**. B, pink; O, red.

Supplementary Table 1. Crystal data and structure refinements for BO1a and BO2

Compound	BO1a	BO2
CCDC number	1954663	1954662
Empirical formula	C ₃₀ H ₂₈ B ₂ O ₂	C ₃₆ H ₃₂ B ₂ O ₂
Formula weight	442.14	518.23
Temperature (K)	293(2) K	193(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	monoclinic	orthorhombic
Space group	P 21/n	P 21 21 21
<i>a</i> (Å)	12.3732(4)	8.0150(3)
<i>b</i> (Å)	8.0799(3)	14.7515(6)
<i>c</i> (Å)	25.7096(10)	24.6982(8)
α (°)	90	90
β (°)	100.6030(10)	90
γ (°)	90	90
Volume (Å ³)	2526.41(16)	2920.15(19)
<i>Z</i>	4	4
<i>F</i> (000)	936	1096
Crystal size (mm ³)	0.200×0.150×0.120	0.200×0.160×0.130
θ (deg) for collection (°)	2.647 to 25.498	2.672 to 25.985
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
Reflections collected	23738	14696
Unique (<i>R</i> _{int})	4665 (0.0349)	5706 (0.0593)
Data / restraints / parameters	4665 / 0 / 314	5706 / 0 / 368
Goodness-of-fit on <i>F</i> ²	1.050	1.032
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> 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
Largest diff. peak and hole (Å ^{−3})	0.155/−0.125	0.201/−0.178

Supplementary Table 2. Crystal data and structure refinements for BO3a, BO3d and BO3b-OH

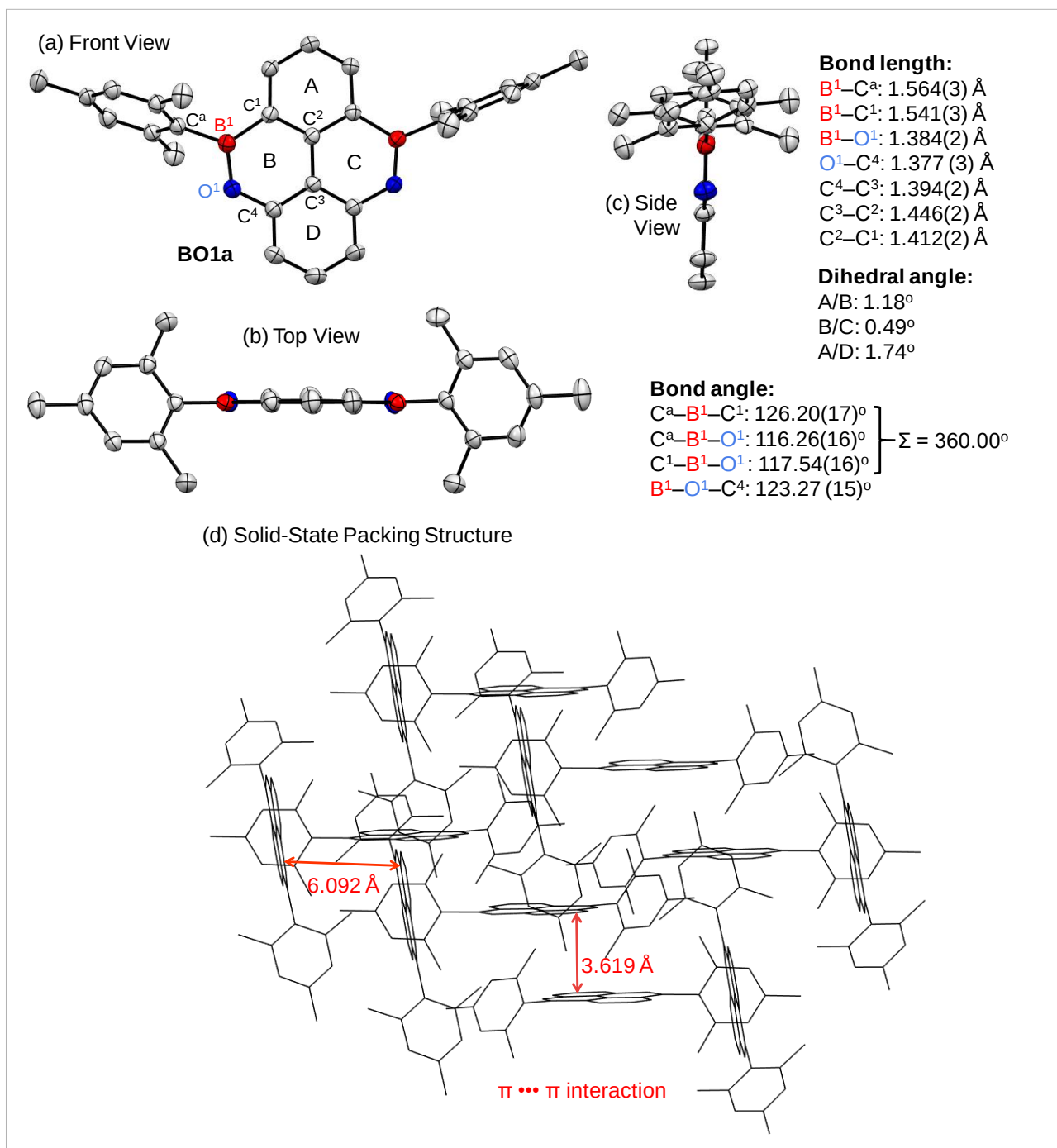
Compound	BO3a	BO3d	BO3b-OH
CCDC number	1954665	1954664	2290997
Empirical formula	C ₃₆ H ₃₂ B ₂ O ₂	C ₄₄ H ₃₆ B ₂ O ₂	C ₂₉ H ₂₇ BO ₂
Formula weight	518.23	618.35	418.31
Temperature (K)	293.04	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	monoclinic	monoclinic	monoclinic
Space group	C 2/c	C 2	P21/n
<i>a</i> (Å)	34.7317(9)	30.8251(8)	17.5960(5)
<i>b</i> (Å)	7.7855(2)	7.5638(2)	7.5552(2)
<i>c</i> (Å)	24.5964(6)	17.0835(4)	19.2892(5)
α (°)	90	90	90
β (°)	98.6690(10)	92.9740(10)	114.5900(10)
γ (°)	90	90	90
Volume (Å ³)	6575.0(3)	3977.74(17)	2331.77(11)
<i>Z</i>	8	4	4
<i>F</i> (000)	2192	1304	888.0
Crystal size (mm ³)	0.2×0.17×0.13	0.200×0.120×0.100	0.2 × 0.14 × 0.1
θ (deg) for collection (°)	2.784 to 25.996	2.388 to 25.499	4.448 to 66.996
Index ranges	$-42 \leq h \leq 42, -9 \leq k \leq 9, -30 \leq l \leq 30$	$-36 \leq h \leq 37, -9 \leq k \leq 9, -19 \leq l \leq 20$	$-19 \leq h \leq 21, -8 \leq k \leq 8, -22 \leq l \leq 23$
Reflections collected	37277	22620	19160
Unique (<i>R</i> _{int})	6409 (0.0409)	9027 (0.0355)	0.0735
Data / restraints / parameters	6409 / 0 / 368	9.27 / 1 / 439	4083 / 1 / 297
Goodness-of-fit on <i>F</i> ²	1.020	1.034	1.031
Final <i>R</i> indices [<i>I</i> >2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0509 w <i>R</i> ₂ = 0.1354	<i>R</i> ₁ = 0.0607 w <i>R</i> ₂ = 0.1635	<i>R</i> ₁ = 0.0718, w <i>R</i> ₂ = 0.2011
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0793 w <i>R</i> ₂ = 0.1561	<i>R</i> ₁ = 0.0928 w <i>R</i> ₂ = 0.1863	<i>R</i> ₁ = 0.0924, w <i>R</i> ₂ = 0.2241
Largest diff. peak and hole (Å ⁻³)	0.21/−0.14	0.25/−0.20	0.39/−0.24

Supplementary Table 3. Crystal data and structure refinements for BO4b, BO4d and BO4e·CH₂Cl₂

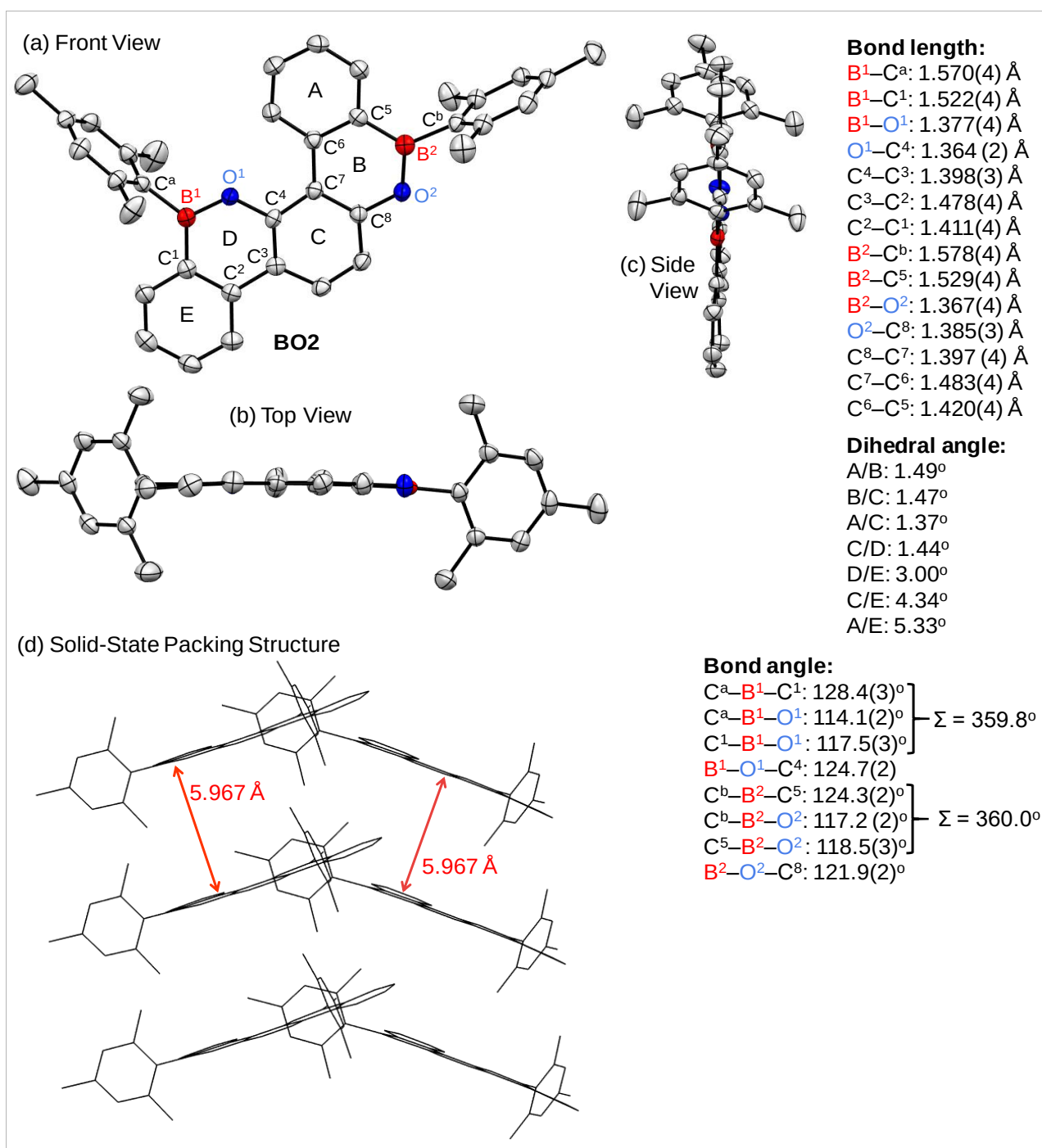
Compound	BO4b	BO4d	BO4e·CH₂Cl₂
CCDC number	1954661	1966566	1968760
Empirical formula	C ₃₈ H ₃₆ B ₂ O ₂	C ₄₄ H ₃₆ B ₂ O ₂	C ₅₅ H ₅₀ B ₂ Cl ₂ O ₂
Formula weight	546.29	618.35	835.47
Temperature (K)	192(2)	170	170
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	orthorhombic	monoclinic	monoclinic
Space 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

Supplementary Table 4. Crystal data and structure refinements for BO5 and BO6

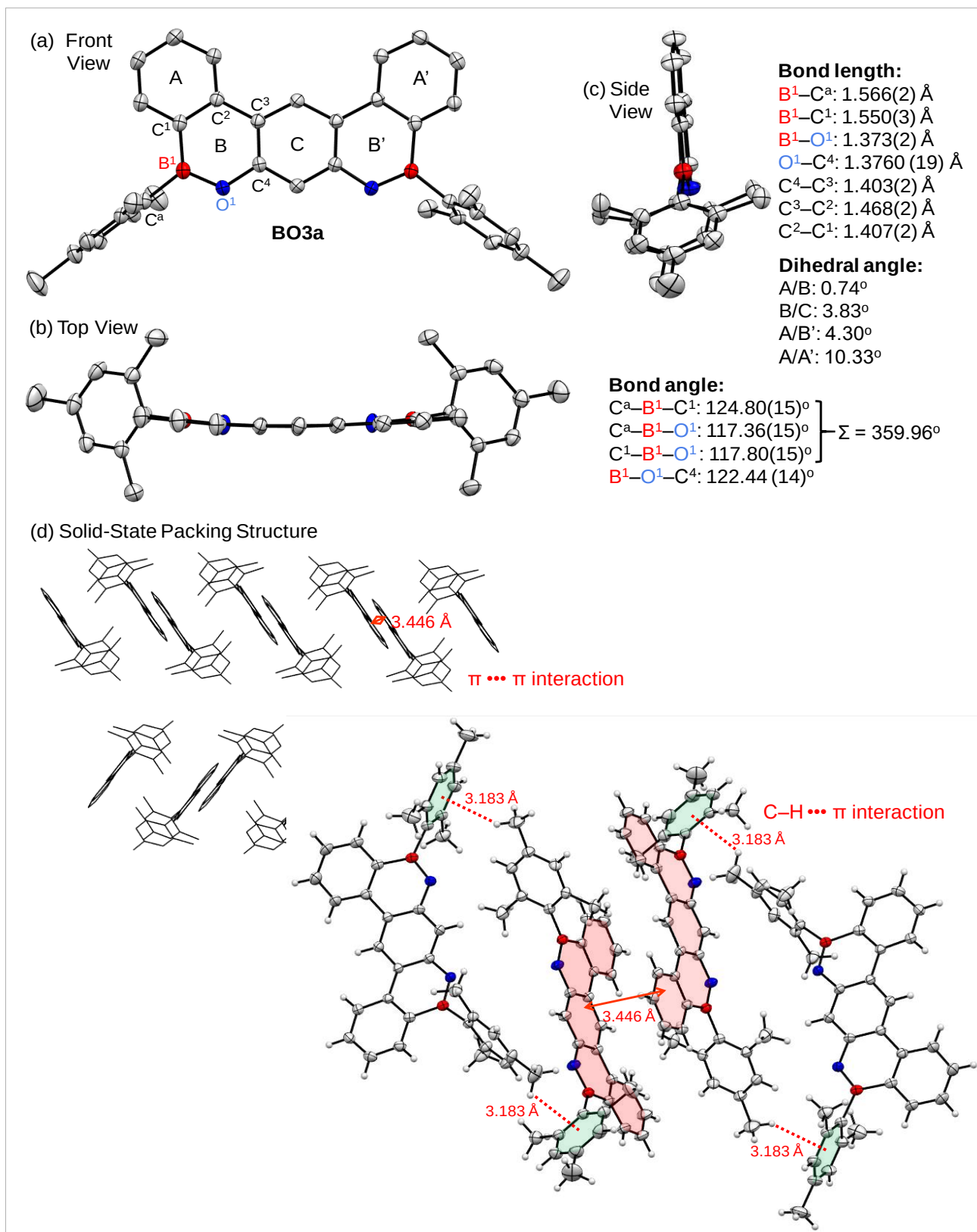
Compound	BO5	BO6
CCDC number	2280610	2029823
Empirical formula	C ₃₆ H ₃₂ B ₂ O ₂	C ₃₆ H ₃₂ B ₂ O ₂
Formula weight	518.23	518.23
Temperature (K)	170.00	192(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	monoclinic	monoclinic
Space group	P2 ₁ /c	P c
<i>a</i> (Å)	9.1072(6)	19.776(2)
<i>b</i> (Å)	10.3791(7)	18.2753(15)
<i>c</i> (Å)	15.0015(10)	16.4263(15)
α (°)	90	90
β (°)	105.825(2)	90.339(3)
γ (°)	90	90
Volume (Å ³)	1364.27(16)	5936.7(9)
<i>Z</i>	2	8
<i>F</i> (000)	548.0	2192.0
Crystal size (mm ³)	0.06 × 0.04 × 0.03	0.18×0.14×0.1
θ (deg) for collection (°)	4.39 to 60.561	1.612 to 24.999
Index ranges	−11 ≤ <i>h</i> ≤ 11, −13 ≤ <i>k</i> ≤ 13, −19 ≤ <i>l</i> ≤ 19	−23 ≤ <i>h</i> ≤ 22, −21 ≤ <i>k</i> ≤ 21, −19 ≤ <i>l</i> ≤ 19
Reflections collected	11533	82048
Unique (<i>R</i> _{int})		19509 (0.1172)
Data / restraints / parameters	3107/0/184	19509 / 2 / 1467
Goodness-of-fit on <i>F</i> ²	1.072	1.016
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0528, <i>wR</i> ₂ = 0.1341	<i>R</i> ₁ = 0.0731 <i>wR</i> ₂ = 0.747
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0738, <i>wR</i> ₂ = 0.1453	<i>R</i> ₁ = 0.1233 <i>wR</i> ₂ = 0.2127
Largest diff. peak and hole (Å ^{−3})	0.26/−0.28	0.22/−0.22



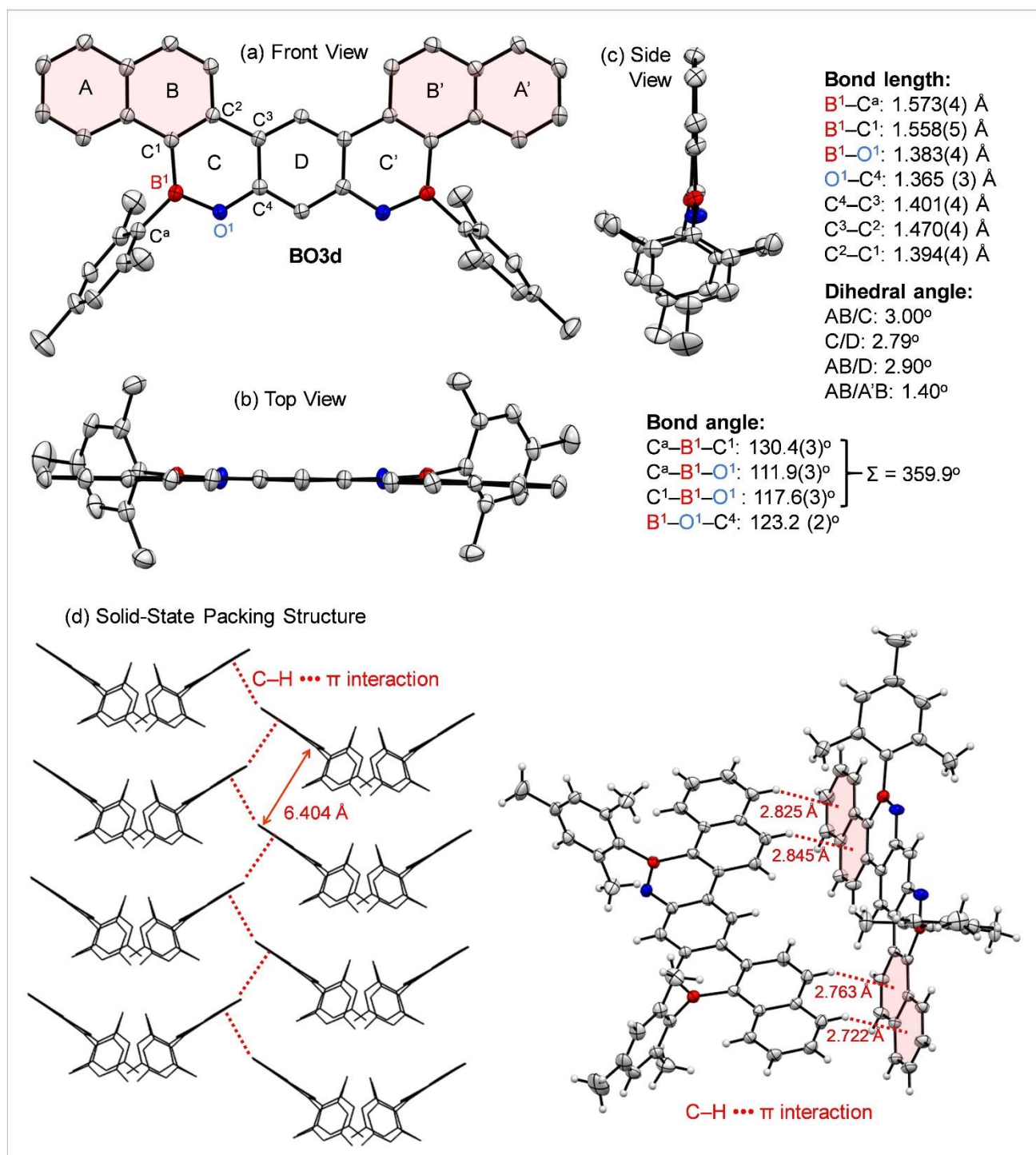
Supplementary Fig. 6. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO1a**. **a** Front View. **b** Top View. **c** Side View. **d** Solide-State Packing Structure. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.



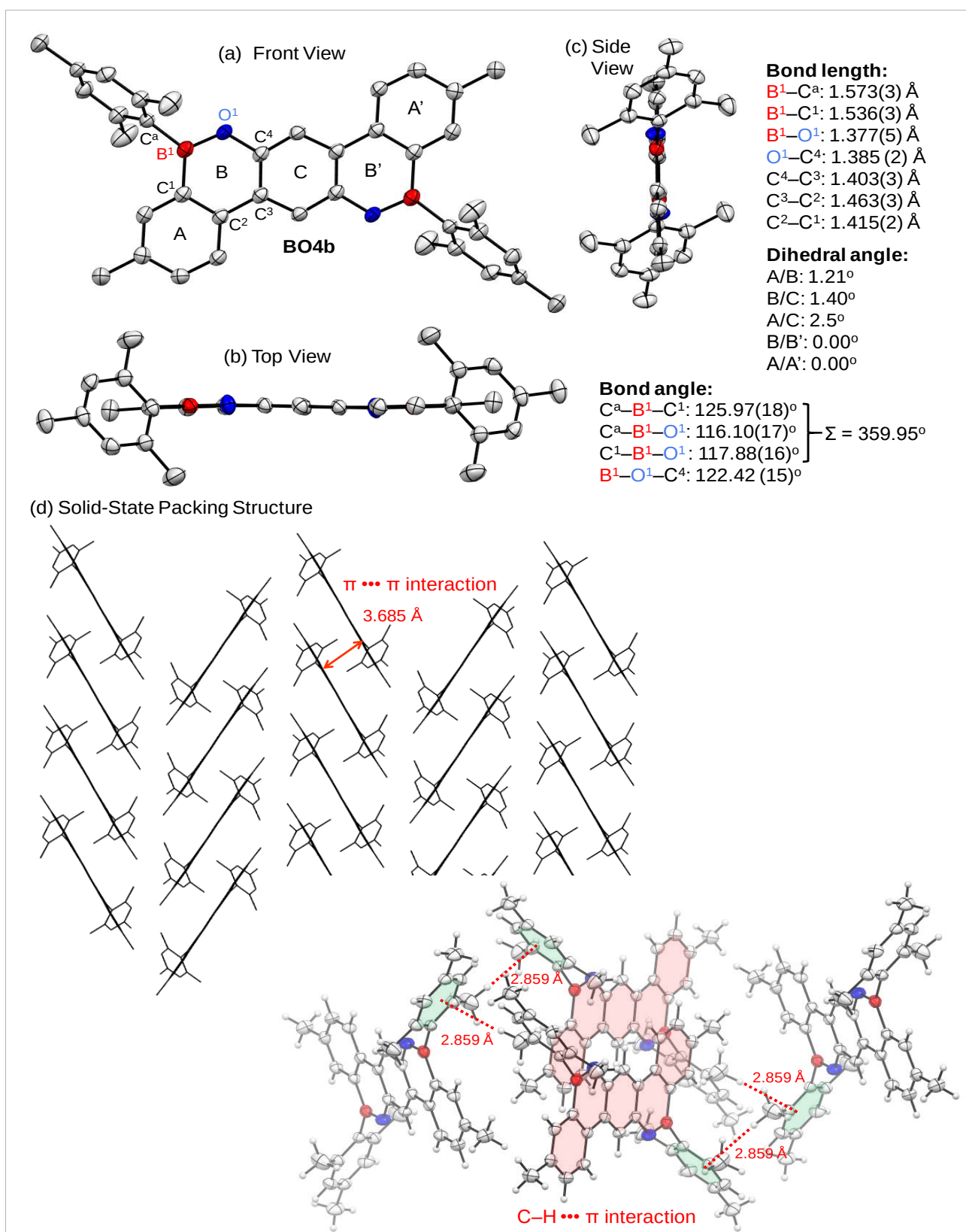
Supplementary Fig. 7. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO2**. **a** Front View. **b** Top View. **c** Side View. **d** Solide-State Packing Structure. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.



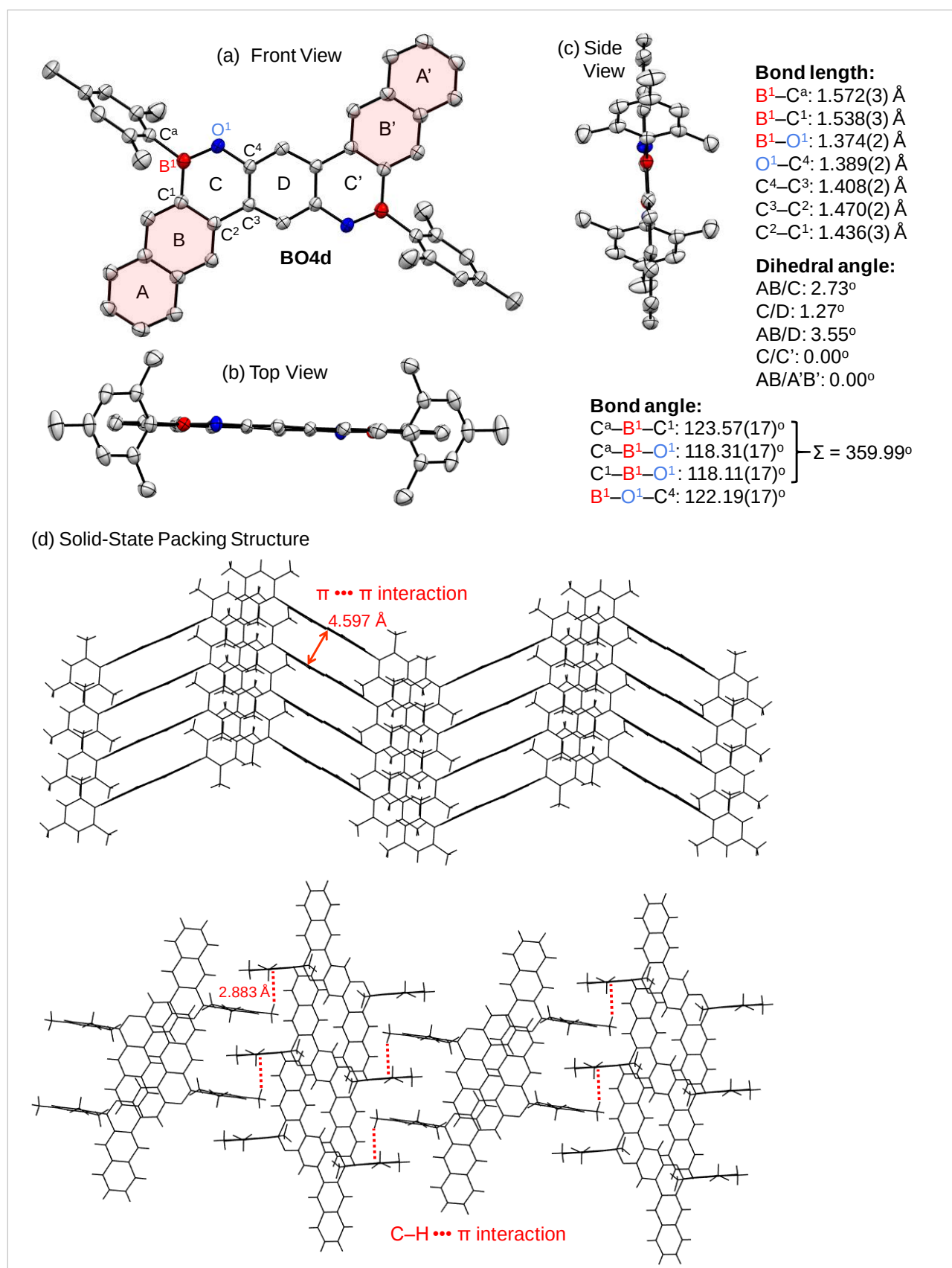
Supplementary Fig. 8. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO3a**. **a** Front View. **b** Top View. **c** Side View. **d** Solid-State Packing Structure. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.



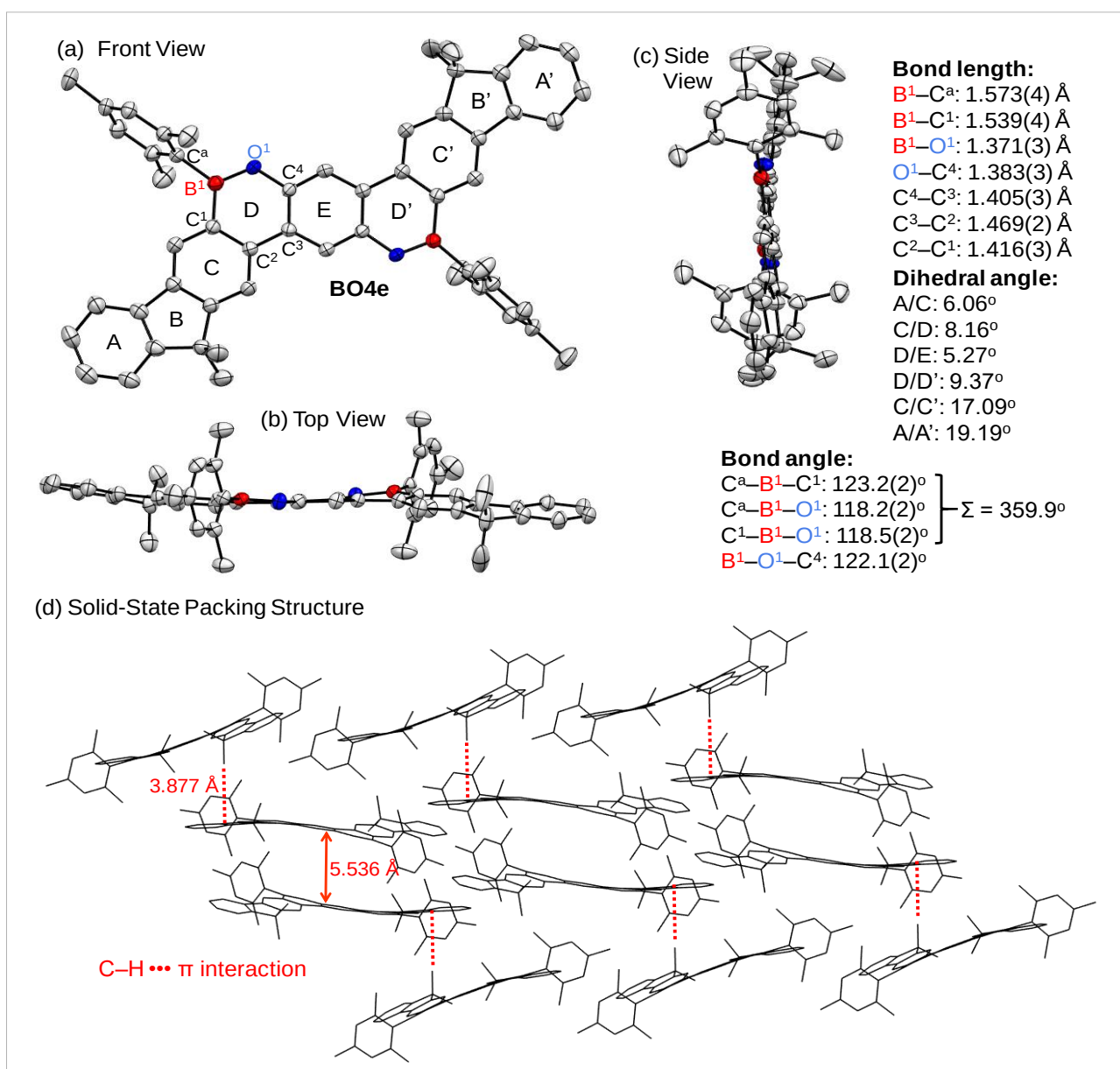
Supplementary Fig. 9. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO3d**. **a** Front View. **b** Top View. **c** Side View. **d** Solide-State Packing Structure. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.



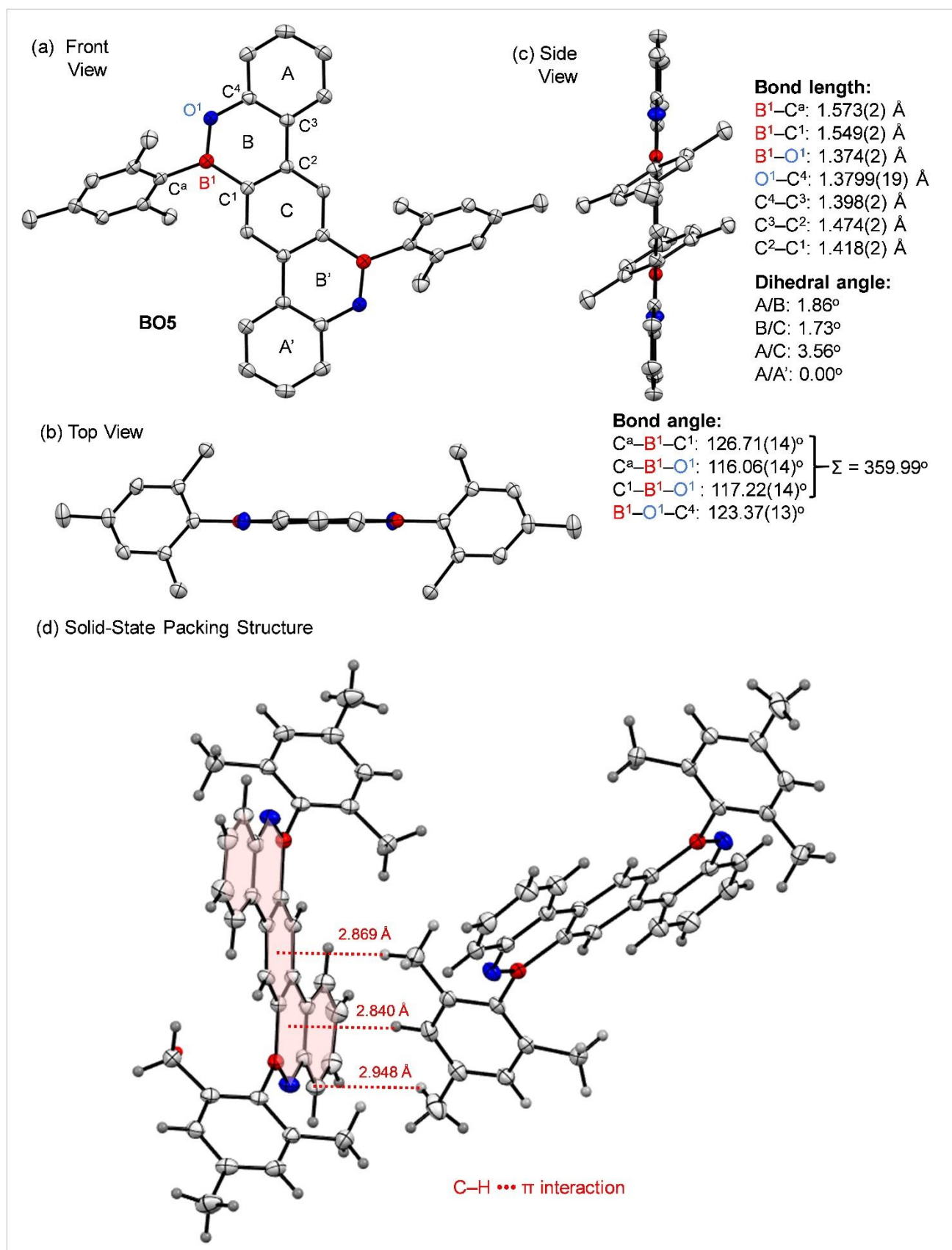
Supplementary Fig. 10. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO4b**. **a** Front View. **b** Top View. **c** Side View. **d** Solide-State Packing Structure. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.



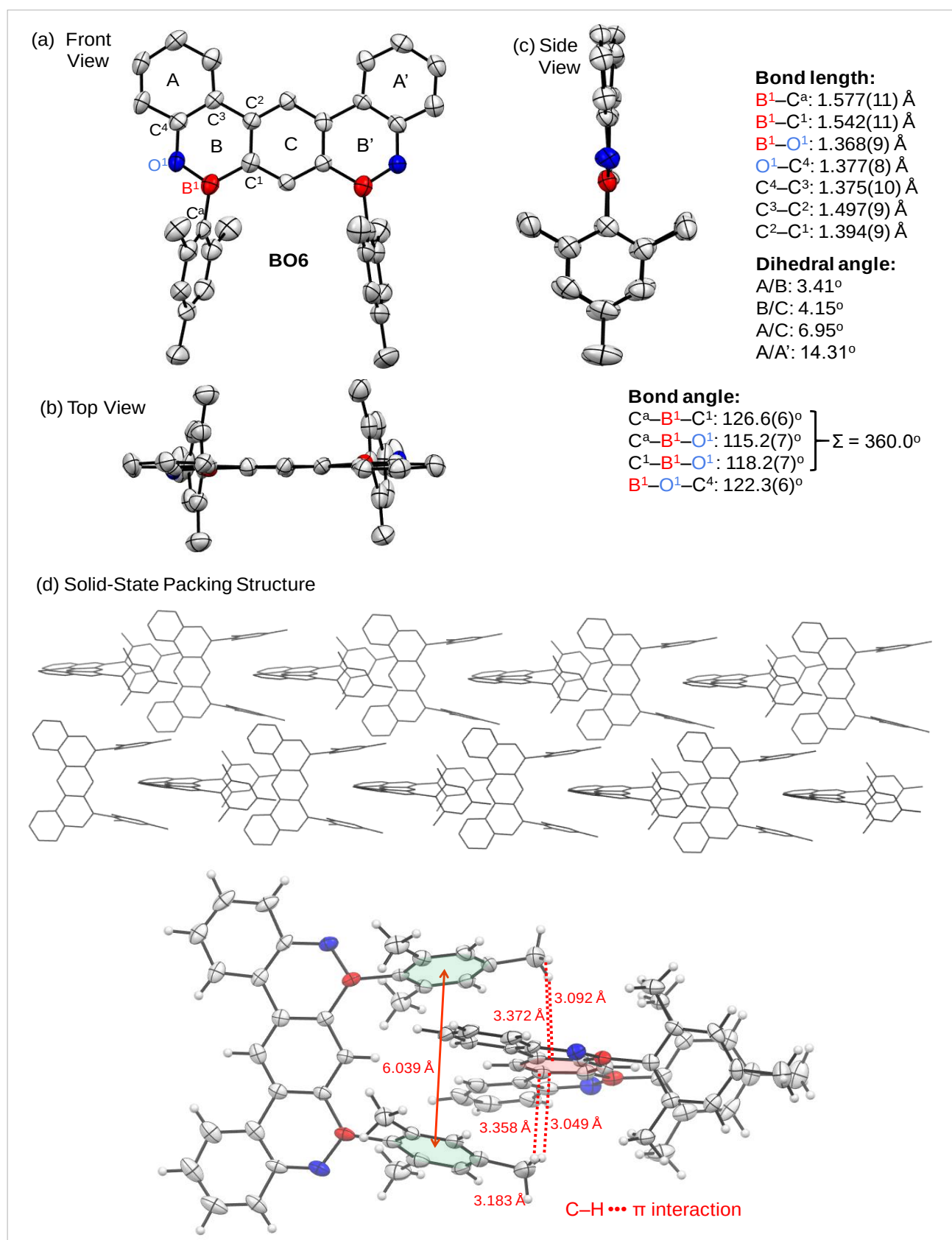
Supplementary Fig. 11. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO4d**. **a** Front View. **b** Top View. **c** Side View. **d** Solide-State Packing Structure. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.



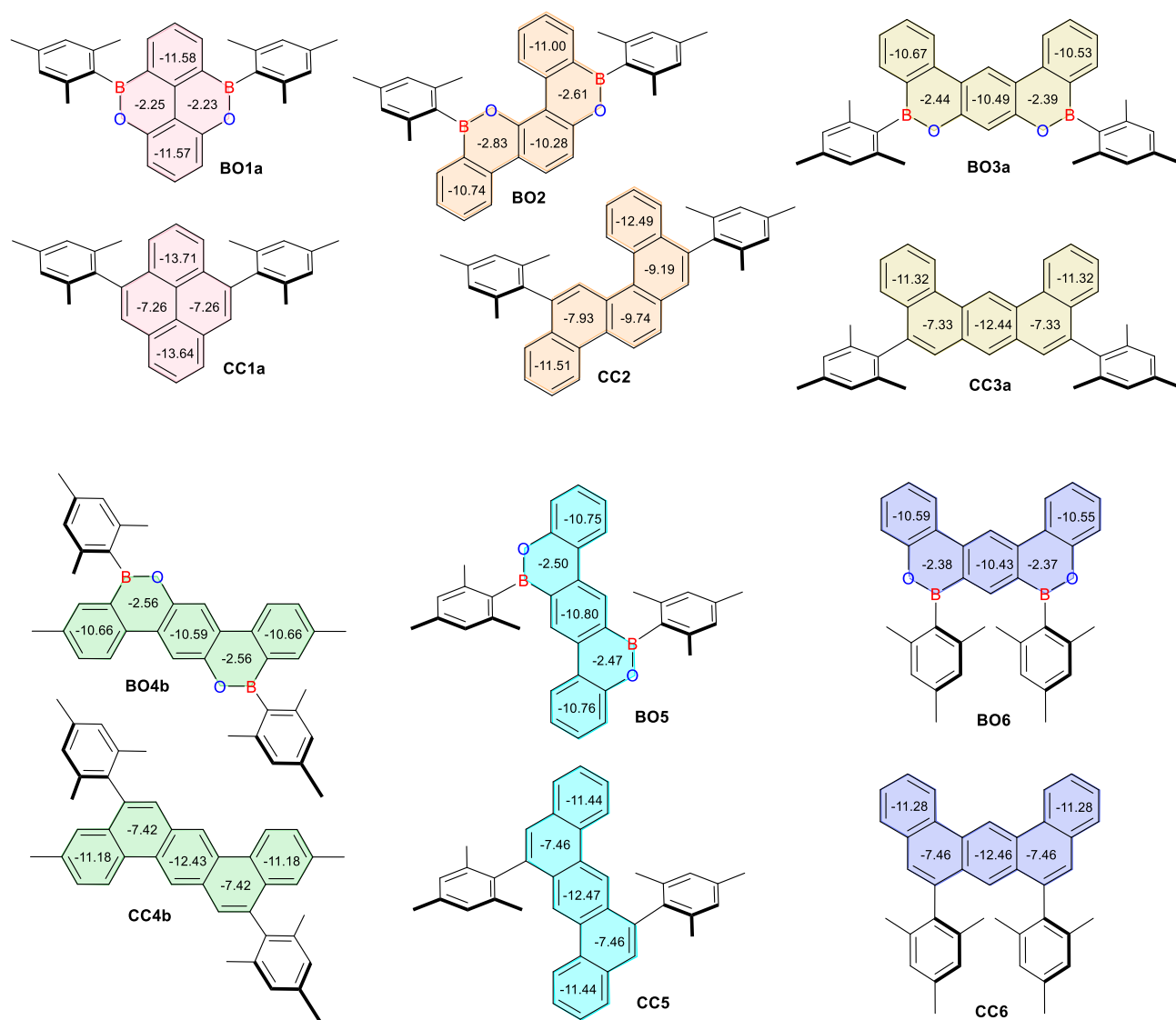
Supplementary Fig. 12. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO4e**. **a** Front View. **b** Top View. **c** Side View. **d** Solide-State Packing Structure. Hydrogen atoms and solvent dichloromethane molecules were omitted for clarity. Ellipsoids are shown at the 50% probability level.



Supplementary Fig. 13. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO5**. **a** Front View. **b** Top View. **c** Side View. **d** Solide-State Packing Structure. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.



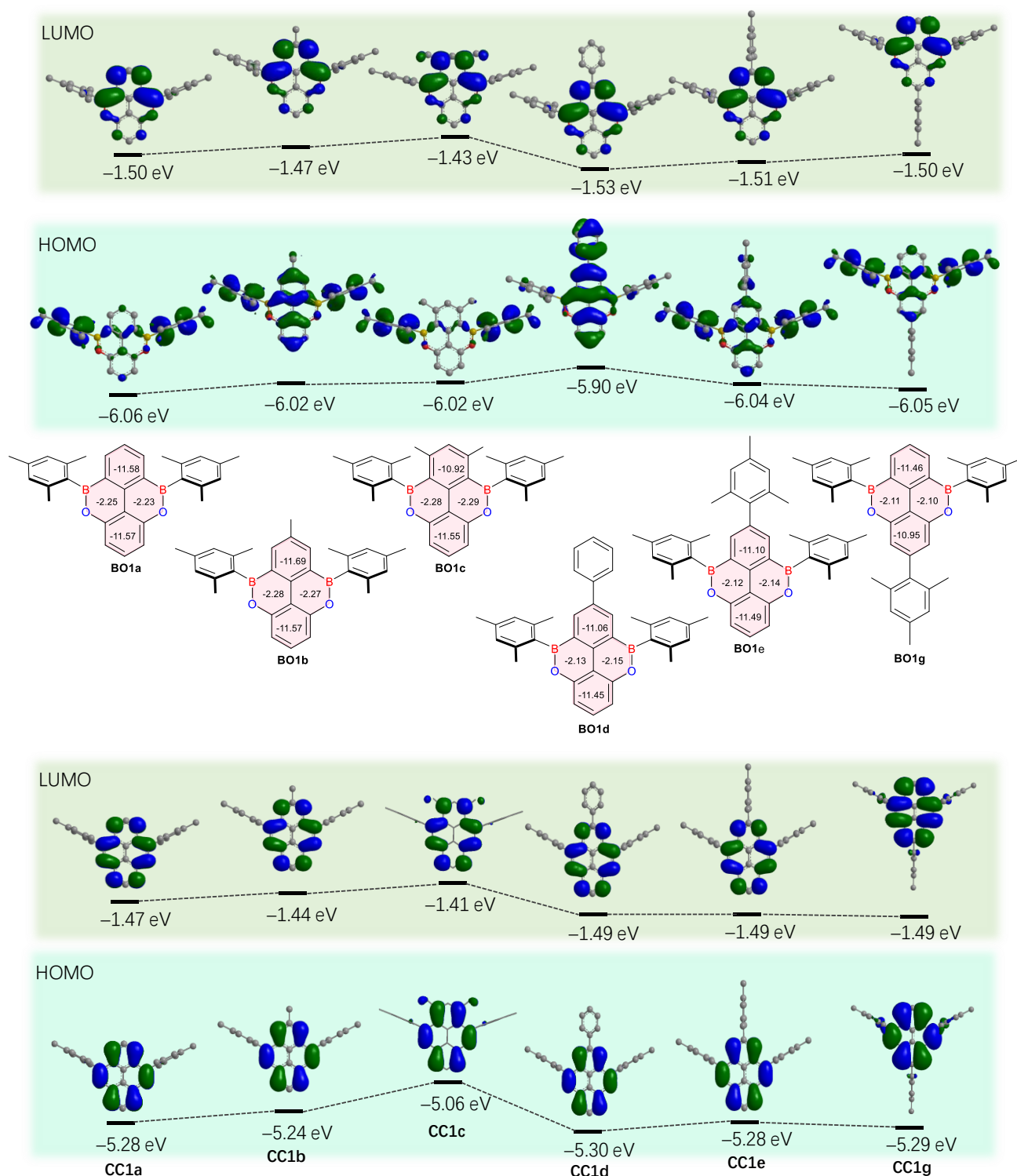
Supplementary Fig. 14. Single crystal structure. X-ray single crystal diffraction structure and crystal packing of **BO6**. **a** Front View. **b** Top View. **c** Side View. **d** Solide-State Packing Structure. Hydrogen atoms were omitted for clarity. Ellipsoids are shown at the 50% probability level.



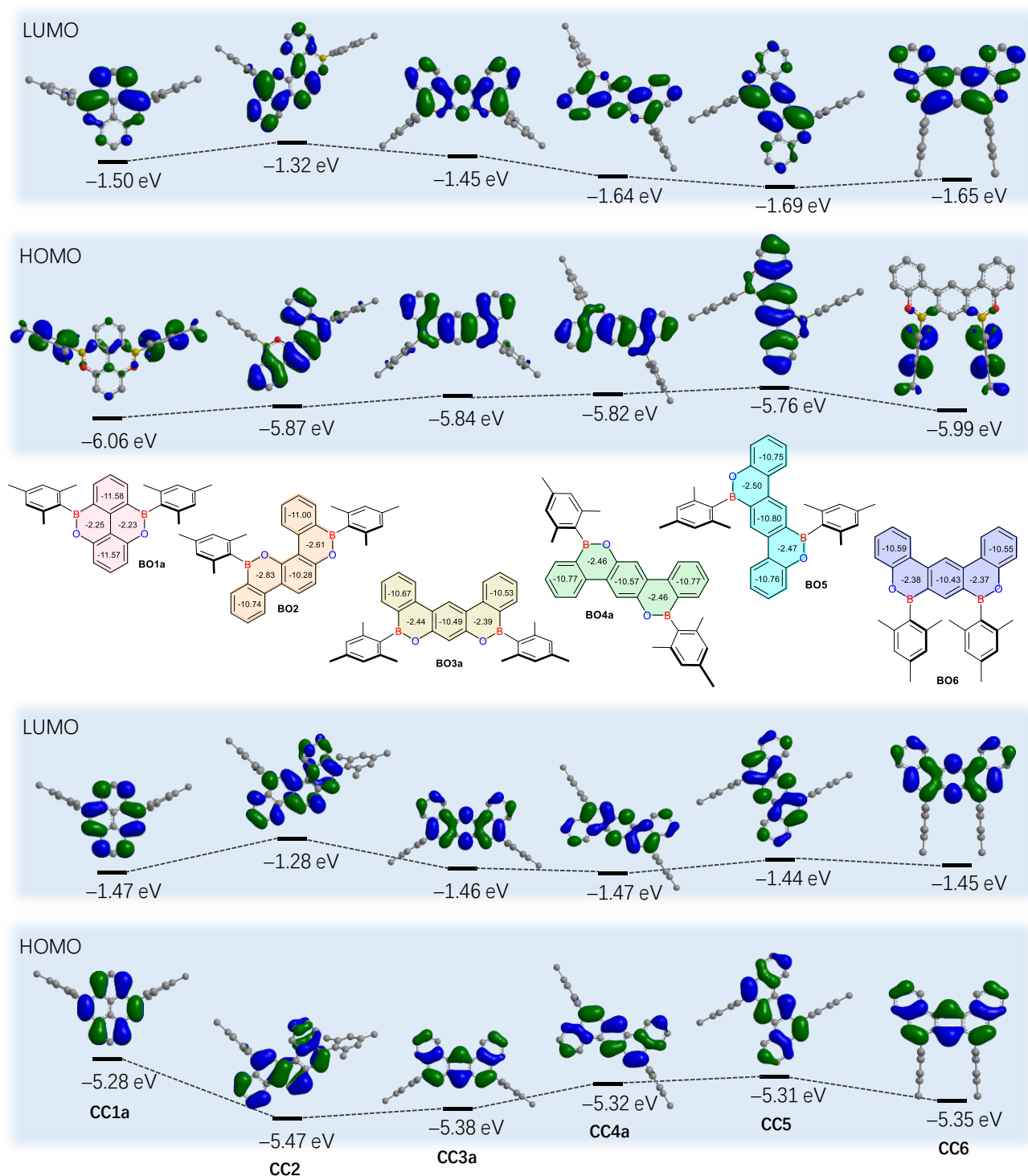
Supplementary Fig. 15. NICS(1) values of dBO-PAHs. Comparison of the calculated NICS(1) values of dBO-PAHs **BO1a**, **BO2**, **BO3a**, **BO4b**, **BO5**, **BO6** and their corresponding PAH analogues **CC1a**, **CC2**, **CC3a**, **CC4b**, **CC5**, **CC6**. The calculations were performed at B3LYP/6-31G* level.

Supplementary Table 5. Comparison of calculated HOMO and LUMO levels and energy gaps of the dBO-PAHs and their corresponding carbon analogues

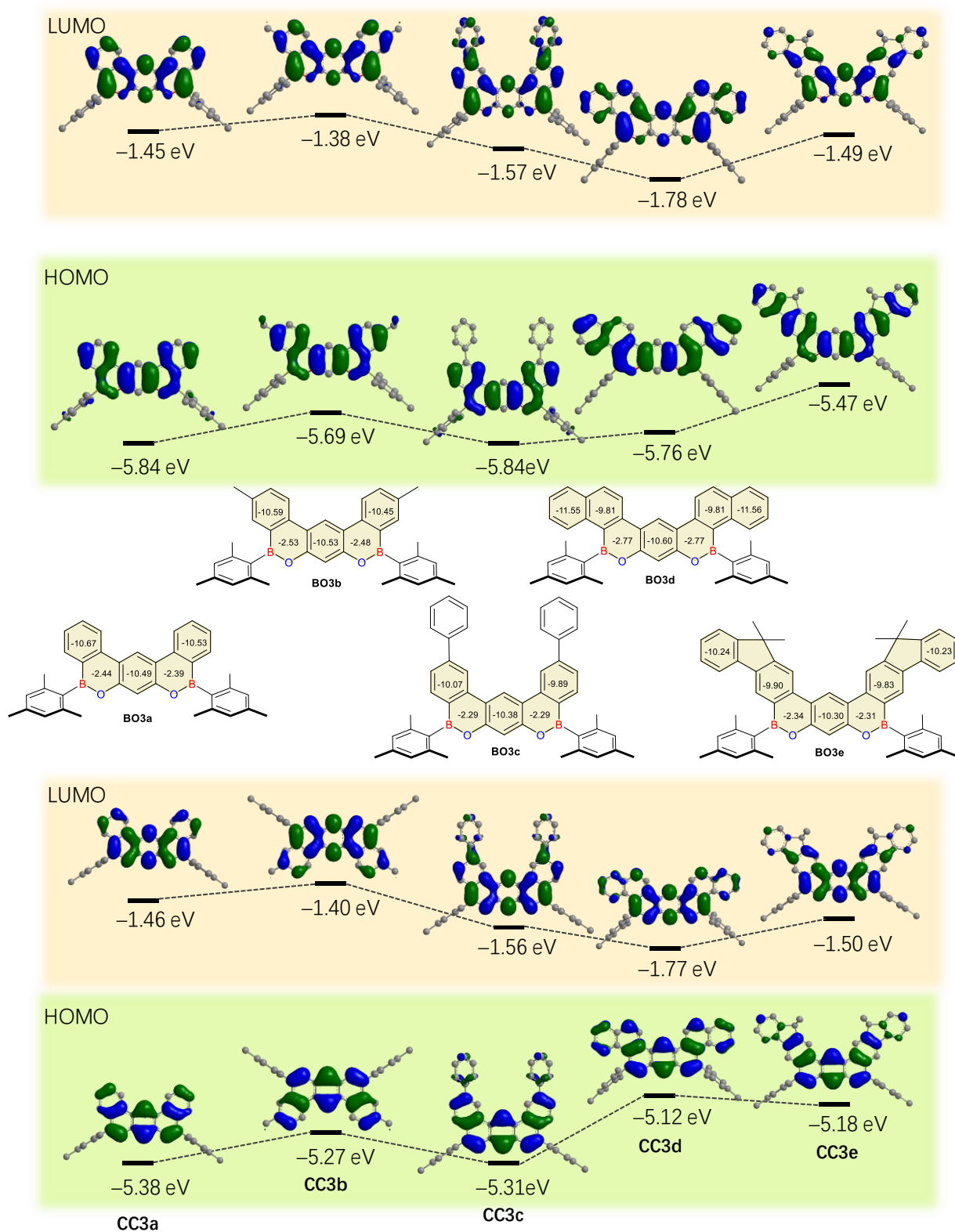
BO-PAH	<i>cat.</i> HOMO/LUMO/ E_g [eV]	BO-PAH	<i>cat.</i> HOMO/LUMO/ E_g [eV]	BO-PAH	<i>cat.</i> HOMO/LUMO/ E_g [eV]
CC1a	−5.28/−1.47/3.81	CC2	−5.47/−1.28/4.19	CC4a	−5.32/−1.49/3.83
BO1a	−6.06/−1.50/4.56	BO2	−5.87/−1.32/4.55	BO4a	−5.82/−1.64/4.18
CC1b	−5.24/−1.44/3.80	CC3a	−5.38/−1.46/3.92	CC4b	−5.24/−1.41/3.83
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



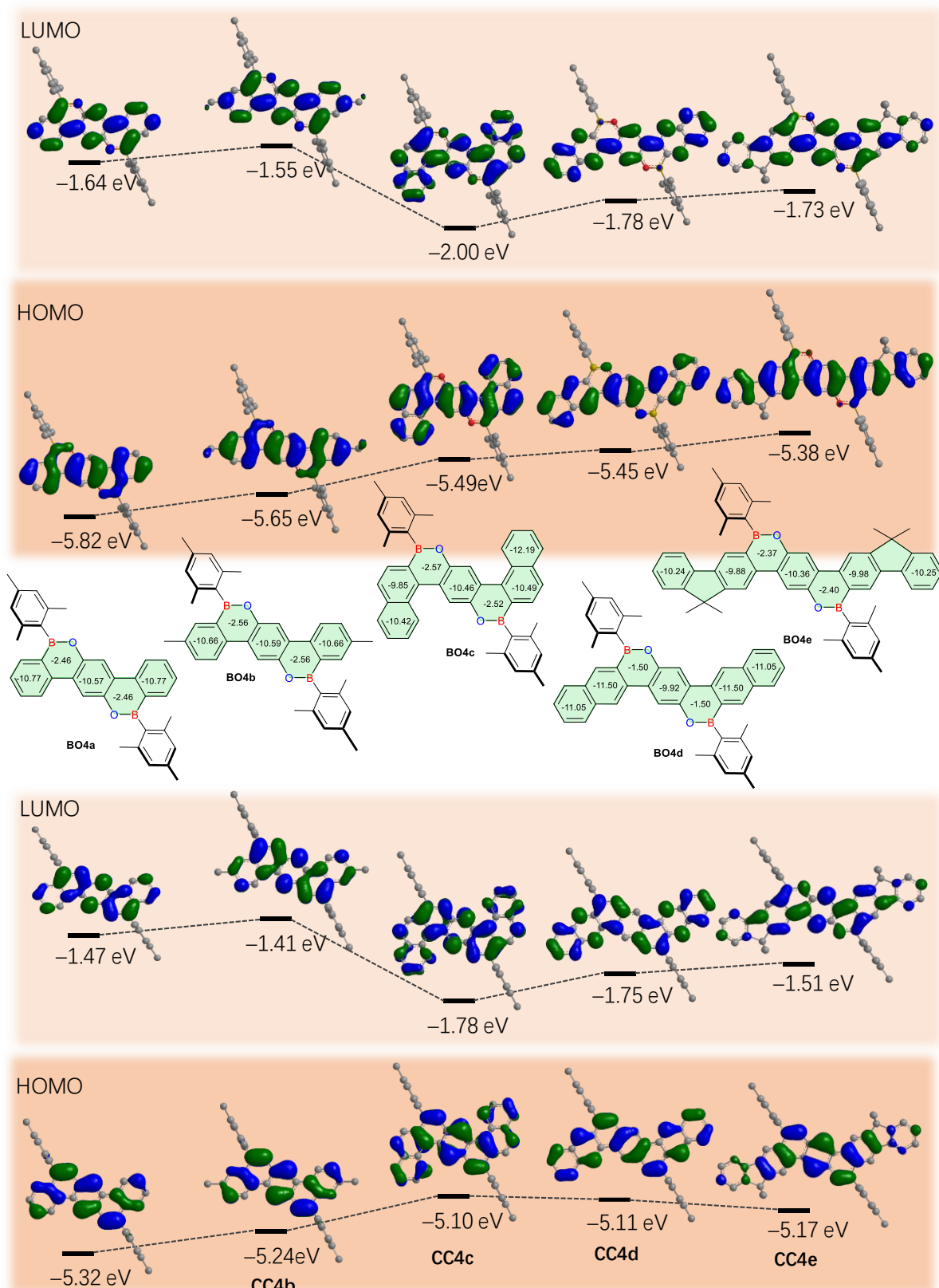
Supplementary Fig. 16. Theoretical calculation. Comparison of frontier orbital distributions, energy levels, and NICS(1) values of dBO-PAHs **BO1a**, **BO1b**, **BO1c**, **BO1d**, **BO1e** and **BO1g**, as well as their corresponding carbon-based PAHs **CC1a**, **CC1b**, **CC1c**, **CC1d**, **CC1e** and **CC1g**. The calculations were performed at B3LYP/6-31G(d) level.



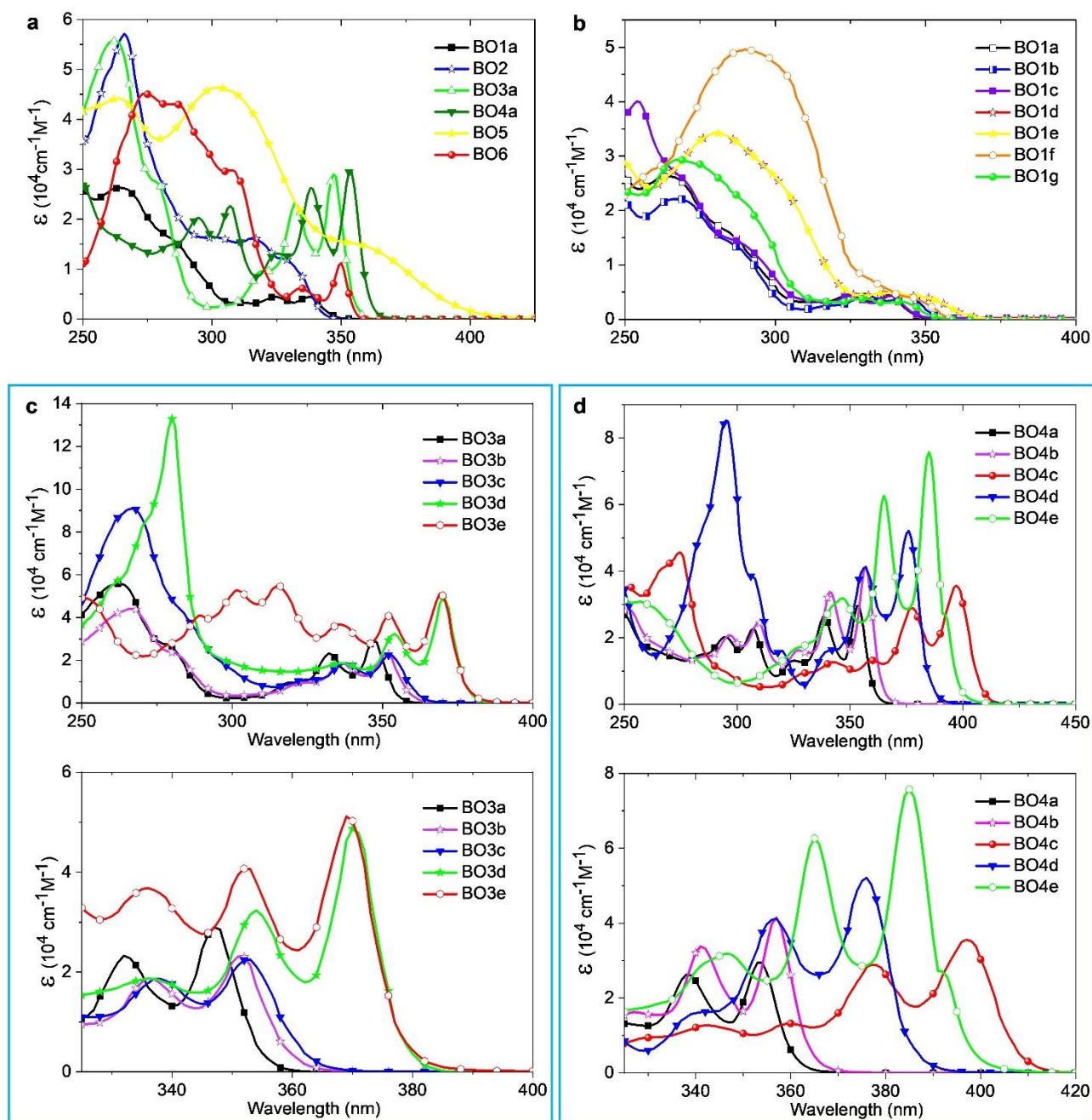
Supplementary Fig. 17. Theoretical calculation. Comparison of frontier orbital distributions, energy levels, and NICS(1) values of dBO-PAHs **BO1a**, **BO2**, **BO3a**, **BO4a**, **BO5** and **BO6**, as well as their corresponding carbon-based PAHs **CC1a**, **CC2**, **CC3a**, **CC4a**, **CC5** and **CC6**. The calculations were performed at B3LYP/6-31G(d) level.



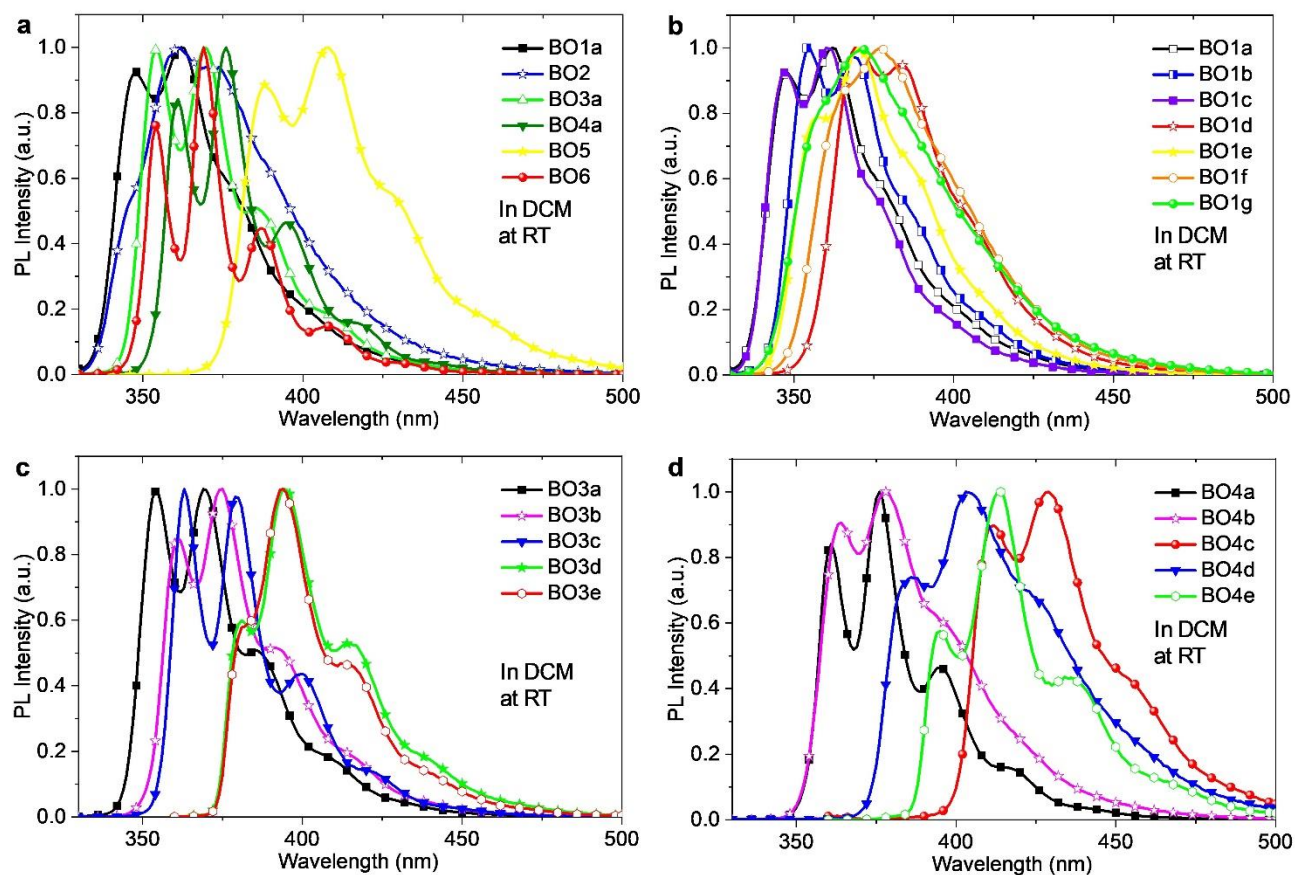
Supplementary Fig. 18. Theoretical calculation. Comparison of frontier orbital distributions, energy levels, and NICS(1) values of dBO-PAHs **BO3a**, **BO3b**, **BO3c**, **BO3d** and **BO3e**, as well as their corresponding carbon-based PAHs **CC3a**, **CC3b**, **CC3c**, **CC3d** and **CC3e**. The calculations were performed at B3LYP/6-31G(d) level.



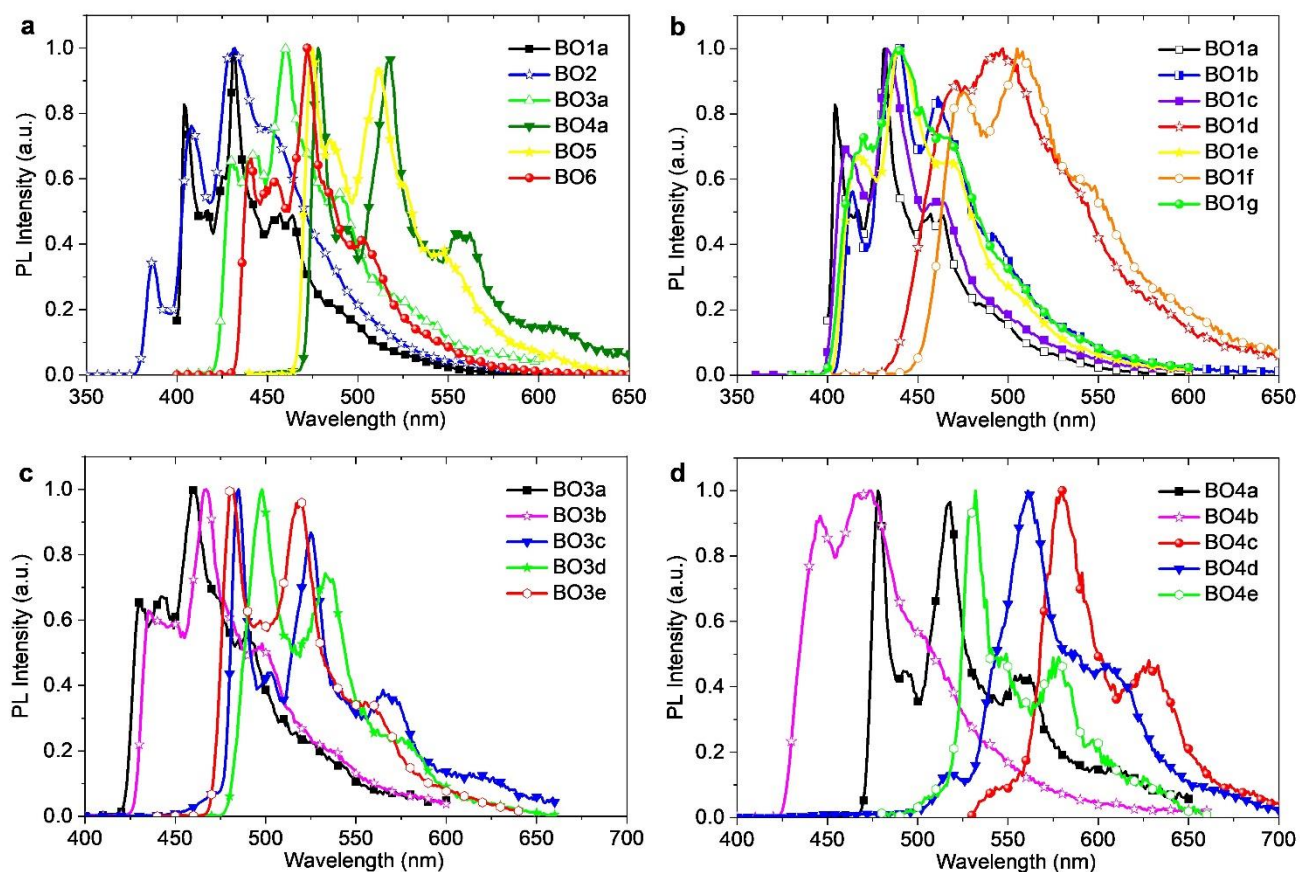
Supplementary Fig. 19. Theoretical calculation. Comparison of frontier orbital distributions, energy levels, and NICS(1) values of dBO-PAHs **BO4a**, **BO4b**, **BO4c**, **BO4d** and **BO4e**, as well as their corresponding carbon-based PAHs **CC5a**, **CC5b**, **CC5c**, **CC5d** and **CC4e**. The calculations were performed at B3LYP/6-31G(d) level.



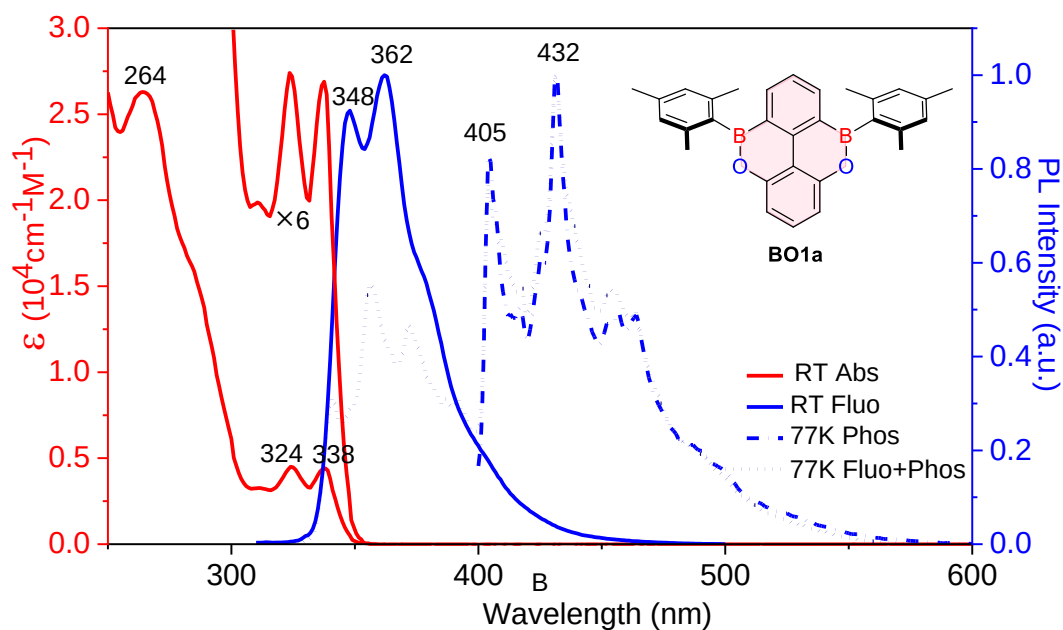
Supplementary Fig. 20. Photophysical properties. Comparison of room-temperature absorption spectra for **a**, BO1a, BO2, BO3a, BO4a, BO5 and BO6; **b**, BO1 series; **c**, BO3 series; **d**, BO4 series in dichloromethane solution.



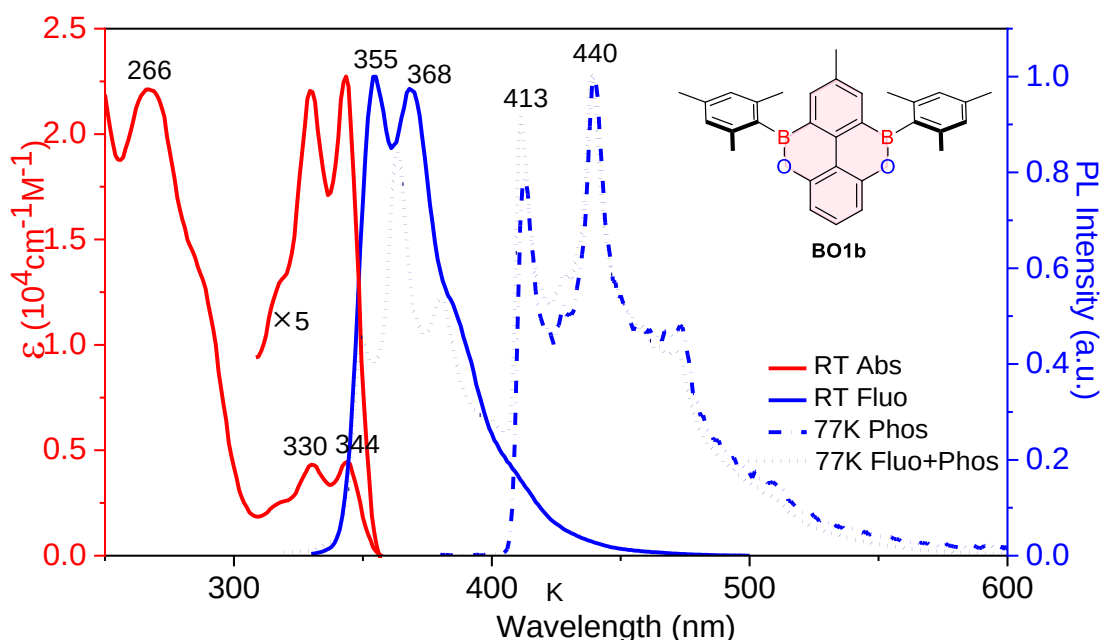
Supplementary Fig. 21. Photophysical properties. Comparison of room-temperature (RT) PL spectra for **a**, BO1a, BO2, BO3a, BO4a, BO5 and BO6; **b**, BO1 series; **c**, BO3 series; **d**, BO4 series in dichloromethane solution.



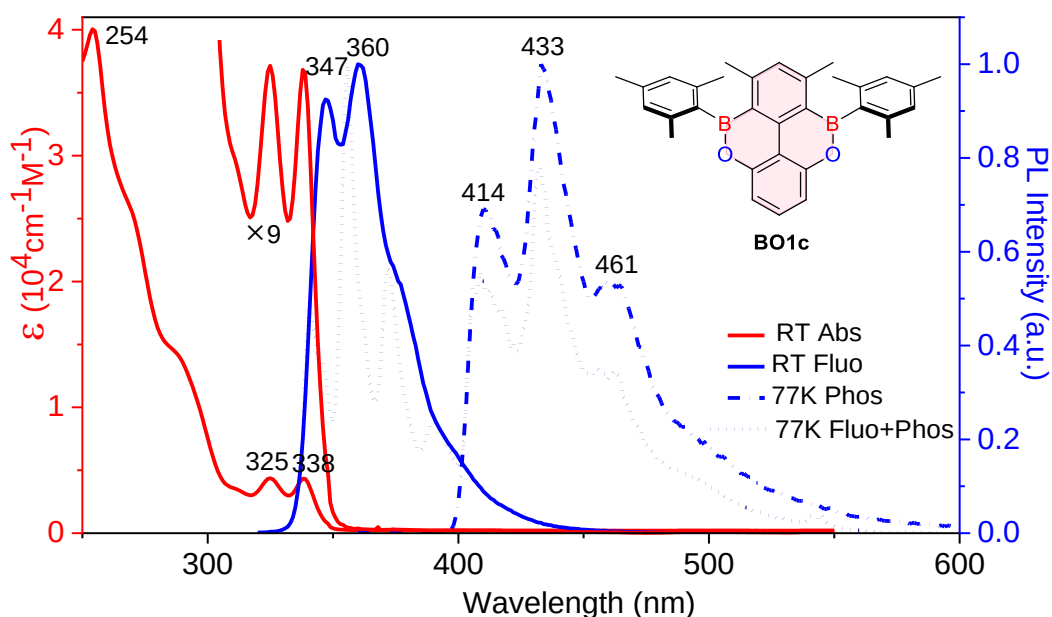
Supplementary Fig. 22. Photophysical properties. Comparison of low-temperature (77 K) phosphorescent spectra for **a**, BO1a, BO2, BO3a, BO4a, BO5 and BO6; **b**, BO1 series, **c**, BO3 series; **d**, BO4 series in 2-MeTHF.



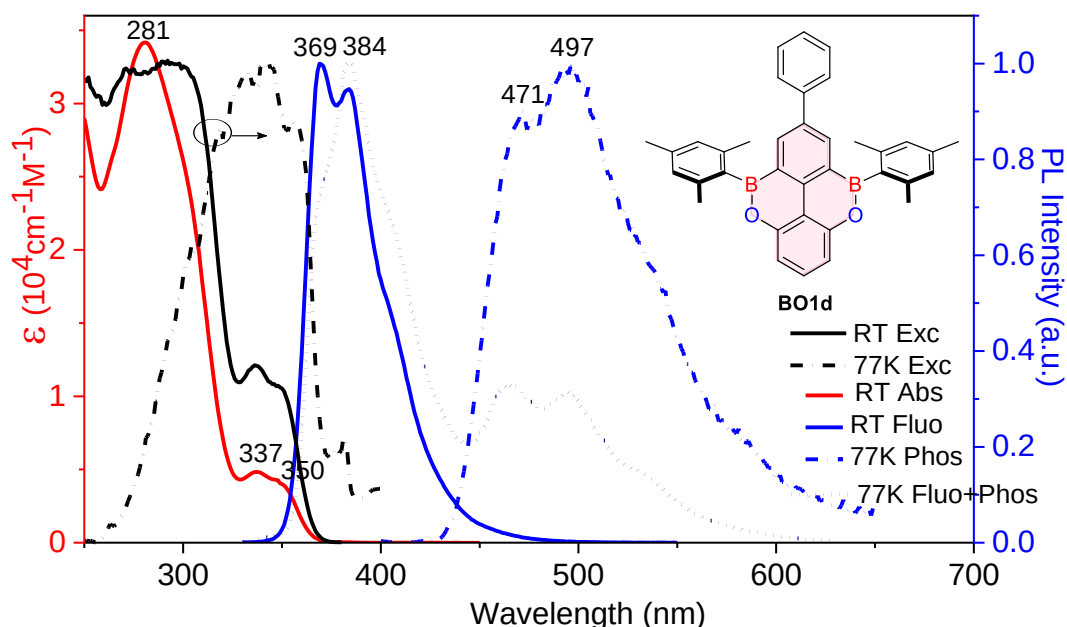
Supplementary Fig. 23. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1a**. The chemical structure is shown in the inset.



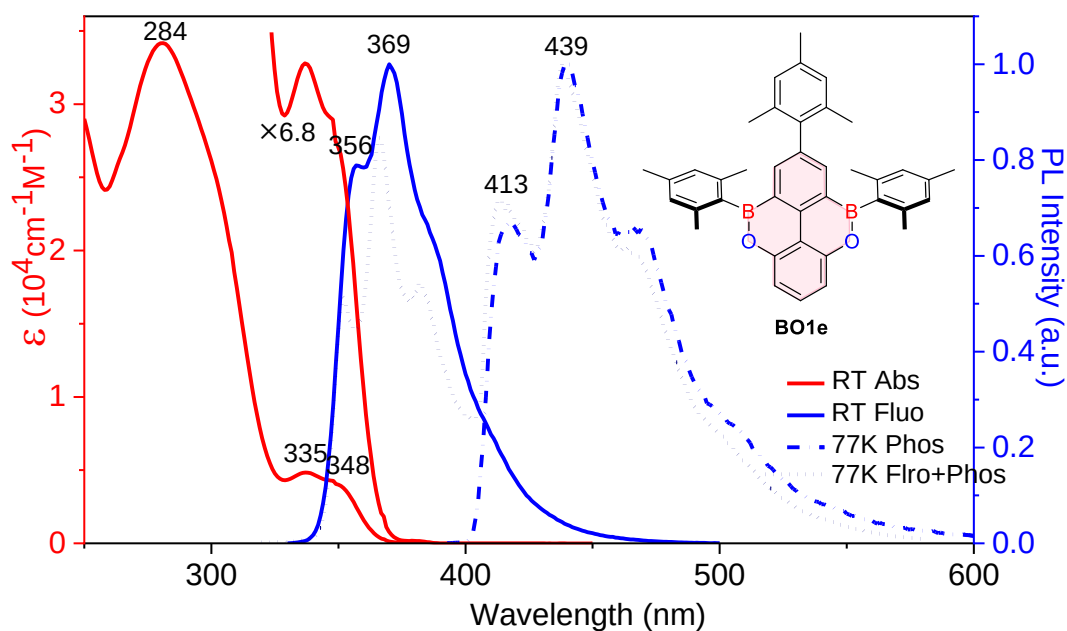
Supplementary Fig. 24. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1b**. The chemical structure is shown in the inset.



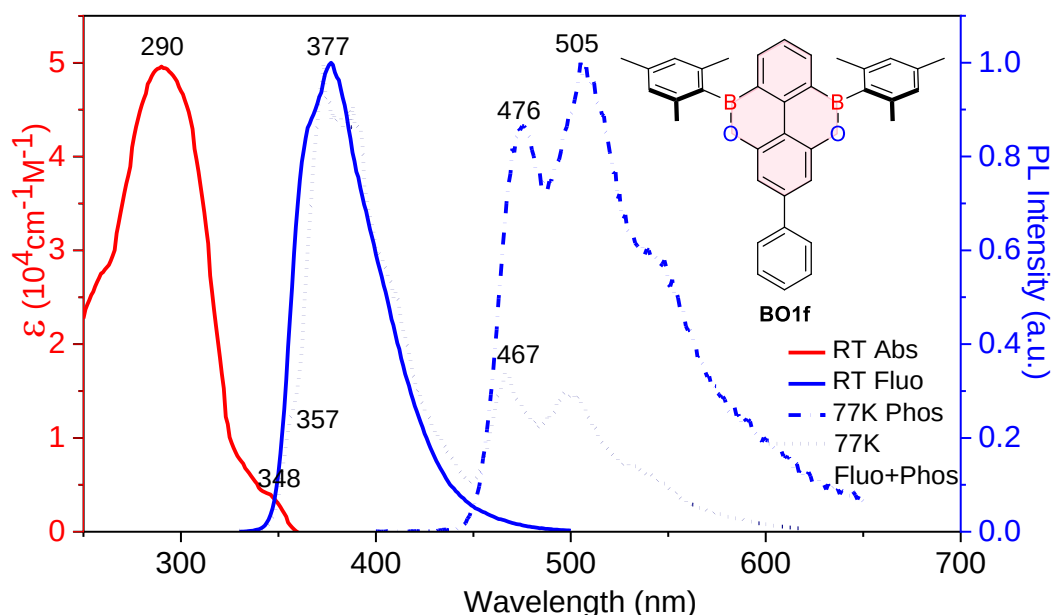
Supplementary Fig. 25. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1c**. The chemical structure is shown in the inset.



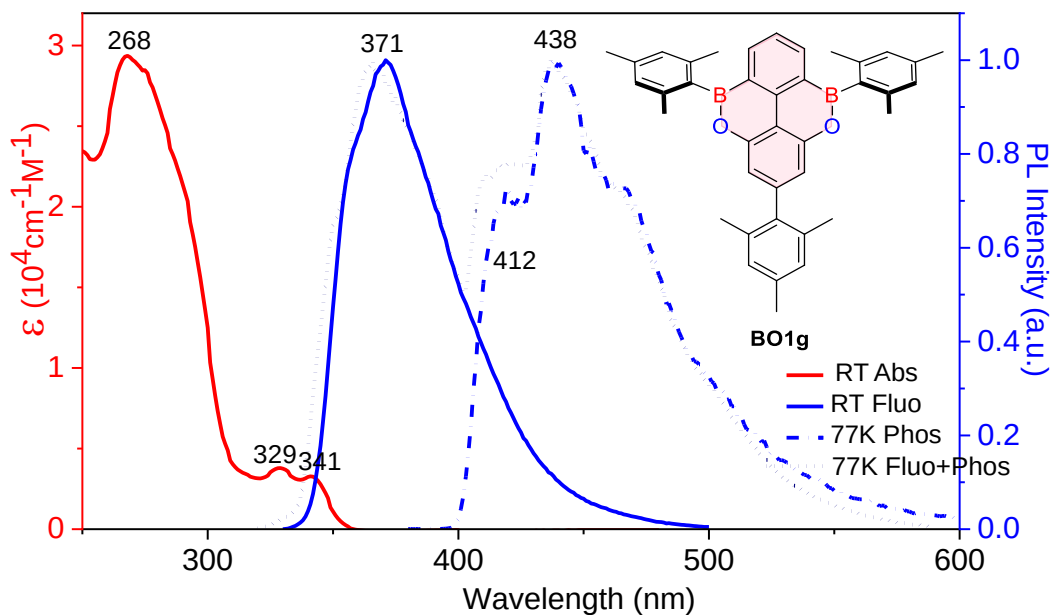
Supplementary Fig. 26. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF and their corresponding excited spectra of **BO1d**. The chemical structure is shown in the inset.



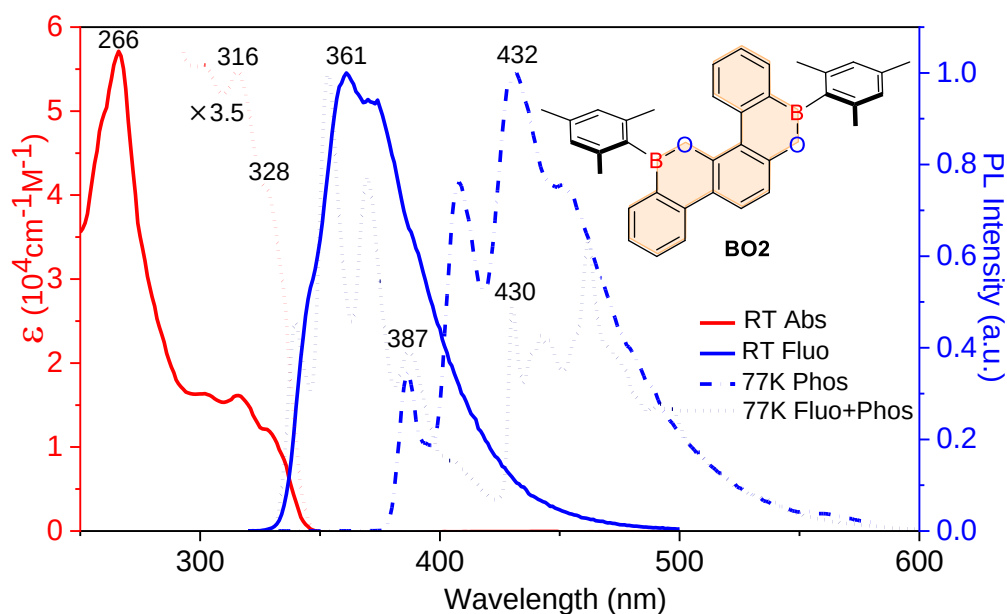
Supplementary Fig. 27. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1e**. The chemical structure is shown in the inset.



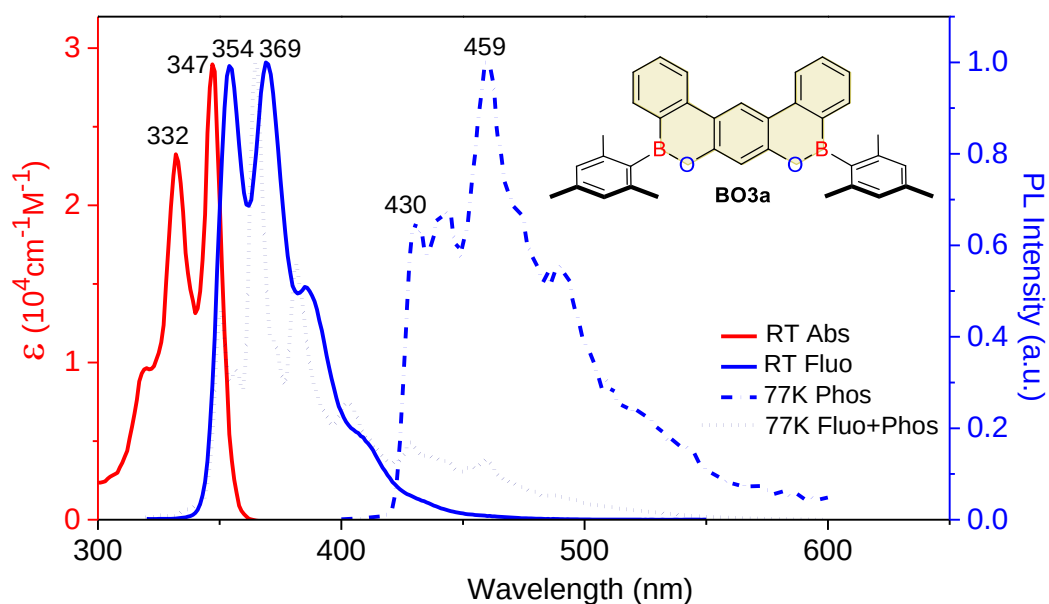
Supplementary Fig. 28. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1f**. The chemical structure is shown in the inset.



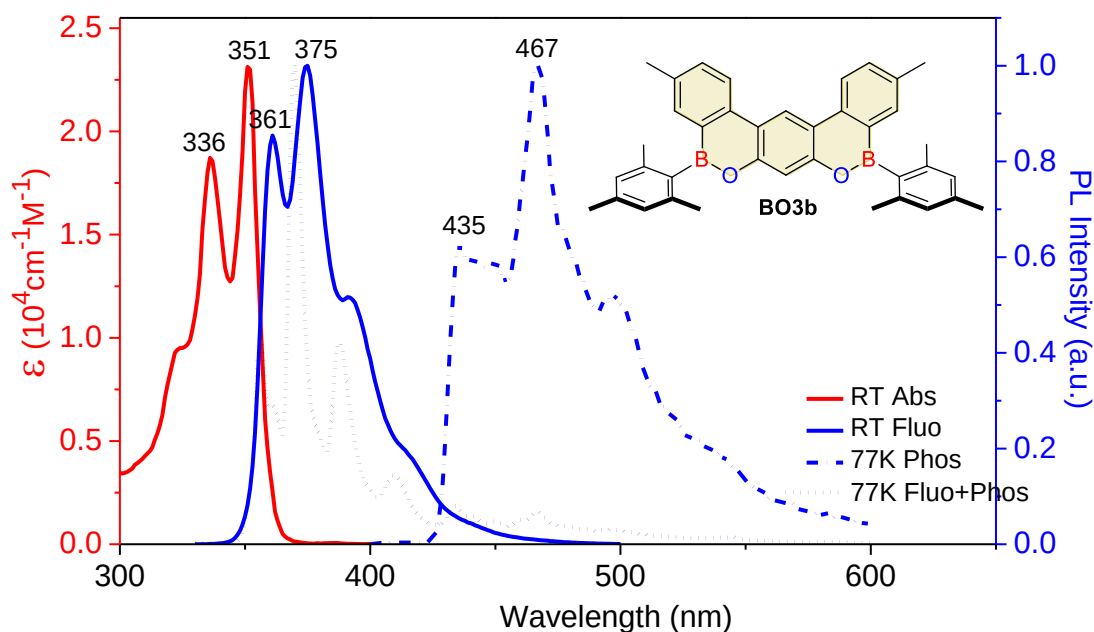
Supplementary Fig. 29. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO1g**. The chemical structure is shown in the inset.



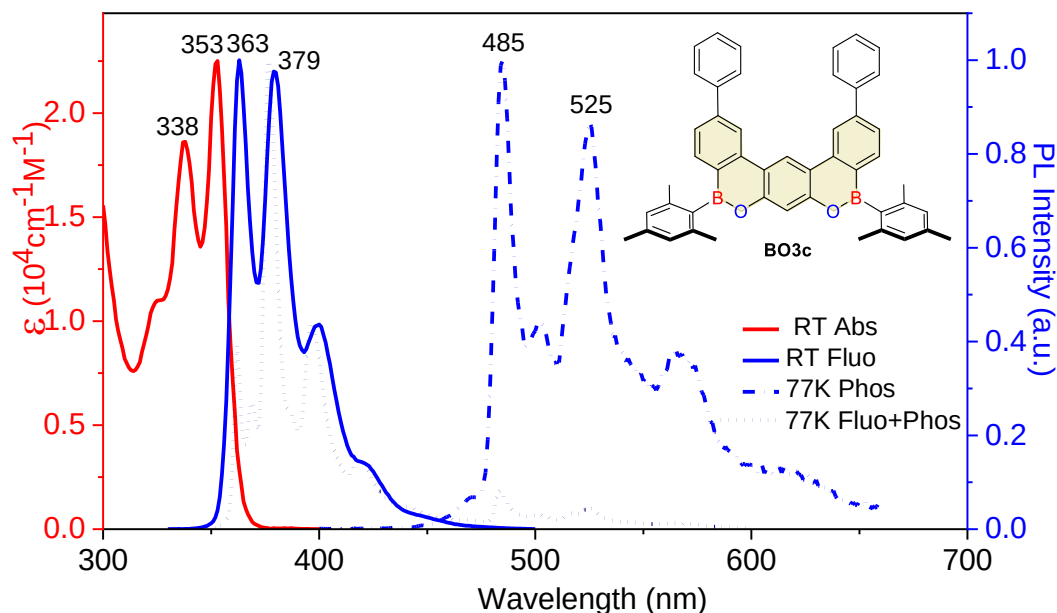
Supplementary Fig. 30. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO2**. The chemical structure is shown in the inset.



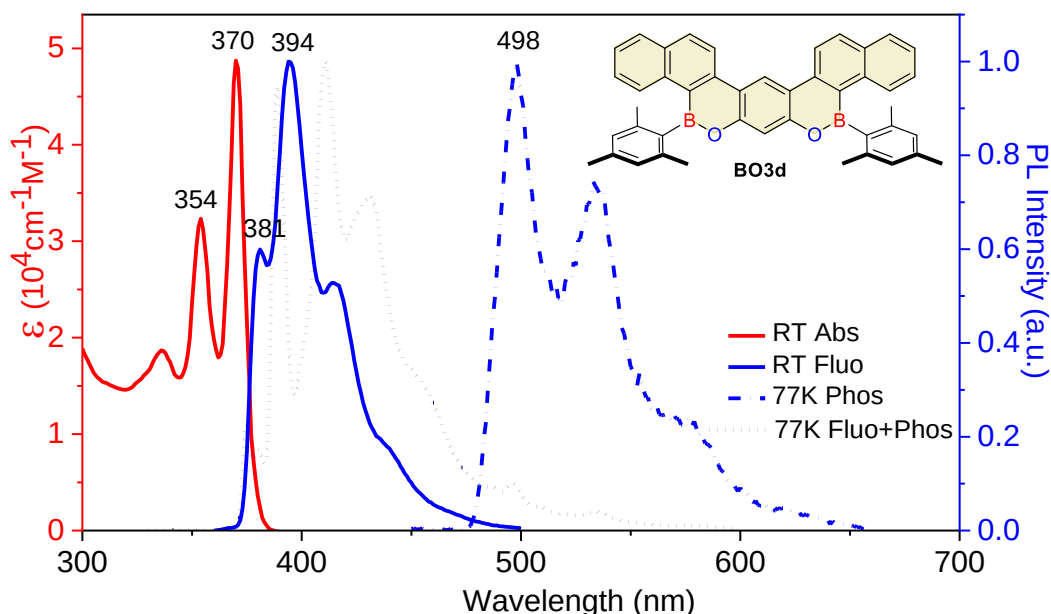
Supplementary Fig. 31. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO3a**. The chemical structure is shown in the inset.



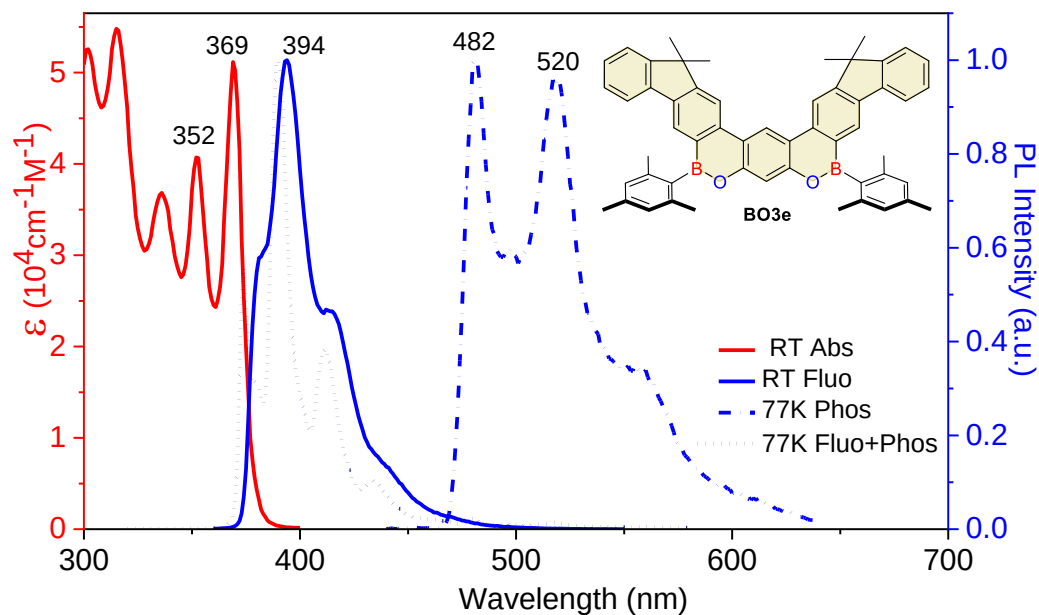
Supplementary Fig. 32. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO3b**. The chemical structure is shown in the inset.



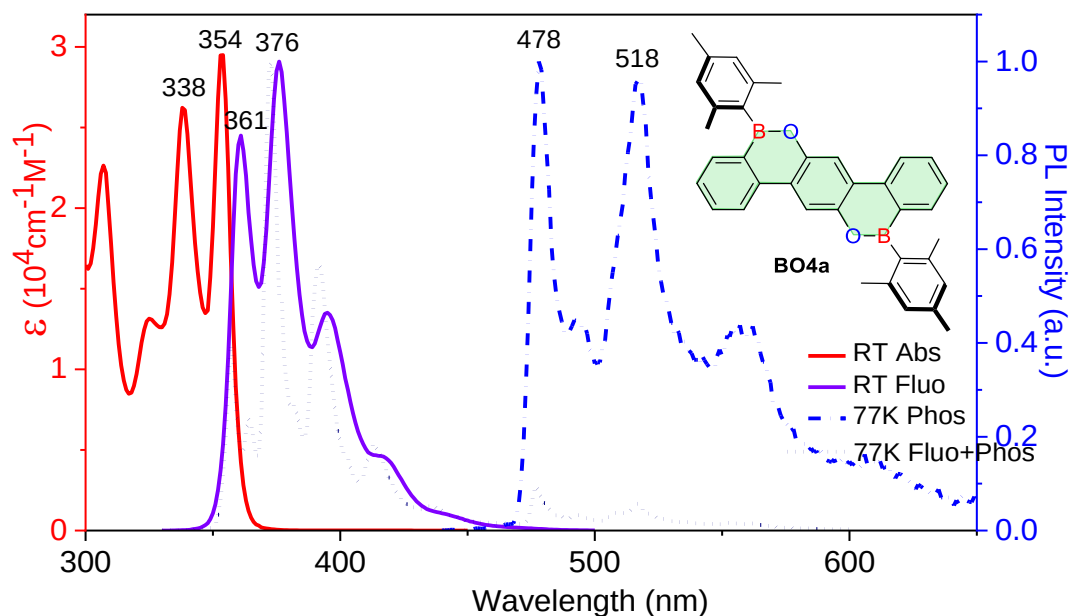
Supplementary Fig. 33. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO3c**. The chemical structure is shown in the inset.



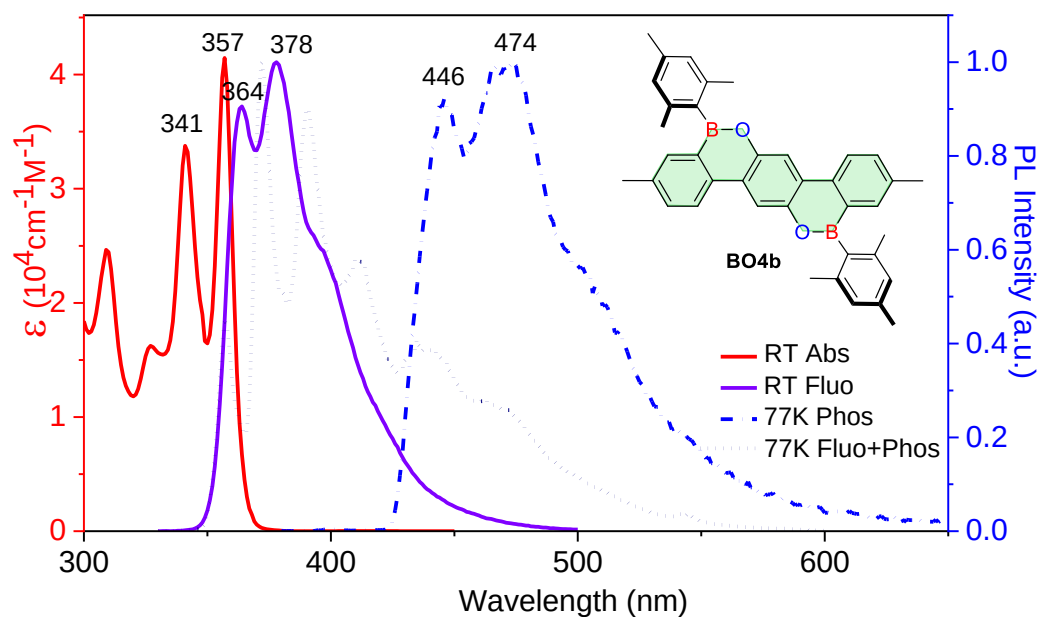
Supplementary Fig. 34. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO3d**. The chemical structure is shown in the inset.



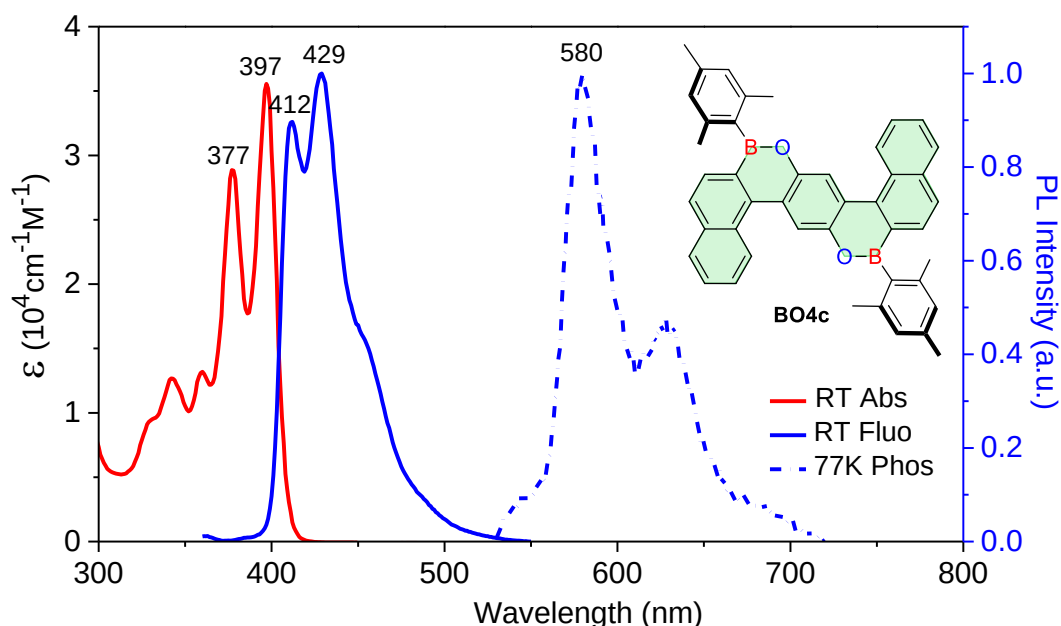
Supplementary Fig. 35. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO3e**. The chemical structure is shown in the inset.



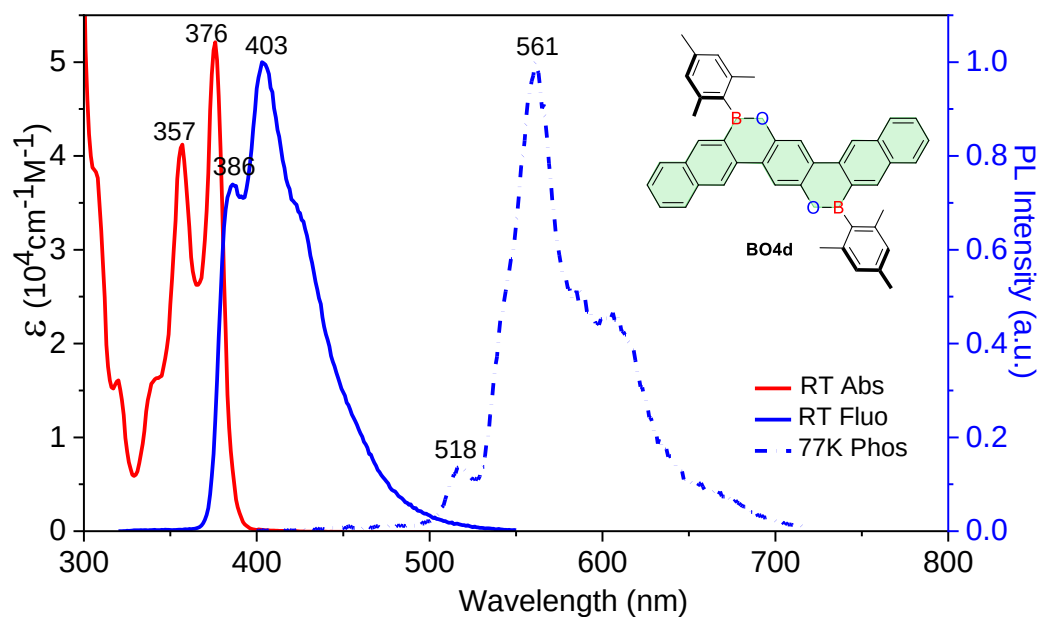
Supplementary Fig. 36. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO4a**. The chemical structure is shown in the inset.



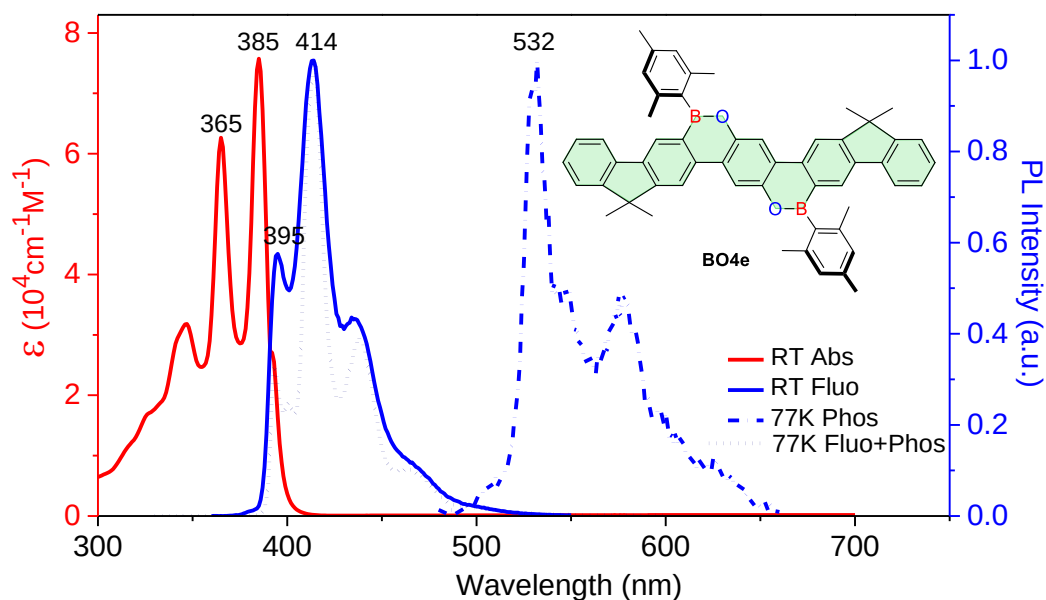
Supplementary Fig. 37. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO4b**. The chemical structure is shown in the inset.



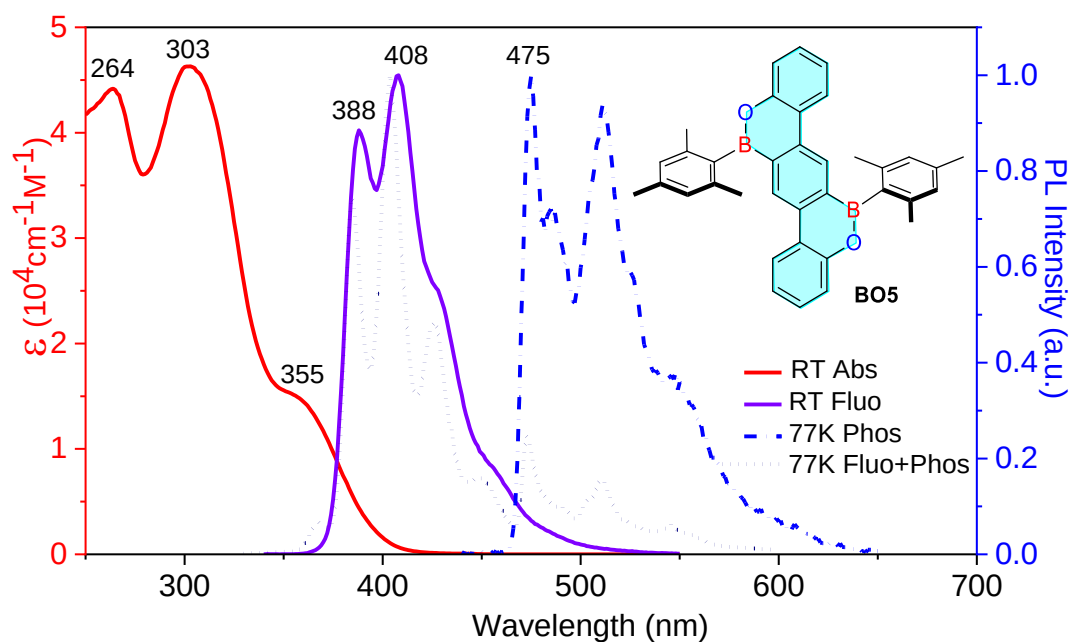
Supplementary Fig. 38. Photophysical properties. Room-temperature absorption spectrum (red solid line) and luminescent spectrum in dichloromethane (blue solid line), and low-temperature (77 K) phosphorescent spectrum (blue dash-dotted line) in 2-MeTHF of **BO4c**. The chemical structure is shown in the inset.



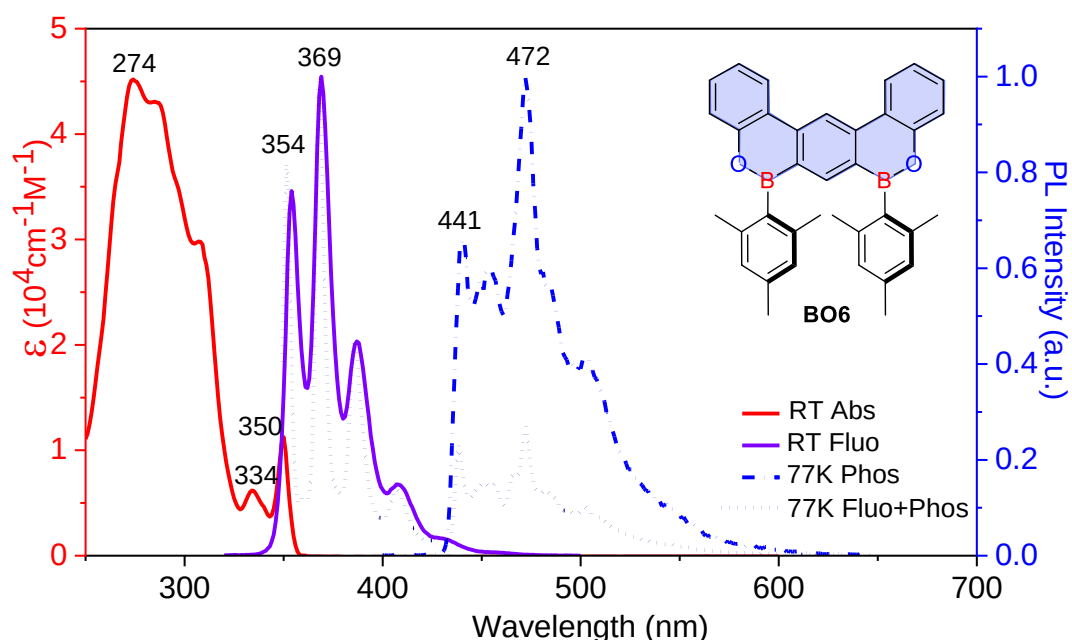
Supplementary Fig. 39. Photophysical properties. Room-temperature absorption spectrum (red solid line) and luminescent spectrum in dichloromethane (blue solid line), and low-temperature (77 K) phosphorescent spectrum (blue dash-dotted line) in 2-MeTHF of **BO4d**. The chemical structure is shown in the inset.



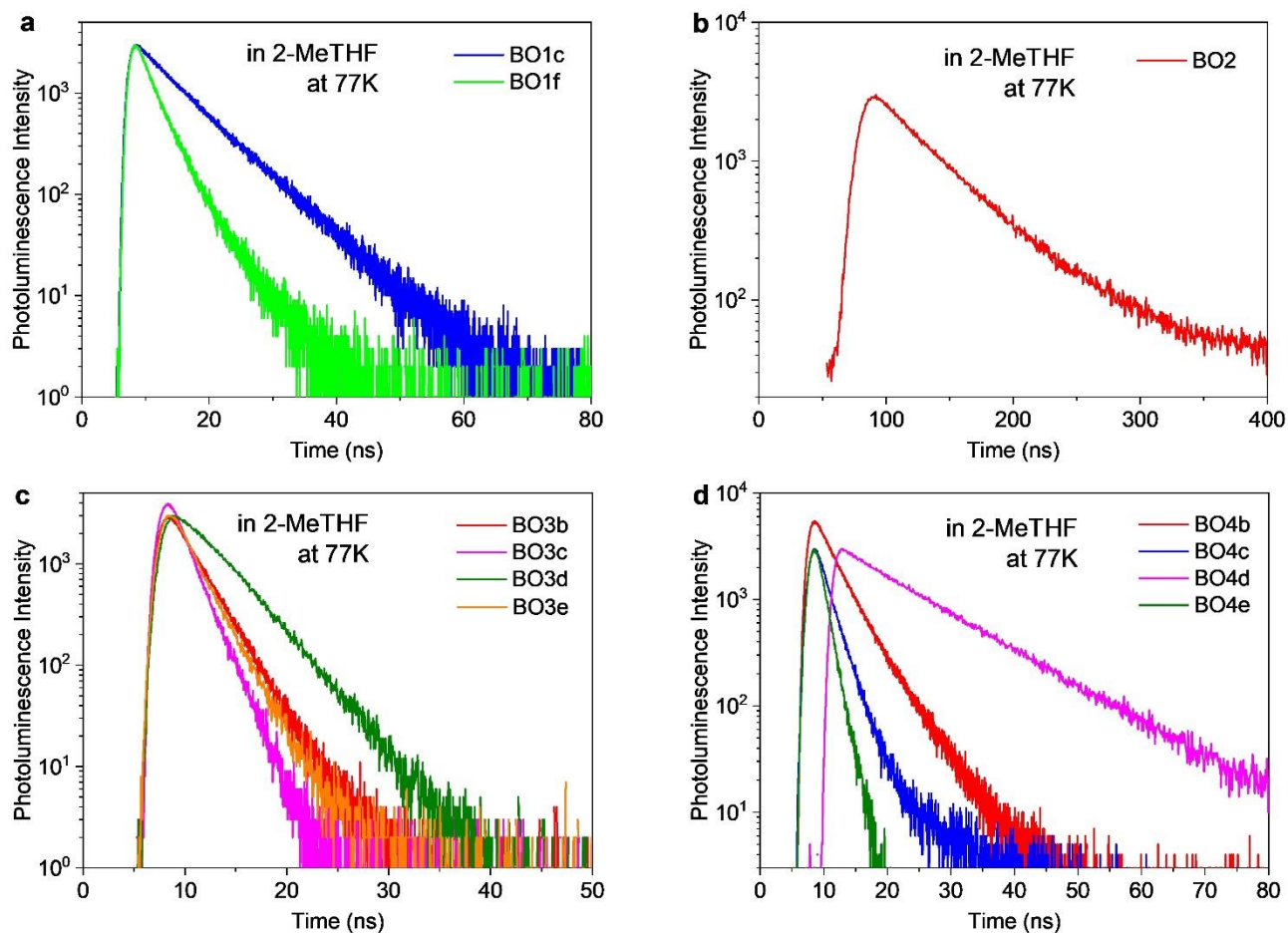
Supplementary Fig. 40. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO4e**. The chemical structure is shown in the inset.



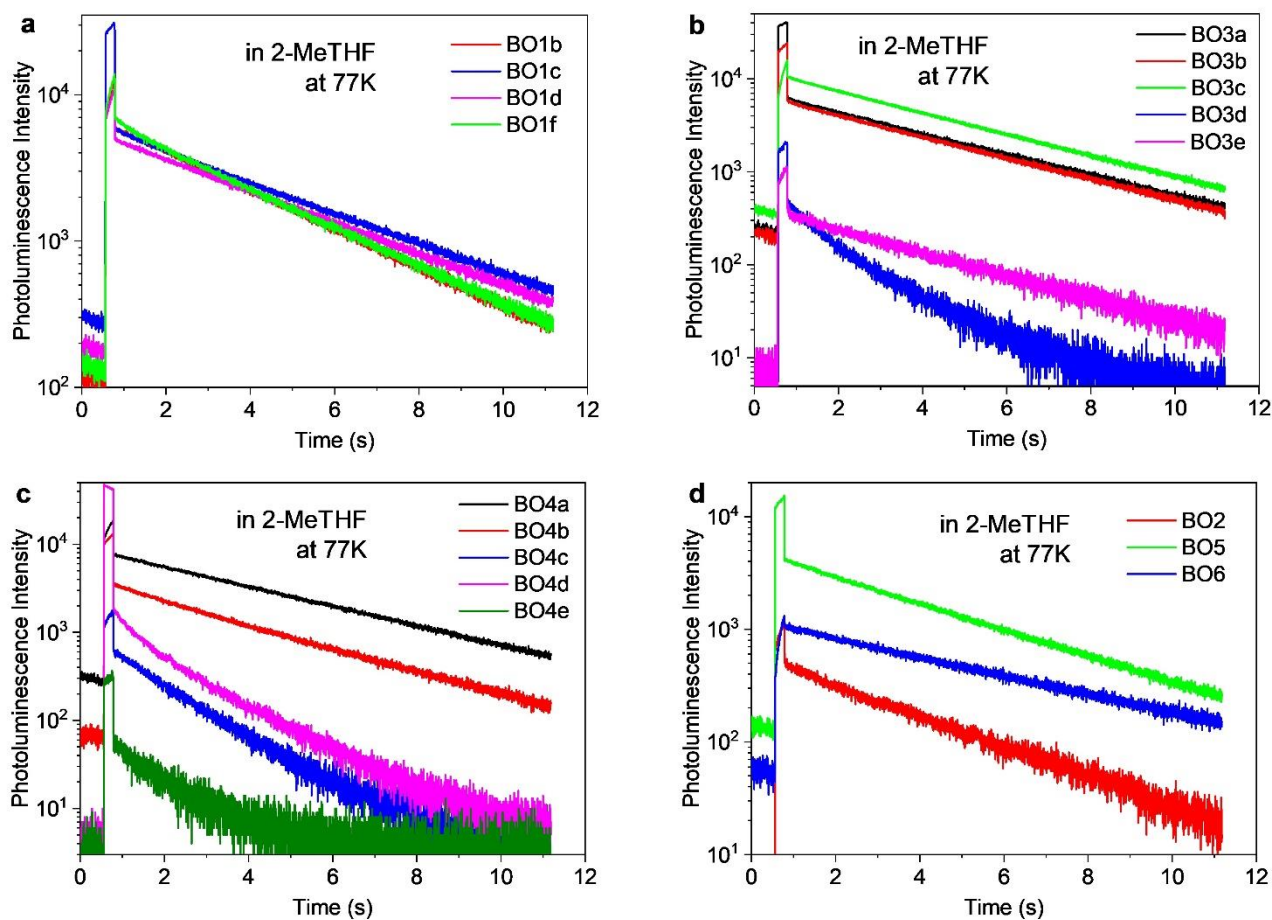
Supplementary Fig. 41. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO5**. The chemical structure is shown in the inset.



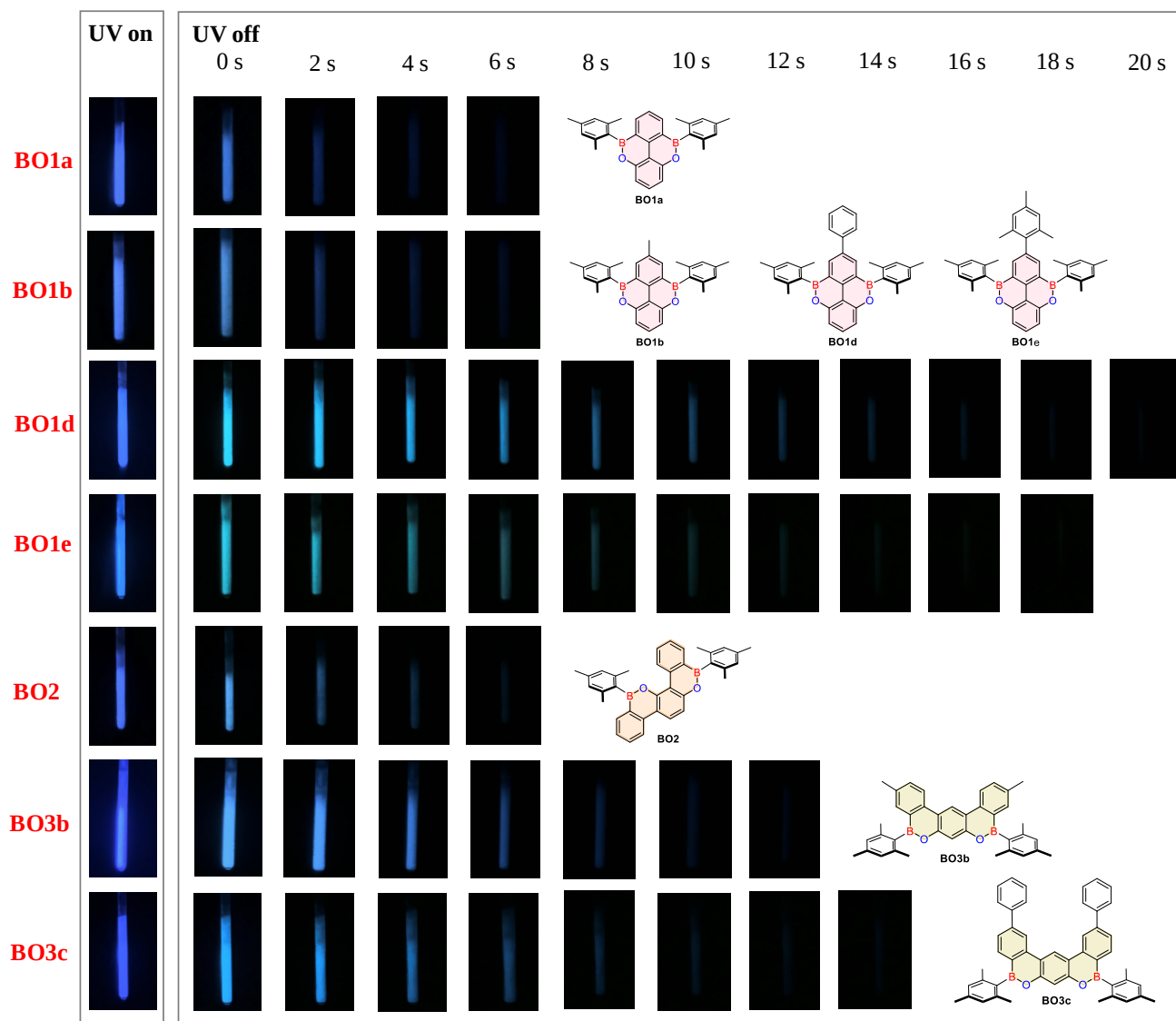
Supplementary Fig. 42. Photophysical properties. Room-temperature absorption spectrum (red solid lines) and fluorescent spectrum (blue solid line) in dichloromethane, and low-temperature (77 K) fluorescent and phosphorescent spectra (blue dash-dotted and navy dotted lines) in 2-MeTHF of **BO6**. The chemical structure is shown in the inset.



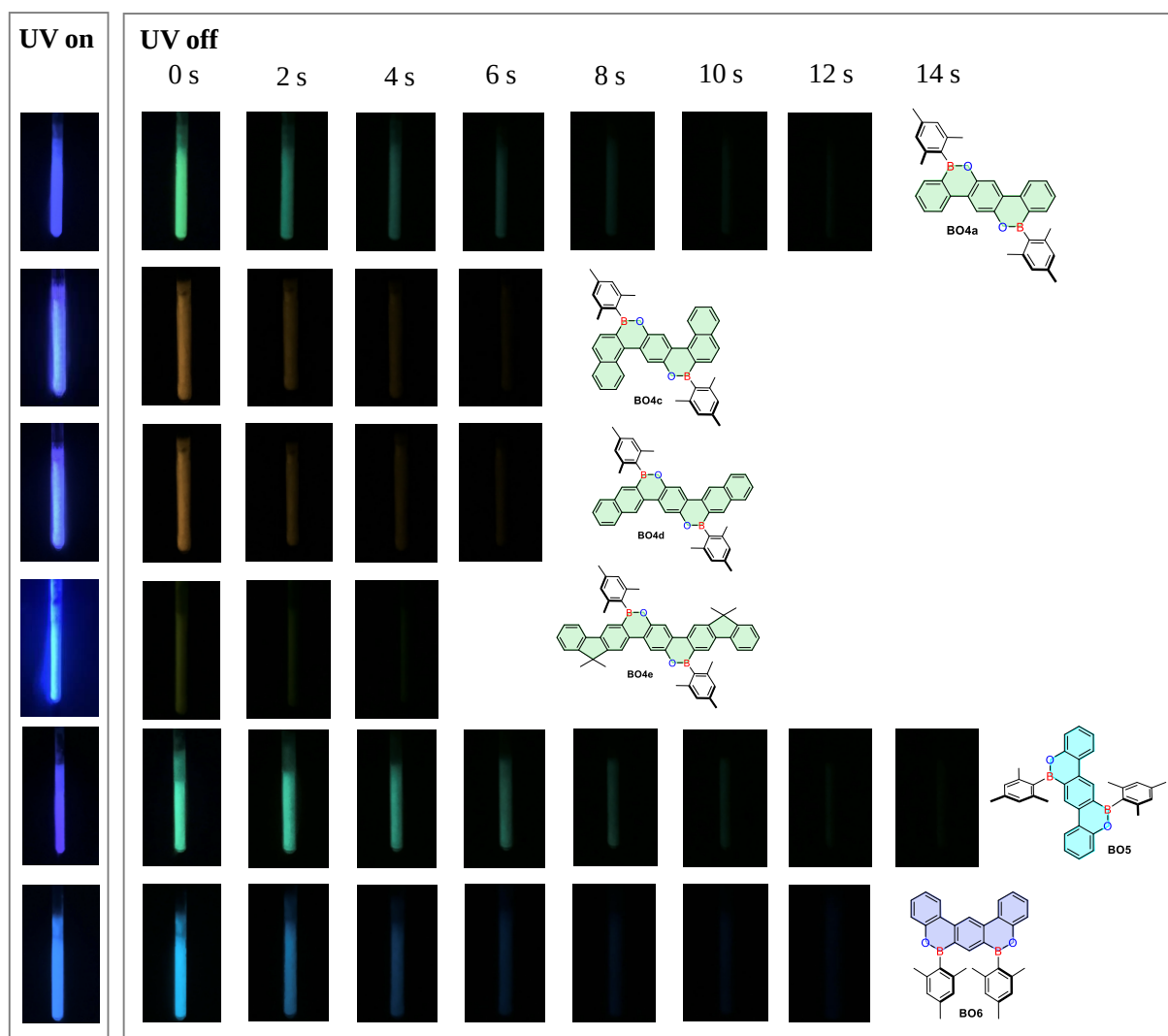
Supplementary Fig. 43. Photophysical properties. Selected PL decay of **a**, BO1c, BO1f; **b**, BO2, **c**, BO3b, BO3c, BO3d, BO3e; **d**, BO4b, BO4c, BO4d, BO4e in 2-MeTHF at 77 K excited at their corresponding first fluorescent peak.



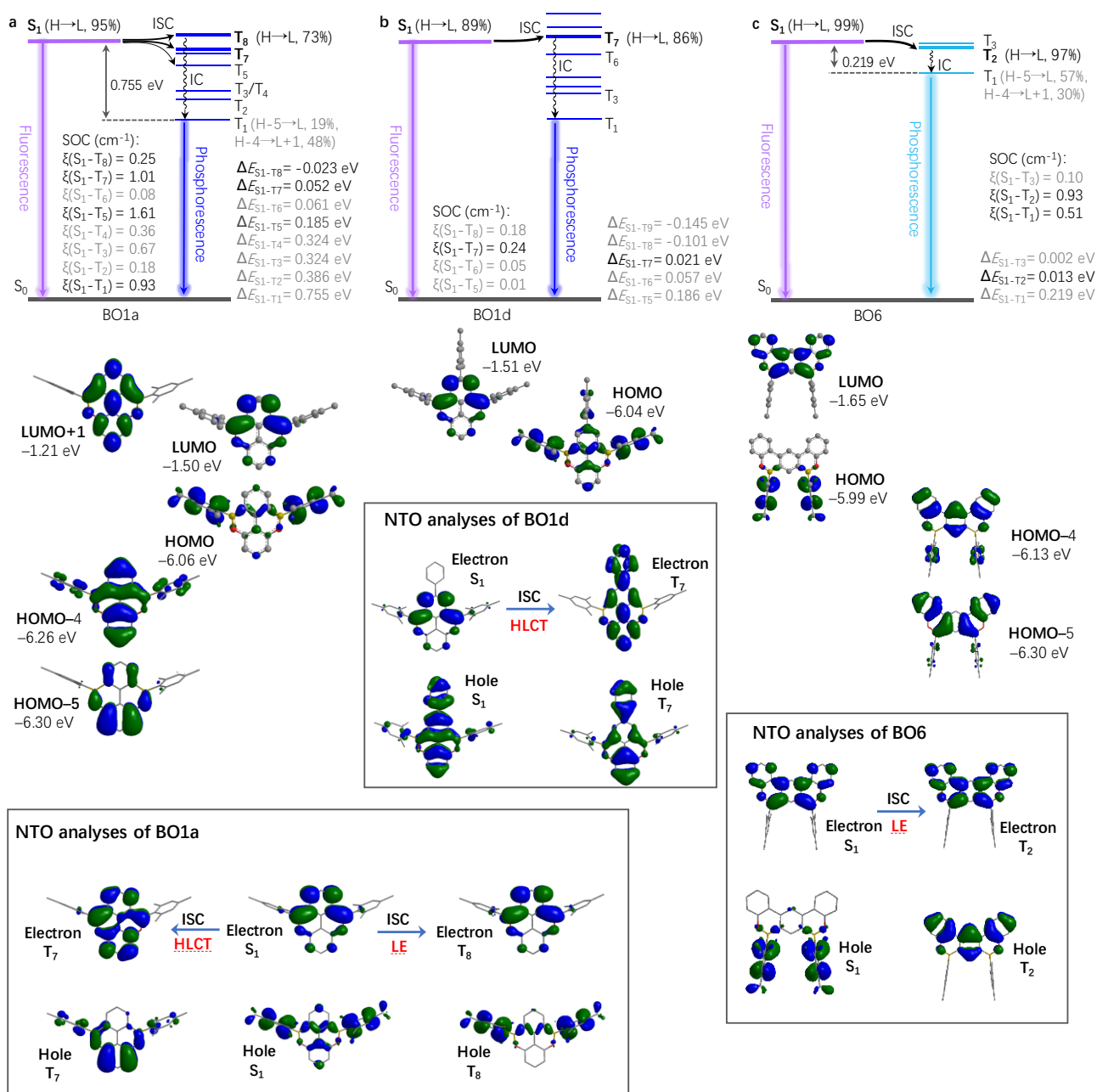
Supplementary Fig. 44. Photophysical properties. Selected PL decay of **a**, BO1b, BO1c, BO1d, BO1f; **b**, BO3a, BO3b, BO3c, BO3d, BO3e; **c**, BO4a, BO4b, BO4c, BO4d, BO4e; **d**, BO2, BO5, BO6 in 2-MeTHF at 77 K excited at their corresponding first phosphorescent peak.



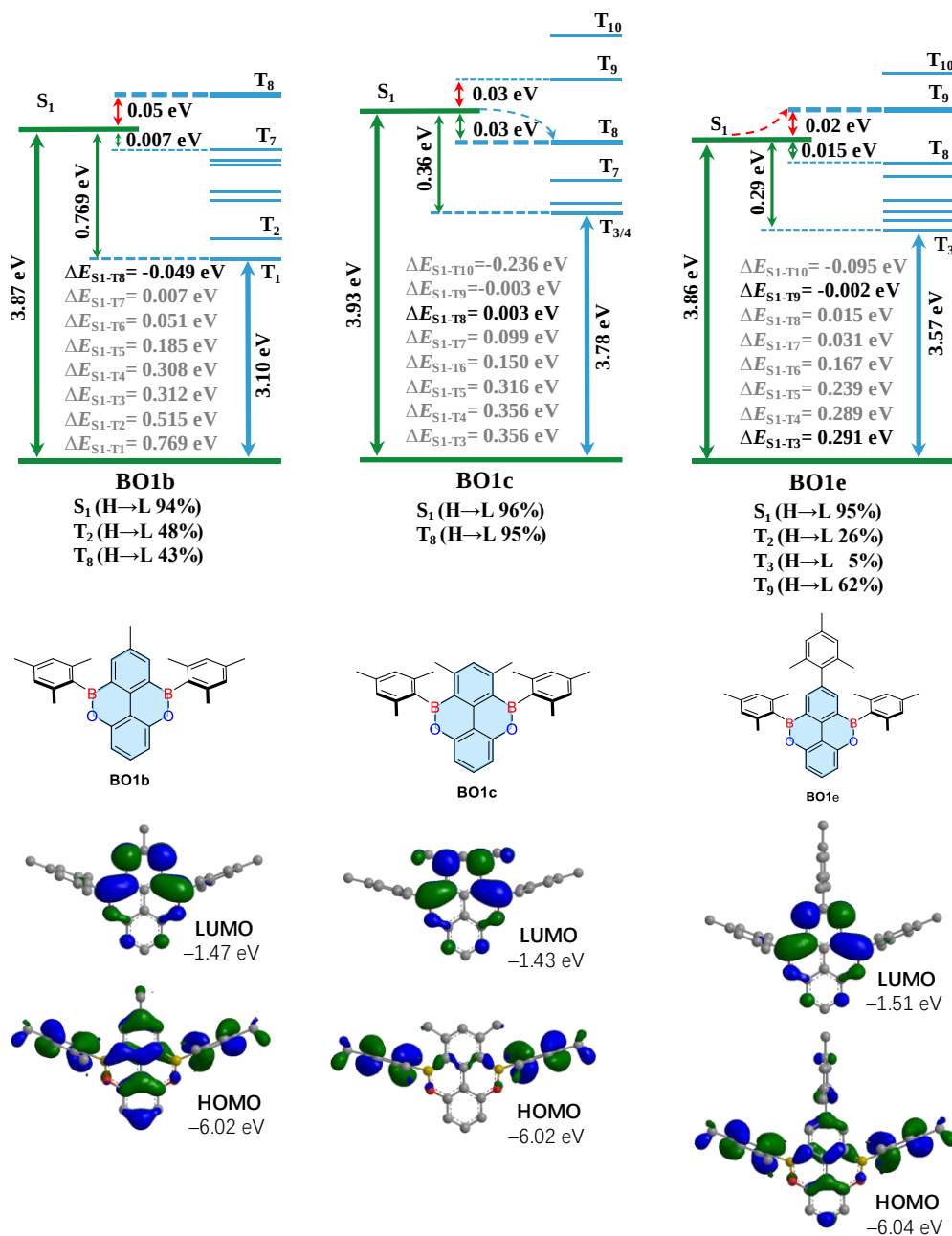
Supplementary Fig. 45. Ultralong phosphorescence. Ultralong phosphorescent photographs of BO1a, BO1b, BO1d, BO1e, BO2, BO3b and BO3c at 77K in THF.



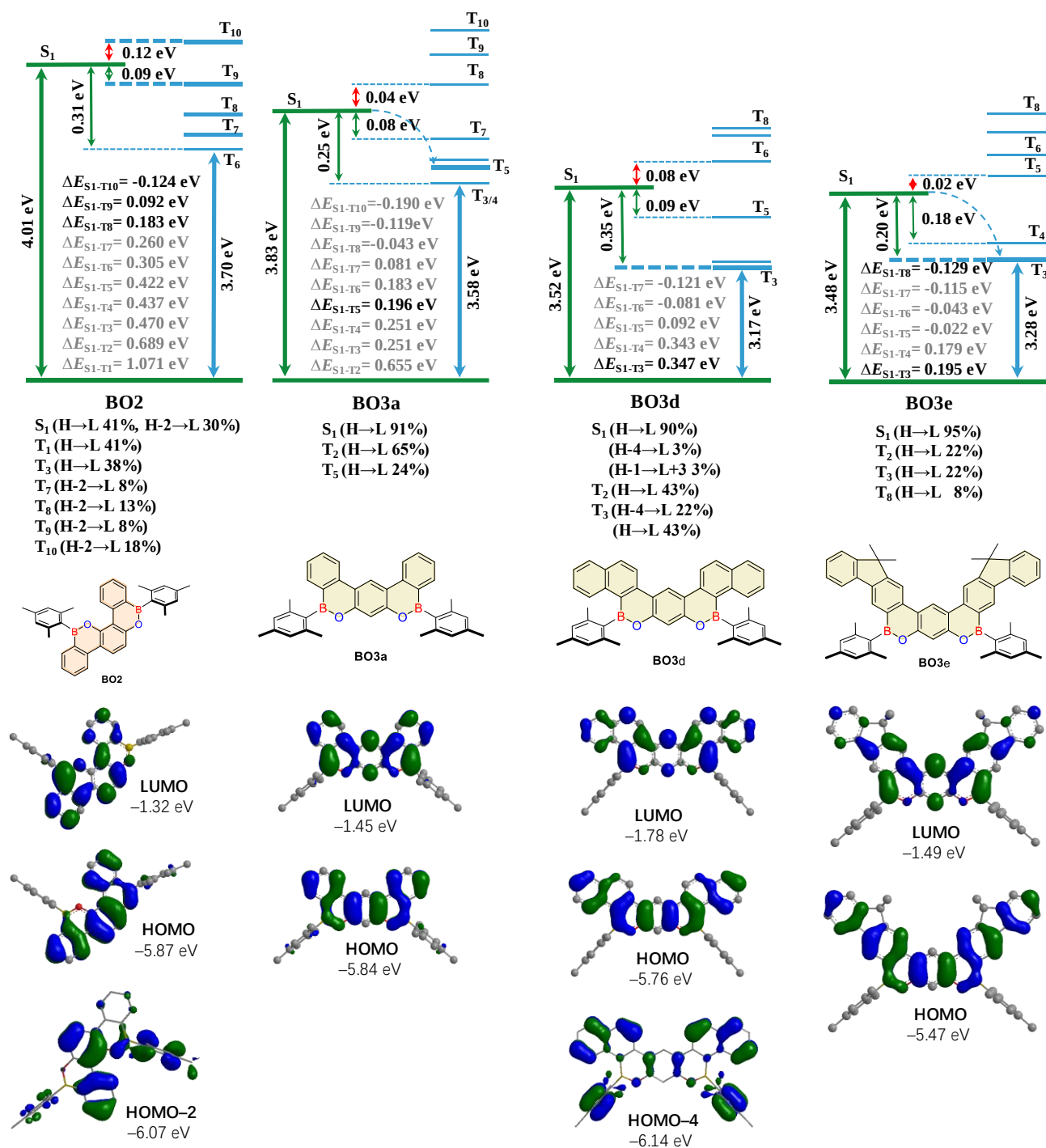
Supplementary Fig. 46. Ultralong phosphorescence. Ultralong phosphorescent photographs of BO4a, BO4c, BO4d, BO4e, BO5 and BO6 at 77K in THF.



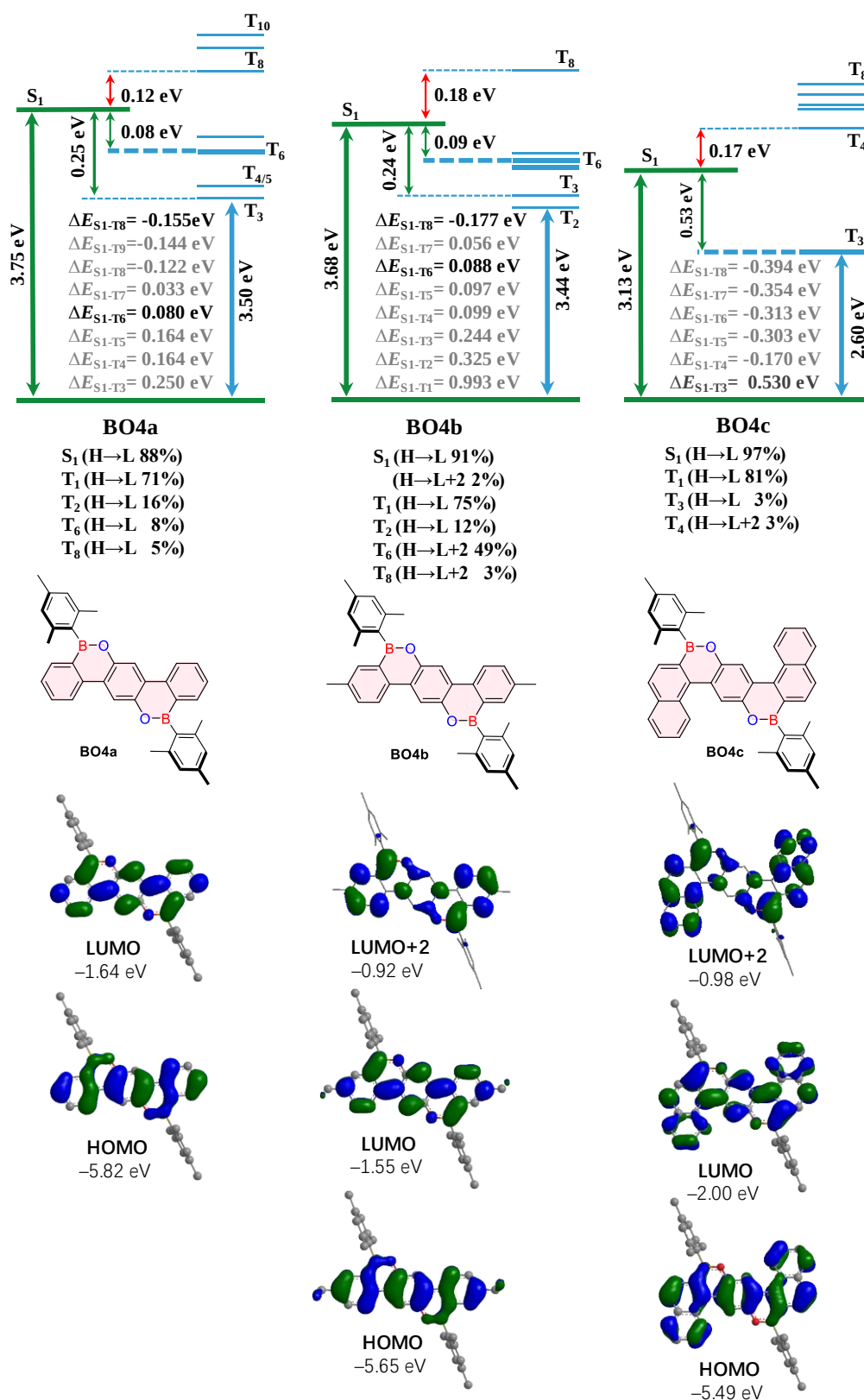
Supplementary Fig. 47. Theoretical calculation. TD-DFT calculated singlet and triplet energy levels, main transition configurations, spin–orbit coupling (SOC) values and natural transition orbital (NTO) analyses of **a**, BO1a; **b**, BO1d; **c**, BO6 at B3LYP/6-31G(d) level based on optimized S_0 geometry. Selected frontier orbital distributions and energy levels are also illustrated.



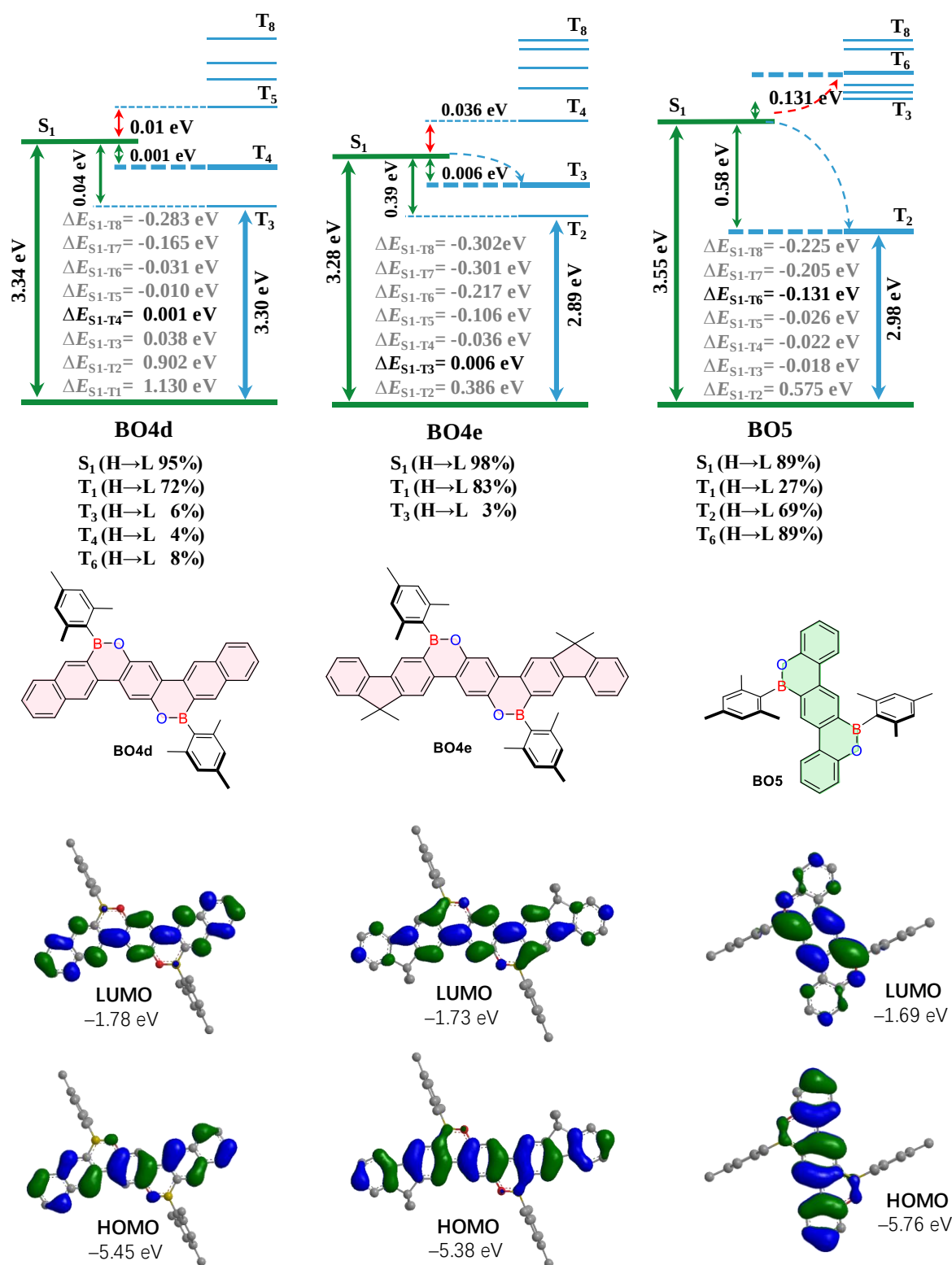
Supplementary Fig. 48. Theoretical calculation. TD-DFT calculated singlet and triplet energy levels, main transition configurations of **BO1b**, **BO1c** and **BO1e** at B3LYP/6-31G(d) level based on optimized S_0 geometry. Selected frontier orbital distributions and energy levels are also illustrated.



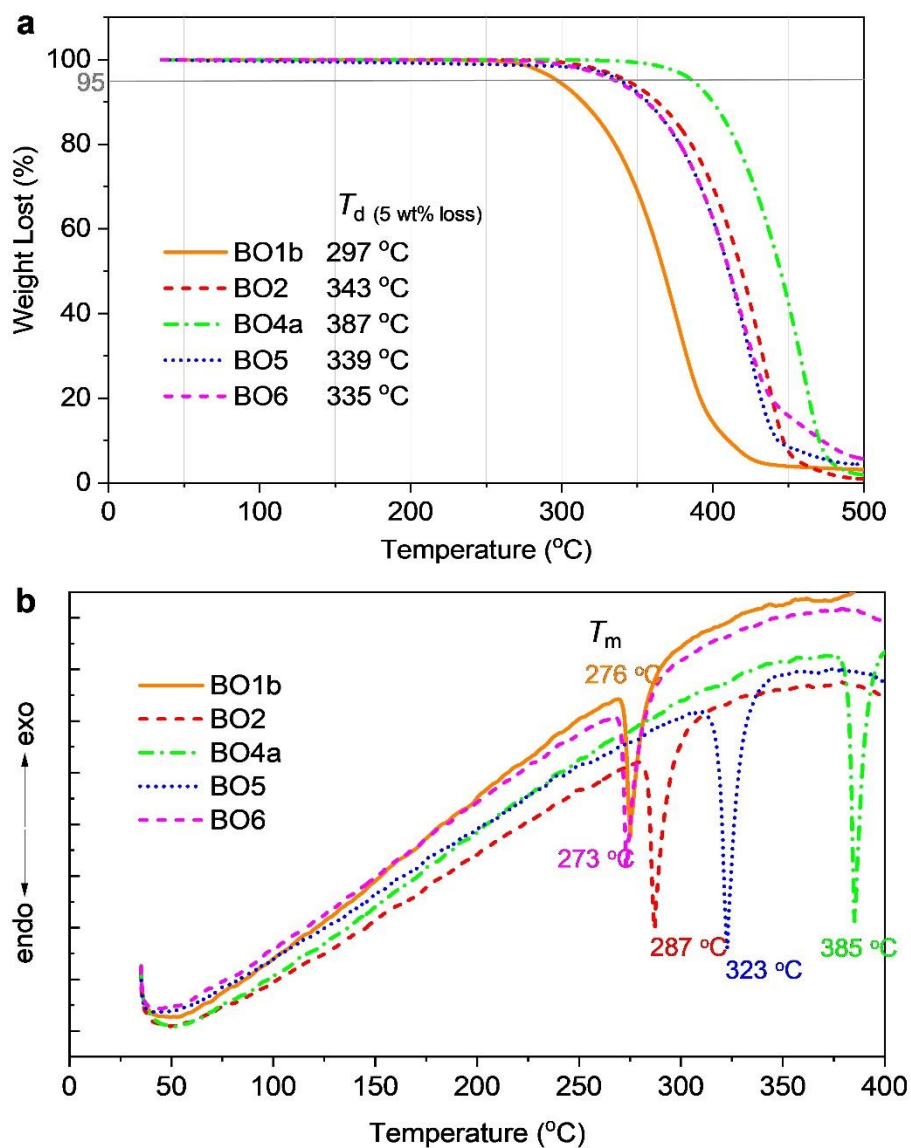
Supplementary Fig. 49. Theoretical calculation. TD-DFT calculated singlet and triplet energy levels, main transition configurations of **BO2**, **BO3a**, **B3d** and **BO3e** at B3LYP/6-31G(d) level based on optimized S_0 geometry. Selected frontier orbital distributions and energy levels are also illustrated.



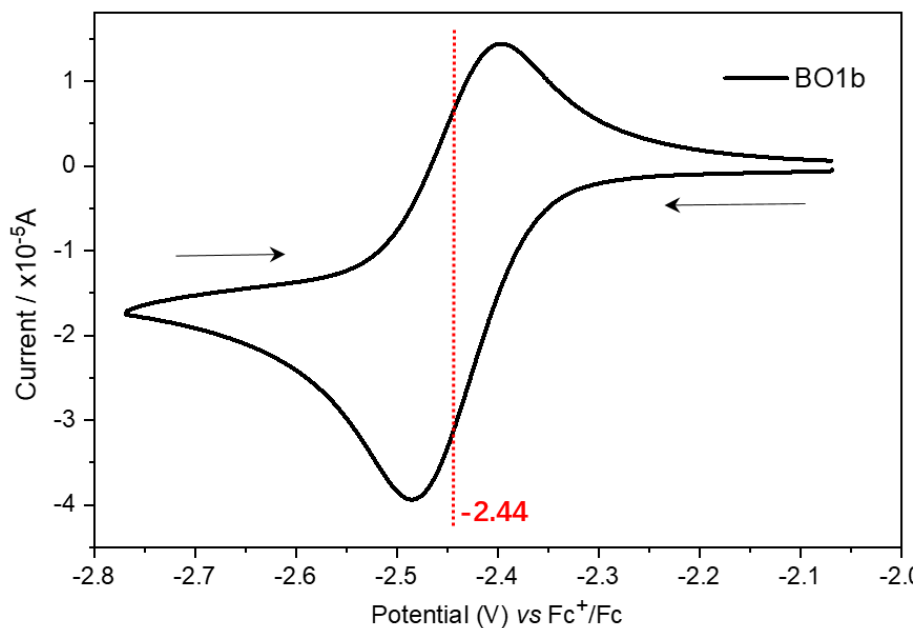
Supplementary Fig. 50. Theoretical calculation. TD-DFT calculated singlet and triplet energy levels, main transition configurations of **BO4a**, **BO4b** and **BO4c** at B3LYP/6-31G(d) level based on optimized S_0 geometry. Selected frontier orbital distributions and energy levels are also illustrated.



Supplementary Fig. 51. 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. Selected frontier orbital distributions and energy levels are also illustrated.



Supplementary Fig. 52. Thermal properties. a, TGA; b, DSC 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.

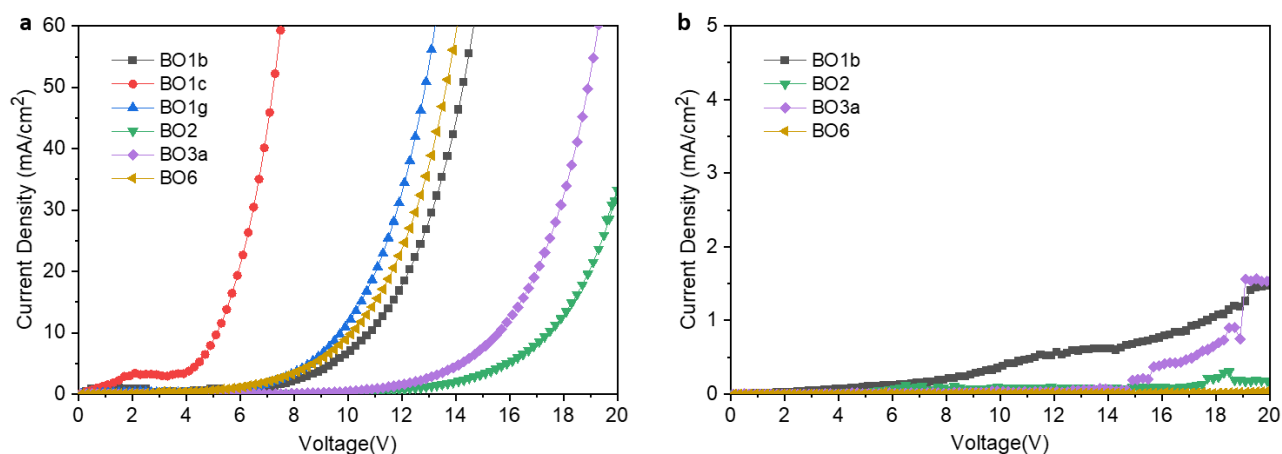


Supplementary Fig. 53. Electrochemical properties. Cyclic voltammogram (CV) of **BO1b** in anhydrous *N,N*-dimethylformamide (DMF).

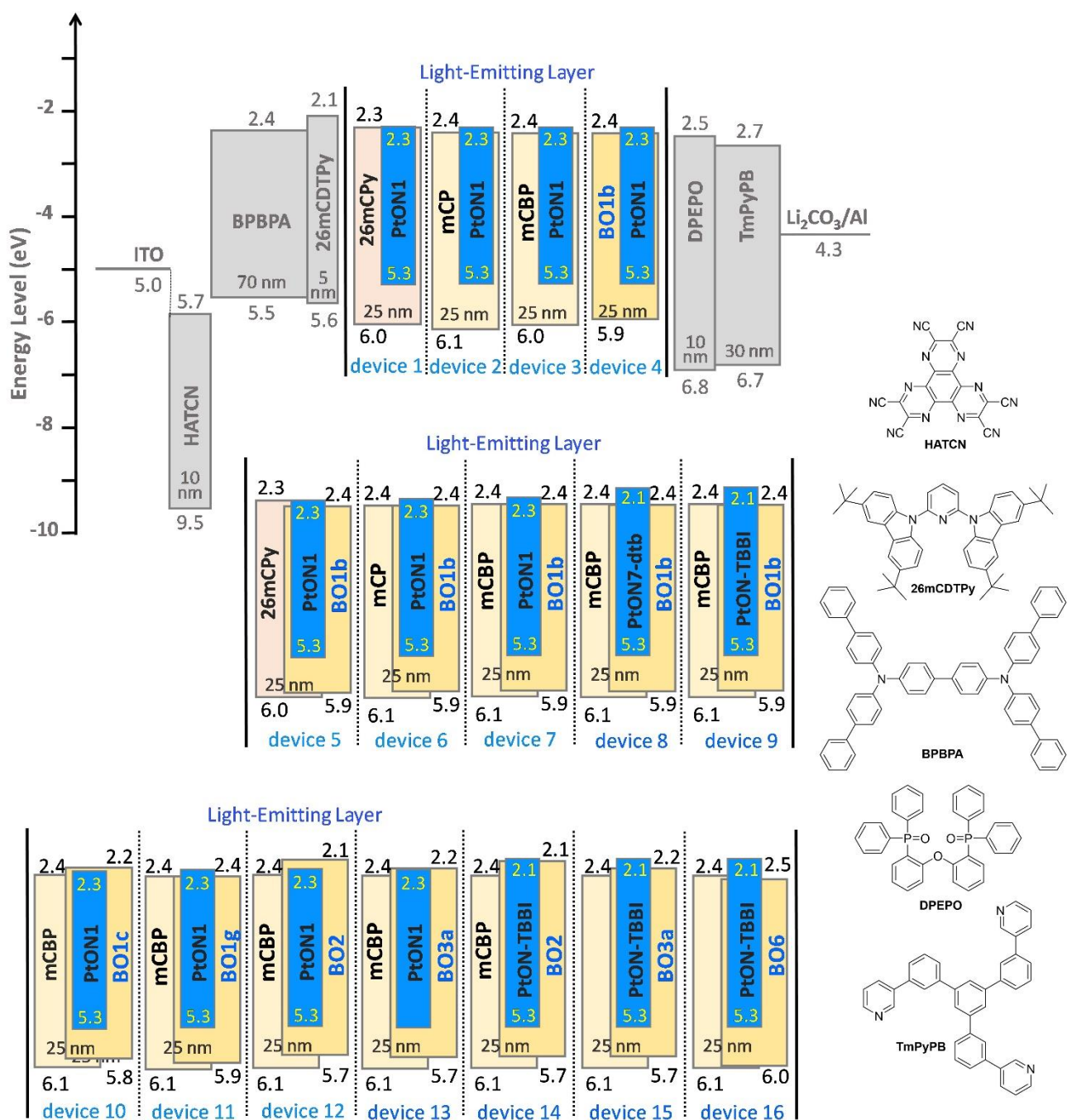
Supplementary Table 6. Electrochemical properties and energy levels of selected dBO-PAHs

Compound	E_{red} (V)	LUMO ^a (eV)	E_g ^b (eV)	HOMO ^c (eV)
BO1b	−2.44	−2.36	3.50	−5.86
BO1c	−2.57	−2.23	3.54	−5.77
BO1g	−2.44	−2.36	3.50	−5.86
BO2	−2.66	−2.14	3.60	−5.74
BO3a	−2.61	−2.19	3.49	−5.68
BO6	−2.33	−2.47	3.48	−5.95

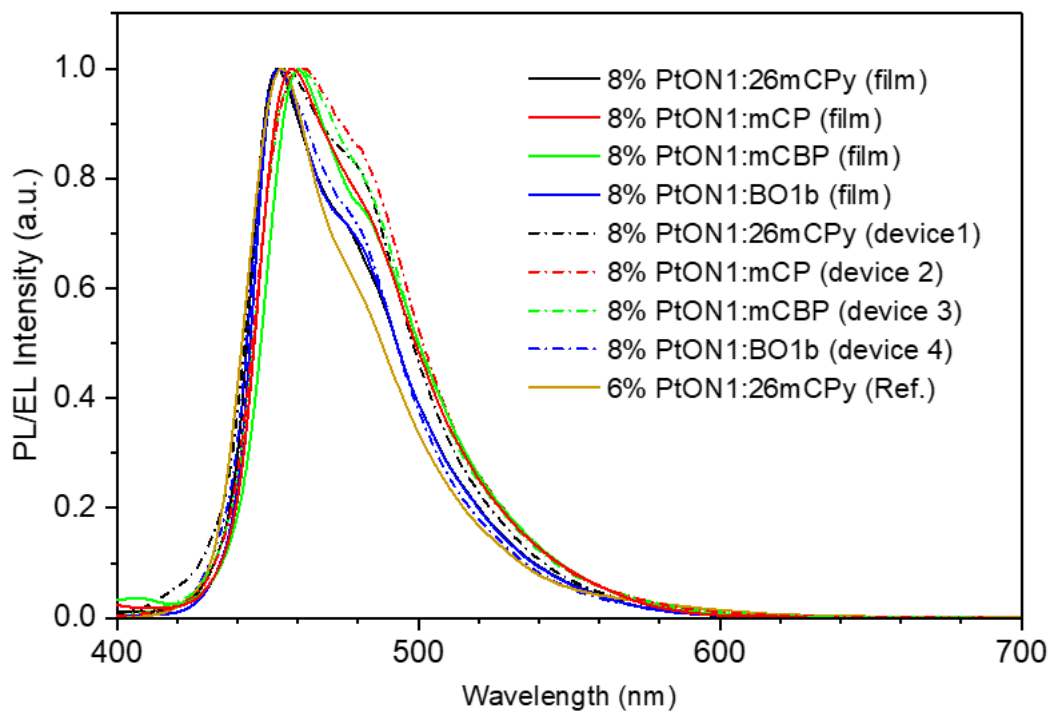
^aLUMO = $-(E_{\text{red}} + 4.8)$ eV. ^bEstimated from the onset wavelength of absorption spectrum measured in dichloromethane. ^cHOMO = LUMO − E_g .



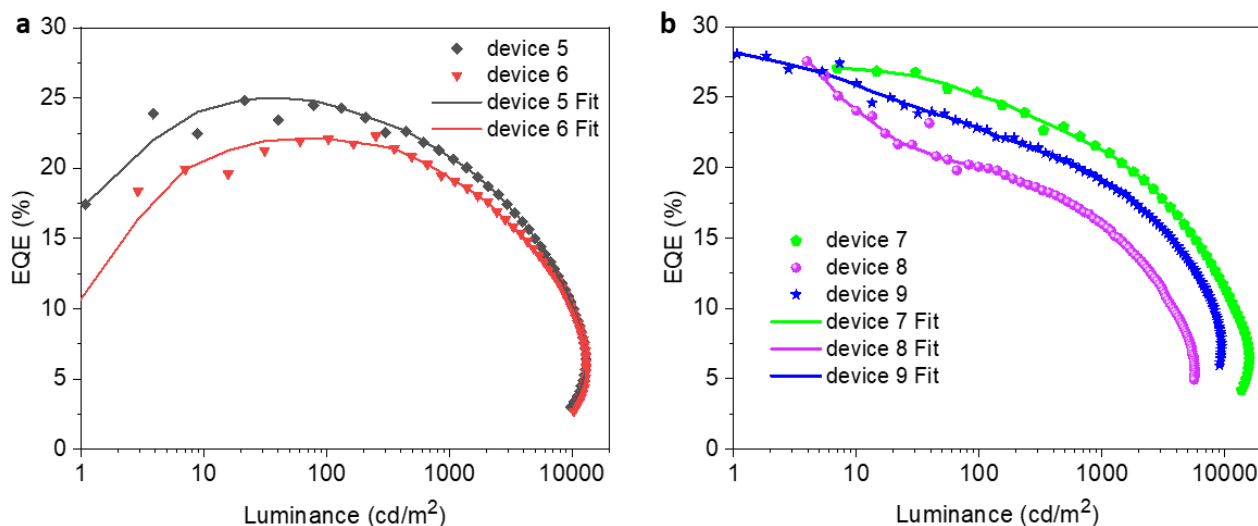
Supplementary Fig. 54. Single carrier devices. **a** Current density–voltage (J – V) characteristics of hole-only device with a structure of ITO/TAPC (10 nm)/dBO-PAH (60 nm)/TAPC (10 nm)/Al. **b** electron-only device with a structure of ITO/TmPyPB (10 nm)/ dBO-PAH (60 nm)/TmPyPB (10 nm)/LiF (1 nm)/Al.



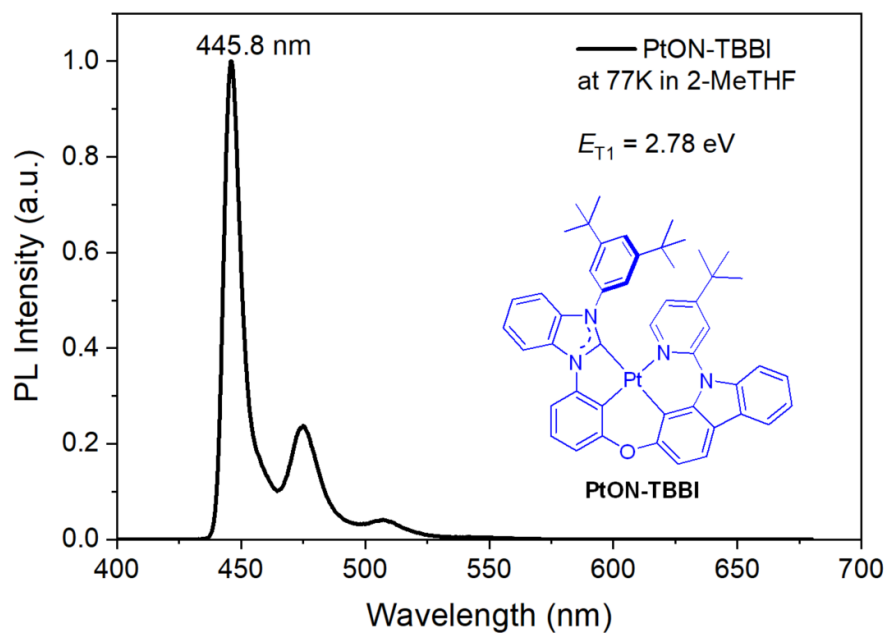
Supplementary Fig. 55. Device and material structures. Energy level diagram of deep-blue OLEDs and chemical structures of materials used.



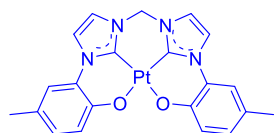
Supplementary Fig. 56. PL and EL spectral comparison. The PL of PtON1-doped thin films versus the EL of PtON1-doped devices. The Ref. is the device with a structure of ITO/HATCN/NPD/TAPC/6%PtON1:26mCPy/DPPS/LiF/Al [Hang, X. C., Fleetham, T., Turner, E., Brooks, J., Li, J. *Angew. Chem. Int. Ed.* **52**, 6753–6756 (2013).



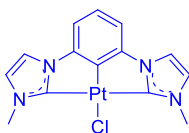
Supplementary Fig. 57. EL properties of deep-blue OLEDs. a, b Fitted EQE vs. luminance plots.



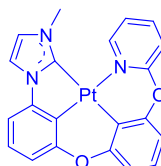
Supplementary Fig. 58. Low-temperature spectrum of PtON-TBBI



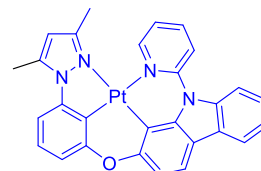
Pt(tetra-NHC) ^[1]
Chem. Commun.
2011, 47, 9075.



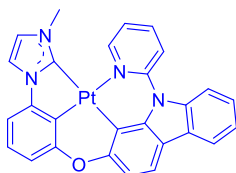
Pt-16 ^[2]
Org. Electron.
2012, 13, 1430.



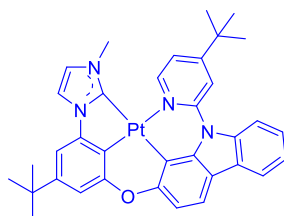
PtO07 ^[3]
Angew. Chem. Int. Ed.
2013, 52, 6753.



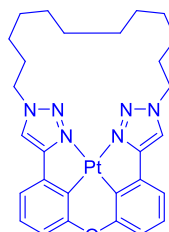
PtON1 ^[3]
Angew. Chem. Int. Ed.
2013, 52, 6753.



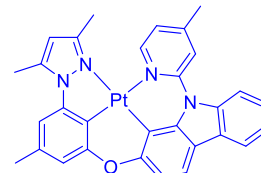
PtON7 ^[3]
Angew. Chem. Int. Ed.
2013, 52, 6753.



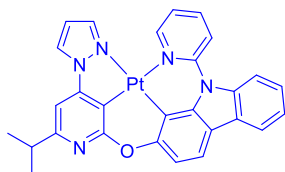
PtON7-dtb ^[4]
Adv. Mater.
2014, 26, 7116.



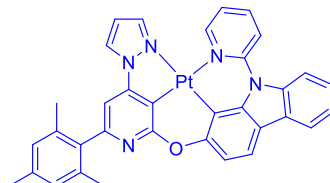
Pt6 ^[5]
Adv. Funct. Mater.
2017, 27, 1604318.



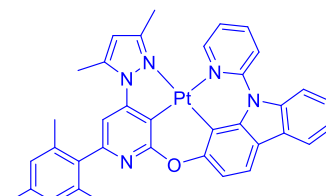
Pt(pzpyOczpy-4m) ^[6]
Mater. Chem. Front.
2019, 3, 2448.



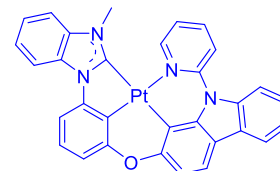
Pt(pzpyOczpy-ⁱPr) ^[7]
Adv. Optical. Mater.
2020, 8, 2000406.



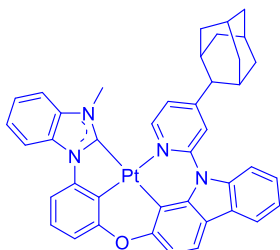
Pt(pzpyOczpy-mes) ^[7]
Adv. Optical. Mater.
2020, 8, 2000406.



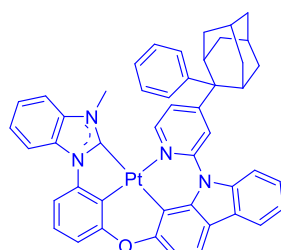
Pt(mpzpyOczpy-mes) ^[8]
ACS Appl. Mater. Interfaces
2021, 13, 52833.



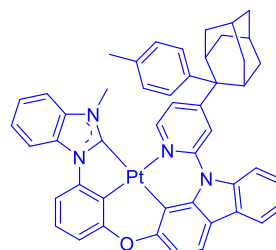
Pt-R ^[9]
Adv. Funct. Mater.
2021, 31, 2100967.



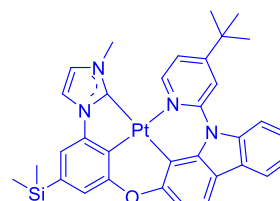
Pt-Ada ^[9]
Adv. Funct. Mater.
2021, 31, 2100967.



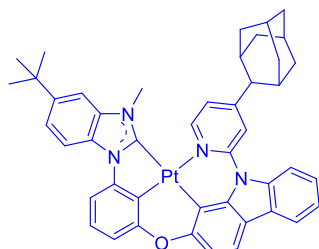
Pt-AdaPh ^[9]
Adv. Funct. Mater.
2021, 31, 2100967.



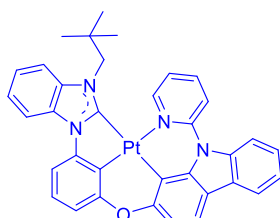
Pt-AdaTol ^[9]
Adv. Funct. Mater.
2021, 31, 2100967.



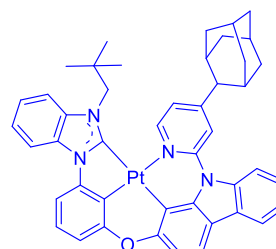
PtON7-TMS ^[10]
ACS Appl. Mater. Interfaces
2022, 14, 34901.



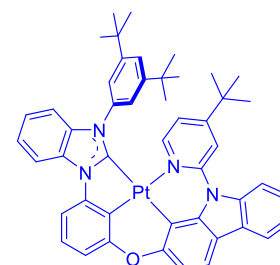
t-Pt-Ad ^[11]
Chem. Eng. J.
2022, 450, 137836.



Pt-NPT ^[11]
Chem. Eng. J.
2022, 450, 137836.



Pt-adNPT ^[11]
Chem. Eng. J.
2022, 450, 137836.



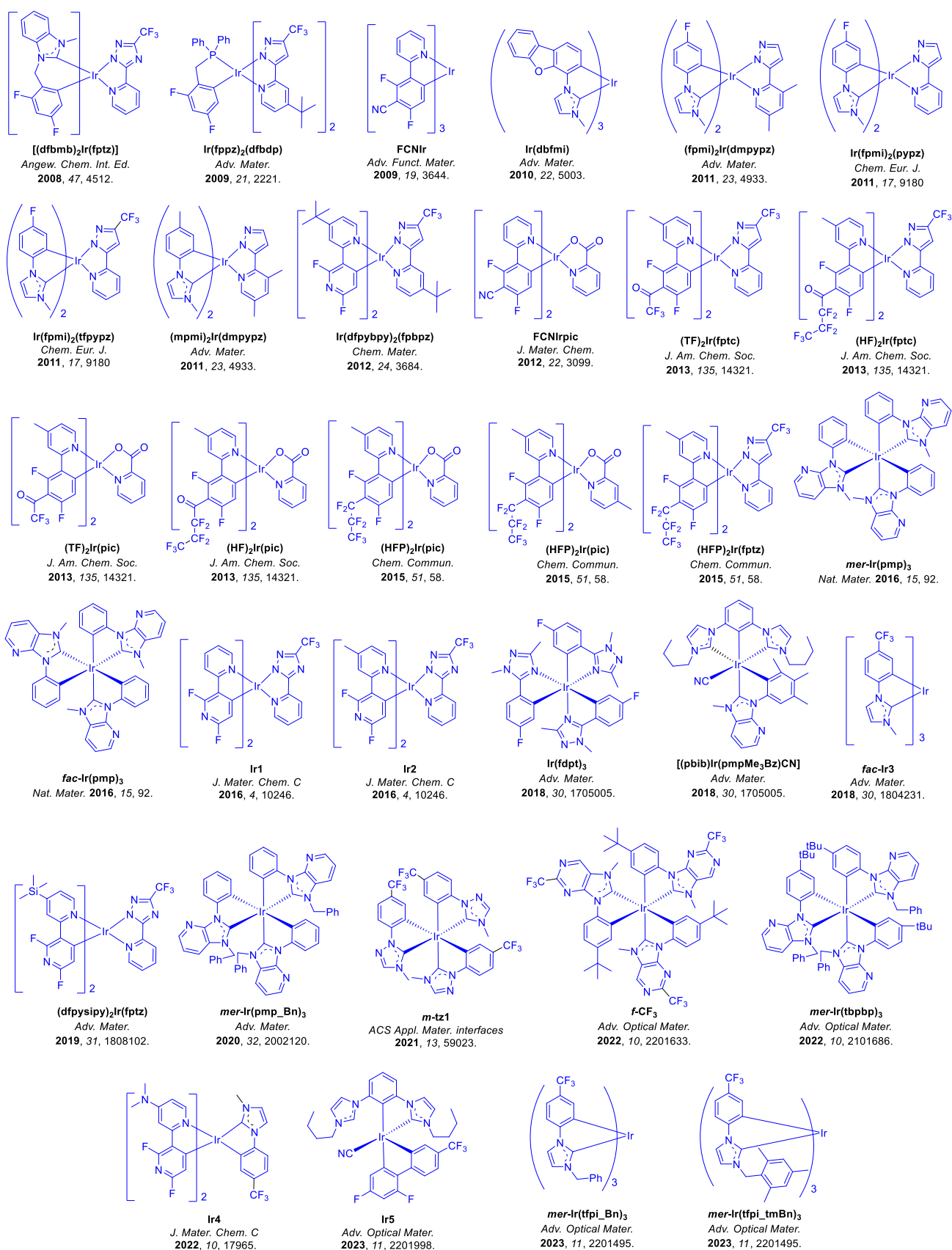
PtON-TBBI ^[12]
Nat. Photonics
2022, 16, 212.

Supplementary Fig. 59. Deep-blue Pt(II) emitters. Chemical structures of dopants for Pt(II)-based deep-blue OLEDs discussed in this work.

Supplementary Table 7. 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
PtON1/ BO1c /mCBP (device 10)	(0.141, 0.168)	456	27219	27.8/24.3/20.0	This work
PtON1/ BO1g /mCBP (device 11)	(0.140, 0.170)	458	22638	25.1/21.9/19.2	This work
PtON-TBBI/ BO2 /mCBP (device 14)	(0.135, 0.103)	458	14481	22.2/18.0/14.9	This work
PtON-TBBI/ BO3a /mCBP(device15)	(0.134, 0.107)	459	15765	19.6/17.0/14.8	This work
PtON-TBBI/ BO6 /mCBP (device 16)	(0.133, 0.111)	459	10071	21.7/16.2/13.4	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.



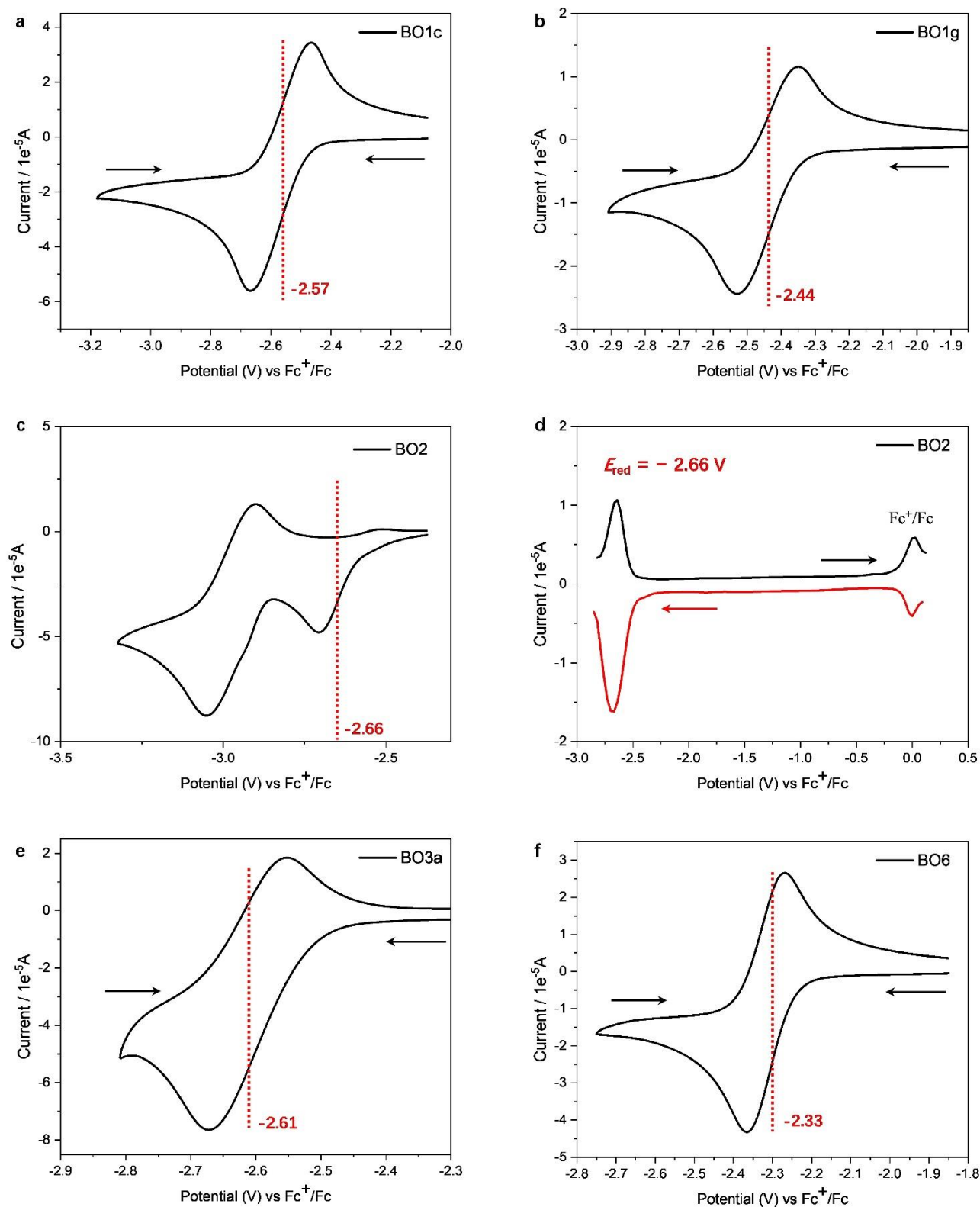
Supplementary Fig. 60. Deep-blue Ir(II) emitters. Chemical structures of dopants for Ir(III)-based deep-blue OLEDs discussed in this work.

Supplementary Table 8. Performance data for Ir(III)-based deep-blue OLEDs with CIE_y < 0.20

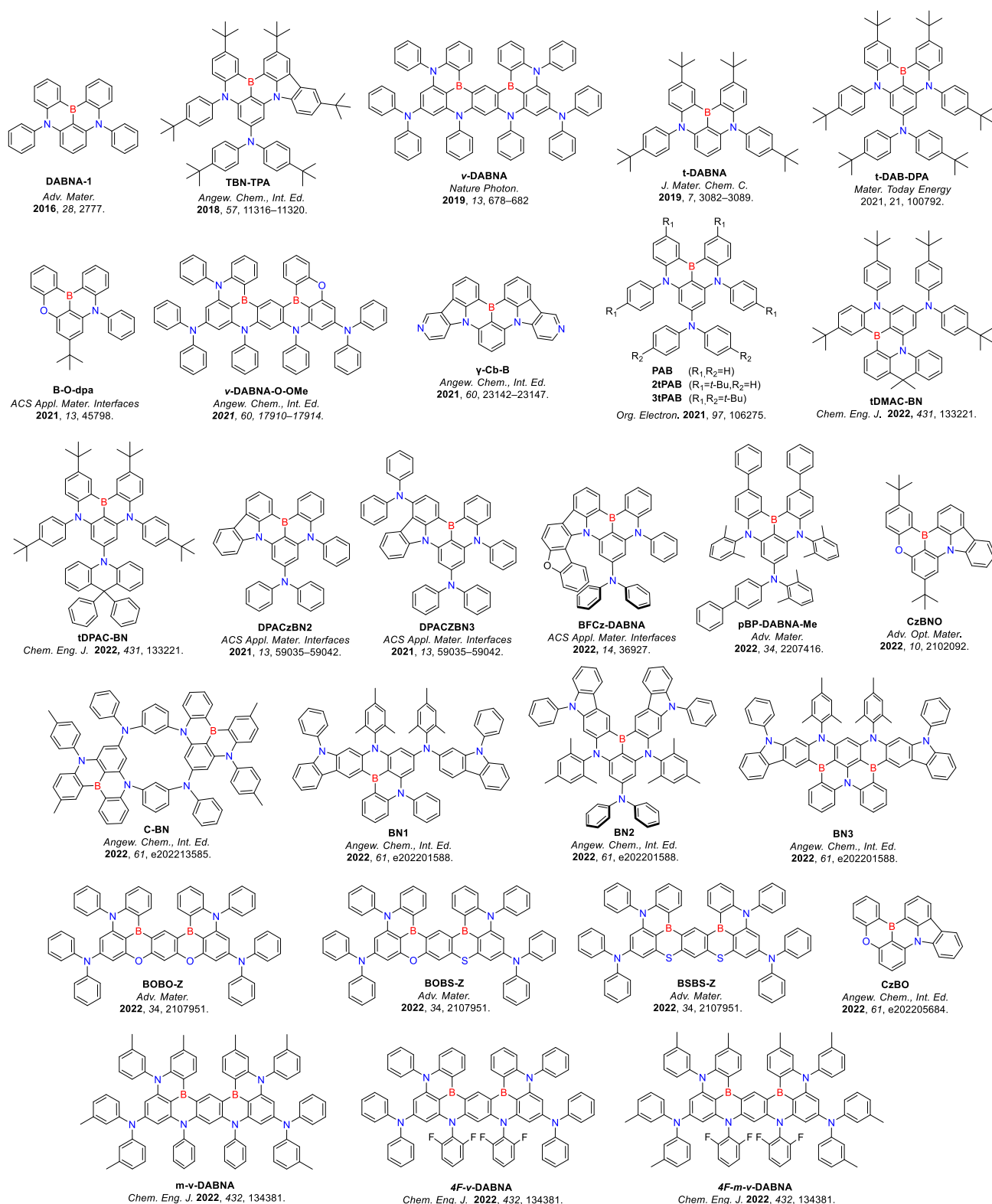
emitter/host	CIE (x, y)	λ_{EL} (nm)	L_{max} (cd/m ²)	EQE(%) max /100/1000	Reference/year
PtON1/ BO1b (device 4)	(0.138, 0.134)	453	8007	22.8/21.5/16.3	This work
PtON1/ BO1b /26mCPy (device 5)	(0.138, 0.130)	454	12982	24.8/24.4/20.9	This work
PtON1/ BO1b /mCP (device 6)	(0.138, 0.154)	460	13098	22.3/20.0/19.2	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
PtON1/ BO1c /mCBP (device 10)	(0.141, 0.168)	456	27219	27.8/24.3/20.0	This work
PtON1/ BO1g /mCBP (device 11)	(0.140, 0.170)	458	22638	25.1/21.9/19.2	This work
PtON-TBBI/ BO2 /mCBP (device 14)	(0.135, 0.103)	458	14481	22.2/18.0/14.9	This work
PtON-TBBI/ BO3a /mCBP(device15)	(0.134, 0.107)	459	15765	19.6/17.0/14.8	This work
PtON-TBBI/ BO6 /mCBP (device 16)	(0.133, 0.111)	459	10071	21.7/16.2/13.4	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 (fpbpz)/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/t-BuCPO	(0.15, 0.13)	430	5080	11.2/10.8/8.3	[29]/2016
Ir2/t-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

<i>mer</i> -Ir(dbfmi) ₃ /TSPO1	(0.14, 0.14)	---	<2000	18.2/---/---	[30]/2017
<i>fac</i> -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(mpPic)/mCBP:TSPO1	(0.14, 0.19)	450	2800	31.9/30.4/24.7	[33]/2019
<i>mer</i> -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
<i>m</i> -tz1/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
<i>f</i> -CF ₃ / <i>t</i> -DABNA/mCBP ^b	(0.13, 0.14)	464	8188	23.8/16.4/10.4	[39]/2022
<i>mer</i> -Ir(tbpbp) ₃ / DPEPO	(0.16, 0.13)	449	2386	24.9/22.1/<10	[40]/2022
Ir/ <i>v</i> -DABNA/mCBP ^b	(0.13, 0.19)	---	11100	15.8/<15.0/10.5	[41]/2023
<i>mer</i> -Ir(tfpi_Bn) ₃ /TSPO1	(0.16, 0.08)	424	632	12.2/10.8/<5	[42]/2023
<i>mer</i> -Ir(tfpi_tmBn) ₃ /TSPO1	(0.16, 0.08)	424	940	14.9/11.7/<5	[42]/2023

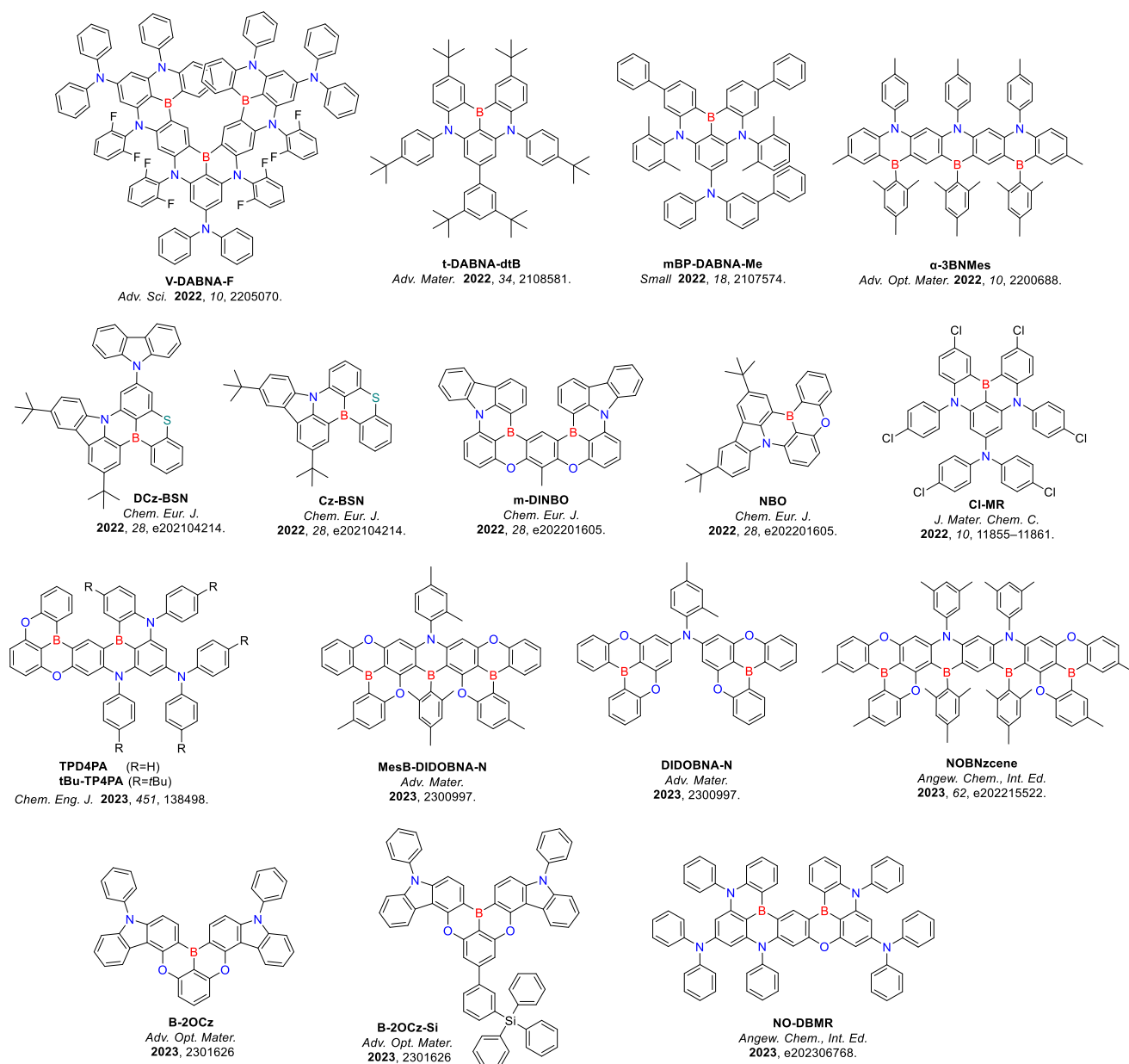
^a EQE @ Max/100/1000 cd m⁻². ^b Hyperfluorescent OLED.



Supplementary Fig. 61. Electrochemical properties. Cyclic voltammogram (CV) of **a**, BO1c; **b**, BO1g; **c**, BO2; **e**, BO3a; **f**, BO6; **d**, differential pulse voltammetry (DPV) of BO2 in anhydrous N,N -dimethylformamide (DMF).



Supplementary Fig. 62. Deep-blue MR-BN-PAH emitters. Chemical structures of dopants for MR-BN-PAH-based deep-blue OLEDs discussed in this work.



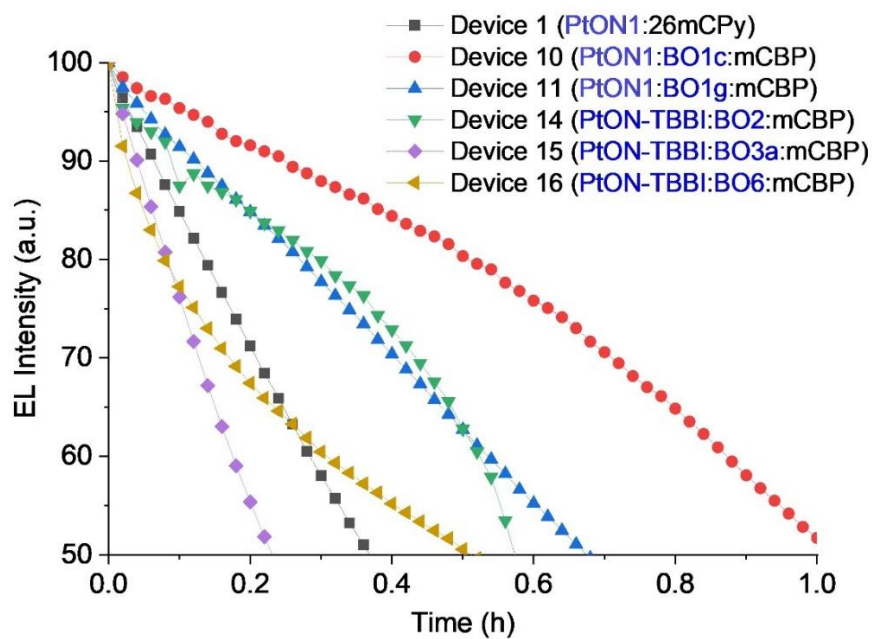
Supplementary Fig. 63. Deep-blue MR-BN-PAH emitters. Chemical structures of dopants for MR-BN-PAH-based deep-blue OLEDs discussed in this work.

Supplementary Table 9. Performance data for BN-based deep-blue OLEDs with CIE_y < 0.20

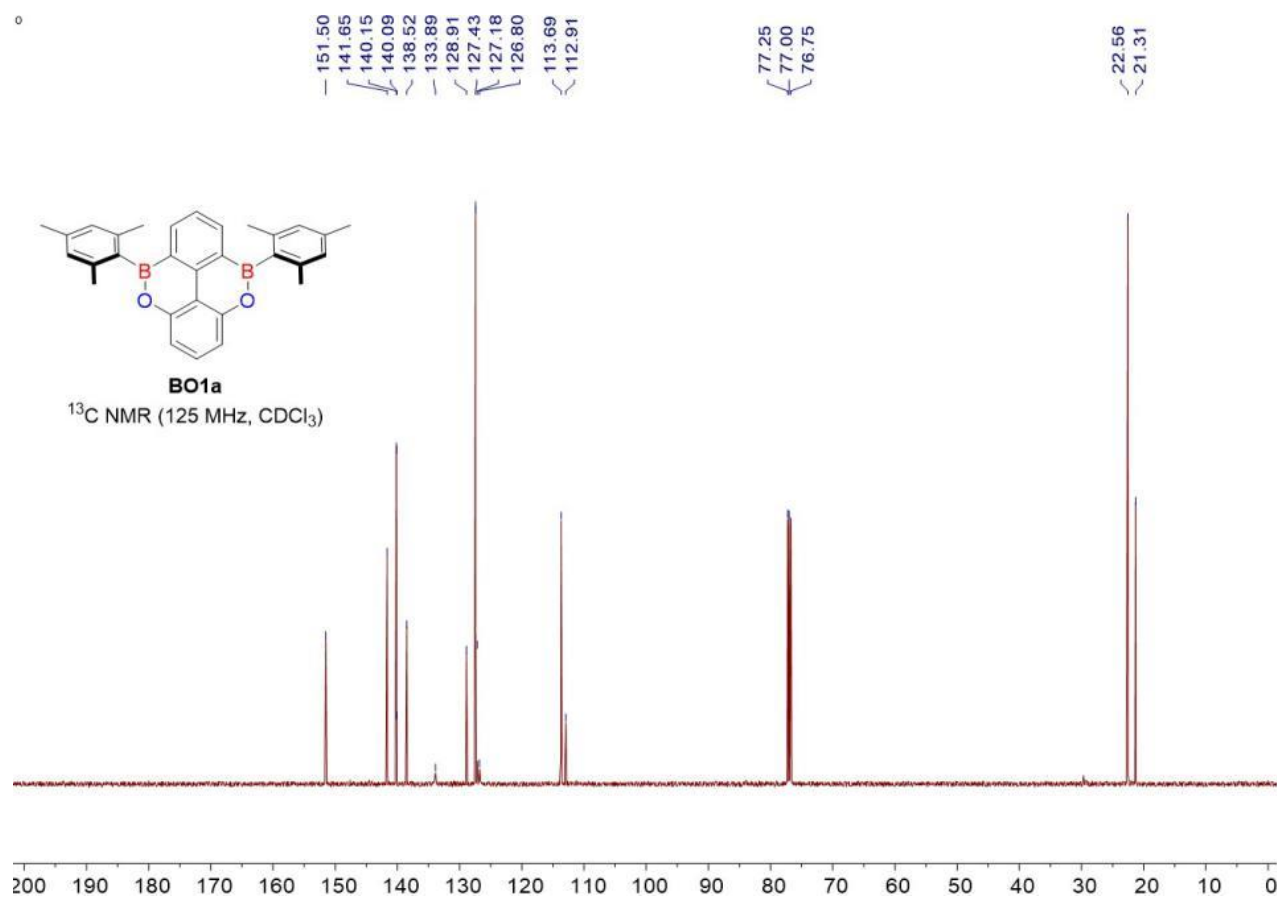
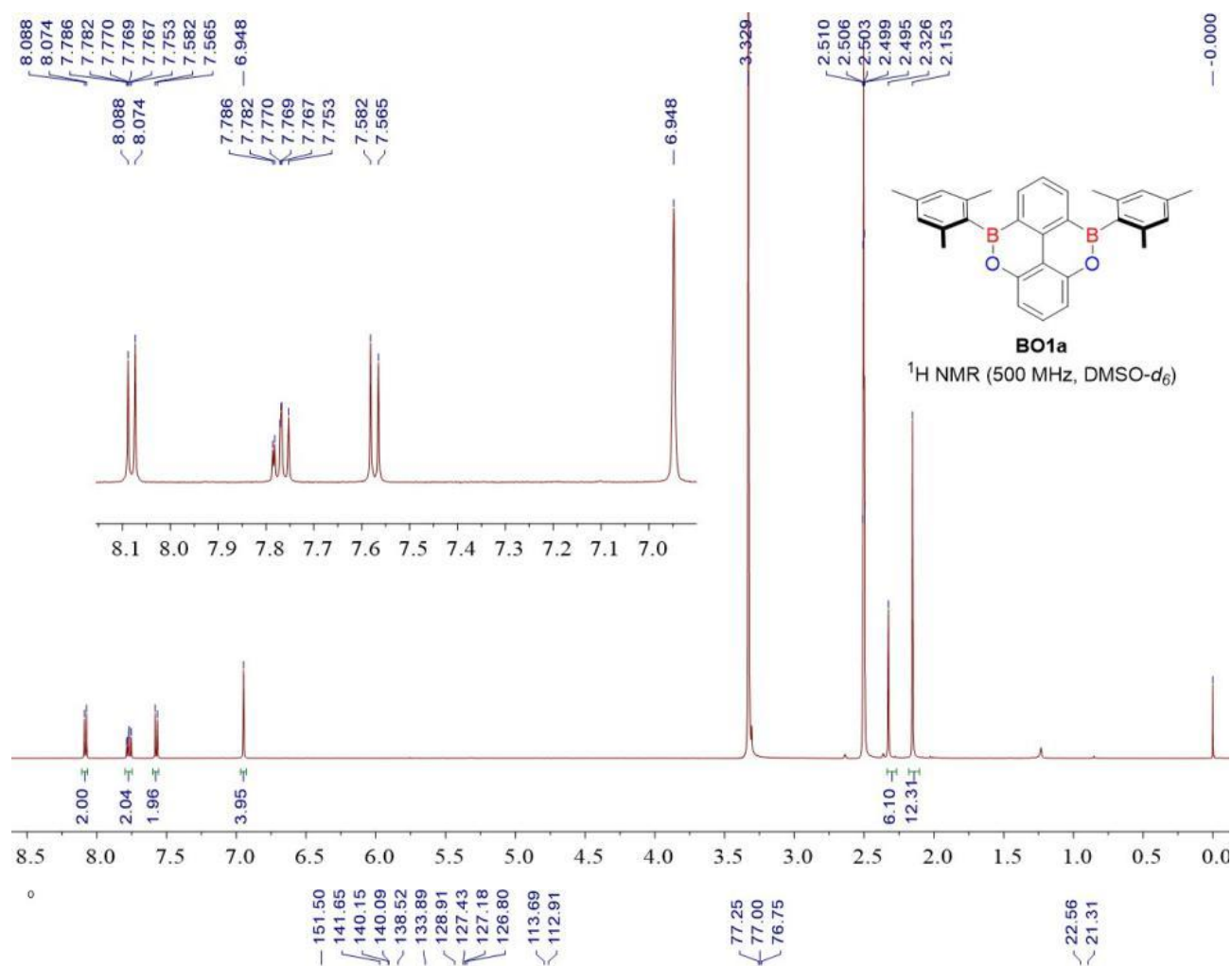
emitter/host	CIE (x, y)	λ_{EL} (nm)	L_{max} (cd/m ²)	EQE(%) ^a max/100/1000	Reference/year
PtON1/ BO1b (device 4)	(0.138, 0.134)	453	8007	22.8/21.5/16.3	This work
PtON1/ BO1b /26mCPy (device 5)	(0.138, 0.130)	454	12982	24.8/24.4/20.9	This work
PtON1/ BO1b /mCP (device 6)	(0.138, 0.154)	460	13098	22.3/20.0/19.2	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
PtON1/ BO1c /mCBP (device 10)	(0.141, 0.168)	456	27219	27.8/24.3/20.0	This work
PtON1/ BO1g /mCBP (device 11)	(0.140, 0.170)	458	22638	25.1/21.9/19.2	This work
PtON-TBBI/ BO2 /mCBP (device 14)	(0.135, 0.103)	458	14481	22.2/18.0/14.9	This work
PtON-TBBI/ BO3a /mCBP(device15)	(0.134, 0.107)	459	15765	19.6/17.0/14.8	This work
PtON-TBBI/ BO6 /mCBP (device 16)	(0.133, 0.111)	459	10071	21.7/16.2/13.4	This work
DABNA-1/mCBP	(0.13, 0.09)	459	<1000	13.5/6.20/---	[43]/2016
TBN-TPA/2,6-DCzppy	(0.12, 0.19)	474	16593	32.1/27.4/13.9	[44]/2018
v-DABNA/DOBNA-OAr	(0.12, 0.11)	469	<3000	34.4/32.8/26.0	[45]/2019
t-DABNA/ DMAC-DPS /DPEPO ^b	(0.13, 0.15)	466	<10000	31.4/27.2/19.8	[46]/2019
t-DAB-DPA/mCBP:mCBP-CN	(0.13, 0.08)	459	<10000	27.9/21.8/8.1	[47]/2021
B-O-dpa/DPEPO	(0.15, 0.05)	443	<1000	16.3/2.2/---	[48]/2021
v-DABNA-O-Me/DOBNA-Tol	(0.13, 0.10)	465	<13000	29.5/28.8/26.9	[49]/2021
γ -Cb-B/mCBP	(0.13, 0.13)	461	<3000	19.0/16.2/7.7	[50]/2021
3tPAB/mCP	(0.14, 0.08)	460	1100	19.3/<15/<5.0	[51]/2021
PAB/mCP	(0.14, 0.08)	456	782	14.7/~10/<5.0	[51]/2021
2tPAB/mCP	(0.14, 0.08)	456	1241	16.8/~10/<5.0	[51]/2021
tDMAC-BN/ DMAC-DP /DPEPO ^b	(0.12, 0.19)	472	1536	22.3/19.0/10.4	[52]/2021
tDPAC-BN/ DMAC-DPS /DPEPO ^b	(0.14, 0.09)	460	1126	21.6/15.3/5.4	[52]/2021
DPACzBN2/26DCzPPy	(0.13, 0.16)	469	15495	24.0/23.5/14.3	[53]/2021
DPACzBN3/26DCzPPy	(0.12, 0.18)	472	14629	27.7/19.3/6.7	[53]/2021
BFCz-DABNA/mCBP-CN	(0.13, 0.09)	463	<6000	28.0/13.4/5.1	[54]/2022
pBP-DABNA-Me/mCBP:DPEPO	(0.13, 0.09)	464	<1200	23.4/20.0/3.2	[55]/2022
C-BN/ p4TzPhBN /mCBP ^b	(0.14, 0.07)	453	<10000	26.6/20.1/8.9	[56]/2022
BN1/ 3Cz2BN /DPFPO ^b	(0.14, 0.08)	457	8323	31.2/18.3/9.3	[57]/2022
BN2/ 3Cz2BN /DPFPO ^b	(0.13, 0.11)	467	14064	33.2/25.5/15.5	[57]/2022
BN3/ 3Cz2BN /DPFPO ^b	(0.14, 0.08)	458	18438	37.6/34.0/26.2	[57]/2022
CzBNO/26DCzPPy	(0.14, 0.08)	454	<8000	13.6/10.1/5.5	[58]/2022
CzBO/mCBP	(0.15, 0.05)	448	<2000	13.4/8.4/3.5	[59]/2022
BOBO-Z/mCBP	(0.15, 0.04)	445	<9000	13.6/9.8/3.3	[60]/2022
BOBS-Z/mCBP	(0.14, 0.06)	456	<9000	26.9/24.0/15.0	[60]/2022
BSBS-Z/mCBP	(0.13, 0.08)	463	<9000	26.8/24.0/15.9	[60]/2022
m-v-DABNA/ DBFPO	(0.12, 0.12)	471	~2000	36.2/---/---	[61]/2022
4F-v-DABNA/DBFPO	(0.13, 0.08)	464	~1000	35.8/26.4/10.2	[61]/2022
4F-m-v-DABNA/DBFPO	(0.13, 0.06)	461	~1000	33.7/25.8/---	[61]/2022
v-DABNA-F/DOBNA-Tol	(0.12, 0.10)	468	<10000	26.6/25.8/23.4	[62]/2022

t-DABNA-dtB/mCBP:mCBP-CN	(0.11, 0.16)	471	<10000	11.4/---/10.5	[63]/2022
mBP-DABNA-Me/mCP:DPEPO	(0.12, 0.14)	468	<1500	24.3/19.5/---	[64]/2022
α -3BNMes/DPEPO	(0.18, 0.08)	443	<900	---/1.70/---	[65]/2022
DCZ-BSN/mCBP	(0.11, 0.17)	473	<9000	22.0/---/---	[66]/2022
CzBSN/mCBP	(0.11, 0.16)	473	<9000	23.1/21.3/15.0	[66]/2022
m-DINBO/mCBP	(0.13, 0.10)	466	<1000	24.2/---/---	[67]/2022
NBO/mCBP	(0.14, 0.14)	459	<1000	16.8/---/---	[67]/2022
Cl-MR/DPEPO	(0.12, 0.19)	472	209	17.0/---/---	[68]/2022
TPD4PA/mCBP-CN	(0.14, 0.06)	455	<6000	30.7/30.6/17.8	[69]/2023
tBu-TPAD4PA/mCBP-CN	(0.14, 0.07)	460	<6000	32.5/30.9/20.5	[69]/2023
Mes-BDIDOBNA-N/CzSi:TSPO1	(0.17, 0.05)	402	<1000	16.2/3.5/---	[70]/2023
DIDOBNA-N/TSPO1	(0.15, 0.07)	429	<1000	15.2/3.8/---	[70]/2023
NOBNacene/TSPO1	(0.17, 0.06)	409	<100	8.5/---/---	[71]/2023
B-2OCz/DPEPO	(0.15, 0.06)	432	<1000	8.4/6.7/---	[72]/2023
B-2Ocz-Si/DPEPO	(0.16, 0.04)	423	<1000	15.2/8.1/---	[72]/2023
NO-DBMR/DBFPO	(0.12, 0.12)	469	<9000	33.7/---/---	[73]/2023

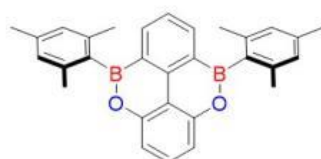
^a EQE @ Max/100/1000 cd m⁻². ^b Hyperfluorescent OLED.



Supplementary Fig. 64. Operational lifetimes of the deep-blue OLEDs ($L_0 = 500 \text{ cd/cm}^2$)

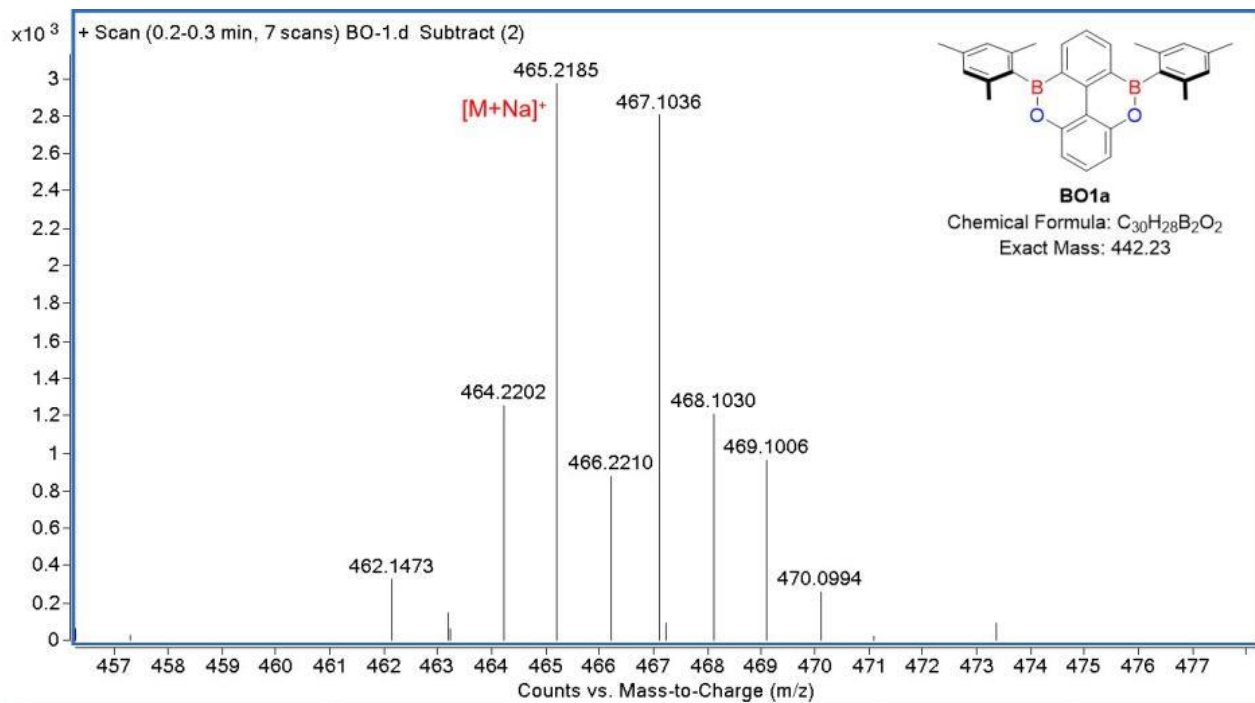
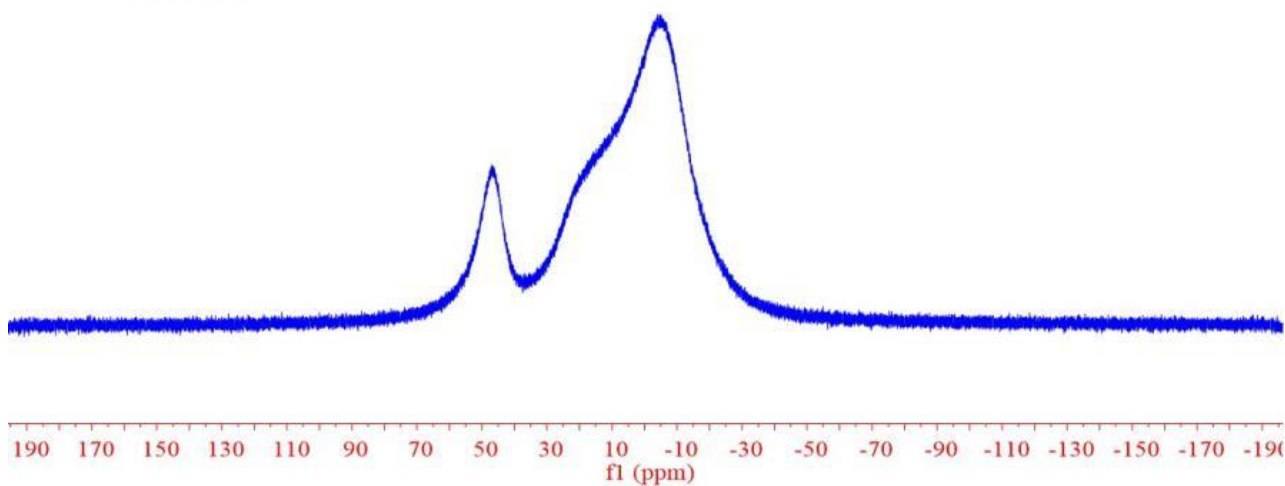


— 46.31



BO1a

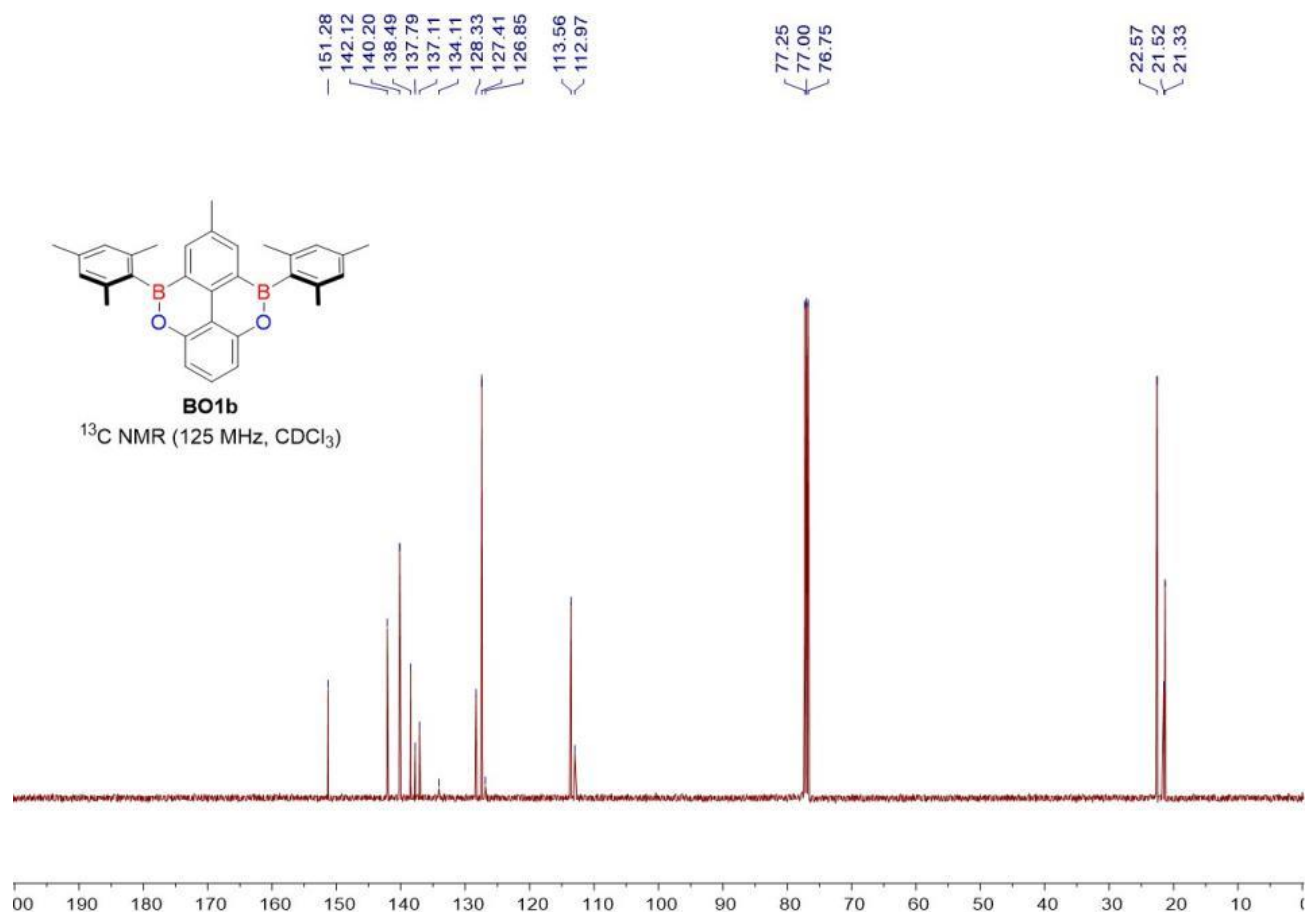
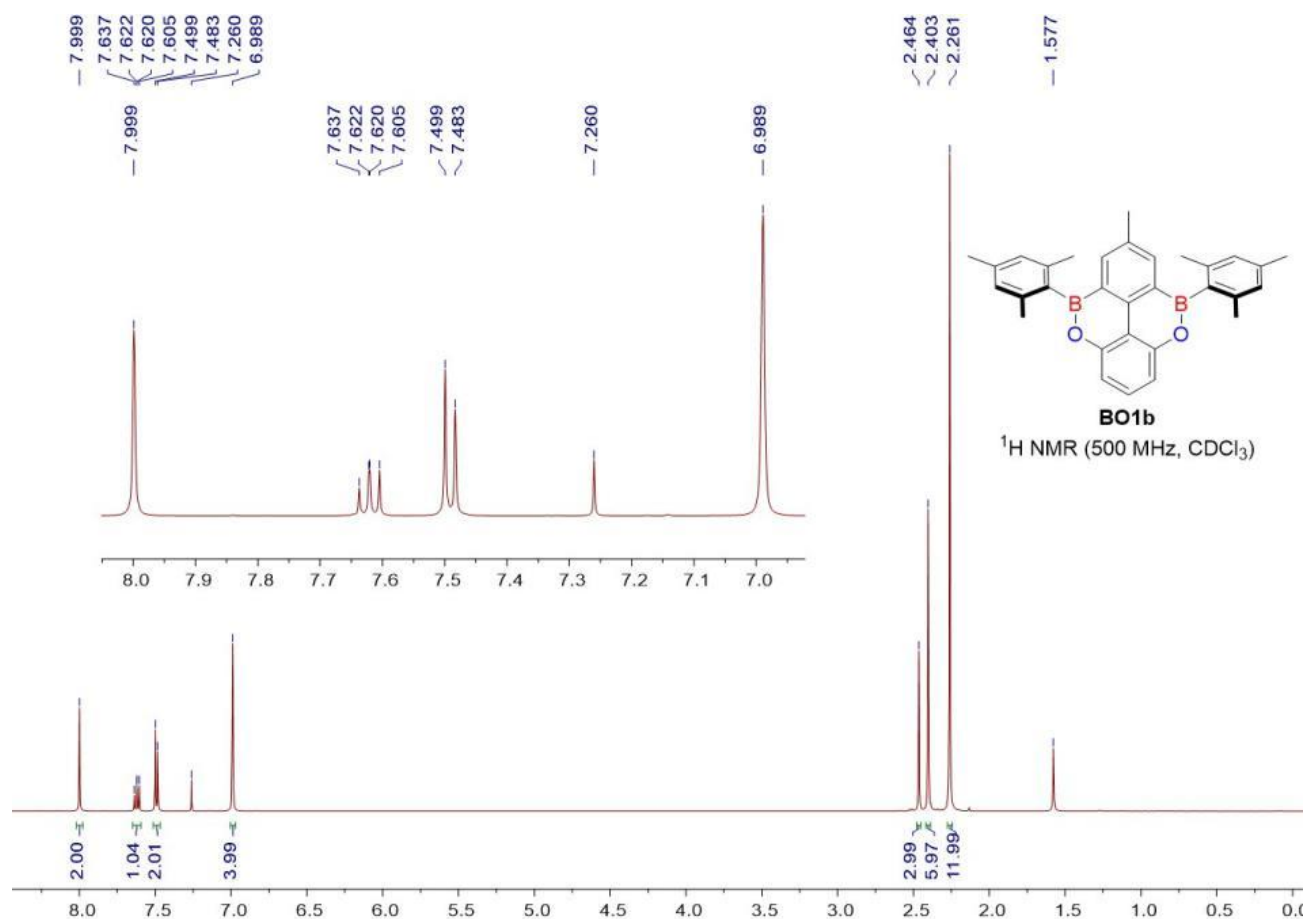
^{11}B NMR (160 MHz, CDCl_3)



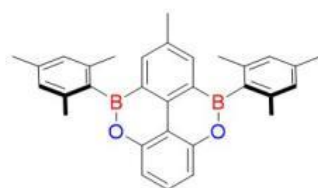
BO1a

Chemical Formula: $\text{C}_{30}\text{H}_{28}\text{B}_2\text{O}_2$
Exact Mass: 442.23

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

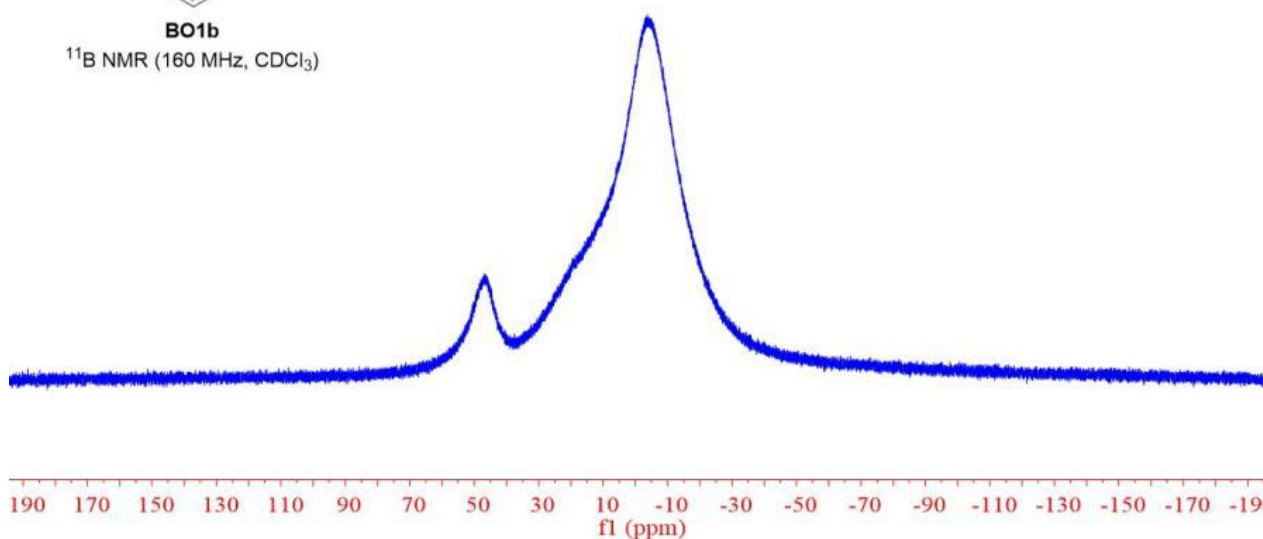


-49.59

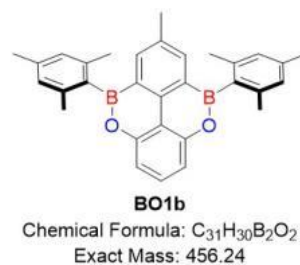
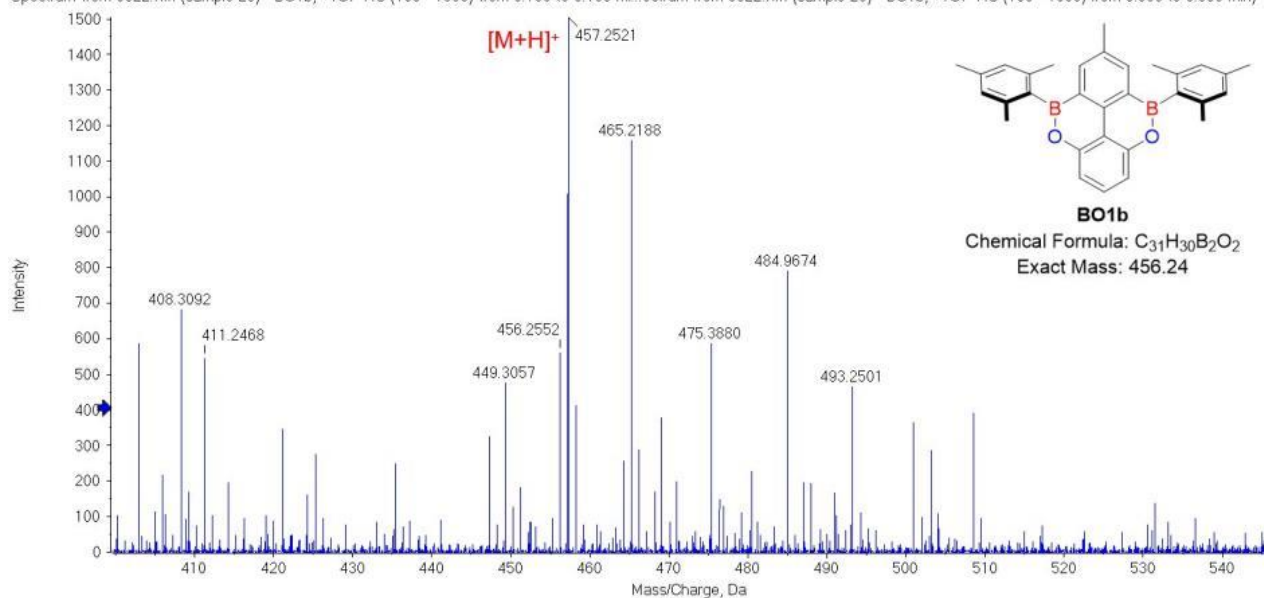


BO1b

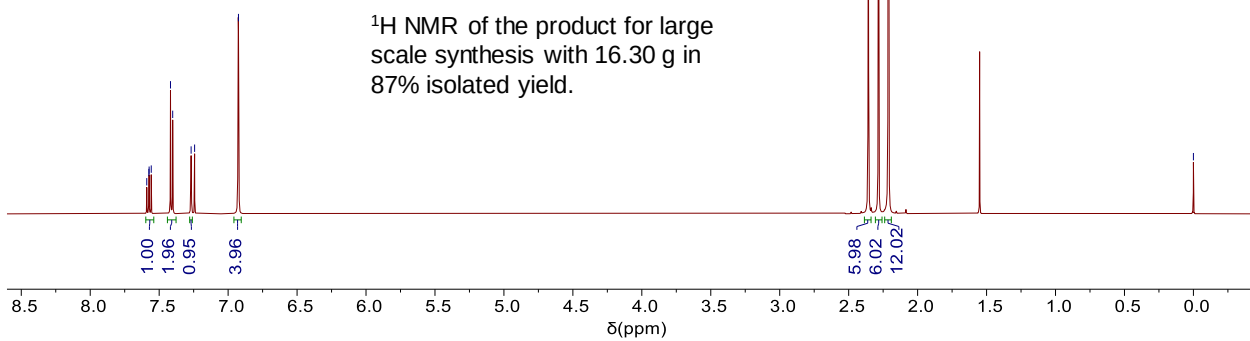
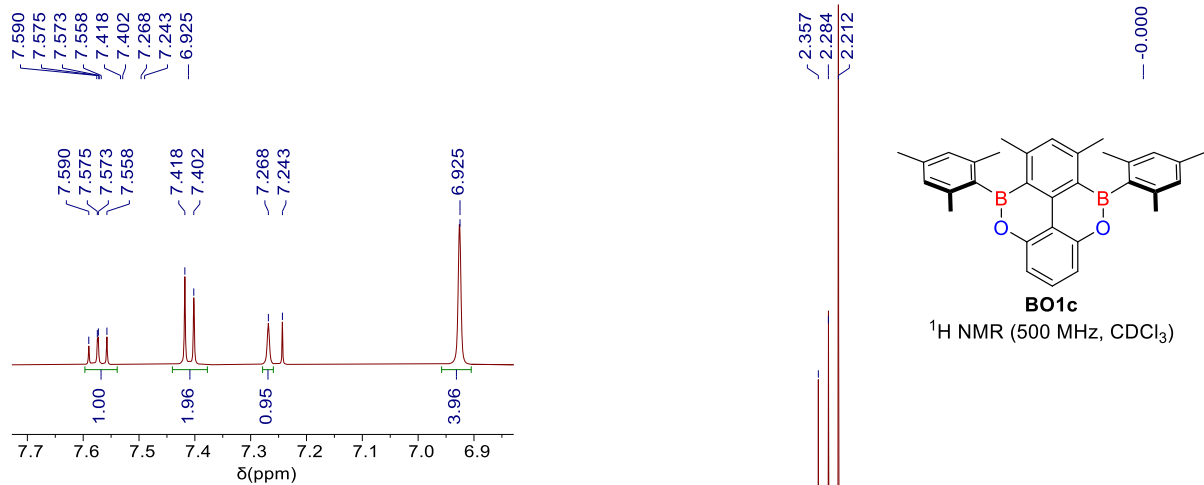
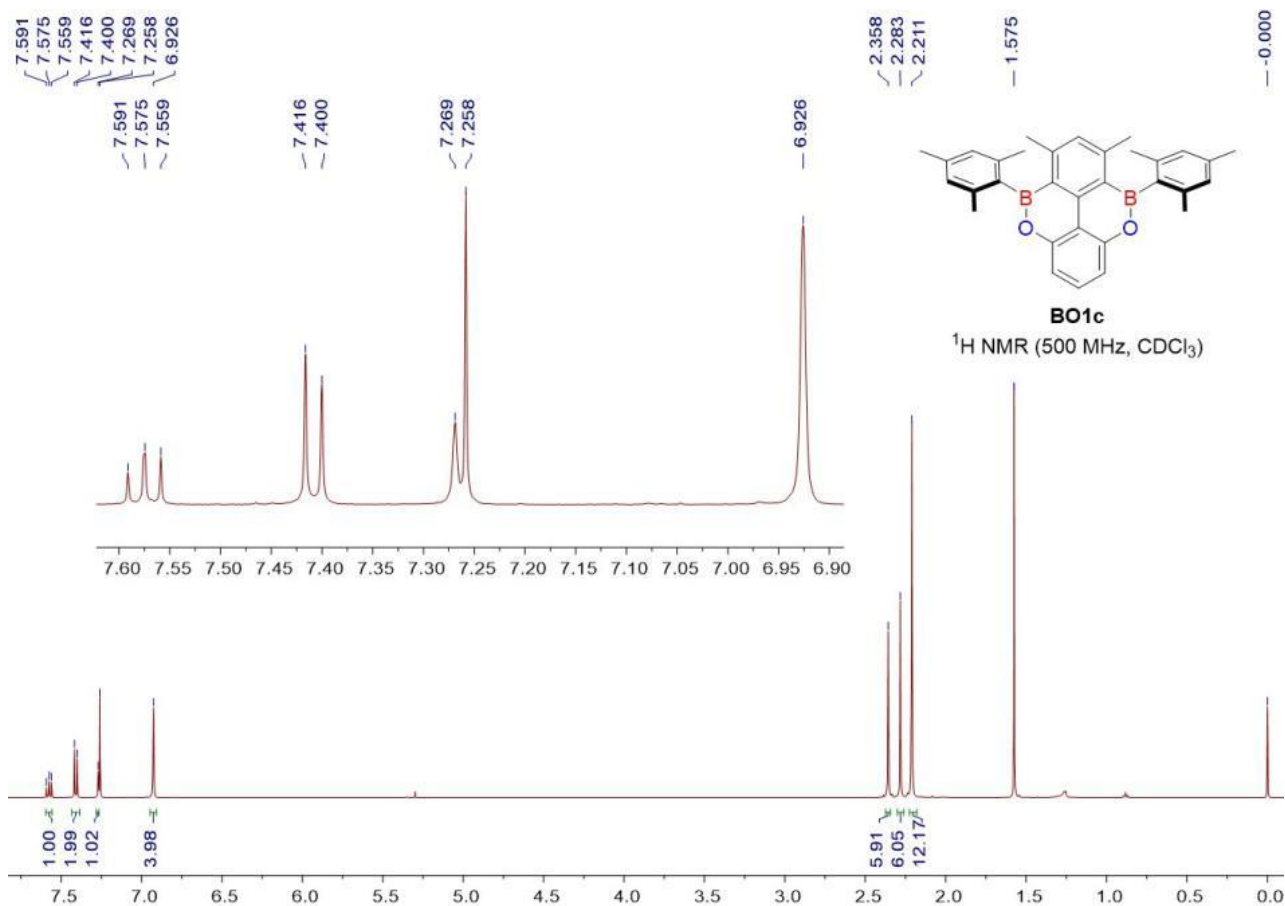
^{11}B NMR (160 MHz, CDCl_3)

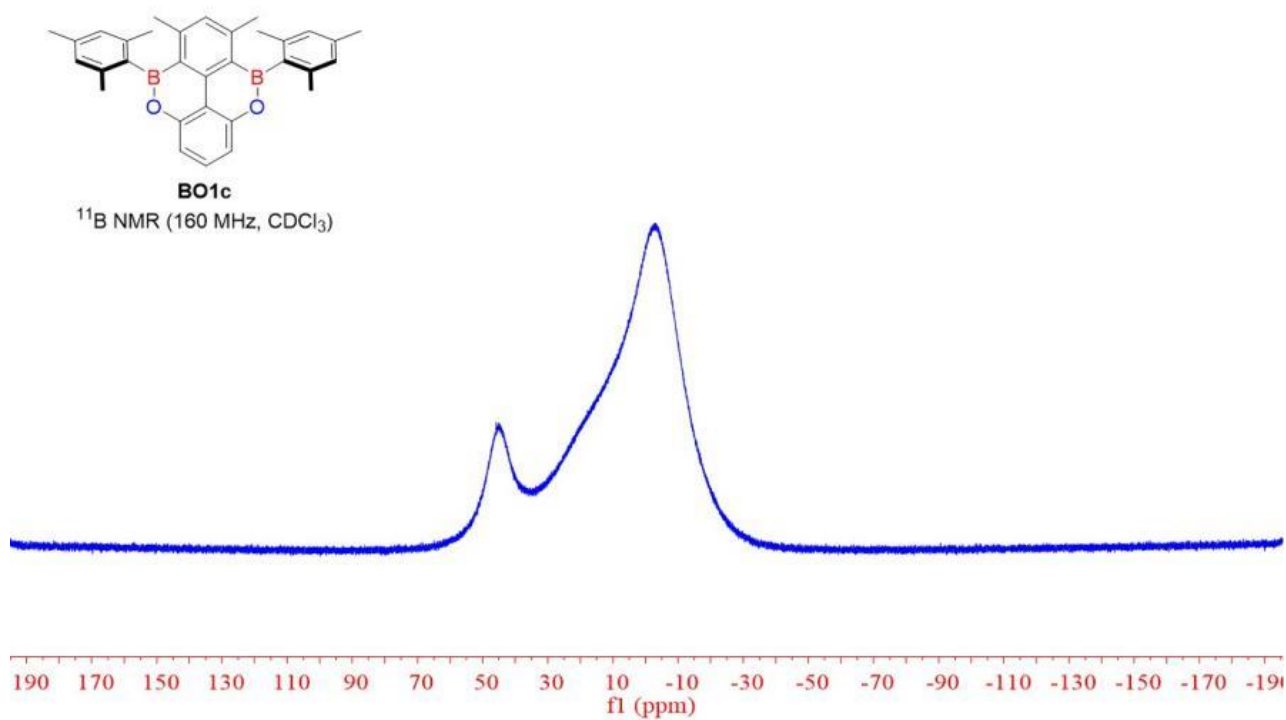
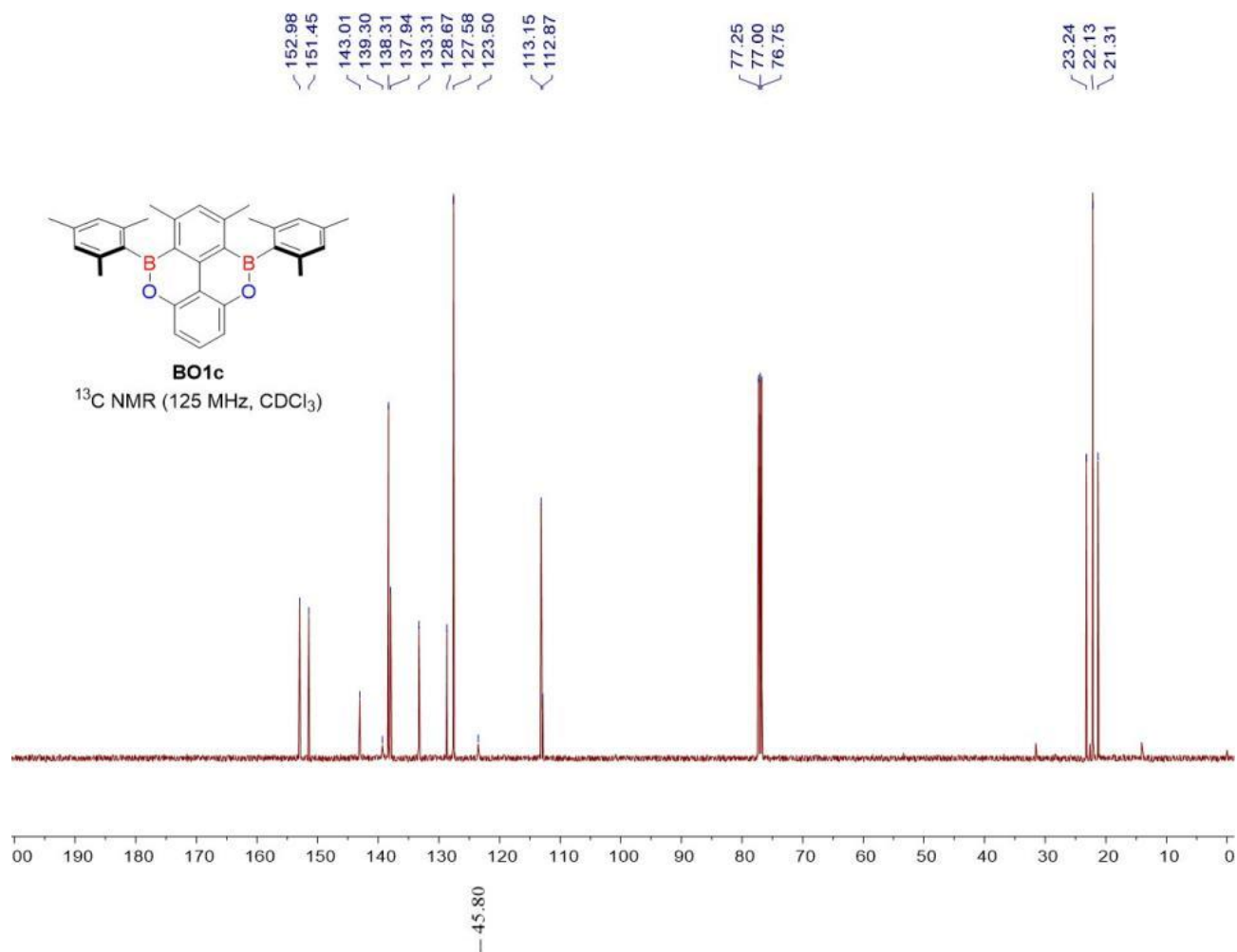


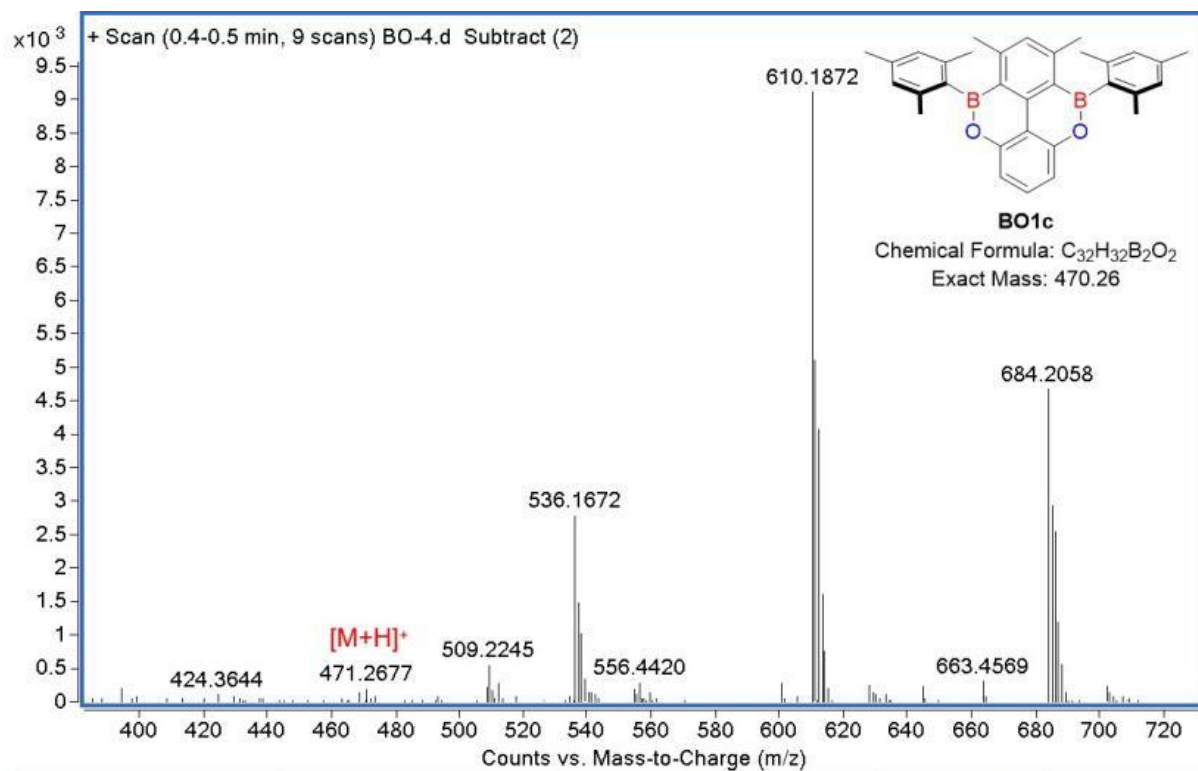
Spectrum from 0922.wiff (sample 26) - BO1b, +TOF MS (100 - 1500) from 0.135 to 0.195 min. Spectrum from 0922.wiff (sample 26) - BO1b, +TOF MS (100 - 1500) from 0.660 to 0.809 min)



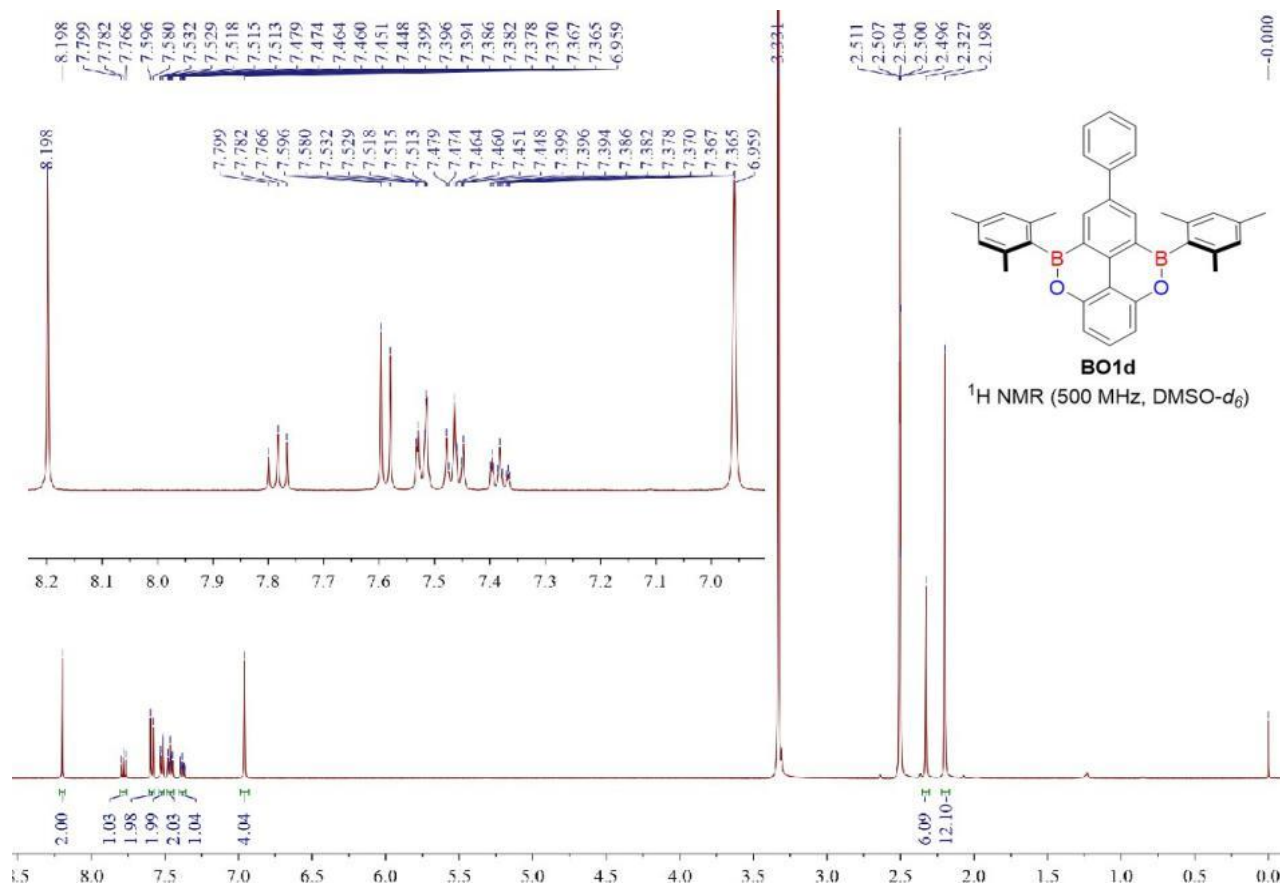
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{31}\text{H}_{30}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{31}\text{H}_{31}[^{11}\text{B}]_2\text{O}_2$	457.2521	457.2505	-3.70

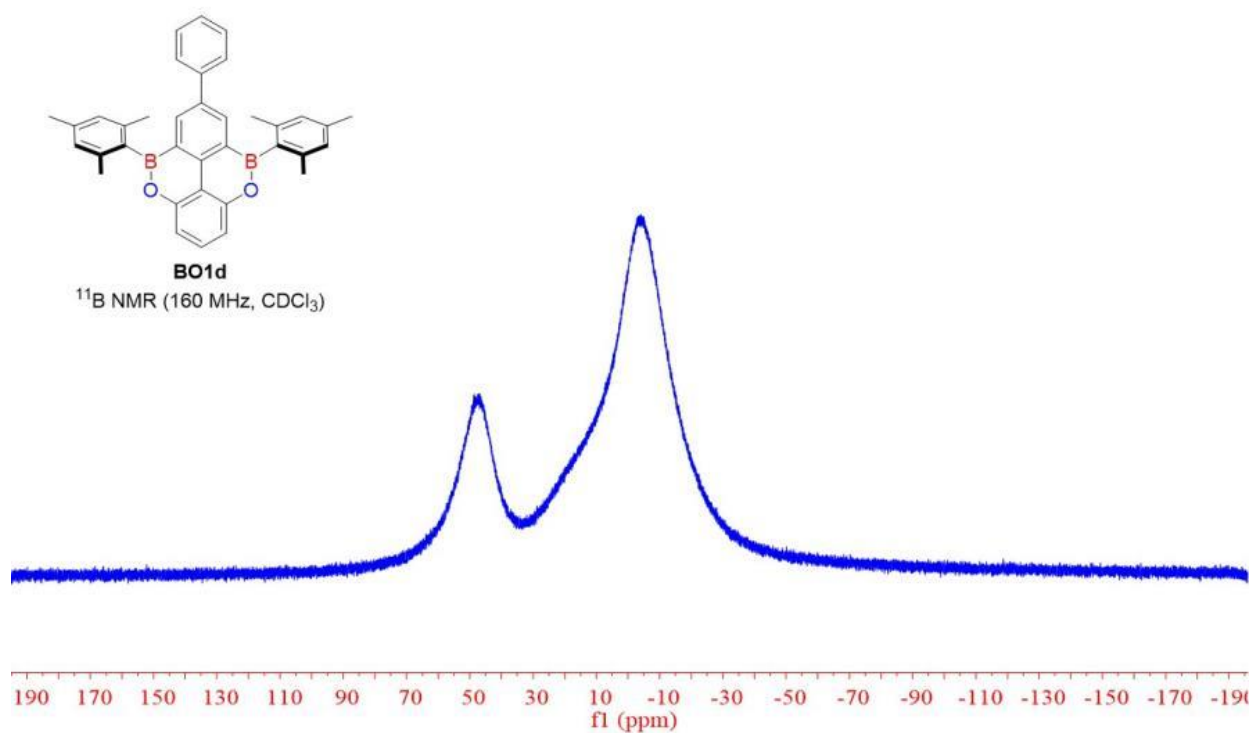
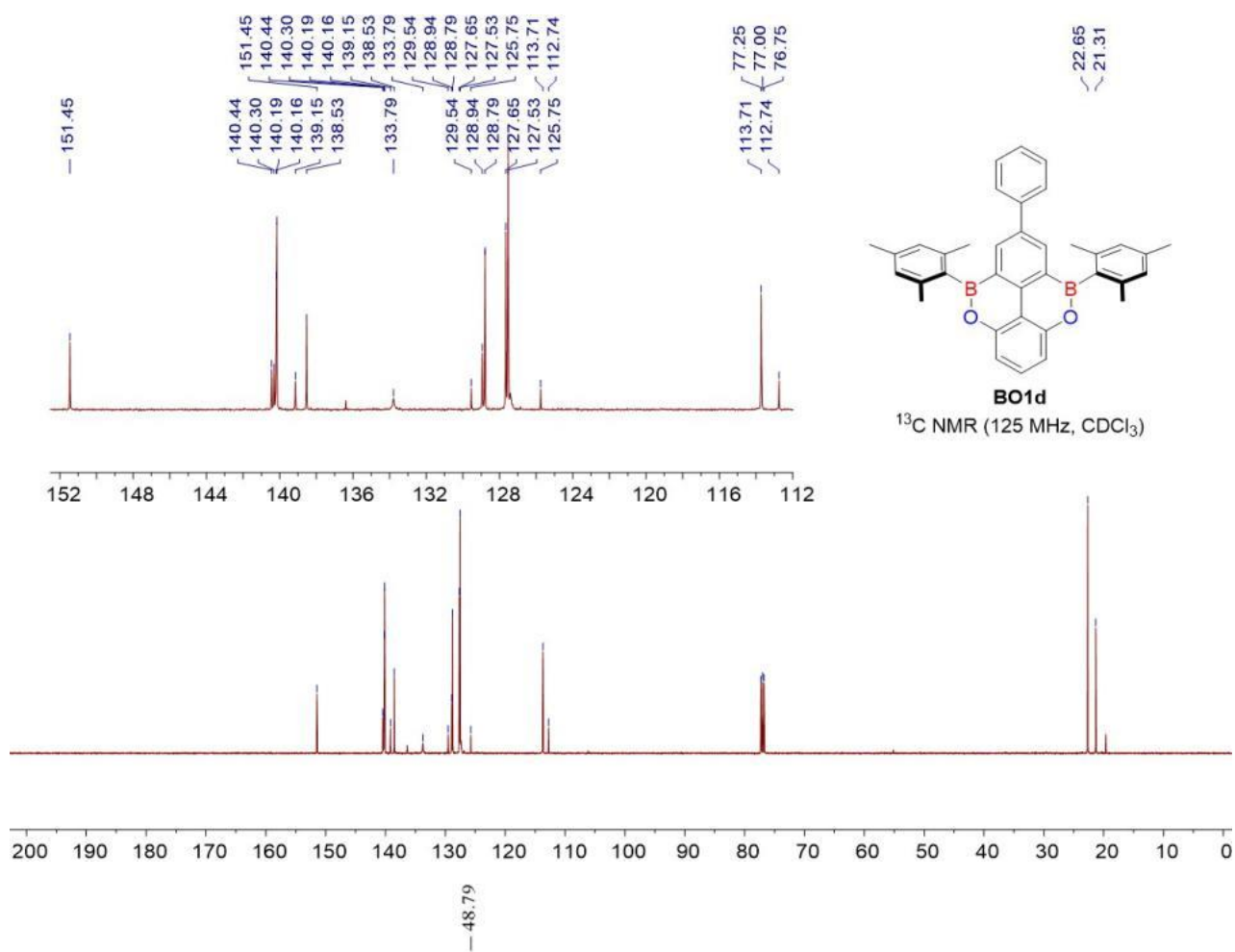


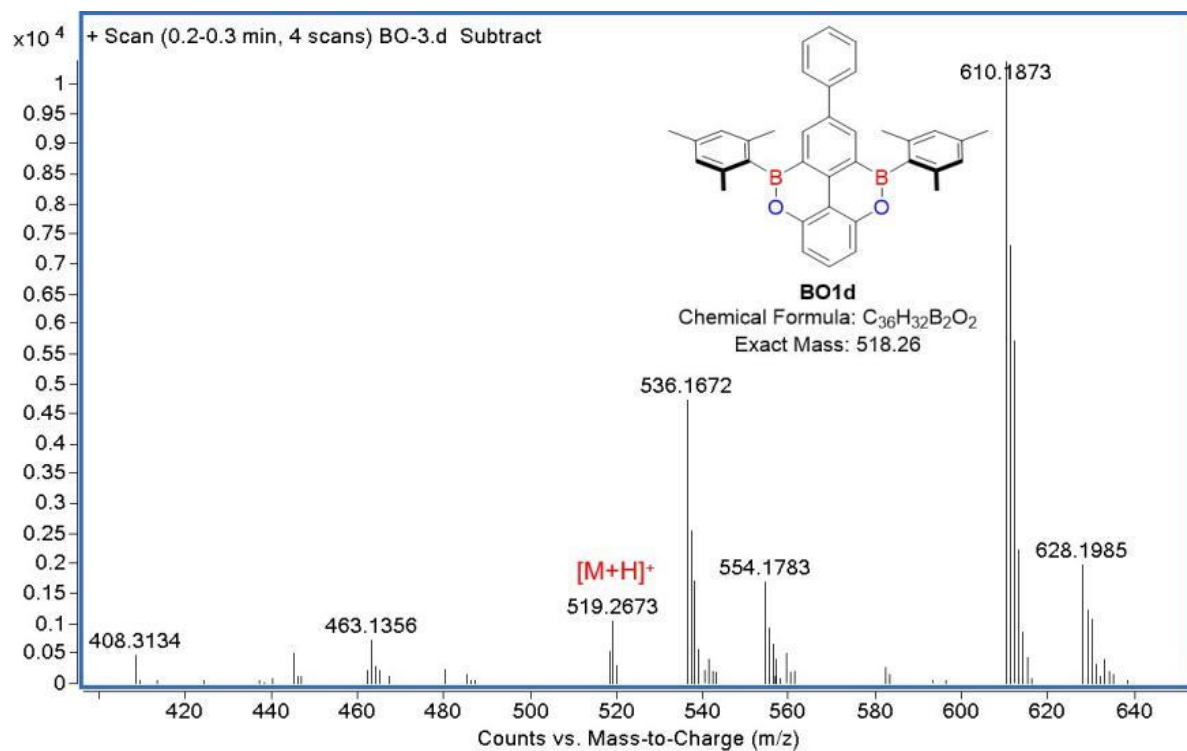




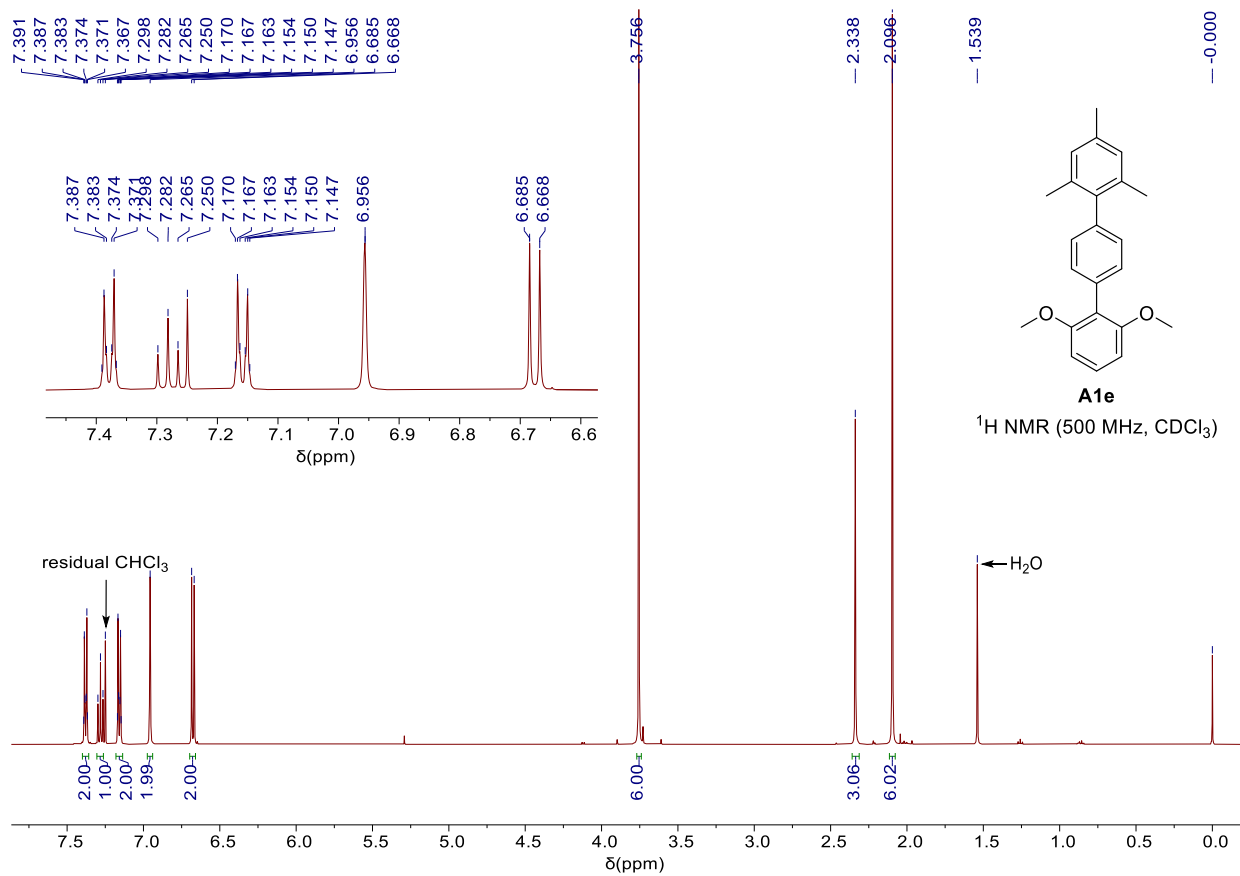
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$C_{32}H_{32}[^{11}B]_2O_2$	$C_{32}H_{33}[^{11}B]_2O_2$	471.2677	471.2661	-3.36	18

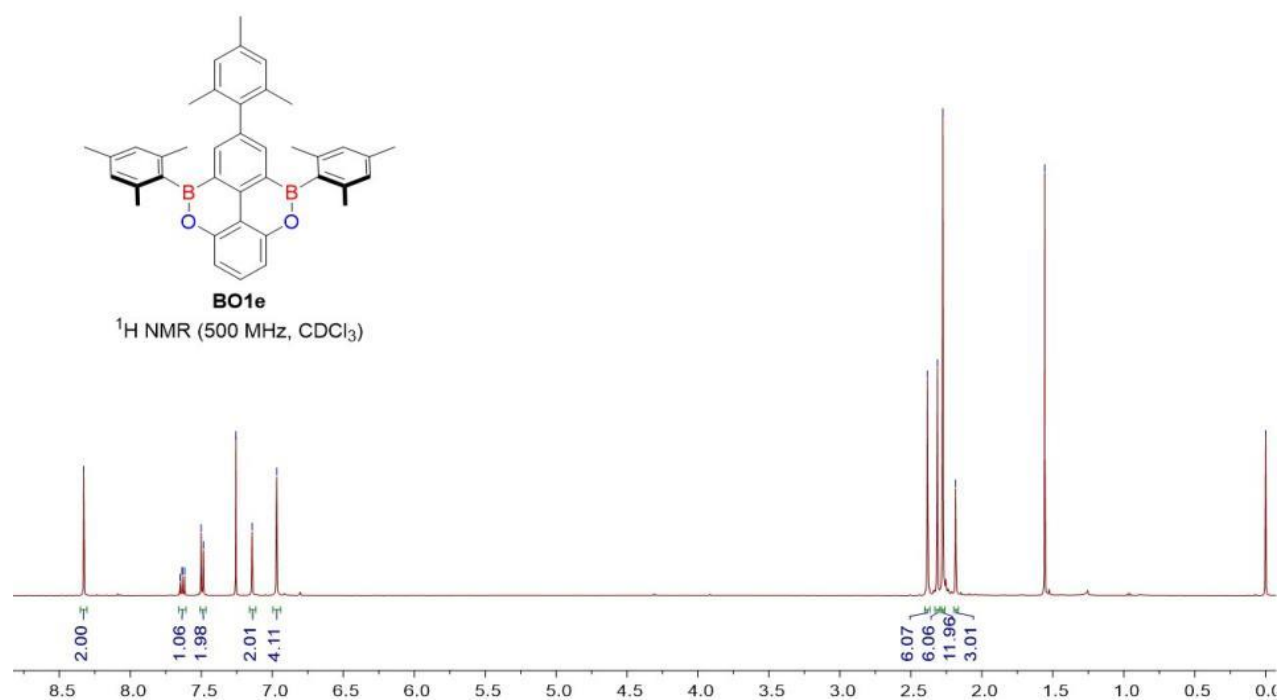
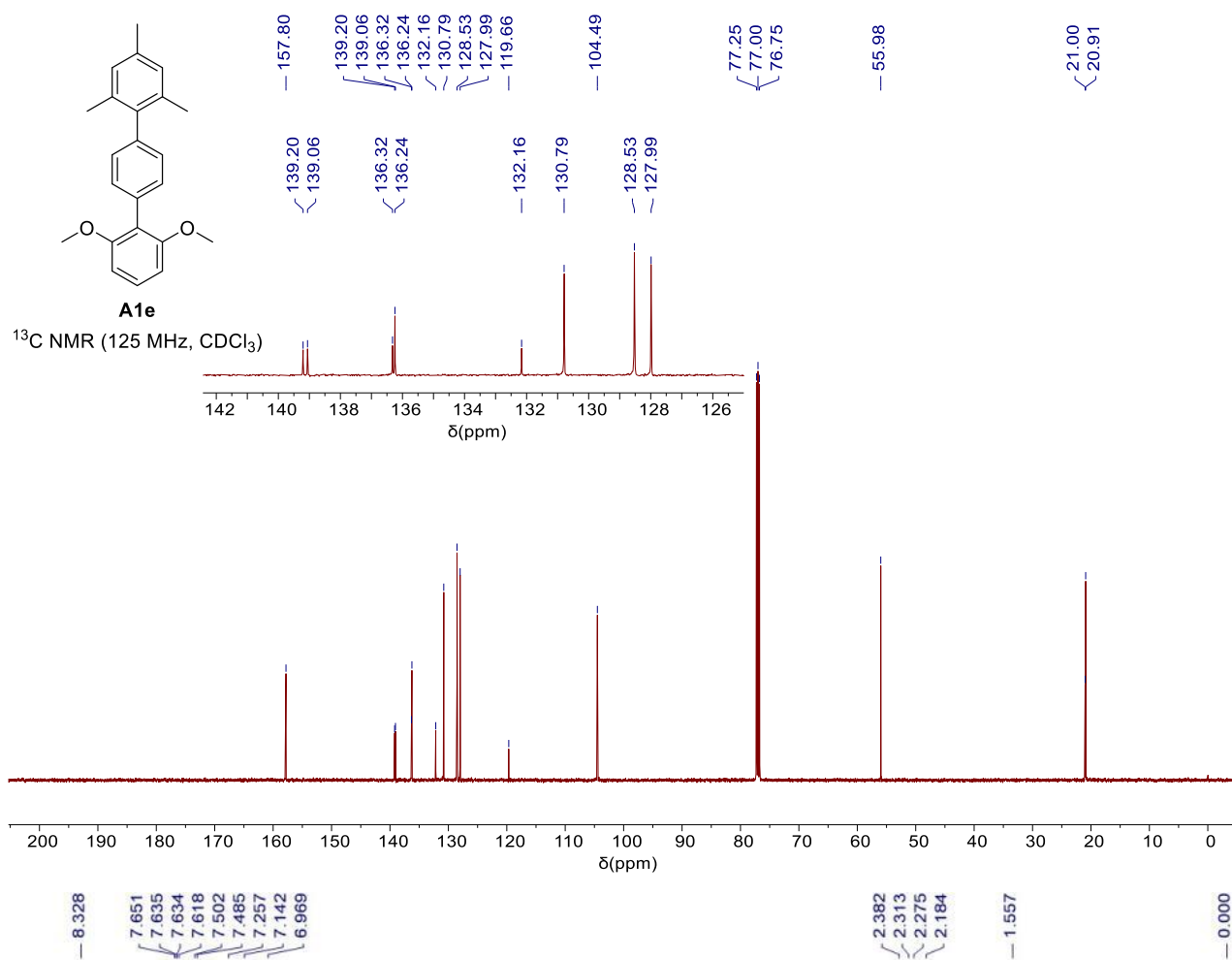


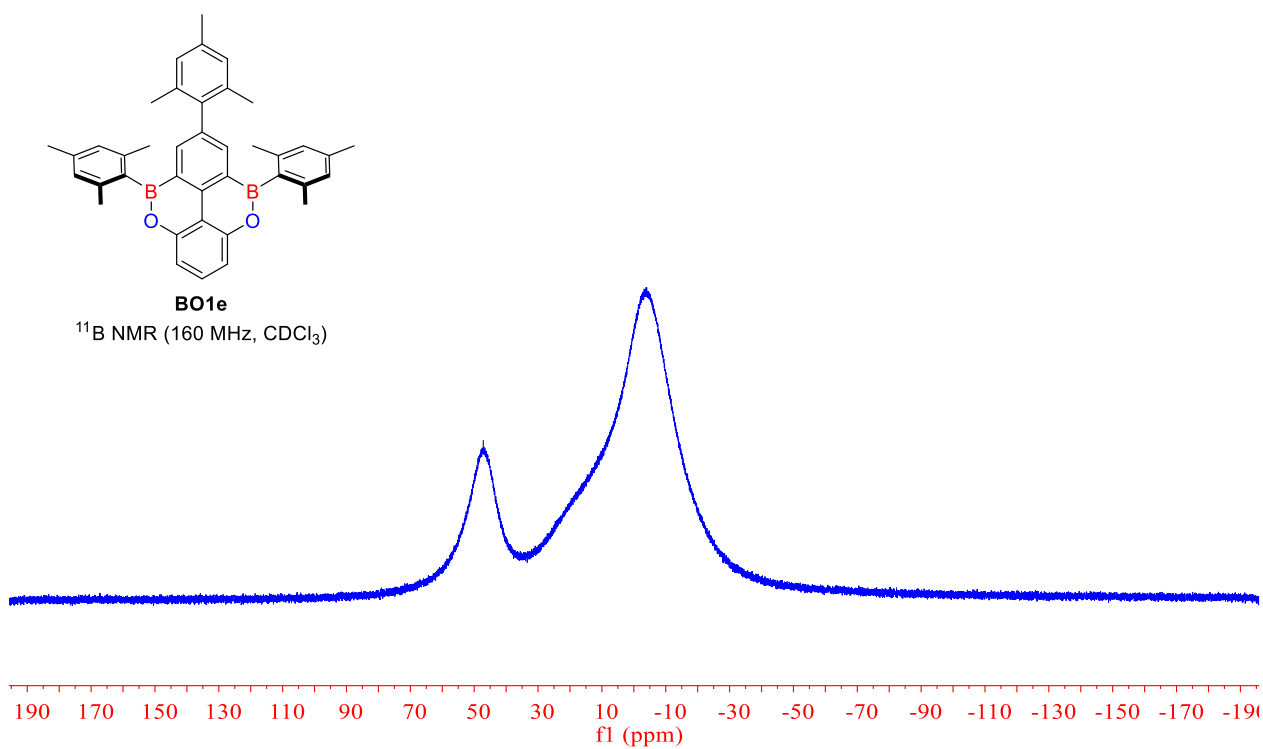
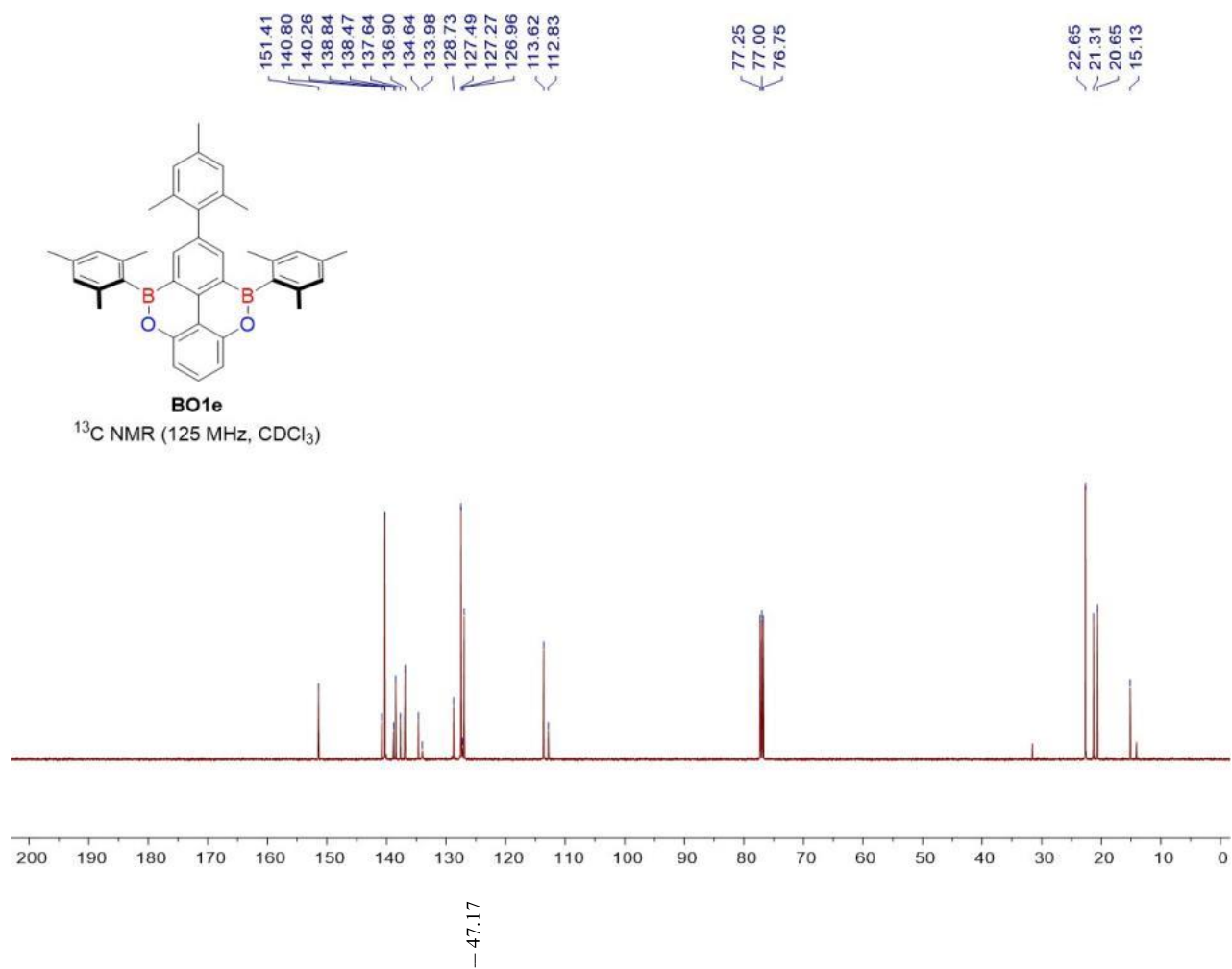


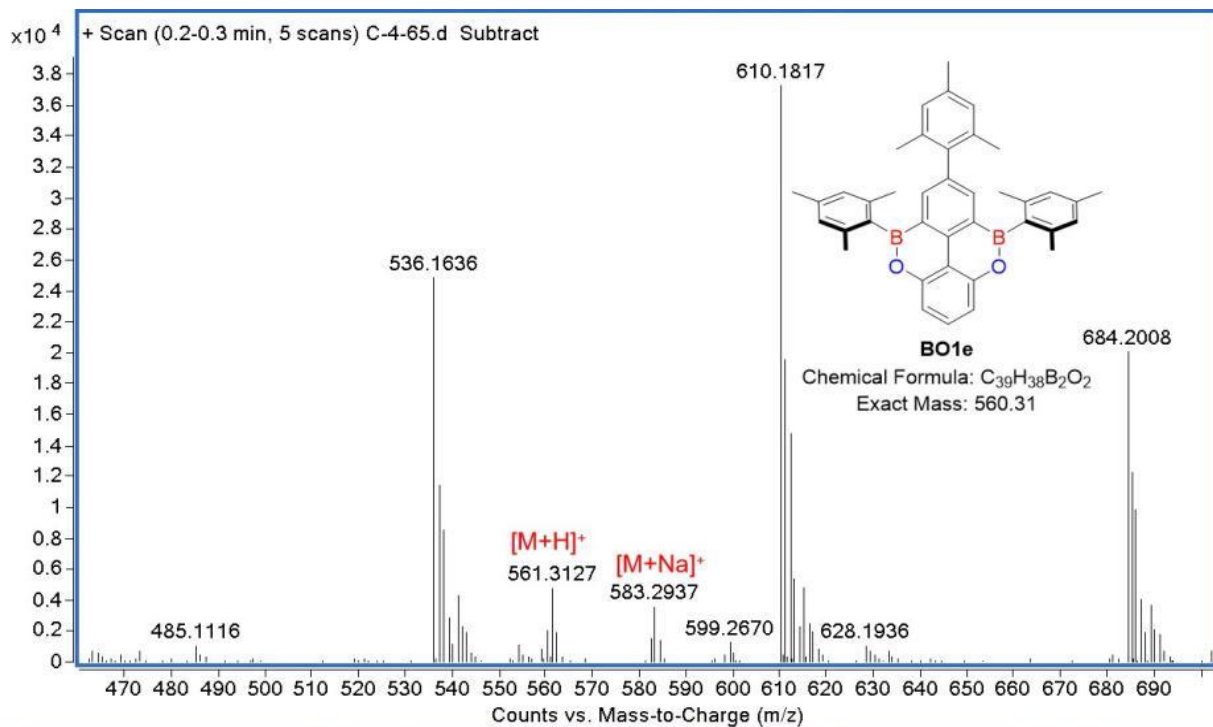


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$C_{36}H_{32}[^{11}B]_2O_2$	$C_{36}H_{33}[^{11}B]_2O_2$	519.2673	519.2661	-2.28	22

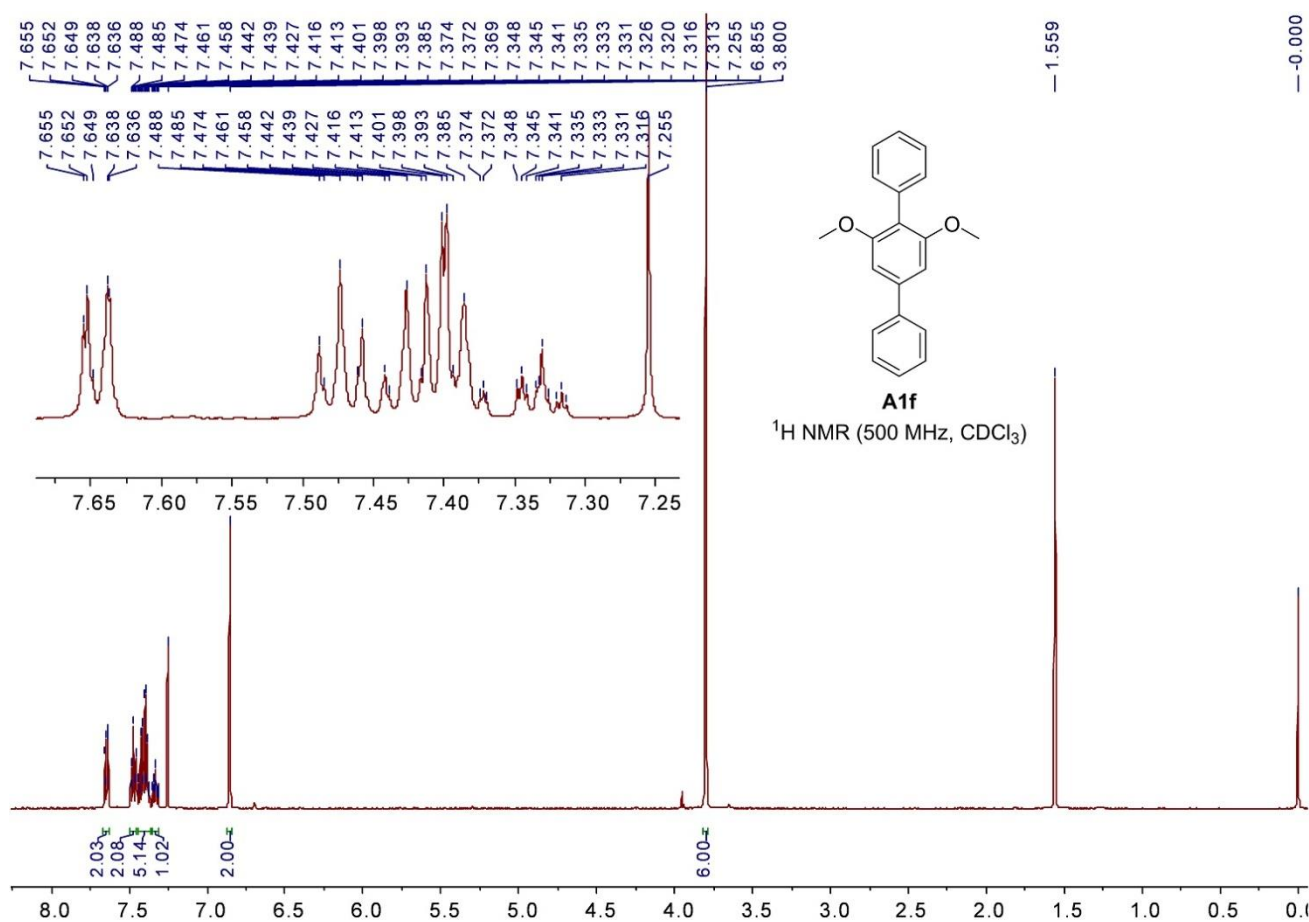


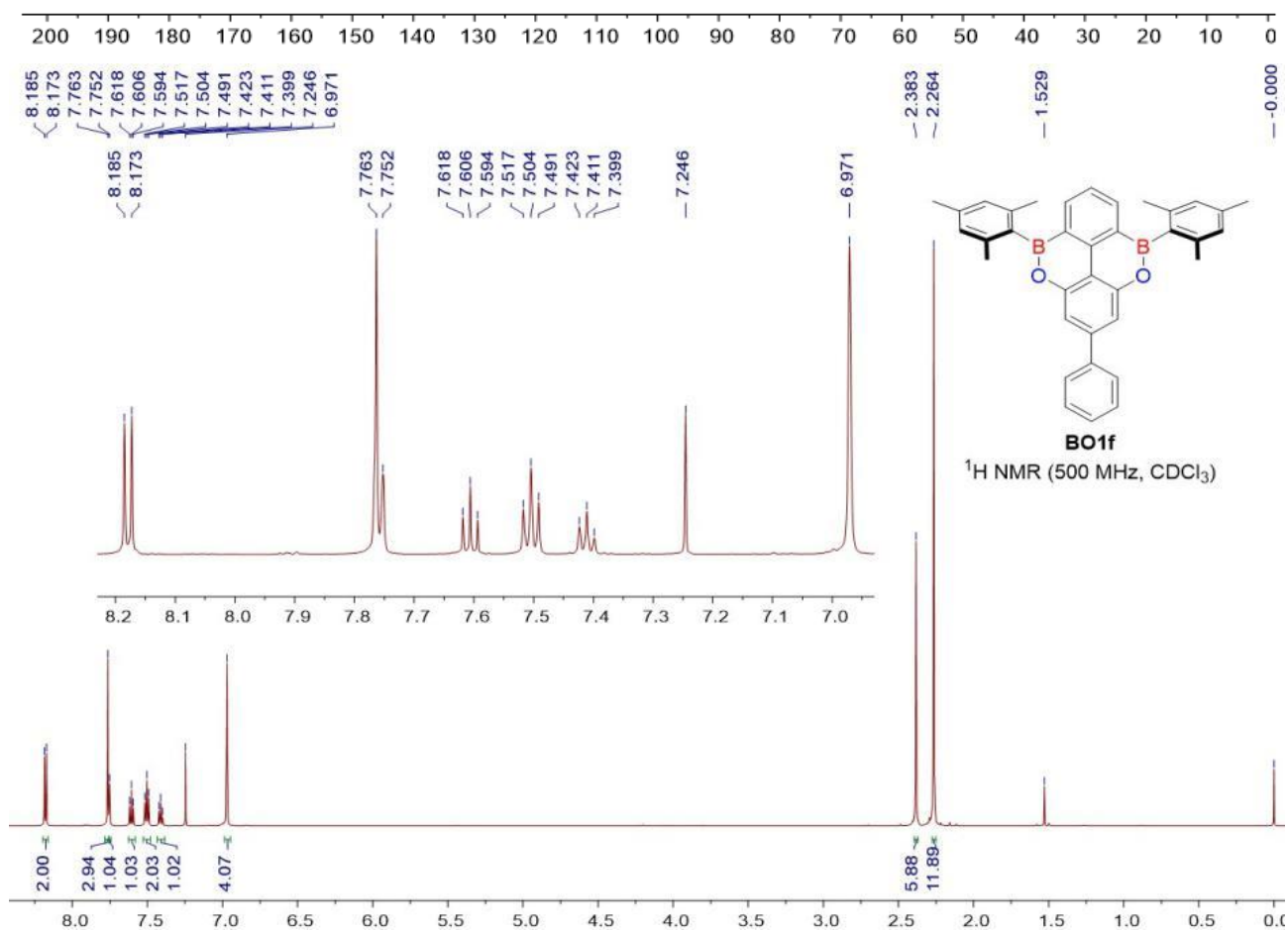
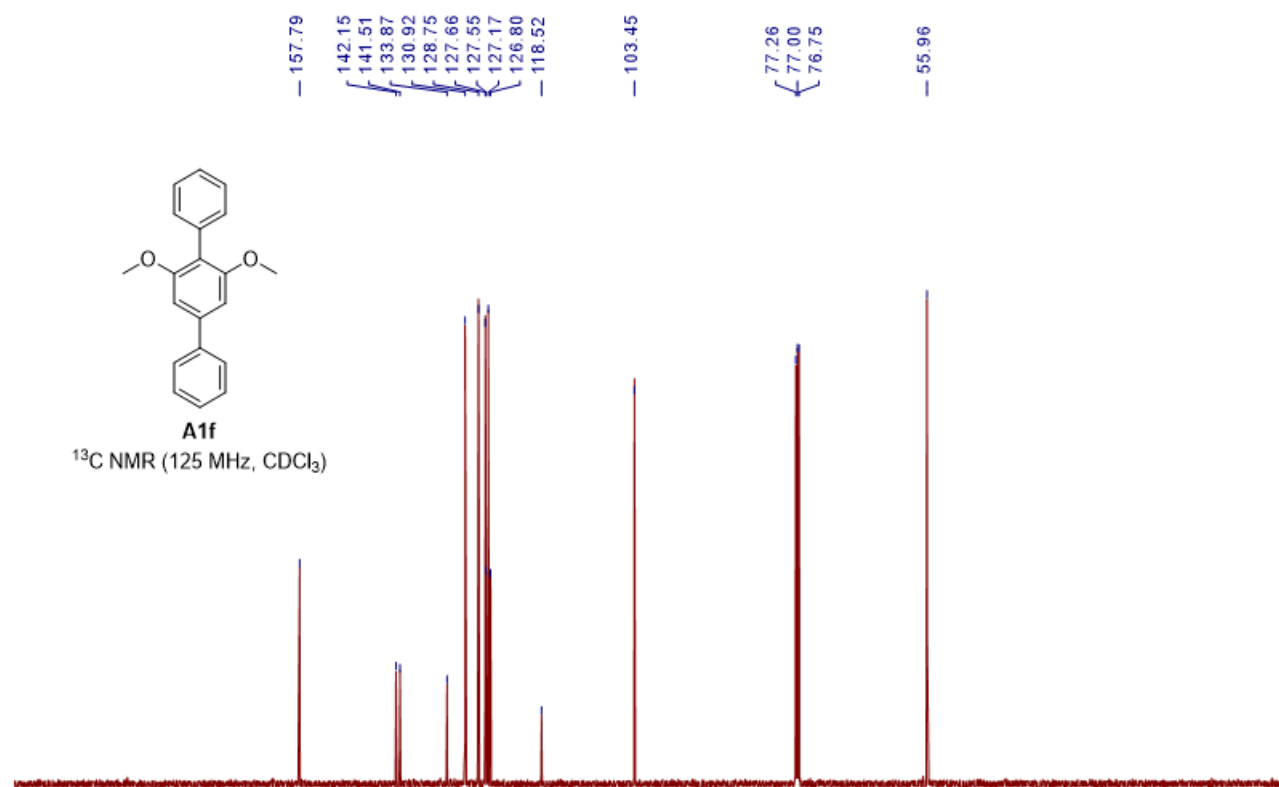


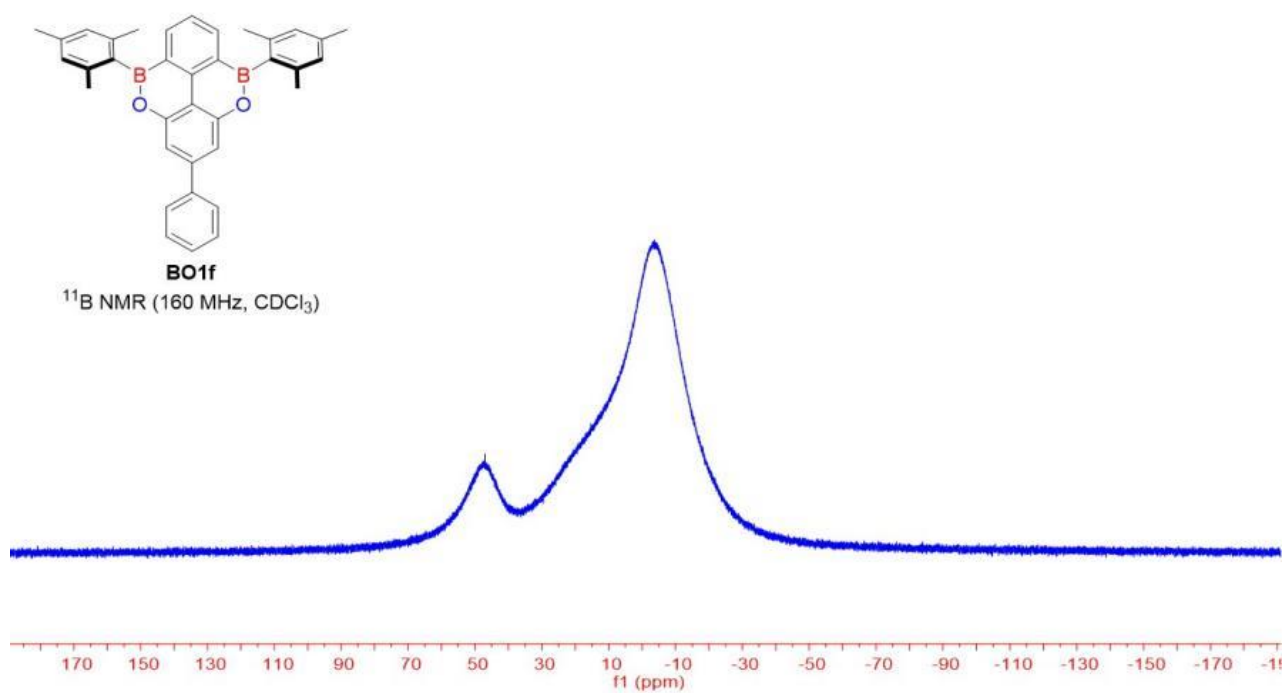
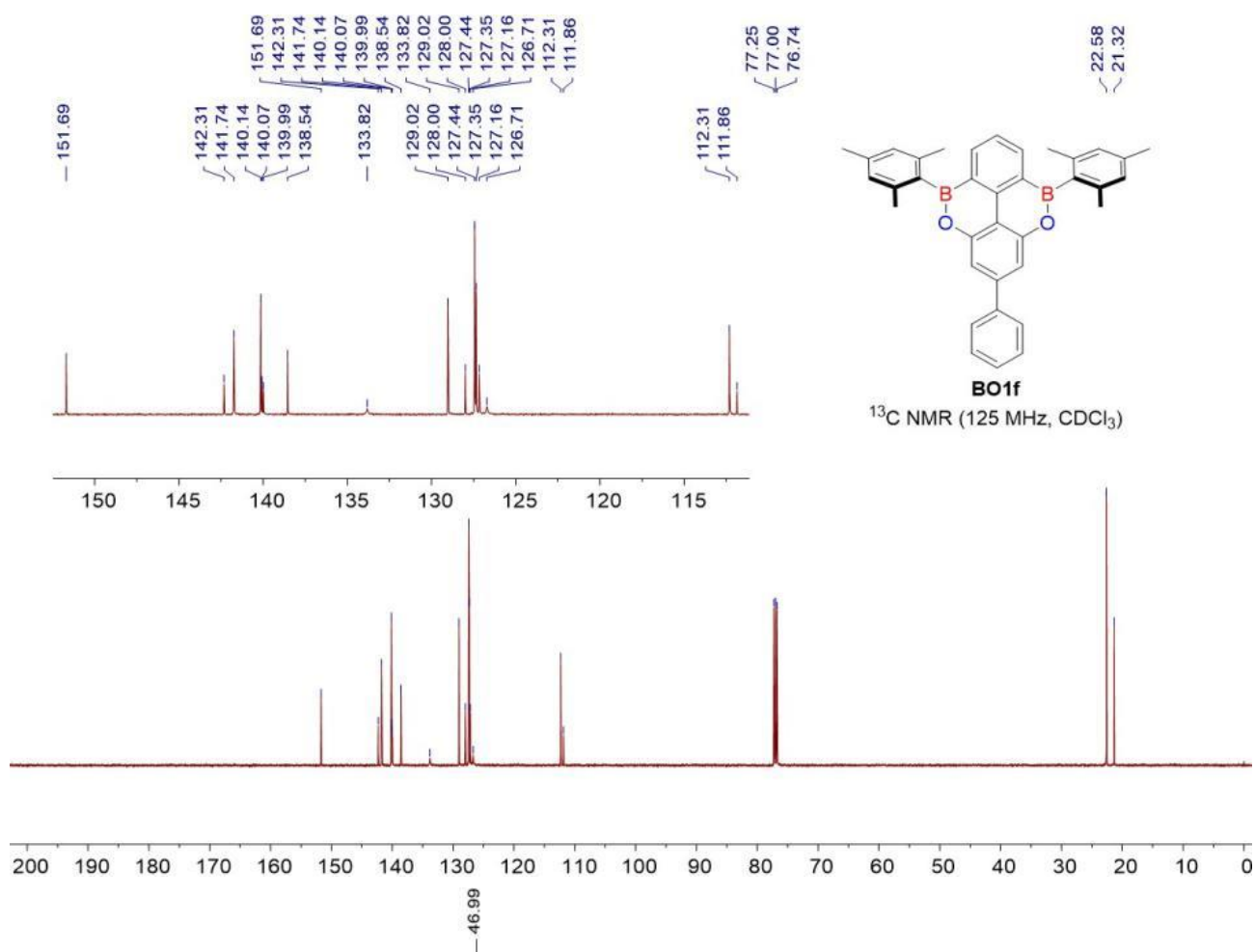




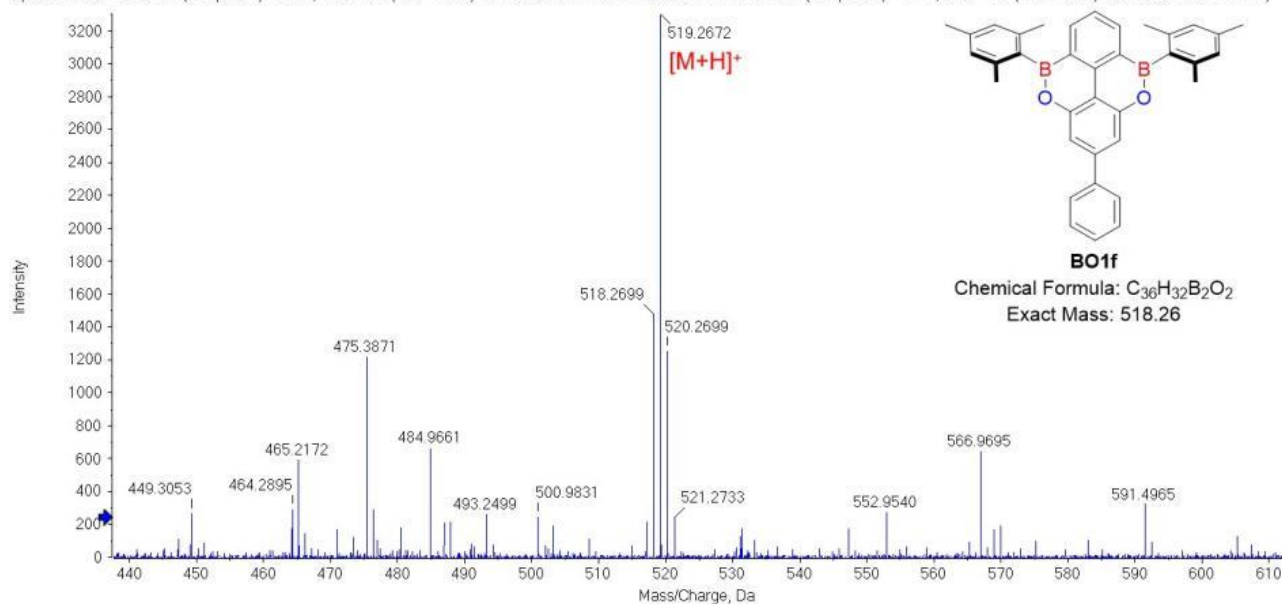
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$C_{39}H_{38}[^{11}B]_2O_2$	$C_{39}H_{39}[^{11}B]_2O_2$	561.3127	561.3131	0.66



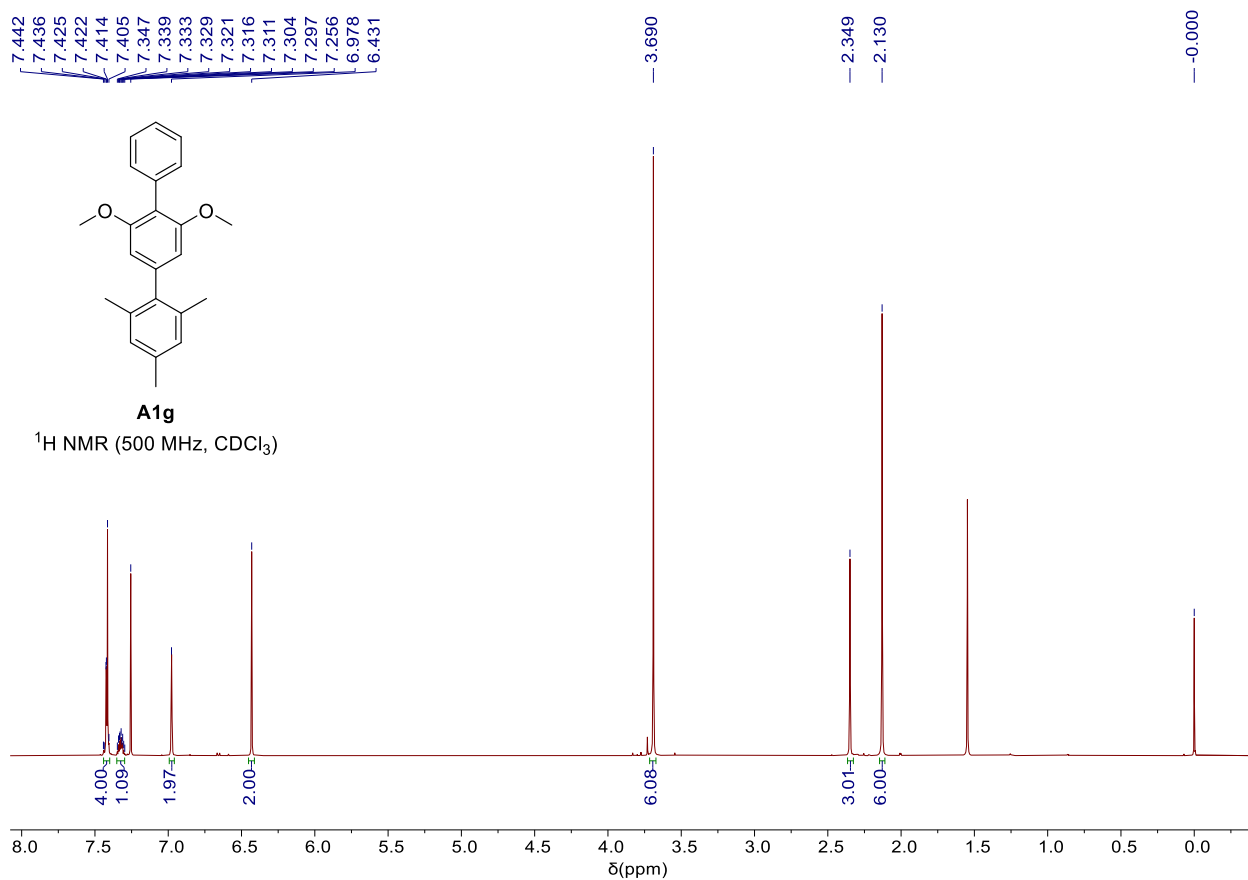


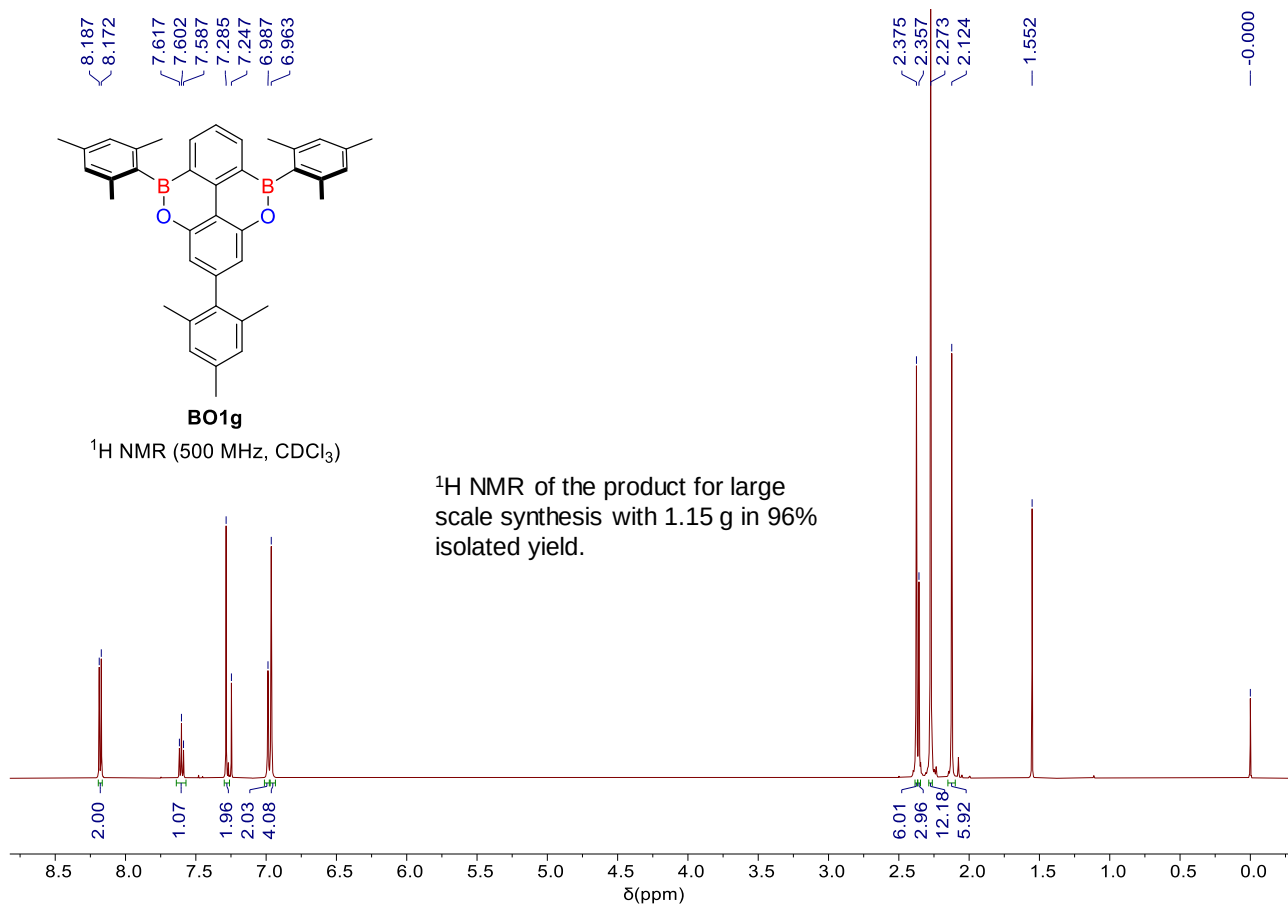
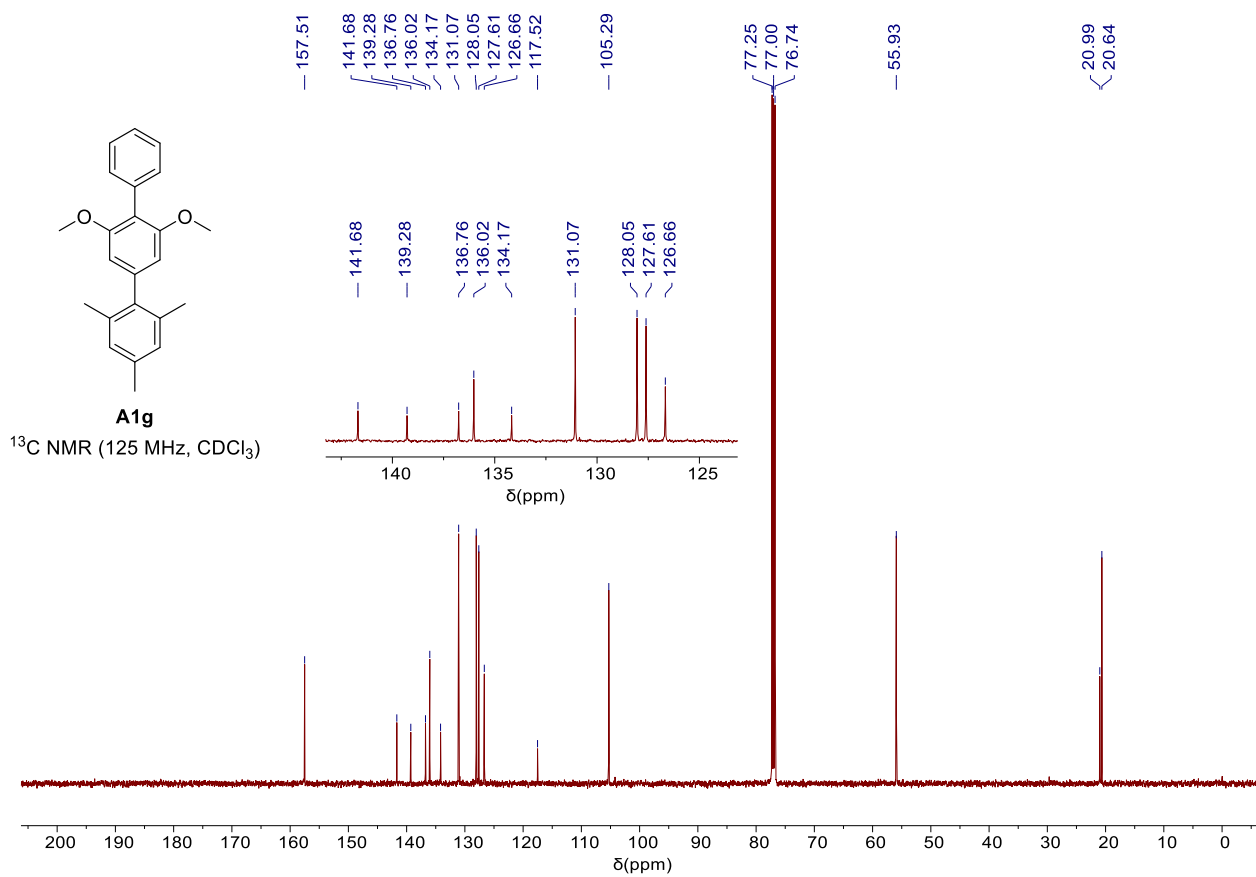


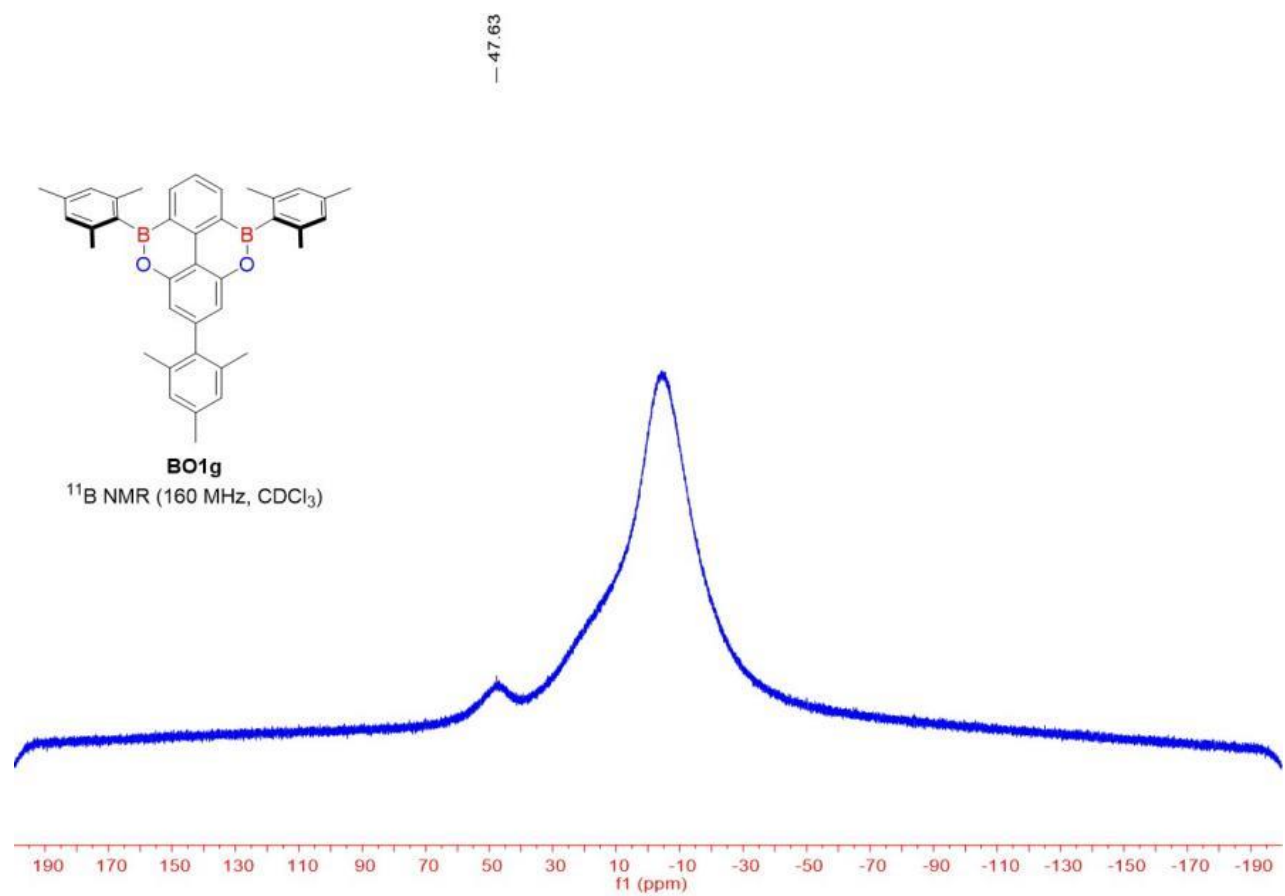
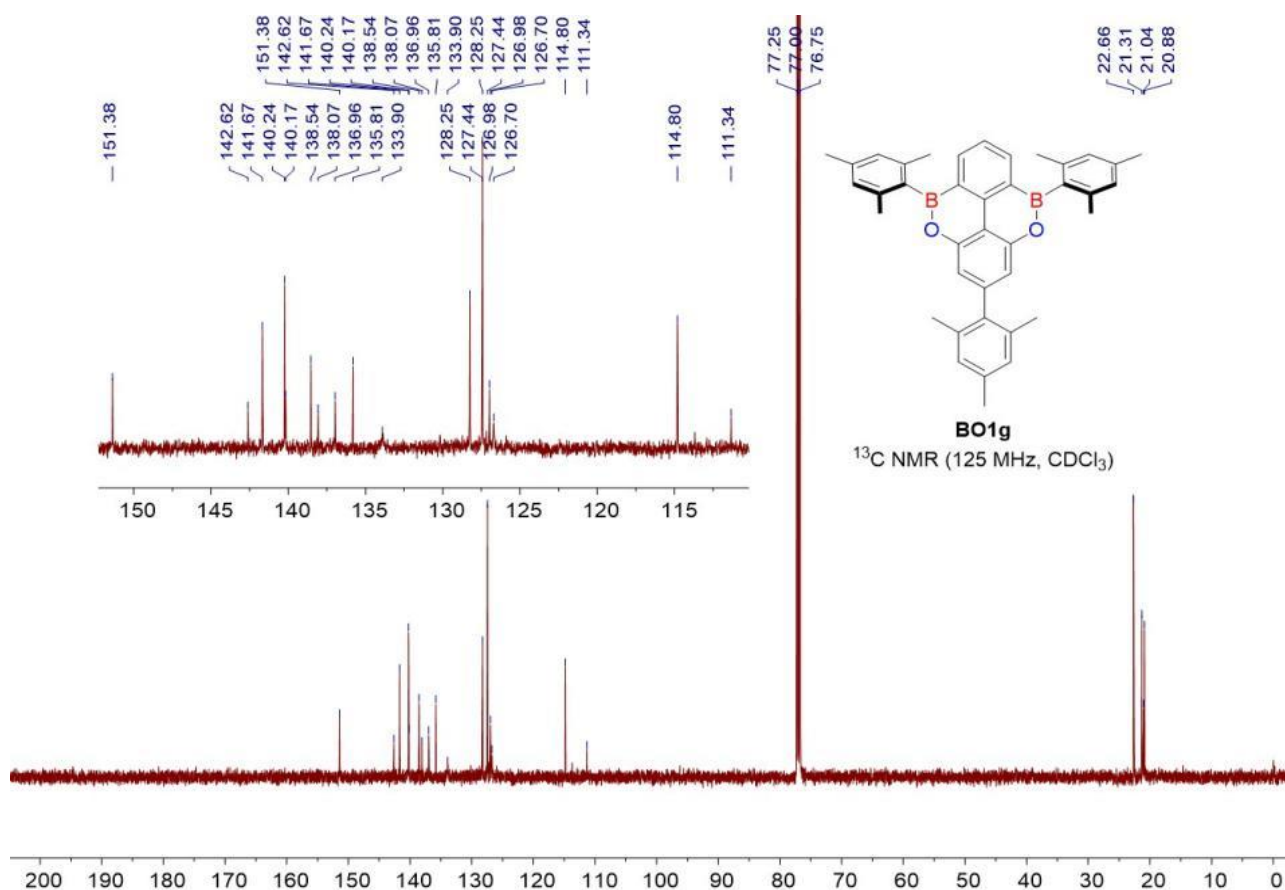
Spectrum from 0922.wiff (sample 27) - BO1f, +TOF MS (100 - 1500) from 0.135 to 0.195 min...pectrum from 0922.wiff (sample 27) - BO1f, +TOF MS (100 - 1500) from 0.326 to 0.479 min)



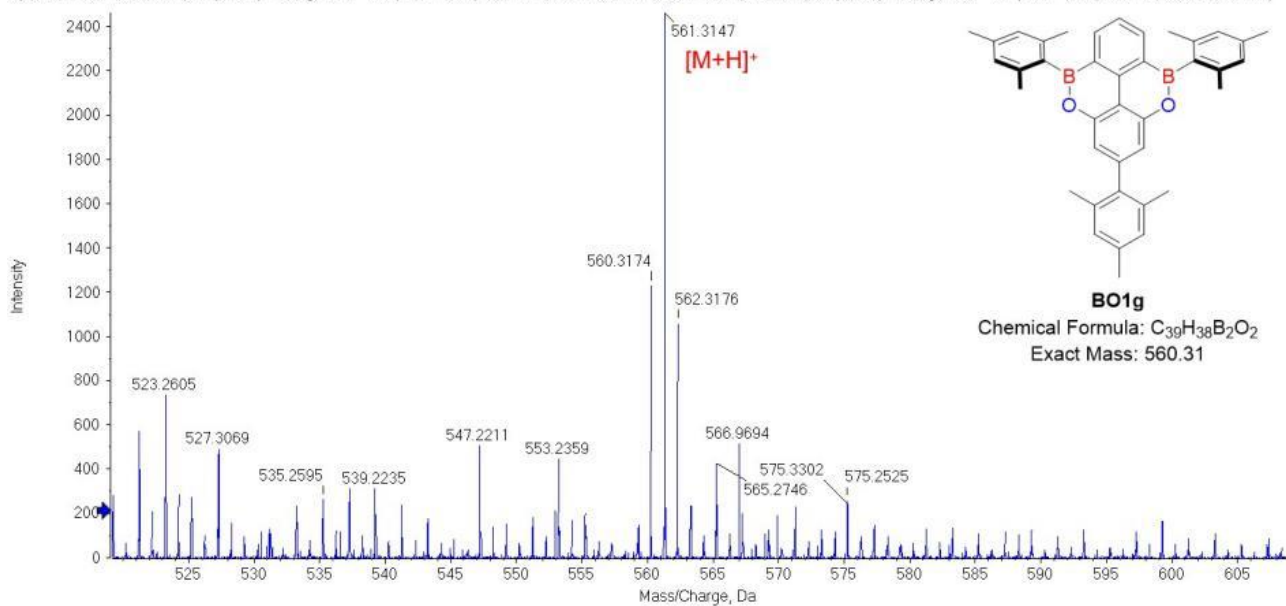
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$C_{36}H_{32}[^{11}B]_2O_2$	$C_{36}H_{33}[^{11}B]_2O_2$	519.2672	519.2661	-2.2



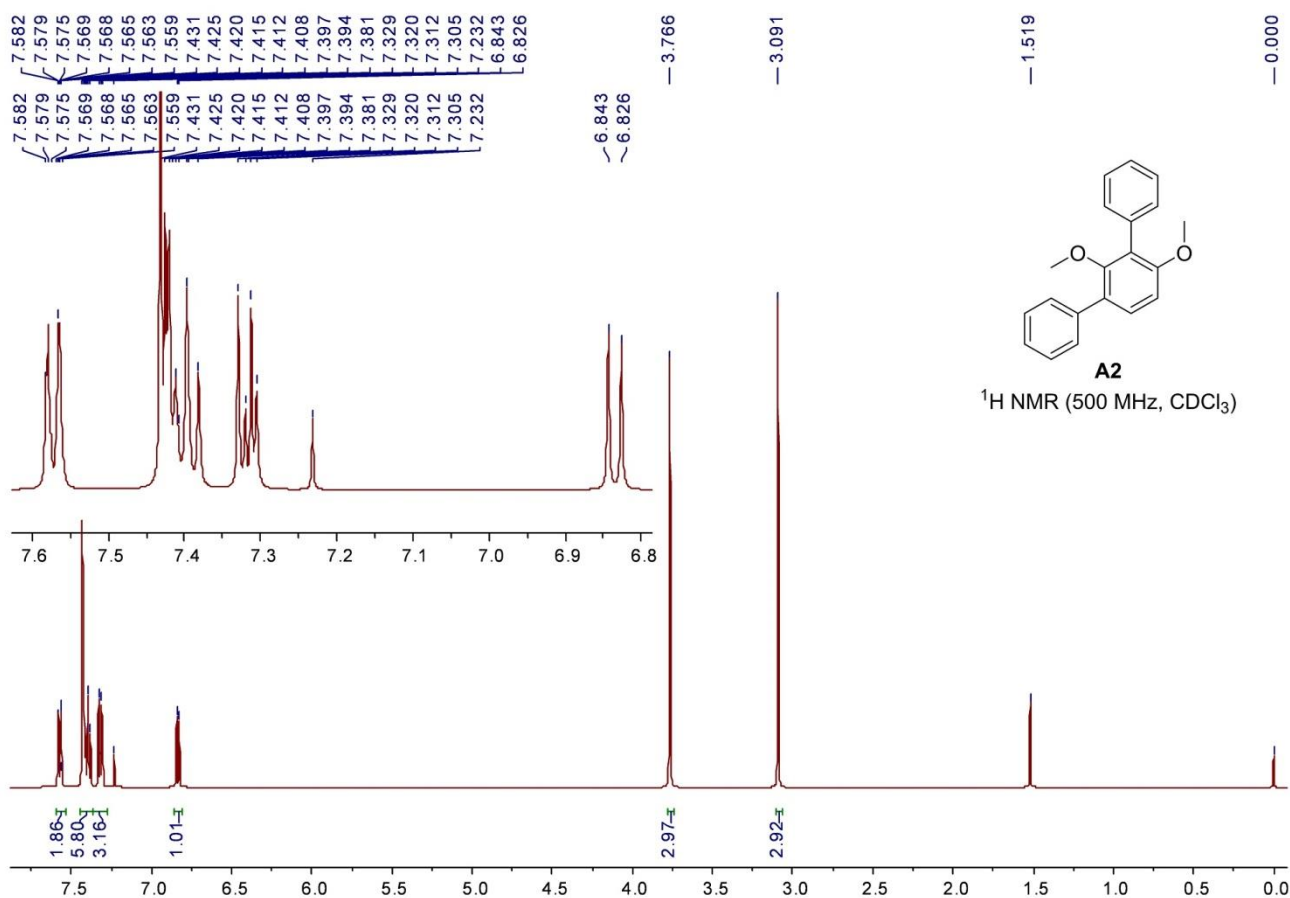


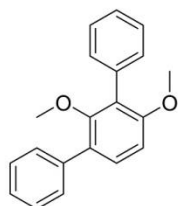


Spectrum from 0922.wiff (sample 28) - BO1g, +TOF MS (100 - 1500) from 0.135 to 0.195 min...pectrum from 0922.wiff (sample 28) - BO1g, +TOF MS (100 - 1500) from 0.326 to 0.479 min)



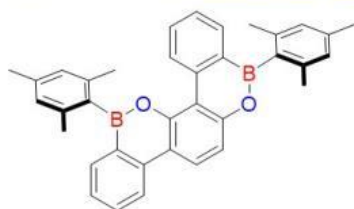
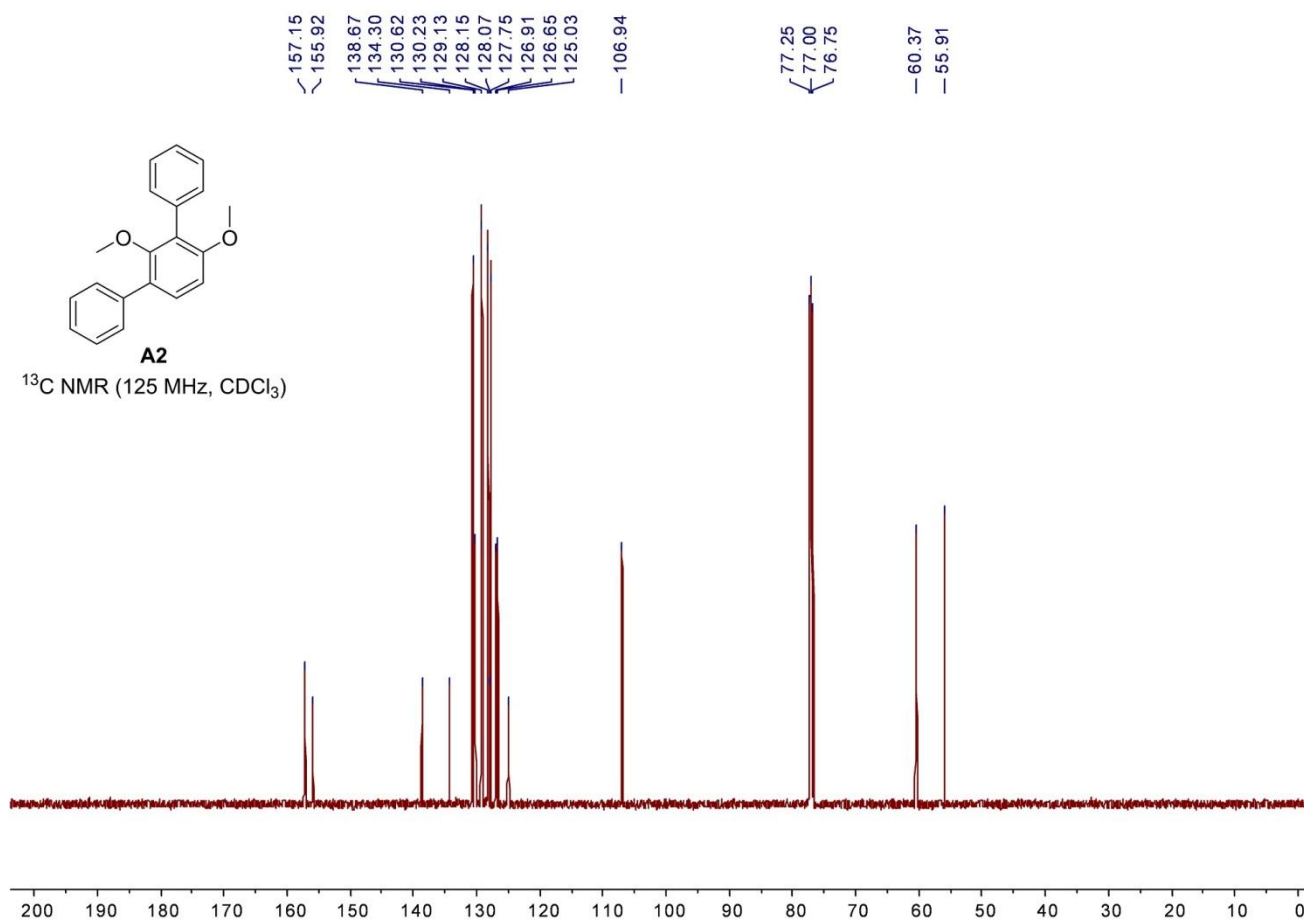
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$C_{39}H_{38}[^{11}B]_2O_2$	$C_{39}H_{39}[^{11}B]_2O_2$	561.3147	561.3131	-2.9





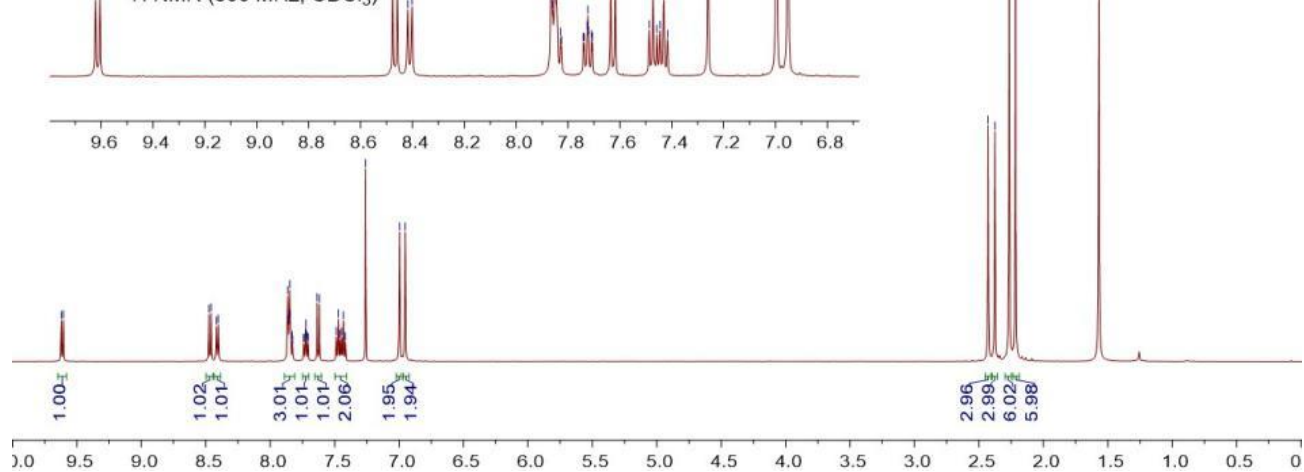
A2

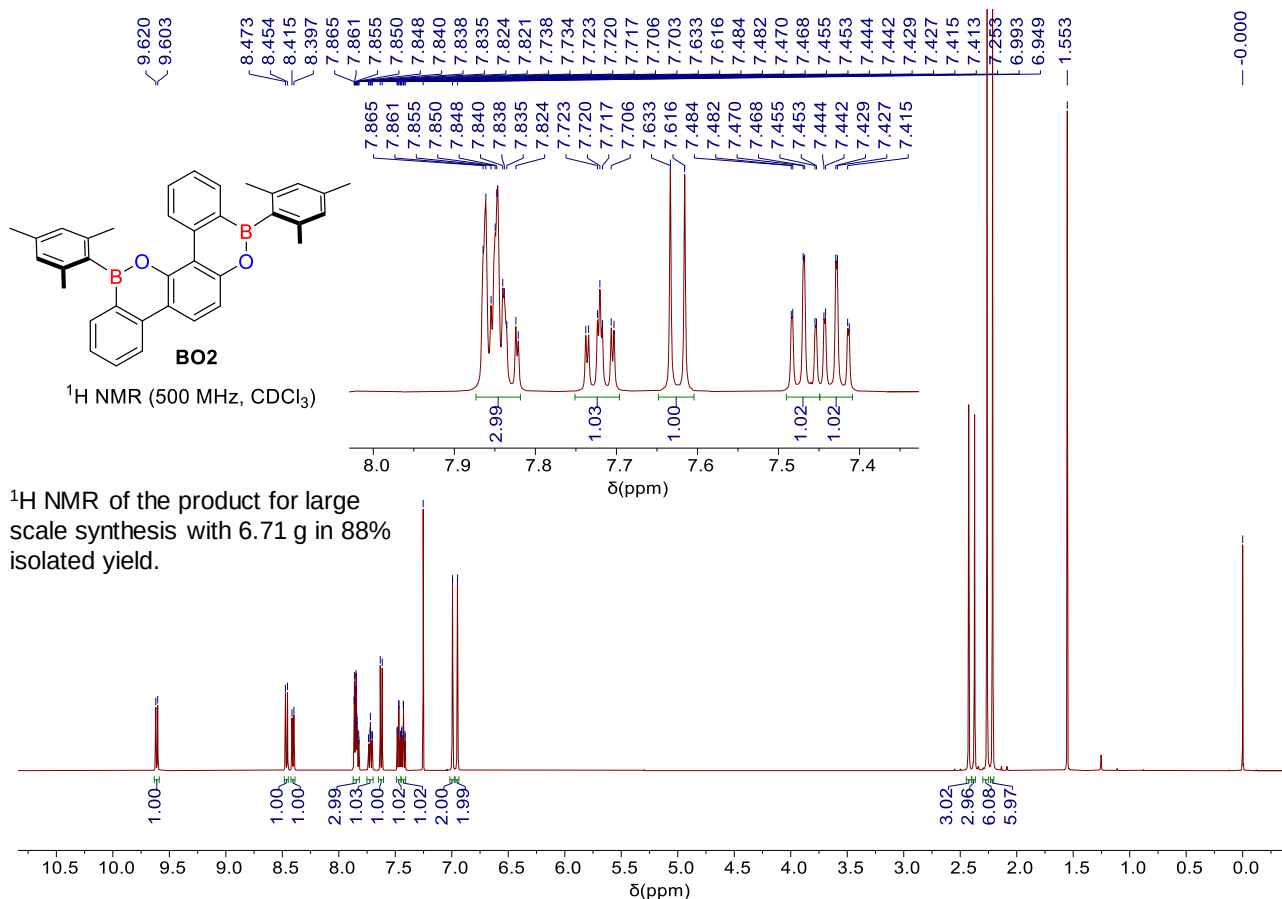
^{13}C NMR (125 MHz, CDCl_3)



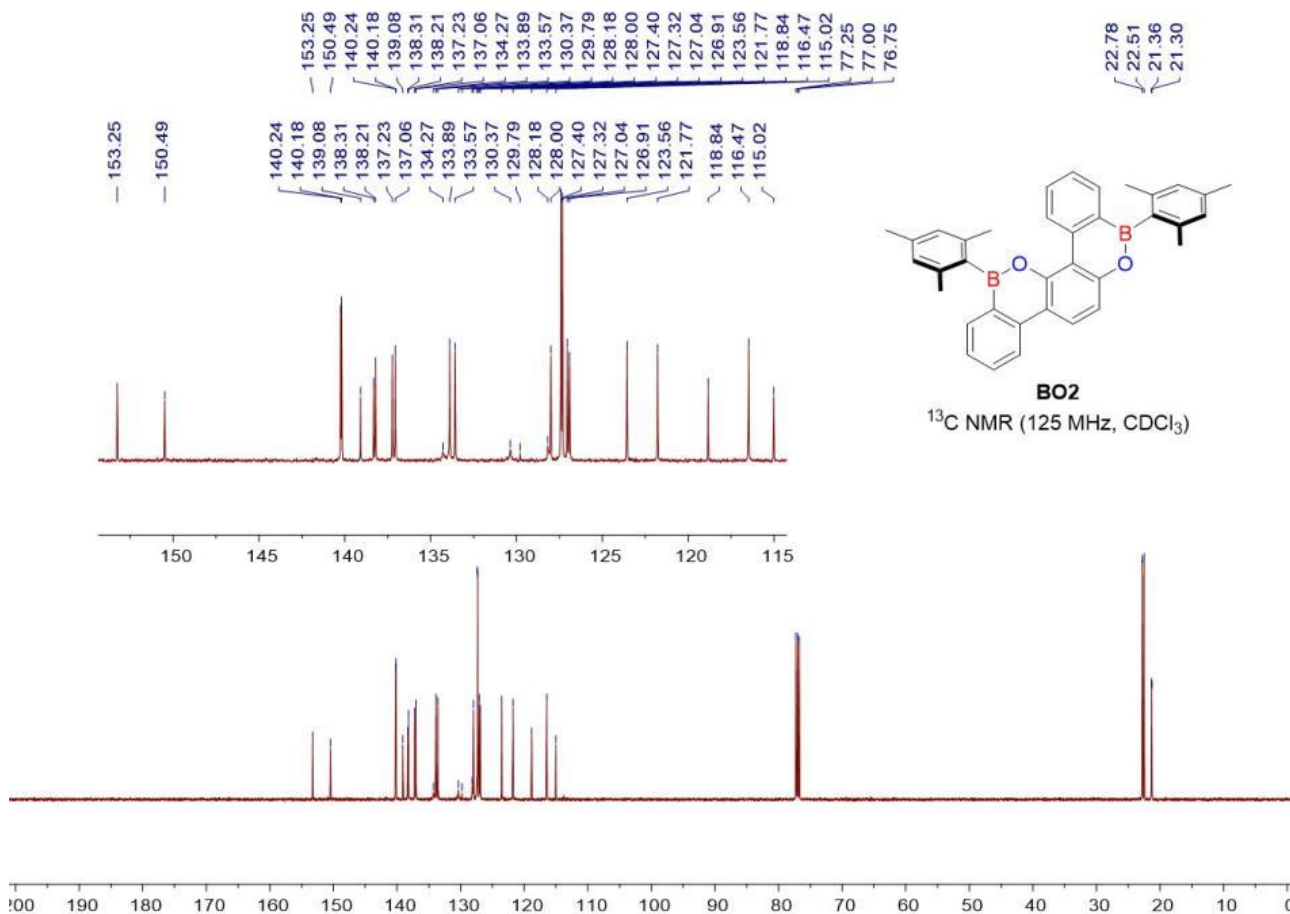
BO2

^1H NMR (500 MHz, CDCl_3)

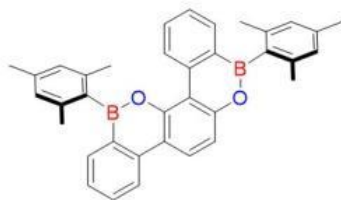




¹H NMR of the product for large scale synthesis with 6.71 g in 88% isolated yield.

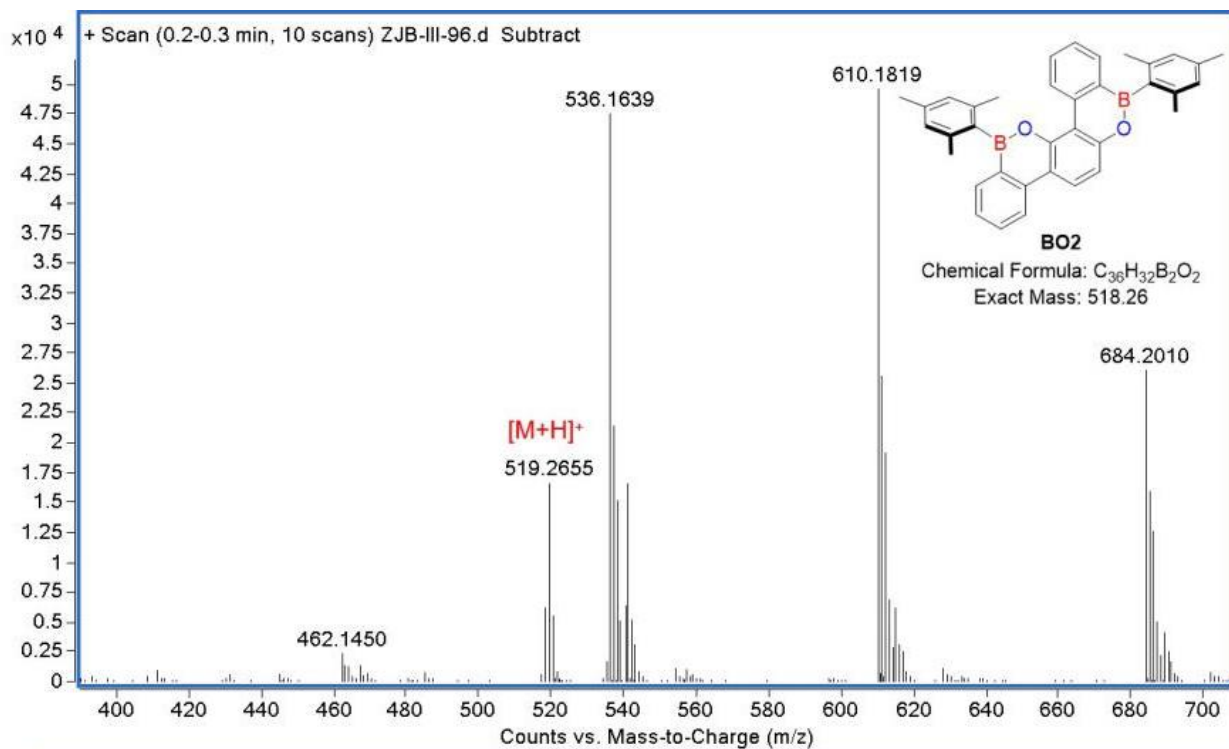
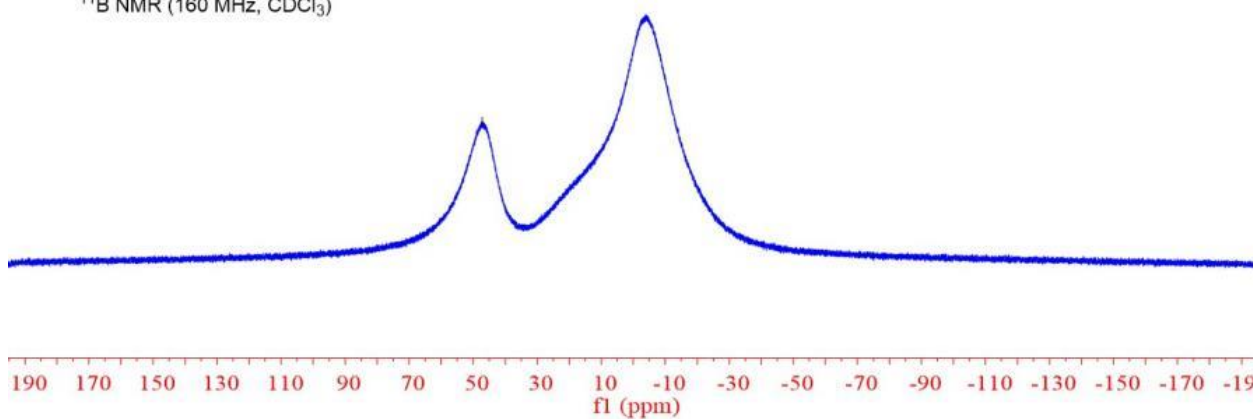


— 47.21

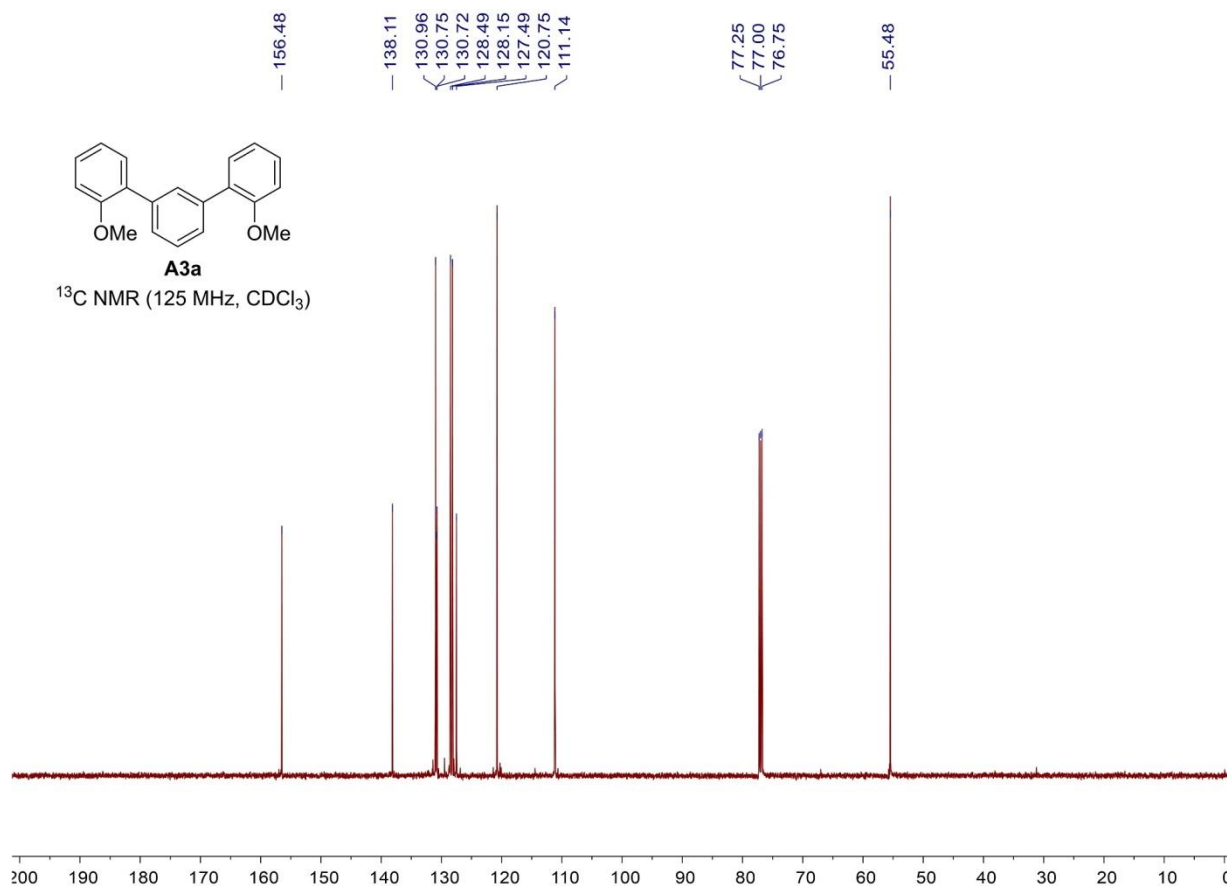
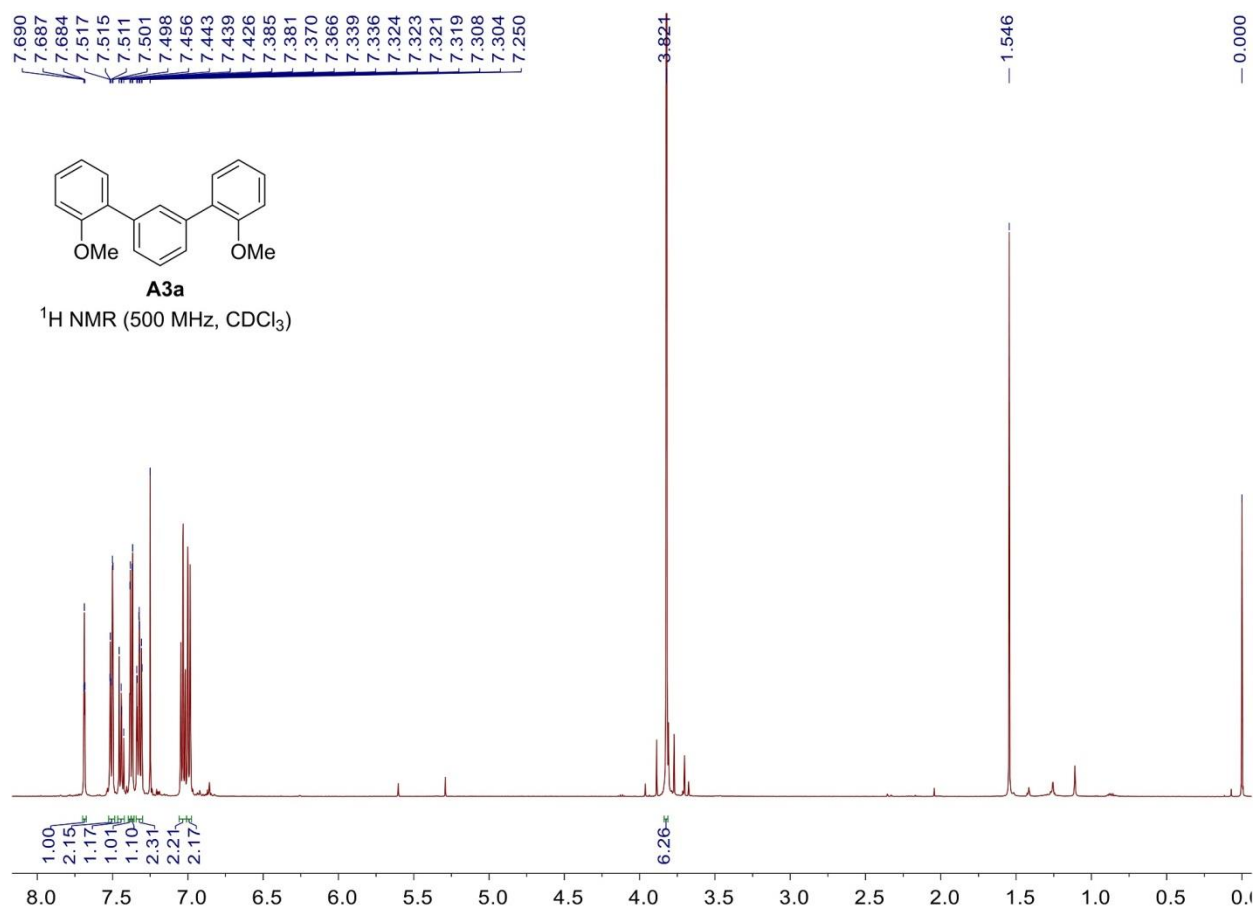


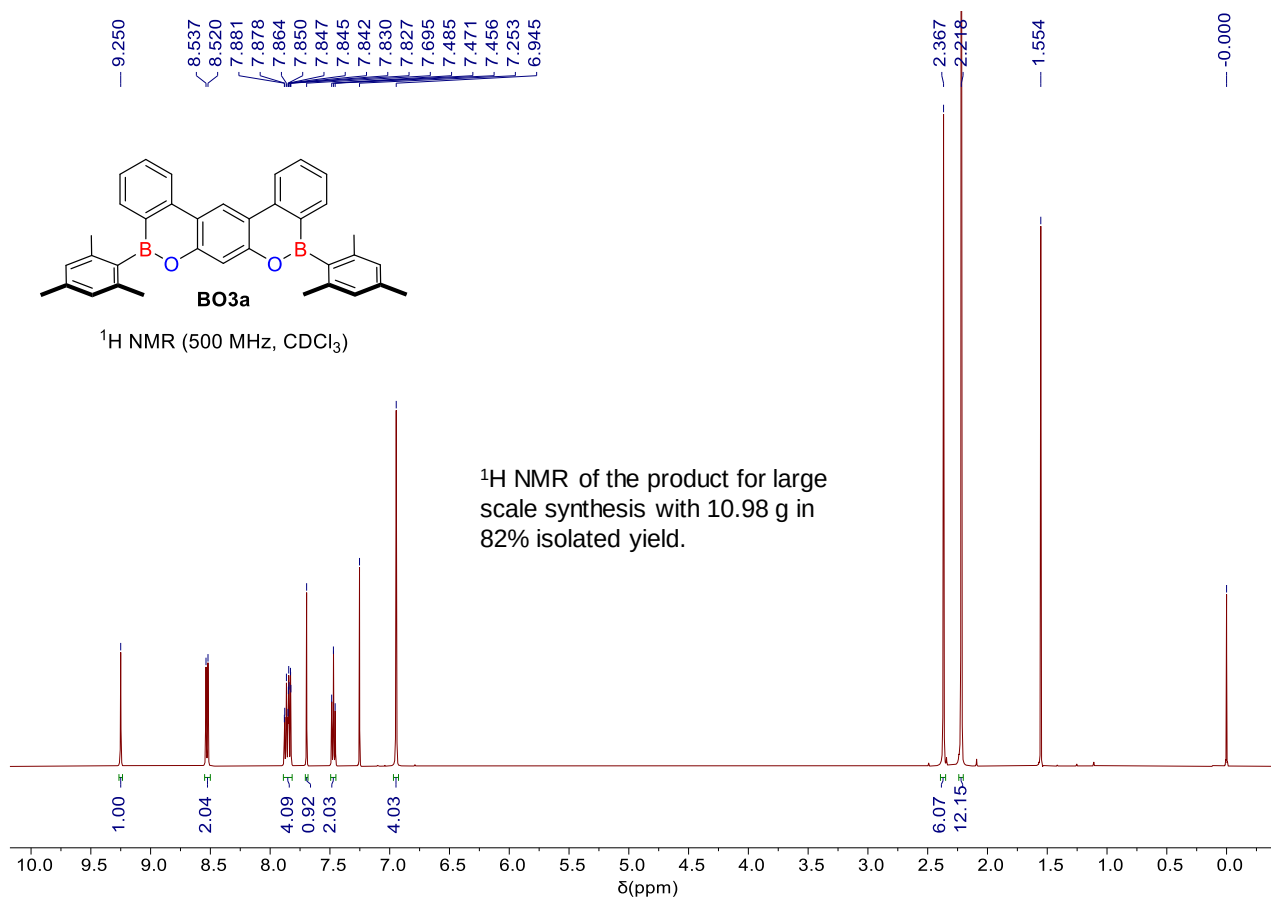
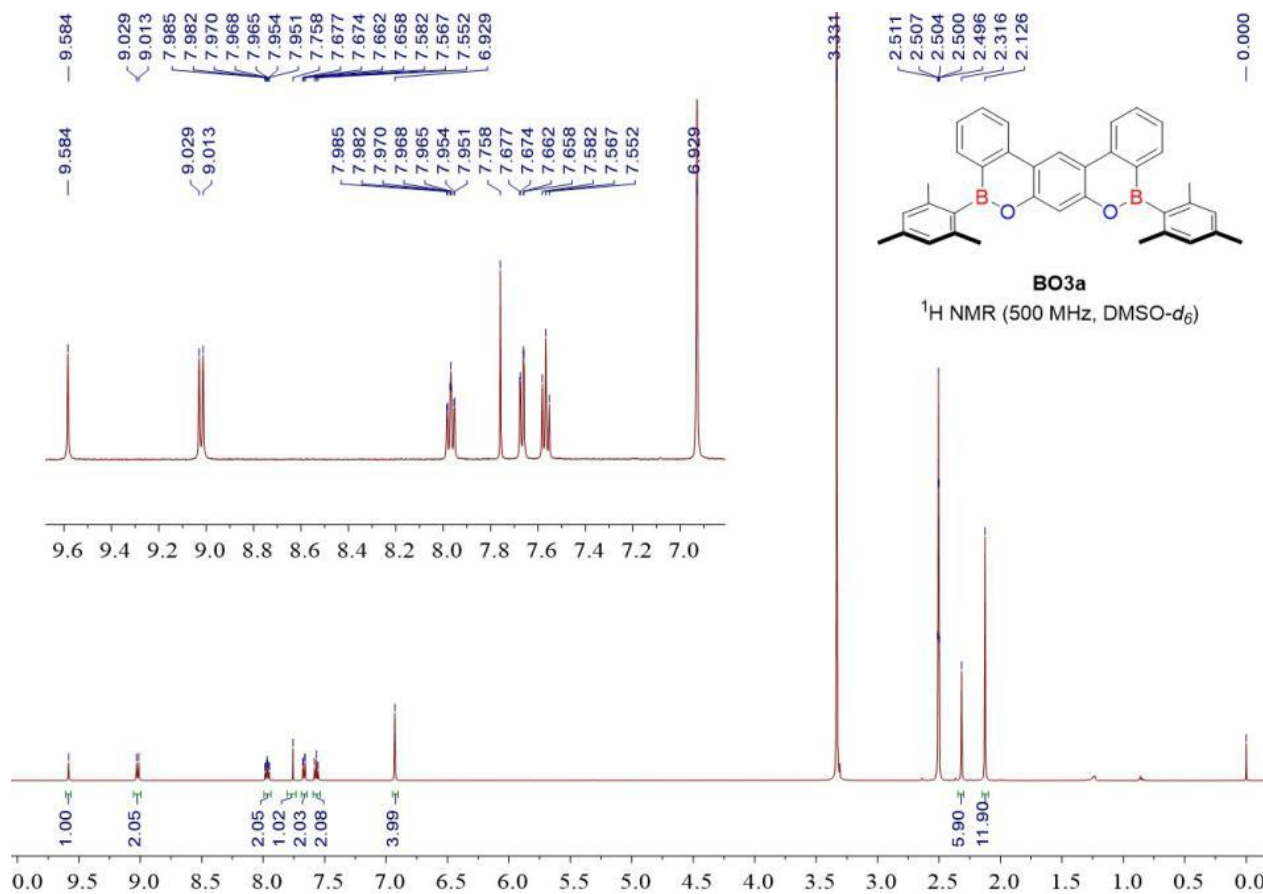
BO2

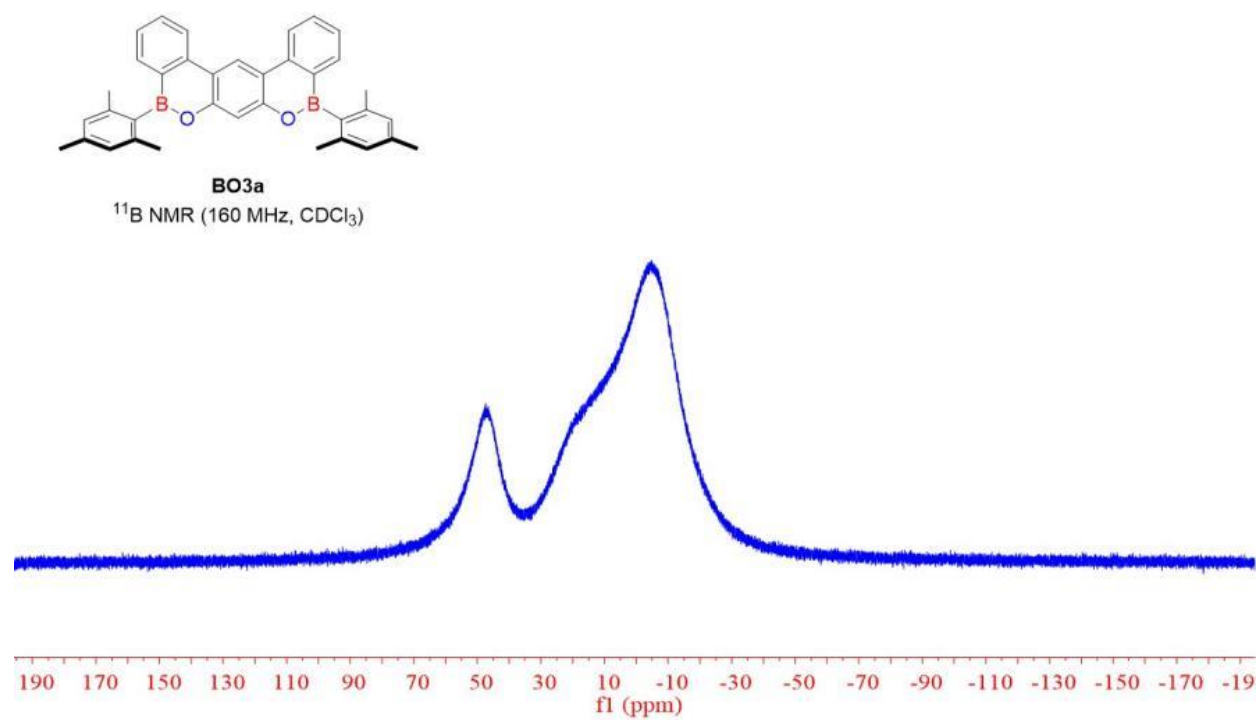
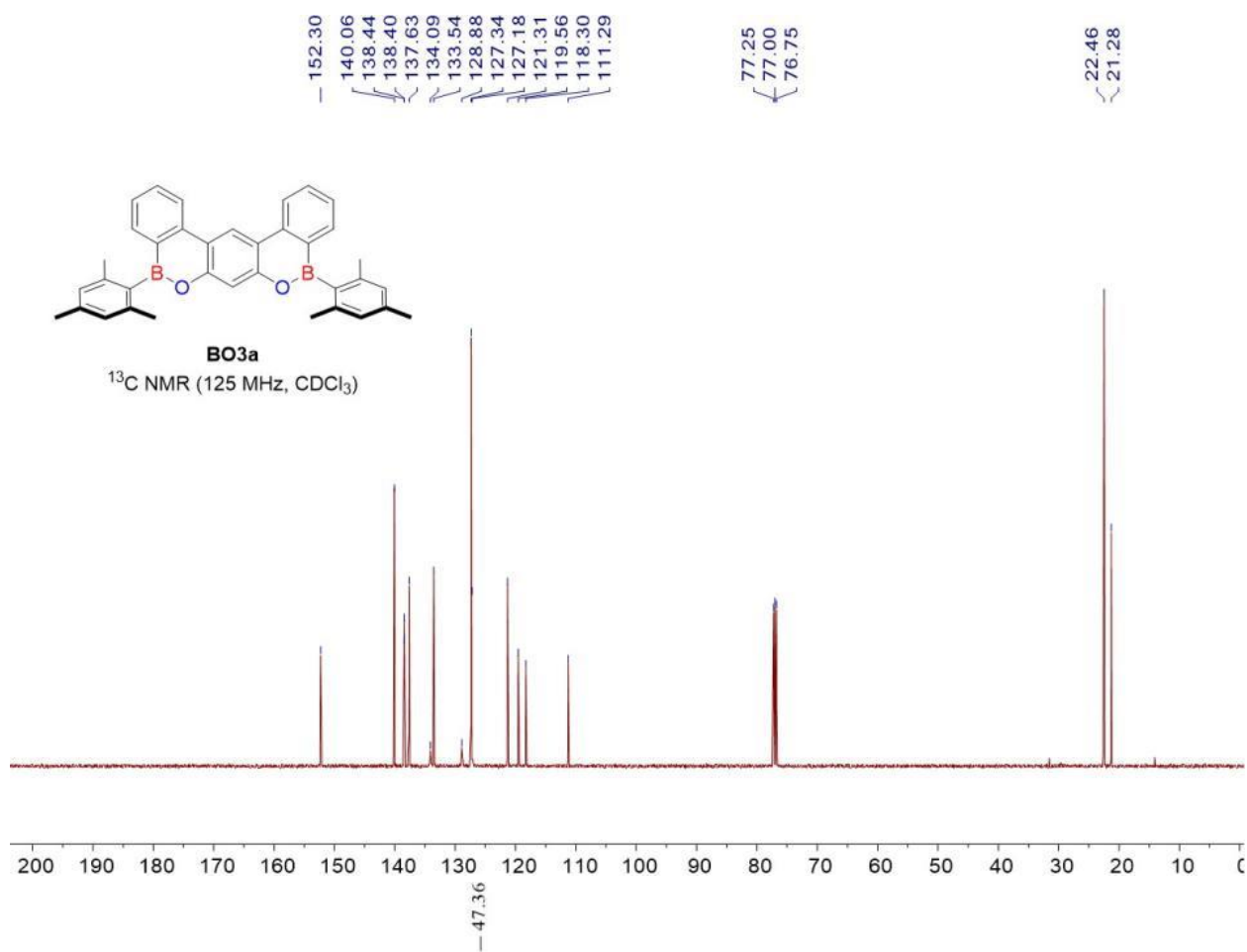
^{11}B NMR (160 MHz, CDCl_3)

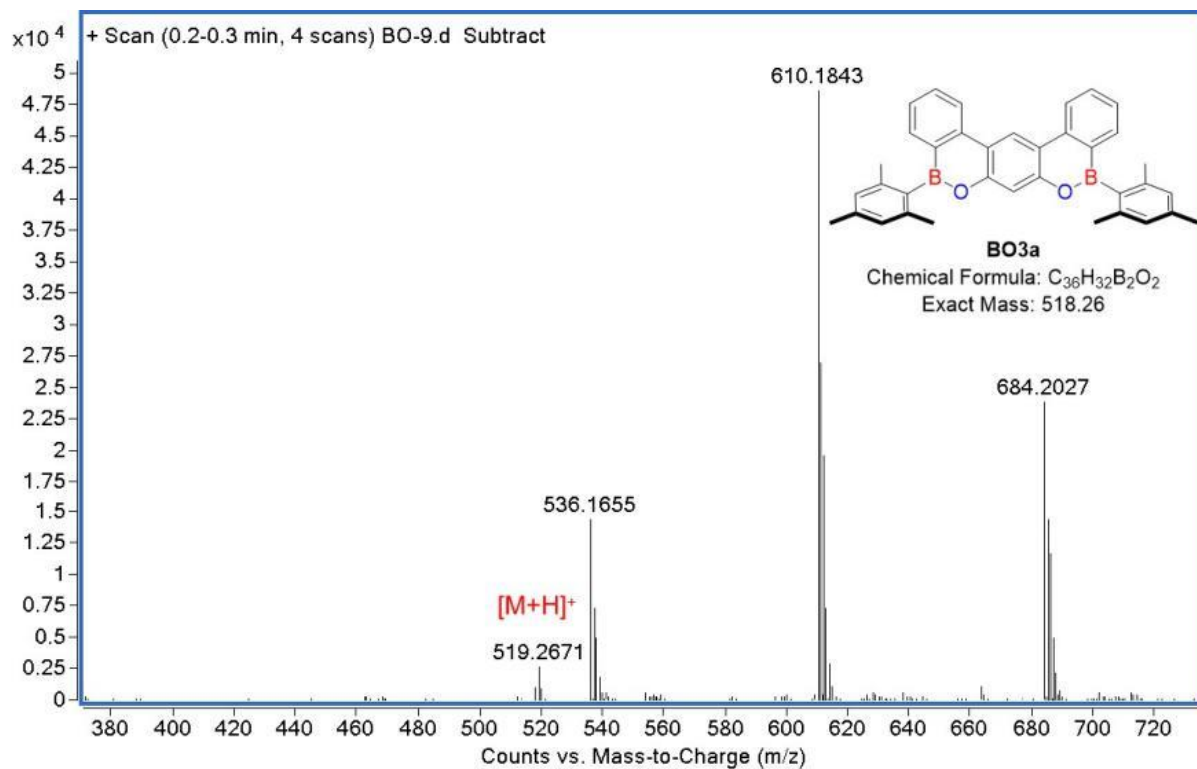


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{36}\text{H}_{32}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{36}\text{H}_{33}[^{11}\text{B}]_2\text{O}_2$	519.2655	519.2661	1.19

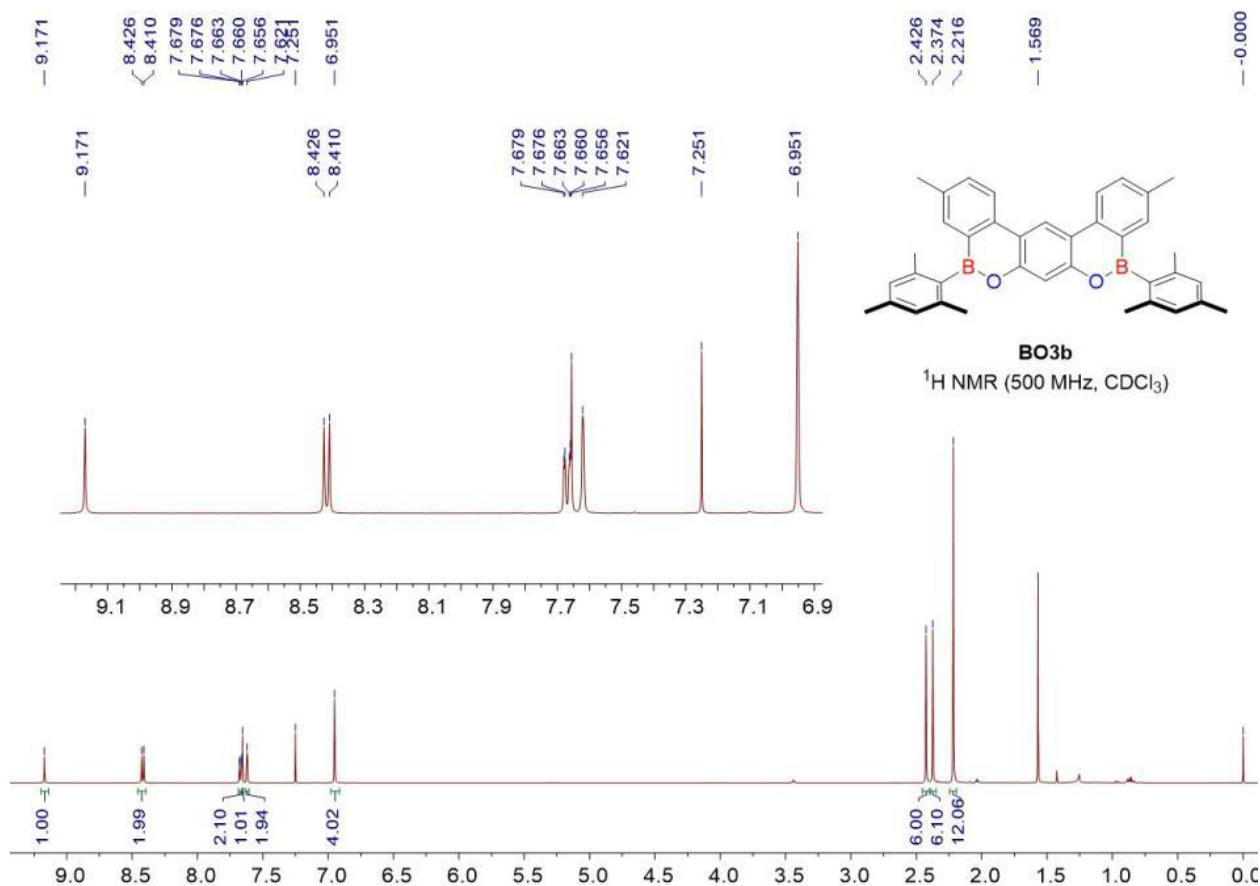


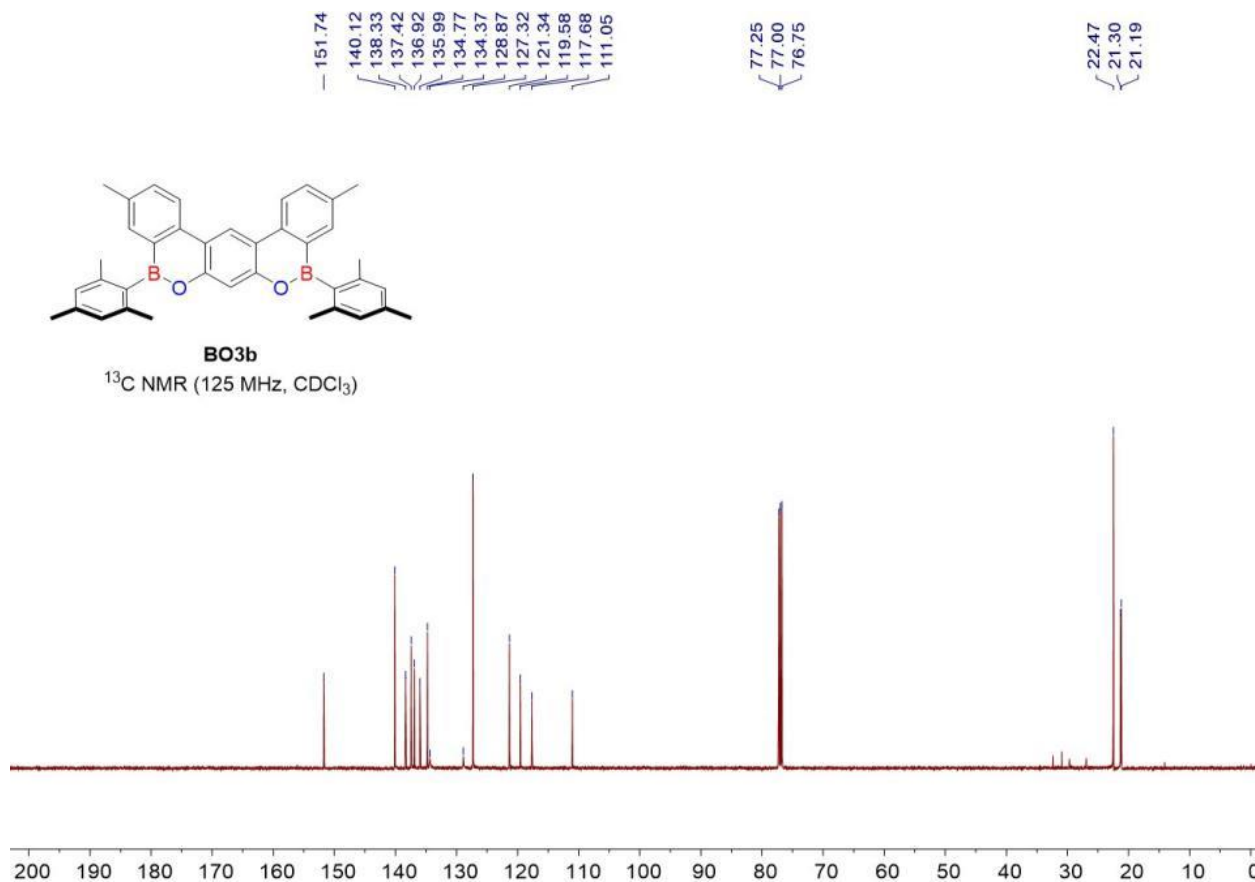
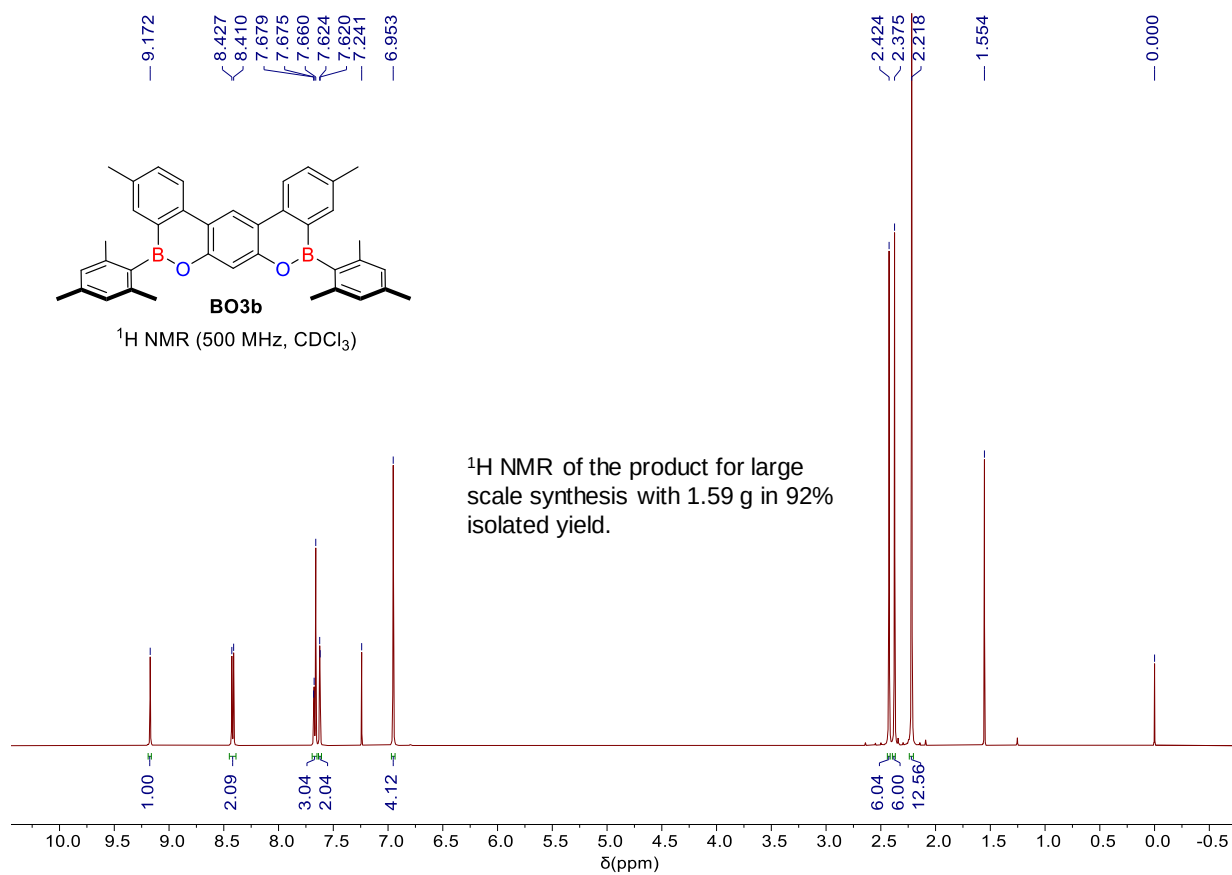


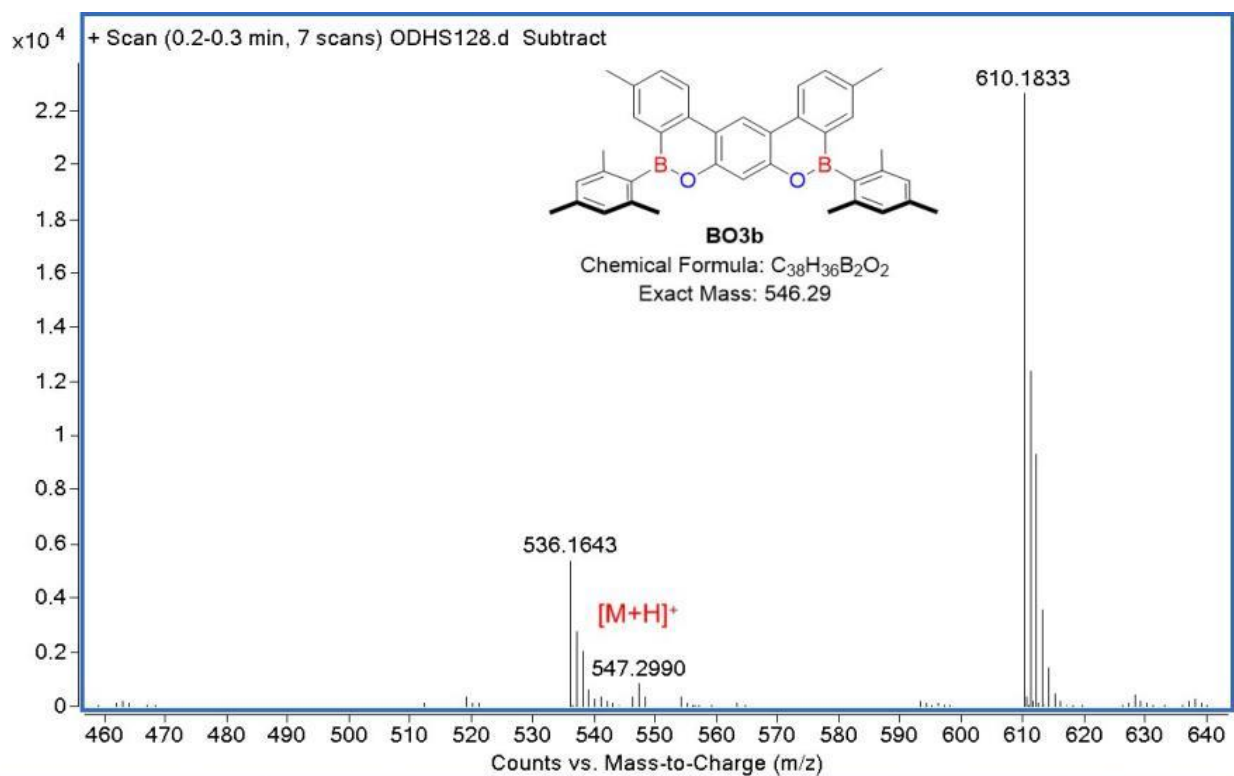
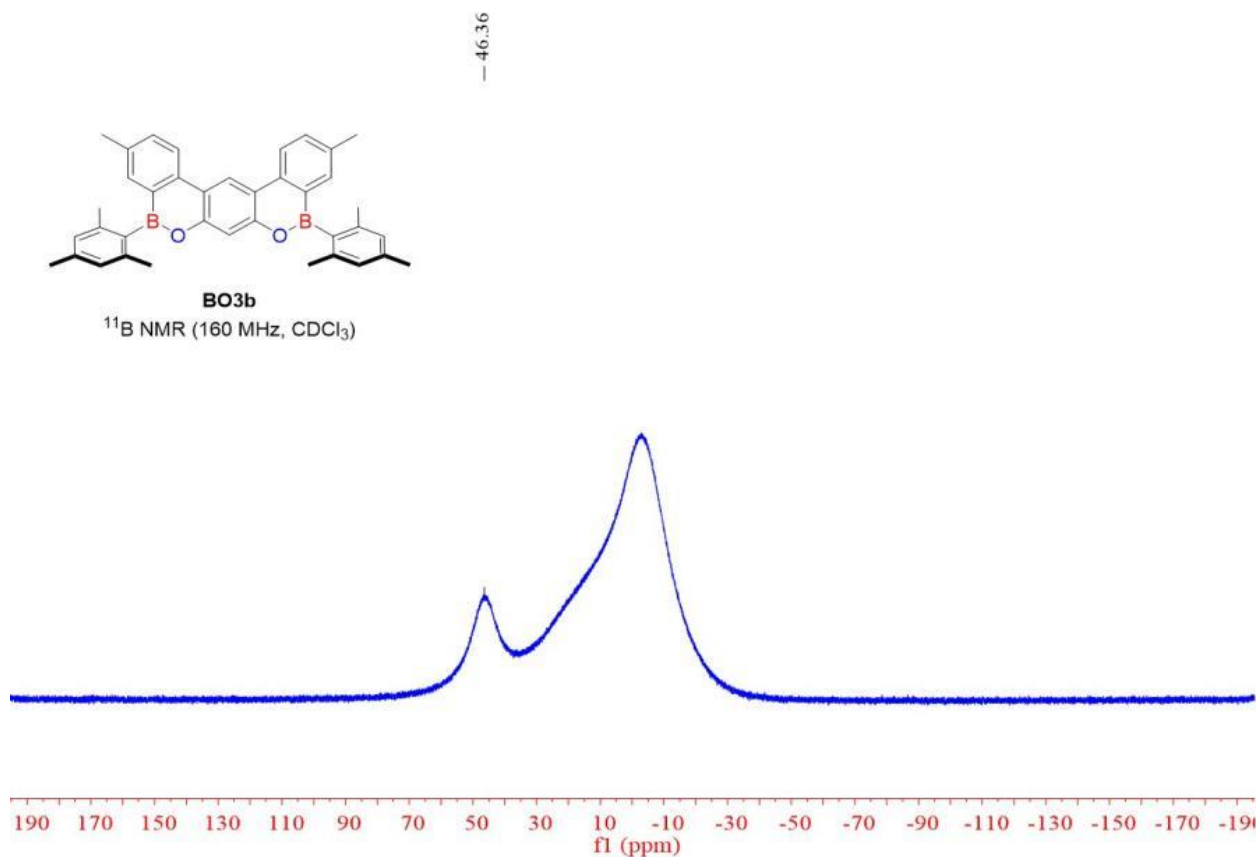




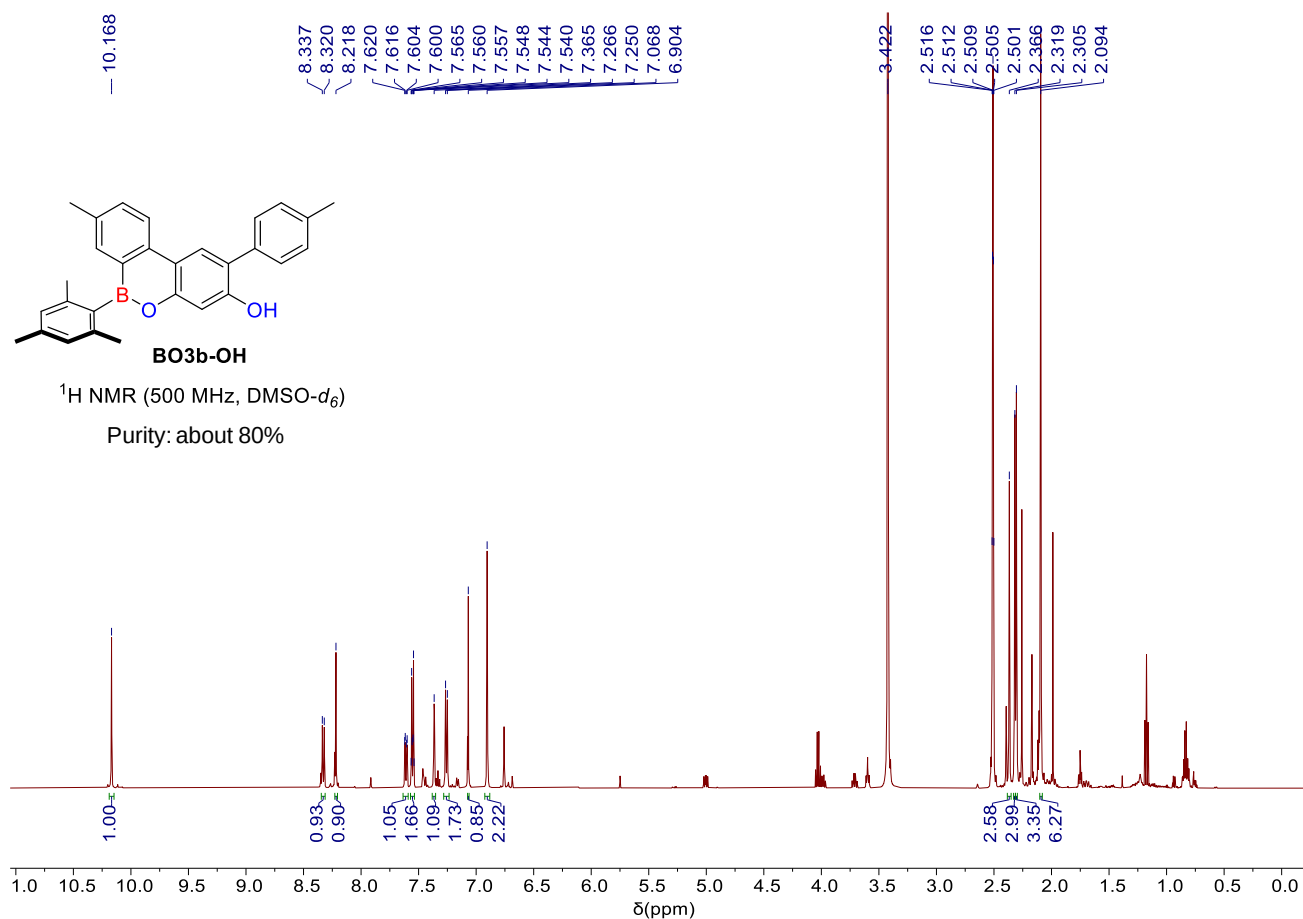
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$C_{36}H_{32}[^{11}B]_2O_2$	$C_{36}H_{33}[^{11}B]_2O_2$	519.2671	519.2661	-1.9	22



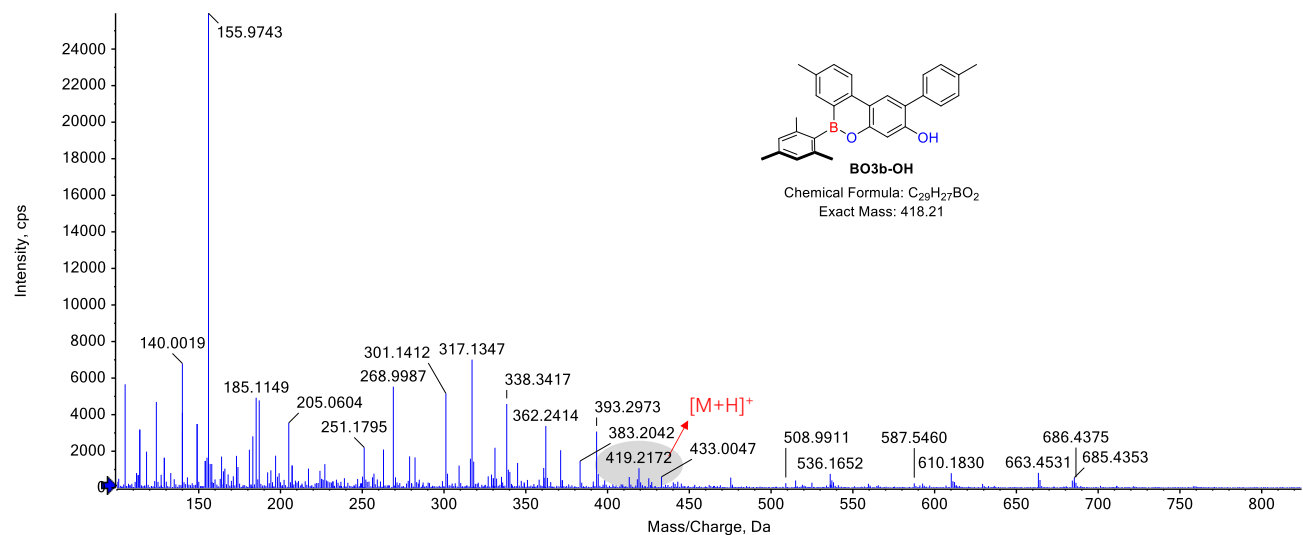


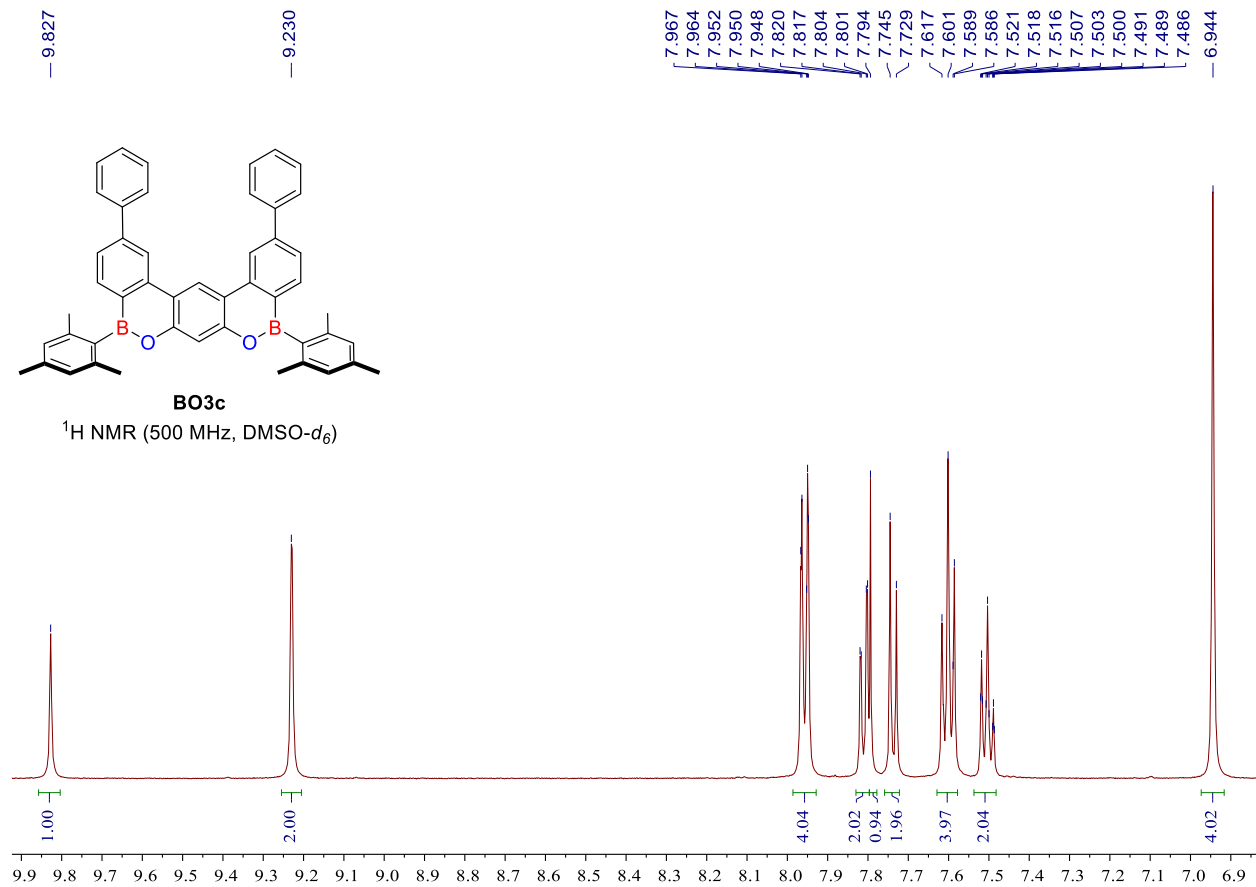
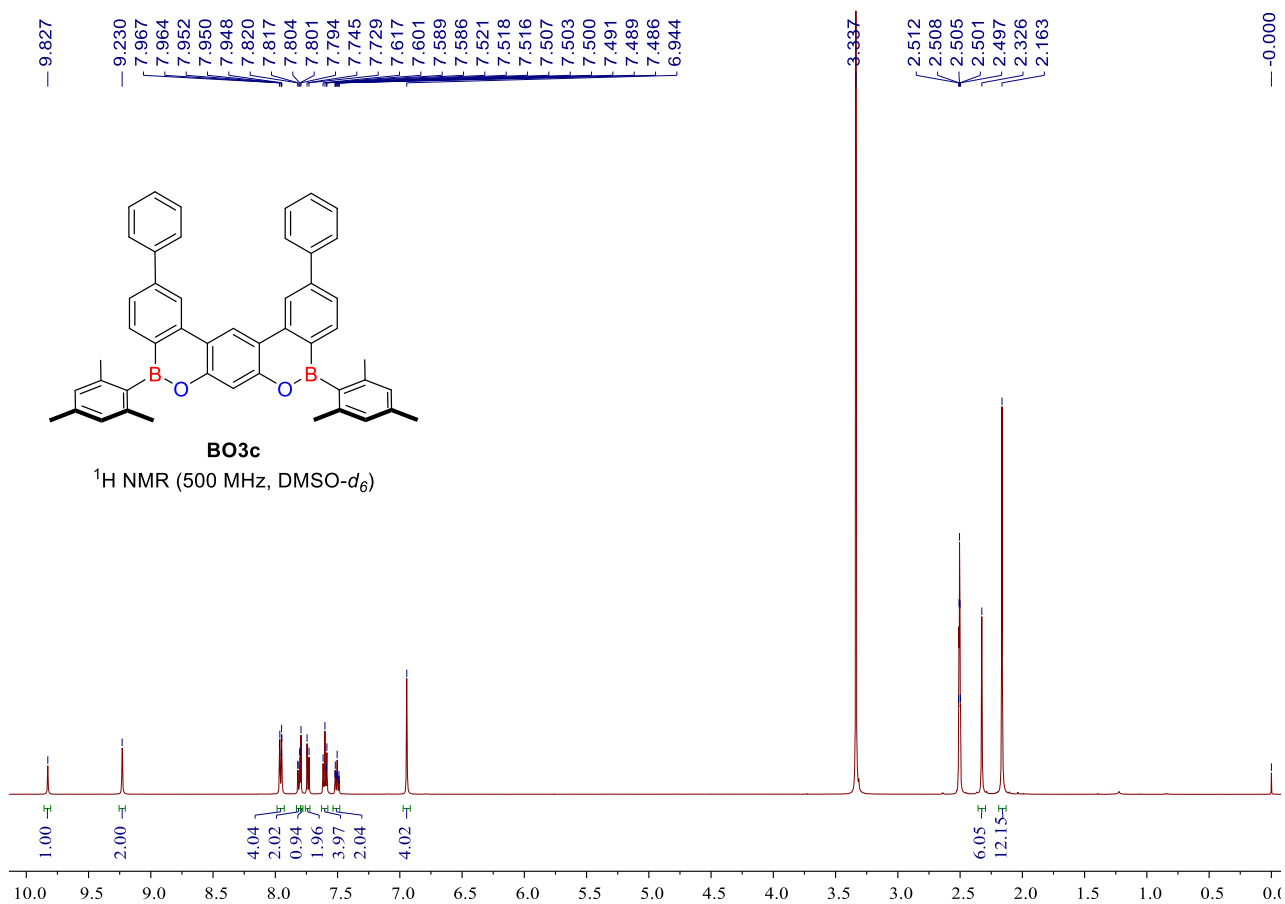


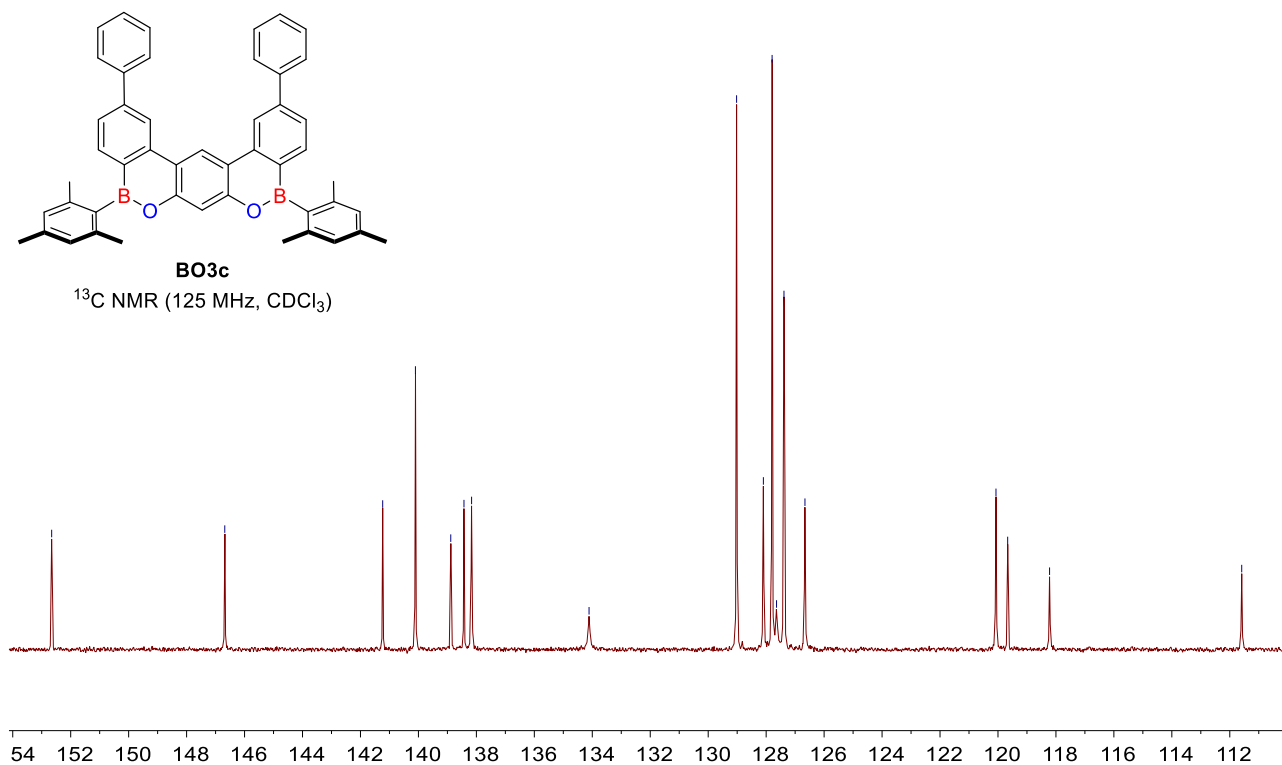
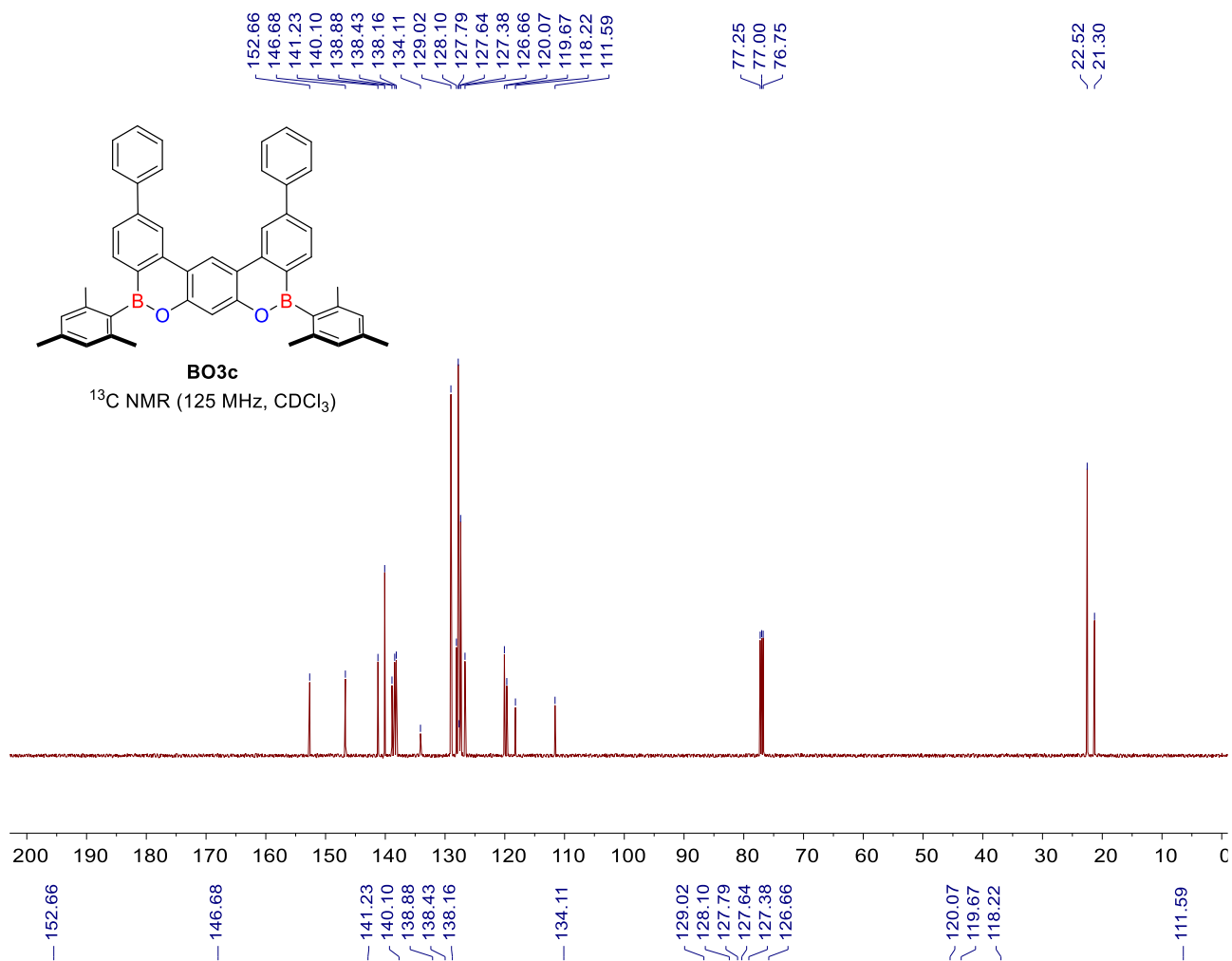
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
C ₃₈ H ₃₆ [¹¹ B] ₂ O ₂	C ₃₈ H ₃₇ [¹¹ B] ₂ O ₂	547.299	547.2974	-2.9	22



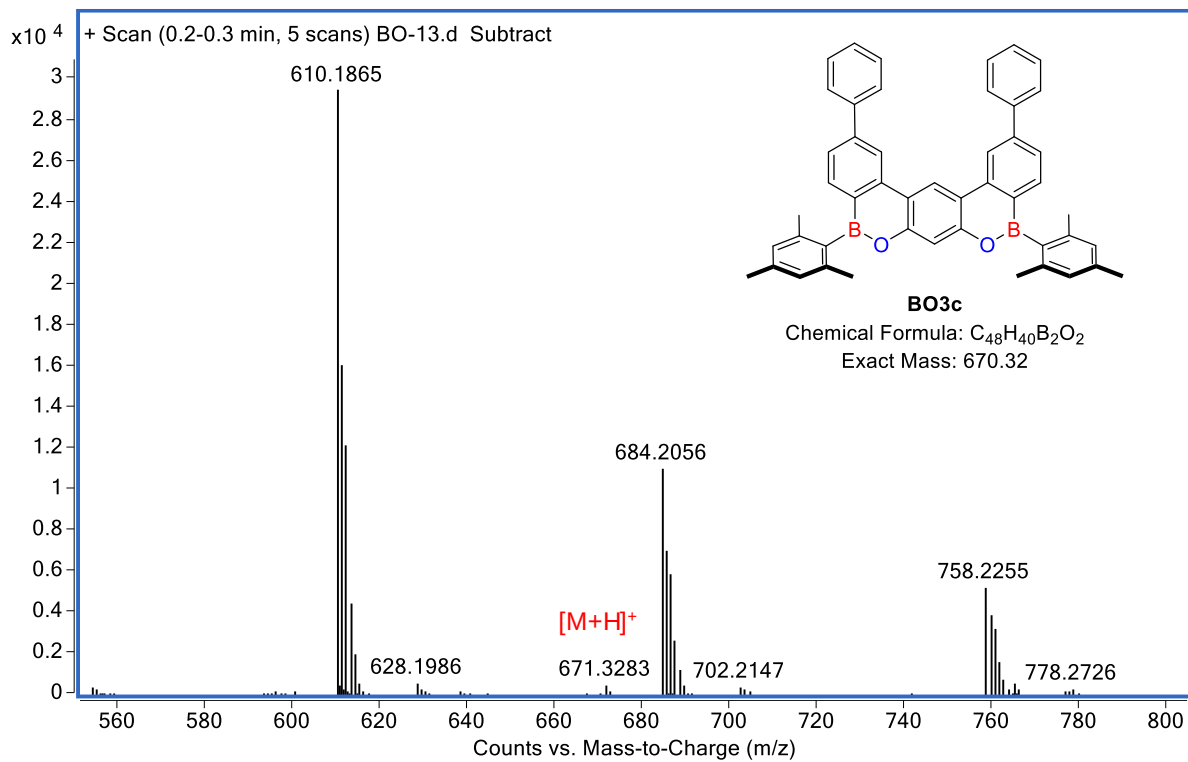
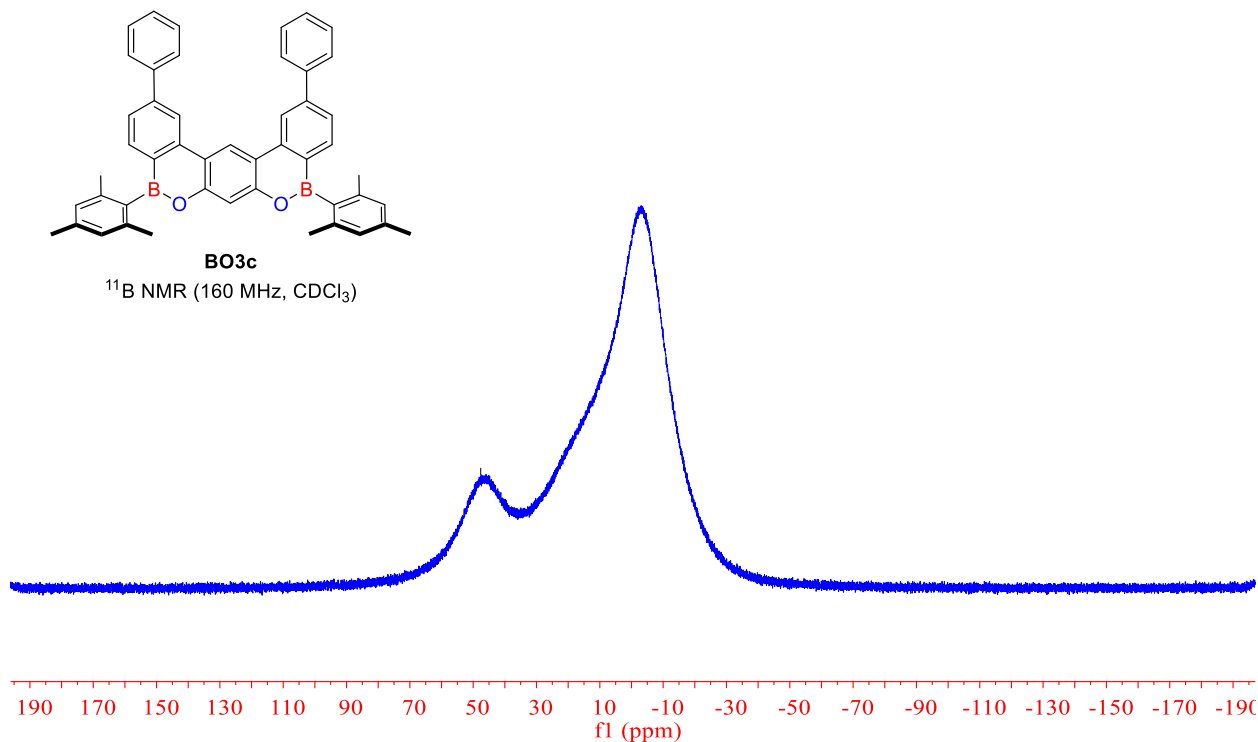
Spectrum from 0809.wiff2 (sample 22) - BO3b-byProduct-1, +TOF MS (100 - 1500) from 0.194 to 0.208 min



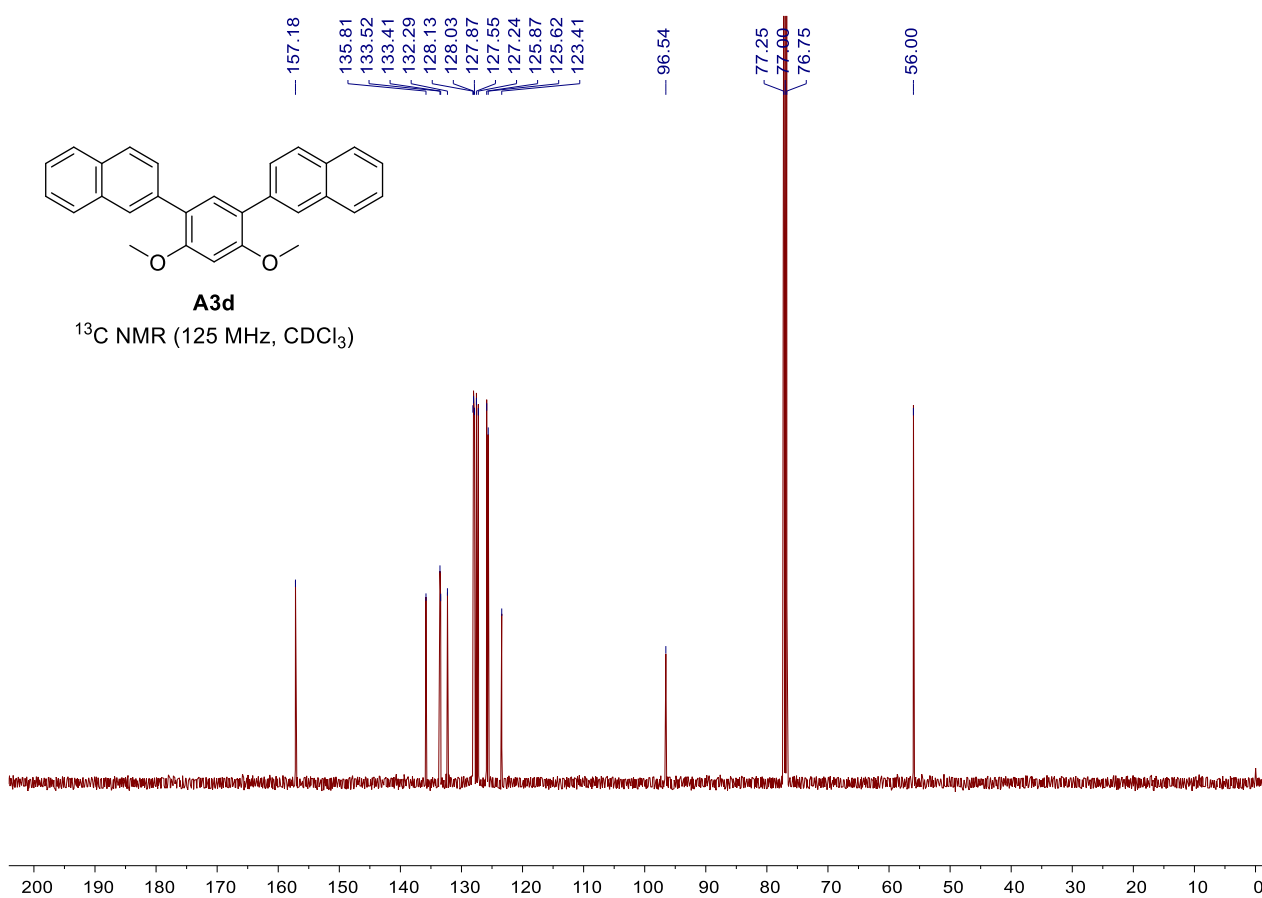
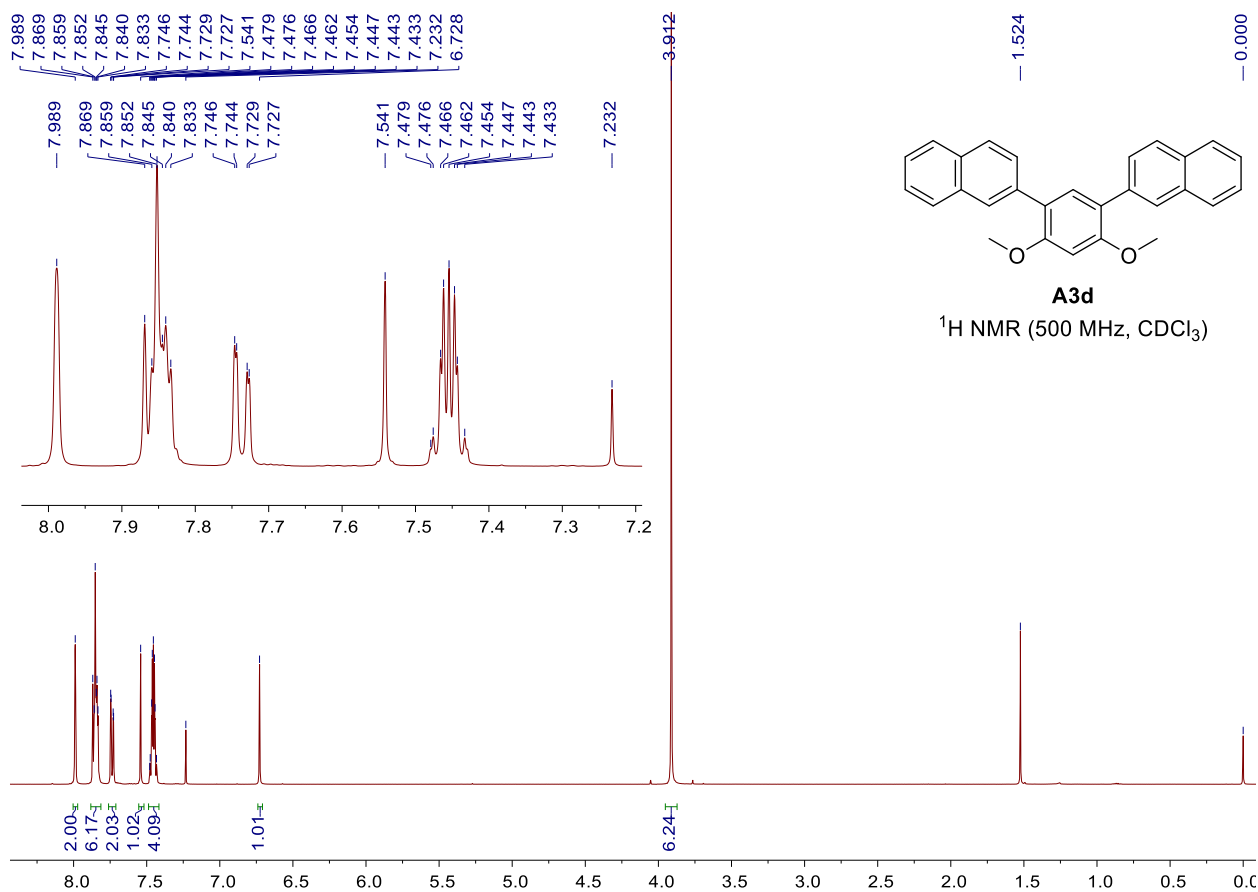


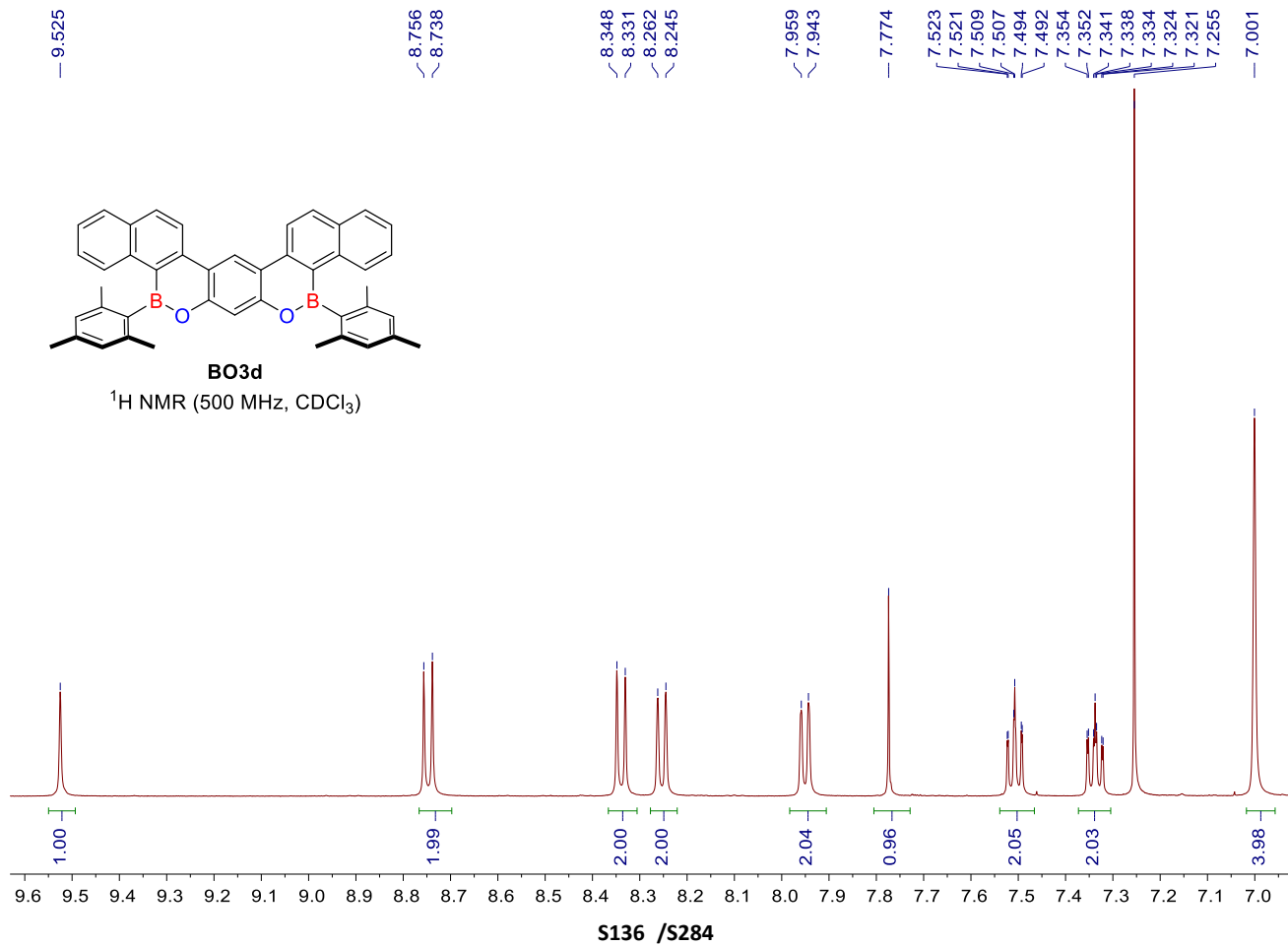
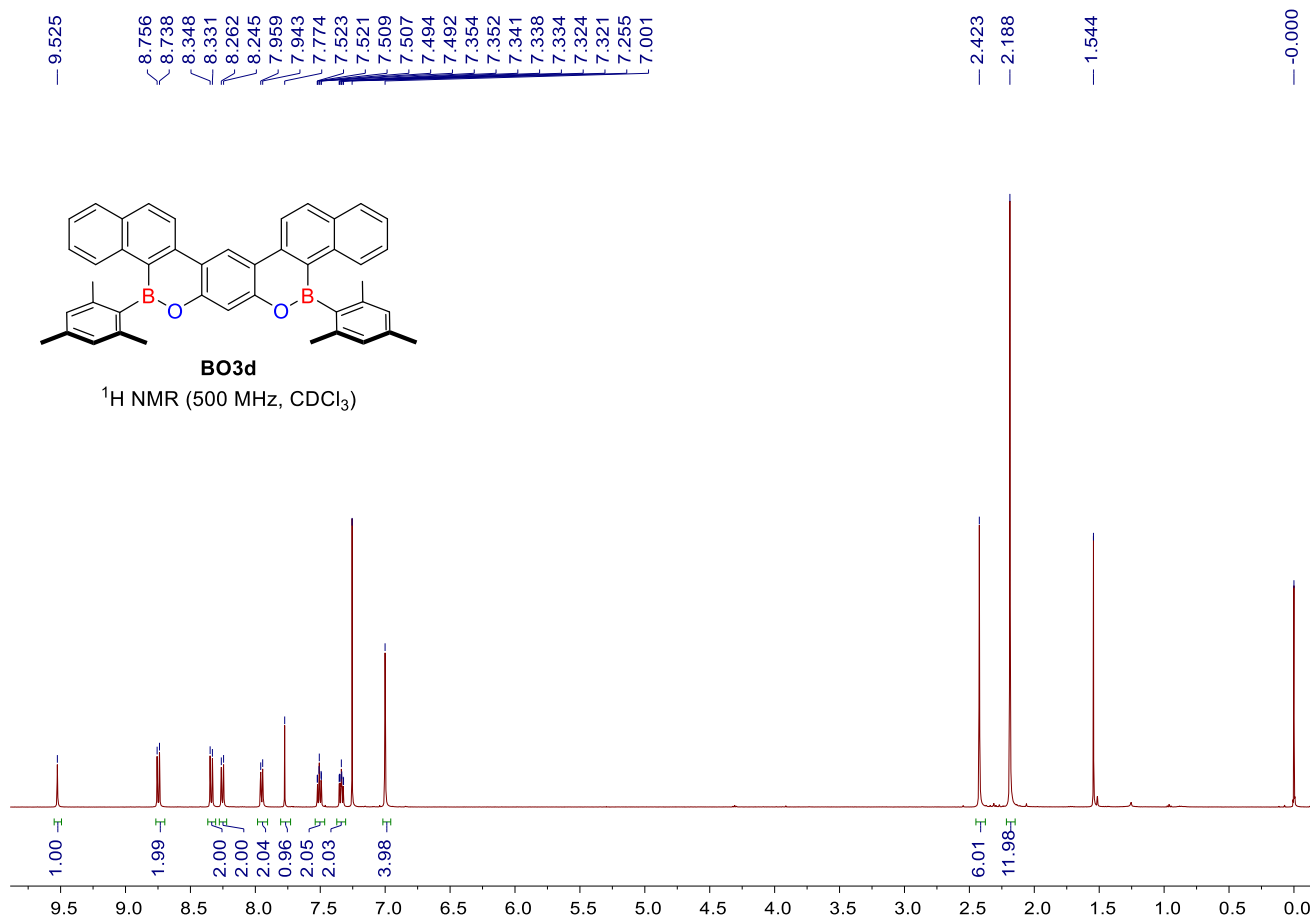


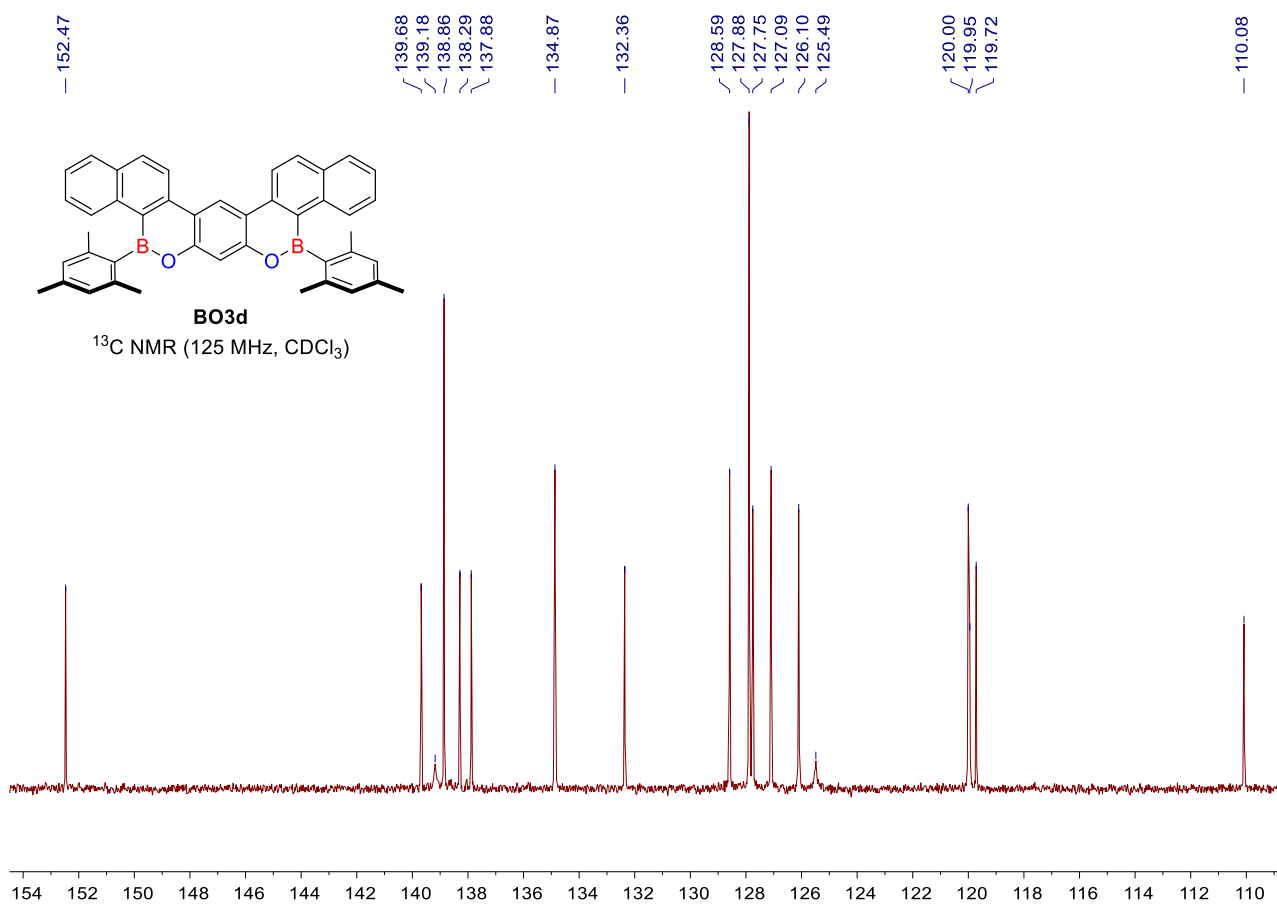
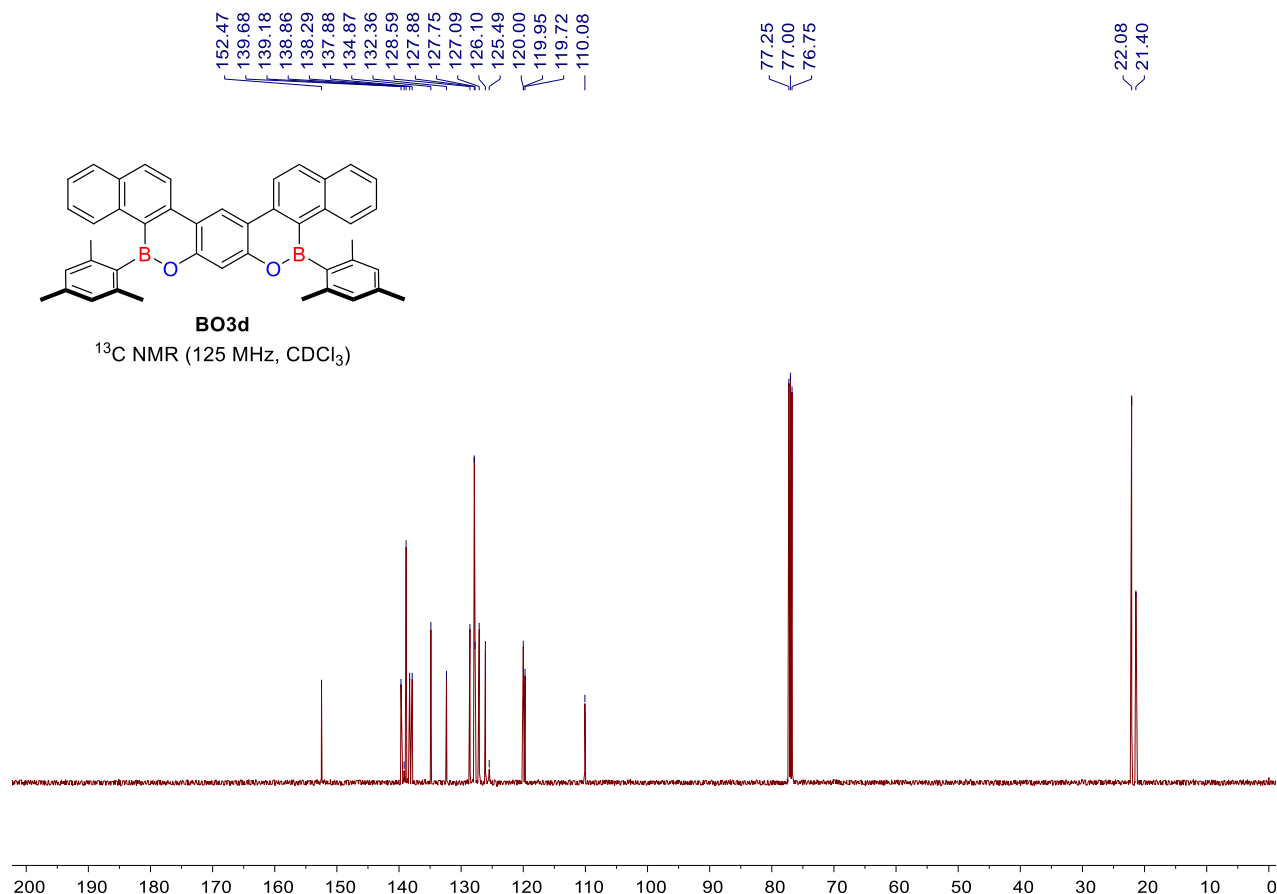
— 47.62



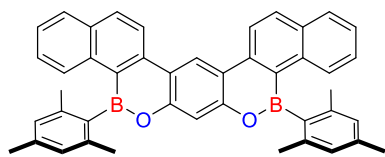
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$\text{C}_{48}\text{H}_{40}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{48}\text{H}_{41}[^{11}\text{B}]_2\text{O}_2$	671.3283	671.3287	0.62	30





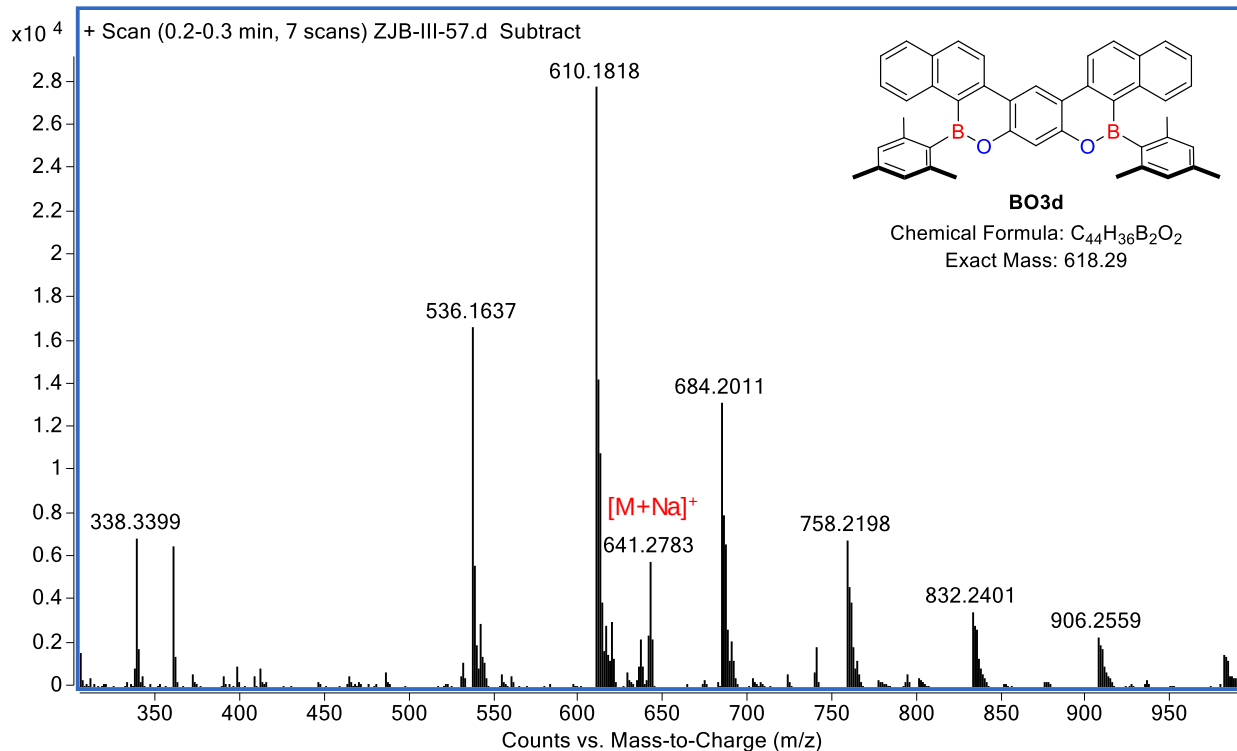
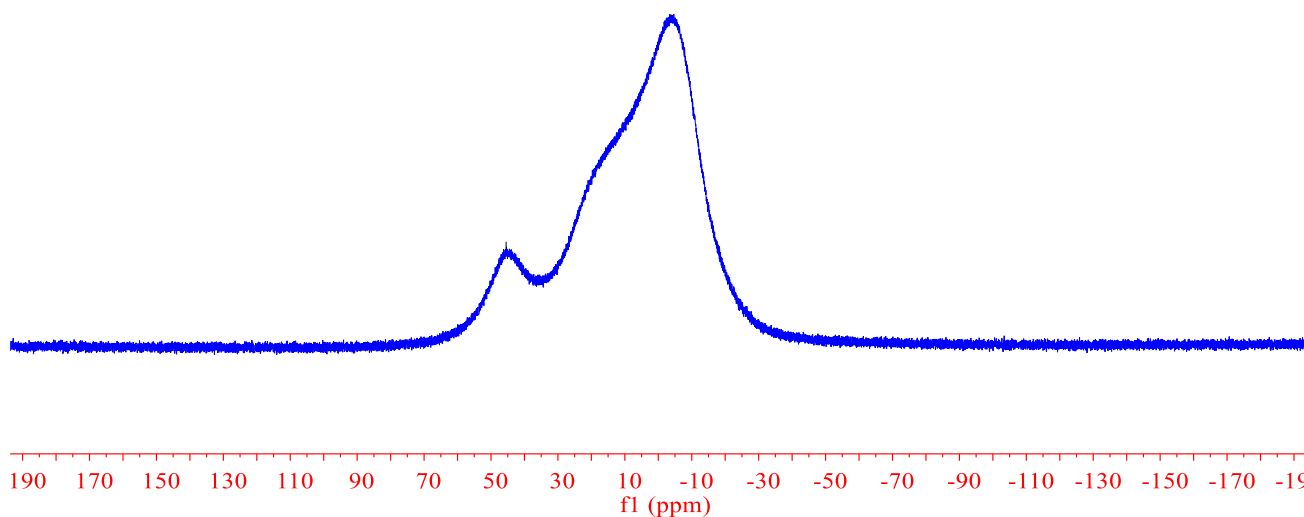


- 45.48

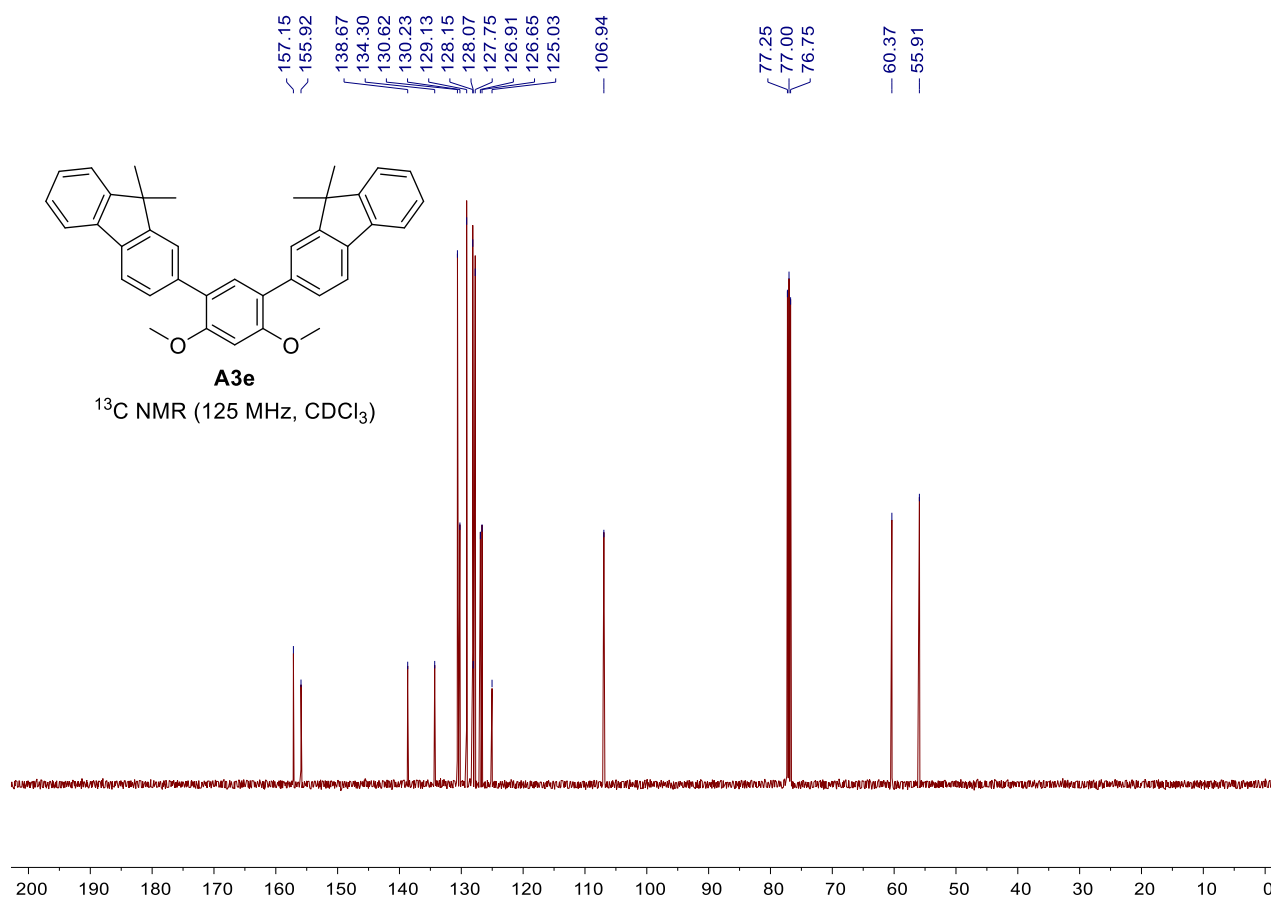
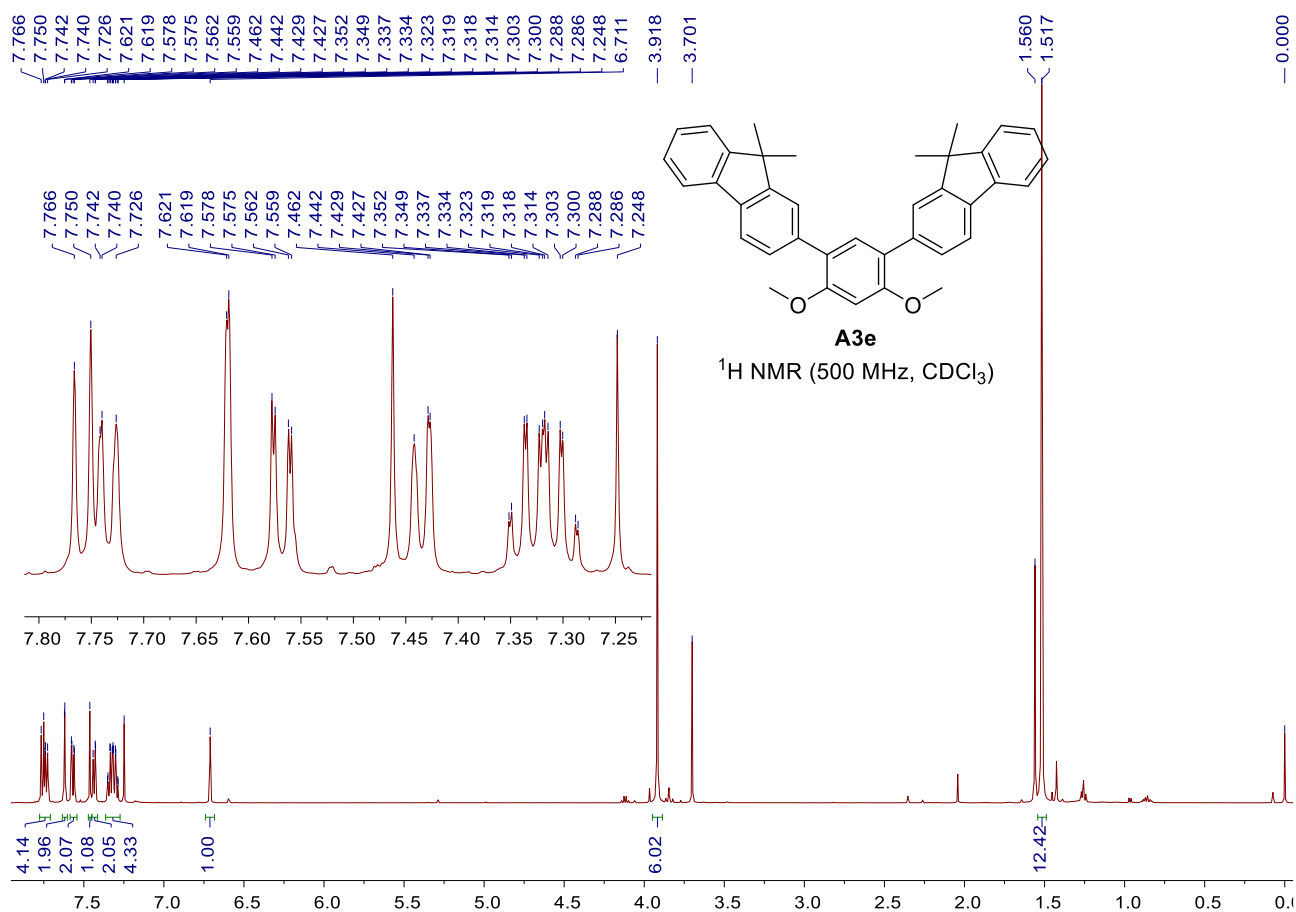


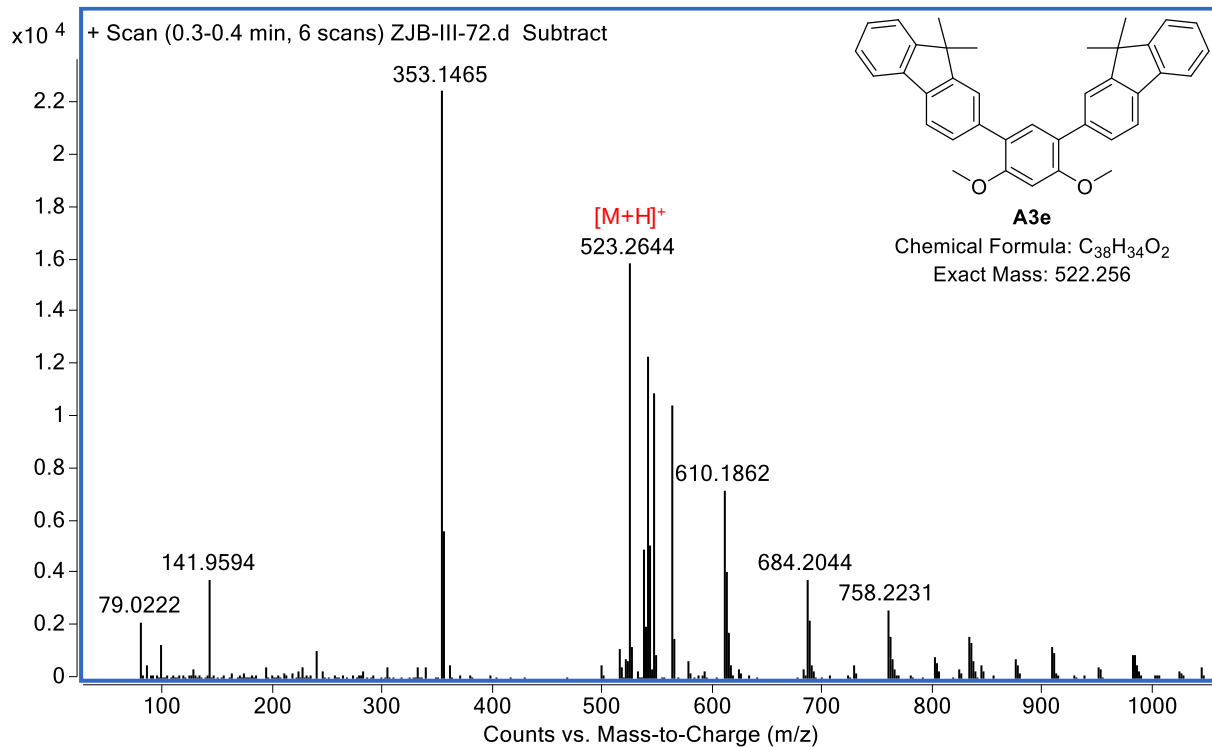
BO3d

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

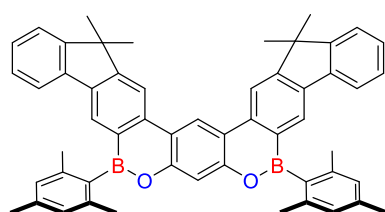


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{NaO}_2$	641.2783	641.2794	1.72



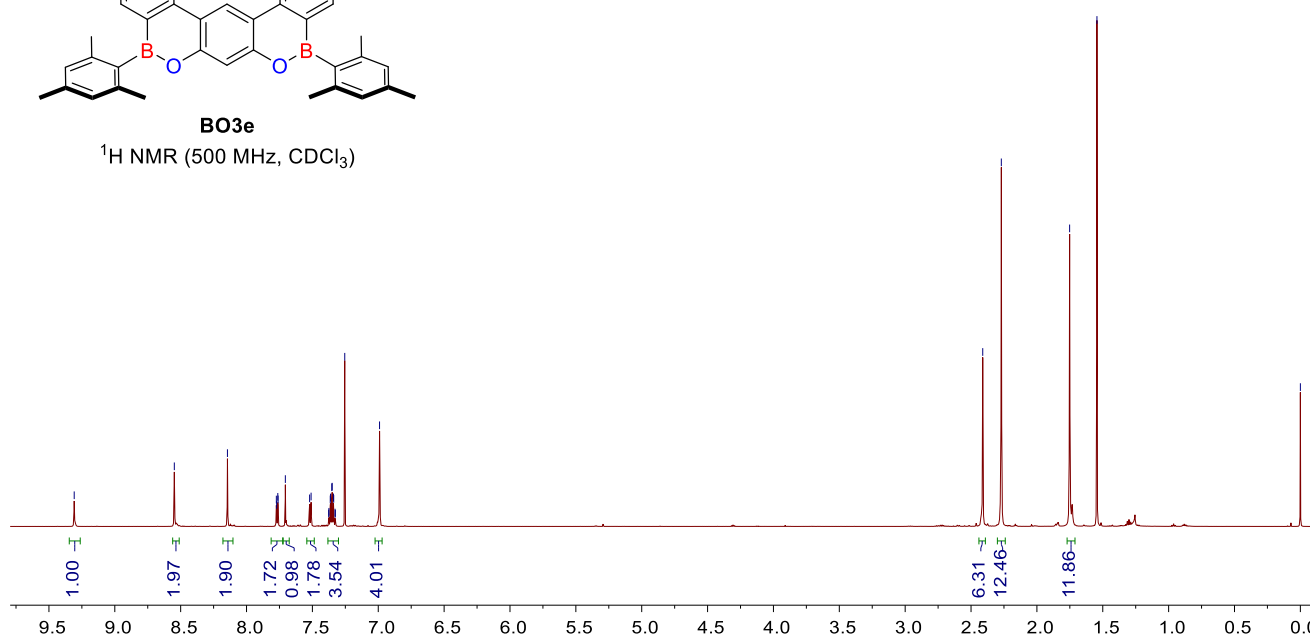


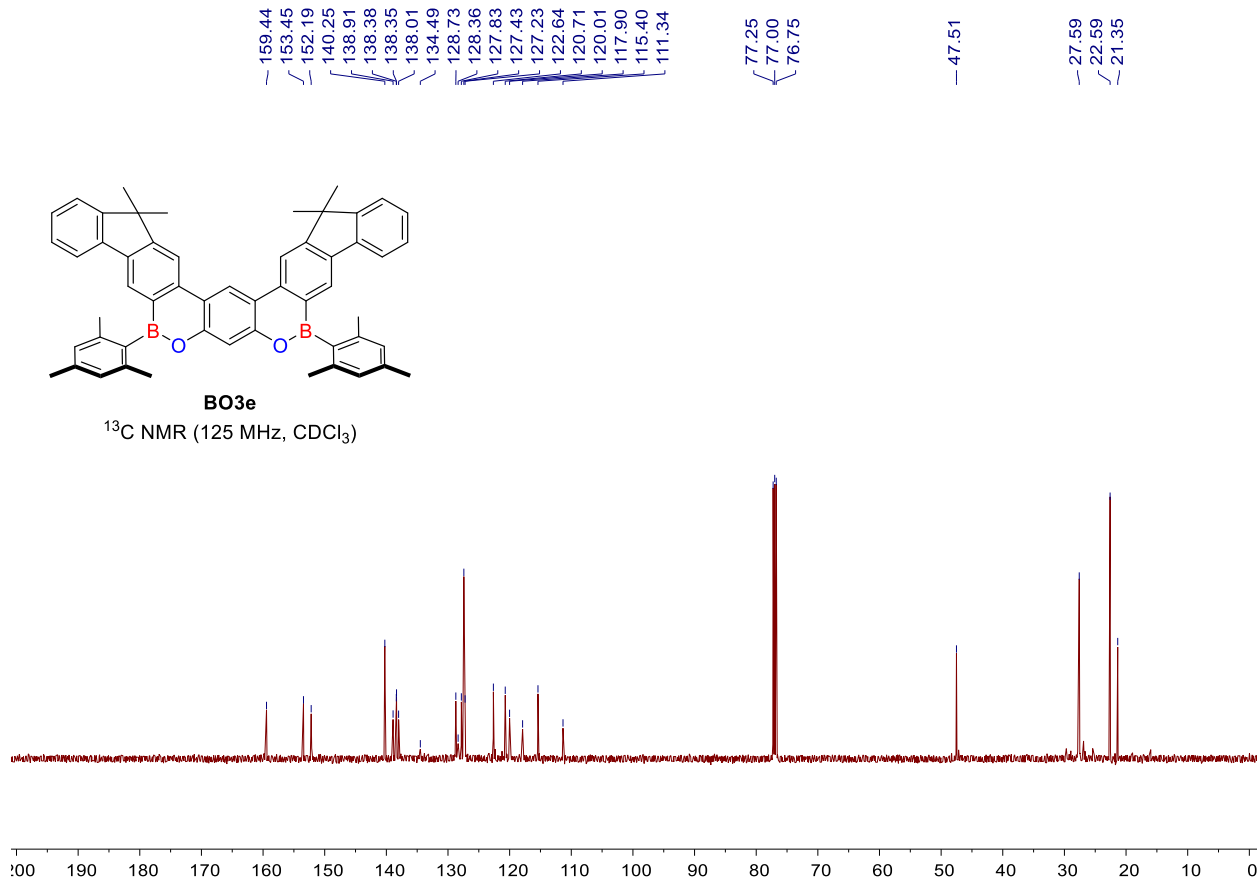
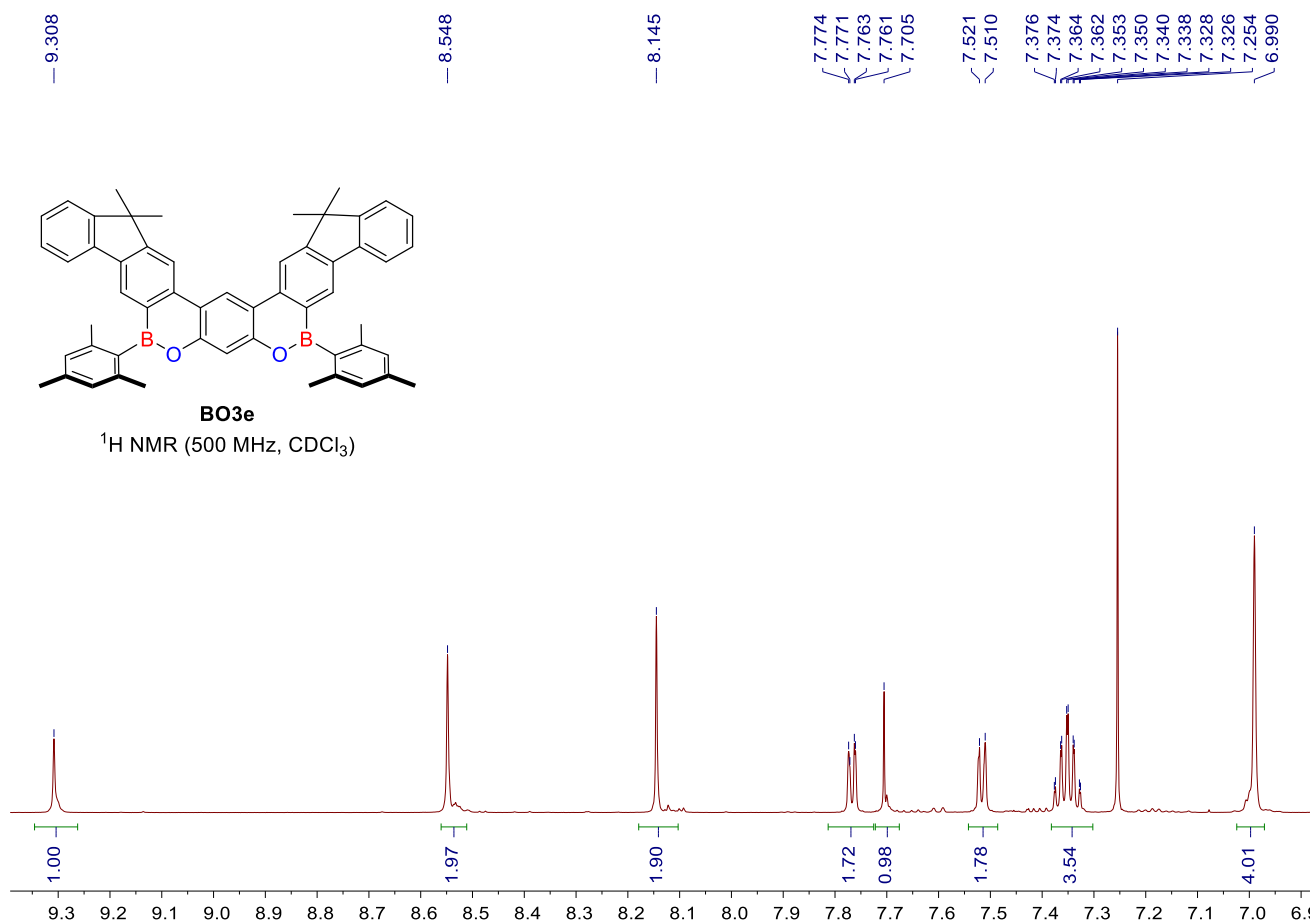
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
$C_{38}H_{34}O_2$	$C_{38}H_{35}O_2$	523.2644	523.2632	-2.38	22

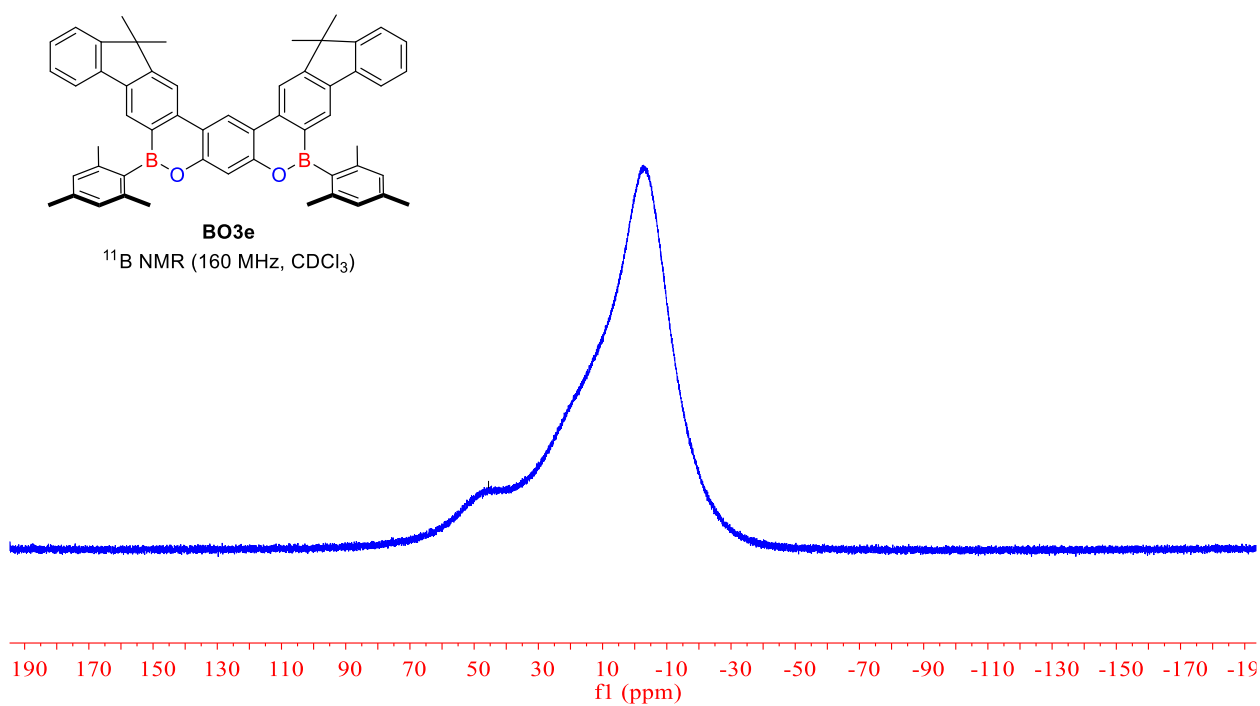
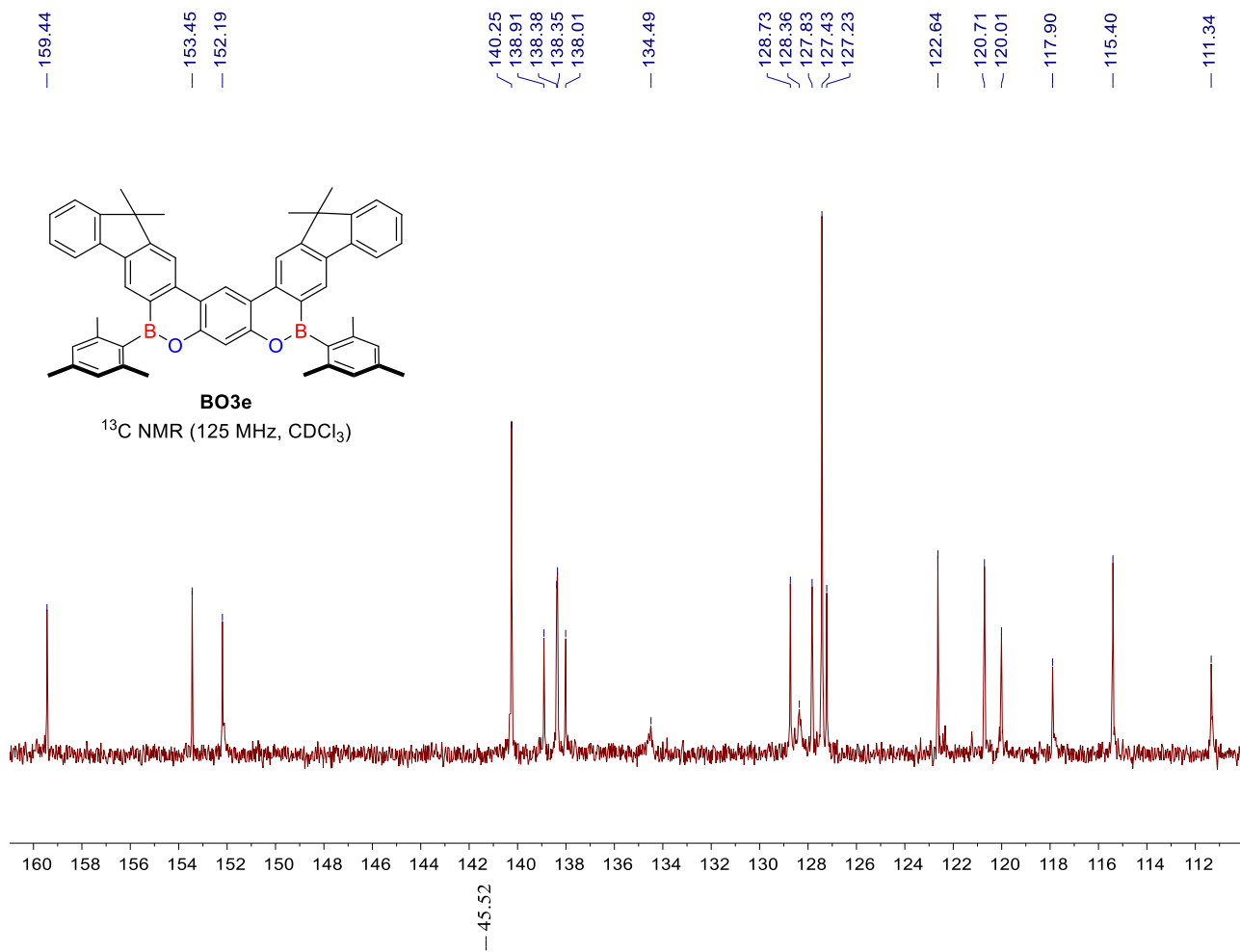


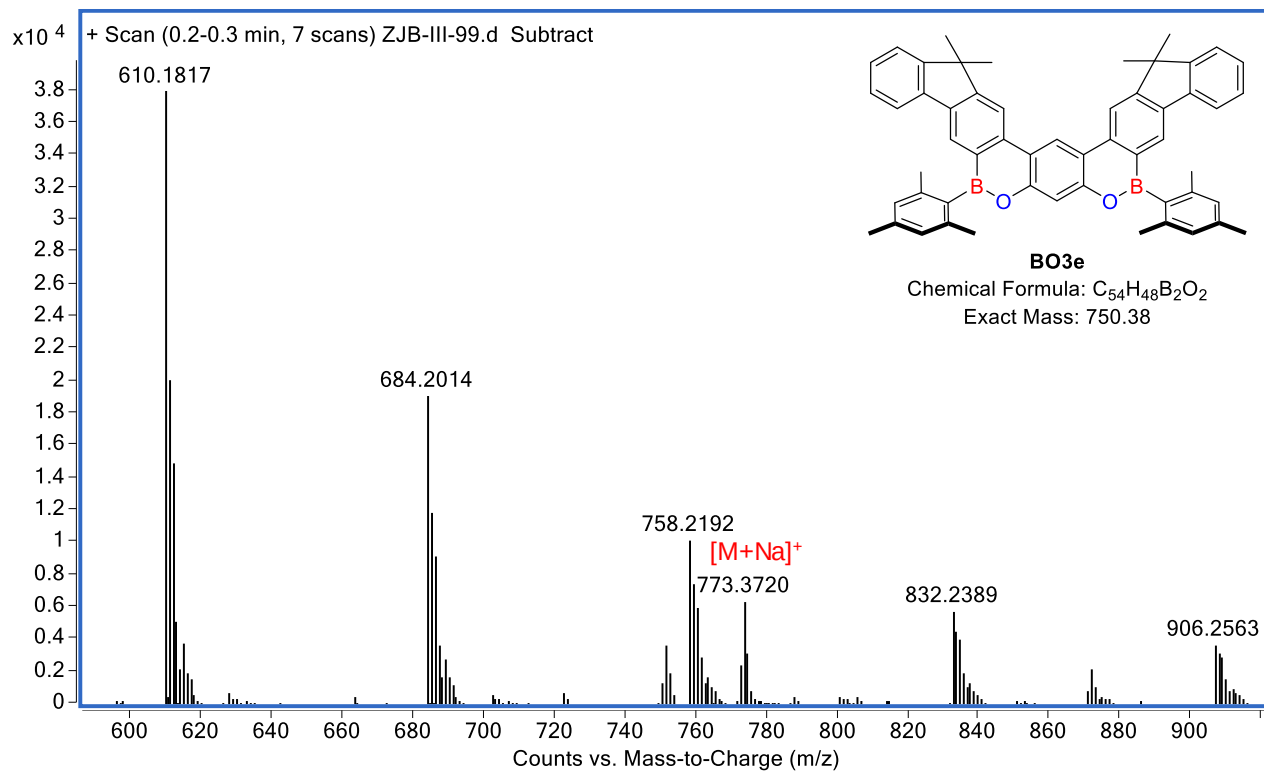
BO3e

1H NMR (500 MHz, $CDCl_3$)

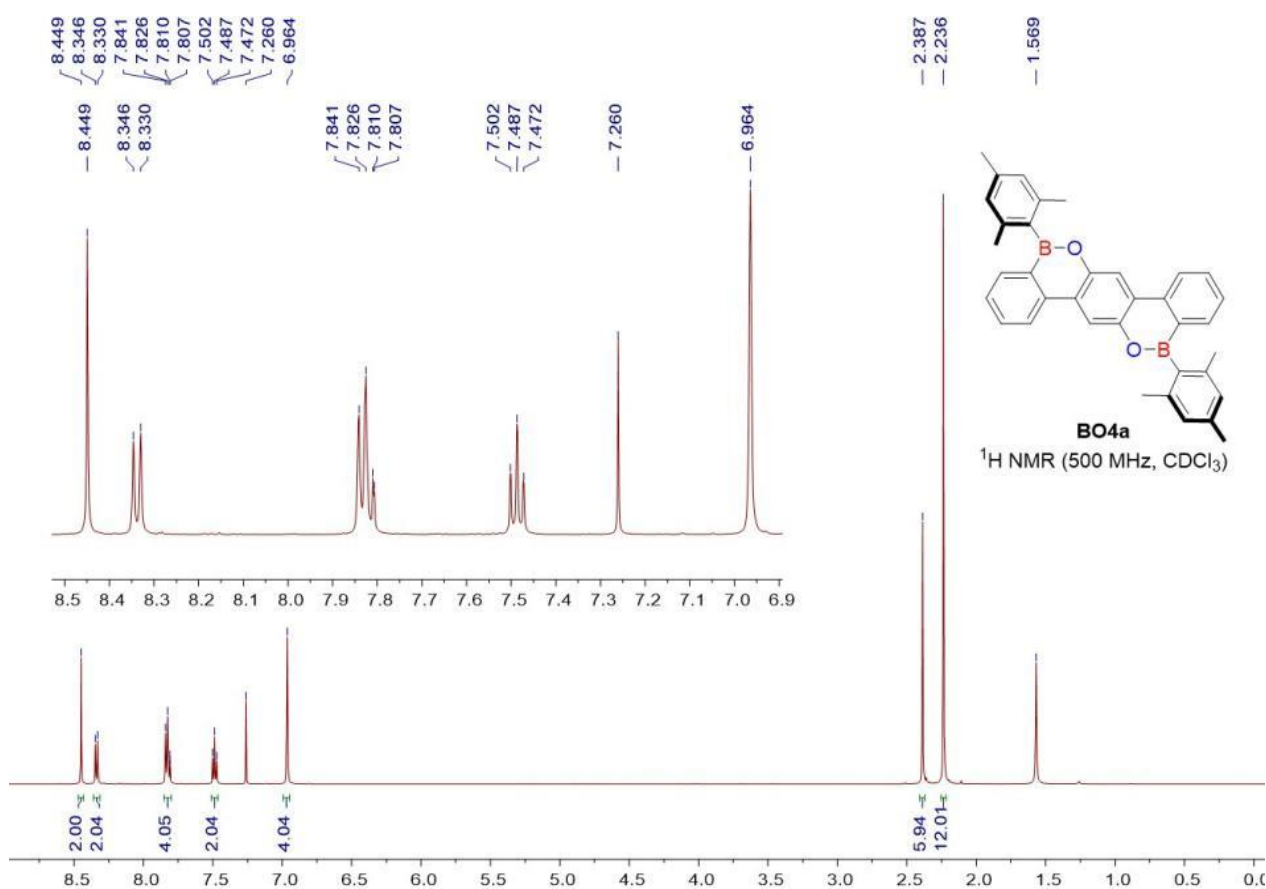


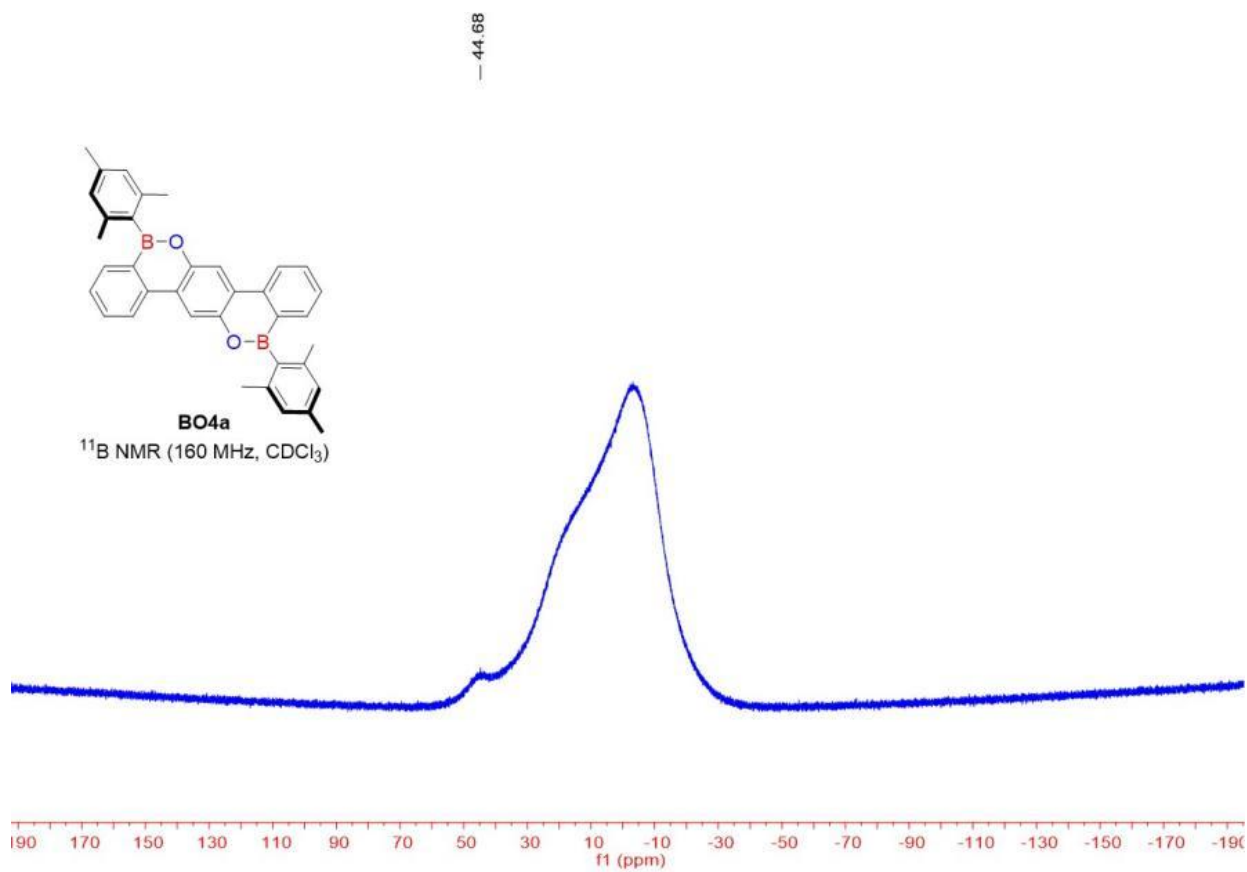
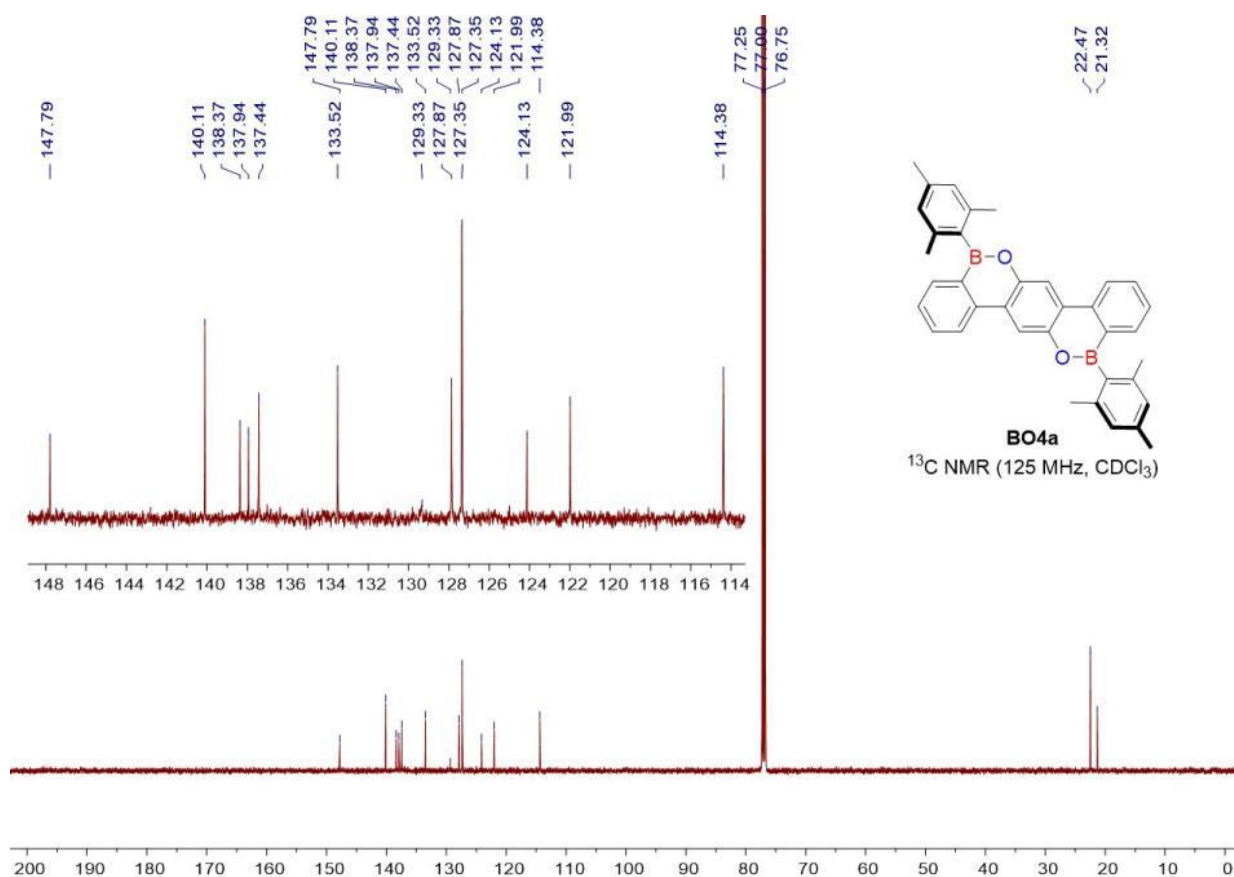




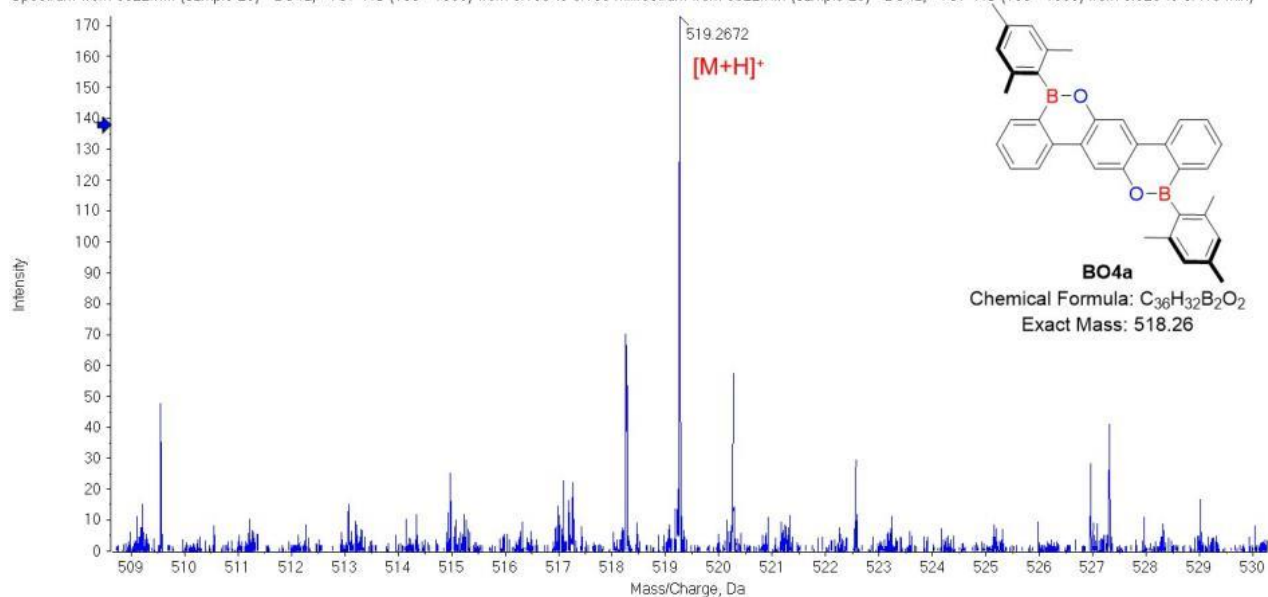


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$C_{54}H_{48}[^{11}B]_2O_2$	$C_{54}H_{48}[^{11}B]_2NaO_2$	773.3720	773.3733	1.68

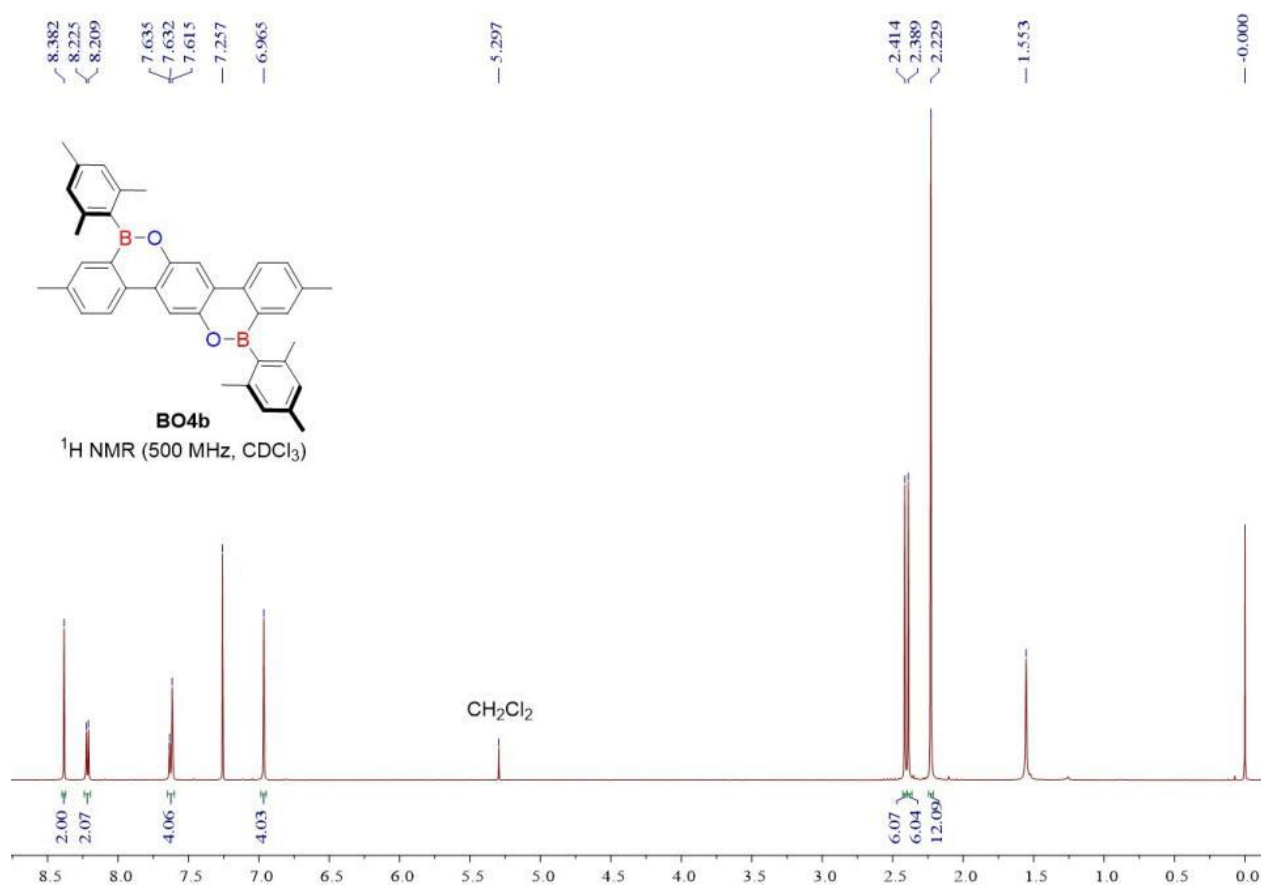


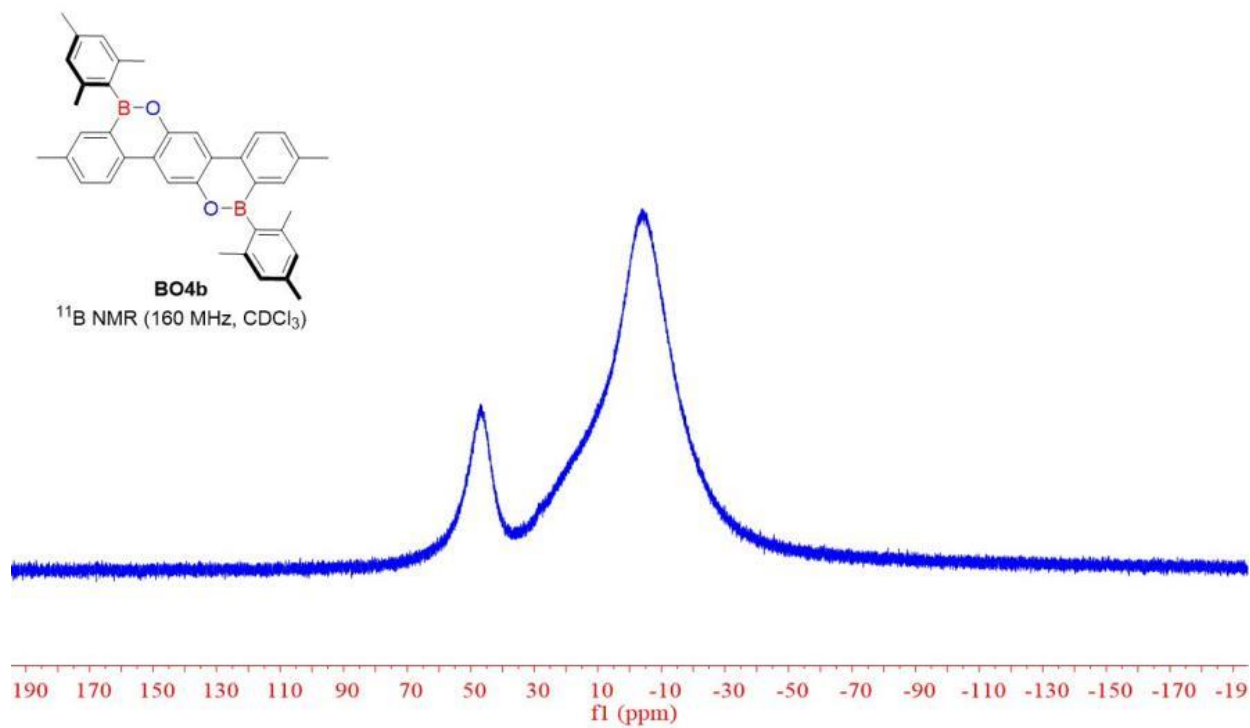
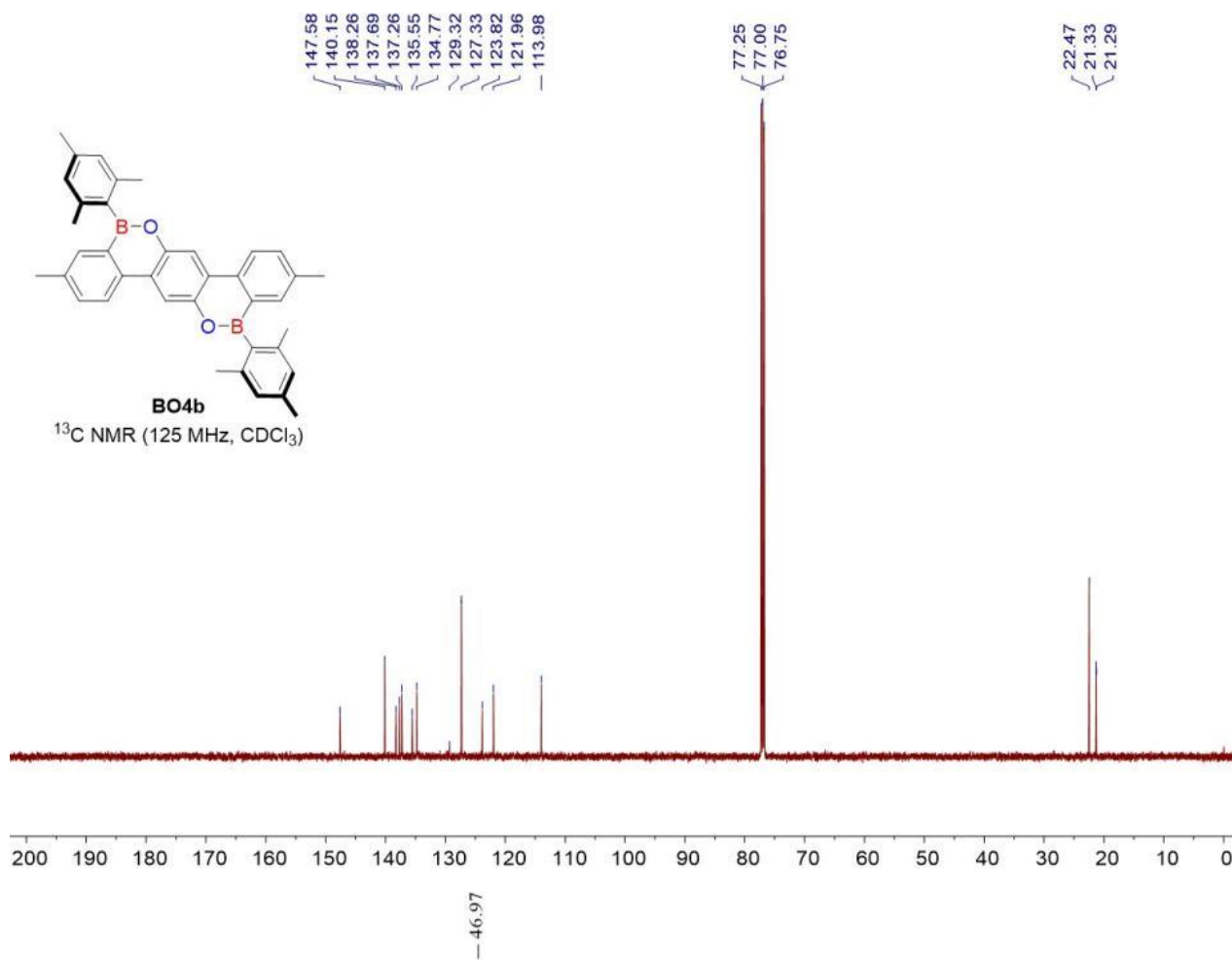


Spectrum from 0922.wiff (sample 29) - BO4a, +TOF MS (100 - 1500) from 0.135 to 0.195 min...pectrum from 0922.wiff (sample 29) - BO4a, +TOF MS (100 - 1500) from 0.325 to 0.479 min)

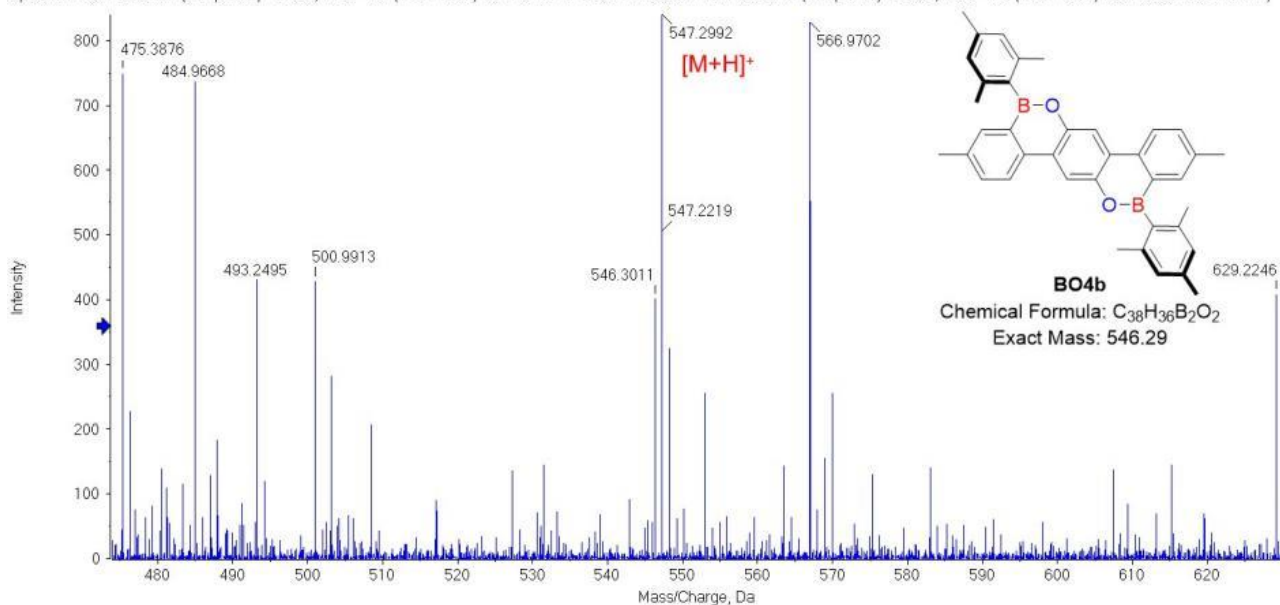


Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$C_{36}H_{32}[^{11}B]_2O_2$	$C_{36}H_{33}[^{11}B]_2O_2$	519.2672	519.2661	-2.1

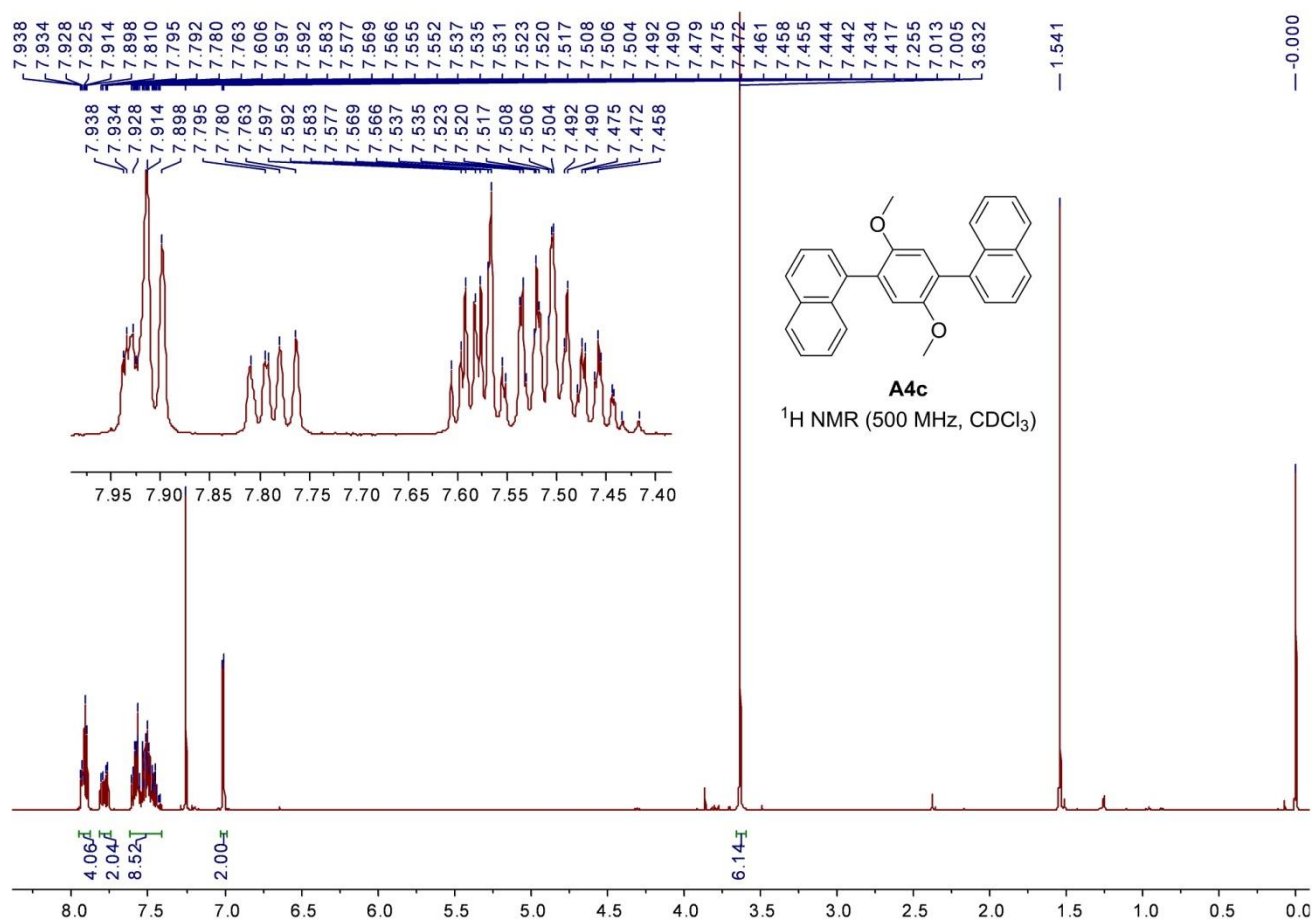


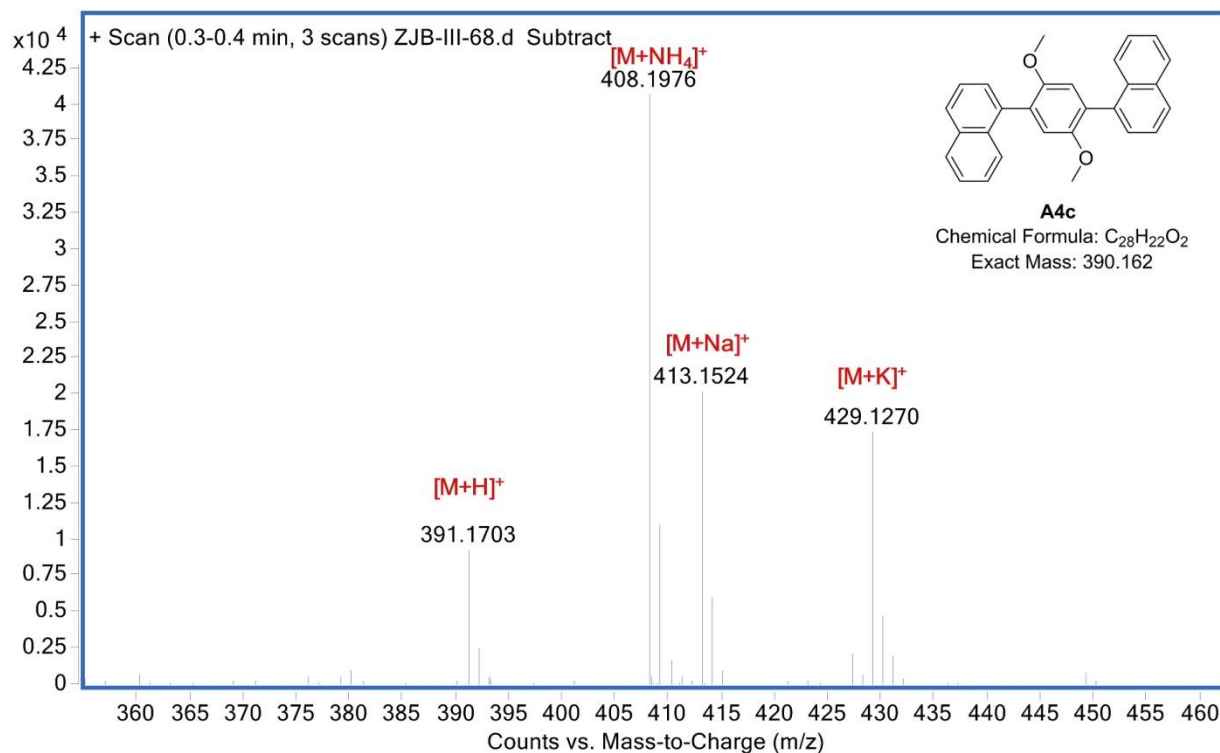
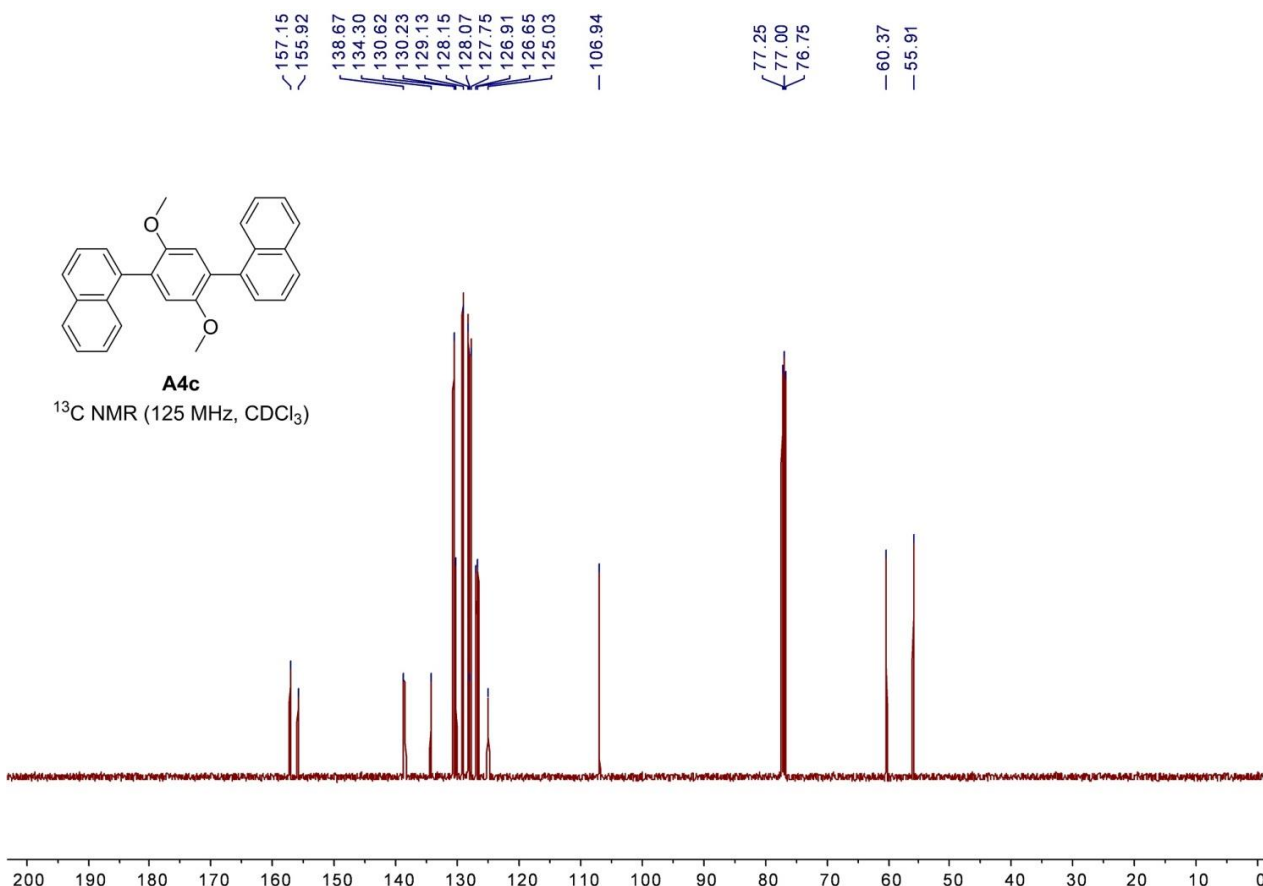


Spectrum from 0922.wiff (sample 30) - BO4b, +TOF MS (100 - 1500) from 0.130 to 0.191 min... Spectrum from 0922.wiff (sample 30) - BO4b, +TOF MS (100 - 1500) from 0.325 to 0.479 min)

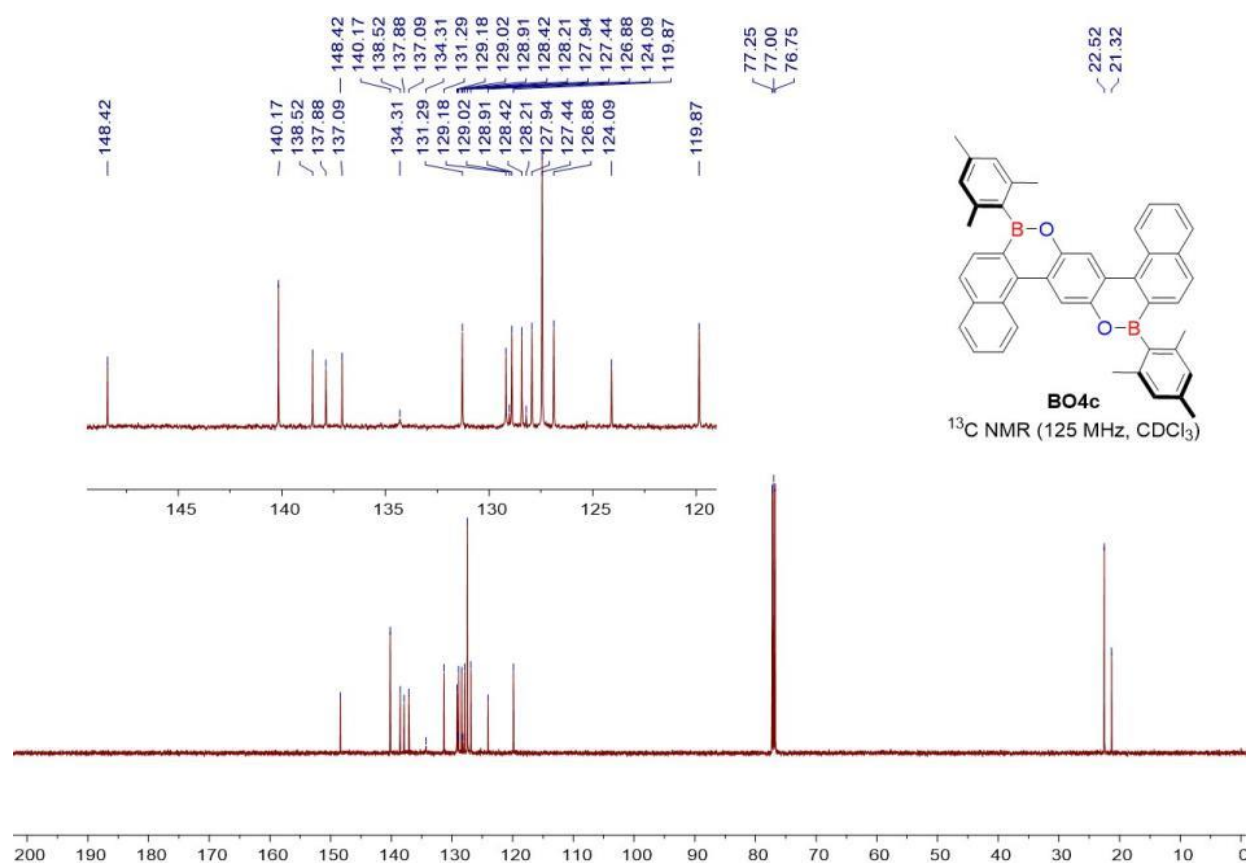
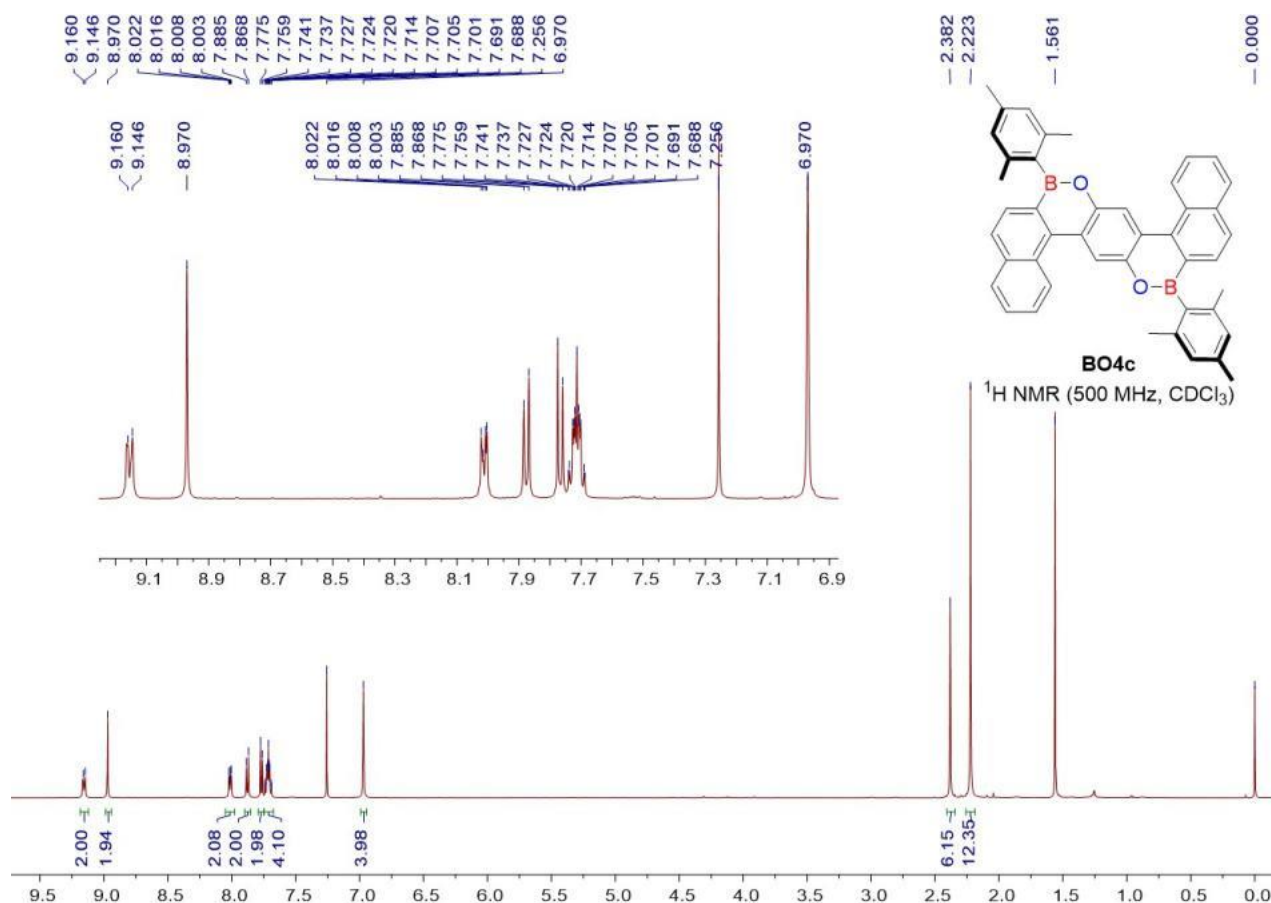


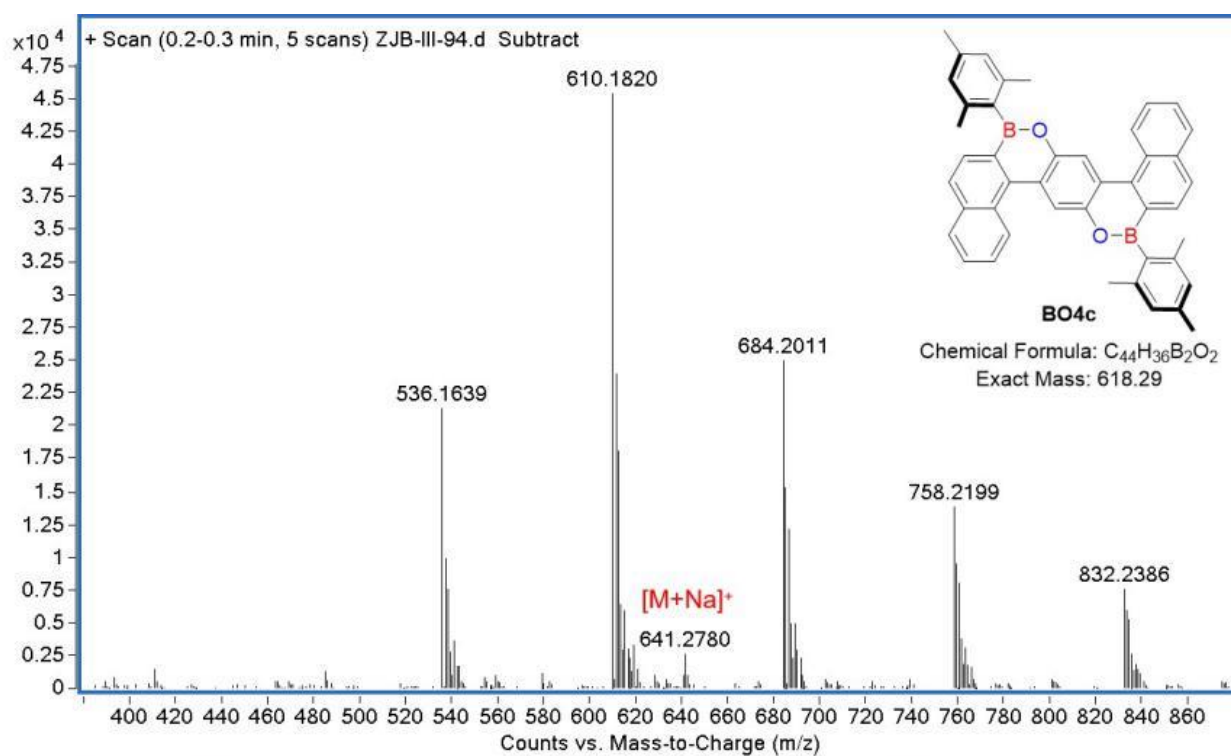
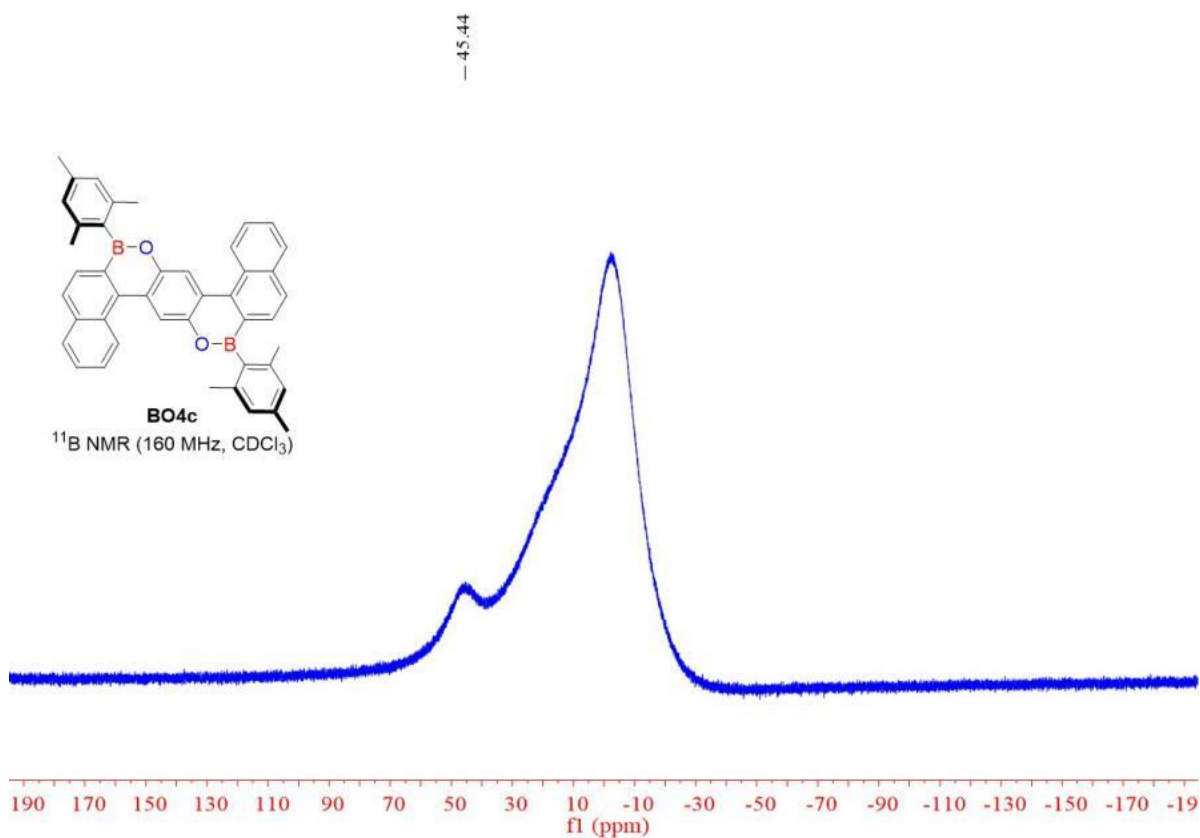
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$C_{38}H_{36}[^{11}B]_2O_2$	$C_{38}H_{37}[^{11}B]_2O_2$	547.2992	547.2974	-3.3



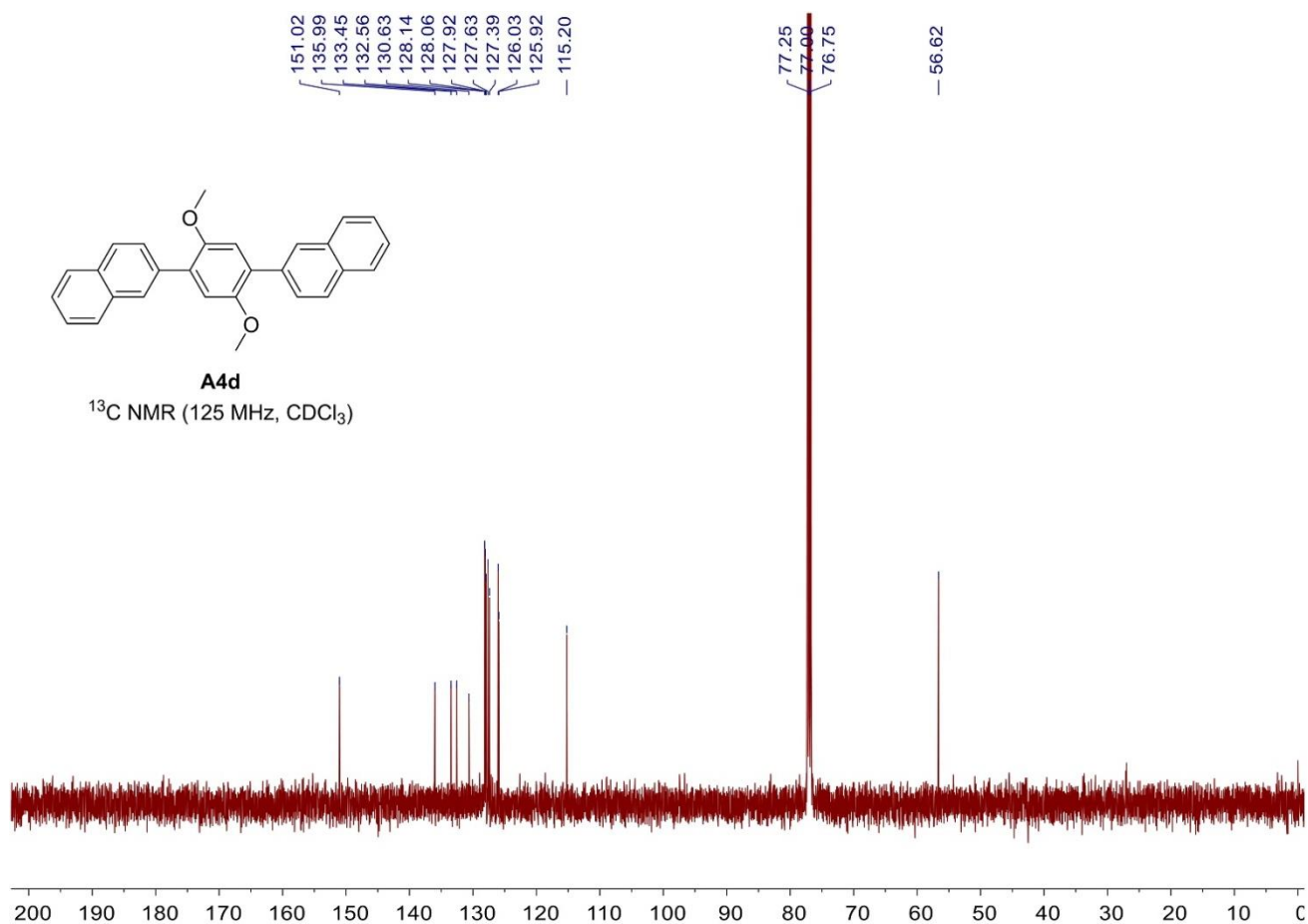
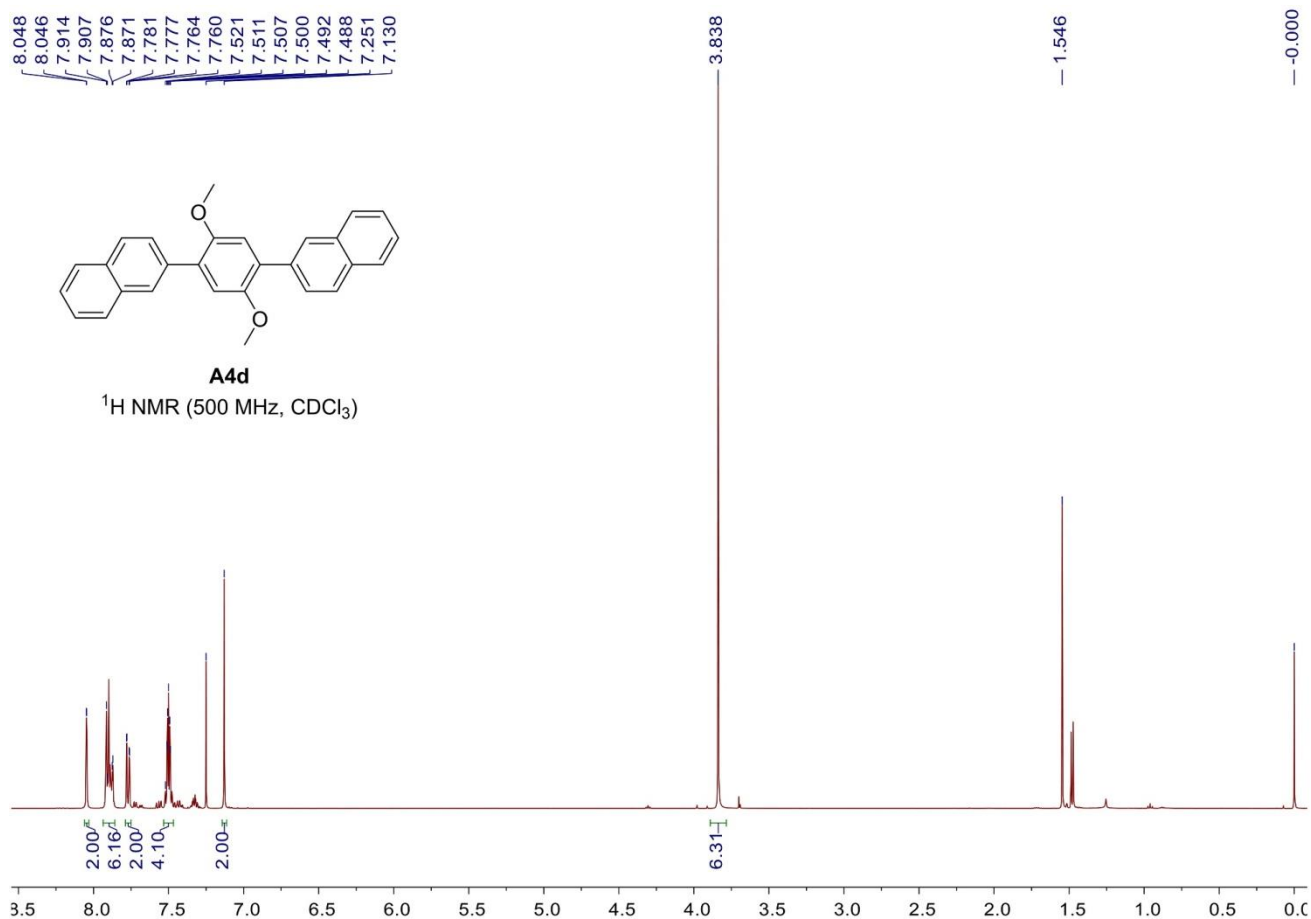


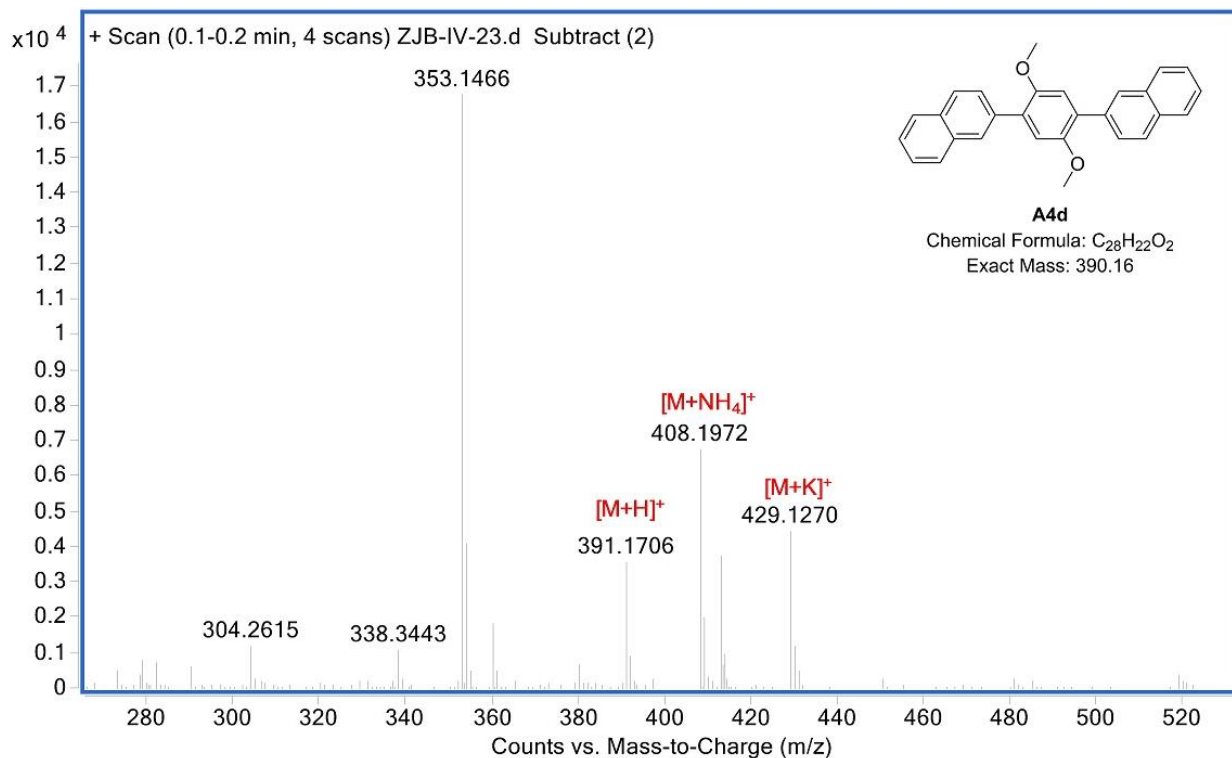
Formula (M)	Ion Formula	m/z	Calc m/z	Diff(ppm)	DBE
C ₂₈ H ₂₂ O ₂	C ₂₈ H ₂₆ NO ₂	408.1976	408.1958	-4.6	18



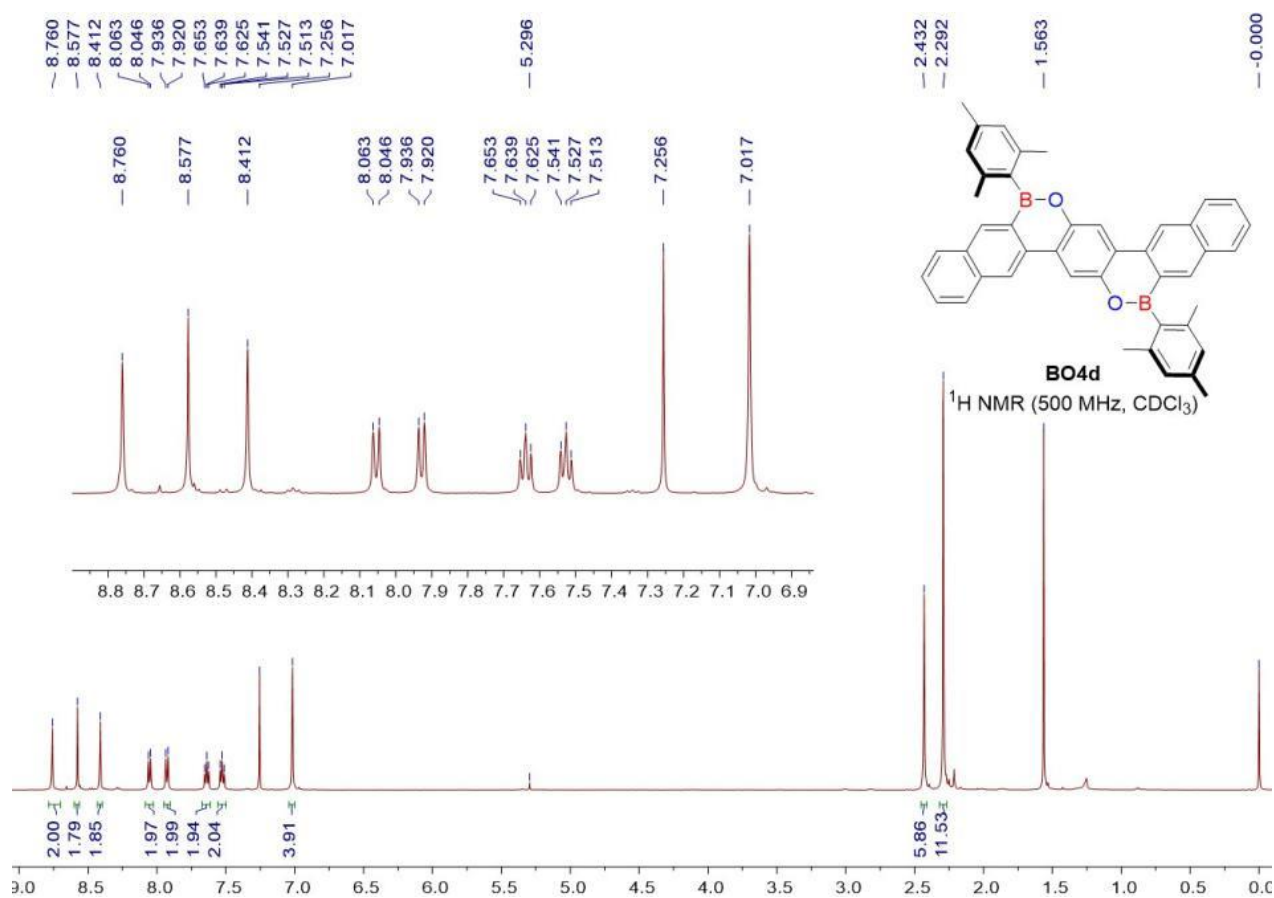


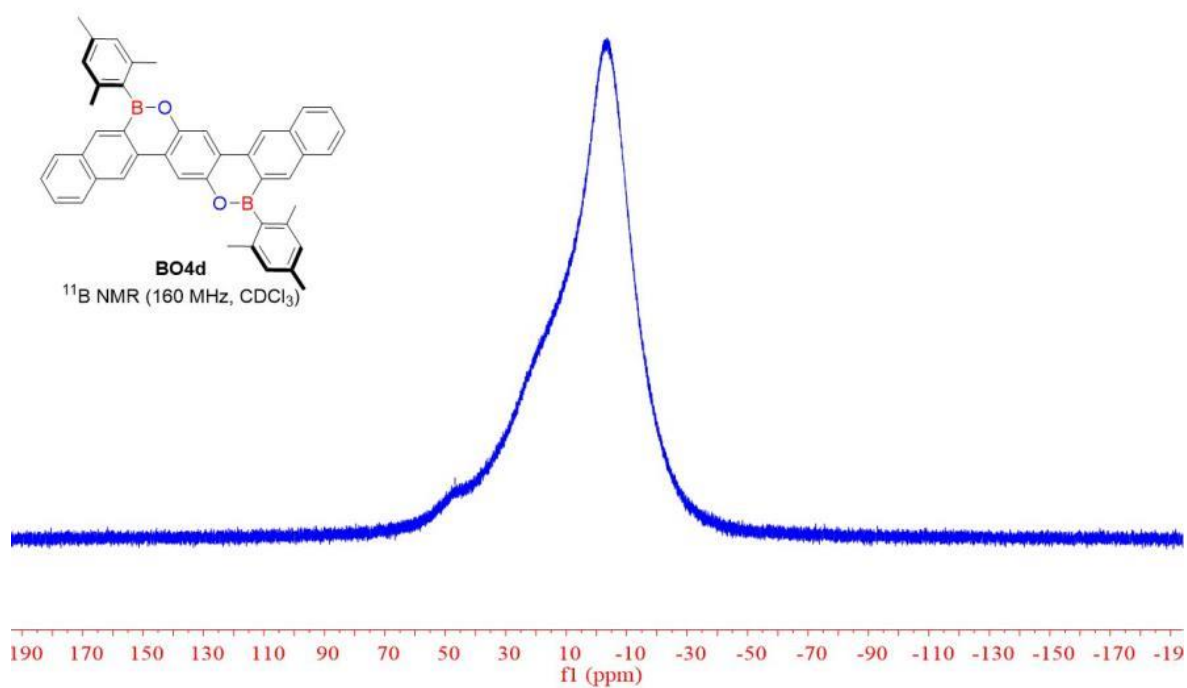
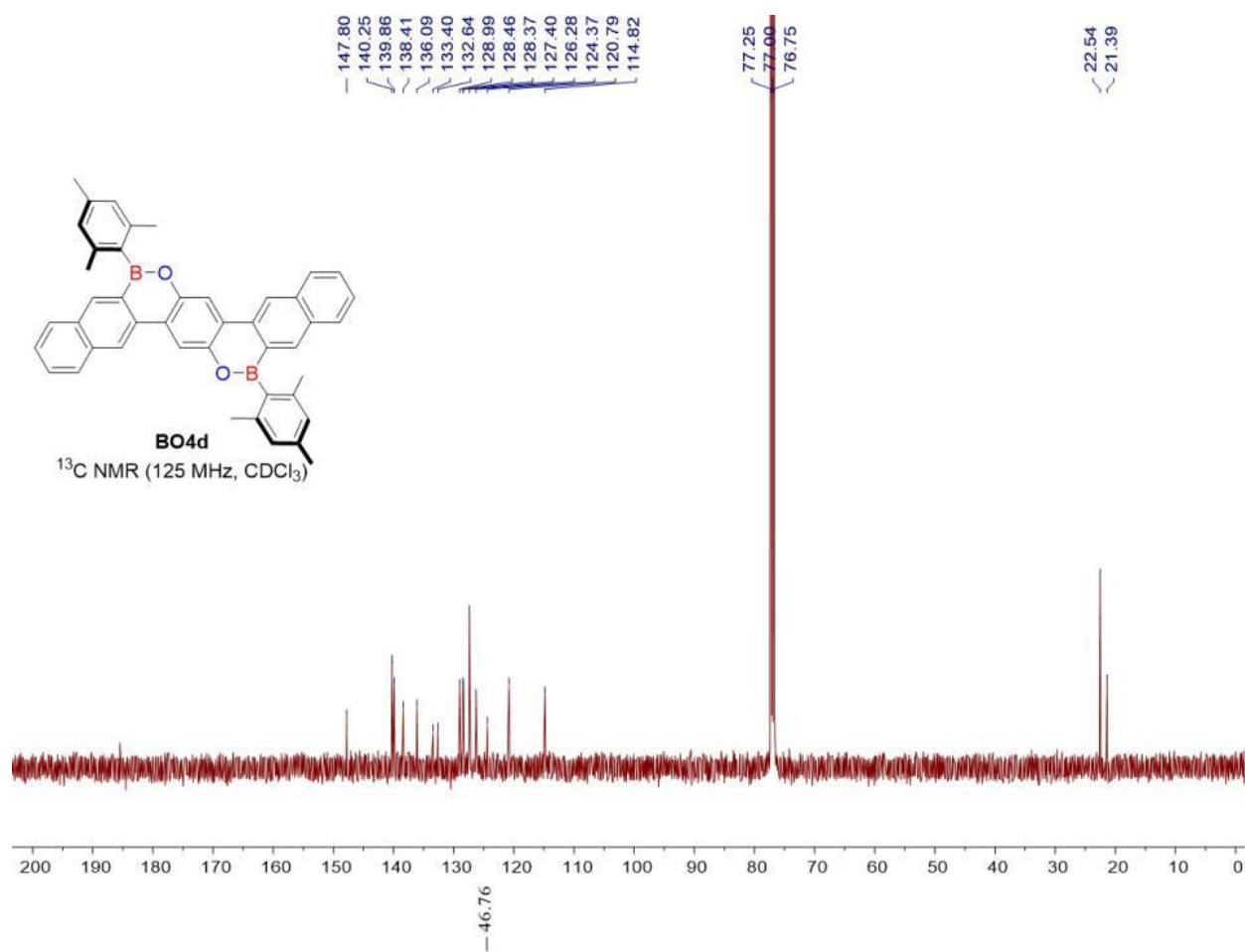
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
$\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{O}_2$	$\text{C}_{44}\text{H}_{36}[^{11}\text{B}]_2\text{NaO}_2$	641.2780	641.2794	2.2

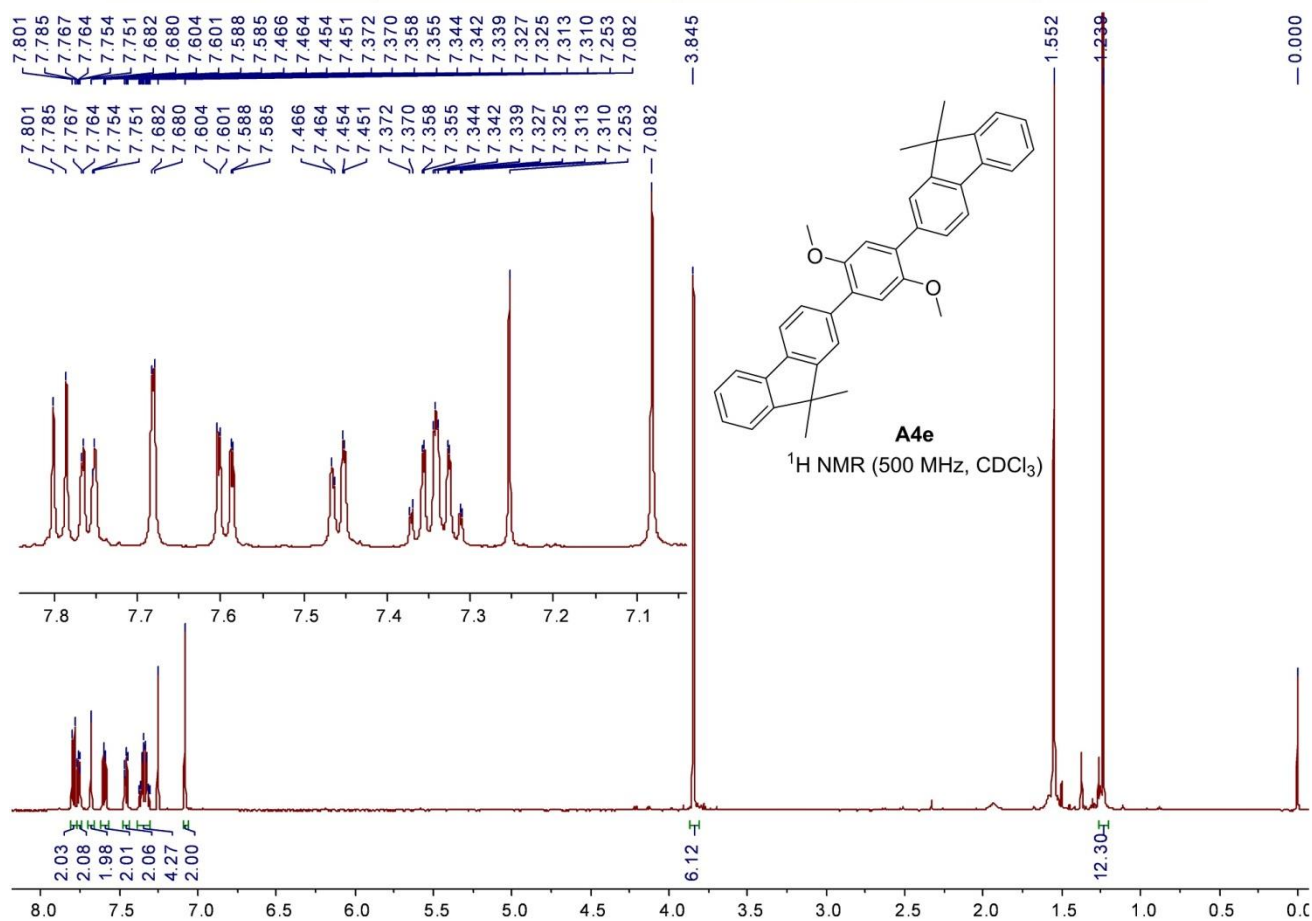
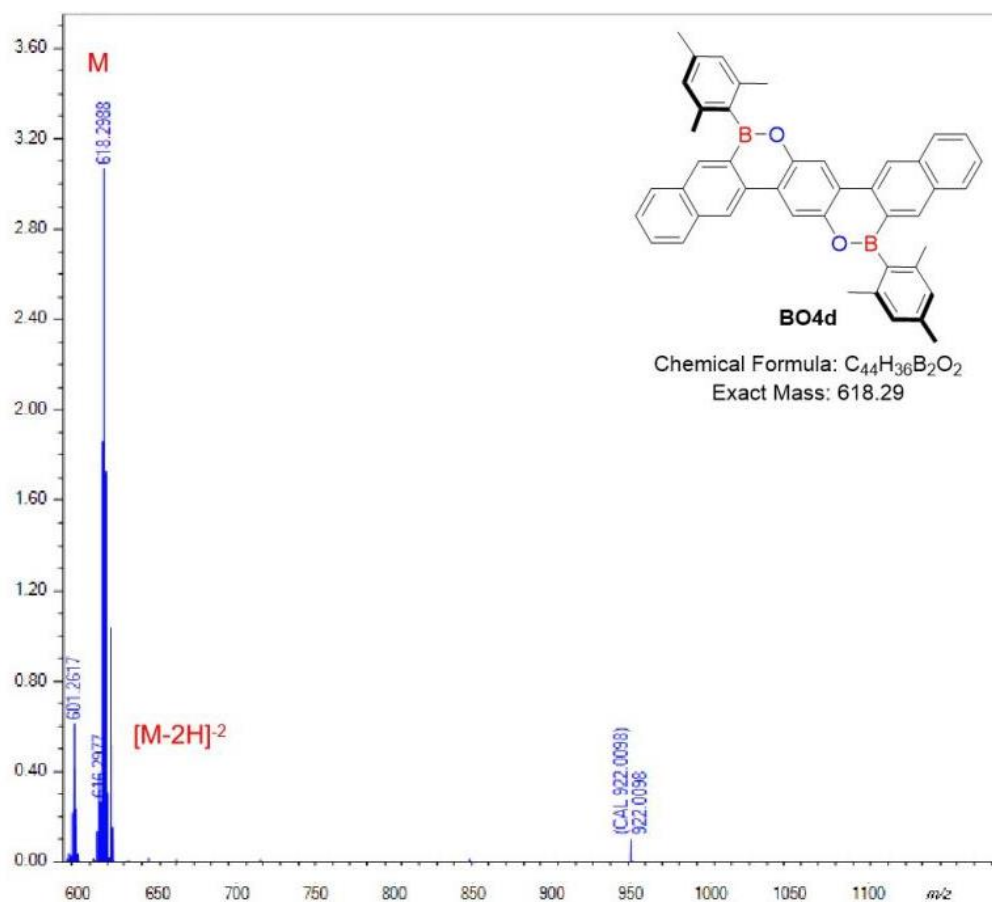


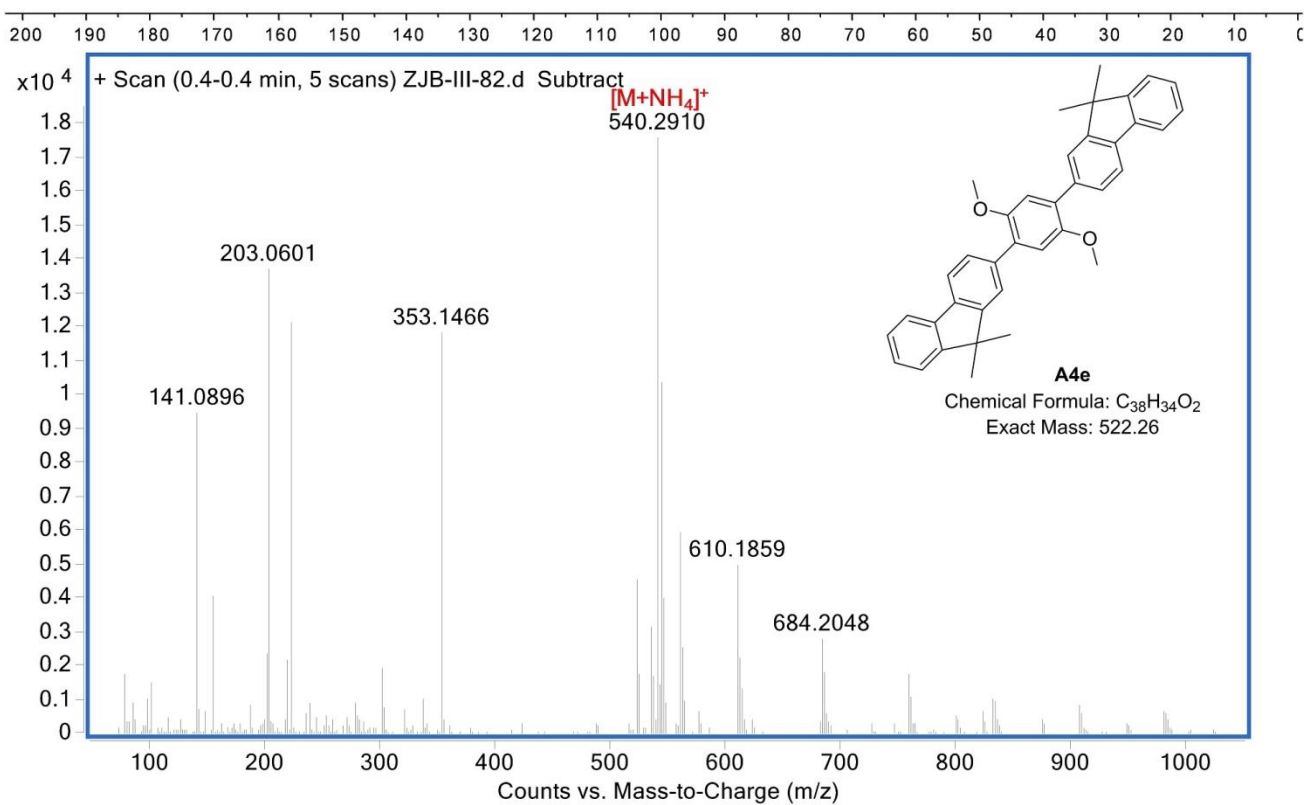
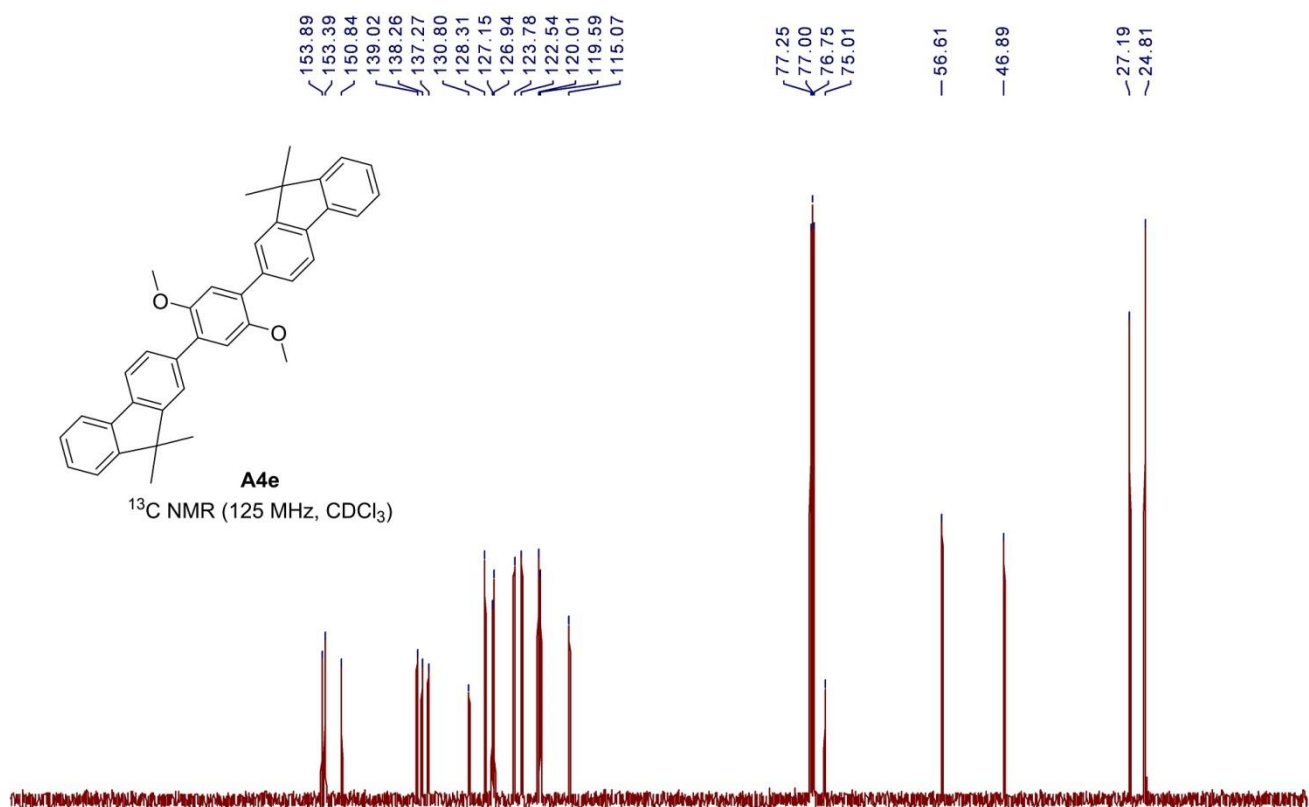


Formula(M)	Ion Formula	m/z	Calc m/z	Diff(ppm)	DBE
$C_{28}H_{22}O_2$	$C_{28}H_{26}NO_2$	408.1972	408.1958	-3.57	18

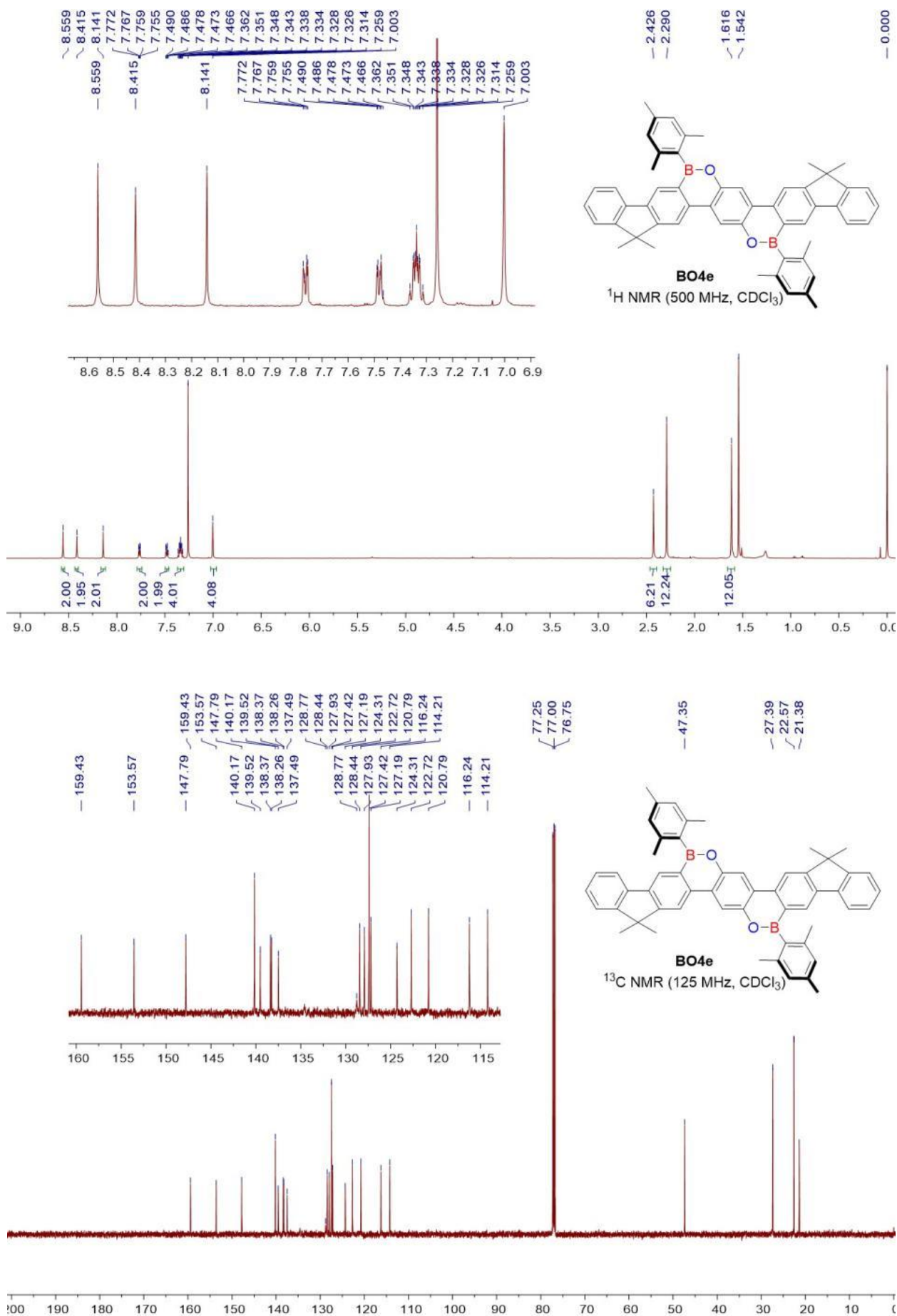




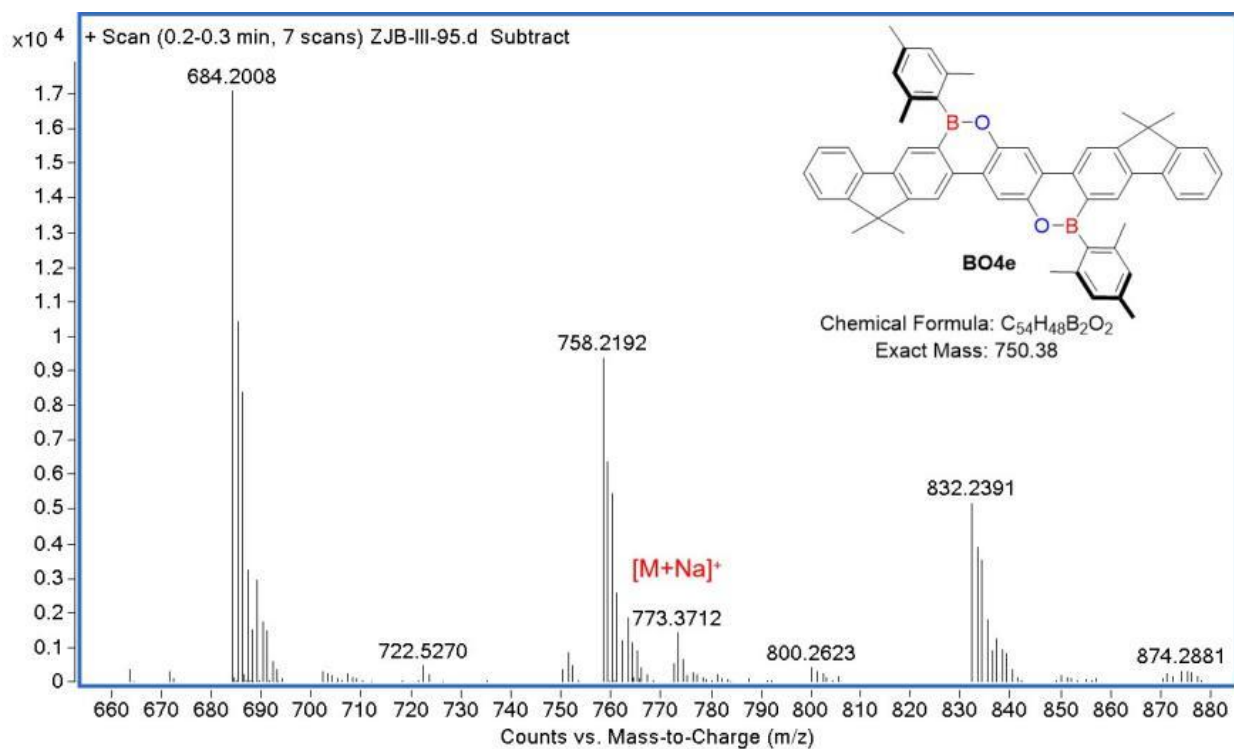
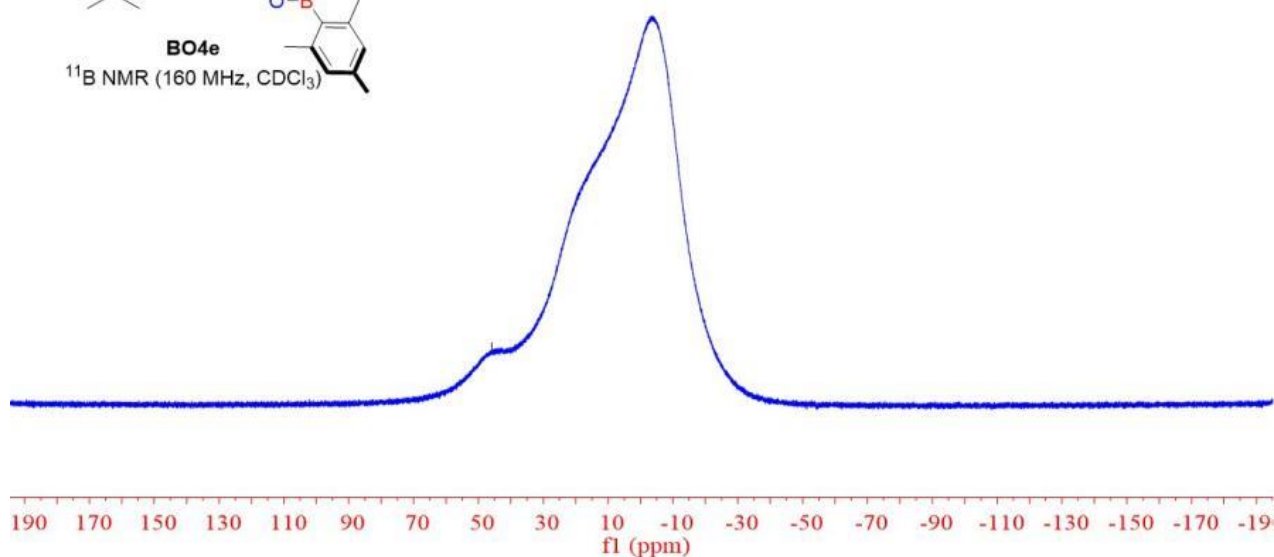
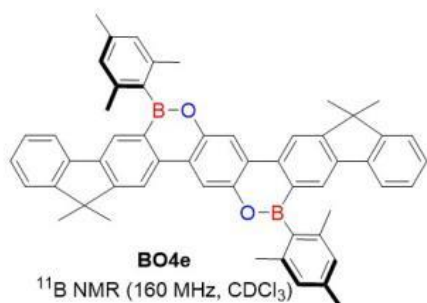




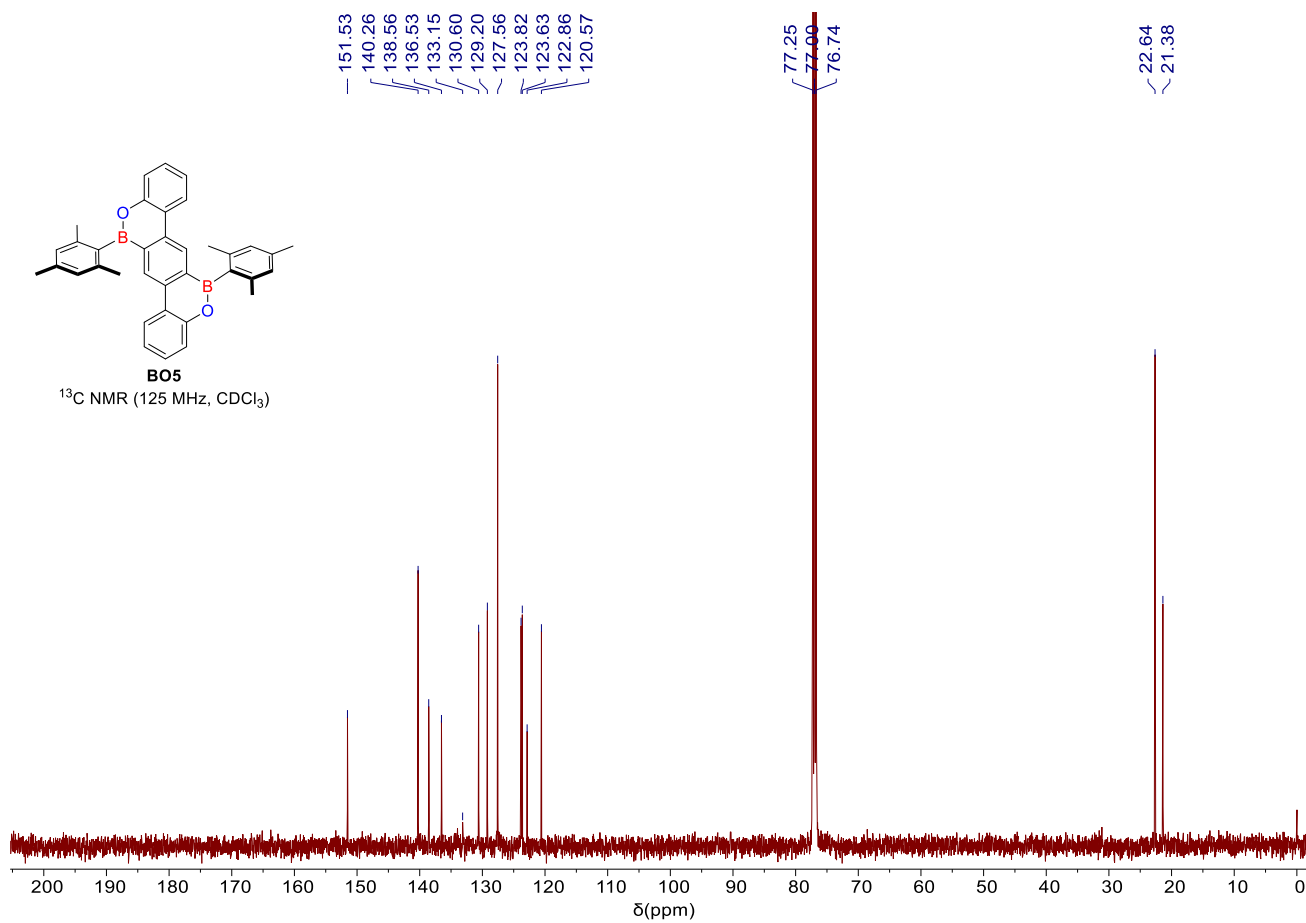
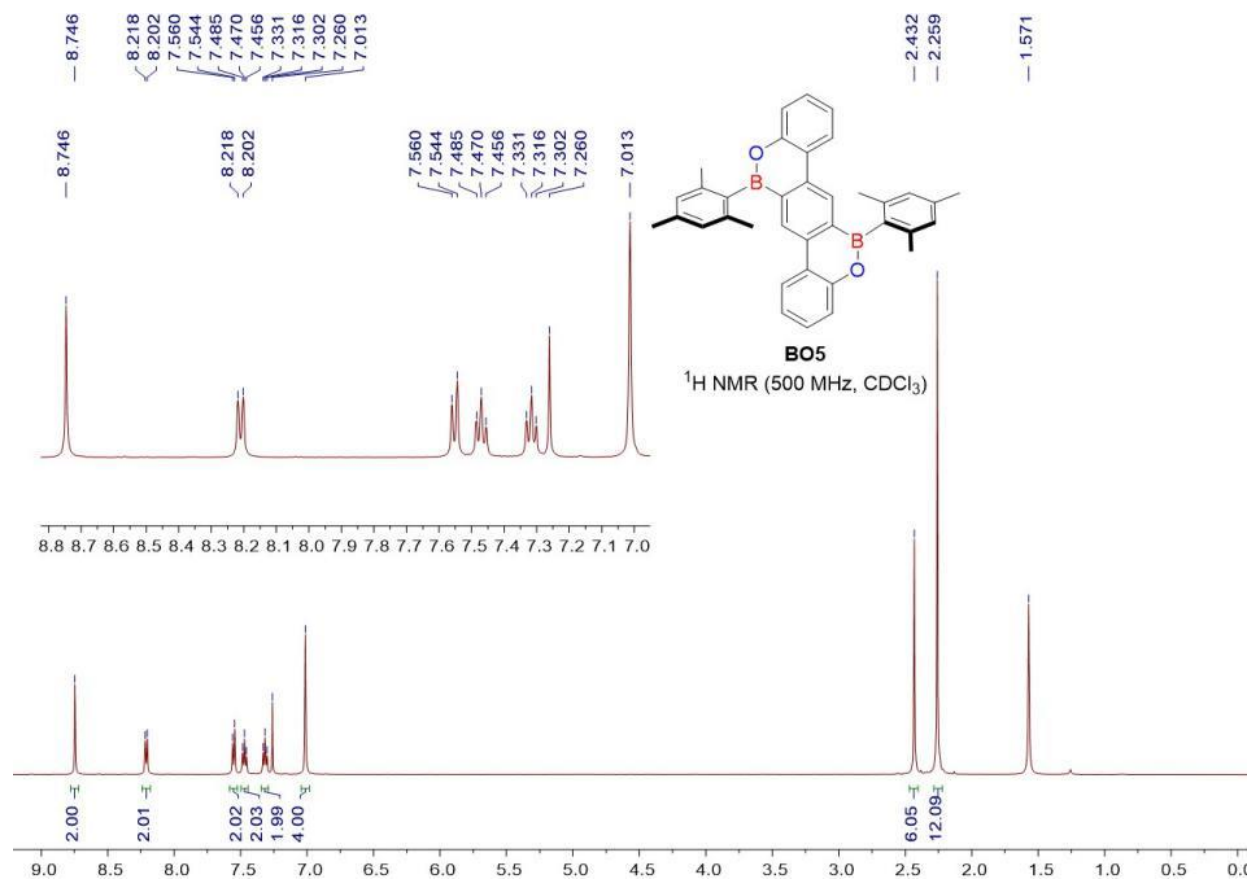
Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
C ₃₈ H ₃₄ O ₂	C ₃₈ H ₃₈ NO ₂	540.2910	540.2897	-2.48	22



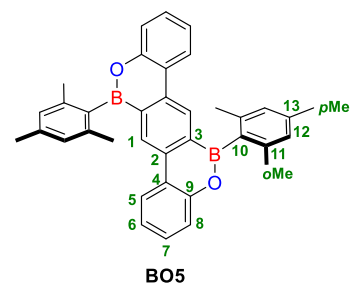
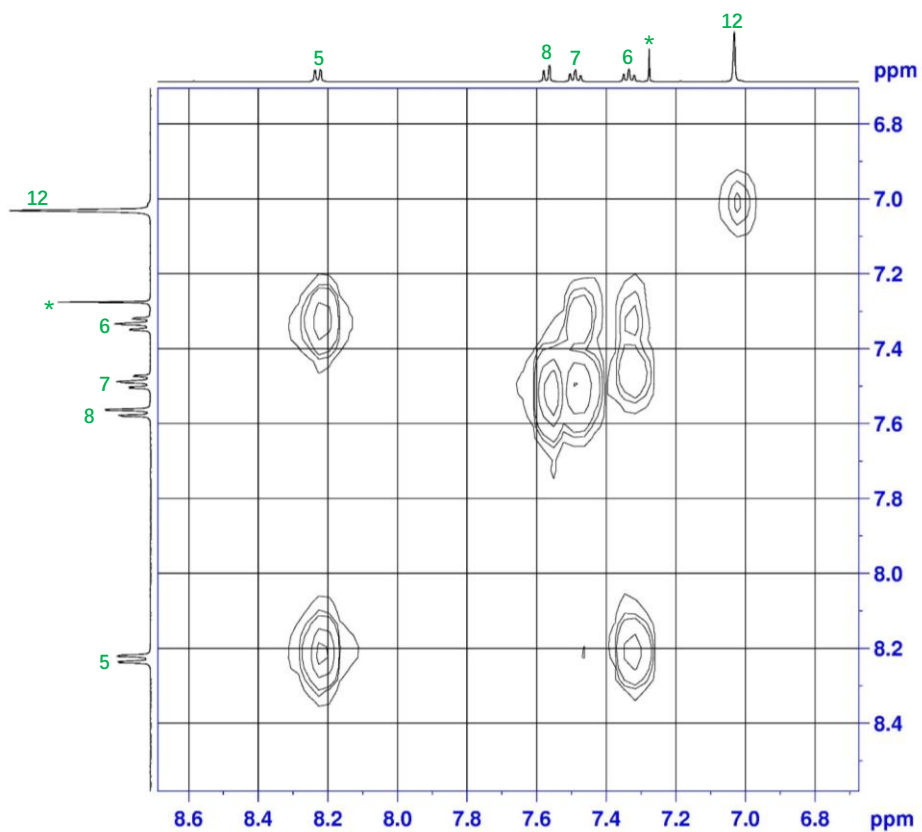
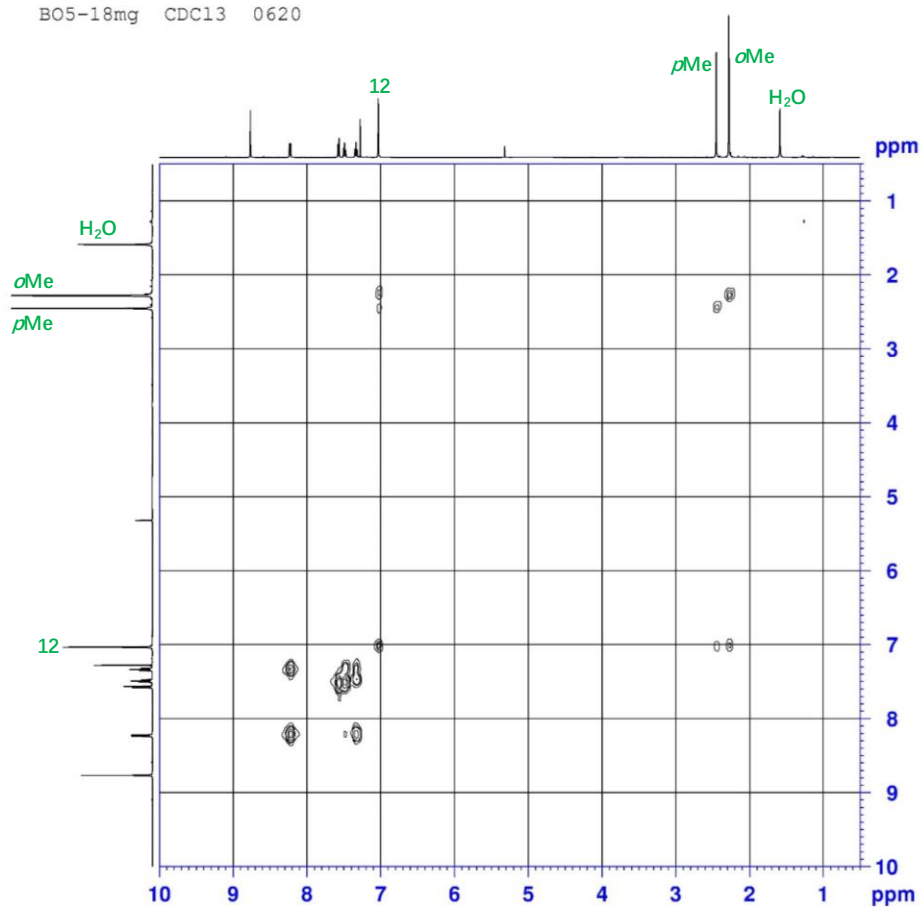
— 45.87



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

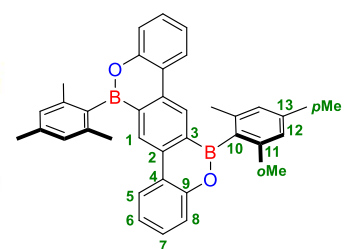
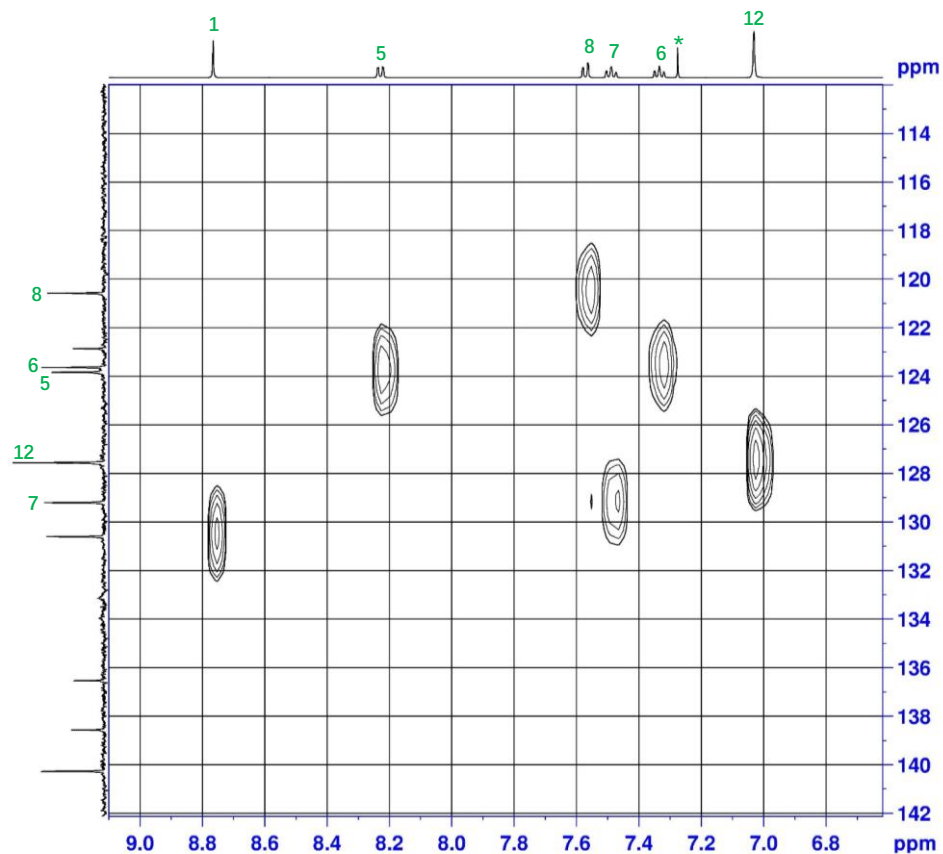
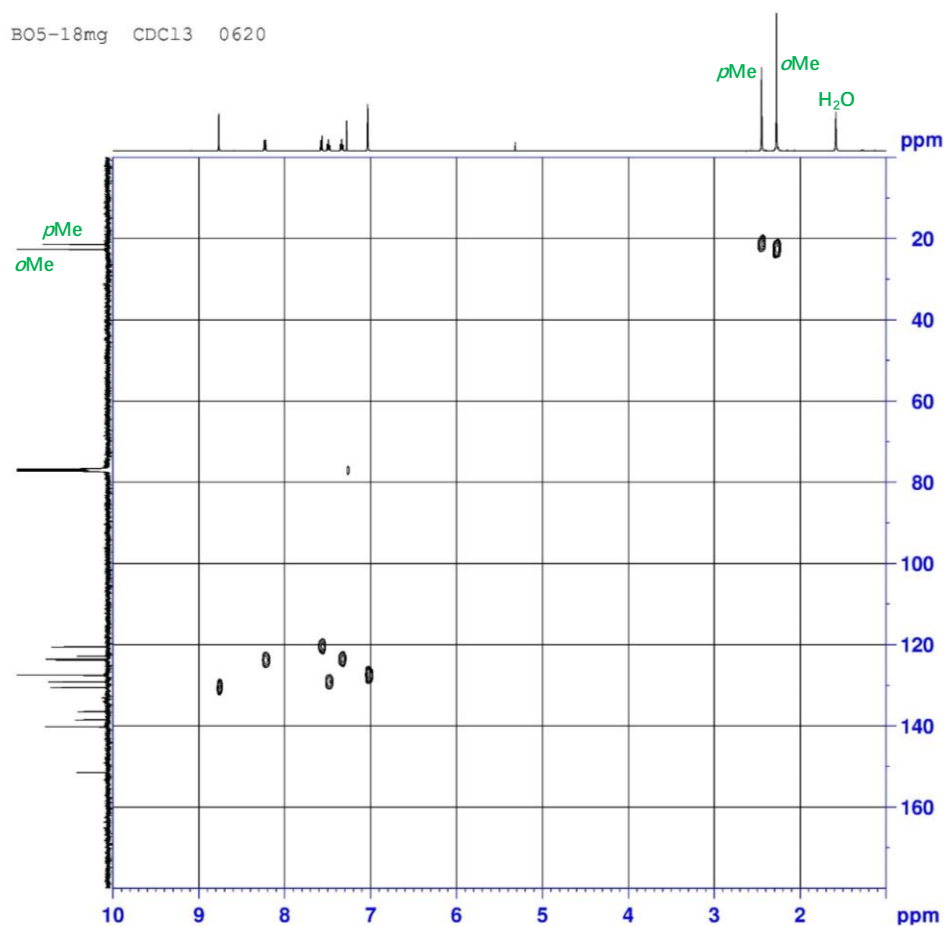


BO5-18mg CDC13 0620

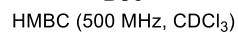
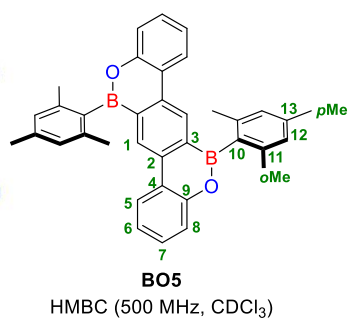


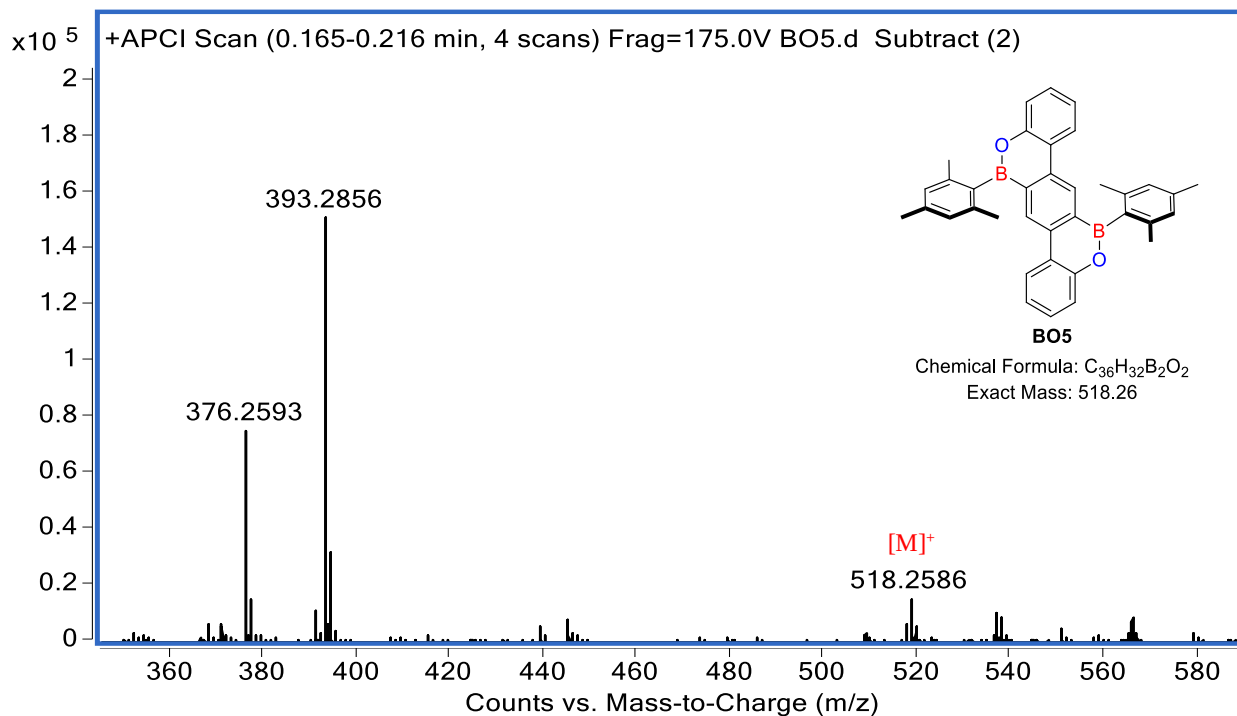
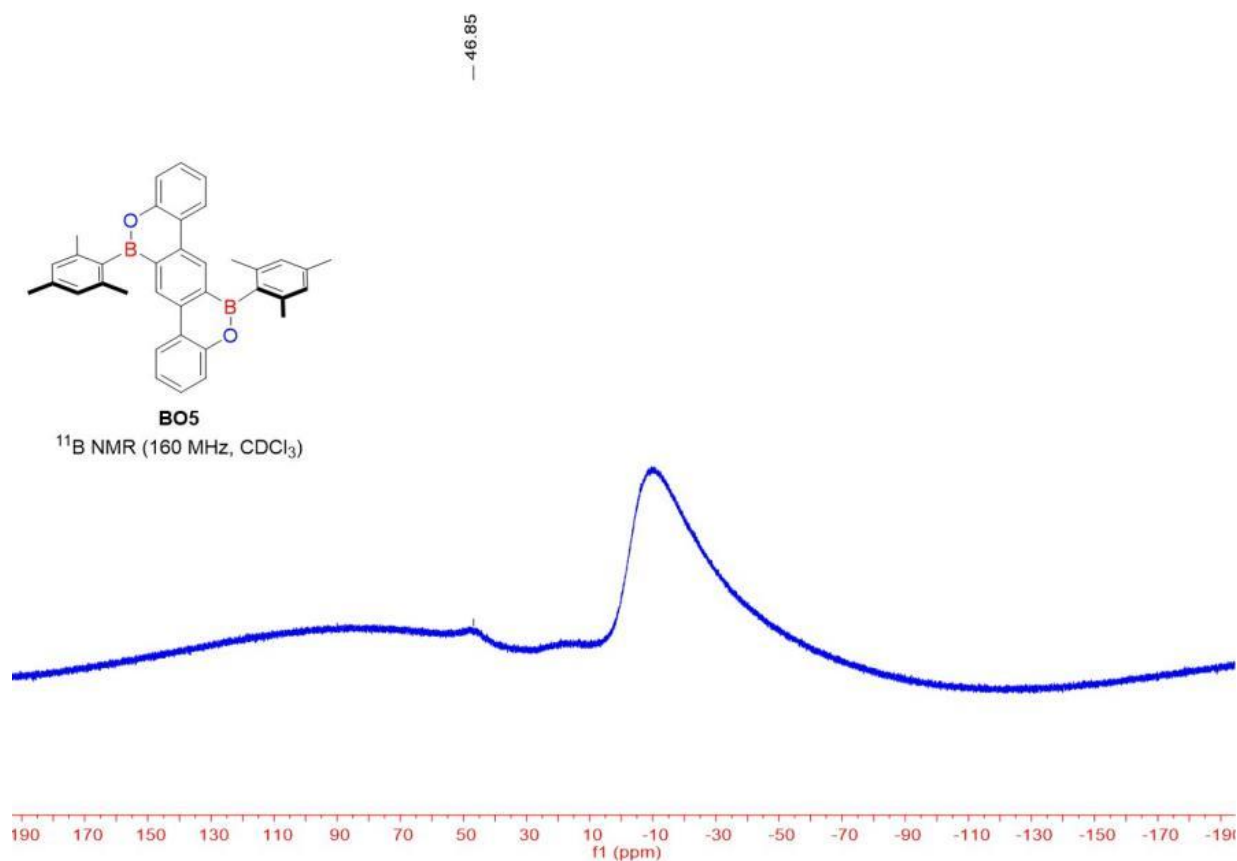
BO5
 ^1H - ^1H COSY (500 MHz, CDCl_3)

BO5-18mg CDC13 0620

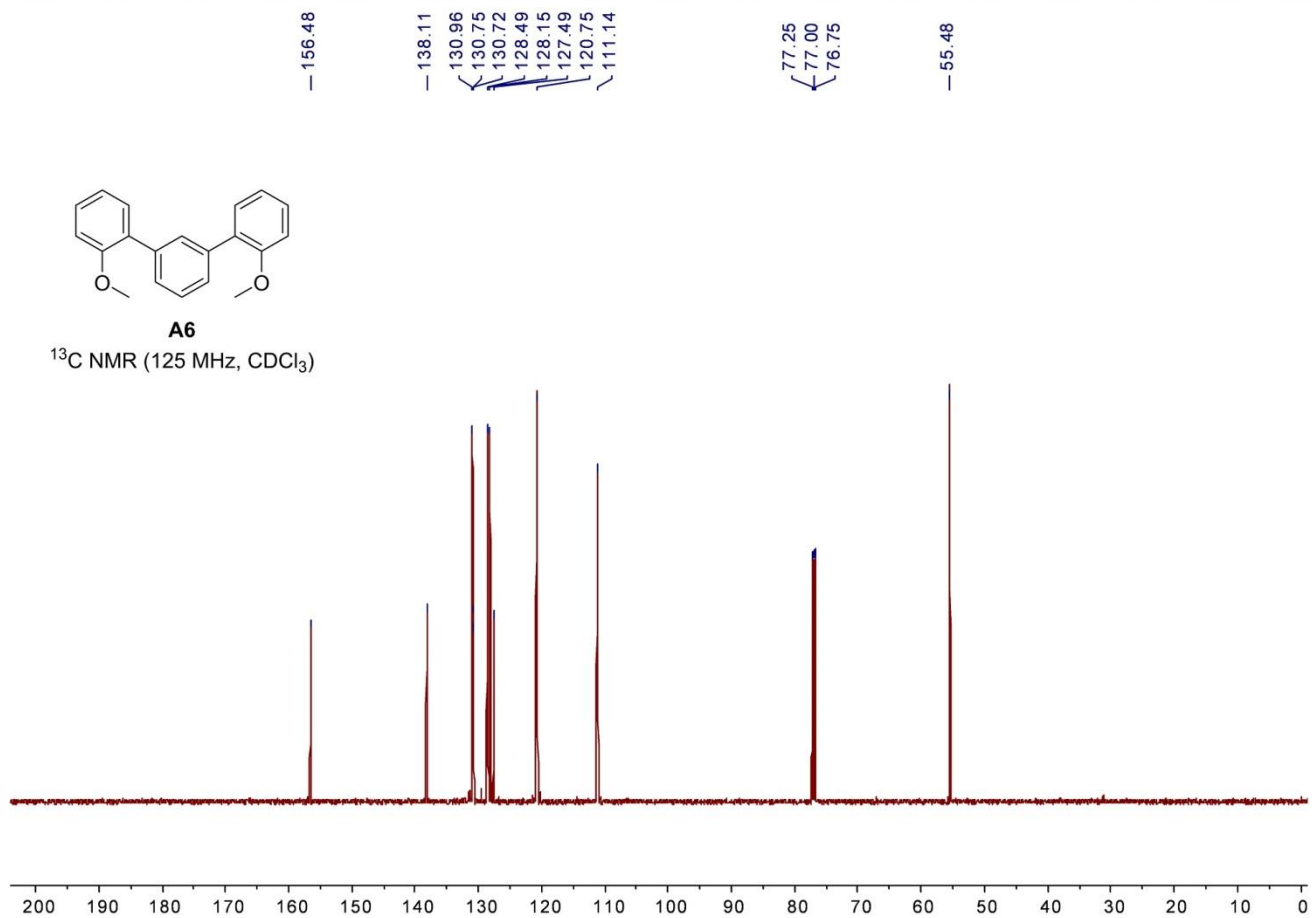
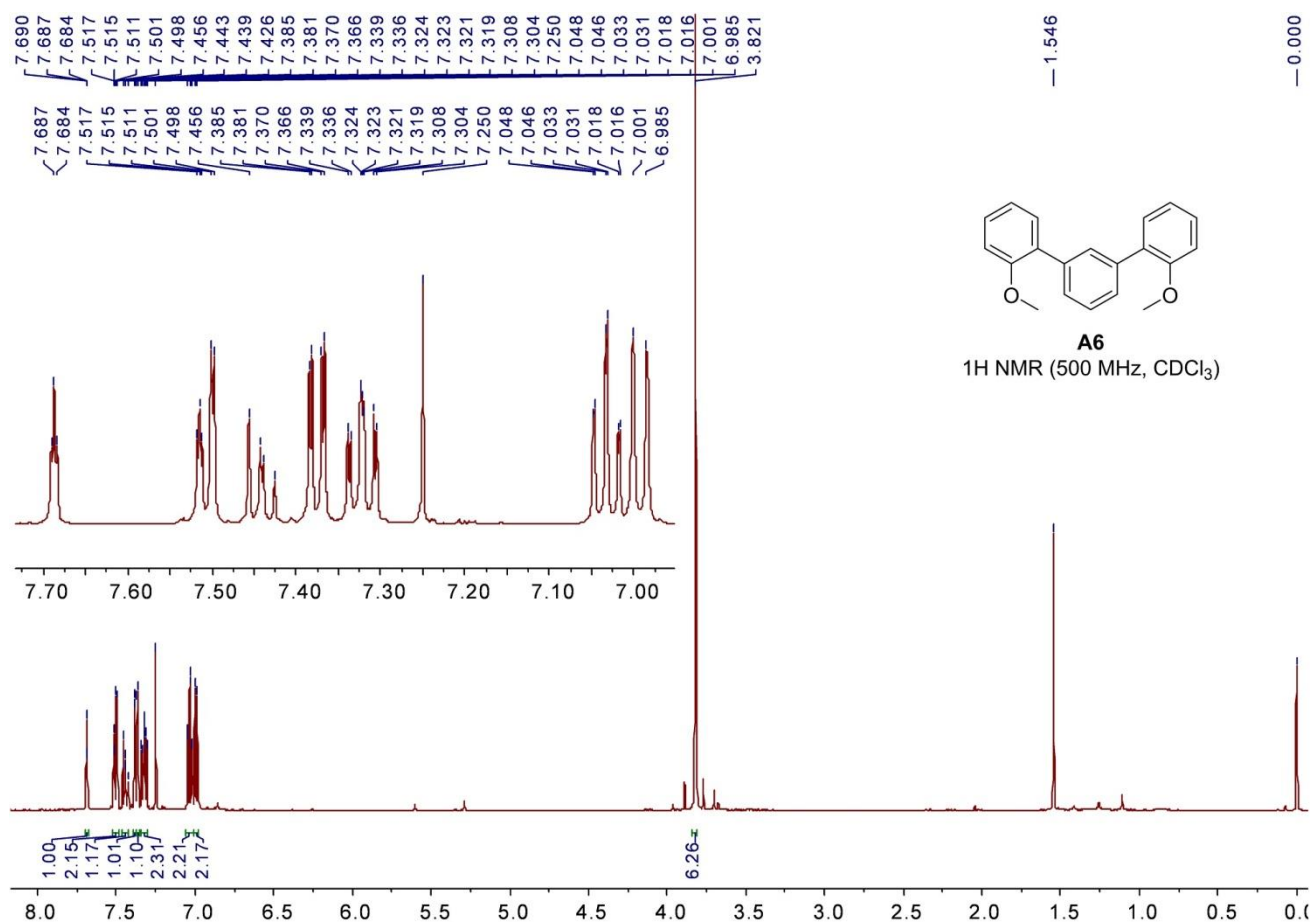


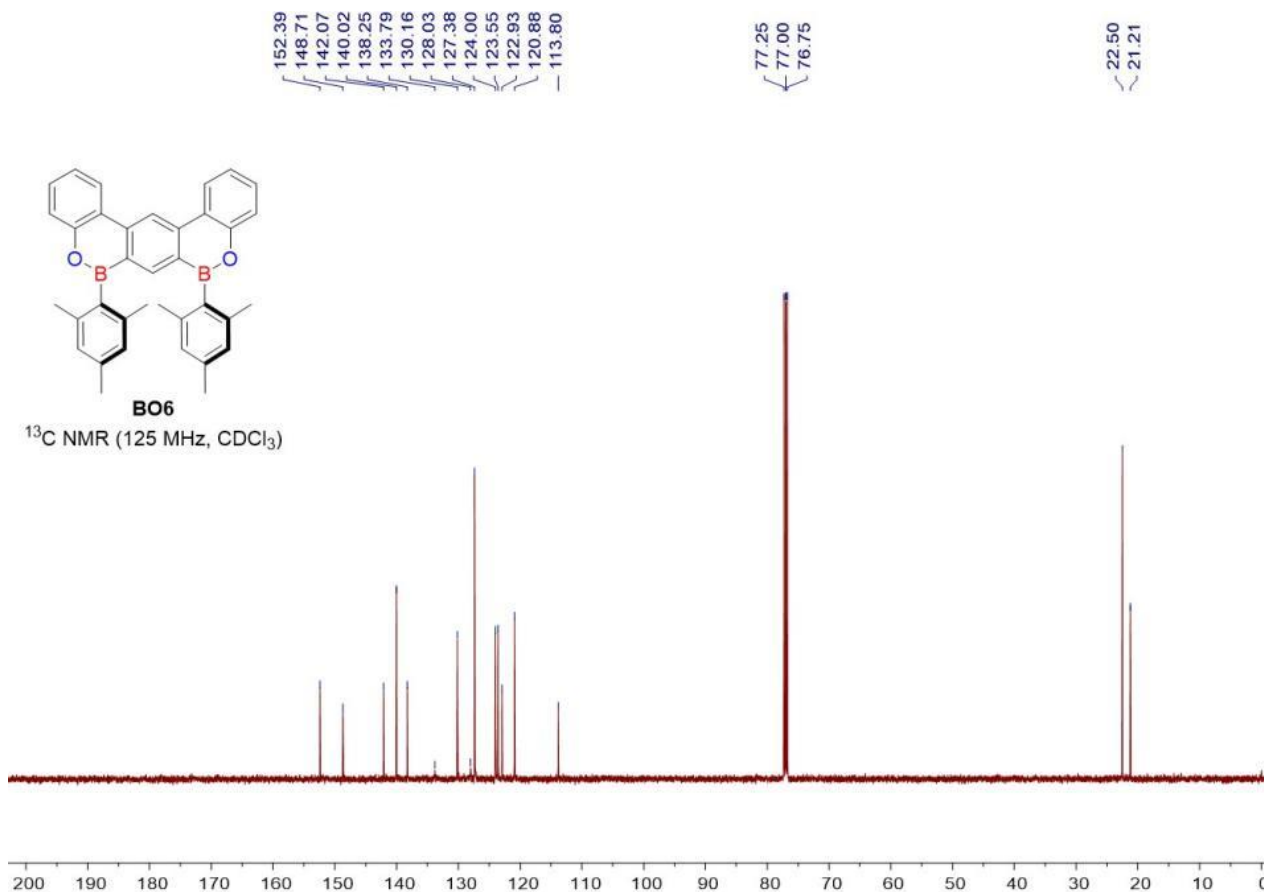
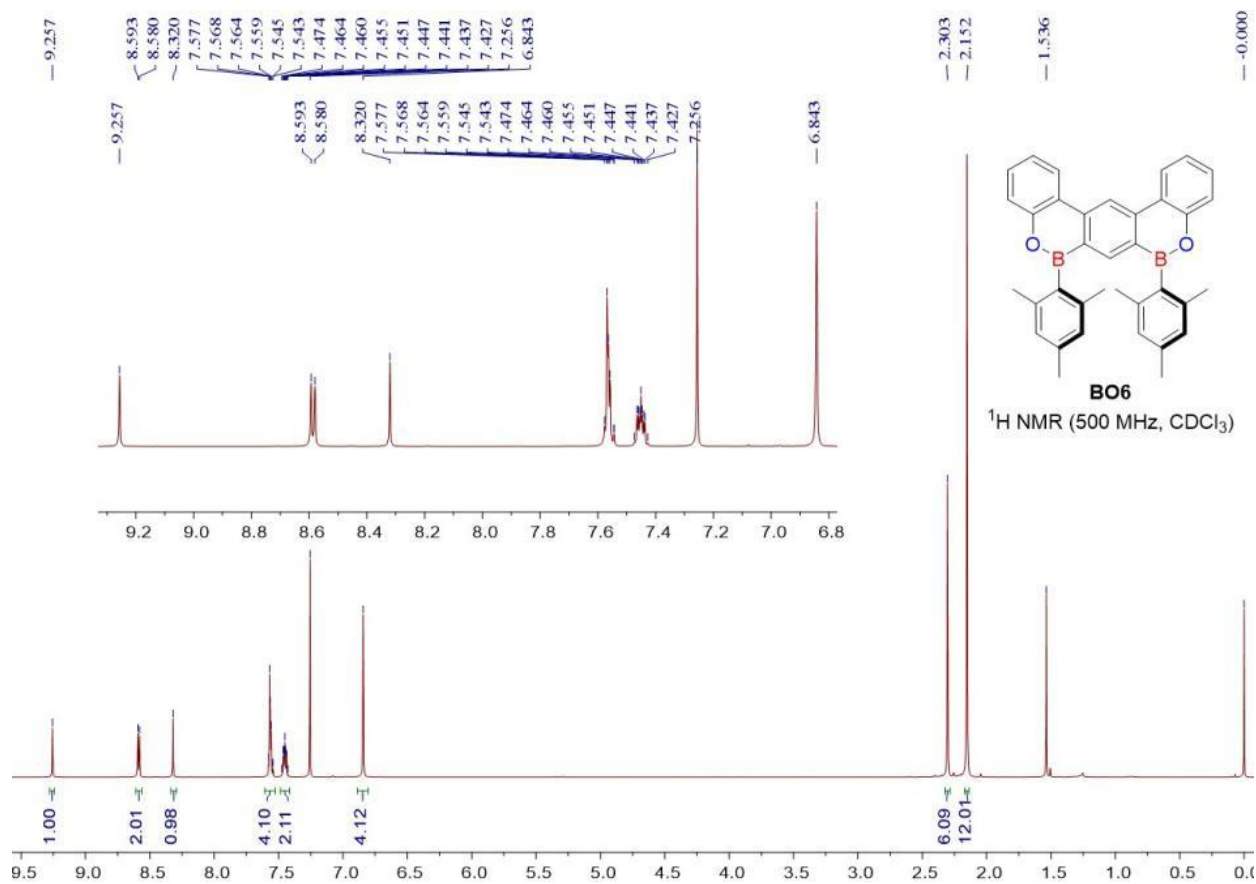
BO5
HSQC (500 MHz, CDCl_3)





Formula (M)	Ion Formula	m/z	Calc m/z	Diff (ppm)
C ₃₆ H ₃₂ [¹¹ B] ₂ O ₂	C ₃₆ H ₃₂ [¹¹ B] ₂ O ₂	518.2586	518.2583	-0.59



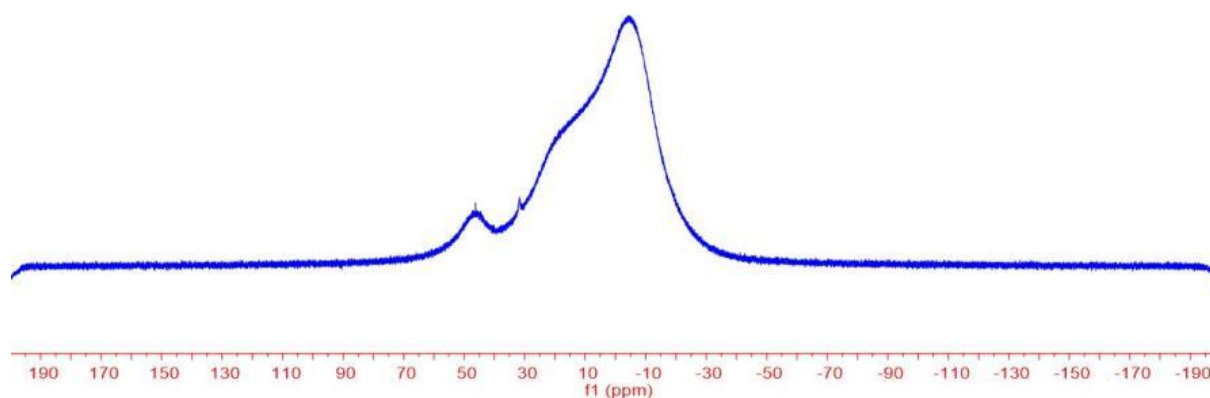


— 46.23

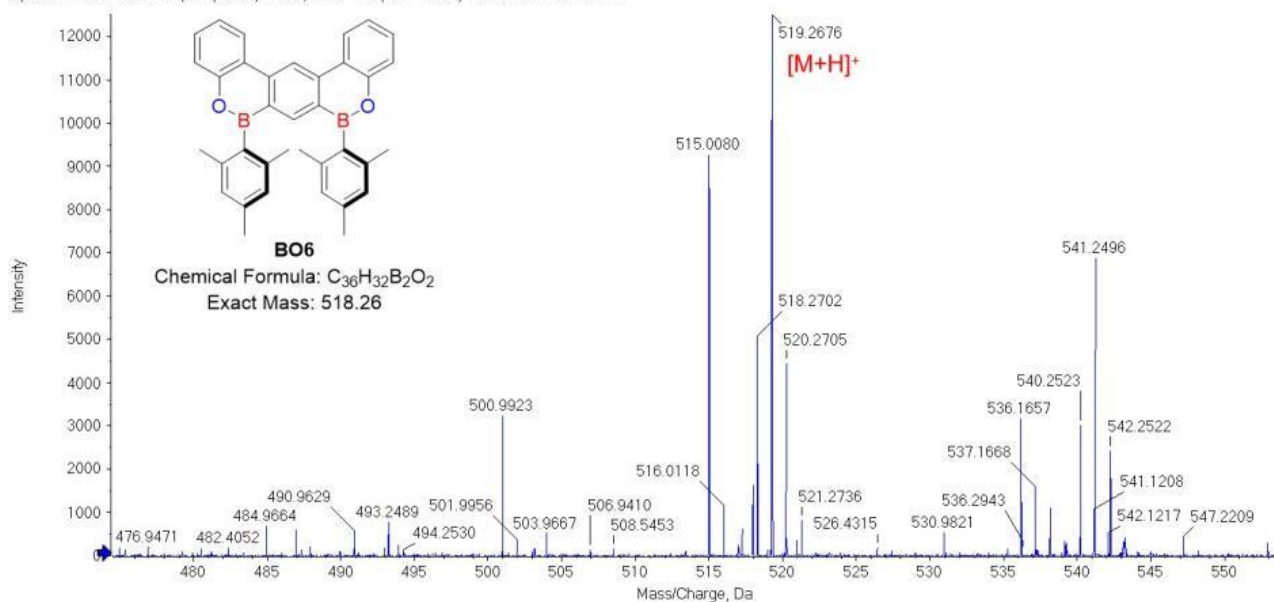


BO6

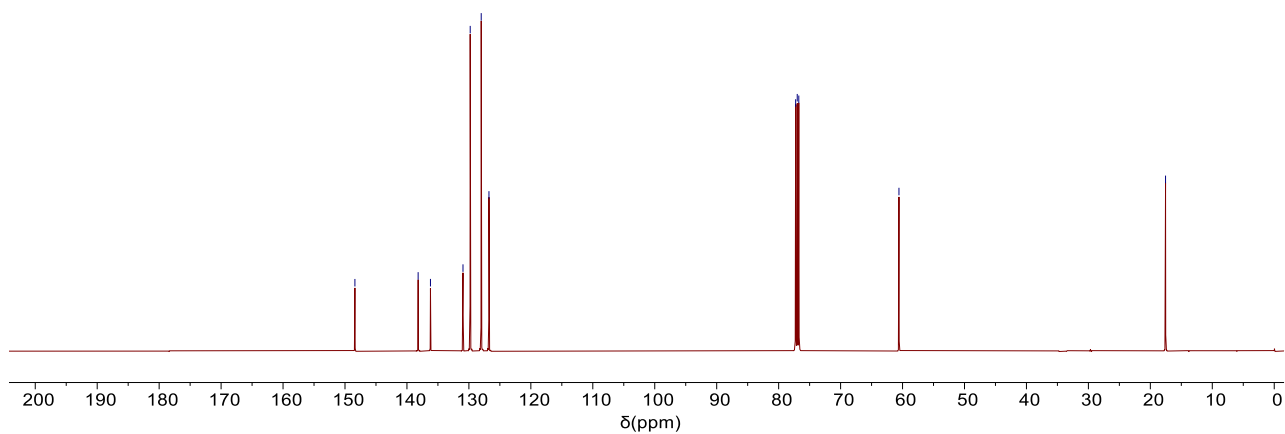
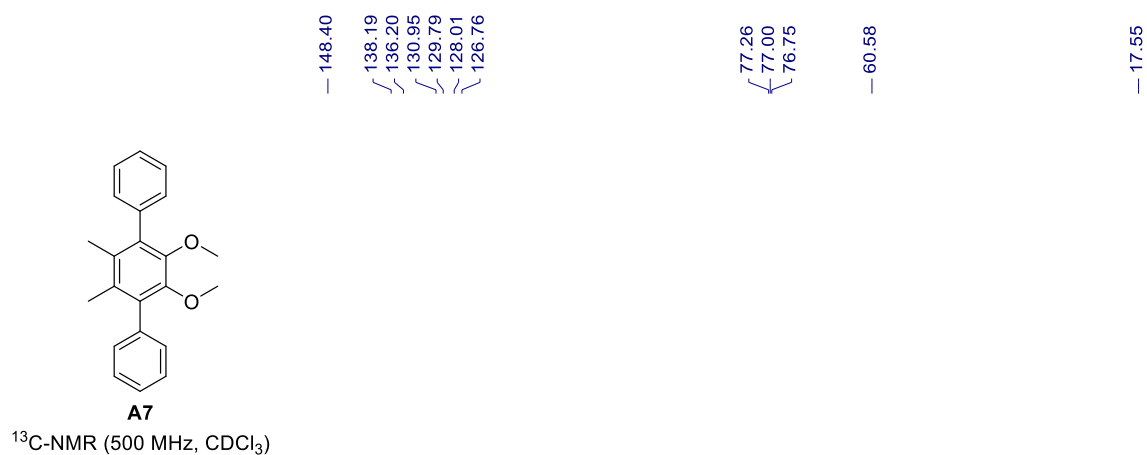
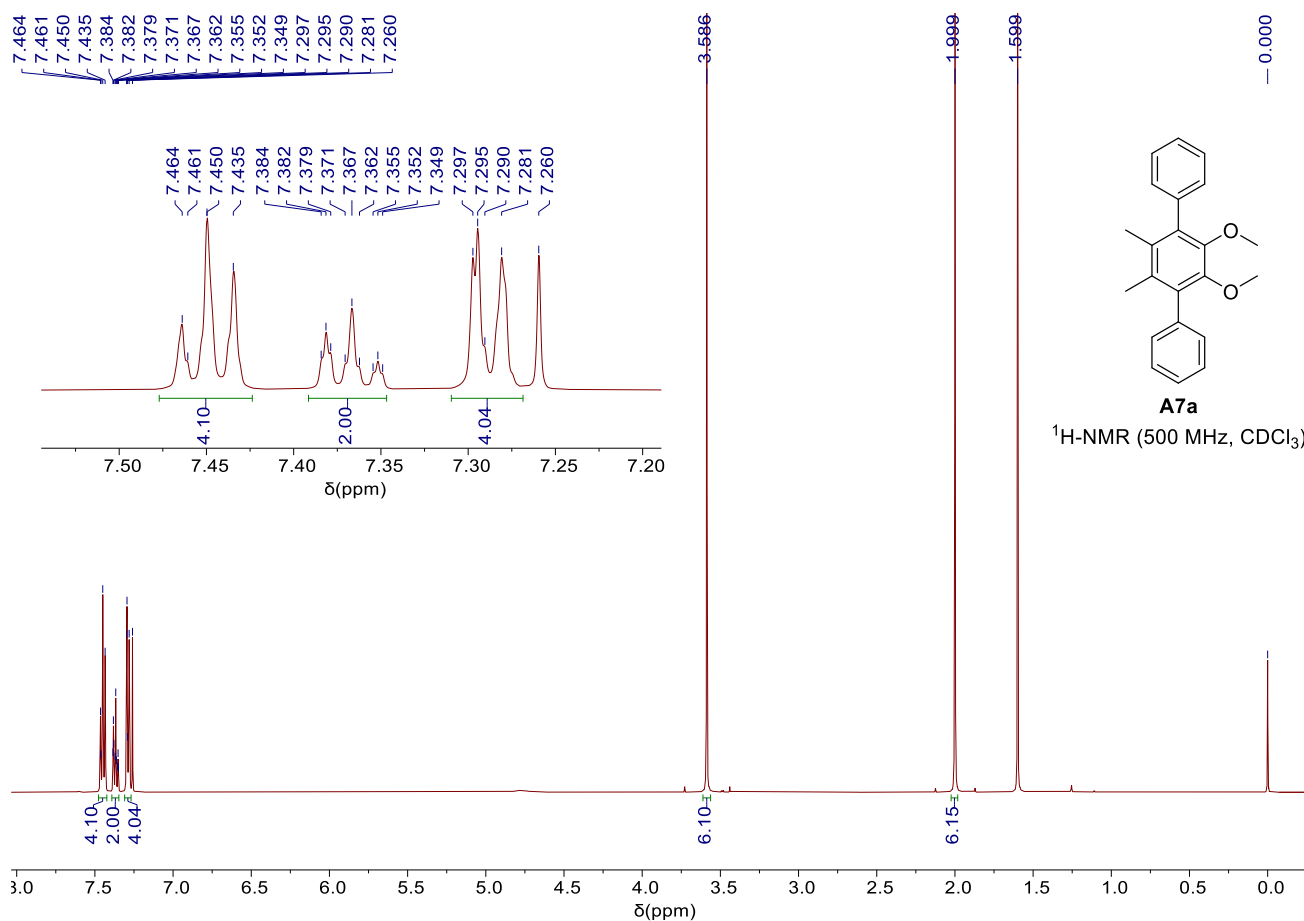
^{11}B NMR (160 MHz, CDCl_3)

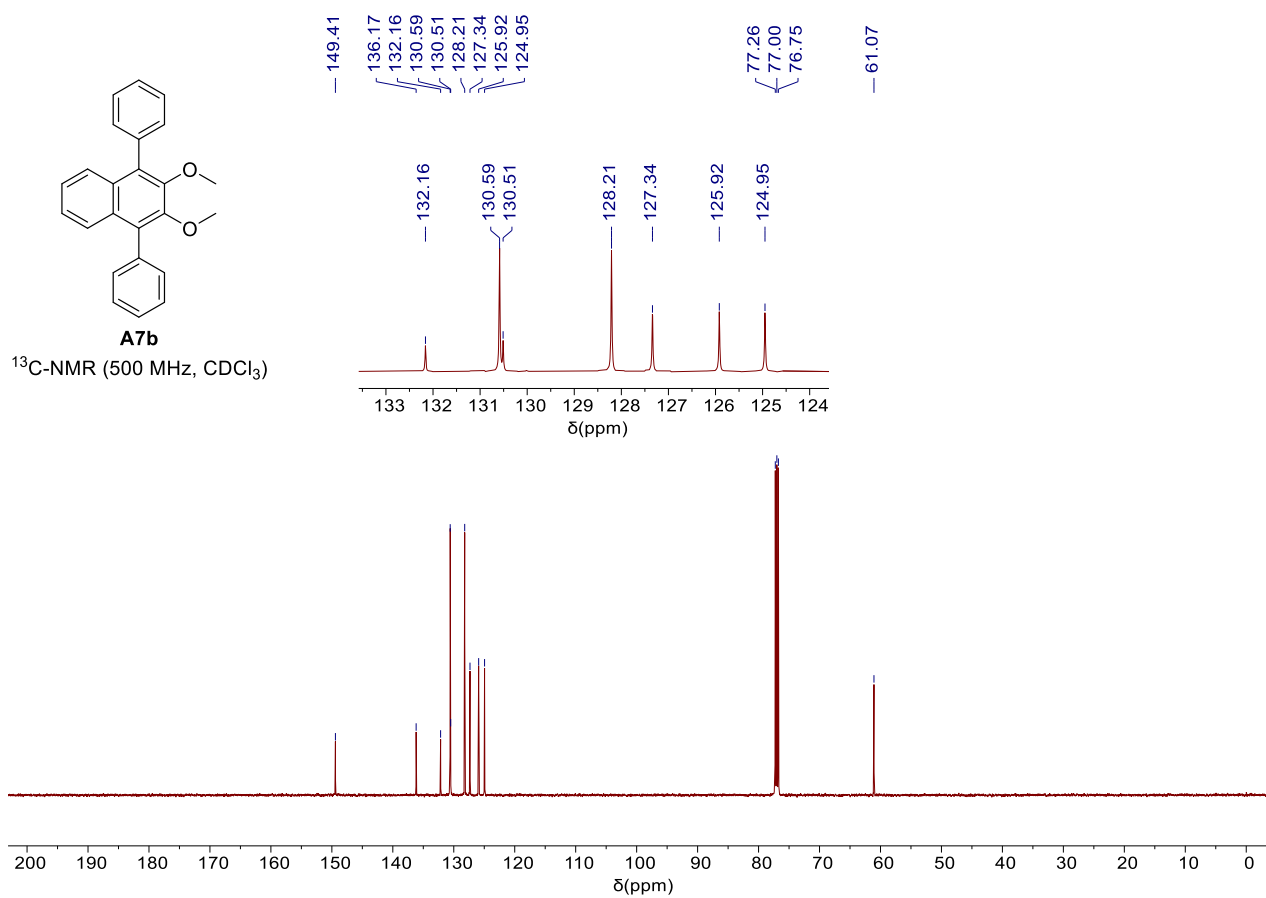
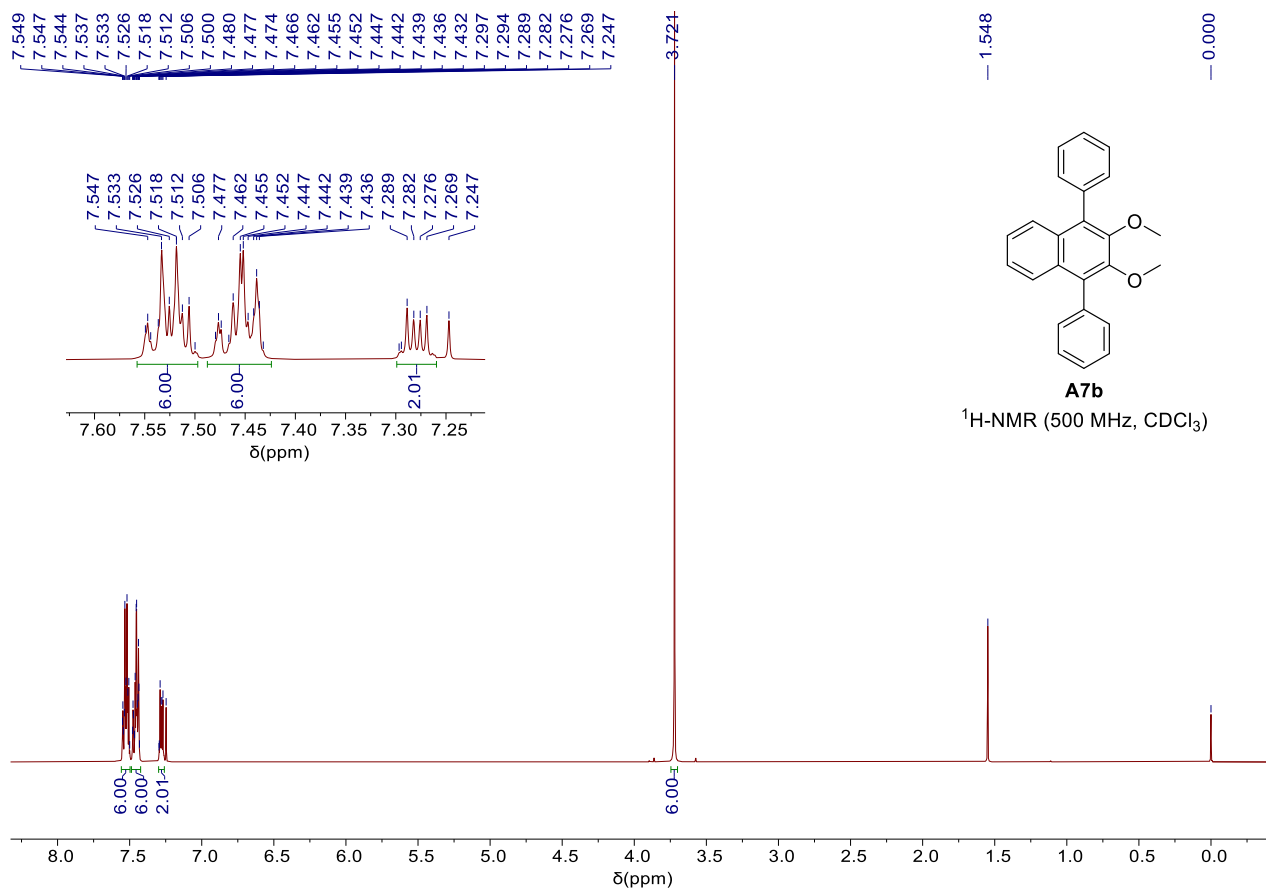


Spectrum from 0922.wiff (sample 32) - BO6, +TOF MS (100 - 1500) from 0.130 to 0.191 min



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
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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

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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
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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

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C	1.20347900	0.15668400	0.00607000
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

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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

CC3d_S₀

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

CC3e_S₀

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

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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

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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

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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

CC5_S₀

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

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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
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
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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

BO6_T1

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

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