Backbone-controlled LUMO energy induces intramolecular C–H activation in *ortho*-bis-9-borafluorene-substituted phenyl and *o*-carboranyl compounds leading to novel 9,10-diboraanthracene derivatives

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Supporting Information

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General experimental details

Unless otherwise noted, the following conditions apply.

All syntheses were carried out using standard Schlenk and glovebox techniques under an argon atmosphere. The solvents used were dried using either a solvent purification system (SPS) from Innovative Technology or were distilled and degassed from appropriate drying agents and stored under argon. Deuterated solvents (CD_2Cl_2 and C_6D_6) used for NMR spectroscopy were purchased from Cambridge Isotope Laboratories. C_6D_6 and CD_2Cl_2 were dried over molecular sieves, degassed by three freeze-pump-thaw cycles and stored under an argon atmosphere prior to use. *n*-Butyllithium (2.5 M solution in hexane) was purchased from Acros Organics and used as received. The compounds 9-bromo-9-borafluorene[1] and 1,2-bis(dichloroboryl)benzene[2] were prepared according to literature procedures. The dilithiated carborane 1,2-Li_2-1,2-$C_2B_{10}H_{10}$ was prepared *in situ* according to a published procedure.[3] Isolation of 1,2-Li_2-1,2-$C_2B_{10}H_{10}$ from lithiation in toluene at 80 °C overnight does not result in a fully dilithiated product, as a significant portion of monolithiated product remains. To lower the amount of side product formation and problems of identification in NMR experiments, we synthesized 1,2-Li_2-1,2-$C_2B_{10}H_{10}$ in Et_2O following a known route.[4] This results in the formation of 1,2-Li_2-1,2-$C_2B_{10}H_{10}\cdot(Et_2O)_2$. All other starting materials were purchased from commercial sources and were used without further purification.

NMR Spectra were recorded on a Bruker Avance 500 FT NMR spectrometer (operating at ^{1}H: 500 MHz, ^{11}B: 160 MHz, ^{13}C{^{1}H}: 126 MHz) or Bruker Avance III HD 300 spectrometer (operating at ^{1}H: 300 MHz, ^{11}B: 96 MHz, ^{13}C{^{1}H}: 75 MHz). Chemical shifts (δ) are given in ppm and ^{11}B{^{1}H} NMR spectra are referenced to external $BF_3\cdot Et_2O$. ^{1}H NMR spectra were referenced via residual proton resonances of CD_2Cl_2 (5.32 ppm), C_6D_6 (7.16 ppm), and THF-d_8 (1.72 ppm). ^{13}C{^{1}H} spectra were referenced to CD_2Cl_2 (53.84 ppm), C_6D_6 (128.06 ppm), and THF-d_8 (25.31 ppm).

HRMS were recorded using a Thermo Scientific Exactive Plus Orbitrap MS system by Liquid Injection Field Desorption Ionization (LIFDI) or an Atmospheric Sample Analysis Probe (ASAP).

Single-crystal X-ray diffraction: Crystals suitable for single-crystal X-ray diffraction were selected, coated in perfluoropolyether oil or polybutyl oil, mounted on a polyimide microloop

(MicroMounts fromMiTeGen) and transferred to a stream of cold nitrogen (Oxford Cryostream 700 or 800, respectively). Diffraction data were collected on a Bruker X8 Apex II 4-circle diffractometer with a CCD area detector, using Mo-K_α radiation generated by a Nonius FR591 rotating anode and monochromated by graphite (**3a**) or by multi-layer focusing mirrors (**2b**). Diffraction data were collected on a Rigaku Oxford Diffraction XtaLAB Synergy diffractometer with a semiconductor HPA-detector (HyPix-6000 or HyPix-Arc-150) and multi-layer mirror monochromated Cu-K_α radiation generated by a PhotonJet (**3a·THF**) or a PhotonJet-R (**3b, 5, 9-(4-bromobutoxy)-9-borafluorene**, **9-(Me_2S)-9-Br-9-borafluorene**, and **1-MeS-2-(Me_2S-9-borafluorene)-1,2-$C_2B_{10}H_{10}$**) source. Data were collected at 100 K or 173 K (**5**). The images were processed and corrected for Lorentz-polarization effects and absorption (empirical scaling) as implemented in the Bruker software packages (**2b** and **3a**) or using the CrysAlis^{Pro} software from Rigaku Oxford Diffraction (**3b**, **3a·THF**, **5**, **9-(4-bromobutoxy)-9-borafluorene**, **9-(Me_2S)-9-Br-9-borafluorene**, and **1-MeS-2-(Me_2S-9-borafluorene)-1,2-$C_2B_{10}H_{10}$**). The structures were solved using the intrinsic phasing method (SHELXT)[5] and Fourier expansion technique. All non-hydrogen atoms were refined in anisotropic approximation, with all hydrogen atoms 'riding' in idealized positions, by full-matrix least squares against F^2 of all data, using SHELXL[6] software and the SHELXLE[7] graphical user interface. In the case of **3a** disordered solvent was masked using SQUEEZE/PLATON.[8] **3b** and **3a·THF** were refined as two-component twins, both with twin fractions of 48%. **1-MeS-2-(Me_2S-9-borafluorene)-1,2-$C_2B_{10}H_{10}$** was refined as two-component twin with a twin fraction of 43%. Diamond software was used for graphical representation.[9] Crystal data and experimental details are listed in Table S1. Full structural information has been deposited with the Cambridge Crystallographic Data Centre. CCDC-2174245 (**2b**), 2174247 (**3a**), 2174246 (**3b**), 2174248 (**3a·THF**), 2174249 (**5**), 2216649 (**9-(4-bromobutoxy)-9-borafluorene**), 2216647 (**9-(Me_2S)-9-Br-9-borafluorene**), and 2216648 (**1-MeS-2-(Me_2S-9-borafluorene)-1,2-$C_2B_{10}H_{10}$**).

Photophysical measurements: All measurements were performed in standard quartz cuvettes (1 cm x 1 cm cross-section). UV–visible absorption spectra were recorded using a Perkin Elmer Lambda 465 UV-visible spectrophotometer. **Emission spectra** were recorded using an Edinburgh Instruments FLSP920 spectrophotometer equipped with a double monochromator for both excitation and emission, operating in right-angle geometry mode, and all spectra were fully corrected for the spectral response of the instrument. **Fluorescence quantum yields** were measured using a calibrated integrating sphere (inner diameter: 150 mm) from Edinburgh Instruments combined with the FLSP920 spectrophotometer described above. For solution-state and solid-state measurements, the longest-wavelength absorption maximum of the

compound in the respective solvent was chosen as the excitation wavelength. **Fluorescence lifetimes** were recorded using the time-correlated single-photon counting (TCSPC) method using the same FLSP920 spectrometer described above. Solutions were excited with a picosecond pulsed diode laser at 376.6 nm. The full width at half maximum (FWHM) of the laser pulses were ca. 70–200 ps, while the instrument response function (IRF) had a FWHM of ca. 1.0 ns, measured from the scatter of a Ludox solution at the excitation wavelength. Decays were recorded to at least 10000 counts in the peak channel with a record length of at least 1000 channels. The band pass of the monochromator was adjusted to give a signal count rate of <10 kHz. Iterative reconvolution of the IRF with one decay function and non-linear least-squares analysis were used to analyze the data. The quality of the fit was judged by the calculated value of the reduced χ^2 and visual inspection of the weighted residuals.

Computational methods

All molecular geometries were fully optimized via DFT calculations at the B3LYP-D(BJ), wB97X-D[10] and M062X[11-13]/6-31G(d,p)[14, 15] level of theory. Frequency calculations at the same level of theory were performed to confirm that all stationary points are local minima (no imaginary frequencies) or transition states (one imaginary frequency) and to provide free energies at 298.15 K. Transition states were located using the Berny algorithm and further confirmed by calculations of intrinsic reaction coordinates (IRC)[16] showing that the transition states indeed connect the two relevant minima. All DFT calculations were performed with the Gaussian 09 (D.01) program.[17]

All calculations regarding the photophysical experiments of **2a**, **2b**, **3a**, and **3b** (DFT and TD-DFT) were carried out with the Gaussian 09 (9.E.01)[18] program package and were performed on a parallel cluster system. GaussView (6.0.16) and multiwfn[19] were used to visualize the results, to measure calculated structural parameters, and to plot orbital surfaces (isovalue: ± 0.030 [e a_0^{-3}]$^{1/2}$). The ground-state geometries were optimized using the B3LYP functional[20] in combination with the 6-31+G(d,p) basis set.[21, 22]

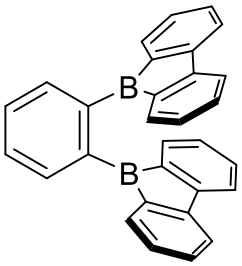
The orbital overlap parameter was calculated with $\Lambda = \frac{\sum_{i,a} c_{i,a}^2 \langle | \varphi_a | | \varphi_i | \rangle}{\sum_{i,a} c_{i,a}^2}$, resulting in $0 \leq \Lambda \leq 1$, where $\Lambda = 0$ corresponds to no overlap and $\Lambda = 1$ corresponds to complete overlap.[23]

The ultrafine integration grid and symmetry constraints were used for all molecules. Frequency calculations were performed on the optimized structures to confirm them to be local minima showing no negative (imaginary) frequencies. Based on these optimized structures, the lowest-energy vertical transitions (using the polarizable continuum model) were calculated (singlets, 25 states) by TD-DFT, using the Coulomb attenuated functional CAM-B3LYP[24] as well as

B3LYP. The CAM-B3LYP functional has been shown to more accurately describe CT systems in comparison to B3LYP.[23] The optimized ground-state geometries were used as starting coordinates for TD-DFT geometry optimizations.

Synthetic procedures

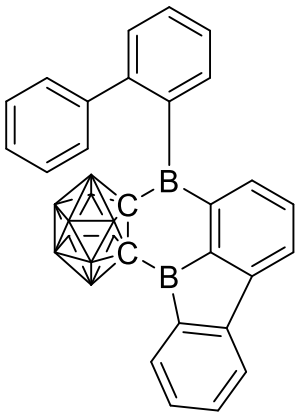
Bis(bis-9-borafluorenyl)benzene (2b)



Via syringe, a solution of 1,2-bis(dichloroboryl)benzene **4** (119 mg, 495 μmol, 1.0 eq.) in 10 mL toluene was slowly added to a solution of dimethyldibenzostannole (300 mg, 990 μmol, 2.0 eq.) in 10 mL toluene at −78 °C in a Schlenk tube. The solution was stirred and allowed to warm to room temperature overnight. After removal of all volatiles including Me_2SnCl_2 *in vacuo*, the residue was washed with hexane (3 x 20 mL) to yield a yellow solid **2b** (158 mg, 393 μmol, 79%).

^{1}H NMR (500.1 MHz, CD_2Cl_2): δ = 8.03 (m, 2H, C*H*$_{Ar}$), 7.70 (m, 2H, C*H*$_{Ar}$), 7.47 (m, 4H, C*H*), 7.29 (m, 4H, C*H*), 7.23 (m, 4H, C*H*), 6.95 (m, 4H, C*H*) ppm.
^{11}B NMR (160.5 MHz, CD_2Cl_2): δ = 67.0 (br) ppm.
^{13}C{^{1}H} NMR (125.8 MHz, CD_2Cl_2): δ = 154.03 ($C_{q,Ar}$), 145.03 ($C_{q,Ar}$), 143.78 ($C_{q,Ar}$), 134.81 (*C*H$_{Ar}$), 134.43 (*C*H$_{Ar}$), 134.16 (*C*H$_{Ar}$), 130.70 (*C*H$_{Ar}$), 128.42 (*C*H$_{Ar}$), 120.06 (*C*H$_{Ar}$) ppm.
HRMS LIFDI calc. for $[C_{30}H_{20}B_2]^+$ = $[M]^+$: 402.1746, found 402.1744.

3-([1,1'-biphenyl]-2-yl)-3*H*-1,2-(1,2-*ortho*-carboranyl)-3,10b-diborafluoranthene (3a)



Ortho-carborane (200 mg, 1.39 mmol, 1.0 eq.) was dissolved in toluene (5 mL) and a 2.5 M *n*BuLi solution in hexane (1.16 mL, 2.91 mmol, 2.1 eq.) was added dropwise at –78 °C. The reaction mixture was slowly warmed to room temperature and stirred at 80 °C overnight to obtain the dilithiated species **1** *in situ*. Then 9-bromo-9-borafluorene (707 mg, 2.91 mmol, 2.1 eq.) in toluene (5 mL) was added dropwise at –78 °C after which the reaction was slowly warmed to room temperature and stirred for 4 d. The suspension was filtered, the solid was washed with toluene (5 mL) and all volatiles were removed from the filtrate *in vacuo*. The crude product was recrystallized from toluene by hexane diffusion at –30 °C to give **3b** as orange crystals (85.0 mg, 182 μmol, 13%).

^{1}H NMR (500.1 MHz, CD_2Cl_2): δ = 7.65 (m, 1H, C*H*$_{Ar}$), 7.59 (m, 1H, C*H*$_{Ar}$), 7.56 (m, 1H, C*H*$_{Ar}$), 7.42 (m, 3H, C*H*$_{Ar}$), 7.36 (m, 1H, C*H*$_{Ar}$), 7.31 (m, 6H, C*H*$_{Ar}$), 7.25 (m, 1H, C*H*$_{Ar}$), 7.18 (m, 1H, C*H*$_{Ar}$), 7.16 (m, 1H, C*H*$_{Ar}$), 3.18–1.53 (br, 10H, B*H*) ppm.

^{1}H{^{11}B} NMR (500.1 MHz, CD_2Cl_2): δ = 7.65 (m, 1H, C*H*$_{Ar}$), 7.59 (m, 1H, C*H*$_{Ar}$), 7.56 (m, 1H, C*H*$_{Ar}$), 7.42 (m, 3H, C*H*$_{Ar}$), 7.36 (m, 1H, C*H*$_{Ar}$), 7.31 (m, 6H, C*H*$_{Ar}$), 7.25 (m, 1H, C*H*$_{Ar}$), 7.18 (m, 1H, C*H*$_{Ar}$), 7.16 (m, 1H, C*H*$_{Ar}$), 2.61(s, 1H, B*H*), 2.45–2.34 (m, 5H, B*H*), 2.27 (s, 1H, B*H*), 2.21(s, 1H, B*H*), 2.05(s, 1H, B*H*), 1.55(s, 1H, B*H*) ppm.

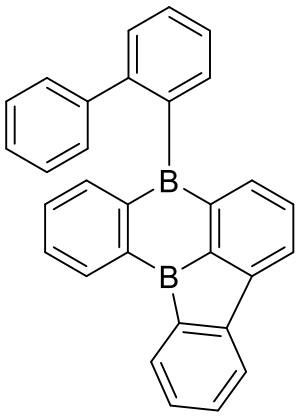
^{11}B NMR (160.5 MHz, CD_2Cl_2): δ = 66.1, 3.2, –4.4, –8.8 ppm.

^{11}B{^{1}H} NMR (160.5 MHz, CD_2Cl_2): δ = 66.1, 2.6, 2.2, –5.0, –5.7, –9.6 ppm.

^{13}C{^{1}H} NMR (125.8 MHz, CD_2Cl_2): δ = 155.8 (*C*$_{q,Ar}$), 152.9 (*C*$_{q,Ar}$), 143.9 (*C*$_{q,Ar}$), 143.8 (*C*$_{q,Ar}$), 138.6 (*C*H$_{Ar}$), 137.1 (*C*H$_{Ar}$), 136.4 (*C*H$_{Ar}$), 136.2 (*C*H$_{Ar}$), 129.9 (*C*H$_{Ar}$), 129.7 (*C*H$_{Ar}$), 129.6 (*C*H$_{Ar}$), 126.5 (*C*H$_{Ar}$), 129.1 (*C*H$_{Ar}$), 129.0 (*C*H$_{Ar}$), 128.1 (*C*H$_{Ar}$), 126.1 (*C*H$_{Ar}$), 125.7 (*C*H$_{Ar}$), 121.7 (*C*H$_{Ar}$) ppm.

HRMS LIFDI calc. for $[C_{26}H_{26}B_{12}]^+$ = $[M]^+$: 468.3219, found 468.3218.

5-([1,1'-biphenyl]-2-yl)-5H-benzo[4,5]borolo[3,2,1-de]boranthrene (3b)



Compound **2b** (37.0 mg, 92.0 μmol) was heated for 3 d at 120 °C in toluene. Removal of all volatiles *in vacuo* led to the isolation of **3b** as an orange solid (34.0 mg, 84.5 μmol, 92%).

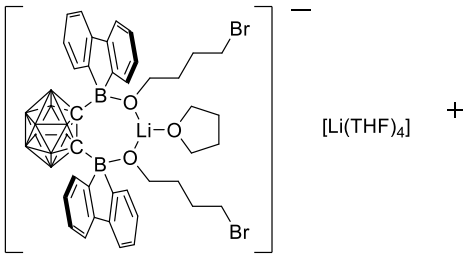
^{1}H NMR (500.1 MHz, CD_2Cl_2): δ = 8.33 (m, 1H, CH_{Ar}), 8.02 (m, 1H, CH_{Ar}), 7.73 (m, 1H, CH_{Ar}), 7.67 (m, 1H, CH_{Ar}), 7.58 (m, 1H, CH_{Ar}), 7.55 (m, 1H, CH_{Ar}) 7.48 (m, 3H, CH_{Ar}), 7.42 (m, 1H, CH_{Ar}), 7.39 (m, 1H, CH_{Ar}), 7.35 (m, 3H, CH_{Ar}), 7.20 (m, 1H, CH_{Ar}), 7.13 (m, 4H, CH_{Ar}), 6.98 (m, 1H, CH_{Ar}) ppm.

^{11}B NMR (160.5 MHz, CD_2Cl_2): δ = 63.9 (br) ppm.

^{13}C{^{1}H} NMR (125.8 MHz, CD_2Cl_2): δ = 156.80 ($C_{q,Ar}$), 153.26 ($C_{q,Ar}$), 150.80 ($C_{q,Ar}$), 149.68 ($C_{q,Ar}$), 145.62 ($C_{q,Ar}$), 144.32 ($C_{q,Ar}$), 144.11 ($C_{q,Ar}$), 143.36 ($C_{q,Ar}$), 141.99 ($C_{q,Ar}$), 141.12 (CH$_{Ar}$), 137.49 (CH$_{Ar}$), 135.79 (CH$_{Ar}$), 135.60 (CH$_{Ar}$), 134.72 (CH$_{Ar}$), 133.97 (CH$_{Ar}$), 133.95 (CH$_{Ar}$), 132.18 (CH$_{Ar}$), 131.51 (CH$_{Ar}$), 129.08 (CH$_{Ar}$), 128.96 (CH$_{Ar}$), 128.93 (CH$_{Ar}$), 128.50 (CH$_{Ar}$), 128.44 (CH$_{Ar}$), 127.52 (CH$_{Ar}$), 126.46 (CH$_{Ar}$), 123.40 (CH$_{Ar}$), 121.14 (CH$_{Ar}$), ppm.

HRMS LIFDI calc. for $[C_{30}H_{20}B_2]^+ = [M]^+$: 402.1746, found 402.1743.

Synthesis of 5



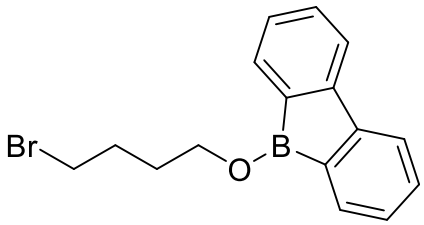
The compound 9-Br-9-borafluorene (10 mg, 41.2 μmol, 2.5 eq) was suspended in THF-d_8 (1 mL) and the mixture was stirred at 60 °C for 1 h. The reaction was monitored by ^{11}B NMR spectroscopy. Then, 1,2-Li_2-1,2-$C_2B_{10}H_{10}\cdot(Et_2O)_2$ (5 mg, 16.4 μmol, 1.0 eq) was added at –30 °C and the reaction was allowed to warm to room temperature. The reaction was monitored by ^{1}H and ^{11}B NMR spectroscopy. Crystals of **5** were obtained from the reaction solution by pentane diffusion at –30 °C.

^{1}H NMR (300.2 MHz, THF-d_8): δ = 7.82 (m, 2H, CH_{Ar}), 7.39 (m, 2H, CH_{Ar}), 6.96 (m, 4H, CH_{Ar}) ppm.

^{11}B{^{1}H} NMR (96.3 MHz, THF-d_8): δ = 4.1, –3.2, –6.7, –8.4 ppm.

^{13}C{^{1}H} NMR (75.5 MHz, THF-d_8): δ = 149.9 ($C_{q,Ar}$), 133.5 (CH$_{Ar}$), 125.6 (CH$_{Ar}$), 124.9 (CH$_{Ar}$), 117.9 (CH$_{Ar}$) ppm.

Synthesis of 9-(4-bromobutoxy)-9-borafluorene



The compound 9-Br-9-borafluorene (10 mg, 41.2 μmol) was suspended in THF (1 mL). The reaction mixture was stirred at 60 °C for 1 h and was monitored by ^{11}B NMR spectroscopy. Removal of all volatiles *in vacuo* led to the isolation of 9-(4-bromobutoxy)-9-borafluorene. Crystals of the product were obtained from a CD_2Cl_2 solution by pentane diffusion at –30 °C.

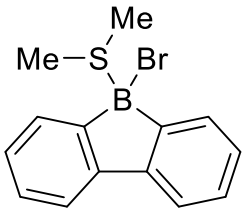
^{1}H NMR (500.1 MHz, CD_2Cl_2): δ = 7.55 (m, 2H, CH_{Ar}), 7.49 (m, 2H, CH_{Ar}), 7.35 (m, 2H, CH_{Ar}), 7.19 (m, 2H, CH_{Ar}), 4.61 (t, $^3J_{HH}$ = 6.24 Hz, 2H, CH_2), 3.54 (t, $^3J_{HH}$ = 6.59 Hz, 2H, CH_2), 2.11 (m, 2H, CH_2), 2.00 (m, 2H, CH_2) ppm.

^{11}B NMR (160.5 MHz, CD_2Cl_2): δ = 45.0 ppm.

^{13}C{^{1}H} NMR (125.8 MHz, CD_2Cl_2): δ = 152.8 ($C_{q,Ar}$), 132.9 (CH$_{Ar}$), 132.3 (CH$_{Ar}$), 128.2 (CH$_{Ar}$), 120.0 (CH$_{Ar}$), 68.0 (CH$_2$), 34.2 (CH$_2$), 30.7 (CH$_2$), 29.8 (CH$_2$) ppm.

HRMS LIFDI calc. for $[C_{16}H_{16}B_1O_1]^+ = [M]^+$: 314.0472, found 314.0463.

Synthesis of 9-(Me_2S)-9-Br-9-borafluorene



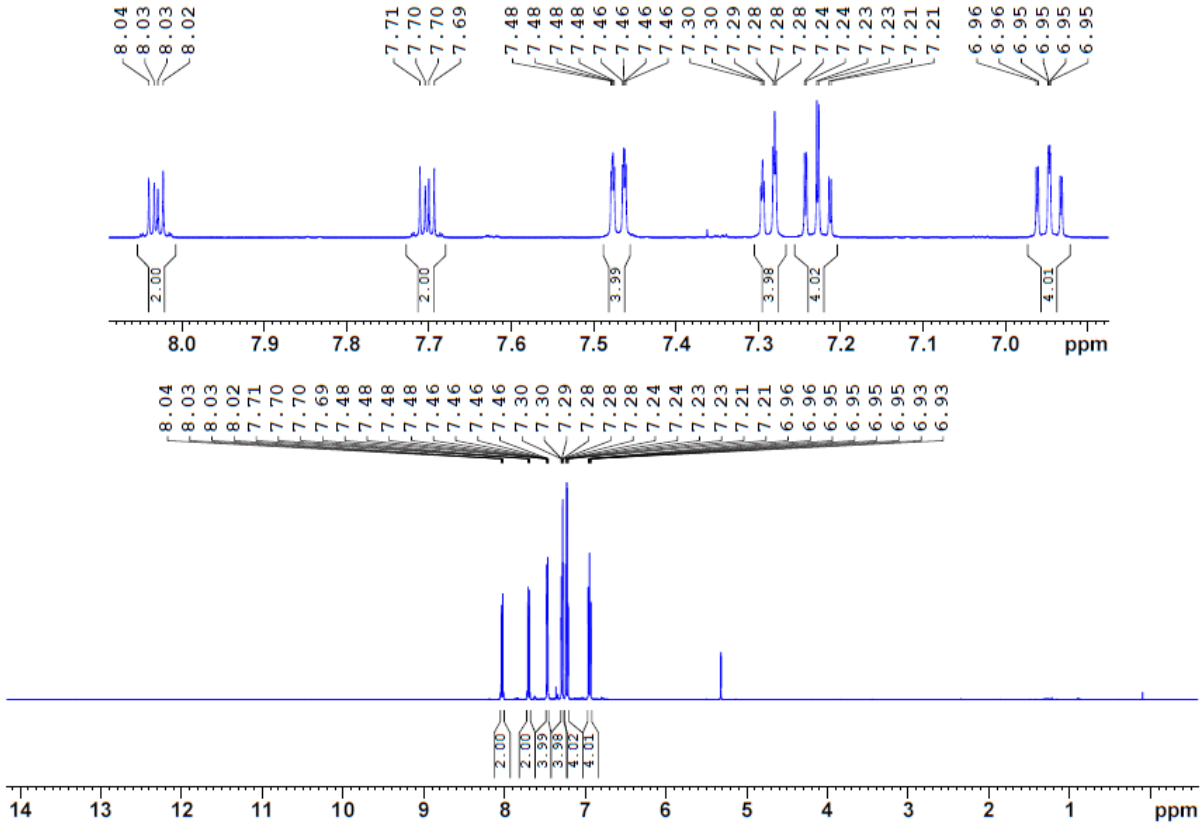
The compound 9-Br-9-borafluorene (10 mg, 41.2 μmol) was dissolved in toluene (1 mL), one drop of Me_2S was added, and a colorless solid precipitated from the solution. The reaction mixture was stirred at room temperature overnight. Removal of all volatiles *in vacuo* led to the formation of the Me_2S adduct in quantitative yield according to ^{1}H and ^{11}B NMR spectroscopy. Crystals of the product were obtained from a Me_2S solution by pentane diffusion at –30 °C.

^{1}H NMR (500.1 MHz, CD_2Cl_2): δ = 7.64 (m, 2H, CH_{Ar}), 7.54 (m, 2H, CH_{Ar}), 7.33 (m, 2H, CH_{Ar}), 7.23 (m, 2H, CH_{Ar}), 2.18 (s, 6H, CH_3) ppm.

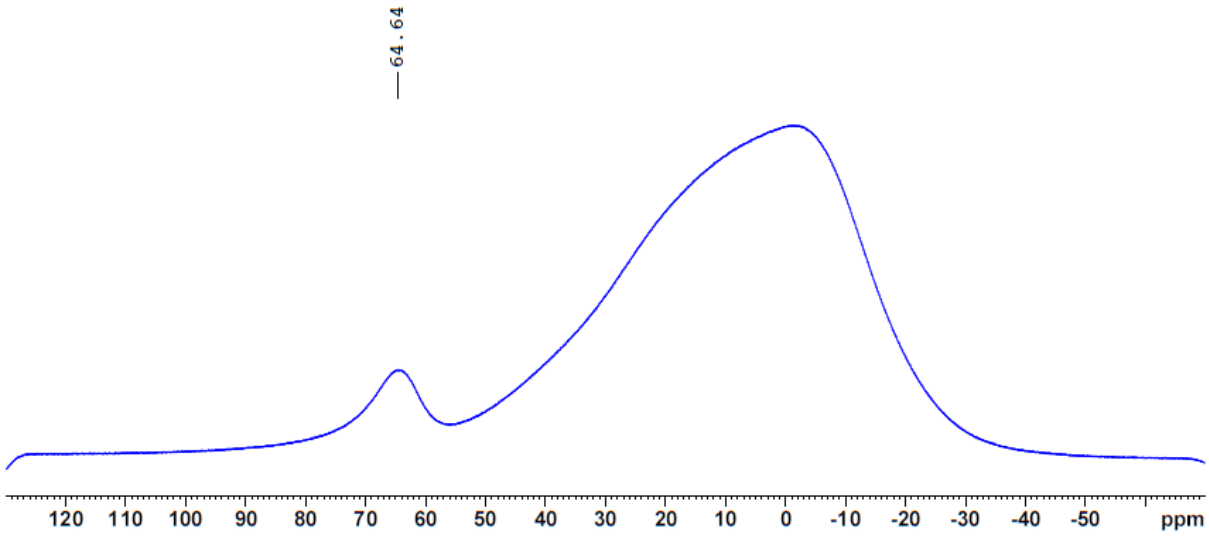
^{11}B NMR (160.5 MHz, CD_2Cl_2): δ = 0.3 ppm.

$^{13}C\{^{1}H\}$ NMR (125.8 MHz, CD_2Cl_2): δ = 148.5 ($C_{q,Ar}$), 131.2 (CH$_{Ar}$), 129.4 (CH$_{Ar}$), 127.6 (CH$_{Ar}$), 120.1 (CH$_{Ar}$), 20.7 (CH$_3$) ppm.

^{1}H NMR spectrum of 2b in CD_2Cl_2



^{11}B NMR spectrum of 2b in CD_2Cl_2



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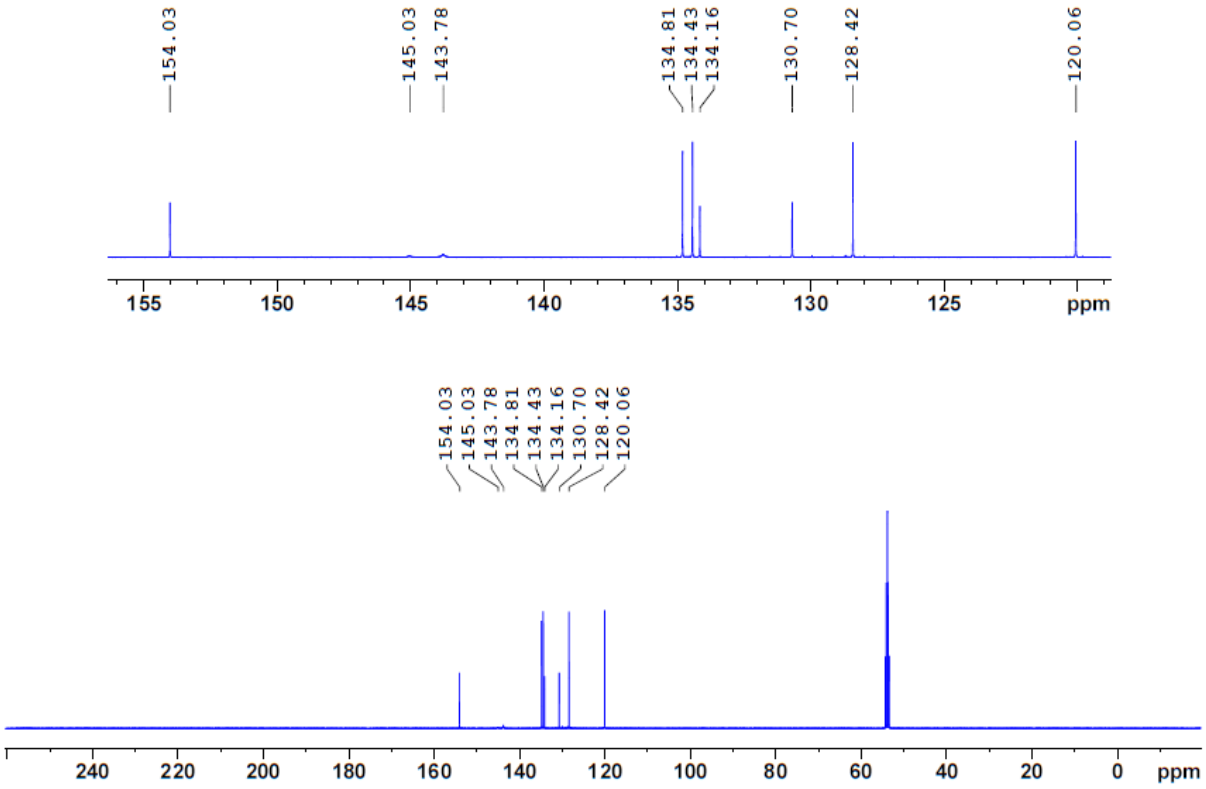

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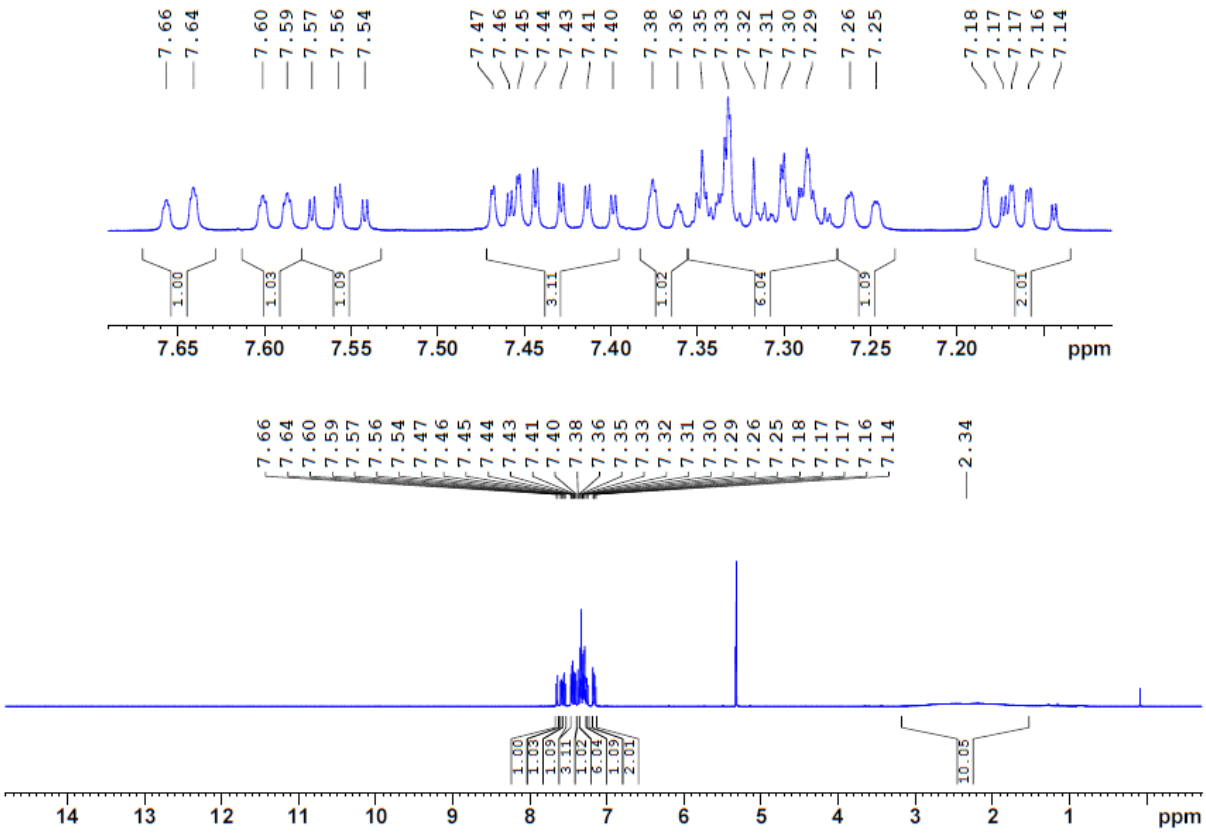
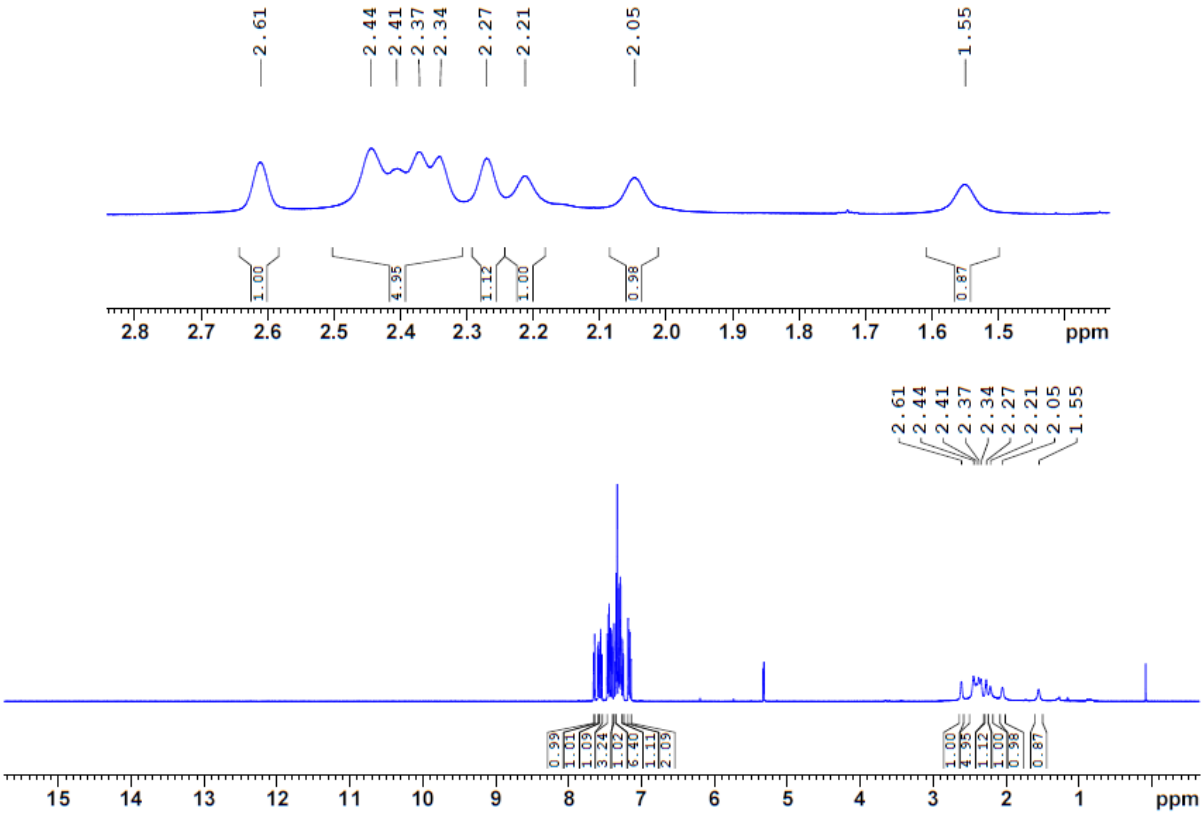
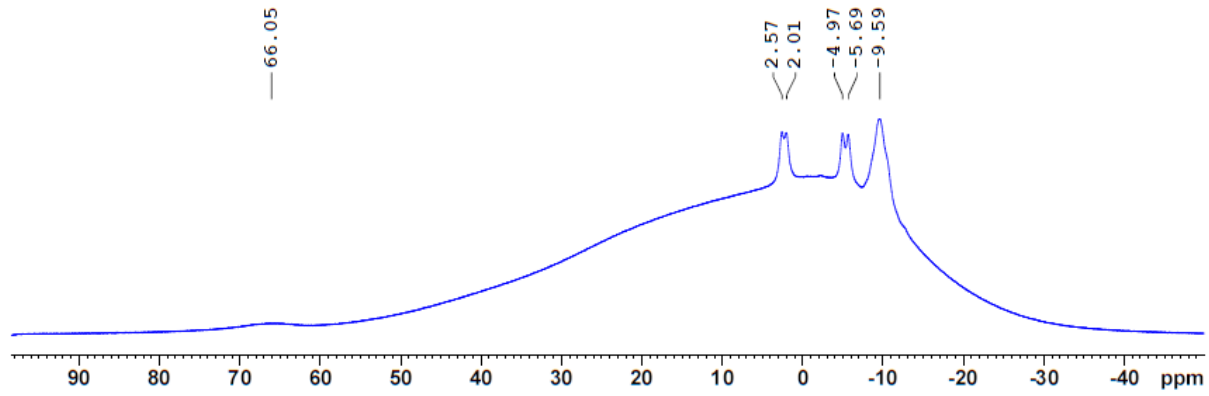


^{1}H {^{11}B} NMR spectrum of 3a in CD_2Cl_2



^{11}B NMR spectrum of 3a in CD_2Cl_2



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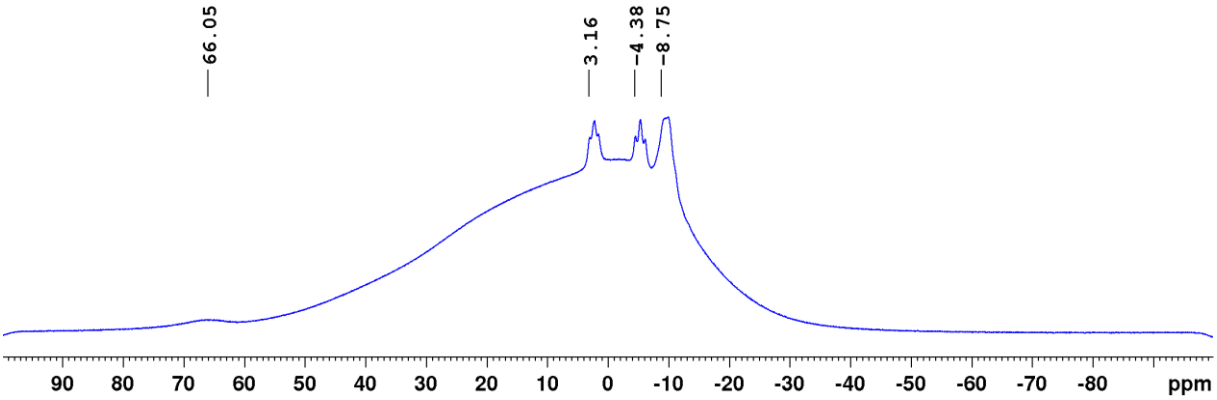
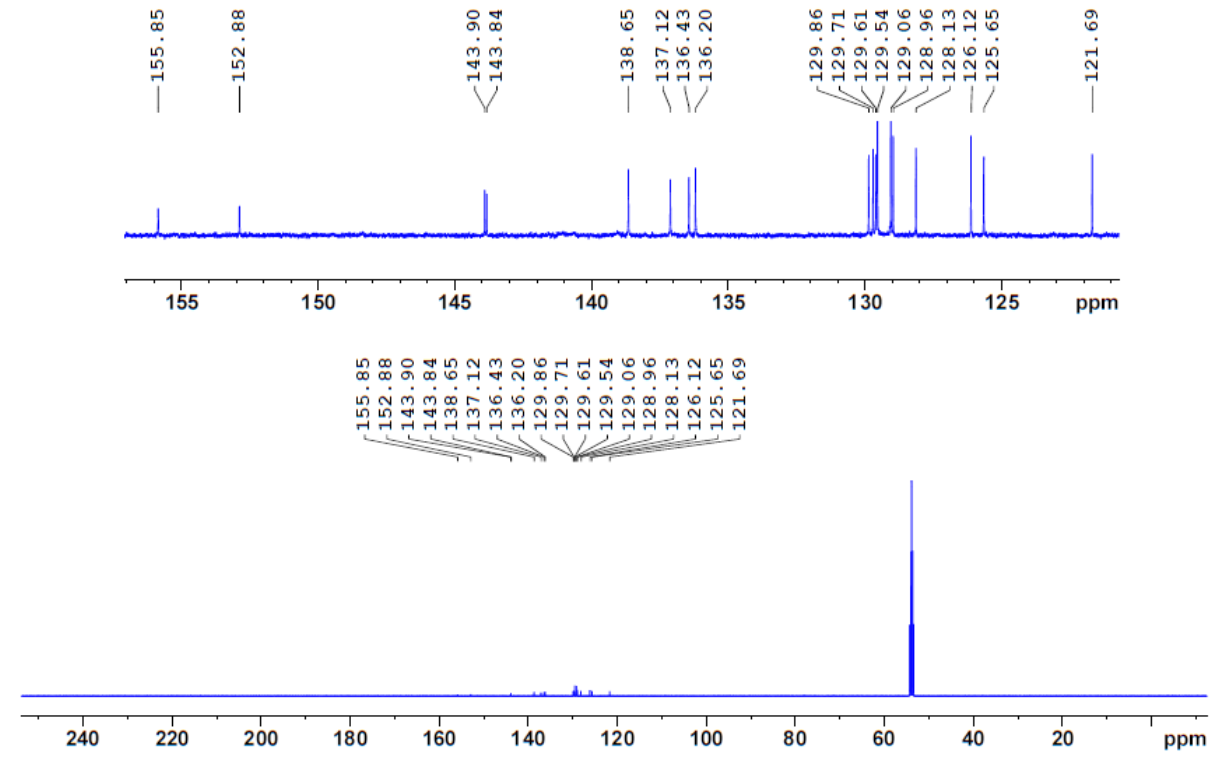
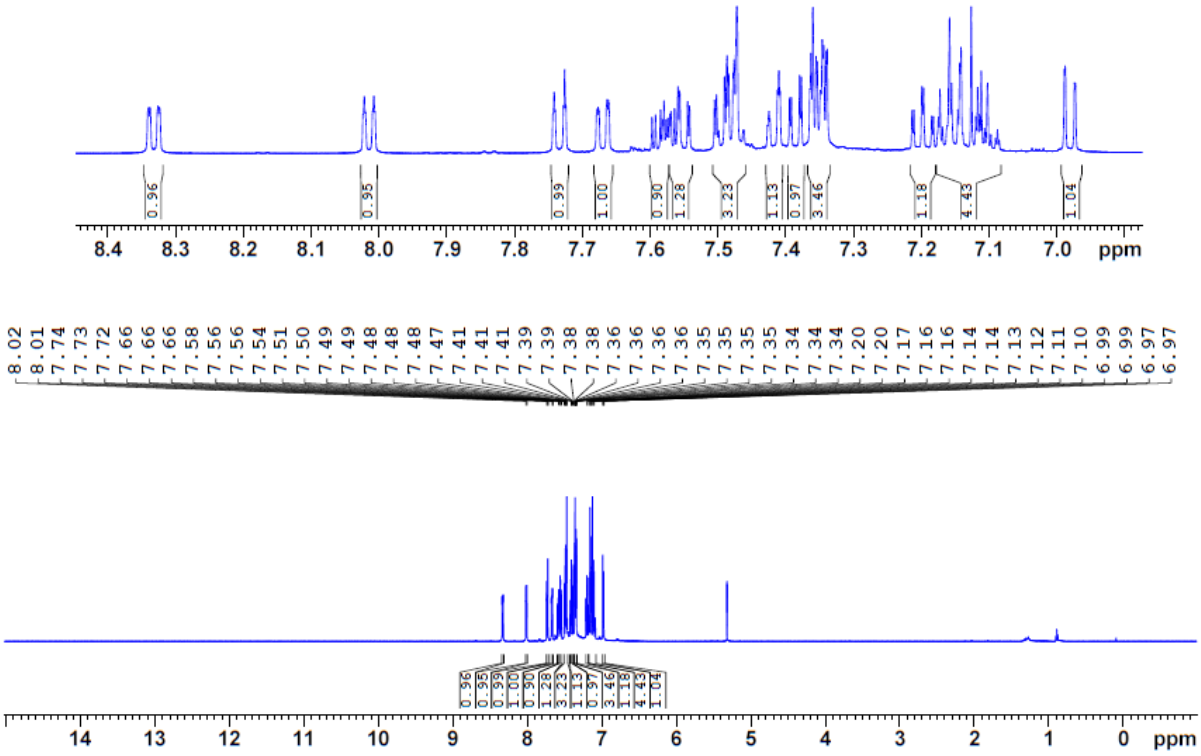


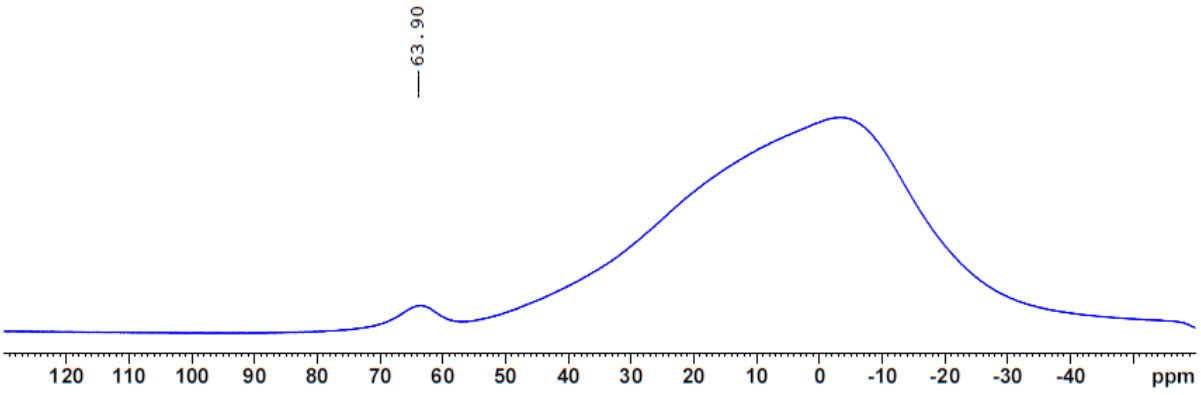
^{13}C{^{1}H} NMR spectrum of 3a in CD_2Cl_2



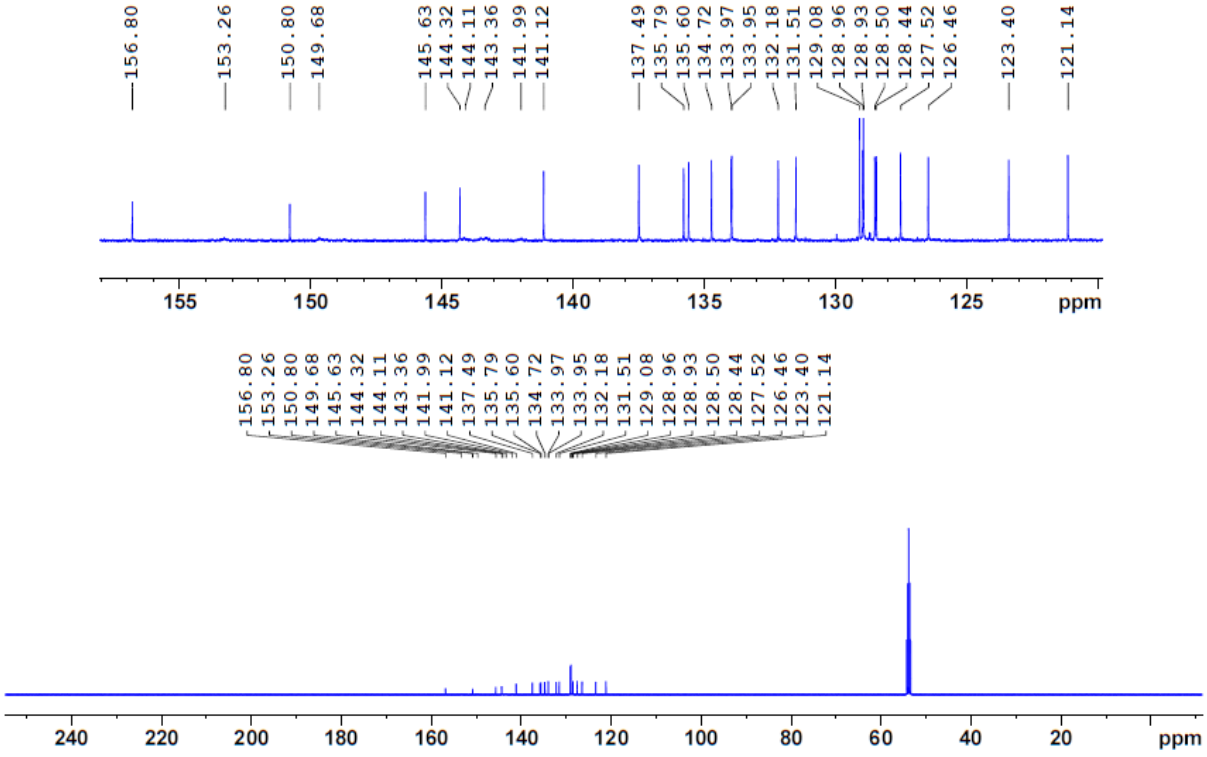
^{1}H NMR spectrum of 3b in CD_2Cl_2



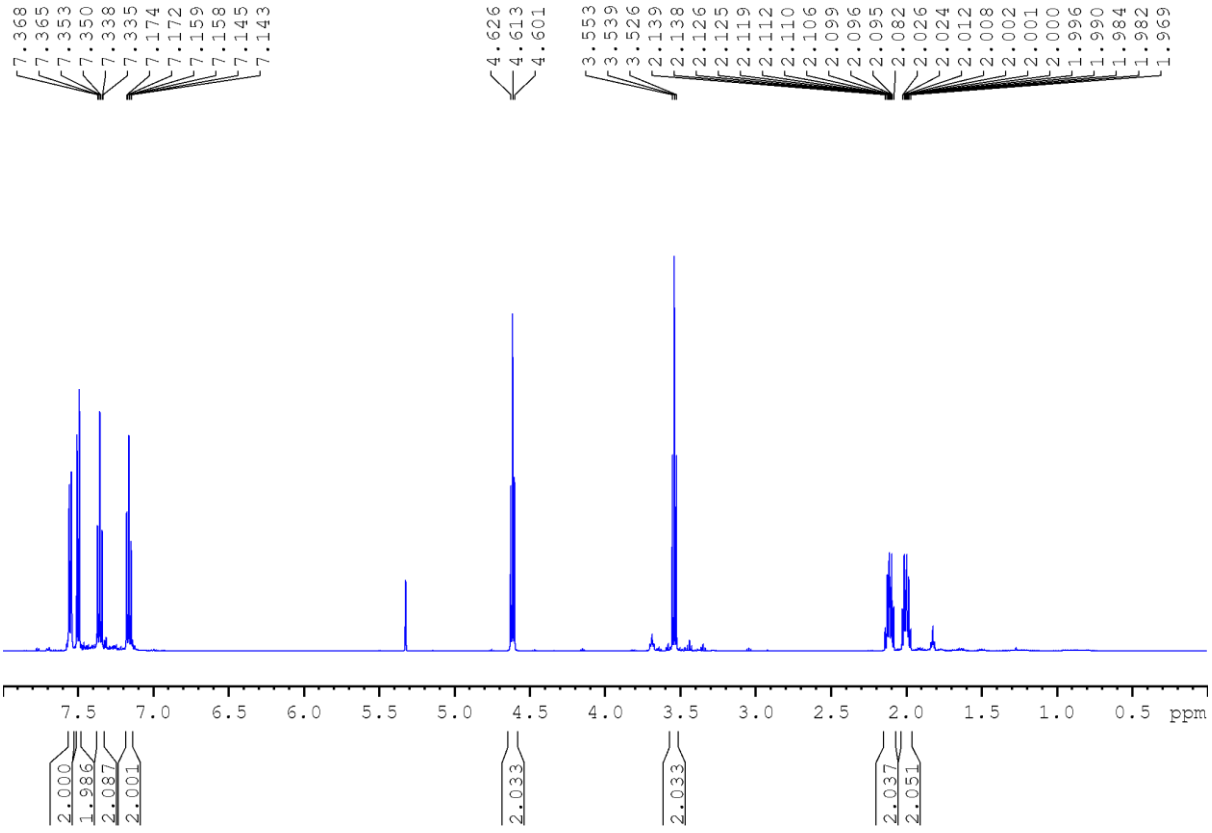
^{11}B NMR spectrum of 3b in CD_2Cl_2



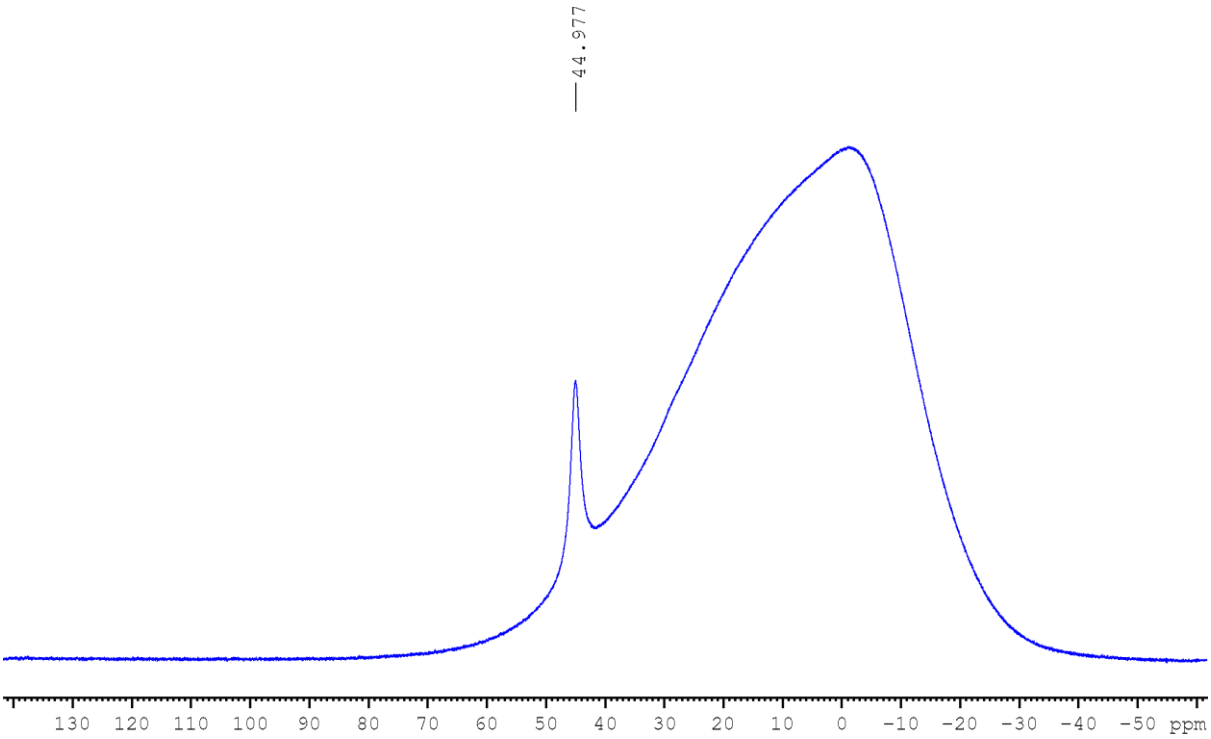
$^{13}C\{^{1}H\}$ NMR spectrum of 3b in CD_2Cl_2



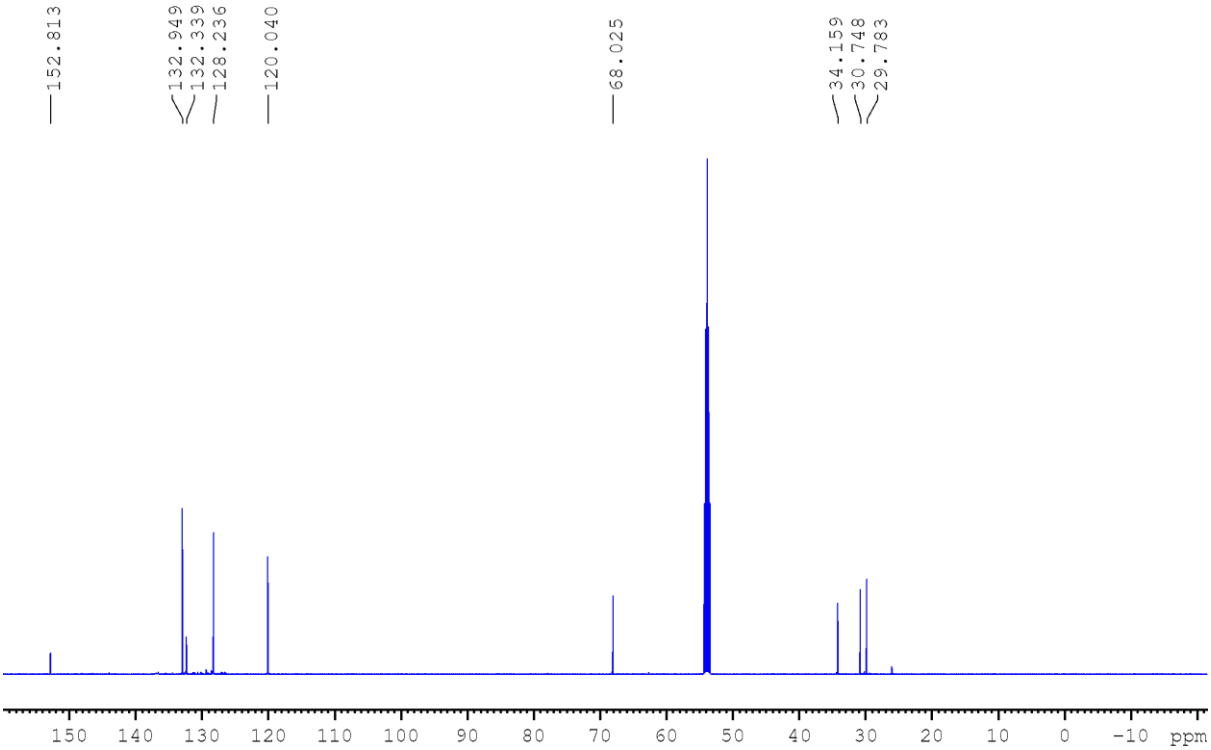
^{1}H NMR spectrum of 9-(4-bromobutoxy)-9-borafluorene in CD_2Cl_2



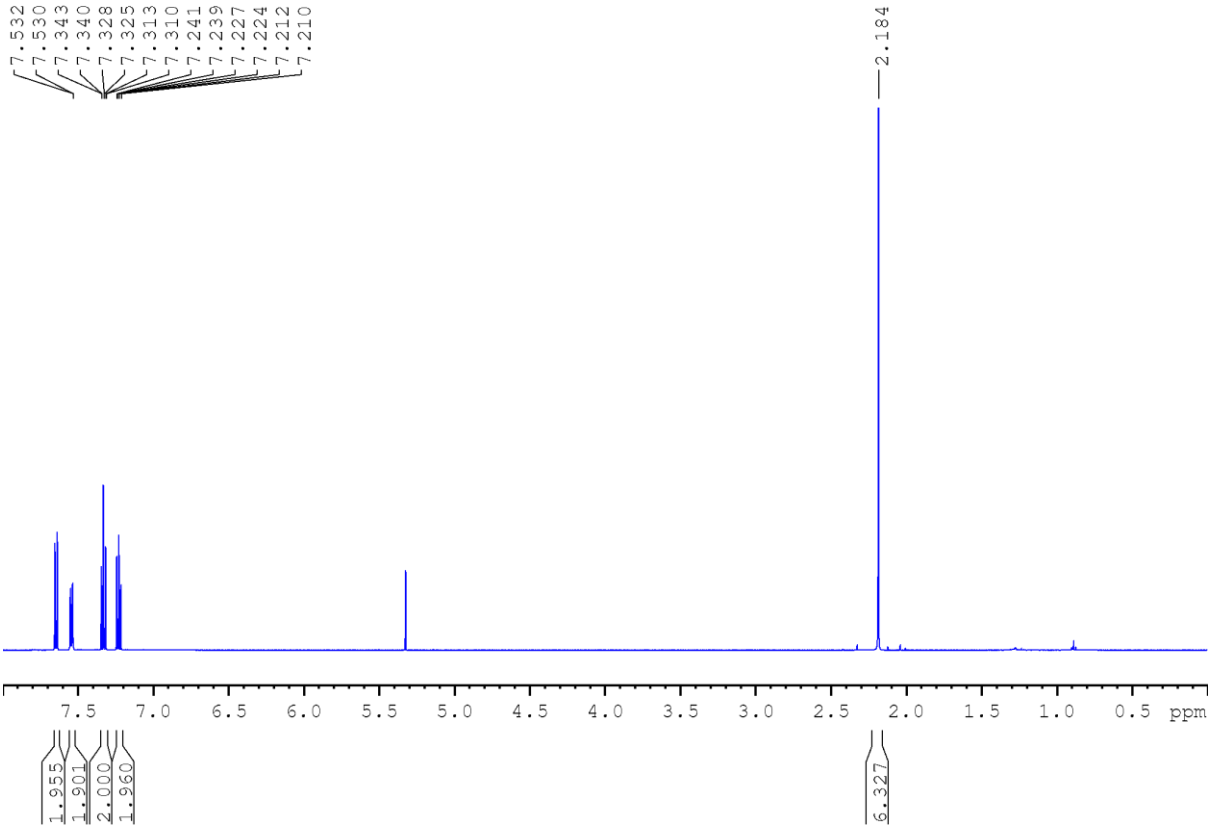
^{11}B NMR spectrum of 9-(4-bromobutoxy)-9-borafluorene in CD_2Cl_2



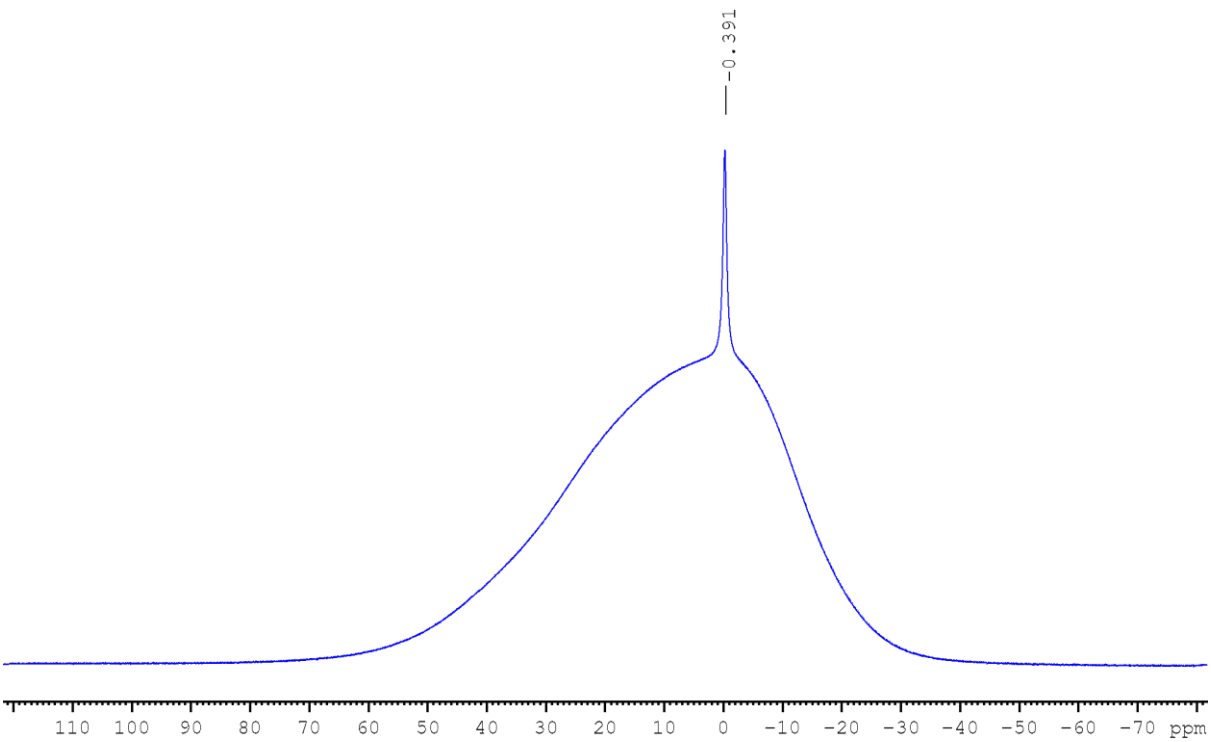
^{13}C{^{1}H} NMR spectrum of 9-(4-bromobutoxy)-9-borafluorene in CD_2Cl_2



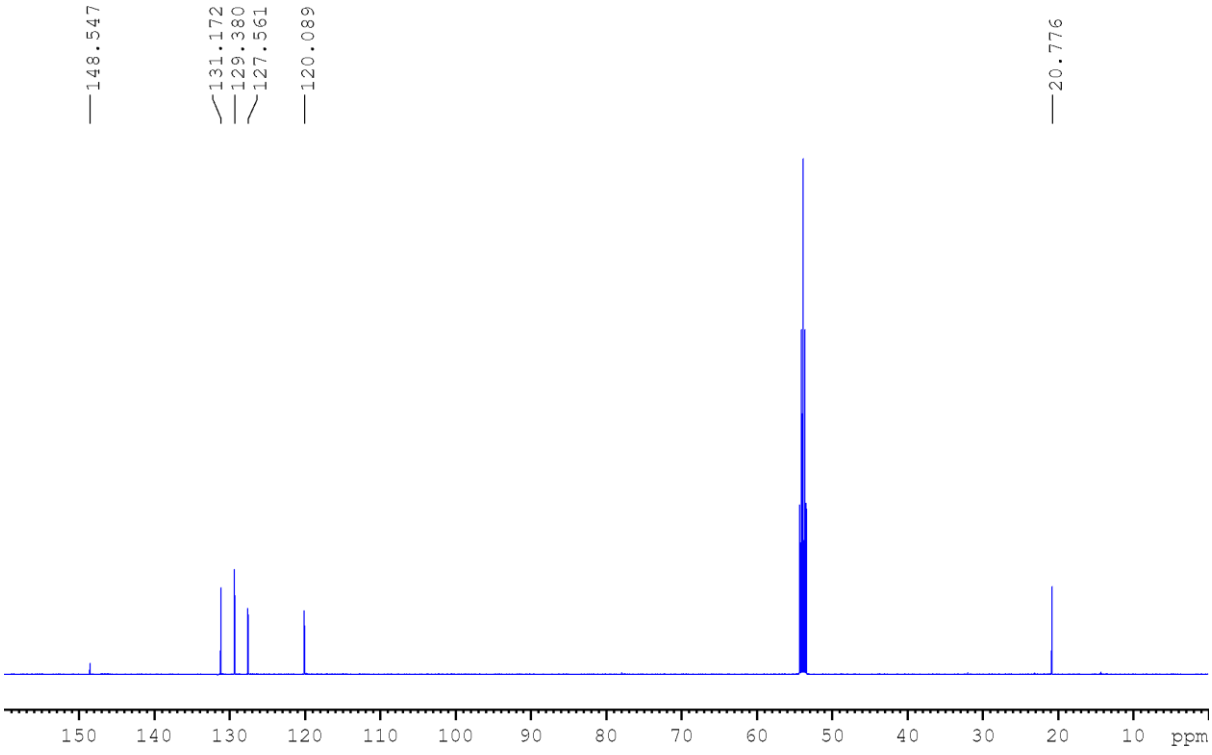
^{1}H NMR spectrum of the 9-(Me_2S)-9-Br-9-borafluorene in CD_2Cl_2



^{11}B NMR spectrum of the 9-(Me_2S)-9-Br-9-borafluorene in CD_2Cl_2



$^{13}C\{^{1}H\}$ NMR spectrum of the 9-(Me_2S)-9-Br-9-borafluorene in CD_2Cl_2



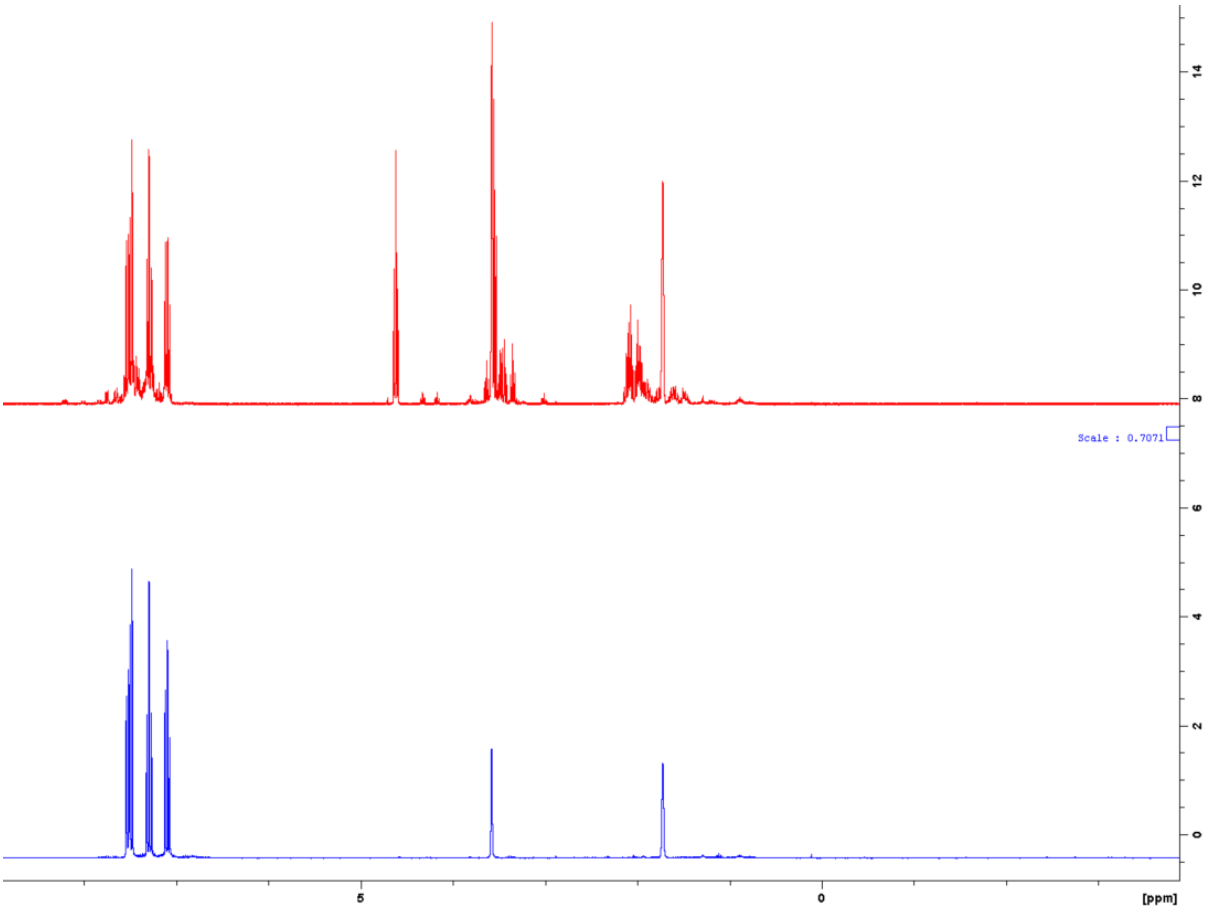
Additional reactions

A clean reaction was observed for the synthesis of **5** when the reaction was carried out in THF-d_8 as a one pot synthesis with an excess of **9-Br-9-borafluorene**, with the formation of a single new species by NMR spectroscopy (see below). As the ring-opened species arises from the deuterated THF solvent, the alkyl chain was not observed in the ^{1}H and ^{13}C NMR spectrum. Compound **5** was not detected by HRMS (LIFDI) as it is an anion.

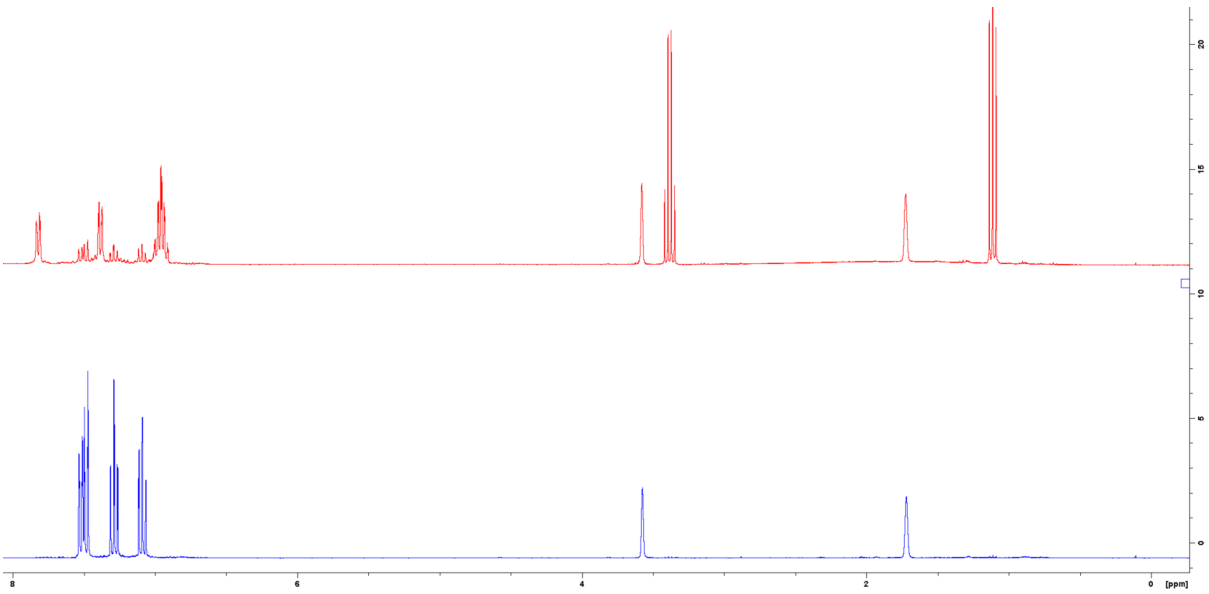
When this reaction was repeated in non-deuterated THF, removal of all volatiles *in vacuo* after the formation of 9-(4-bromobutoxy)-9-borafluorene led to the formation of some impurities. Continuing the reaction in THF-d_8 resulted in a mixture of compounds in the ^{1}H and ^{11}B NMR spectra.

The following NMR spectra show a comparison of the deuterated and non-deuterated 9-(4-bromobutoxy)-9-borafluorene and the reaction of the deuterated 9-(4-bromobutoxy)-9-borafluorene monitored by ^{1}H and ^{11}B NMR spectra.

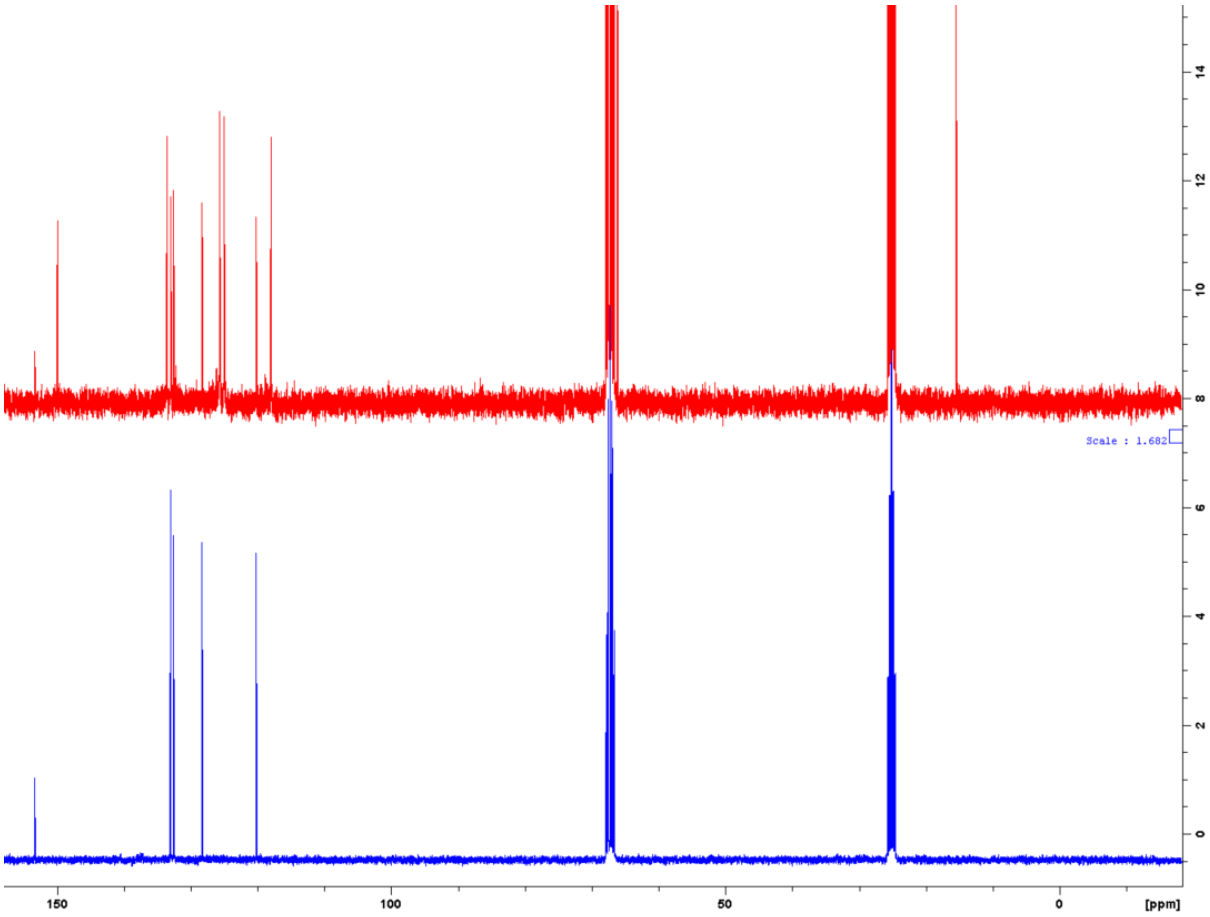
^{1}H NMR spectrum (300.2 MHz, THF-d_8): Comparison of the deuterated (blue) and non-deuterated (red) **9-(4-bromobutoxy)-9-borafluorene**.



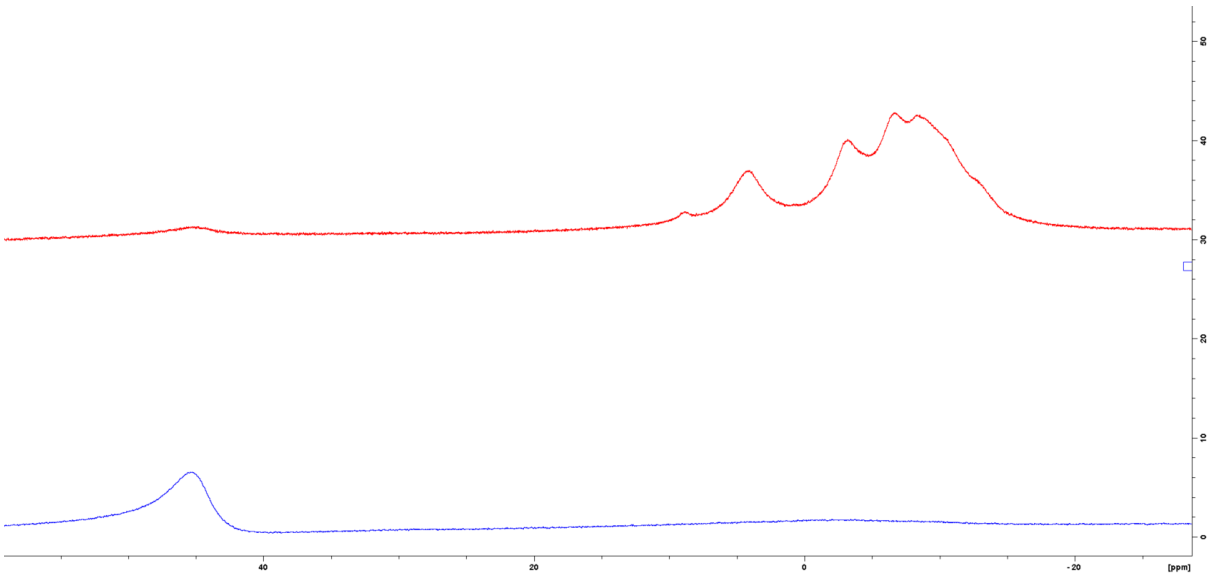
^{1}H NMR spectrum (300.2 MHz, THF-d_8): Reaction before (blue) and after (red) the addition of 1,2-Li_2-1,2-$C_2B_{10}H_{10}$·$(Et_2O)_2$.



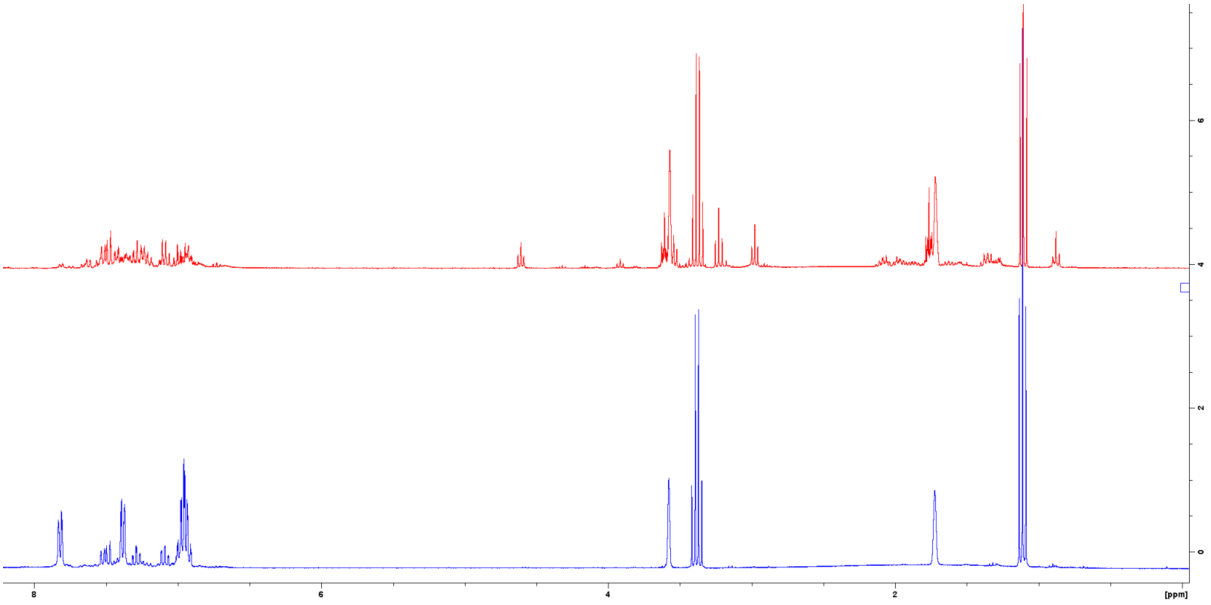
$^{13}C\{^1H\}$ NMR spectrum (75.5 MHz, THF-d_8): Reaction before (blue) and after (red) the addition of 1,2-Li_2-1,2-$C_2B_{10}H_{10}\cdot(Et_2O)_2$.



$^{11}B\{^1H\}$ NMR spectrum (96.3 MHz, THF-d_8): Reaction before (blue) and after (red) the addition of 1,2-Li_2-1,2-$C_2B_{10}H_{10}\cdot(Et_2O)_2$.

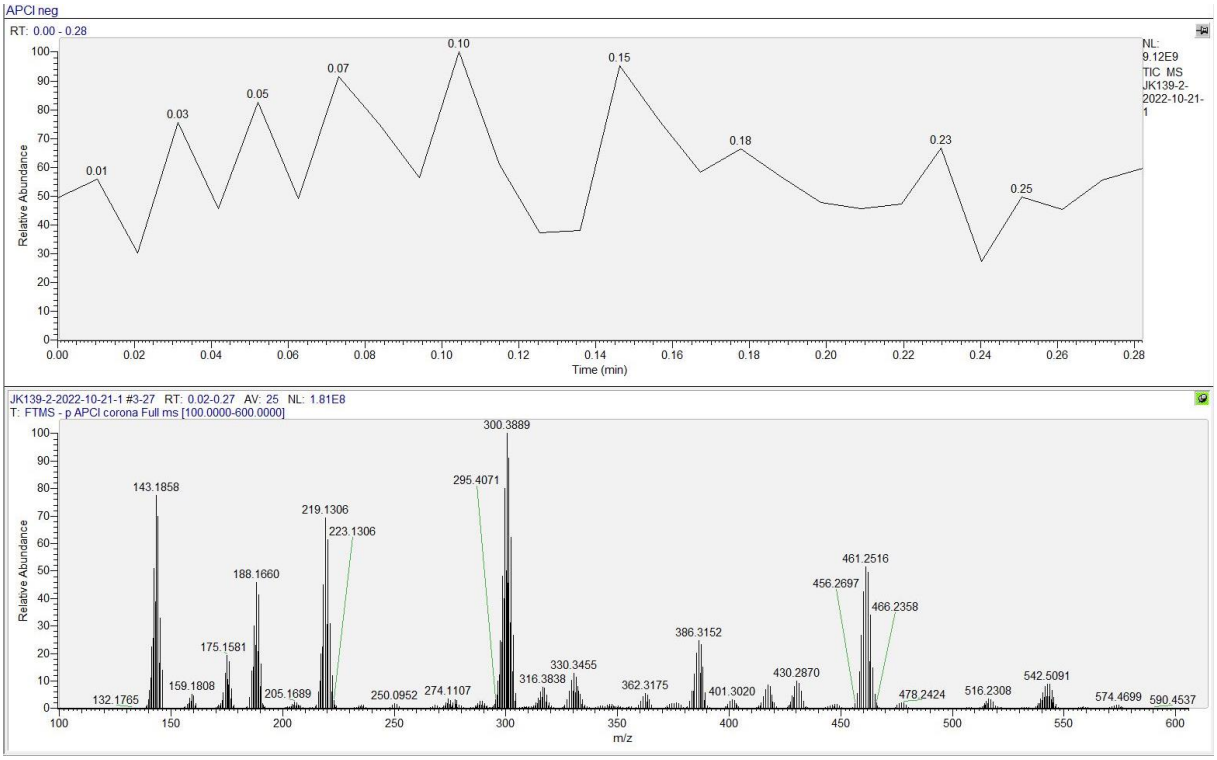


^{1}H NMR spectrum (300.2 MHz, THF-d_8): Difference between the reaction of (impure) non-deuterated **9-(4-bromobutoxy)-9-borafluorene** (red) and deuterated **9-(4-bromobutoxy)-9-borafluorene** (blue) after the addition of 1,2-Li_2-1,2-$C_2B_{10}H_{10}$·$(Et_2O)_2$.

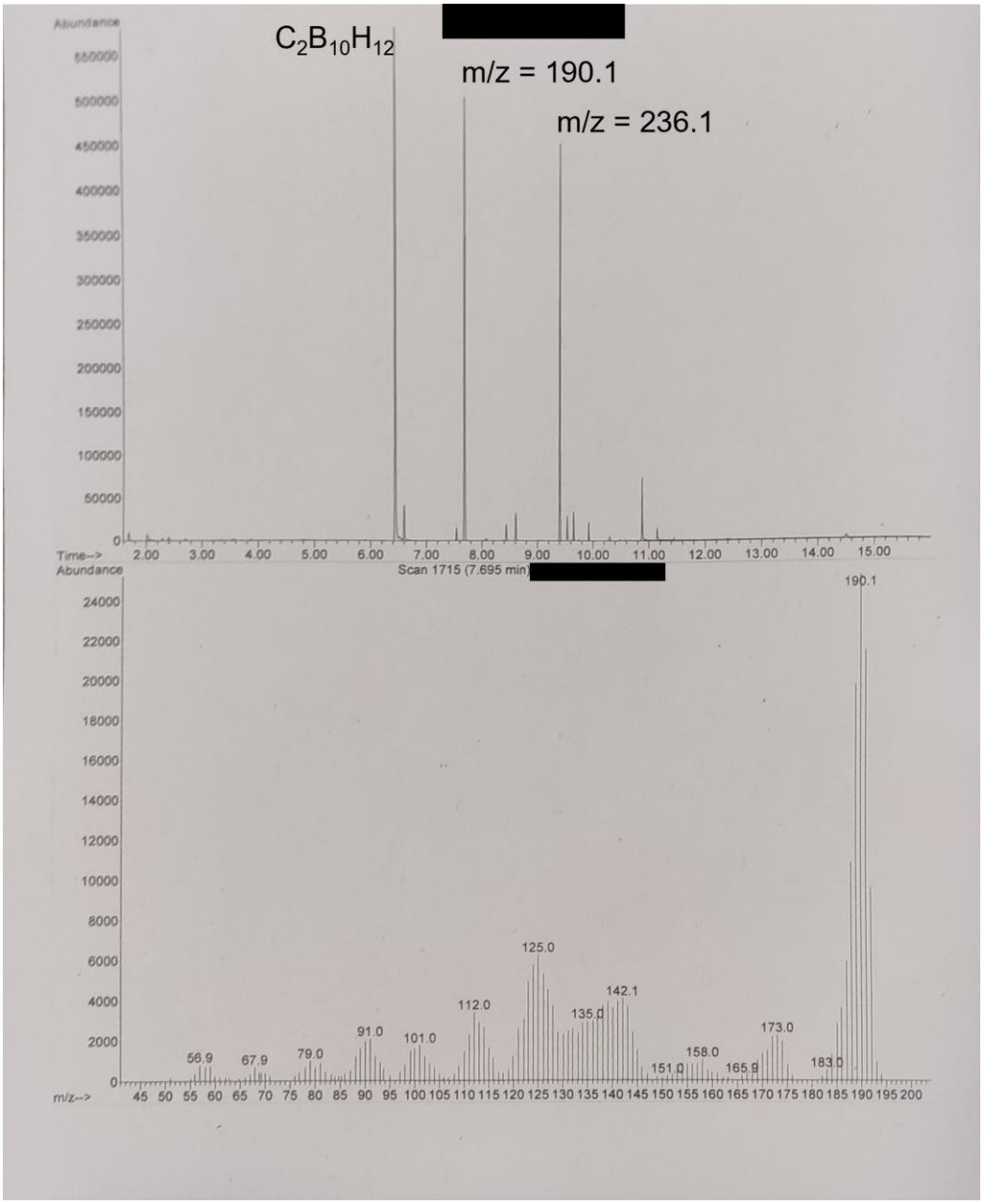


When **9-(Me_2S)-9-Br-9-borafluorene** was reacted with 1,2-Li_2-1,2-$C_2B_{10}H_{10}$·$(Et_2O)_2$ in C_6D_6, solubility was low and the reaction led to a complex mixture, as observed by NMR spectroscopy and HRMS. When the same reaction was carried out in Me_2S, reaction between the solvent and 1,2-Li_2-1,2-$C_2B_{10}H_{10}$·$(Et_2O)_2$ formed a complex mixture from which a crystal of **1-MeS-2-(Me_2S-9-borafluorene)-1,2-$C_2B_{10}H_{10}$** was isolated and characterized by single-crystal X-ray diffraction. To confirm the reaction between the solvent and dilithium salt, as similar reactions are known for *n*-butyllithium,[25] 1,2-Li_2-1,2-$C_2B_{10}H_{10}$·$(Et_2O)_2$ was dissolved in Me_2S. In this experiment **1-MeS-1,2-$C_2B_{10}H_{11}$** (calc. for $[C_3H_{14}B_{10}S]$ = [M]: 190.2, found 190.1), **1,2-($MeS)_2$-1,2-$C_2B_{10}H_{10}$** (calc. for $[C_4H_{16}B_{10}S_2]$ = [M]: 236.2, found 236.1) were visible in GCMS, and **μ-1,2-CH_2-(1,2-$C_2B_{10}H_{11}$)** (calc. for $[C_5H_{24}B_{20}]^-$ = $[M]^-$: 300.3884, found 300.3889), as well as compounds of higher mass were visible in the HRMS.

HRMS (APCI neg) of the reaction of Me_2S with 1,2-Li_2-1,2-$C_2B_{10}H_{10}(Et_2O)_2$



GCMS of the reaction of Me_2S with 1,2-Li_2-1,2-$C_2B_{10}H_{10}(Et_2O)_2$



Single-crystal X-ray diffraction

Table S1. Single-crystal X-ray diffraction data and structure refinements of **2b**, **3a**, **3b**, **3a·THF**, **5**, **9-(Me$_2$S)-9-Br-9-borafluorene**, **1-MeS-2-(Me$_2$S-9-borafluorene)-1,2-C$_2$B$_{10}$H$_{10}$**, and **9-(4-bromobutoxy)-9-borafluorene**.

	2b	**3a**	**3b**	**3a·THF**
CCDC	2174245	2174247	2174246	2174248
Empirical formula	$C_{30}H_{20}B_2$	$C_{26}H_{26}B_{12}$	$C_{30}H_{20}B_2$ [+solvent]	2(C_{30} H_{34} B_{12} O), C_7 H_8
ρ_{calc}/g·cm^{-3}	1.260	1.213	1.065	1.207
F(000)	840	968	1680	614
Crystal size/mm^3	0.22×0.20×0.16	0.68×0.32×0.27	0.15×0.04×0.02	0.31×0.18×0.13
Crystal colour, habit	yellow block	orange block	orange block	colourless block
μ/mm^{-1}	0.070	0.062	0.445	0.476
M_r/g·mol^{-1}	402.08	468.19	402.08	1172.71
Temperature/K	100(2)	100(2)	100(2)	100(2)
Radiation, λ/Å	MoK$_\alpha$, 0.71073	MoK$_\alpha$, 0.71073	CuK$_\alpha$, 1.54184	CuK$_\alpha$, 1.54184
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1$	$P\bar{1}$
a/Å	10.040(3)	11.6705(5)	9.81472(6)	10.0646(3)
b/Å	14.612(6)	11.4351(5)	30.3107(2)	11.5240(4)
c/Å	14.451(4)	19.4944(8)	16.86116(12)	15.6916(5)
α/°	90	90	90	105.086(3)
β/°	90.177(9)	99.7240(10)	90.0056(6)	98.763(3)
γ/°	90	90	90	108.320(3)
Volume/Å^3	2120.0(12)	2564.21(19)	5016.04(6)	1612.85(9)
Z	4	4	8	4
2Θ/°	3.96–53.46	3.54–52.08	5.24–150.63	6.03–153.86
Reflections collected	40200	32404	255080	32353
Unique reflections	4510	5057	20250	12402
Parameters / restraints	289/0	383/0	1154/1	463/122
GooF on F^2	1.076	1.032	1.039	1.046
R_1 [I>=2σ (I)]	0.0443	0.0432	0.0575	0.0654
wR_2 [all data]	0.1072	0.1134	0.1629	0.1955
Max./min. res. electron density/ e Å^{-3}	0.33 / –0.26	0.30 / –0.26	0.39 / –0.28	0.30 / –0.35

Table S1. Continued.

	5	**9-(Me_2S)-9-Br-9-borafluorene**	**1-MeS-2-(Me_2S-9-borafluorene)-1,2-$C_2B_{10}H_{10}$**	**9-(4-bromobutoxy)-9-borafluorene**
CCDC	2174249	2216647	2216648	2216649
Empirical formula	$C_{38}H_{50}B_{12}Br_2LiO_3$, $C_{16}H_{32}LiO_4$	$C_{14}H_{14}BBrS$	$C_{17}H_{27}B_{11}S_2$	$C_{16}H_{16}BBrO$
ρ_{calc}/g·cm^{-3}	1.132	1.525	1.256	1.513
F(000)	2392	616	864	640
Crystal size/mm^3	0.24×0.13×0.12	0.28×0.20×0.16	0.34×0.04×0.02	0.21×0.03×0.03
Crystal colour, habit	yellow block	colourless block	colourless needle	colourless needle
μ/mm^{-1}	2.082	5.445	2.180	3.933
M_r/g·mol^{-1}	1146.60	305.03	414.41	315.01
Temperature/K	173.01(10)	100(2)	100(2)	100(2)
Radiation, λ/Å	CuK$_\alpha$, 1.54184	CuK$_\alpha$, 1.54184	CuK$_\alpha$, 1.54184	CuK$_\alpha$, 1.54184
Crystal system	orthorhombic	monoclinic	monoclinic	monoclinic
Space group	$P2_12_12_1$	$P2_1$/n	$P2_1$/c	$P2_1/c$
a/Å	10.14540(10)	11.8821(4)	13.0013(3)	16.3598(3)
b/Å	15.55010(10)	6.7210(2)	19.0378(4)	5.11900(10)
c/Å	37.9243(2)	17.0968(5)	8.8640(2)	16.5080(3)
α/°	90	90	90	90
β/°	90	103.399(3)	93.062(2)	90.050(2)
γ/°	90	90	90	90
Volume/Å^3	5983.02(8)	1328.18(7)	2190.85(9)	1382.48(4)
Z	4	4	4	4
2Θ/°	4.66–151.03	4.12–75.19	3.40–74.50	2.70–74.94
Reflections collected	131709	11292	35742	8247
Unique reflections	12305	2694	8080	2619
Parameters / restraints	919 / 624	156 / 0	275 / 0	172 / 0
GooF on F^2	1.020	1.083	1.089	1.084
R_1 [I>=2σ (I)]	0.0519	0.0268	0.0574	0.0633
wR_2 [all data]	0.1512	0.0718	0.1634	0.0643
Max./min. res. electron density/ e Å^{-3}	0.65 / –0.60	0.75 / –0.66	0.93 / –0.60	0.36 / –0.28

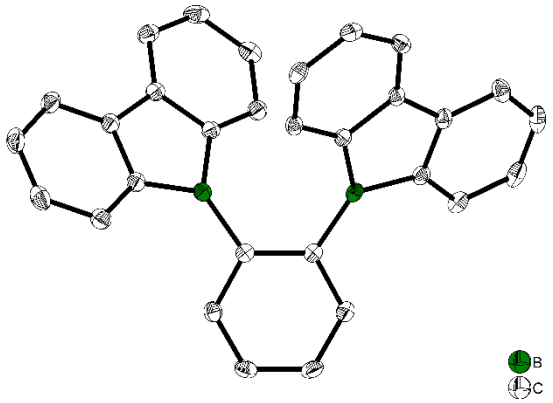


Figure S1. Solid state molecular structure of **2b** from single-crystal X-ray diffraction at 100 K. Atomic displacement ellipsoids are drawn at the 50% probability level and hydrogen atoms are omitted for clarity.

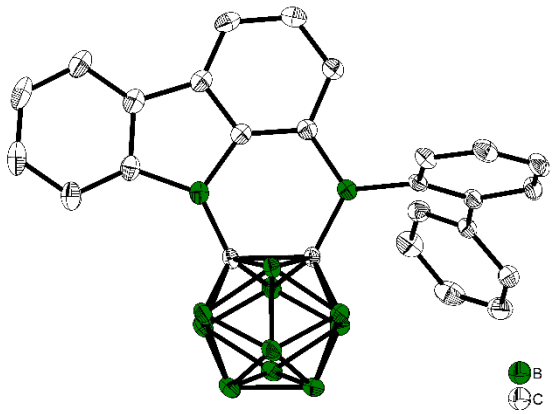


Figure S2. Solid state molecular structure of **3a** from single-crystal X-ray diffraction at 100 K. Atomic displacement ellipsoids are drawn at the 50% probability level and hydrogen atoms are omitted for clarity.

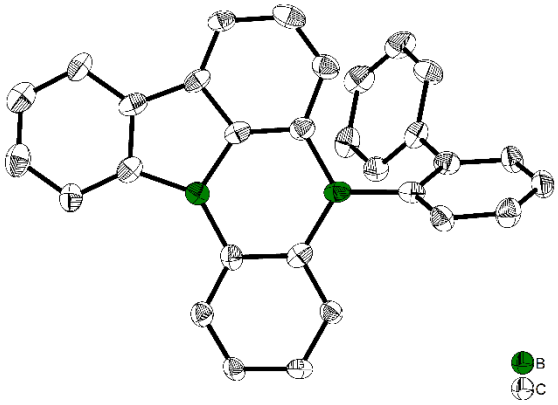


Figure S3. Solid state molecular structure of **3b** from single-crystal X-ray diffraction at 100 K. Atomic displacement ellipsoids are drawn at the 50% probability level and hydrogen atoms and solvent molecules are omitted for clarity. Only one of four symmetry-independent molecules is shown.

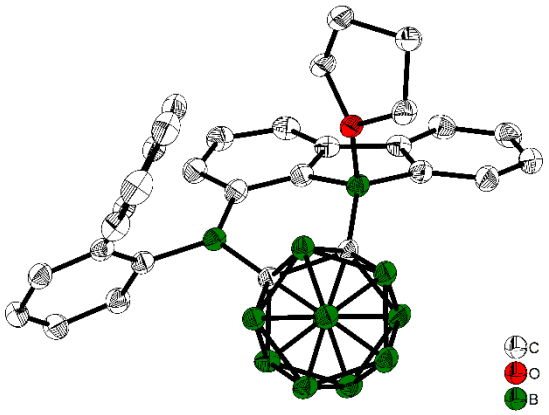


Figure S4. Solid state molecular structure of **3a·THF** from single-crystal X-ray diffraction at 100 K. Atomic displacement ellipsoids are drawn at the 50% probability level and solvent molecules and hydrogen atoms are omitted for clarity.

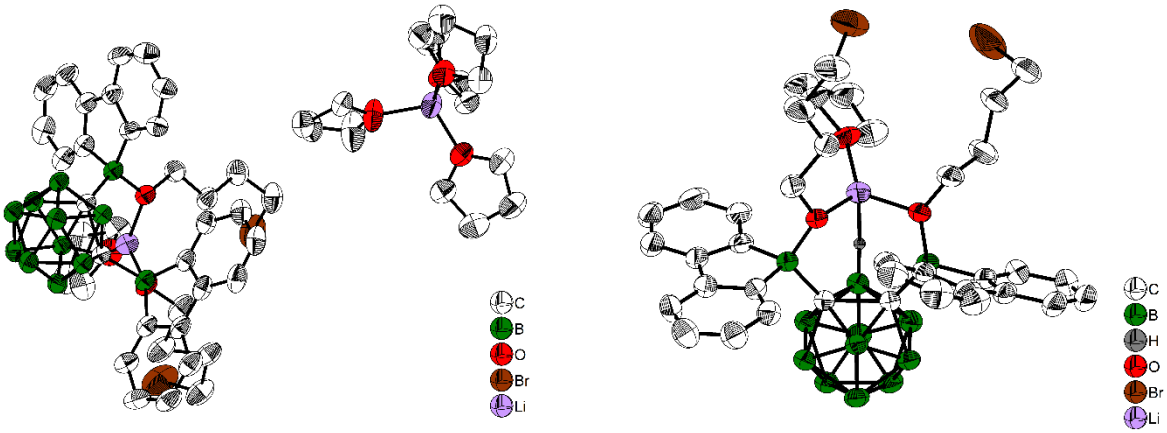


Figure S5. Solid state molecular structure of **5** from single-crystal X-ray diffraction at 100 K, on the left with the lithium counterion and on the right from a different angle. Atomic displacement ellipsoids are drawn at the 50% probability level, and hydrogen atoms and the minor occupied components of disordered THF and alkyl groups are omitted for clarity. Only one of two symmetry-independent anions and cations are shown.

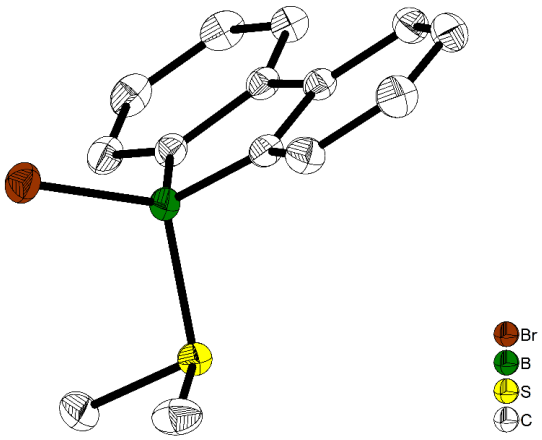


Figure S6. Solid state molecular structure of the dimethyl sulfide adduct of 9-Br-9-borafluorene, **9-(Me$_2$S)-9-Br-9-borafluorene**, from single-crystal X-ray diffraction at 100 K. Atomic displacement ellipsoids are drawn at the 50% probability level and hydrogen atoms are omitted for clarity.

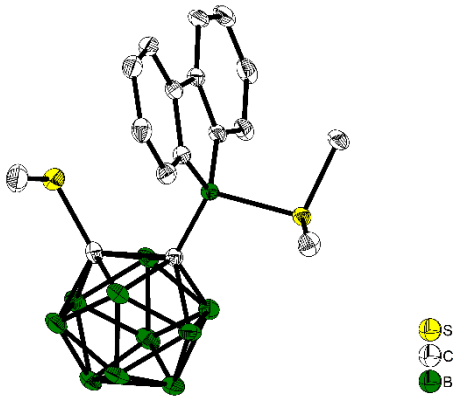


Figure S7. Solid state molecular structure of an isolated product **1-MeS-2-(Me_2S-9-borafluorene)-1,2-$C_2B_{10}H_{10}$** from the reaction in SMe_2 described above from single-crystal X-ray diffraction at 100 K. Atomic displacement ellipsoids are drawn at the 50% probability level and hydrogen atoms are omitted for clarity.

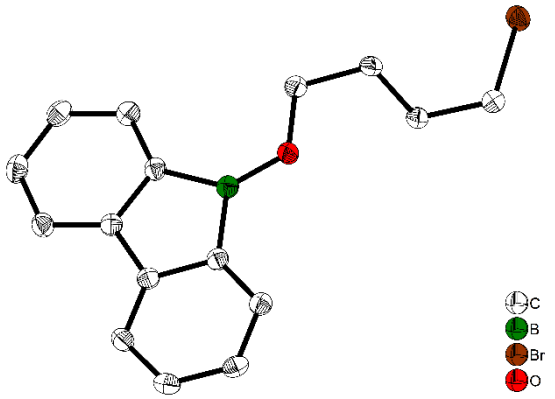
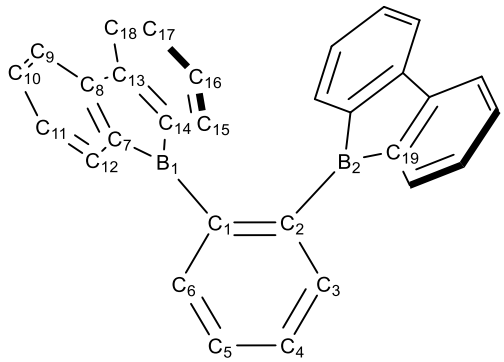


Figure S8. Solid state molecular structure of **9-(4-bromobutoxy)-9-borafluorene** from single-crystal X-ray diffraction at 100 K. Atomic displacement ellipsoids are drawn at the 50% probability level and hydrogen atoms are omitted for clarity.

Geometry tables



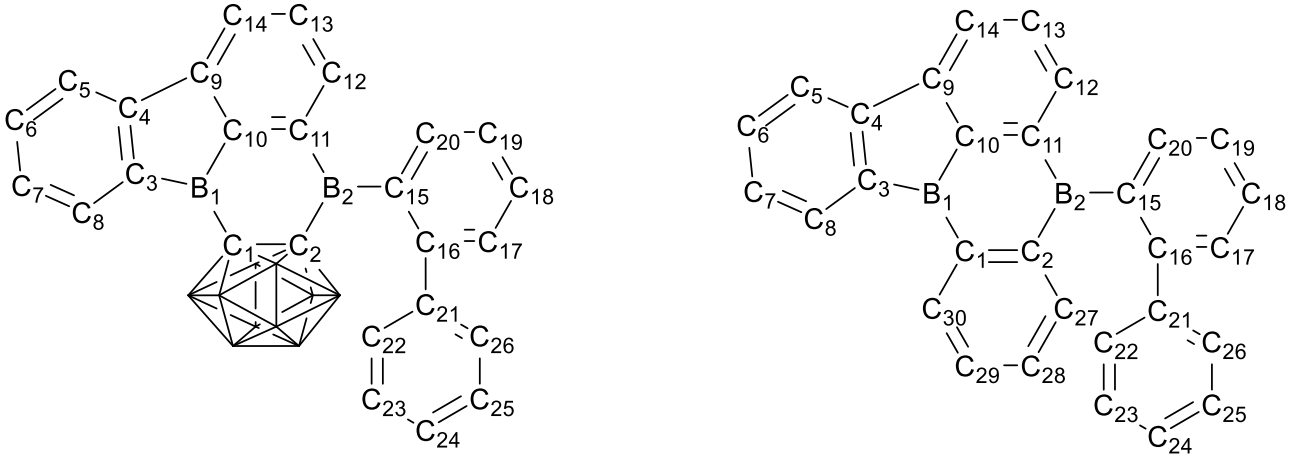
Scheme S1. Atom labeling in compound **2b**.

Table S2. Selected bond lengths [Å], distances [Å], and angles [°] in the crystal and calculated at the B3LYP-d3bj and ωB97X-D level of theory (starting molecule).

	2a calc. B3LYP-d3bj	**2a** calc. ωB97X-D	**2b** crystal	**2b** calc. B3LYP-d3bj	**2b** calc. ωB97X-D
C_1–C_2	1.674	1.674	1.426(2)	1.426	1.420
C_1–C_6 / C_2–C_3	–	–	1.402(2) / 1.405(2)	1.404	1.402
C_5–C_6 / C_3–C_4	–	–	1.388(2) / 1.389(2)	1.396	1.393
C_4–C_5	–	–	1.386(2)	1.395	1.393
B_1–C_1[a]	1.591	1.600	1.554(2) / 1.551(2)	1.550	1.556
B_1–C_{14}[a]	1.566	1.570	1.571(2) / 1.571(2)	1.564	1.568
B_1–C_7[a]	1.562	1.566	1.568(2) / 1.571(2)	1.565	1.570
B_1–B_2	3.025	3.054	3.186(2)	3.005	3.083
B_2–C_{15}[a]	3.428	3.487	3.252(2) / 3.354(2)	3.153	3.231
C_{14}–C_{13}[a]	1.426	1.418	1.417(2) / 1.415(2)	1.421	1.414
C_7–C_8[a]	1.421	1.413	1.416(2) / 1.419(2)	1.422	1.413
C_8–C_{13}[a]	1.480	1.483	1.487(2) / 1.489(2)	1.485	1.489
C_1–B_1–C_{14}[a]	129.0	128.8	128.1(1) / 128.5(1)	126.7	127.9
C_{14}–B_1–C_7[a]	105.1	105.0	103.9(1) / 103.7(1)	104.2	103.9
C_7–B_1–C_1[a]	125.1	125.1	127.5(1) / 127.5(1)	128.9	128.2
ΣC–B_1–C[a]	359.2	358.9	359.5(3) / 359.8(3)	359.8	359.8
C_2–C_1–B_1, C_1–C_2–B_2	115.0	115.6	124.9(1) / 123.6(1)	120.4	122.1
B_1–C_1–C_2–B_2	5.8	6.3	13.2(2)	8.5	9.4

C_2–C_1–B_1–C_{14}[a]	58.8	59.5	43.6(2) / 39.2(2)	43.3	43.5
C_{15}–C_{14}–B_1–C_1[a]	11.2	12.8	4.7(2) / 2.7(2)	8.1	2.6

[a] Values are given for both borafluorene moieties of B1 and B2, respectively, for the crystal of **2b**.



Scheme S2. Atom labeling in compounds **3a** and **3b**.

Table S3. Selected bond lengths [Å], distances [Å], and angles [°] in the crystals and calculated structures of **3a** and **3b** at the B3LYP-d3bj and ωB97X-D level of theory.

	3a crystal	**3a** B3LYP-d3bj	**3a** ωB97X-D	**3b** crystal[a]	**3b** B3LYP-d3bj	**3b** ωB97X-D	**3a·THF** crystal
C_1–C_2	1.718(2)	1.712	1.693	1.460(8), 1.409(7), 1.425(7), 1.425(7)	1.435	1.429	1.717(2)
C_2–C_{27}	–	–	–	1.399(7), 1.401(7), 1.423(7), 1.402(7)	1.402	1.399	–
C_{27}–C_{28}	–	–	–	1.393(7), 1.389(8), 1.380(8), 1.396(7)	1.397	1.394	–
C_{28}–C_{29}	–	–	–	1.403(7), 1.360(9), 1.403(9), 1.390(8)	1.394	1.390	–
C_{29}–C_{30}	–	–	–	1.364(8), 1.402(9), 1.417(8), 1.376(8)	1.396	1.393	–
C_{30}–C_1	–	–	–	1.379(7), 1.407(8), 1.384(8), 1.391(8)	1.403	1.398	–
B_1–C_1	1.551(2)	1.549	1.555	1.555(8), 1.548(8), 1.565(8), 1.554(8)	1.541	1.547	1.624(3)
B_1–C_3	1.546(2)	1.549	1.551	1.545(9), 1.591(9),	1.570	1.574	1.622(2)

				1.553(9), 1.604(9)			
B_1–C_{10}	1.538(2)	1.541	1.544	1.567(9), 1.554(9), 1.561(9), 1.533(9)	1.549	1.553	1.595(3)
B_2–C_2	1.607(2)	1.599	1.604	1.587(9), 1.597(8), 1.570(8), 1.573(8)	1.583	1.588	1.603(3)
B_2–C_{11}	1.557(2)	1.557	1.562	1.558(8), 1.577(8), 1.557(8), 1.564(8)	1.563	1.567	1.541(2)
B_2–C_{15}	1.572(2)	1.562	1.568	1.593(8), 1.577(8), 1.556(9), 1.604(8)	1.567	1.574	1.572(2)
C_3–C_4	1.424(2)	1.430	1.422	1.401(9), 1.431(9), 1.457(9), 1.423(8)	1.432	1.424	1.419(3)
C_9–C_{10}	1.406(2)	1.410	1.403	1.415(9), 1.421(9), 1.414(8), 1.396(8)	1.405	1.399	1.399(2)
C_4–C_9	1.492(2)	1.492	1.495	1.470(10), 1.450(10), 1.440(10), 1.545(8)	1.491	1.493	1.485(2)
B_1–C_1–C_2	114.4(1)	114.2	114.3	116.6(5), 117.9(5), 117.5(4), 116.9(5)	117.3	117.2	114.0(1)
B_2–C_2–C_1	118.5(1)	118.5	118.8	122.3(5), 122.9(4), 124.0(5), 122.3(5)	122.7	122.7	119.6(1)
C_1–B_1–C_{10} / C_{10}–B_1–C_3 / C_3–B_1–C_1	119.5(1) / 105.5(1) / 135.0(1)	120.0 / 105.2 / 134.8	119.9 / 105.1 / 134.9	118.4(5) / 104.0(5) / 137.6(5), 117.5(5) / 103.8(5) / 138.7(5), 116.9(5) / 102.4(5) / 140.6(5), 118.8(5) / 103.7(5) / 137.5(5)	118.5 / 103.5 / 138.0	118.5 / 103.3 / 138.2	112.1(1) / 100.0(1) / 123.9(1)
ΣC–B_1–C	360.0	360.0	359.9	360.0	360.0	360.0	336.0
C_2–B_2–C_{15} / C_{15}–B_2–C_{11} / C_{15}–B_2–C_2	119.6(1) / 120.0(1) / 119.2(1)	120.1 / 119.6 / 119.7	119.9 / 119.9 / 119.6	120.6(5) / 119.3(5) / 120.1(5), 117.8(5) / 120.9(5) / 121.3(5), 119.1(5) / 119.2(5) / 121.7(5),	120.9 / 119.9 / 119.2	120.9 / 119.8 / 119.2	118.3(1) / 122.2(2) / 118.1(1)

				120.2(5) / 119.5(5) / 120.3(5)			
ΣC–B_2–C	358.8	359.4	359.4	360.0	360.0	359.9	358.6
B_1–C_1–C_2–B_2	2.6(2)	5.5	3.6	3.3(8), 3.3(7), 1.9(7), 3.4(7)	2.2	2.7	0.9(2)
C_2–B_2–C_{15}–C_{16}	82.4(1)	76.2	79.4	58.2(6), 60.2(6), 60.7(6), 58.2(6)	61.1	63.3	78.6(2)
C_2–C_1–B_1–C_3	176.1(1)	176.6	177.9	175.4(6), 176.7(6), 176.0(7), 176.1(6)	179.4	179.5	142.5(2)
C_1–C_2–B_2–C_{15}	159.7(2)	166.3	170.4	178.0(5), 178.1(5), 177.1(5), 179.4(5)	175.3	176.1	176.0(1)
C_{15}–C_{16}–C_{21}–C_{26}	140.8(2)	141.6	136.6	126.0(6), 128.6(6), 128.9(6), 126.0(6)	136.7	133.4	133.3(2)

[a] Four symmetry-independent molecules are present in the crystal structure of **3b**. Values are given for all four molecules.

Table S4. Selected bond lengths [Å], distances (B–B, B–C_{15} [Å]), and angles [°] of the calculated transition state structures at the ωB97X-D level of theory.

	2a-3a	**2b-3b**
C_1–C_1*	1.689	1.422
B_1–B_1	3.229	3.101
B_1–C_1	1.551	1.534
B_1–C_3	1.551	1.577
B_1–C_{10}	1.548	1.554
B_1–C_2	1.638	1.610
B_1–C_{15}	1.596	1.597
B_1–C_{22}	1.723	1.733
B_1–C_{11}	1.771	1.750
B_1–C_1–C_2	114.6	118.1
B_2–C_2–C_1	123.0	126.4
B_1–C_1–C_2–B_2	2.6	4.7
C_2–C_1–B_1–C_3	175.0	172.6
C_{15}–C_{16}–C_{21}–C_{22}	176.2	176.6

Photophysical data

2b

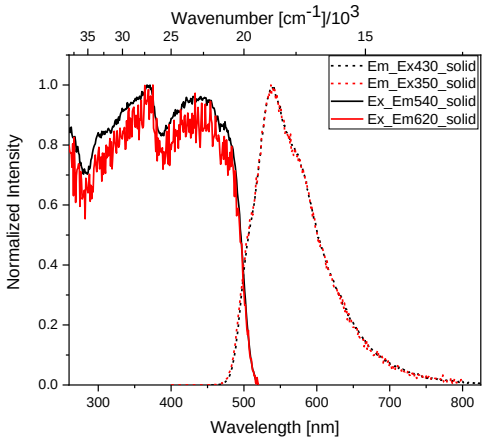


Figure S9. Excitation (solid) and emission (dashed) spectra of **2b** in the solid state.

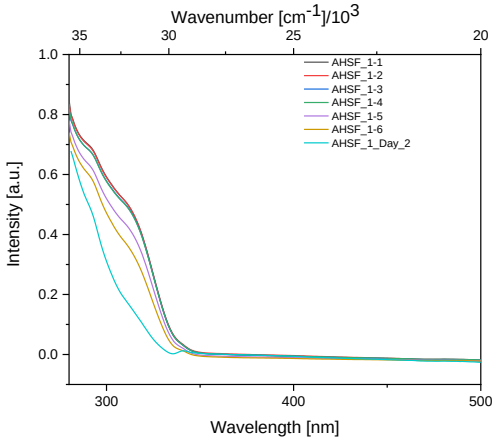


Figure S10. Absorption spectra of compound **2b** in toluene.

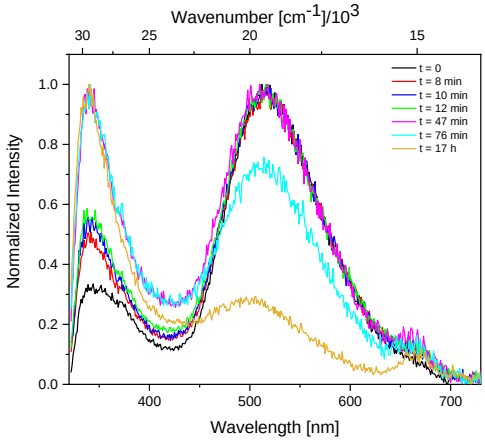


Figure S11. Normalized emission spectra of compound **2b** in toluene.

3a

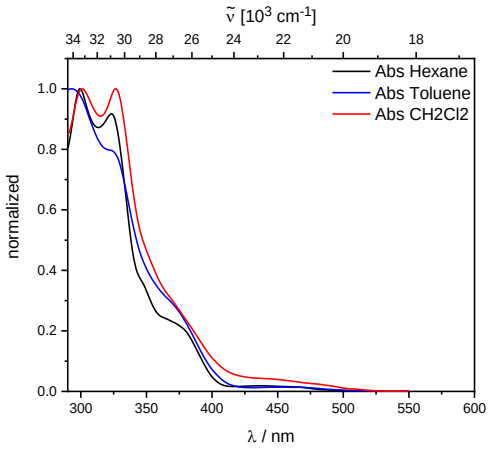


Figure S12. Absorption spectra of **3a** in hexane (black), toluene (blue) and CH_2Cl_2 (red).

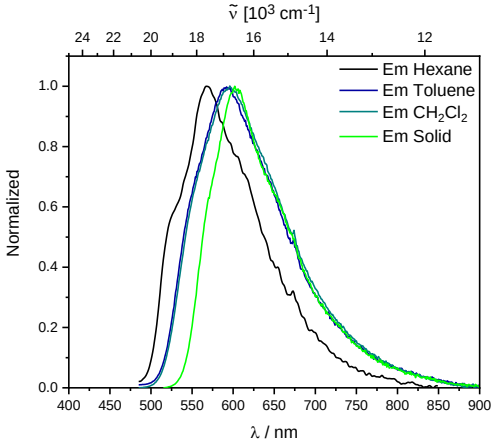


Figure S13. Emission spectra of **3a** in hexane (black), toluene (blue), CH_2Cl_2 (turquoise) and in the solid state (green).

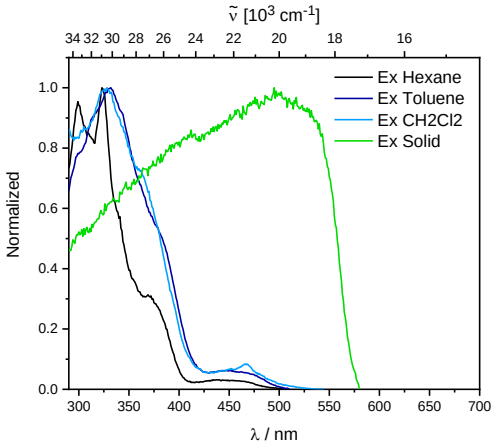


Figure S14. Excitation spectra of **3a** in hexane (black), toluene (blue), CH_2Cl_2 (turquoise) and in the solid state (green).

3b

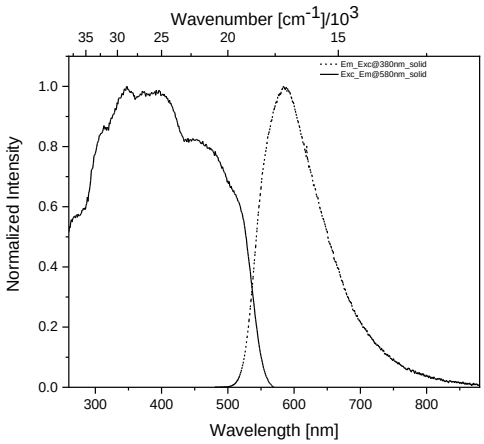


Figure S15. Excitation (solid) and emission (dashed) spectra of **3b** in the solid state.

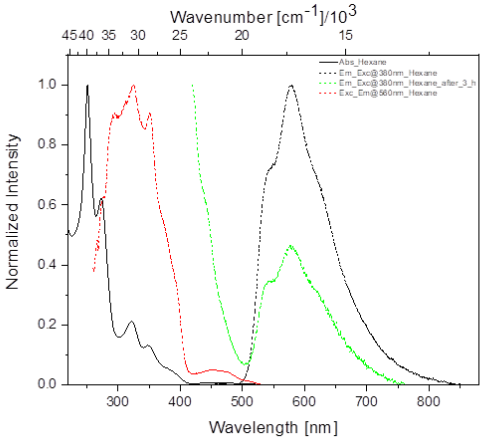


Figure S16. Absorption (black, solid), emission (black, dashed) and excitation (red, dashed) spectra of **3b** in hexane initially and after 3 h (green, dashed).

Cyclic voltammetry

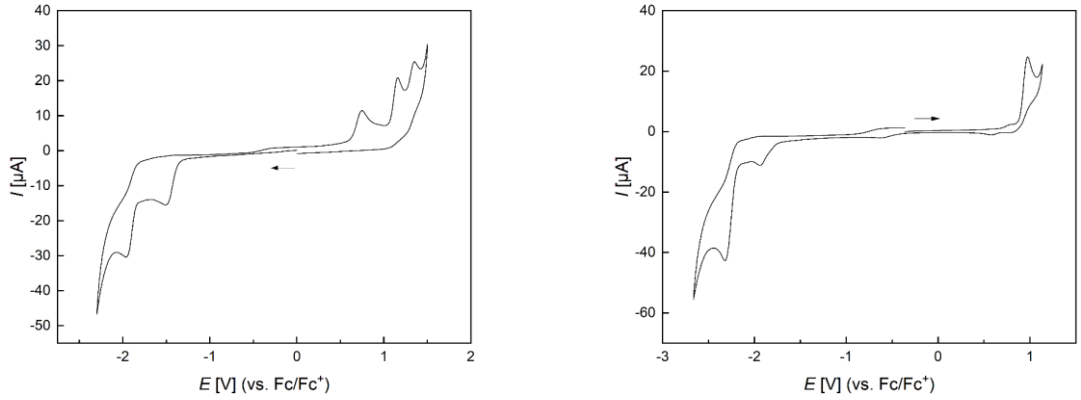


Figure S17. Cyclic voltammograms of **2b** measured in CH_2Cl_2 with $[nBu_4N][PF_6]$ as the electrolyte with a scan rate of 250 mVs^{-1}. All measurements are referenced to the Fc/Fc^+ ion couple.

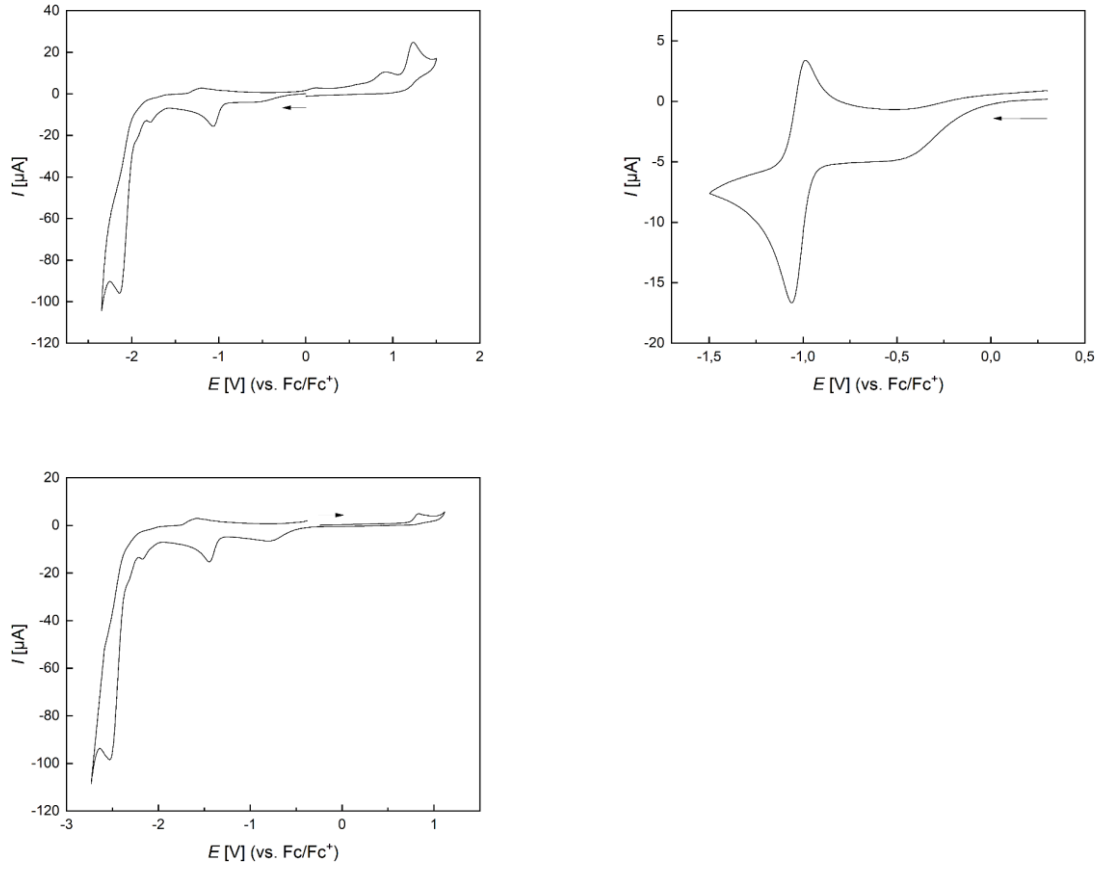


Figure S18. Cyclic voltammograms of **3a** measured in CH_2Cl_2 with $[nBu_4N][PF_6]$ as the electrolyte with a scan rate of 250 mVs^{-1}. All measurements are referenced to the Fc/Fc^+ ion couple.

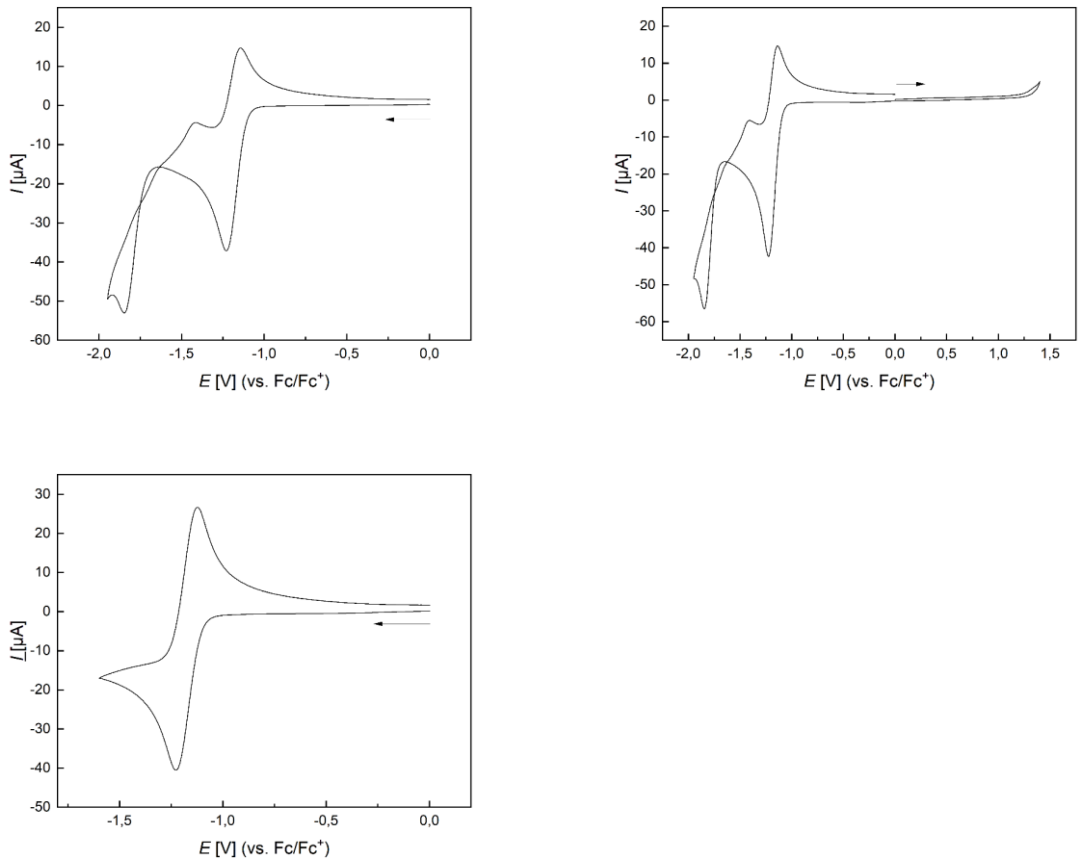


Figure S19. Cyclic voltammograms of **3b** measured in CH_2Cl_2 with $[nBu_4N][PF_6]$ as the electrolyte with a scan rate of 250 mVs^{-1}. All measurements are referenced to the Fc/Fc^+ ion couple.

Table S5. Reduction and oxidation potentials of **2b**, **3a** and **3b**.

compound	**1st reduction**	**2nd reduction**	**1st oxidation**
2a	E_{pc} = –1.50 V	E_{pc} = –1.96 V	E_{pa} = 0.98 V
3a	$E_{1/2}$[a] = –1.03 V	E_{pc} = –2.14 V	E_{pa} = 0.84 V
3b	$E_{1/2}$ = –1.17 V	E_{pc} = –1.85 V	

[a] partially reversible.

DFT and TD-DFT results

Cartesian coordinates of the optimized structures of 2a, 2b, 3a and 3b in the transition state calculations

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M062X_**2a** (E = –1304.381314 a.u.)			
H	-1.674587000	-1.681467000	1.646903000
B	-2.396994000	1.018008000	-1.001561000
C	1.869236000	-1.188931000	-1.413385000
B	-0.488890000	1.138247000	1.004461000
H	-1.674526000	1.681308000	-1.646761000
H	-3.097740000	-0.663864000	-2.776306000
B	-0.488843000	-1.138328000	-1.004368000
C	-0.470187000	3.699129000	0.057367000
H	-1.532345000	3.760452000	-0.152272000
C	-1.930180000	-0.588996000	-0.581832000
B	-3.273957000	-1.630229000	-0.394163000
H	-4.727725000	1.750487000	-1.743227000
C	0.076294000	-2.554611000	-0.634751000
B	-3.274014000	1.630023000	0.394213000
H	-5.689258000	1.081175000	1.091802000
H	-5.689201000	-1.081406000	-1.091865000
C	-1.930200000	0.588828000	0.581919000
B	-2.397014000	-1.018184000	1.001649000
C	0.353989000	-4.780703000	0.268711000
H	-0.075436000	-5.673148000	0.711697000
H	-4.727743000	-1.750707000	1.743230000
B	-4.151941000	1.018463000	-1.012159000
H	-3.097837000	0.663680000	2.776354000
B	-4.699826000	-0.623079000	-0.630222000
C	1.723278000	-4.714991000	0.031173000
H	2.355234000	-5.558486000	0.292214000
B	-3.255077000	-0.380962000	-1.638639000
C	2.295324000	-3.570392000	-0.532886000
H	3.367848000	-3.520197000	-0.696435000
B	-4.151956000	-1.018677000	1.012172000
H	-3.143274000	2.760189000	0.711041000
C	1.470733000	-2.507193000	-0.861689000
B	-3.255139000	0.380768000	1.638686000
H	-3.143175000	-2.760385000	-0.710982000
C	0.738957000	-0.349423000	-1.592295000
B	-4.699859000	0.622850000	0.630207000
C	3.150651000	-0.752242000	-1.696508000
H	4.009764000	-1.396208000	-1.532270000
C	3.329029000	0.548045000	-2.183464000
H	4.330528000	0.907349000	-2.400518000
C	2.236141000	1.377337000	-2.397943000
H	2.381679000	2.382910000	-2.778738000
C	0.942537000	0.929599000	-2.108852000
H	0.114487000	1.605678000	-2.280019000
C	0.076197000	2.554520000	0.634723000
C	0.353610000	4.780656000	-0.268714000
H	-0.075928000	5.673035000	-0.711724000
C	1.722891000	4.715156000	-0.031075000
H	2.354737000	5.558743000	-0.292087000
C	2.295083000	3.570647000	0.533017000
H	3.367604000	3.520624000	0.696623000
C	1.470634000	2.507321000	0.861769000
C	1.869285000	1.189098000	1.413428000
C	3.150758000	0.752438000	1.696353000
H	4.009827000	1.396457000	1.532069000
C	3.329236000	-0.547861000	2.183246000
H	4.330770000	-0.907135000	2.400187000
C	2.236402000	-1.377217000	2.397737000
H	2.381991000	-2.382801000	2.778483000
C	0.942748000	-0.929528000	2.108772000
H	0.114756000	-1.605647000	2.280092000
C	0.739044000	0.349571000	1.592463000

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M062X_TS1-**2a**/**3a** (E = -1304.336144 a.u.)			
H	-0.407581000	1.437831000	2.240836000
B	-0.519596000	1.543845000	-1.575714000
C	-3.686268000	-1.628311000	0.248783000
C	0.004446000	-1.521727000	0.288362000
B	1.125593000	-0.174233000	-0.007547000
H	-0.662877000	0.641241000	-2.324598000
H	-2.894468000	2.458684000	-1.659471000
B	-2.083181000	0.138270000	0.178967000
C	1.825746000	-0.998305000	-2.490076000
H	0.815854000	-0.903676000	-2.877115000
C	-1.294936000	1.451894000	-0.070048000
B	-1.744010000	2.941521000	0.592188000
H	-0.398761000	3.665765000	-3.022050000
C	-1.349904000	-1.221432000	0.310396000
B	1.004912000	2.382210000	-1.261320000
H	1.342505000	4.904448000	-0.821578000
H	-1.700638000	5.183233000	-0.691664000
C	0.369241000	1.272795000	-0.135796000
B	-0.353586000	2.026678000	1.217381000
C	0.393805000	-2.874638000	0.274566000
H	1.449955000	-3.132851000	0.267471000
H	-0.115609000	4.509082000	1.845563000
B	-0.386647000	3.276088000	-1.904186000
H	2.131714000	2.569271000	1.045538000
B	-1.138165000	4.150789000	-0.548007000
C	-0.570873000	-3.874530000	0.268312000
H	-0.257261000	-4.913626000	0.254717000
B	-1.846269000	2.643815000	-1.141426000
C	-1.941413000	-3.570071000	0.270891000
H	-2.674379000	-4.371511000	0.251418000
B	-0.220940000	3.766967000	0.928819000
H	1.959389000	2.052741000	-1.874271000
C	-2.324852000	-2.239507000	0.285473000
B	1.106242000	2.683938000	0.470689000
H	-2.721684000	2.961231000	1.260079000
C	-3.597266000	-0.212907000	0.194468000
B	0.620439000	3.986793000	-0.622600000
C	-4.914631000	-2.264422000	0.249784000
H	-4.989351000	-3.347471000	0.285902000
C	-6.075425000	-1.480409000	0.202386000
H	-7.046154000	-1.966783000	0.204738000
C	-6.003887000	-0.092312000	0.149497000
H	-6.916415000	0.493106000	0.111856000
C	-4.759530000	0.547258000	0.141258000
H	-4.701353000	1.631237000	0.092939000
C	2.103014000	-0.689436000	-1.159400000
C	2.848790000	-1.425382000	-3.334062000
H	2.633197000	-1.648187000	-4.374304000
C	4.150561000	-1.571409000	-2.851066000
H	4.938988000	-1.907153000	-3.517210000
C	4.440083000	-1.298532000	-1.518490000
H	5.449780000	-1.429648000	-1.139958000
C	3.414496000	-0.859143000	-0.681768000
C	3.502922000	-0.545519000	0.751904000
C	4.645550000	-0.522237000	1.548123000
H	5.616117000	-0.759498000	1.122732000
C	4.537233000	-0.180999000	2.893869000
H	5.427229000	-0.159974000	3.514874000
C	3.298731000	0.131363000	3.450890000
H	3.224583000	0.388808000	4.502040000
C	2.152156000	0.111609000	2.658275000
H	1.189869000	0.340253000	3.104792000

H	-1.532117000	-3.760823000	0.152091000
C	-0.469954000	-3.699310000	-0.057445000

C	2.248987000	-0.207208000	1.303946000
H	0.982758000	-0.948858000	1.057637000

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M062X_**3a** (E = -1304.39502822 a.u.)

H	-0.247664000	1.206098000	1.836781000
B	-0.474233000	1.325253000	-1.982113000
C	-4.024259000	-1.229137000	0.407632000
C	-0.385690000	-1.667725000	-0.118726000
B	0.743728000	-0.643482000	-0.469964000
H	-0.774805000	0.448397000	-2.718164000
H	-2.657528000	2.644387000	-2.006354000
B	-2.214437000	0.238233000	-0.119020000
C	2.111577000	-1.850692000	-2.191904000
H	1.165526000	-1.973492000	-2.715520000
C	-1.220843000	1.389605000	-0.448705000
B	-1.375890000	2.934602000	0.207296000
H	-0.028559000	3.387521000	-3.451227000
C	-1.689838000	-1.206490000	0.030900000
B	1.183880000	1.894463000	-1.717123000
H	1.963567000	4.320016000	-1.312826000
H	-0.972805000	5.123273000	-1.104078000
C	0.391335000	0.922182000	-0.562573000
B	-0.150843000	1.788563000	0.812039000
C	-0.175148000	-3.051901000	0.055107000
H	0.823602000	-3.466300000	-0.055052000
H	0.544447000	4.193540000	1.397836000
B	-0.050509000	3.007077000	-2.330489000
H	2.386320000	1.900670000	0.562422000
B	-0.598563000	4.008626000	-0.961893000
C	-1.240897000	-3.891256000	0.367524000
H	-1.059333000	-4.953222000	0.502206000
B	-1.578863000	2.645794000	-1.518341000
C	-2.550980000	-3.402167000	0.509829000
H	-3.359888000	-4.087154000	0.749009000
B	0.280328000	3.474887000	0.494934000
H	2.042812000	1.386228000	-2.350651000
C	-2.773702000	-2.045040000	0.335717000
B	1.385509000	2.179934000	0.007695000
H	-2.315386000	3.133376000	0.899600000
C	-3.745623000	0.140153000	0.139290000
B	1.099575000	3.542902000	-1.083954000
C	-5.311783000	-1.648905000	0.687106000
H	-5.531295000	-2.692379000	0.894094000
C	-6.341464000	-0.697538000	0.700556000
H	-7.356367000	-1.014970000	0.919811000
C	-6.084782000	0.643602000	0.438646000
H	-6.898176000	1.361297000	0.454802000
C	-4.780657000	1.066707000	0.156151000
H	-4.579288000	2.114882000	-0.048220000
C	2.131691000	-1.188304000	-0.953924000
C	3.276819000	-2.335463000	-2.776249000
H	3.236080000	-2.826178000	-3.743215000
C	4.488557000	-2.198725000	-2.104738000
H	5.402747000	-2.589333000	-2.540069000
C	4.523245000	-1.581291000	-0.860931000
H	5.461069000	-1.513776000	-0.317216000
C	3.360044000	-1.069438000	-0.275622000
C	3.426195000	-0.426606000	1.058499000
C	4.494953000	0.416238000	1.386987000
H	5.282514000	0.583526000	0.658432000
C	4.518396000	1.090666000	2.601152000

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M062X_**2b** (E = -1204.509805 a.u.)

C	2.067705000	-1.333805000	1.333483000
B	-1.480458000	0.838310000	-0.467083000
B	1.480458000	0.838242000	0.466672000
C	-3.880835000	1.090549000	0.780815000
H	-3.668830000	2.069722000	1.204696000
C	2.937324000	0.455194000	0.017885000
C	5.105068000	0.464650000	-1.046108000
H	5.848036000	0.958299000	-1.664308000
C	5.370104000	-0.795912000	-0.520886000
H	6.320912000	-1.276035000	-0.732393000
C	4.425801000	-1.458971000	0.272168000
H	4.643742000	-2.447427000	0.667077000
C	3.219352000	-0.831133000	0.535232000
C	1.021143000	-0.383950000	1.338606000
C	1.945793000	-2.537411000	2.007885000
H	2.747397000	-3.270879000	2.001455000
C	0.760145000	-2.799215000	2.705100000
H	0.649485000	-3.740637000	3.234901000
C	-0.273768000	-1.868921000	2.733310000
H	-1.182442000	-2.087666000	3.284576000
C	-0.140168000	-0.652616000	2.054155000
H	-0.948360000	0.075669000	2.091405000
C	-2.937256000	0.455296000	-0.018026000
C	-5.104807000	0.464858000	1.046339000
H	-5.847701000	0.958606000	1.664549000
C	-5.369853000	-0.795843000	0.521460000
H	-6.320591000	-1.275981000	0.733249000
C	-4.425652000	-1.459025000	-0.271617000
H	-4.643603000	-2.447588000	-0.666249000
C	-3.219291000	-0.831165000	-0.535034000
C	-2.067743000	-1.333923000	-1.333380000
C	-1.945910000	-2.537593000	-2.007689000
H	-2.747488000	-3.271088000	-2.001038000
C	-0.760389000	-2.799419000	-2.705105000
H	-0.649812000	-3.740874000	-3.234866000
C	0.273481000	-1.869083000	-2.733626000
H	1.182053000	-2.087862000	-3.285047000
C	0.139949000	-0.652701000	-2.054603000
H	0.948111000	0.075609000	-2.092033000
C	-1.021232000	-0.384014000	-1.338851000
H	3.669012000	2.069364000	-1.205118000
C	3.880998000	1.090306000	-0.780964000
C	1.354787000	3.369438000	0.298231000
C	0.692500000	2.141997000	0.157228000
C	-0.692536000	2.142054000	-0.157605000
C	-1.354773000	3.369531000	-0.298352000
C	-0.678942000	4.579300000	-0.150709000
C	0.679006000	4.579258000	0.150818000
H	2.413921000	3.376429000	0.545841000
H	-2.413918000	3.376612000	-0.545905000
H	-1.210775000	5.518331000	-0.269463000
H	1.210848000	5.518260000	0.269764000

H	5.342206000	1.759171000	2.829741000
C	3.475352000	0.932181000	3.512285000
H	3.487539000	1.470954000	4.453890000
C	2.421768000	0.075346000	3.209774000
H	1.615097000	-0.069181000	3.921353000
C	2.402963000	-0.606815000	1.996016000
H	1.595766000	-1.306740000	1.788480000

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M062X_TS1-**2b**/**3b** (E = -1204.45650 a.u.)

C	-3.785849000	-1.019905000	0.247945000
C	-0.107126000	-1.195513000	0.210714000
B	1.027562000	0.080829000	-0.201693000
B	-2.031335000	0.607994000	-0.069465000
C	2.152414000	-1.113076000	-2.342356000
H	1.220726000	-1.092008000	-2.902049000
C	-1.436604000	-0.801293000	0.214552000
C	0.192209000	-2.564075000	0.344989000
H	1.226874000	-2.897207000	0.356096000
C	-0.842440000	-3.487014000	0.454383000
H	-0.605092000	-4.542279000	0.548745000
C	-2.188828000	-3.086839000	0.442151000
H	-2.974010000	-3.833487000	0.524184000
C	-2.480303000	-1.736772000	0.317342000
C	-3.587564000	0.373134000	0.044825000
C	-5.056770000	-1.560505000	0.355961000
H	-5.200854000	-2.626927000	0.506189000
C	-6.162475000	-0.707454000	0.273310000
H	-7.163829000	-1.117867000	0.361150000
C	-5.991340000	0.659255000	0.082520000
H	-6.859119000	1.308435000	0.024595000
C	-4.704931000	1.197611000	-0.034542000
H	-4.591091000	2.268130000	-0.181781000
C	2.202306000	-0.582562000	-1.055016000
C	3.296951000	-1.665134000	-2.915058000
H	3.259540000	-2.065932000	-3.923398000
C	4.494978000	-1.708273000	-2.198319000
H	5.379132000	-2.145679000	-2.651548000
C	4.561951000	-1.196186000	-0.906456000
H	5.493968000	-1.237802000	-0.349360000
C	3.416644000	-0.632730000	-0.343584000
C	3.274346000	-0.024268000	0.989546000
C	4.267130000	0.238642000	1.931551000
H	5.296854000	-0.051838000	1.743522000
C	3.931404000	0.896304000	3.113177000
H	4.703419000	1.102557000	3.848096000
C	2.619368000	1.302399000	3.359806000
H	2.377279000	1.822202000	4.280911000
C	1.622250000	1.040962000	2.421720000
H	0.595856000	1.351045000	2.605656000
C	1.948073000	0.378956000	1.241165000
H	0.816636000	-0.511642000	0.967057000
C	-1.566629000	2.998184000	-0.926334000
C	-1.092895000	1.732224000	-0.530699000
C	0.297191000	1.449849000	-0.620096000
C	1.146783000	2.459546000	-1.096025000
C	0.657096000	3.700919000	-1.482015000
C	-0.709012000	3.979306000	-1.396272000
H	-2.632343000	3.203336000	-0.867940000
H	2.214251000	2.262615000	-1.170810000
H	1.341148000	4.457135000	-1.856579000
H	-1.090429000	4.948931000	-1.700266000

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M062X_**3b** (E = -1204.514213 a.u.)

C	-3.991220000	-0.668217000	0.316456000
C	-0.430327000	-1.569282000	-0.081726000
B	0.745748000	-0.656694000	-0.575238000
B	-2.025074000	0.488753000	-0.475153000
C	2.442952000	-2.323225000	-1.491441000
H	1.606118000	-2.769344000	-2.024948000
C	-1.683226000	-0.965387000	-0.047856000
C	-0.349446000	-2.896671000	0.382027000
H	0.606983000	-3.413914000	0.395907000
C	-1.493730000	-3.554526000	0.831794000
H	-1.414843000	-4.579137000	1.183243000
C	-2.748867000	-2.925327000	0.851718000
H	-3.618902000	-3.467452000	1.213395000
C	-2.837366000	-1.611876000	0.409389000
C	-3.572866000	0.593452000	-0.195714000
C	-5.312063000	-0.901603000	0.659146000
H	-5.627117000	-1.865933000	1.048109000
C	-6.246300000	0.128659000	0.496486000
H	-7.285152000	-0.044233000	0.761201000
C	-5.858889000	1.368087000	0.001033000
H	-6.595477000	2.155970000	-0.118462000
C	-4.521916000	1.598837000	-0.343876000
H	-4.235696000	2.574204000	-0.728052000
C	2.207142000	-1.234022000	-0.639327000
C	3.723182000	-2.832682000	-1.688295000
H	3.879318000	-3.666423000	-2.365524000
C	4.798950000	-2.271879000	-1.006064000
H	5.799537000	-2.670538000	-1.140663000
C	4.585979000	-1.212741000	-0.130407000
H	5.416967000	-0.800296000	0.435419000
C	3.303624000	-0.688883000	0.061747000
C	3.092248000	0.418918000	1.027451000
C	3.969770000	1.507398000	1.083412000
H	4.815733000	1.543512000	0.402413000
C	3.746432000	2.553751000	1.971763000
H	4.429758000	3.396845000	1.994077000
C	2.642462000	2.529000000	2.821527000
H	2.467269000	3.347508000	3.512088000
C	1.766018000	1.448764000	2.779876000
H	0.907614000	1.416457000	3.443017000
C	1.992843000	0.400560000	1.893914000
H	1.324384000	-0.457853000	1.892326000
C	-1.096243000	2.676959000	-1.508239000
C	-0.887244000	1.379701000	-1.029747000
C	0.424334000	0.814362000	-1.080168000
C	1.452978000	1.588674000	-1.628194000
C	1.223751000	2.880434000	-2.102332000
C	-0.051894000	3.430058000	-2.041124000
H	-2.094440000	3.105107000	-1.468955000
H	2.456797000	1.176593000	-1.690342000
H	2.043855000	3.455700000	-2.521702000
H	-0.232467000	4.435166000	-2.409968000

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ωB97XD_**2a** (E = -1304.491995 a.u.)

H	-1.685704000	-1.708345000	1.635607000
B	-2.402087000	1.034531000	-0.994320000
C	1.867605000	-1.152075000	-1.443993000
B	-0.485910000	1.130211000	1.027132000
H	-1.684770000	1.709594000	-1.635704000
H	-3.103054000	-0.631434000	-2.791309000
B	-0.486951000	-1.129900000	-1.027296000
C	-0.438285000	3.692735000	0.096527000
H	-1.501847000	3.772193000	-0.097389000
C	-1.927513000	-0.586496000	-0.592066000
B	-3.279381000	-1.629566000	-0.411749000
H	-4.736667000	1.774373000	-1.728857000
C	0.094167000	-2.537591000	-0.661380000
B	-3.278086000	1.632045000	0.412026000
H	-5.699640000	1.075539000	1.108030000
H	-5.700569000	-1.071284000	-1.107445000
C	-1.926991000	0.588015000	0.592106000
B	-2.402661000	-1.032714000	0.994419000
C	0.393703000	-4.763041000	0.233250000
H	-0.027905000	-5.663416000	0.668129000
H	-4.737718000	-1.770925000	1.729330000
B	-4.157709000	1.032813000	-1.003566000
H	-3.102092000	0.633881000	2.791522000
B	-4.707932000	-0.616447000	-0.638751000
C	1.763853000	-4.675481000	0.010975000
H	2.407214000	-5.509026000	0.276790000
B	-3.258160000	-0.363476000	-1.646312000
C	2.323541000	-3.522471000	-0.547048000
H	3.396215000	-3.457705000	-0.702699000
B	-4.158291000	-1.029731000	1.004051000
H	-3.148024000	2.763626000	0.735065000
C	1.488089000	-2.470924000	-0.881565000
B	-3.257653000	0.365915000	1.646591000
H	-3.150160000	-2.761239000	-0.734824000
C	0.725011000	-0.333343000	-1.627263000
B	-4.707380000	0.619952000	0.639274000
C	3.138962000	-0.696397000	-1.738938000
H	4.011187000	-1.320494000	-1.569606000
C	3.291812000	0.596116000	-2.251893000
H	4.285917000	0.968796000	-2.480115000
C	2.184120000	1.402700000	-2.475672000
H	2.310924000	2.402319000	-2.877657000
C	0.902735000	0.939167000	-2.165570000
H	0.059305000	1.594267000	-2.338620000
C	0.096251000	2.537479000	0.661182000
C	0.397561000	4.762492000	-0.233970000
H	-0.023333000	5.663095000	-0.669068000
C	1.767635000	4.673896000	-0.011682000
H	2.411679000	5.506846000	-0.277711000
C	2.326405000	3.520576000	0.546620000
H	3.399029000	3.454988000	0.702260000
C	1.490124000	2.469765000	0.881379000
C	1.868651000	1.150711000	1.443975000
C	3.139651000	0.694313000	1.739394000
H	4.012290000	1.317902000	1.570305000
C	3.291553000	-0.598254000	2.252483000
H	4.285368000	-0.971543000	2.480966000
C	2.183303000	-1.404131000	2.476014000
H	2.309397000	-2.403778000	2.878157000
C	0.902272000	-0.939809000	2.165604000
H	0.058375000	-1.594339000	2.338523000
C	0.725494000	0.332758000	1.627105000
H	-1.504908000	-3.771125000	0.097036000
C	-0.441291000	-3.692530000	-0.096945000

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ωB97XD_TS1-**2a/3a** (E = -1304.445008 a.u.)

H	-0.427245000	1.404341000	2.246144000
B	-0.503023000	1.564474000	-1.584556000
C	-3.690406000	-1.631677000	0.219113000
C	0.000199000	-1.532538000	0.239302000
B	1.125183000	-0.188401000	-0.015577000
H	-0.638125000	0.679179000	-2.358202000
H	-2.883212000	2.490896000	-1.674968000
B	-2.083919000	0.128084000	0.152548000
C	1.879000000	-0.944516000	-2.503283000
H	0.877996000	-0.837066000	-2.908686000
C	-1.299522000	1.445225000	-0.081546000
B	-1.750654000	2.931693000	0.601437000
H	-0.365240000	3.715980000	-2.995496000
C	-1.353983000	-1.232105000	0.268618000
B	1.023354000	2.397787000	-1.238382000
H	1.360753000	4.917489000	-0.753976000
H	-1.690097000	5.199940000	-0.649359000
C	0.378912000	1.264716000	-0.134382000
B	-0.363886000	2.004960000	1.228165000
C	0.385322000	-2.885578000	0.203905000
H	1.439953000	-3.145956000	0.189553000
H	-0.129102000	4.482000000	1.899129000
B	-0.364473000	3.303942000	-1.881171000
H	2.132207000	2.549991000	1.085212000
B	-1.130338000	4.159944000	-0.515088000
C	-0.580158000	-3.883796000	0.187239000
H	-0.268457000	-4.923149000	0.156199000
B	-1.836495000	2.661085000	-1.141964000
C	-1.949027000	-3.577338000	0.202935000
H	-2.683785000	-4.376555000	0.179069000
B	-0.225575000	3.750056000	0.968144000
H	1.986742000	2.082466000	-1.849623000
C	-2.330170000	-2.246829000	0.237157000
B	1.108519000	2.671988000	0.503699000
H	-2.737856000	2.946814000	1.260991000
C	-3.595519000	-0.217124000	0.175475000
B	0.633102000	3.994916000	-0.575183000
C	-4.921987000	-2.260196000	0.231243000
H	-5.004366000	-3.342771000	0.261990000
C	-6.078793000	-1.469865000	0.204701000
H	-7.051819000	-1.951400000	0.217121000
C	-6.000586000	-0.082047000	0.160224000
H	-6.910721000	0.508369000	0.137755000
C	-4.753192000	0.550092000	0.141525000
H	-4.687474000	1.633457000	0.100191000
C	2.127448000	-0.670313000	-1.160424000
C	2.919264000	-1.348083000	-3.336556000
H	2.726177000	-1.543181000	-4.386864000
C	4.210446000	-1.504107000	-2.829967000
H	5.013317000	-1.822104000	-3.487816000
C	4.471392000	-1.261048000	-1.486293000
H	5.473873000	-1.398621000	-1.091303000
C	3.428450000	-0.844716000	-0.660404000
C	3.487342000	-0.559946000	0.779986000
C	4.612736000	-0.540467000	1.599009000
H	5.594280000	-0.757660000	1.188975000
C	4.474305000	-0.228036000	2.948824000
H	5.351739000	-0.210671000	3.587978000
C	3.222171000	0.059889000	3.487150000
H	3.122948000	0.292728000	4.542058000
C	2.093715000	0.047363000	2.670685000
H	1.120543000	0.259604000	3.100025000
C	2.220804000	-0.243279000	1.313282000
H	0.969012000	-0.978849000	1.028422000

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ωB97XD_**3a** (E = -1304.502156 a.u.)

H	-0.127483000	1.114217000	1.830602000
B	-0.534850000	1.462531000	-1.976628000
C	-3.950859000	-1.309275000	0.300669000
C	-0.326823000	-1.648966000	-0.376622000
B	0.787474000	-0.579518000	-0.611548000
H	-0.860463000	0.632036000	-2.757458000
H	-2.732807000	2.766358000	-1.820027000
B	-2.175101000	0.224435000	-0.129999000
C	2.358694000	-1.517804000	-2.338804000
H	1.479725000	-1.576722000	-2.977014000
C	-1.216998000	1.418214000	-0.402918000
B	-1.351009000	2.923026000	0.356277000
H	-0.169808000	3.621605000	-3.332344000
C	-1.629788000	-1.219480000	-0.143451000
B	1.134944000	2.030834000	-1.747005000
H	1.912384000	4.443593000	-1.227492000
H	-1.023725000	5.200096000	-0.836742000
C	0.403408000	0.977537000	-0.616668000
B	-0.086262000	1.756080000	0.837246000
C	-0.100983000	-3.040574000	-0.356424000
H	0.897770000	-3.430690000	-0.531709000
H	0.616487000	4.133212000	1.538994000
B	-0.139189000	3.167179000	-2.235218000
H	2.441089000	1.903402000	0.471277000
B	-0.633901000	4.078905000	-0.779890000
C	-1.150300000	-3.920188000	-0.109884000
H	-0.957430000	-4.988675000	-0.096739000
B	-1.631657000	2.741959000	-1.378381000
C	-2.458012000	-3.462441000	0.123027000
H	-3.253846000	-4.177852000	0.310655000
B	0.317043000	3.465038000	0.603603000
H	1.973278000	1.576694000	-2.450121000
C	-2.695736000	-2.097768000	0.103979000
B	1.411611000	2.212177000	-0.015429000
H	-2.260717000	3.073904000	1.103432000
C	-3.691277000	0.081991000	0.166000000
B	1.065119000	3.639799000	-1.007395000
C	-5.226151000	-1.766990000	0.574638000
H	-5.433445000	-2.827721000	0.681487000
C	-6.260451000	-0.831306000	0.716539000
H	-7.266281000	-1.179740000	0.931030000
C	-6.021099000	0.531714000	0.585129000
H	-6.837695000	1.237377000	0.697514000
C	-4.729529000	0.993139000	0.308323000
H	-4.539268000	2.057403000	0.203448000
C	2.229488000	-1.031031000	-1.029445000
C	3.592020000	-1.904798000	-2.850490000
H	3.669028000	-2.262403000	-3.872290000
C	4.721616000	-1.839198000	-2.040762000
H	5.687743000	-2.152250000	-2.423853000
C	4.607567000	-1.388831000	-0.731504000
H	5.483156000	-1.371625000	-0.088956000
C	3.374727000	-0.980121000	-0.212557000
C	3.282075000	-0.511324000	1.193375000
C	4.241937000	0.363561000	1.716639000
H	5.061925000	0.692340000	1.085272000
C	4.118410000	0.864097000	3.006242000
H	4.858822000	1.561394000	3.385300000
C	3.035524000	0.494643000	3.802146000
H	2.932060000	0.897915000	4.804275000
C	2.089858000	-0.394086000	3.303815000
H	1.251327000	-0.702089000	3.920538000
C	2.216956000	-0.899265000	2.012472000
H	1.491423000	-1.622690000	1.651968000

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ωB97XD_**2b** (E = -1204.612990 a.u.)

C	1.932513000	-1.341403000	1.355123000
B	-1.442675000	0.874441000	-0.543661000
B	1.442348000	0.873712000	0.543440000
C	-3.862693000	1.069906000	0.667450000
H	-3.692783000	2.069309000	1.060832000
C	2.888605000	0.448968000	0.105474000
C	5.061191000	0.403607000	-0.945680000
H	5.828174000	0.886426000	-1.543230000
C	5.269478000	-0.883330000	-0.460587000
H	6.201123000	-1.395731000	-0.682167000
C	4.292761000	-1.531278000	0.305066000
H	4.467454000	-2.540318000	0.667753000
C	3.112283000	-0.863193000	0.583422000
C	0.931835000	-0.344533000	1.388287000
C	1.742949000	-2.563919000	1.976214000
H	2.506088000	-3.336397000	1.946340000
C	0.536704000	-2.796821000	2.647976000
H	0.373606000	-3.754034000	3.134434000
C	-0.450685000	-1.819369000	2.705241000
H	-1.378573000	-2.016026000	3.232704000
C	-0.249026000	-0.584837000	2.080170000
H	-1.022501000	0.177107000	2.131209000
C	-2.888807000	0.449527000	-0.105481000
C	-5.060998000	0.403621000	0.946470000
H	-5.827843000	0.886218000	1.544378000
C	-5.269201000	-0.883317000	0.461342000
H	-6.200659000	-1.395923000	0.683237000
C	-4.292634000	-1.530993000	-0.304735000
H	-4.467246000	-2.540031000	-0.667464000
C	-3.112399000	-0.862639000	-0.583472000
C	-1.932779000	-1.340613000	-1.355541000
C	-1.743161000	-2.563061000	-1.976736000
H	-2.506170000	-3.335663000	-1.946752000
C	-0.537013000	-2.795737000	-2.648756000
H	-0.373860000	-3.752914000	-3.135268000
C	0.450219000	-1.818139000	-2.706183000
H	1.378026000	-2.014655000	-3.233841000
C	0.248512000	-0.583670000	-2.080998000
H	1.021856000	0.178402000	-2.132117000
C	-0.932246000	-0.343598000	-1.388857000
H	3.692642000	2.069019000	-1.060399000
C	3.862645000	1.069619000	-0.667046000
C	1.331900000	3.414835000	0.385746000
C	0.680570000	2.187332000	0.203070000
C	-0.680548000	2.187801000	-0.203115000
C	-1.331259000	3.415688000	-0.385149000
C	-0.667051000	4.624771000	-0.193684000
C	0.668324000	4.624344000	0.194833000
H	2.373651000	3.424116000	0.697909000
H	-2.373030000	3.425692000	-0.697223000
H	-1.190238000	5.563990000	-0.346051000
H	1.191963000	5.563242000	0.347625000

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ωB97XD_TS1-**2b**/**3b** (E = -1204.558240 a.u.)

C	-3.784105000	-1.019414000	0.227679000
C	-0.107061000	-1.211044000	0.178587000
B	1.028634000	0.062209000	-0.210383000
B	-2.022785000	0.599729000	-0.088230000
C	2.209730000	-1.118985000	-2.328961000
H	1.287694000	-1.115080000	-2.904152000
C	-1.435475000	-0.813611000	0.182665000
C	0.185328000	-2.581193000	0.307235000
H	1.217894000	-2.918498000	0.320805000
C	-0.852061000	-3.500755000	0.410120000
H	-0.619454000	-4.557429000	0.501129000
C	-2.196155000	-3.094838000	0.399685000
H	-2.984076000	-3.838847000	0.477606000
C	-2.482042000	-1.743559000	0.283094000
C	-3.578105000	0.373525000	0.037343000
C	-5.057959000	-1.550900000	0.340985000
H	-5.209821000	-2.617297000	0.482203000
C	-6.157835000	-0.688991000	0.277585000
H	-7.161235000	-1.093693000	0.370794000
C	-5.978042000	0.678148000	0.100369000
H	-6.841048000	1.335338000	0.057176000
C	-4.689239000	1.207553000	-0.022978000
H	-4.566736000	2.278140000	-0.160830000
C	2.227950000	-0.584305000	-1.042980000
C	3.372166000	-1.654920000	-2.878883000
H	3.358718000	-2.063166000	-3.885092000
C	4.557606000	-1.674406000	-2.141275000
H	5.456828000	-2.099362000	-2.576891000
C	4.592892000	-1.156272000	-0.850861000
H	5.516425000	-1.180630000	-0.278838000
C	3.428630000	-0.611976000	-0.309637000
C	3.250223000	-0.008576000	1.021234000
C	4.218396000	0.271202000	1.982833000
H	5.257914000	0.005412000	1.814227000
C	3.846816000	0.916032000	3.160745000
H	4.600646000	1.136157000	3.910540000
C	2.522385000	1.292102000	3.385037000
H	2.251667000	1.800282000	4.304943000
C	1.550446000	1.016333000	2.426081000
H	0.514680000	1.302254000	2.591310000
C	1.912153000	0.366212000	1.249624000
H	0.801901000	-0.531815000	0.950221000
C	-1.552132000	2.989171000	-0.946336000
C	-1.082986000	1.721212000	-0.550663000
C	0.306251000	1.433886000	-0.644068000
C	1.157897000	2.439551000	-1.123653000
C	0.671944000	3.681975000	-1.509144000
C	-0.692003000	3.965828000	-1.419423000
H	-2.616006000	3.201013000	-0.884606000
H	2.223901000	2.241118000	-1.203227000
H	1.358722000	4.435437000	-1.884793000
H	-1.071532000	4.937065000	-1.721701000

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ωB97XD_**3b** (E = -1204.614720 a.u.)

C	-3.958707000	-0.693975000	0.299040000
C	-0.401778000	-1.593150000	-0.124292000
B	0.770918000	-0.672476000	-0.607882000
B	-1.995690000	0.470444000	-0.485136000
C	2.537532000	-2.305671000	-1.480571000
H	1.735662000	-2.760190000	-2.057995000
C	-1.653777000	-0.988686000	-0.078714000
C	-0.320014000	-2.924255000	0.326792000
H	0.635608000	-3.442122000	0.330589000
C	-1.461796000	-3.585585000	0.776025000
H	-1.381261000	-4.613764000	1.117172000
C	-2.715437000	-2.954702000	0.809039000
H	-3.584041000	-3.498079000	1.171729000
C	-2.804823000	-1.638170000	0.379143000
C	-3.541254000	0.571518000	-0.202443000
C	-5.279625000	-0.930425000	0.637685000
H	-5.594800000	-1.897437000	1.019785000
C	-6.214778000	0.099272000	0.480187000
H	-7.254518000	-0.076986000	0.739522000
C	-5.827751000	1.342055000	-0.006897000
H	-6.565570000	2.129697000	-0.123601000
C	-4.490798000	1.576562000	-0.346787000
H	-4.204736000	2.553313000	-0.727374000
C	2.243455000	-1.228078000	-0.632306000
C	3.833041000	-2.793704000	-1.618347000
H	4.035278000	-3.618424000	-2.294792000
C	4.865352000	-2.222277000	-0.880552000
H	5.877787000	-2.603796000	-0.970860000
C	4.593525000	-1.172977000	-0.010013000
H	5.391232000	-0.748715000	0.593515000
C	3.296070000	-0.669714000	0.122853000
C	3.021987000	0.440527000	1.071065000
C	3.837111000	1.576808000	1.100417000
H	4.686214000	1.638885000	0.425458000
C	3.545916000	2.637321000	1.950992000
H	4.181234000	3.517856000	1.950982000
C	2.434967000	2.579089000	2.789380000
H	2.204162000	3.409742000	3.448829000
C	1.622845000	1.449292000	2.777111000
H	0.759731000	1.390519000	3.432743000
C	1.918016000	0.386791000	1.929120000
H	1.293764000	-0.503138000	1.945386000
C	-1.068308000	2.675297000	-1.489449000
C	-0.862100000	1.368858000	-1.035192000
C	0.445179000	0.796820000	-1.114564000
C	1.468189000	1.569456000	-1.674547000
C	1.240569000	2.868109000	-2.127618000
C	-0.027683000	3.427674000	-2.029841000
H	-2.060043000	3.114256000	-1.423735000
H	2.466875000	1.151186000	-1.759891000
H	2.057368000	3.442174000	-2.555126000
H	-0.206820000	4.440698000	-2.377553000

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B3LYP(D3bj)_**2a** (E = -1305.062609 a.u.)

H	-1.682754000	-1.665185000	1.670280000
B	-2.399629000	1.008795000	-1.014170000
C	1.872121000	-1.183944000	-1.441671000
B	-0.483638000	1.139021000	0.994873000
H	-1.684064000	1.663502000	-1.670101000
H	-3.100396000	-0.696848000	-2.773636000
B	-0.482348000	-1.139507000	-0.994681000
C	-0.452458000	3.696325000	0.053238000
H	-1.512950000	3.758136000	-0.158379000
C	-1.922319000	-0.604042000	-0.580396000
B	-3.275633000	-1.641496000	-0.375726000
H	-4.730469000	1.730979000	-1.768125000
C	0.091775000	-2.545623000	-0.628921000
B	-3.277274000	1.638218000	0.375573000
H	-5.695113000	1.093046000	1.081415000
H	-5.693871000	-1.098635000	-1.081995000
C	-1.923001000	0.602048000	0.580453000
B	-2.398831000	-1.011229000	1.014166000
C	0.380457000	-4.780453000	0.265474000
H	-0.044875000	-5.675054000	0.709465000
H	-4.729103000	-1.735618000	1.767718000
B	-4.152887000	1.008301000	-1.027995000
H	-3.101551000	0.693753000	2.773497000
B	-4.703388000	-0.635071000	-0.625847000
C	1.751036000	-4.711401000	0.017508000
H	2.388269000	-5.553411000	0.272207000
B	-3.253021000	-0.403169000	-1.638152000
C	2.317491000	-3.562953000	-0.553953000
H	3.388194000	-3.513419000	-0.728381000
B	-4.152096000	-1.012395000	1.027671000
H	-3.151629000	2.773528000	0.672130000
C	1.489914000	-2.497010000	-0.875686000
B	-3.253687000	0.399925000	1.637987000
H	-3.148819000	-2.776679000	-0.672251000
C	0.727916000	-0.347413000	-1.595313000
B	-4.704110000	0.630437000	0.625431000
C	3.143448000	-0.739046000	-1.766225000
H	4.011275000	-1.375788000	-1.622712000
C	3.300392000	0.559528000	-2.274325000
H	4.293595000	0.921056000	-2.524714000
C	2.194507000	1.383413000	-2.463330000
H	2.323413000	2.386471000	-2.856455000
C	0.911419000	0.930115000	-2.129362000
H	0.072968000	1.595978000	-2.277005000
C	0.088972000	2.545714000	0.629014000
C	0.375330000	4.780950000	-0.265076000
H	-0.050936000	5.675158000	-0.708965000
C	1.745971000	4.713315000	-0.017063000
H	2.382325000	5.556029000	-0.271633000
C	2.313612000	3.565371000	0.554248000
H	3.384359000	3.516921000	0.728710000
C	1.487140000	2.498522000	0.875802000
C	1.870703000	1.185799000	1.441699000
C	3.142525000	0.742149000	1.766016000
H	4.009699000	1.379753000	1.622377000
C	3.300872000	-0.556317000	2.273956000
H	4.294488000	-0.916850000	2.524144000
C	2.195867000	-1.381359000	2.463042000
H	2.325859000	-2.384314000	2.856073000
C	0.912273000	-0.929325000	2.129335000
H	0.074513000	-1.596031000	2.277076000
C	0.727365000	0.348062000	1.595416000
H	-1.508896000	-3.759674000	0.158523000
C	-0.448464000	-3.696751000	-0.053031000

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B3LYP(D3bj)_TS1-**2a**/**3a** (E = -1305.011695 a.u.)

H	-0.402181000	1.455954000	2.233658000
B	-0.531938000	1.535375000	-1.583443000
C	-3.686519000	-1.644200000	0.256708000
C	0.007164000	-1.516859000	0.263408000
B	1.125354000	-0.171838000	-0.008559000
H	-0.674131000	0.637336000	-2.334165000
H	-2.911334000	2.457912000	-1.671891000
B	-2.089107000	0.129983000	0.178542000
C	1.840420000	-0.976849000	-2.488853000
H	0.835947000	-0.859332000	-2.881014000
C	-1.317698000	1.446182000	-0.073053000
B	-1.756326000	2.946818000	0.582820000
H	-0.421817000	3.650892000	-3.047381000
C	-1.351037000	-1.221431000	0.296536000
B	0.995972000	2.382222000	-1.281793000
H	1.328816000	4.910746000	-0.854709000
H	-1.717860000	5.185437000	-0.715564000
C	0.375561000	1.270043000	-0.145925000
B	-0.357912000	2.031895000	1.205157000
C	0.403541000	-2.871779000	0.243667000
H	1.458906000	-3.125734000	0.228281000
H	-0.121625000	4.521124000	1.826976000
B	-0.404621000	3.265568000	-1.927009000
H	2.128977000	2.589184000	1.023278000
B	-1.154353000	4.153154000	-0.567817000
C	-0.557471000	-3.878696000	0.242135000
H	-0.238992000	-4.916690000	0.222869000
B	-1.864131000	2.639521000	-1.152719000
C	-1.933219000	-3.580558000	0.257376000
H	-2.661567000	-4.386095000	0.242785000
B	-0.229163000	3.772931000	0.914321000
H	1.947736000	2.059281000	-1.899337000
C	-2.325676000	-2.249897000	0.278916000
B	1.102874000	2.692862000	0.451349000
H	-2.729434000	2.976801000	1.255911000
C	-3.597489000	-0.221557000	0.207076000
B	0.609173000	3.991715000	-0.648365000
C	-4.918377000	-2.279709000	0.264817000
H	-4.993548000	-3.362892000	0.295796000
C	-6.083101000	-1.494683000	0.229645000
H	-7.053629000	-1.982185000	0.237022000
C	-6.011836000	-0.102907000	0.181917000
H	-6.924880000	0.483273000	0.153035000
C	-4.764499000	0.537862000	0.166712000
H	-4.708006000	1.621082000	0.122898000
C	2.111821000	-0.679995000	-1.152801000
C	2.864458000	-1.415684000	-3.330695000
H	2.653062000	-1.626533000	-4.374804000
C	4.162819000	-1.586853000	-2.837336000
H	4.951477000	-1.931666000	-3.499416000
C	4.447523000	-1.323313000	-1.498778000
H	5.452932000	-1.470655000	-1.115057000
C	3.422076000	-0.871088000	-0.662850000
C	3.508492000	-0.554574000	0.766413000
C	4.651343000	-0.533520000	1.569152000
H	5.619669000	-0.788870000	1.149712000
C	4.545154000	-0.169565000	2.912251000
H	5.435036000	-0.150569000	3.534398000
C	3.307455000	0.171729000	3.463580000
H	3.235505000	0.450711000	4.509879000
C	2.159420000	0.152472000	2.667872000
H	1.199533000	0.404245000	3.104218000
C	2.254810000	-0.191408000	1.318107000
H	0.991489000	-0.932768000	1.064237000

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B3LYP(D3bj)_**3a** (E = -1305.071413 a.u.)

H	-0.206371000	1.165523000	1.828978000
B	-0.484754000	1.388922000	-1.982685000
C	-3.987081000	-1.274596000	0.345834000
C	-0.351801000	-1.659385000	-0.270970000
B	0.770762000	-0.616958000	-0.546880000
H	-0.791831000	0.541113000	-2.745950000
H	-2.674010000	2.714323000	-1.946516000
B	-2.195212000	0.232178000	-0.137054000
C	2.251538000	-1.687493000	-2.275045000
H	1.340623000	-1.798583000	-2.857796000
C	-1.228246000	1.405118000	-0.436195000
B	-1.366444000	2.935039000	0.266409000
H	-0.064415000	3.496442000	-3.401567000
C	-1.659028000	-1.210699000	-0.075686000
B	1.180188000	1.958645000	-1.725049000
H	1.956176000	4.377652000	-1.256141000
H	-0.981765000	5.165546000	-0.986260000
C	0.412156000	0.940592000	-0.587332000
B	-0.128048000	1.769288000	0.819220000
C	-0.133203000	-3.054490000	-0.180251000
H	0.865678000	-3.454272000	-0.325001000
H	0.571122000	4.160026000	1.473928000
B	-0.071674000	3.080791000	-2.292144000
H	2.408833000	1.899635000	0.537730000
B	-0.604013000	4.047039000	-0.881913000
C	-1.191795000	-3.918577000	0.097383000
H	-1.004233000	-4.986260000	0.165763000
B	-1.592234000	2.696859000	-1.467939000
C	-2.503956000	-3.443121000	0.291797000
H	-3.305855000	-4.144500000	0.505452000
B	0.296491000	3.466059000	0.553879000
H	2.031951000	1.479075000	-2.386974000
C	-2.736711000	-2.076393000	0.201738000
B	1.402345000	2.191653000	0.007095000
H	-2.293088000	3.119197000	0.978545000
C	-3.713936000	0.114622000	0.148074000
B	1.097824000	3.589565000	-1.039819000
C	-5.271276000	-1.710745000	0.628802000
H	-5.486838000	-2.764422000	0.781274000
C	-6.304566000	-0.761546000	0.717966000
H	-7.314393000	-1.094103000	0.940192000
C	-6.053727000	0.596000000	0.525898000
H	-6.867090000	1.310981000	0.599153000
C	-4.753134000	1.037134000	0.239372000
H	-4.557075000	2.094721000	0.090672000
C	2.184579000	-1.107191000	-0.995353000
C	3.464370000	-2.094849000	-2.827434000
H	3.491353000	-2.519668000	-3.826199000
C	4.637765000	-1.960789000	-2.084801000
H	5.586982000	-2.289128000	-2.497327000
C	4.587166000	-1.427292000	-0.799997000
H	5.493631000	-1.366430000	-0.205738000
C	3.374818000	-0.996012000	-0.241393000
C	3.340475000	-0.461200000	1.138258000
C	4.361641000	0.378210000	1.612801000
H	5.186896000	0.633974000	0.956133000
C	4.289930000	0.936316000	2.885695000
H	5.077287000	1.602149000	3.225881000
C	3.198266000	0.664243000	3.714706000
H	3.138264000	1.110280000	4.702484000
C	2.189812000	-0.186906000	3.265775000
H	1.345638000	-0.420107000	3.907462000
C	2.266831000	-0.753398000	1.993624000
H	1.501064000	-1.453883000	1.676625000

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B3LYP(D3bj)_**2b** (E = -1205.152114 a.u.)

C	1.580164000	-1.353433000	1.358457000
B	-1.341114000	0.946254000	-0.677871000
B	1.340988000	0.946106000	0.677699000
C	-3.848603000	1.009088000	0.354970000
H	-3.799699000	2.049232000	0.667726000
C	2.773617000	0.430836000	0.314998000
C	4.991447000	0.246414000	-0.636744000
H	5.835095000	0.695648000	-1.152197000
C	5.041504000	-1.096944000	-0.263777000
H	5.925635000	-1.685223000	-0.493146000
C	3.962359000	-1.703054000	0.398249000
H	4.012476000	-2.753727000	0.670095000
C	2.840079000	-0.939255000	0.689761000
C	0.682037000	-0.255221000	1.431656000
C	1.221166000	-2.599693000	1.851409000
H	1.894809000	-3.449252000	1.780291000
C	-0.042691000	-2.754210000	2.444723000
H	-0.335493000	-3.727367000	2.828834000
C	-0.921221000	-1.677219000	2.553705000
H	-1.892384000	-1.814234000	3.018980000
C	-0.553401000	-0.420482000	2.052643000
H	-1.242904000	0.414093000	2.132234000
C	-2.773707000	0.430918000	-0.315116000
C	-4.991401000	0.246321000	0.636914000
H	-5.835032000	0.695499000	1.152443000
C	-5.041360000	-1.097068000	0.264046000
H	-5.925395000	-1.685430000	0.493572000
C	-3.962230000	-1.703107000	-0.398073000
H	-4.012260000	-2.753808000	-0.669826000
C	-2.840075000	-0.939204000	-0.689786000
C	-1.580173000	-1.353317000	-1.358550000
C	-1.221117000	-2.599562000	-1.851496000
H	-1.894699000	-3.449165000	-1.780333000
C	0.042725000	-2.754007000	-2.444864000
H	0.335573000	-3.727153000	-2.828967000
C	0.921182000	-1.676962000	-2.553909000
H	1.892330000	-1.813931000	-3.019228000
C	0.553305000	-0.420240000	-2.052852000
H	1.242742000	0.414384000	-2.132488000
C	-0.682119000	-0.255055000	-1.431811000
H	3.799557000	2.049198000	-0.667816000
C	3.848536000	1.009080000	-0.354986000
C	1.287270000	3.508125000	0.528693000
C	0.656431000	2.278649000	0.278827000
C	-0.656548000	2.278769000	-0.278948000
C	-1.287268000	3.508353000	-0.528550000
C	-0.644990000	4.719678000	-0.265163000
C	0.645098000	4.719564000	0.265567000
H	2.288246000	3.517018000	0.953105000
H	-2.288234000	3.517428000	-0.952983000
H	-1.149138000	5.659309000	-0.472542000
H	1.149324000	5.659108000	0.473156000

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B3LYP(D3bj)_TS1-**2b**/**3b** (E = -1205.095101 a.u.)

C	-3.799739000	-1.007244000	0.246068000
C	-0.118978000	-1.231184000	0.177492000
B	1.022846000	0.027051000	-0.219990000
B	-2.021200000	0.591618000	-0.100551000
C	2.236836000	-1.196115000	-2.292591000
H	1.319806000	-1.218916000	-2.875378000
C	-1.447089000	-0.819804000	0.185484000
C	0.164015000	-2.606064000	0.323647000
H	1.192836000	-2.952842000	0.333374000
C	-0.884504000	-3.516441000	0.446326000
H	-0.660315000	-4.574552000	0.546909000
C	-2.229303000	-3.098235000	0.440959000
H	-3.022736000	-3.834699000	0.535194000
C	-2.507259000	-1.742697000	0.307223000
C	-3.574913000	0.387666000	0.032213000
C	-5.084409000	-1.519515000	0.368152000
H	-5.250514000	-2.581971000	0.524026000
C	-6.176032000	-0.642132000	0.291345000
H	-7.185138000	-1.032116000	0.389480000
C	-5.978227000	0.723520000	0.092442000
H	-6.833333000	1.390681000	0.038422000
C	-4.679156000	1.235087000	-0.039843000
H	-4.543490000	2.302028000	-0.193816000
C	2.237088000	-0.627335000	-1.018795000
C	3.413633000	-1.730599000	-2.823618000
H	3.413026000	-2.160698000	-3.821140000
C	4.597047000	-1.715756000	-2.076146000
H	5.505693000	-2.138103000	-2.495339000
C	4.616147000	-1.163740000	-0.795910000
H	5.535293000	-1.160411000	-0.216468000
C	3.438762000	-0.619860000	-0.272964000
C	3.248866000	0.019644000	1.035960000
C	4.215459000	0.345511000	1.991532000
H	5.257262000	0.082929000	1.831905000
C	3.836635000	1.030627000	3.147919000
H	4.588650000	1.285746000	3.888938000
C	2.504883000	1.403420000	3.358797000
H	2.228639000	1.944110000	4.258775000
C	1.532362000	1.080566000	2.408902000
H	0.494510000	1.363904000	2.564124000
C	1.902236000	0.391448000	1.255466000
H	0.790761000	-0.532393000	0.961680000
C	-1.537220000	2.961543000	-1.003286000
C	-1.077173000	1.693018000	-0.584524000
C	0.315284000	1.391476000	-0.682508000
C	1.173185000	2.380847000	-1.190690000
C	0.694661000	3.622959000	-1.598723000
C	-0.669668000	3.922321000	-1.502998000
H	-2.598636000	3.183300000	-0.939892000
H	2.235802000	2.169142000	-1.272949000
H	1.384547000	4.362145000	-1.997455000
H	-1.041470000	4.891762000	-1.821668000

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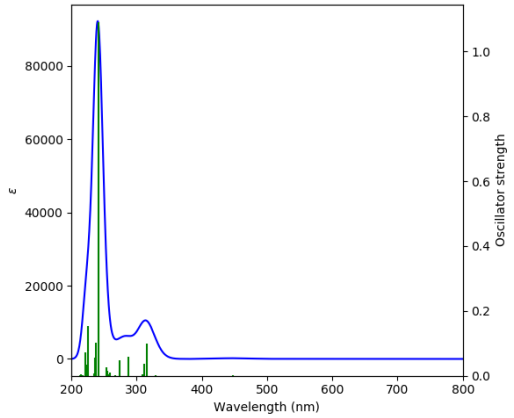
B3LYP(D3bj)_**3b** (E = -1205.154418 a.u.)

C	-3.952661000	-0.700893000	0.290209000
C	-0.394073000	-1.619271000	-0.135573000
B	0.782374000	-0.702322000	-0.601000000
B	-1.980916000	0.450522000	-0.500079000
C	2.566158000	-2.355076000	-1.400508000
H	1.775108000	-2.832425000	-1.973389000
C	-1.647586000	-1.007048000	-0.094472000
C	-0.320872000	-2.955418000	0.316764000
H	0.632458000	-3.475971000	0.327252000
C	-1.470873000	-3.614361000	0.759274000
H	-1.397739000	-4.644400000	1.097566000
C	-2.725436000	-2.975870000	0.790223000
H	-3.597396000	-3.516800000	1.148963000
C	-2.808107000	-1.653570000	0.363597000
C	-3.519783000	0.568439000	-0.210927000
C	-5.277804000	-0.920130000	0.637237000
H	-5.603978000	-1.884879000	1.016109000
C	-6.202104000	0.126946000	0.493804000
H	-7.241660000	-0.036167000	0.763836000
C	-5.800671000	1.371047000	0.011205000
H	-6.527649000	2.170985000	-0.092362000
C	-4.459936000	1.589005000	-0.339871000
H	-4.162291000	2.565131000	-0.713350000
C	2.251044000	-1.249791000	-0.590024000
C	3.870987000	-2.833959000	-1.511309000
H	4.088223000	-3.678690000	-2.158440000
C	4.893157000	-2.226227000	-0.781019000
H	5.910717000	-2.599805000	-0.848323000
C	4.602043000	-1.150225000	0.054661000
H	5.388818000	-0.701359000	0.653990000
C	3.294658000	-0.655223000	0.160979000
C	2.995760000	0.475725000	1.070381000
C	3.832597000	1.600491000	1.126262000
H	4.719880000	1.633395000	0.501082000
C	3.509927000	2.689126000	1.933403000
H	4.160864000	3.558405000	1.950486000
C	2.345465000	2.672947000	2.704597000
H	2.091331000	3.525104000	3.327550000
C	1.512706000	1.554535000	2.670215000
H	0.609977000	1.526456000	3.272979000
C	1.839635000	0.463671000	1.866741000
H	1.202928000	-0.415932000	1.871280000
C	-1.048929000	2.642142000	-1.524275000
C	-0.848248000	1.335848000	-1.053910000
C	0.464462000	0.759697000	-1.118493000
C	1.493612000	1.529437000	-1.679939000
C	1.270347000	2.827180000	-2.147204000
C	-0.002240000	3.390331000	-2.065500000
H	-2.041755000	3.080081000	-1.471761000
H	2.492107000	1.110572000	-1.750498000
H	2.091320000	3.397710000	-2.572605000
H	-0.177958000	4.400576000	-2.424157000

Cartesian coordinates of optimized structures of 2a, 2b, 3a and 3b for the TD-DFT calculations, orbital energies, and transitions

TD-DFT calculations 2a:

Calculated absorption spectrum



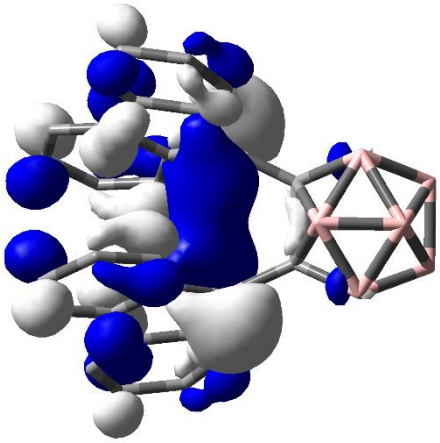
Orbital	Energy [eV]	Symmetry
L+4	-0.41	A
L+3	-0.09	A
L+2	-0.29	A
L+1	-1.72	A
LUMO	-2.04	A
HOMO	-7.53	A
H-1	-7.86	A
H-2	-8.57	A
H-3	-8.58	A
H-4	-8.94	A

TD-DFT CAMB3LYP/6-31+G(d,p), gas phase

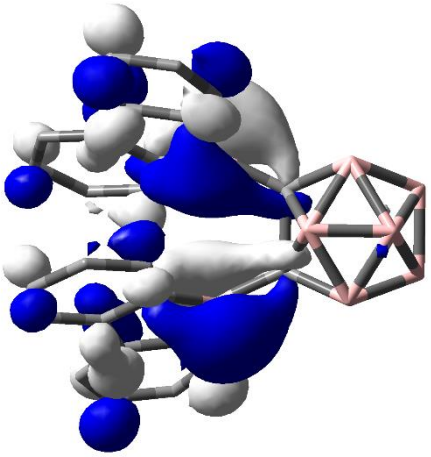
Table S6: Lowest energy singlet electronic transition of **2a** (TD-DFT CAM-B3LYP/6-31+G(d,p), gas phase).

State	E [eV]	λ [nm]	*f*	Symmetry	Major contributions	Λ
1	2.77	448.08	0.0026	Singlet-A	H-1→L+1 (22%), HOMO→LUMO (75%)	0.60
2	2.88	430.84	0.0002	Singlet-A	H-1→LUMO (51%), HOMO→L+1 (46%)	0.60
3	3.77	329.00	0.0019	Singlet-A	H-2→LUMO (12%), H-1→LUMO (35%), HOMO→L+1 (45%)	0.60
4	3.93	315.36	0.1006	Singlet-A	H-3→LUMO (14%), H-1→L+1 (54%), HOMO→LUMO (20%)	0.60
5	3.97	312.18	0.0363	Singlet-A	H-3→LUMO (54%), H-1→L+1 (21%)	0.61
6	4.02	308.27	0.0042	Singlet-A	H-3→L+1 (17%), H-2→LUMO (50%), H-1→LUMO (11%)	0.62
7	4.31	287.89	0.0582	Singlet-A	H-4→LUMO (50%), H-3→LUMO (11%), H-2→L+1 (22%)	0.63
8	4.53	273.71	0.0468	Singlet-A	H-5→LUMO (13%), H-4→L+1 (21%), H-3→L+1 (44%), H-2→LUMO (10%)	0.62
9	4.65	266.87	0.0024	Singlet-A	H-5→LUMO (44%), H-3→L+1 (25%), H-2→LUMO (10%)	0.65
10	4.78	259.22	0.0104	Singlet-A	H-5→L+1 (20%), H-4→LUMO (14%), H-3→LUMO (13%), H-2→L+1 (32%)	0.63
11	4.85	255.87	0.0047	Singlet-A	H-15→LUMO (17%), H-14→L+1 (17%), H-12→LUMO (22%), H-7→LUMO (11%)	0.44
12	4.85	255.67	0.016	Singlet-A	H-14→LUMO (22%), H-12→L+1 (11%), H-9→LUMO (10%), HOMO→L+2 (14%)	0.50
13	4.90	253.02	0.0265	Singlet-A	H-1→L+3 (10%), HOMO→L+2 (52%)	0.68
14	5.15	240.97	1.0913	Singlet-A	H-2→L+1 (18%), H-1→L+2 (26%), HOMO→L+3 (46%)	0.71
15	5.21	237.82	0.1028	Singlet-A	H-8→LUMO (16%), H-5→L+1 (13%), H-4→LUMO (20%)	0.63
16	5.24	236.69	0.0552	Singlet-A	H-6→LUMO (12%), H-5→LUMO (12%), H-4→L+1 (50%)	0.68
17	5.29	234.50	0.0072	Singlet-A	H-10→LUMO (30%)	0.45
18	5.30	233.89	0.0003	Singlet-A	H-16→LUMO (10%), H-11→LUMO (14%), H-10→L+1 (17%), H-9→LUMO (20%)	0.44
19	5.49	225.84	0.1545	Singlet-A	H-6→LUMO (59%)	0.71
20	5.52	224.63	0.0341	Singlet-A	H-8→LUMO (20%), H-6→L+1 (24%), H-5→L+1 (36%)	0.68
21	5.53	224.13	0.0296	Singlet-A	H-1→L+2 (44%), HOMO→L+3 (33%)	0.71
22	5.59	221.98	0.0722	Singlet-A	H-3→L+2 (18%), H-1→L+3 (39%), HOMO→L+2 (12%)	0.68
23	5.71	216.98	0.0023	Singlet-A	H-4→L+2 (12%), H-1→L+3 (13%), HOMO→L+9 (10%)	0.64
24	5.78	214.34	0.0021	Singlet-A	H-3→L+3 (17%), H-2→L+2 (16%), HOMO→L+6 (11%)	0.59
25	5.79	214.05	0.0034	Singlet-A	H-7→LUMO (71%)	0.34

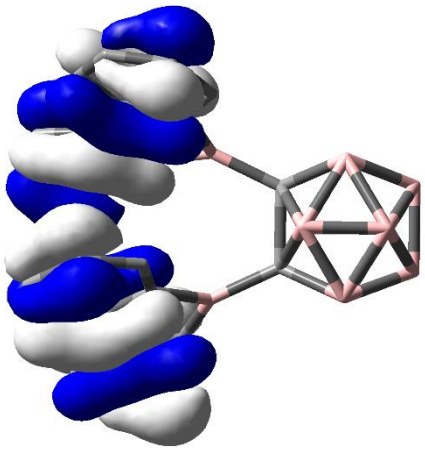
Orbitals relevant to the $S_1 \leftarrow S_o$ and $S_2 \leftarrow S_o$ transitions



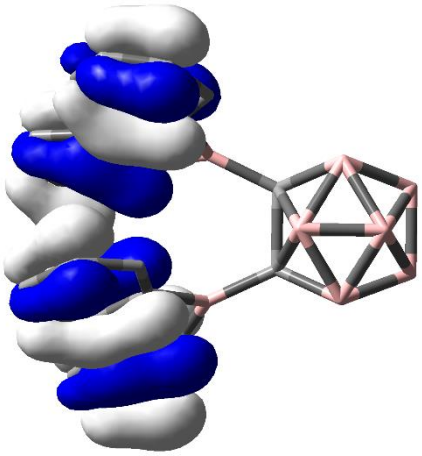
LUMO: -2.04 **eV**



LUMO+1: -1.72 **eV**



HOMO: -7.53 **eV**



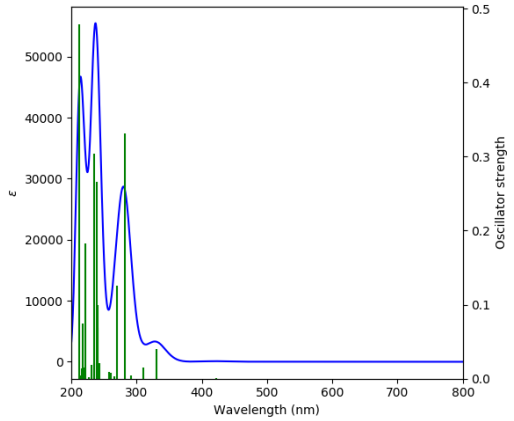
HOMO-1: -7.86 **eV**

Isovalue= 0.03

H	1.67283600	-1.59448300	-1.73728900
B	2.39100200	0.96788900	1.05534700
C	-1.86961000	-1.27415200	1.45252200
B	0.47775900	1.18248700	-0.95459200
H	1.67353600	1.59337700	1.73714400
H	3.09116100	-0.81109500	2.74327500
B	0.47710700	-1.18289000	0.95444800
C	0.46092200	3.72384700	0.03663700
H	1.51649800	3.76663000	0.27480700
C	1.91379900	-0.62775600	0.55460600
B	3.26922600	-1.65564400	0.30781500
H	4.72219000	1.65807500	1.83973700
C	-0.08688500	-2.59046100	0.57024500
B	3.27007100	1.65374100	-0.30788300
H	5.68768900	1.13862100	-1.03602400
H	5.68707000	-1.14173900	1.03606200
C	1.91414200	0.62654000	-0.55474200
B	2.39056300	-0.96935200	-1.05545900
C	-0.35909300	-4.81983800	-0.34863200
H	0.07130700	-5.70032800	-0.81544200
H	4.72144000	-1.66070900	-1.83974000
B	4.14515900	0.96649100	1.06989900
H	3.09169400	0.80928200	-2.74335500
B	4.69642100	-0.65964800	0.59946200
C	-1.72503400	-4.77973000	-0.06381300
H	-2.35331500	-5.63012300	-0.31252000
B	3.24461500	-0.47061000	1.62112100
C	-2.29640400	-3.64805300	0.53775400
H	-3.36271200	-3.62134200	0.74174300
B	4.14472200	-0.96883500	-1.06992900
H	3.14537200	2.80001300	-0.55591500
C	-1.47930900	-2.57037500	0.85220300
B	3.24492400	0.46872000	-1.62119400
H	3.14395100	-2.80184800	0.55585000
C	-0.73747400	-0.41836000	1.58792600
B	4.69677800	0.65702800	-0.59946900
C	-3.13914000	-0.86262500	1.82926600
H	-3.99803100	-1.51529100	1.70471400
C	-3.30623400	0.42239000	2.37019000
H	-4.29712100	0.75693600	2.66335600
C	-2.21097700	1.26752900	2.53479000
H	-2.34637500	2.25962100	2.95313700
C	-0.93033400	0.84771500	2.14757200
H	-0.10179600	1.52895700	2.27820800
C	-0.08531200	2.59037300	-0.57024900
C	-0.35598300	4.81983900	0.34885300
H	0.07503600	5.70001900	0.81567800
C	-1.72199100	4.78060700	0.06423000
H	-2.34970300	5.63137400	0.31309600
C	-2.29415800	3.64933900	-0.53735300
H	-3.36050900	3.62332100	-0.74121100
C	-1.47778300	2.57117500	-0.85200700
C	-1.86895700	1.27526900	-1.45243700
C	-3.13878700	0.86460700	-1.82911300
H	-3.99725100	1.51779700	-1.70437000
C	-3.30675000	-0.42020500	-2.37024500
H	-4.29787800	-0.75407500	-2.66336900
C	-2.21203700	-1.26598800	-2.53513700
H	-2.34810100	-2.25791400	-2.95366000
C	-0.93108700	-0.84704400	-2.14799000
H	-0.10300700	-1.52878200	-2.27887500
C	-0.73736100	0.41879500	-1.58810100
H	1.51405500	-3.76781100	-0.27494300
C	0.45854400	-3.72433200	-0.03662900

TD-DFT calculations 3a:

Calculated absorption spectrum



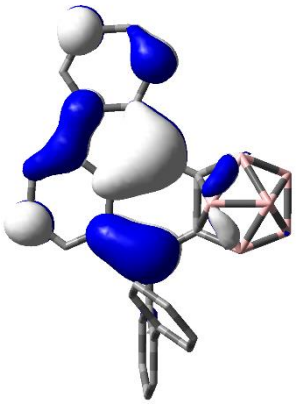
Orbital	Energy [eV]	Symmetry
L+4	0.37	A
L+3	0.15	A
L+2	-0.05	A
L+1	-1.19	A
LUMO	-2.13	A
HOMO	-7.83	A
H-1	-7.92	A
H-2	-8.52	A
H-3	-8.58	A
H-4	-8.87	A

TD-DFT CAMB3LYP/6-31+G(d,p), gas phase

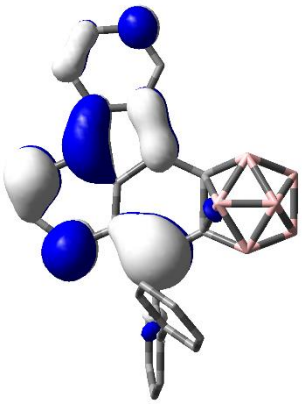
Table S7: Lowest energy singlet electronic transition of **3a** (TD-DFT CAM-B3LYP/6-31+G(d,p), gas phase).

State	E [eV]	λ [nm]	*f*	Symmetry	Major contributions	Λ
1	2.93	422.45	0.0014	Singlet-A	H-1→LUMO (85%)	0.55
2	3.74	331.07	0.0403	Singlet-A	HOMO→LUMO (64%), HOMO→L+1 (13%)	0.29
3	3.99	310.81	0.0153	Singlet-A	H-4→LUMO (39%), H-1→L+1 (39%)	0.65
4	4.25	291.41	0.004	Singlet-A	H-2→LUMO (59%), H-2→L+1 (13%), HOMO→LUMO (12%)	0.23
5	4.39	282.10	0.3311	Singlet-A	H-4→LUMO (39%), H-1→L+1 (33%)	0.65
6	4.61	269.21	0.1259	Singlet-A	H-6→LUMO (63%), H-3→LUMO (11%)	0.65
7	4.67	265.75	0.0038	Singlet-A	H-15→LUMO (12%), H-11→LUMO (25%), H-7→LUMO (14%), HOMO→L+1 (17%)	0.38
8	4.76	260.51	0.0084	Singlet-A	H-3→LUMO (62%)	0.28
9	4.81	257.75	0.0091	Singlet-A	HOMO→L+1 (46%)	0.36
10	5.09	243.52	0.0208	Singlet-A	H-5→LUMO (16%), H-2→L+2 (11%), HOMO→L+5 (18%)	0.47
11	5.12	242.11	0.0008	Singlet-A	H-14→LUMO (21%), H-13→LUMO (29%)	0.42
12	5.15	240.63	0.0688	Singlet-A	H-5→LUMO (13%), H-2→L+2 (10%)	0.46
13	5.17	239.65	0.0991	Singlet-A	H-6→L+1 (14%), H-4→L+1 (13%)	0.56
14	5.20	238.29	0.2662	Singlet-A	H-5→LUMO (10%), HOMO→L+2 (57%)	0.68
15	5.28	235.03	0.0206	Singlet-A	H-9→LUMO (15%), H-8→LUMO (22%)	0.50
16	5.28	234.80	0.3035	Singlet-A	H-6→LUMO (12%), H-4→L+1 (38%)	0.61
17	5.37	230.98	0.0188	Singlet-A	H-9→LUMO (13%), H-5→LUMO (28%), H-3→L+2 (11%)	0.39
18	5.39	230.19	0.0023	Singlet-A	H-2→LUMO (13%), H-2→L+1 (44%)	0.29
19	5.46	227.26	0.0021	Singlet-A	H-11→LUMO (24%), H-7→LUMO (50%)	0.35
20	5.62	220.79	0.1826	Singlet-A	H-10→LUMO (16%), H-9→LUMO (15%), H-1→L+3 (26%)	0.56
21	5.67	218.63	0.0146	Singlet-A	H-15→LUMO (37%), H-9→LUMO (13%)	0.48
22	5.69	217.86	0.011	Singlet-A	H-10→LUMO (46%), H-8→LUMO (15%), H-3→L+1 (14%)	0.50
23	5.70	217.35	0.0744	Singlet-A	H-10→LUMO (20%), H-3→L+1 (49%)	0.36
24	5.75	215.55	0.0142	Singlet-A	H-12→LUMO (79%)	0.42
25	5.81	213.56	0.0047	Singlet-A	H-14→LUMO (23%), H-13→LUMO (38%)	0.38

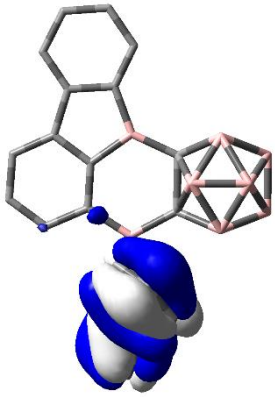
Orbitals relevant to the $S_1 \leftarrow S_o$ and $S_2 \leftarrow S_o$ transitions



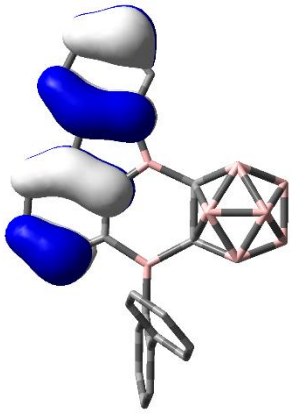
LUMO: -2.13 **eV**



LUMO+1: -1.19 **eV**



HOMO: -7.83 **eV**



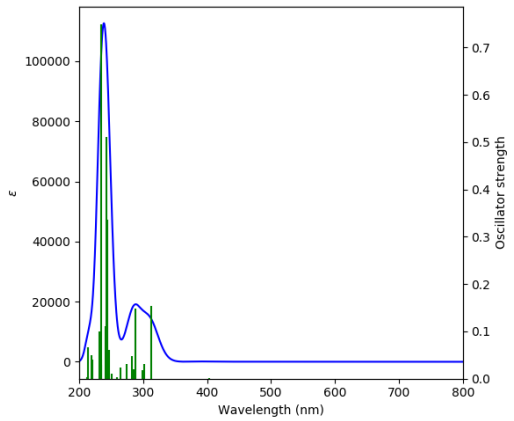
HOMO-1: -7.92 **eV**

Isovalue= 0.03

H	-0.11437800	1.00249100	1.90953000
B	-0.66272300	1.70243700	-1.83068800
C	-3.94761000	-1.40795800	0.21882800
C	-0.31763500	-1.55962400	-0.55747600
B	0.77129200	-0.44580200	-0.69711300
H	-0.99693100	0.95728500	-2.68533400
H	-2.87763800	2.94547900	-1.48300900
B	-2.22158200	0.23059900	-0.07412900
C	2.36030800	-1.11549000	-2.52665200
H	1.47682400	-1.10399400	-3.16134200
C	-1.30477100	1.48123600	-0.24723600
B	-1.43151900	2.91268700	0.66071900
H	-0.38941200	3.99032900	-2.98385800
C	-1.63424000	-1.19017600	-0.25562200
B	1.00646300	2.29015700	-1.60384400
H	1.75081900	4.65951800	-0.87036500
H	-1.18719000	5.30375200	-0.31109700
C	0.34311000	1.09949000	-0.55994900
B	-0.12464600	1.72832300	0.97855400
C	-0.05962400	-2.94633100	-0.69729900
H	0.94301300	-3.29059800	-0.93364200
H	0.55371400	4.04042900	1.89621900
B	-0.31197800	3.43530900	-1.93861800
H	2.38989500	1.97381700	0.55092900
B	-0.77361700	4.19382500	-0.37950100
C	-1.08415600	-3.88041500	-0.53543800
H	-0.86341700	-4.93831500	-0.64812700
B	-1.76706600	2.89584600	-1.07576900
C	-2.40167900	-3.48515800	-0.22775500
H	-3.17552100	-4.23910700	-0.10877100
B	0.23788500	3.46281900	0.90991500
H	1.82589900	1.93845900	-2.37892000
C	-2.67523700	-2.12821700	-0.08796600
B	1.33994100	2.30494500	0.12986400
H	-2.31116500	2.97699800	1.45061100
C	-3.73055000	0.00507400	0.23887600
B	0.92918500	3.81988200	-0.70463000
C	-5.20787700	-1.93710000	0.46170900
H	-5.38151100	-3.00971200	0.44737900
C	-6.27409500	-1.05939500	0.73076200
H	-7.26338500	-1.46553000	0.92242500
C	-6.07860400	0.32204200	0.75395400
H	-6.91402000	0.98335100	0.96296500
C	-4.80371200	0.85646300	0.50677800
H	-4.65702700	1.93255400	0.52511000
C	2.23206500	-0.81651300	-1.15402000
C	3.59598900	-1.40005300	-3.10850100
H	3.65963900	-1.60986700	-4.17223600
C	4.74161600	-1.41624500	-2.31134800
H	5.71043700	-1.64713600	-2.74476700
C	4.63442400	-1.15611500	-0.94639400
H	5.52058800	-1.21100600	-0.32090200
C	3.39702800	-0.85659300	-0.34784400
C	3.35372900	-0.63108600	1.12467200
C	4.32654900	0.16512400	1.75712700
H	5.08720700	0.65507300	1.15651200
C	4.30370600	0.36637000	3.13688100
H	5.05664700	0.99776400	3.59997700
C	3.30870600	-0.22738700	3.92031500
H	3.28978100	-0.06838400	4.99443600
C	2.34118300	-1.02648500	3.30907500
H	1.57023400	-1.50417700	3.90707100
C	2.36604100	-1.22850400	1.92636000
H	1.63072900	-1.88633000	1.47437100

TD-DFT calculations 2b:

Calculated absorption spectrum



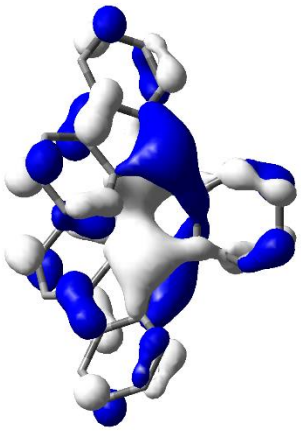
Orbital	Energy [eV]	Symmetry
L+4	0.67	A
L+3	0.18	A
L+2	0.06	A
L+1	-1.10	A
LUMO	-1.54	A
HOMO	-7.32	A
H-1	-7.37	A
H-2	-8.11	A
H-3	-8.25	A
H-4	-8.29	A

TD-DFT CAMB3LYP/6-31+G(d, p), gas phase

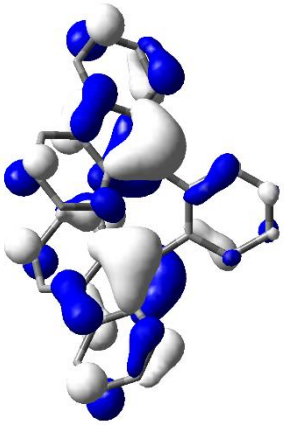
Table S8: Lowest energy singlet electronic transition of **2b** (TD-DFT CAM-B3LYP/6-31+G(d,p), gas phase).

State	E [eV]	λ [nm]	*f*	Symmetry	Major contributions	Λ
1	3.07	403.46	0.0016	Singlet-A	H-1→L+1 (30%), HOMO→LUMO (66%)	0.61
2	3.10	400.57	0.0001	Singlet-A	H-1→LUMO (62%), HOMO→L+1 (35%)	0.61
3	3.97	312.68	0.1529	Singlet-A	H-2→LUMO (83%)	0.61
4	4.11	301.61	0.0315	Singlet-A	H-4→L+1 (10%), H-3→LUMO (46%), H-1→L+1 (14%)	0.66
5	4.15	298.63	0.0173	Singlet-A	H-4→LUMO (45%), H-3→L+1 (17%), HOMO→L+2 (11%)	0.68
6	4.31	287.37	0.1489	Singlet-A	H-5→LUMO (67%)	0.56
7	4.34	285.63	0.0197	Singlet-A	H-1→LUMO (34%), HOMO→L+1 (52%)	0.62
8	4.39	282.70	0.0481	Singlet-A	H-1→L+1 (51%), HOMO→LUMO (29%)	0.63
9	4.53	273.78	0.0319	Singlet-A	H-2→L+1 (70%)	0.56
10	4.68	265.18	0.0236	Singlet-A	H-7→L+1 (12%), H-6→LUMO (50%)	0.72
11	4.79	258.88	0.0038	Singlet-A	H-7→LUMO (41%), H-6→L+1 (25%)	0.75
12	4.95	250.37	0.0103	Singlet-A	H-10→LUMO (19%), H-5→L+1 (42%), H-4→L+1 (17%)	0.56
13	5.03	246.43	0.0616	Singlet-A	H-4→LUMO (28%), H-1→L+3 (21%), HOMO→L+2 (28%)	0.69
14	5.08	243.91	0.3361	Singlet-A	H-10→LUMO (39%), H-3→LUMO (12%), H-1→L+2 (12%), HOMO→L+3 (11%)	0.60
15	5.10	242.93	0.5115	Singlet-A	H-10→LUMO (17%), H-5→L+1 (15%), H-3→LUMO (17%), H-1→L+2 (17%), HOMO→L+3 (15%)	0.64
16	5.14	241.28	0.1113	Singlet-A	H-3→L+1 (46%), HOMO→L+2 (15%)	0.69
17	5.29	234.49	0.0401	Singlet-A	H-12→LUMO (36%), H-11→L+1 (24%), H-4→L+1 (11%)	0.60
18	5.30	233.92	0.0296	Singlet-A	H-13→LUMO (20%), H-12→L+1 (13%), H-11→LUMO (29%), H-10→L+1 (23%)	0.53
19	5.30	233.91	0.7495	Singlet-A	H-5→L+1 (20%), H-4→L+1 (31%)	0.66
20	5.36	231.29	0.0998	Singlet-A	H-13→LUMO (19%), H-11→LUMO (14%), H-10→L+1 (20%), H-3→L+1 (13%)	0.58
21	5.62	220.63	0.0395	Singlet-A	H-12→LUMO (11%), H-9→LUMO (26%), H-8→L+1 (11%), H-6→LUMO (19%)	0.69
22	5.64	219.69	0.0496	Singlet-A	H-11→LUMO (11%), H-9→L+1 (10%), H-8→LUMO (35%)	0.70
23	5.78	214.32	0.0665	Singlet-A	H-6→L+1 (13%), H-5→LUMO (11%), H-2→L+5 (22%)	0.64
24	5.80	213.68	0.0049	Singlet-A	H-7→LUMO (13%), H-4→L+3 (13%), H-3→L+2 (21%)	0.69
25	5.82	212.99	0.0029	Singlet-A	H-9→LUMO (23%), H-7→L+1 (11%), H-6→LUMO (17%)	0.73

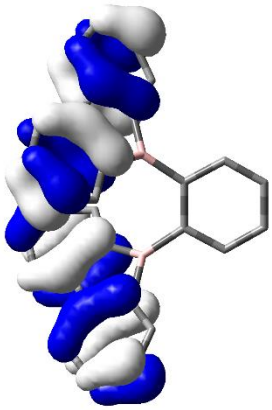
Orbitals relevant to the $S_1 \leftarrow S_o$ and $S_2 \leftarrow S_o$ transitions



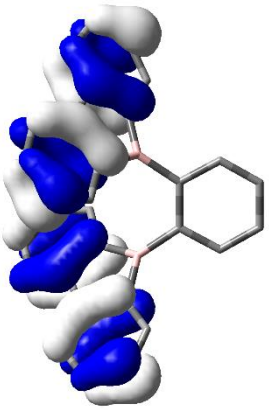
LUMO: -1.54 **eV**



LUMO+1: -1.10 **eV**



HOMO: -7.32 **eV**



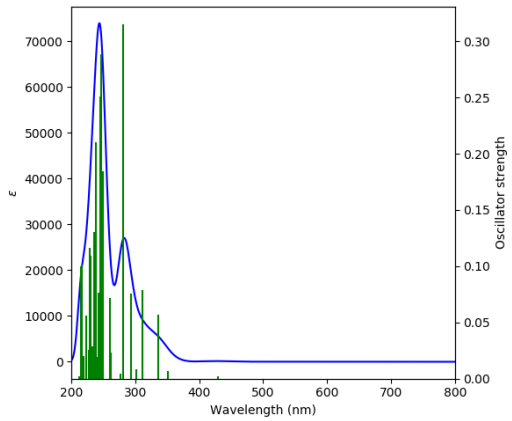
HOMO-1: -7.37 **eV**

Isovalue= 0.03

B	1.54656300	0.77025200	-0.41969800
B	-1.54649400	0.77027300	0.41962900
C	-1.22882400	-0.41785100	1.39776300
C	-0.15304600	-0.69239100	2.24415100
H	0.69777000	-0.01752600	2.28951800
C	-0.16236500	-1.84501700	3.04618100
H	0.67868800	-2.06119900	3.69850700
C	-1.25508500	-2.71284300	3.00801500
H	-1.25856500	-3.60242600	3.63212200
C	-2.35713800	-2.44647100	2.17736100
H	-3.20419500	-3.12743600	2.16910000
C	-2.34039000	-1.30543500	1.38302600
C	-3.38749800	-0.80584900	0.45080200
C	-4.61142600	-1.38151300	0.12620200
H	-4.92710300	-2.32250700	0.56901800
C	-5.44732500	-0.72855500	-0.79564200
H	-6.40550100	-1.17066700	-1.05515500
C	-5.05932000	0.47661400	-1.38447400
H	-5.71512600	0.96594600	-2.09892000
C	-3.82090500	1.05130700	-1.05464000
H	-3.52004100	1.98444400	-1.52519700
C	-2.97966100	0.42513200	-0.13307000
C	-0.70297100	2.04896900	0.13047400
C	-1.36575600	3.28918200	0.24157500
H	-2.43360800	3.30368800	0.44478800
C	-0.68642300	4.50447900	0.12372100
H	-1.22717400	5.44185300	0.22205500
C	0.68647100	4.50451100	-0.12366600
H	1.22719200	5.44191100	-0.22192300
C	1.36584400	3.28924800	-0.24161700
H	2.43369300	3.30380400	-0.44485100
C	0.70311400	2.04900900	-0.13060800
C	1.22879800	-0.41793300	-1.39772400
C	0.15298000	-0.69248400	-2.24405800
H	-0.69779500	-0.01757000	-2.28946400
C	0.16219900	-1.84518900	-3.04597500
H	-0.67888700	-2.06138000	-3.69825500
C	1.25486400	-2.71308100	-3.00775600
H	1.25826700	-3.60272700	-3.63177500
C	2.35696100	-2.44669800	-2.17716500
H	3.20397400	-3.12771800	-2.16886300
C	2.34030800	-1.30558700	-1.38293700
C	3.38748500	-0.80597000	-0.45080500
C	4.61140900	-1.38165300	-0.12623000
H	4.92701900	-2.32270400	-0.56897200
C	5.44739400	-0.72863800	0.79549700
H	6.40556600	-1.17076700	1.05499700
C	5.05947800	0.47660600	1.38423300
H	5.71534900	0.96598300	2.09858900
C	3.82106600	1.05132000	1.05442100
H	3.52026600	1.98450800	1.52491500
C	2.97973900	0.42509200	0.13296200

TD-DFT calculations 3b:

Calculated absorption spectrum



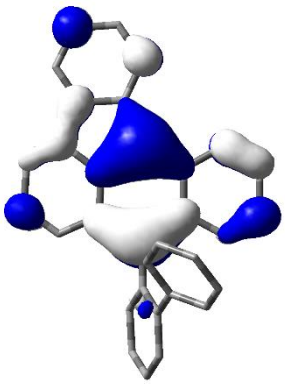
Orbital	Energy [eV]	Symmetry
L+4	0.63	A
L+3	0.37	A
L+2	0.16	A
L+1	-0.67	A
LUMO	-1.81	A
HOMO	-7.38	A
H-1	-7.62	A
H-2	-8.11	A
H-3	-8.24	A
H-4	-8.32	A

TD-DFT CAMB3LYP/6-31+G(d,p), gas phase

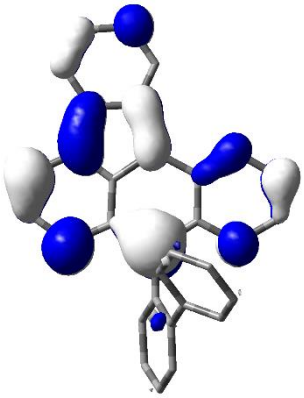
Table S9: Lowest energy singlet electronic transition of **3b** (TD-DFT CAM-B3LYP/6-31+G(d,p), gas phase).

State	E [eV]	λ [nm]	*f*	Symmetry	Major contributions	Λ
1	2.89	429.67	0.0022	Singlet-A	HOMO→LUMO (91%)	0.51
2	3.54	350.44	0.0066	Singlet-A	H-2→LUMO (89%)	0.60
3	3.70	335.18	0.0571	Singlet-A	H-3→LUMO (16%), H-1→LUMO (62%)	0.34
4	3.98	311.74	0.0791	Singlet-A	H-4→LUMO (56%), HOMO→L+1 (23%)	0.60
5	4.11	301.52	0.008	Singlet-A	H-9→LUMO (28%), H-3→LUMO (26%), H-1→LUMO (14%)	0.50
6	4.23	293.04	0.0753	Singlet-A	H-6→LUMO (24%), H-3→LUMO (13%), HOMO→L+1 (23%)	0.54
7	4.41	281.31	0.3153	Singlet-A	H-6→LUMO (25%), H-4→LUMO (17%), HOMO→L+1 (24%)	0.62
8	4.49	276.13	0.0047	Singlet-A	H-9→LUMO (29%), H-3→LUMO (22%)	0.53
9	4.74	261.55	0.0231	Singlet-A	H-11→LUMO (46%), H-5→LUMO (27%)	0.47
10	4.77	260.19	0.0716	Singlet-A	H-11→LUMO (30%), H-5→LUMO (41%)	0.43
11	4.96	249.72	0.1841	Singlet-A	H-8→LUMO (16%), H-2→L+1 (10%), H-1→L+1 (18%), HOMO→L+1 (11%)	0.55
12	5.03	246.61	0.2885	Singlet-A	H-2→L+1 (45%), H-1→L+1 (23%)	0.50
13	5.05	245.74	0.2508	Singlet-A	H-12→LUMO (10%), H-8→LUMO (14%), H-1→L+1 (17%)	0.55
14	5.10	243.01	0.0764	Singlet-A	H-12→LUMO (20%), H-7→LUMO (12%), H-3→L+2 (10%), H-1→L+5 (12%)	0.53
15	5.16	240.19	0.019	Singlet-A	H-12→LUMO (37%), H-1→L+5 (10%)	0.51
16	5.21	238.12	0.2103	Singlet-A	H-1→L+2 (48%)	0.67
17	5.26	235.51	0.1306	Singlet-A	H-3→L+2 (12%), H-1→L+2 (26%)	0.760
18	5.31	233.29	0.0288	Singlet-A	H-10→LUMO (23%), H-9→LUMO (14%), H-8→LUMO (29%)	0.67
19	5.38	230.27	0.1095	Singlet-A	H-7→LUMO (16%), H-6→LUMO (13%), H-4→L+1 (17%)	0.56
20	5.43	228.32	0.1167	Singlet-A	H-9→L+1 (12%), H-7→LUMO (27%), H-3→L+1 (12%)	0.47
21	5.46	227.00	0.0253	Singlet-A	H-13→LUMO (16%), H-9→L+1 (12%), H-1→L+1 (11%)	0.51
22	5.55	223.40	0.056	Singlet-A	H-4→L+1 (36%), HOMO→L+3 (23%)	0.58
23	5.66	219.15	0.0198	Singlet-A	H-13→LUMO (36%), H-3→L+1 (36%)	0.42
24	5.73	216.23	0.1017	Singlet-A	H-6→L+1 (40%), H-5→L+1 (12%)	0.59
25	5.77	214.90	0.0996	Singlet-A	H-10→LUMO (11%), H-8→L+1 (10%), HOMO→L+3 (11%), HOMO→L+12 (14%)	0.64

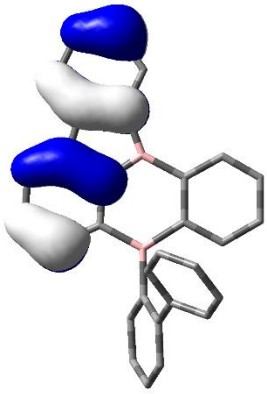
Orbitals relevant to the $S_1 \leftarrow S_o$ and $S_2 \leftarrow S_o$ transitions



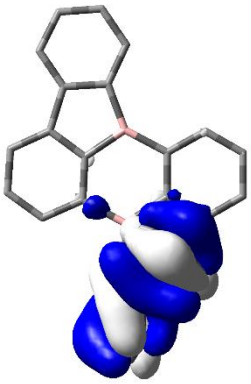
LUMO: -1.81 **eV**



LUMO+1: -0.67 **eV**



HOMO: -7.38 **eV**



HOMO-1: -7.62 **eV**

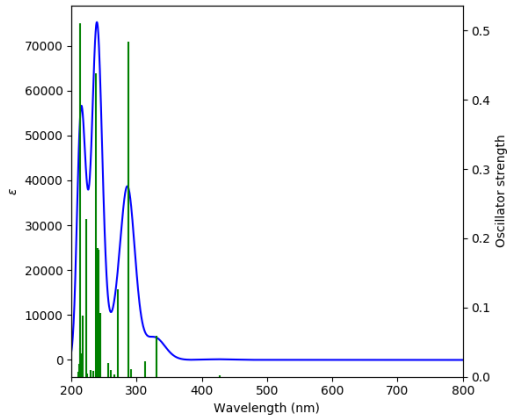
Isovalue= 0.03

C	4.01006900	0.68943100	0.36383000
C	0.43005200	1.52432700	-0.11335700
B	-0.72385700	0.59121100	-0.62791500
B	2.07660800	-0.50699000	-0.46751900
C	-2.42304500	2.16556000	-1.68631600
H	-1.58168500	2.55512800	-2.25524300
C	1.69948800	0.94017200	-0.05059200
C	0.32325100	2.86154600	0.33657100
H	-0.63747700	3.36955700	0.32423400
C	1.45075300	3.54495100	0.80503200
H	1.34787400	4.57312300	1.14219000
C	2.71901500	2.93337800	0.85787100
H	3.57148600	3.49494100	1.23237100
C	2.83832900	1.61316500	0.42747400
C	3.61951900	-0.58611600	-0.15761500
C	5.32570300	0.94015000	0.73557400
H	5.62167500	1.90858600	1.13050600
C	6.28265100	-0.07982200	0.59657600
H	7.31294900	0.10909800	0.88568100
C	5.92283400	-1.33020600	0.09283600
H	6.67255900	-2.10962700	-0.00831600
C	4.59264400	-1.58016200	-0.28289800
H	4.33068700	-2.56049800	-0.67231200
C	-2.19730000	1.14785000	-0.73612400
C	-3.69872200	2.67110800	-1.94304400
H	-3.83693100	3.44418000	-2.69375600
C	-4.78977800	2.18316900	-1.22083000
H	-5.78660100	2.57807500	-1.39582500
C	-4.59084600	1.19922100	-0.25299100
H	-5.43396400	0.85026700	0.33672200
C	-3.31256700	0.67067100	0.00095000
C	-3.15444000	-0.35827900	1.06633300
C	-4.06195200	-1.42723200	1.17941700
H	-4.87238300	-1.51724400	0.46154200
C	-3.91702800	-2.39027000	2.17887500
H	-4.62354200	-3.21351900	2.23877300
C	-2.86164800	-2.30496500	3.09225100
H	-2.74799700	-3.05520400	3.86932900
C	-1.95637400	-1.24578000	2.99744000
H	-1.13822800	-1.16167600	3.70713800
C	-2.10379200	-0.28187900	1.99735400
H	-1.41305600	0.55524000	1.95850200
C	1.20746100	-2.71651800	-1.52831800
C	0.96756400	-1.41801900	-1.04798300
C	-0.36214800	-0.87388400	-1.12798300
C	-1.36286800	-1.67178400	-1.70884200
C	-1.09920700	-2.96147600	-2.18536800
C	0.18806400	-3.48987800	-2.09209700
H	2.21008000	-3.13093600	-1.46776500
H	-2.37211100	-1.28086800	-1.79502800
H	-1.89946500	-3.54926900	-2.62715700
H	0.39830400	-4.49103400	-2.45857400

CAM-B3LYP-Hexane

TD-DFT calculations 3a:

Calculated absorption spectrum



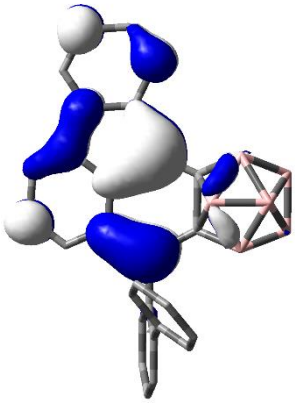
Orbital	Energy [eV]	Symmetry
L+4	0.42	A
L+3	0.20	A
L+2	-0.04	A
L+1	-1.15	A
LUMO	-2.10	A
HOMO	-7.81	A
H-1	-7.87	A
H-2	-8.51	A
H-3	-8.57	A
H-4	-8.81	A

TD-DFT CAMB3LYP/6-31+G(d, p), n-Hexane

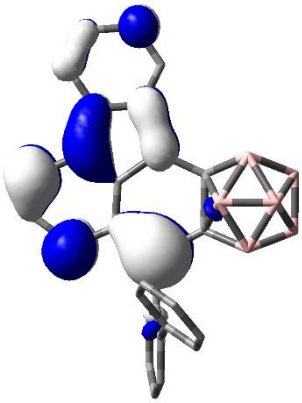
Table S10: Lowest energy singlet electronic transition of **3a** (TD-DFT CAM-B3LYP/6-31+G(d, p), n-hexane).

State	E [eV]	λ [nm]	*f*	Symmetry	Major contributions	Λ
1	2.90	427.41	0.0021	Singlet-A	H-1→LUMO (68%), HOMO→LUMO (25%)	0.51
2	3.75	330.81	0.059	Singlet-A	H-1→LUMO (16%), HOMO→LUMO (52%), HOMO→L+1 (12%)	0.41
3	3.97	312.24	0.0231	Singlet-A	H-4→LUMO (40%), H-1→L+1 (33%)	0.62
4	4.26	291.15	0.0106	Singlet-A	H-2→LUMO (59%), H-2→L+1 (13%), HOMO→LUMO (10%)	0.25
5	4.32	286.97	0.4836	Singlet-A	H-4→LUMO (39%), H-1→L+1 (30%), HOMO→L+1 (10%)	0.63
6	4.57	271.09	0.1269	Singlet-A	H-6→LUMO (69%)	0.68
7	4.67	265.29	0.0036	Singlet-A	H-15→LUMO (10%), H-11→LUMO (24%), H-8→LUMO (24%), HOMO→L+1 (12%)	0.42
8	4.77	259.90	0.0097	Singlet-A	H-3→LUMO (66%)	0.29
9	4.83	256.73	0.02	Singlet-A	H-1→L+1 (10%), HOMO→L+1 (41%)	0.47
10	5.09	243.65	0.0928	Singlet-A	H-5→LUMO (11%), H-2→L+2 (10%), HOMO→L+2 (19%), HOMO→L+5 (12%)	0.53
11	5.12	242.17	0.1836	Singlet-A	H-7→LUMO (29%), H-6→L+1 (21%), H-4→L+1 (14%)	0.65
12	5.13	241.49	0.0104	Singlet-A	H-14→LUMO (17%), H-13→LUMO (34%)	0.42
13	5.16	240.37	0.1856	Singlet-A	H-2→L+2 (11%), HOMO→L+2 (20%)	0.61
14	5.17	239.72	0.1557	Singlet-A	H-5→LUMO (28%), HOMO→L+2 (21%)	0.47
15	5.23	236.85	0.4388	Singlet-A	H-7→LUMO (13%), H-6→LUMO (11%), H-4→L+1 (35%)	0.62
16	5.31	233.54	0.0083	Singlet-A	H-9→LUMO (24%), H-5→LUMO (19%)	0.34
17	5.39	230.01	0.0096	Singlet-A	H-9→LUMO (16%), H-5→LUMO (22%), H-3→L+2 (11%)	0.37
18	5.41	228.97	0.0015	Singlet-A	H-9→LUMO (19%), H-2→LUMO (10%), H-2→L+1 (35%)	0.30
19	5.54	223.80	0.005	Singlet-A	H-11→LUMO (33%), H-8→LUMO (34%)	0.41
20	5.56	222.95	0.2281	Singlet-A	H-7→LUMO (39%), H-1→L+3 (22%)	0.65
21	5.71	217.06	0.0881	Singlet-A	H-3→L+1 (58%)	0.31
22	5.74	216.09	0.0345	Singlet-A	H-15→LUMO (34%), H-9→LUMO (24%)	0.43
23	5.80	213.86	0.0415	Singlet-A	H-10→LUMO (85%)	0.40
24	5.80	213.66	0.5111	Singlet-A	H-6→L+1 (36%), H-4→L+1 (10%)	0.60
25	5.85	212.11	0.019	Singlet-A	H-12→LUMO (82%)	0.33

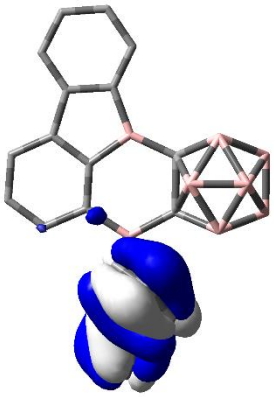
Orbitals relevant to the $S_1 \leftarrow S_o$ and $S_2 \leftarrow S_o$ transitions



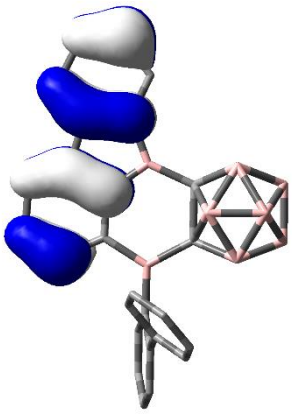
LUMO: -2.10 **eV**



LUMO+1: -1.15 **eV**



HOMO: -7.81 **eV**



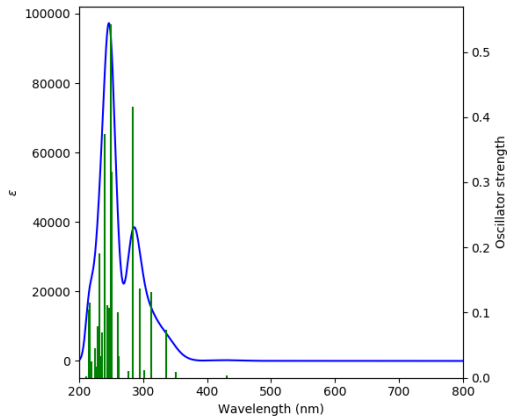
HOMO-1: -7.87 **eV**

Isovalue= 0.03

H	-0.11437800	1.00249100	1.90953000
B	-0.66272300	1.70243700	-1.83068800
C	-3.94761000	-1.40795800	0.21882800
C	-0.31763500	-1.55962400	-0.55747600
B	0.77129200	-0.44580200	-0.69711300
H	-0.99693100	0.95728500	-2.68533400
H	-2.87763800	2.94547900	-1.48300900
B	-2.22158200	0.23059900	-0.07412900
C	2.36030800	-1.11549000	-2.52665200
H	1.47682400	-1.10399400	-3.16134200
C	-1.30477100	1.48123600	-0.24723600
B	-1.43151900	2.91268700	0.66071900
H	-0.38941200	3.99032900	-2.98385800
C	-1.63424000	-1.19017600	-0.25562200
B	1.00646300	2.29015700	-1.60384400
H	1.75081900	4.65951800	-0.87036500
H	-1.18719000	5.30375200	-0.31109700
C	0.34311000	1.09949000	-0.55994900
B	-0.12464600	1.72832300	0.97855400
C	-0.05962400	-2.94633100	-0.69729900
H	0.94301300	-3.29059800	-0.93364200
H	0.55371400	4.04042900	1.89621900
B	-0.31197800	3.43530900	-1.93861800
H	2.38989500	1.97381700	0.55092900
B	-0.77361700	4.19382500	-0.37950100
C	-1.08415600	-3.88041500	-0.53543800
H	-0.86341700	-4.93831500	-0.64812700
B	-1.76706600	2.89584600	-1.07576900
C	-2.40167900	-3.48515800	-0.22775500
H	-3.17552100	-4.23910700	-0.10877100
B	0.23788500	3.46281900	0.90991500
H	1.82589900	1.93845900	-2.37892000
C	-2.67523700	-2.12821700	-0.08796600
B	1.33994100	2.30494500	0.12986400
H	-2.31116500	2.97699800	1.45061100
C	-3.73055000	0.00507400	0.23887600
B	0.92918500	3.81988200	-0.70463000
C	-5.20787700	-1.93710000	0.46170900
H	-5.38151100	-3.00971200	0.44737900
C	-6.27409500	-1.05939500	0.73076200
H	-7.26338500	-1.46553000	0.92242500
C	-6.07860400	0.32204200	0.75395400
H	-6.91402000	0.98335100	0.96296500
C	-4.80371200	0.85646300	0.50677800
H	-4.65702700	1.93255400	0.52511000
C	2.23206500	-0.81651300	-1.15402000
C	3.59598900	-1.40005300	-3.10850100
H	3.65963900	-1.60986700	-4.17223600
C	4.74161600	-1.41624500	-2.31134800
H	5.71043700	-1.64713600	-2.74476700
C	4.63442400	-1.15611500	-0.94639400
H	5.52058800	-1.21100600	-0.32090200
C	3.39702800	-0.85659300	-0.34784400
C	3.35372900	-0.63108600	1.12467200
C	4.32654900	0.16512400	1.75712700
H	5.08720700	0.65507300	1.15651200
C	4.30370600	0.36637000	3.13688100
H	5.05664700	0.99776400	3.59997700
C	3.30870600	-0.22738700	3.92031500
H	3.28978100	-0.06838400	4.99443600
C	2.34118300	-1.02648500	3.30907500
H	1.57023400	-1.50417700	3.90707100
C	2.36604100	-1.22850400	1.92636000
H	1.63072900	-1.88633000	1.47437100

TD-DFT calculations 3b:

Calculated absorption spectrum



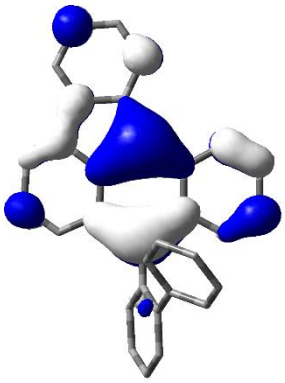
Orbital	Energy [eV]	Symmetry
L+4	0.63	A
L+3	0.34	A
L+2	0.13	A
L+1	-0.70	A
LUMO	-1.84	A
HOMO	-7.41	A
H-1	-7.65	A
H-2	-8.15	A
H-3	-8.27	A
H-4	-8.35	A

TD-DFT CAMB3LYP/6-31+G(d,p), n-Hexane

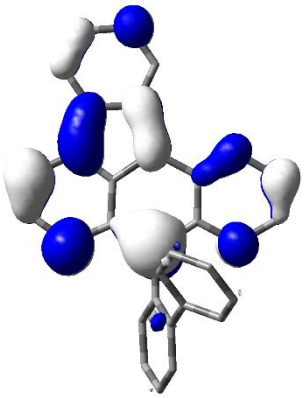
Table S11: Lowest energy singlet electronic transition of **3b** (TD-DFT CAM-B3LYP/6-31+G(d,p), *n*-Hexane).

State	E [eV]	λ [nm]	*f*	Symmetry	Major contributions	Λ
1	2.88	430.44	0.0031	Singlet-A	HOMO→LUMO (91%)	0.51
2	3.53	350.79	0.0091	Singlet-A	H-2→LUMO (89%)	0.60
3	3.69	335.95	0.0738	Singlet-A	H-3→LUMO (16%), H-1→LUMO (62%)	0.34
4	3.96	313.04	0.1311	Singlet-A	H-4→LUMO (61%), HOMO→L+1 (19%)	0.60
5	4.11	301.89	0.0114	Singlet-A	H-9→LUMO (30%), H-3→LUMO (25%), H-1→LUMO (13%)	0.50
6	4.21	294.42	0.1364	Singlet-A	H-6→LUMO (17%), H-3→LUMO (12%), HOMO→L+1 (31%)	0.54
7	4.37	283.97	0.4162	Singlet-A	H-6→LUMO (32%), H-4→LUMO (14%), HOMO→L+1 (21%)	0.62
8	4.48	276.50	0.0099	Singlet-A	H-9→LUMO (30%), H-3→LUMO (22%)	0.53
9	4.73	261.88	0.0332	Singlet-A	H-11→LUMO (43%), H-5→LUMO (28%)	0.47
10	4.76	260.65	0.1	Singlet-A	H-11→LUMO (33%), H-5→LUMO (38%)	0.45
11	4.93	251.34	0.3167	Singlet-A	H-8→LUMO (13%), H-2→L+1 (31%), HOMO→L+1 (11%)	0.59
12	4.98	249.08	0.5429	Singlet-A	H-8→LUMO (10%), H-2→L+1 (39%), H-1→L+1 (12%)	0.55
13	5.03	246.34	0.1075	Singlet-A	H-1→L+1 (39%)	0.46
14	5.09	243.47	0.1119	Singlet-A	H-12→LUMO (24%), H-7→LUMO (10%), H-1→L+5 (10%)	0.54
15	5.16	240.42	0.0123	Singlet-A	H-12→LUMO (34%), H-1→L+5 (11%)	0.51
16	5.16	240.04	0.3739	Singlet-A	H-1→L+2 (62%)	0.72
17	5.25	236.02	0.0694	Singlet-A	H-5→L+2 (10%), H-3→L+2 (15%)	0.53
18	5.29	234.53	0.0334	Singlet-A	H-10→LUMO (25%), H-9→LUMO (12%), H-8→LUMO (31%)	0.70
19	5.37	231.05	0.1904	Singlet-A	H-6→LUMO (12%), H-4→L+1 (22%), HOMO→L+3 (11%)	0.60
20	5.42	228.71	0.0785	Singlet-A	H-9→L+1 (12%), H-7→LUMO (40%), H-3→L+1 (11%)	0.43
21	5.46	227.27	0.0174	Singlet-A	H-13→LUMO (18%), H-9→L+1 (14%), H-1→L+1 (11%)	0.51
22	5.52	224.48	0.0452	Singlet-A	H-10→LUMO (11%), H-4→L+1 (39%), HOMO→L+3 (24%)	0.58
23	5.65	219.41	0.0255	Singlet-A	H-13→LUMO (32%), H-3→L+1 (37%)	0.41
24	5.71	217.24	0.1148	Singlet-A	H-13→LUMO (12%), H-6→L+1 (43%), H-5→L+1 (12%)	0.60
25	5.76	215.40	0.1041	Singlet-A	H-10→LUMO (13%), H-8→L+1 (11%), HOMO→L+11 (16%)	64

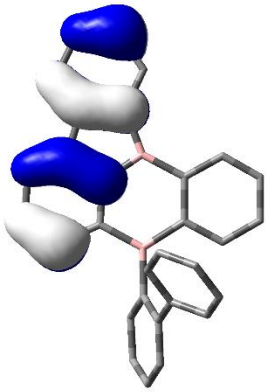
Orbitals relevant to the $S_1 \leftarrow S_o$ and $S_2 \leftarrow S_o$ transitions



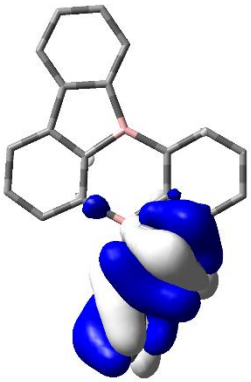
LUMO: -1.84 **eV**



LUMO+1: -0.70**eV**



HOMO: -7.41 **eV**



HOMO-1: -7.65 **eV**

Isovalue= 0.03

C	4.01006900	0.68943100	0.36383000
C	0.43005200	1.52432700	-0.11335700
B	-0.72385700	0.59121100	-0.62791500
B	2.07660800	-0.50699000	-0.46751900
C	-2.42304500	2.16556000	-1.68631600
H	-1.58168500	2.55512800	-2.25524300
C	1.69948800	0.94017200	-0.05059200
C	0.32325100	2.86154600	0.33657100
H	-0.63747700	3.36955700	0.32423400
C	1.45075300	3.54495100	0.80503200
H	1.34787400	4.57312300	1.14219000
C	2.71901500	2.93337800	0.85787100
H	3.57148600	3.49494100	1.23237100
C	2.83832900	1.61316500	0.42747400
C	3.61951900	-0.58611600	-0.15761500
C	5.32570300	0.94015000	0.73557400
H	5.62167500	1.90858600	1.13050600
C	6.28265100	-0.07982200	0.59657600
H	7.31294900	0.10909800	0.88568100
C	5.92283400	-1.33020600	0.09283600
H	6.67255900	-2.10962700	-0.00831600
C	4.59264400	-1.58016200	-0.28289800
H	4.33068700	-2.56049800	-0.67231200
C	-2.19730000	1.14785000	-0.73612400
C	-3.69872200	2.67110800	-1.94304400
H	-3.83693100	3.44418000	-2.69375600
C	-4.78977800	2.18316900	-1.22083000
H	-5.78660100	2.57807500	-1.39582500
C	-4.59084600	1.19922100	-0.25299100
H	-5.43396400	0.85026700	0.33672200
C	-3.31256700	0.67067100	0.00095000
C	-3.15444000	-0.35827900	1.06633300
C	-4.06195200	-1.42723200	1.17941700
H	-4.87238300	-1.51724400	0.46154200
C	-3.91702800	-2.39027000	2.17887500
H	-4.62354200	-3.21351900	2.23877300
C	-2.86164800	-2.30496500	3.09225100
H	-2.74799700	-3.05520400	3.86932900
C	-1.95637400	-1.24578000	2.99744000
H	-1.13822800	-1.16167600	3.70713800
C	-2.10379200	-0.28187900	1.99735400
H	-1.41305600	0.55524000	1.95850200
C	1.20746100	-2.71651800	-1.52831800
C	0.96756400	-1.41801900	-1.04798300
C	-0.36214800	-0.87388400	-1.12798300
C	-1.36286800	-1.67178400	-1.70884200
C	-1.09920700	-2.96147600	-2.18536800
C	0.18806400	-3.48987800	-2.09209700
H	2.21008000	-3.13093600	-1.46776500
H	-2.37211100	-1.28086800	-1.79502800
H	-1.89946500	-3.54926900	-2.62715700
H	0.39830400	-4.49103400	-2.45857400

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