Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

for the paper

Effects of boron doping on the structural and optoelectronic properties of 9,10-diarylanthracenes

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Content:

1) Syntheses and Spectroscopic Characterisation of 2a, 2b, Li_2[2a] and 4a-c

Experimental Methods. Unless otherwise specified, all reactions were carried out under dry nitrogen or argon using carefully dried and degassed solvents, flame-dried glassware and Schlenk or glove box techniques. Toluene, C_6D_6, Et_2O, THF and THF-d_8 were dried over Na/benzophenone. Solvents used for UV/vis spectroscopic measurements were purchased as spectroscopic grade, dried over Na/K alloy (C_6H_{12}, C_6H_6, THF) or CaH_2 (CH_2Cl_2) and degassed prior to use. Other solvents (pentane, hexane, $CHCl_3$, CH_2Cl_2, MeOH) were purchased as reagent grade and used without further purification. Column chromatography was performed using silica gel 60 (Macherey-Nagel). NMR spectra were recorded with Bruker Avance 300 or Avance 400 spectrometers at r. t. Chemical shifts are referenced to (residual) solvent signals ($^1H/^{13}C\{^1H\}$; C_6D_6: δ = 7.16/128.06; THF-d_8: δ = 3.58/25.30), external $BF_3{\cdot}Et_2O$ (^{11}B, $^{11}B\{^1H\}$) or external LiCl ($^7Li\{^1H\}$; 1.0 M in H_2O). Abbreviations: s = singlet, d = doublet, dd = doublet of doublets, t = triplet, m = multiplet, app. = apparent, *i* = *ipso*, *o* = *ortho*, *m* = *meta*, *p* = *para*. Electrochemical measurements were performed at r. t. by using an EG&G Princeton Applied Research 263A potentiostat with a platinum disc working electrode (diameter 2.00 mm). The reference electrode was a silver wire on which AgCl had been deposited by immersing the wire into HCl/HNO_3 (3:1). The solvent (THF) was dried over Na/K alloy without added benzophenone at r. t. and degassed by five freeze-pump-thaw cycles. [*n*Bu_4N][PF_6] (0.1 M) was employed as the supporting electrolyte. All potential values are referenced against the FcH/FcH^+ couple ($E_{1/2}$ = 0 V). UV/vis absorption spectra were recorded with a Varian Cary 50 Scan UV/vis spectrophotometer; for *in situ* UV/vis monitoring experiments an immersion probe from Hellma (10.00 mm) was employed. UV/vis emission spectra were recorded with a Spectrofluorometer FP-8300 (Jasco). The absolute fluorescence quantum yields (ϕ_f) were determined using a calibrated integrating sphere system (ILF-835 100 mm dia. Integrating Sphere; Jasco), a quantum yield calculation program (FWQE-880; Jasco) and highly diluted samples of ten different optical densities in each measurement. Mass spectra were recorded with a Fisons Instruments VG TofSpec mass spectrometer. The compounds **1**[1] and 10-bromo-9-phenyl-2,7-di-*tert*-butylanthracene[2] were prepared according to literature procedures. Combustion analyses were performed by the Microanalytical Laboratory of the Goethe-University.

Synthesis of 2a. A solution (0.45 M) of the Grignard reagent MesMgBr was prepared in THF. An aliquot (4.4 mL, 2.0 mmol) was transferred into a Schlenk vessel, all volatiles were removed under reduced pressure, the resulting brown oil was dissolved in toluene (10 mL) and the solution added dropwise with stirring at 0 °C to a solution of **1** (300 mg, 0.899 mmol) in toluene (50 mL). The reaction mixture was allowed to warm to r. t. overnight, whereupon a colourless precipitate formed. After filtration, all volatiles were removed from the filtrate in vacuo to yield a yellow solid. Deionised H_2O (20 mL) and $CHCl_3$ (50 mL) were added, the resulting two liquid phases were separated and the aqueous layer was extracted with $CHCl_3$ (3 × 15 mL). The combined organic layers were dried over $MgSO_4$, filtered and the filtrate was evaporated in vacuo. The crude product was purified by column chromatography (silica gel 60; $CHCl_3$) and dried for 4 h at r. t. under dynamic vacuum (single crystals of **2a** suitable for X-ray diffraction were obtained by slow evaporation of a toluene solution). Yield: 277 mg, 75 % (Found: C, 87.22; H, 7.13. Calc. for $C_{30}H_{30}B_2$ [412.16]: C, 87.42; H, 7.34). R_f = 0.91 (silica gel; $CHCl_3$).

^{1}H NMR (300.0 MHz, C_6D_6): δ = 2.12 (s, 12 H, CH_3-*o*), 2.34 (s, 6 H, CH_3-*p*), 6.92 (s, 4 H, Mes-*m*), 7.14 (m, 4 H, H-b), 7.80 (m, 4 H, H-a); ^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6): δ = 21.4 (CH_3-*p*), 22.8 (CH_3-*o*), 127.6 (Mes-*m*), 134.0 (C-b), 137.0 (Mes-*p*), 138.1 (Mes-*o*), 139.4 (C-a) , 141.3 (Mes-*i*), 145.8 (C-c); ^{11}B{^{1}H} NMR (96.3 MHz, C_6D_6): δ = 73 ($h_{1/2}$ = 2000 Hz).

^{1}H NMR (400.1 MHz, THF-d_8): δ = 2.02 (s, 12 H, CH_3-*o*), 2.35 (s, 6 H, CH_3-*p*), 6.89 (s, 4 H, Mes-*m*), 7.46 (m, 4 H, H-b), 7.59 (m, 4 H, H-a); ^{13}C{^{1}H} NMR (100.6 MHz, THF-d_8): δ = 21.4 (CH_3-*p*), 22.7 (CH_3-*o*), 127.8 (Mes-*m*), 134.3 (C-b), 137.4 (Mes-*p*), 138.3 (Mes-*o*), 139.6 (C-a), 141.6 (Mes-*i*), 146.1 (C-c); ^{11}B{^{1}H} NMR (128.4 MHz, THF-d_8): δ = 72.3 ($h_{1/2}$ = 2000 Hz); UV/vis (C_6H_6): λ_{max} (ε) = 349 nm (10400 $dm^3mol^{-1}cm^{-1}$); fluorescence (C_6H_6): λ_{max} = 460 nm (λ_{ex} = 350 nm).

Synthesis of Li_2[2a]. A lithium granule (7 mg, 1 mmol) was added to a clear, bright yellow solution of **2a** (6.5 mg, 0.016 mmol) in THF (0.5 mL) under an atmosphere of argon, whereupon the colour of the solution instantaneously turned red. After the mixture had been kept at r. t. for 12 h, the residual lithium was removed. Dark red single crystals of $[Li(THF)_2]_2$[**2a**] formed by slow evaporation of the solvent (24 h). Yield: 10 mg, 87 %. $[Li(Et_2O)]_2$[**2a**] was obtained in the form of orange crystals through the reduction of **2a** in Et_2O instead of THF.

^{1}H NMR (300.0 MHz, THF-d_8): δ = 2.23 (s, 12 H, CH_3-*o*), 2.32 (s, 6 H, CH_3-*p*), 6.56 (m, 4 H, H-b), 6.88 (s, 4 H, Mes-*m*), 7.69 (m, 4 H, H-a); ^{13}C{^{1}H} NMR (75.5 MHz, THF-d_8): δ = 21.4

(CH_3-*p*), 25.1 (CH_3-*o*), 118.8 (C-b), 127.7 (Mes-*m*), 133.3 (Mes-*p*), 134.9 (C-c), 137.5 (C-a), 141.5 (Mes-*o*), 148.3 (Mes-*i*); $^{11}B\{^1H\}$ NMR (96.3 MHz, THF-d_8): δ = 28 ($h_{1/2}$ = 500 Hz). $^7Li\{^1H\}$ NMR (97.2 MHz, THF-d_8): δ = 0.4, −7.2.

Synthesis of 2b. 1,2-Dibromoethane (0.100 mL, 0.218 mg, 1.16 mmol) was added to a mixture of Mg turnings (169 mg, 6.96 mmol) and 1-bromo-2-methylnaphthalene (95 % purity; 162 mg, 0.696 mmol) in THF (20 mL). The mixture was heated at reflux temperature for 3 h and then allowed to cool to r. t. The Grignard solution was transferred via syringe into another flask to separate it from residual Mg turnings. All volatiles were removed under reduced pressure and the pale fawn solid residue was dissolved in Et_2O-toluene (1:1, 30 mL). **1** (100 mg, 0.300 mmol) in toluene (15 mL) was added at 0 °C, the resulting bright yellow mixture was stirred for 15 min and allowed to warm to r. t. overnight. All volatiles were removed in vacuo, the crude solid product was washed with non-dried MeOH (3 × 3 mL) and further purified by flash column chromatography (silica gel 60; hexane, then hexane-$CHCl_3$ = 2:1). In analytically pure form, **2b** is a yellow solid (single crystals of *anti*-**2b** were grown by gas-phase diffusion of hexane into a concentrated C_6H_6 solution). Yield: 98 mg, 72 % (Found: C, 89.58; H, 5.83. Calc. for $C_{34}H_{26}B_2$ [456.19]: C, 89.52; H, 5.74). R_f = 0.64 (silica gel; hexane-$CHCl_3$ = 2:1).

^1H NMR (300.0 MHz, C_6D_6): δ = 2.25 (s, 6 H, CH_3), 2.30 (s, 6 H, CH_3'), 6.95 (m, 8 H, H-b,b'), 7.04 (m, 2 H, H-7), 7.10 (m, 2 H, H-7'), 7.21 (m, 2 H, H-6), 7.27 (m, 2 H, H-6'), 7.34 (d, $^3J_{HH}$ = 8.3 Hz, 2 H, H-3), 7.36 (d, $^3J_{HH}$ = 8.3 Hz, 2 H, H-3'), 7.60–7.69 (m, 12 H, H-8,8',a,a'), 7.79–7.84 (m, 8 H, H-4,4',5,5'); ^{11}B NMR (96.3 MHz, C_6D_6): δ = 71 ($h_{1/2}$ = 1200 Hz); $^{13}C\{^1H\}$ NMR (75.4 MHz, C_6D_6): δ = 23.1 (CH_3), 23.3 (CH_3'), 2 × 125.2 (C-6,6'), 2 × 125.8 (C-7,7'), 127.9 (C-4,4'), 128.6 (C-5,5'), 128.8 (C-3,3'), 129.7 (C-8), 129.8 (C-8'), 132.1 (C-4a,4a'), 134.3 (C-b,b'), 135.9 (C-2 or 2'), 136.0 (C-2 or 2'), 136.5 (C-8a or 8a'), 136.6 (C-8a or 8a'), 140.2 (C-a,a'), 142.1 (C-1,1'), 146.0 (C-c, C-c'); UV/vis (C_6H_6): λ_{max} (ε) = 357 (8600), 422 nm (1300 $mol^{-1}dm^3cm^{-1}$); fluorescence (C_6H_6): λ_{max} = 513 nm (λ_{ex} = 420 nm); MS (MALDI): *m*/*z* (%): 456 (100) [M^+].

Synthesis of 4a. *n*BuLi in hexane (1.53 M, 29 mL, 44 mmol) was added dropwise with stirring at −78 °C to a solution of 2-bromomesitylene (5.74 g, 28.8 mmol) in Et_2O (40 mL). Stirring was continued for 15 min, the reaction mixture was allowed to warm to r. t. within 1 h and stirred for another 1 h. The resulting turbid yellow solution was cooled to −78 °C again, a suspension of **3** (3.00 g, 14.4 mmol) in THF (80 mL) was added slowly with stirring and the

intensely red-coloured mixture obtained was allowed to warm to r. t. overnight. Aqueous HCl (10 %, 40 mL), saturated with $SnCl_2$, was added dropwise with stirring, stirring was continued for 24 h at r. t., deionised H_2O (500 mL) was added and the aqueous suspension was extracted with $CHCl_3$ (5 × 100 mL). The combined extracts were dried over anhydrous $MgSO_4$, filtered, and the filtrate was evaporated to dryness under vacuum. The solid residue was dissolved in $CHCl_3$ (30 mL) and added to MeOH (300 mL) without stirring, whereupon pale yellow crystalline needles formed. Analytically pure **4a** was obtained by column chromatography (silica gel 60; hexane-$CHCl_3$ = 5:1) as a colourless solid. Yield: 2.24 g, 38 % (Found: C, 92.68; H, 7.32. Calc. for $C_{32}H_{30}$ [414.56]: C, 92.71; H, 7.29). R_f = 0.67 (silica gel; hexane-$CHCl_3$ = 3:1).

^{1}H NMR (300.0 MHz, C_6D_6): δ = 1.84 (s, 12 H, CH_3-*o*), 2.35 (s, 6 H, CH_3-*p*), 7.03 (s, 4 H, Mes-*m*), 7.13 (m, 4 H, H-b), 7.76 (m, 4 H, H-a); ^{13}C{^{1}H} NMR (75.4 MHz, C_6D_6): δ = 20.2 (CH_3-*o*), 21.3 (CH_3-*p*), 126.0 (C-b), 126.8 (C-a), 128.9 (Mes-*m*), 130.4 (C-c), 135.4 (Mes-*i*), 136.0 (C-d), 137.2 (Mes-*p*), 137.8 (Mes-*o*). UV/vis (C_6H_6): λ_{max} (ε) = 399 nm (22300 $mol^{-1}dm^3cm^{-1}$); fluorescence (C_6H_6): λ_{max} = 403 nm (λ_{ex} = 358 nm); MS (MALDI): *m*/*z* (%): 414 (100) [M^+].

Synthesis of 4b. *n*BuLi in hexane (1.72 M, 17.9 mL, 30.8 mmol) was added dropwise with stirring at −78 °C to a solution of 1-bromo-2-methylnaphthalene (95 % purity, 5.26 g, 22.6 mmol) in Et_2O (35 mL). Stirring was continued for 15 min before the reaction mixture was warmed to r. t. within 1 h. The resulting turbid solution was cooled to −78 °C again, a suspension of **3** (2.14 g, 10.3 mmol) in THF (30 mL) was added dropwise with stirring and the reaction mixture was allowed to warm to r. t. overnight. The reaction was quenched with glacial acetic acid (10 mL), whereupon an off-white precipitate formed. The precipitate was isolated by filtration, the filtrate was extracted with $CHCl_3$ (3 × 20 mL) and the combined extracts were evaporated to dryness under vacuum. The solid residue and the precipitate were placed into a round-bottom flask and treated with glacial acetic acid (60 mL), aqueous H_3PO_2 (50 %, 10 mL) and aqueous HI (57 %, 3 mL). The resulting turbid suspension was heated to 80 °C for 2 h. After cooling to r. t., all insolubles were collected on a frit and washed with MeOH (3 × 50 mL) and pentane (2 × 50 mL) to obtain a 1:1 mixture of *anti*-**4b** and *syn*-**4b** as a pale fawn solid.

In order to separate the two isomers, the isomer mixture was recrystallised from a hot saturated C_6H_6 solution, which gave single crystals of *anti*-**4b** within 12 h at r. t. The mother liquor was isolated, evaporated to dryness and the residue was recrystallised again. After 5-6

such recrystallisation steps, the mother liquor was sufficiently enriched in *syn*-**4b** to provide single crystals of this isomer, too. Combined yield of *anti*-**4b** and *syn*-**4b**: 4.29 g, 91 % (Found: C, 93.49; H, 5.84. Calc. for $C_{36}H_{26}$ [458.59] × 0.05 CH_2Cl_2 [84.93]: C, 93.55; H, 5.68; the relative amount of CH_2Cl_2 present in the sample was confirmed by ^{1}H NMR spectroscopy).

anti-**4b**: ^{1}H NMR (300.0 MHz, C_6D_6): δ = 2.05 (s, 6 H, CH_3), 6.90–6.98 (m, 6 H, H-7,b), 7.20 (m, 2 H, H-6), 7.29 (d, $^3J_{HH}$ = 8.5 Hz, 2 H, H-8), 7.46 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, H-3), 7.57 (m, 4 H, H-a), 7.82 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, H-5), 7.88 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, H-4); ^{13}C{^{1}H} NMR (75.4 MHz, C_6D_6): δ = 20.6 (CH_3), 125.5 (C-6), 126.2 (C-b), 126.8 (C-7 or 8), 126.9 (C-7 or 8), 127.2 (C-a), 128.6 (C-4,5), 129.2 (C-3), 131.1 (C-c), 133.0 (C-4a), 134.6 (C-8a), 135.0 (C-d), 135.2 (C-1), 136.0 (C-2); UV/vis (C_6H_6): λ_{max} (ε) = 399 (17900 $mol^{-1}dm^3cm^{-1}$); fluorescence (C_6H_6): λ_{max} = 404 nm (λ_{ex} = 358 nm); MS (MALDI): *m*/*z* (%): 458 (100) [M^+].

syn-**4b**: ^{1}H NMR (400.1 MHz, C_6D_6): δ = 1.97 (s, 6 H, CH_3), 6.93 (m, 4 H, H-b), 7.01 (m, 2 H, H-7), 7.24 (m, 2 H, H-6), 7.41 (d, $^3J_{HH}$ = 8.8 Hz, 2 H, H-8), 7.44 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, H-3), 7.57 (m, 4 H, H-a), 7.84 (d, $^3J_{HH}$ = 8.0 Hz, 2 H, H-5), 7.88 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, H-4); ^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6): δ = 20.4 (CH_3), 125.6 (C-6), 126.2 (C-b), 126.9 (C-7), 127.0 (C-8), 127.2 (C-a), 128.6 (C-4,5), 129.2 (C-3), 131.1 (C-c), 132.9 (C-4a), 134.5 (C-8a), 135.0 (C-d), 135.2 (C-1), 135.9 (C-2).

Synthesis of 4c. *n*BuLi in hexane (1.53 M, 1.10 mL, 1.68 mmol) was diluted with hexane (3 mL) and added dropwise with stirring at −78 °C to a solution of 10-bromo-9-phenyl-2,7-di-*tert*-butylanthracene (500 mg, 1.12 mmol) in Et_2O (40 mL). Stirring was continued for 15 min before the reaction mixture was warmed to r. t. within 1 h. The resulting turbid yellow solution was cooled to −78 °C again, a suspension of **3** (117 mg, 0.562 mmol) in THF (20 mL) was added dropwise with stirring and the intensely red-coloured reaction mixture was allowed to warm to r. t. overnight. Aqueous HCl (10 %, 20 mL), saturated with $SnCl_2$, was added dropwise with stirring, stirring was continued for 12 h at r. t., deionised H_2O (30 mL) was added and the aqueous suspension was extracted with CH_2Cl_2 (5 × 20 mL). The combined extracts were washed with water (2 × 20 mL), dried over anhydrous $MgSO_4$, filtered, and the filtrate was evaporated to dryness under vacuum. The solid residue was washed with MeOH (4 × 10 mL), followed by flash column chromatography (silica gel 60; hexane, then hexane-$CHCl_3$ = 2:1) to obtain **4c** as a pale fawn solid. Yield: 365 mg, 72 % (Found: C, 92.64; H, 7.36. Calc. for $C_{70}H_{66}$ [907.27]: C, 92.67; H, 7.33). R_f = 0.74 (silica gel, hexane-$CHCl_3$ = 2:1).

^{1}H NMR (400.1 MHz, C_6D_6): δ = 1.21 (s, 36 H, C(CH_3)$_3$), 6.86 (m, 4 H, H-b), 7.24 (dd, $^{3}J_{HH}$ = 9.2 Hz, $^{4}J_{HH}$ = 1.0 Hz, 4 H, H-3,6), 7.42 (t, $^{3}J_{HH}$ = 7.6 Hz, 2 H, H-*p*), 7.54 (app. t, 4 H, H-*m*), 7.72 (m, 4 H, H-a), 7.79 (d, $^{3}J_{HH}$ = 9.2 Hz, 4 H, H-4,5), 7.89 (d, $^{3}J_{HH}$ = 7.2 Hz, 4 H, H-*o*), 8.19 (d, $^{4}J_{HH}$ = 1.0 Hz, 4 H, H-1,8); ^{13}C{^{1}H} NMR (75.4 MHz, C_6D_6): δ = 30.9 (C(CH_3)$_3$), 35.1 (C(CH_3)$_3$), 122.0 (C-1,8), 125.7 (C-3,6), 126.4 (C-b), ≈127.5* (C-4,5), ≈127.7* (C-*p*, C-a), 128.9 (C-*m*), 130.7 (C-4a,10a), 131.2 (C-8a,9a), 132.0 (C-*o*), 132.4 (C-c), 133.4 (C-10), 135.2 (C-d), 138.0 (C-9), 140.4 (C-*i*), 147.9 (C-2,7); UV/vis (C_6H_6): λ_{max} (ε) = 406 (47700 mol^{-1}dm^{3}cm^{-1}); fluorescence (C_6H_6): λ_{max} = 442 nm (λ_{ex} = 380 nm); MS (MALDI): *m*/*z* (%): 907 (100) [M^{+}]. *These resonances are hidden underneath the solvent signal; their chemical shift values were taken from the cross peaks in an HSQC spectrum.

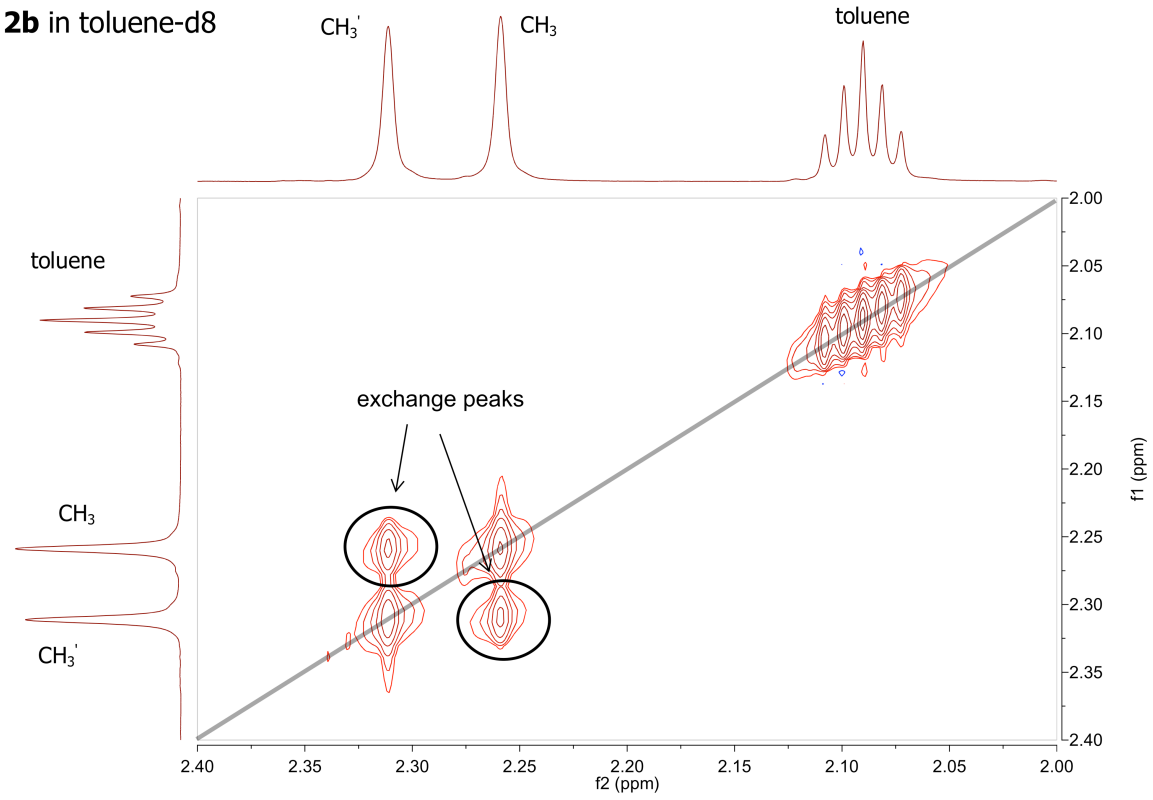


Figure S1: ROESY NMR spectrum of *syn/anti*-**2b** in toluene-d_8 at r.t. showing the exchange peaks between the resonances of the methyl groups of *syn/anti*-**2b** (CH_3, CH_3').

2) Details of the X-ray Crystal Structure Analyses of 2a, $[Li(THF)_2]_2$[2a], $[Li(Et_2O)]_2$[2a], *anti*-2b, 4a, *anti*-4b, and *syn*-4b

Crystal structure analyses: Data collections for **2a**, $[Li(THF)_2]_2$[**2a**], $[Li(Et_2O)]_2$[**2a**] and *anti*-**2b** were performed on a Stoe IPDS-II two-circle diffractometer with graphite-monochromated MoK_α radiation (λ = 0.71073 Å). Data for **4a**, *anti*-**4b** and *syn*-**4b** were collected on a STOE IPDS II two-circle diffractometer with a Genix Microfocus X-ray source with mirror optics using MoK_α radiation (λ = 0.71073 Å). Equivalent reflections were averaged. The structures were solved by direct methods using the program SHELXS[3] and refined with full-matrix least-squares on F^2 using the program SHELXL-97[4]. All H atoms were geometrically positioned and refined using a riding model. All methyl groups were allowed to rotate but not to tip.

In $[Li(THF)_2]_2$[**2a**] one methylene group in a THF molecule is disordered over two sites with a site occupation factor of 0.512(9) for the major occupied site. The disordered atoms were isotropically refined.

CCDC reference numbers: CCDC-922259 (**2a**), 922260 ($[Li(THF)_2]_2$[**2a**]), 922261 ($[Li(Et_2O)]_2$[**2a**]), 922262 (*anti*-**2b**), 922263 (**4a**), 922264 (*anti*-**4b**), 922265 (*syn*-**4b**).

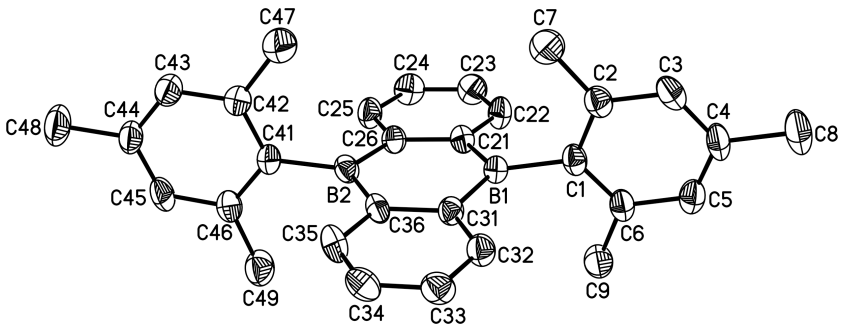


Figure S2: Molecular structure of **2a** in the solid state; displacement ellipsoids at the 50 % probability level, H atoms omitted for clarity. Selected bond lengths (Å), (bond) angles (deg) and dihedral angles (deg): B(1)−C(1) 1.580(5), B(1)−C(21) 1.562(4), B(1)−C(31) 1.560(5), B(2)−C(41) 1.578(5), B(2)−C(26) 1.566(5), B(2)−C(36) 1.562(5), C(21)−C(26) 1.418(4), C(31)−C(36) 1.426(4); C(1)−B(1)−C(21) 120.9(3), C(1)−B(1)−C(31) 119.7(3), C(21)−B(1)−C(31) 119.4(3), C(26)−B(2)−C(36) 118.9(3), C(26)−B(2)−C(41) 120.2(3), C(36)−B(2)−C(41) 120.9(3), C(1)···COG···C(41) 169.2; Ar(C1)//C(21)B(1)C(31) 89.3(2), Ar(C41)//C(26)B(2)C(36) 87.3(2), Ar(C1)//Ar(C41) 5.9(2), Ar(C21)//Ar(C31) 6.6(1); Ar = phenyl/phenylene.

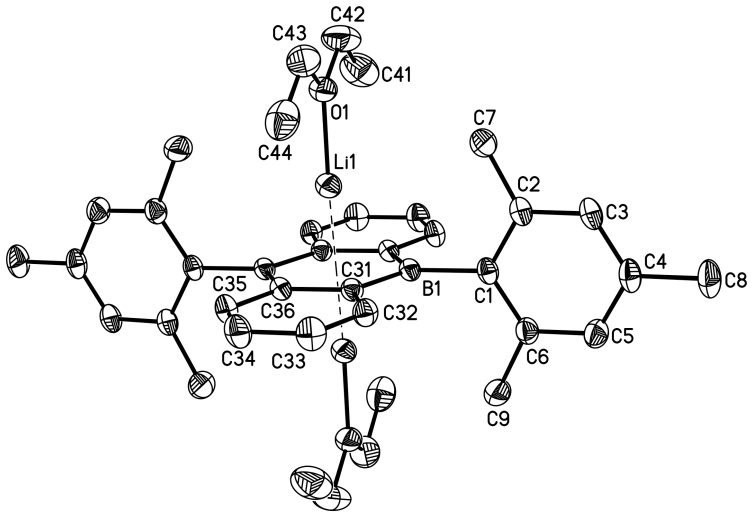


Figure S3: Molecular structure of $[Li(Et_2O)_2]_2$[**2a**] in the solid state; displacement ellipsoids at the 50 % probability level, H atoms omitted for clarity. Selected bond lengths (Å), bond angles (deg) and dihedral angle (deg): B(1)−C(1) 1.606(2), B(1)−C(31) 1.534(2), B(1)−C(36A) 1.533(2), C(31)−C(36) 1.473(2), C(31)−C(32) 1.443(2), C(32)−C(33) 1.359(2), C(33)−C(34) 1.423(2), C(34)−C(35) 1.359(2), C(35)−C(36) 1.442(2), Li(1)···COG(B_2C_4) 1.740; C(1)−B(1)−C(31) 120.4(1), C(1)−B(1)−C(36A) 123.5(1), C(31)−B(1)−C(36A) 116.2(1); Ar(C1)//C(31)B(1)C(36A) 87.8(1); Ar = phenyl. Symmetry transformation used to generate equivalent atoms: A: −x+3/2, −y+1/2, −z+1.

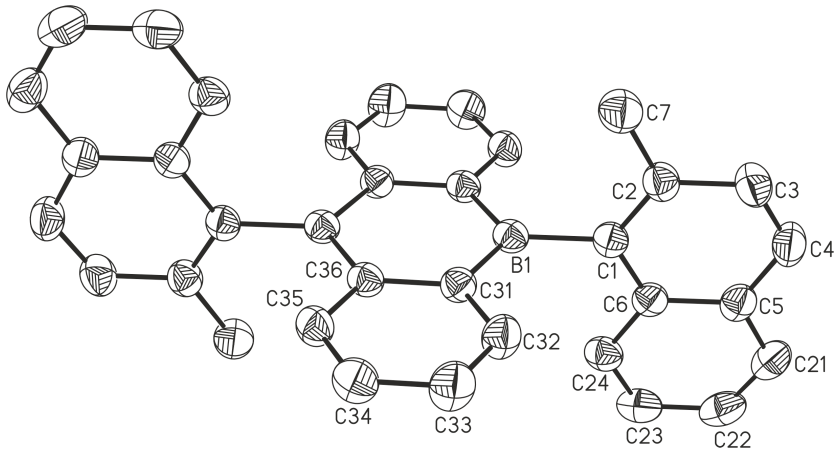


Figure S4: Molecular structure of *anti*-**2b** in the solid state; displacement ellipsoids at the 50 % probability level, H atoms omitted for clarity. Selected bond lengths (Å), bond angles (deg) and dihedral angle (deg): B(1)−C(1) 1.581(2), B(1)−C(31) 1.563(2), B(1)−C(36A) 1.559(2), C(31)−C(36) 1.422(2); C(1)−B(1)−C(31) 120.2(1), C(1)−B(1)−C(36A) 120.4(1), C(31)−B(1)−C(36A) 119.4(1); Ar(C1)//C(31)B(1)C(36A) 85.5(1); Ar = phenyl. Symmetry transformation used to generate equivalent atoms: A: −x+1, −y+1, −z+2.

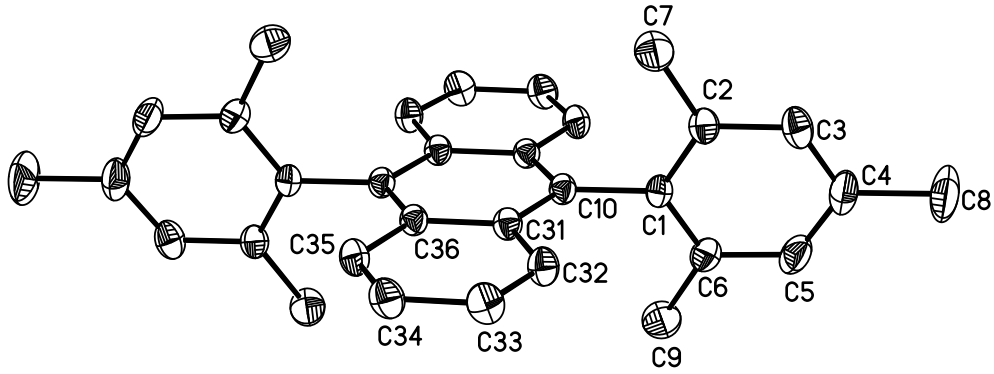


Figure S5: Molecular structure of **4a** in the solid state; displacement ellipsoids at the 50 % probability level, H atoms omitted for clarity. Selected bond lengths (Å), bond angles (deg) and dihedral angle (deg): C(1)−C(10) 1.496(2), C(10)−C(31) 1.406(2), C(10)−C(36A) 1.406(2), C(31)−C(32) 1.429(2), C(31)−C(36) 1.434(2), C(32)−C(33) 1.361(2), C(33)−C(34) 1.416(2), C(34)−C(35) 1.361(2), C(35)−C(36) 1.429(2); C(1)−C(10)−C(31) 120.3(1), C(1)−C(10)−C(36A) 120.2(1), C(31)−C(10)−C(36A) 119.5(1); Ar(C1)//C(31)C(10)C(36A) 81.4(1); Ar = phenyl. Symmetry transformation used to generate equivalent atoms: A: −x+1, −y+1, −z+1.

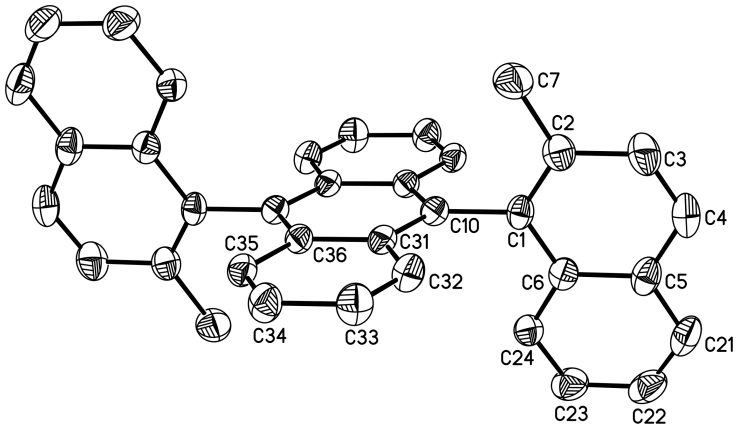


Figure S6: Molecular structure of *anti*-**4b** in the solid state; displacement ellipsoids at the 50 % probability level, H atoms omitted for clarity. Selected bond lengths (Å), bond angles (deg) and dihedral angle (deg): C(1)−C(10) 1.494(5), C(10)−C(31) 1.406(5), C(10)−C(36A) 1.409(5), C(31)−C(36) 1.444(5); C(1)−C(10)−C(31) 120.6(3), C(1)−C(10)−C(36A) 119.9(3), C(31)−C(10)−C(36A) 119.5(3); Ar(C1)//C(31)C(10)C(36A) 82.8(3); Ar = phenyl. Symmetry transformation used to generate equivalent atoms: A: −x, −y+1, −z.

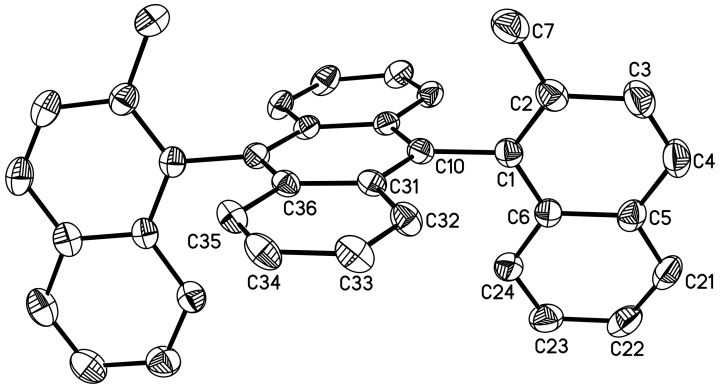


Figure S7: Molecular structure of *syn*-**4b** in the solid state; displacement ellipsoids at the 50 % probability level, H atoms omitted for clarity. Selected bond lengths (Å), bond angles (deg) and dihedral angles (deg): C(1)−C(10) 1.497(2), C(10)−C(31) 1.410(2), C(10)−C(36A) 1.407(2), C(31)−C(36) 1.435(2); C(1)−C(10)−C(31) 120.0(1), C(1)−C(10)−C(36A) 120.1(1), C(31)−C(10)−C(36A) 119.8(1); Ar(C31)//Ar(C36A) 5.0(1), Ar(C1)//C(31)C(10)C(36A) 80.0(1), Ar(C1)//Ar(C1A) 21.4(1); Ar = phenyl/phenylene. Symmetry transformation used to generate equivalent atoms: A: −x+1, y, −z+3/2.

Table S1. Crystallographic Data for **2a**, $[Li(THF)_2]_2$[**2a**] and $[Li(Et_2O)]_2$[**2a**]

	2a	$[Li(THF)_2]_2$[**2a**]	$[Li(Et_2O)]_2$[**2a**]
formula	$C_{30}H_{30}B_2$	$C_{46}H_{62}B_2Li_2O_4$	$C_{38}H_{50}B_2Li_2O_2$
M_r	412.16	714.46	574.28
colour, shape	yellow, block	red, block	orange, block
T [K]	173(2)	173(2)	173(2)
radiation, λ [Å]	$Mo_{K\alpha}$, 0.71073	$Mo_{K\alpha}$, 0.71073	$Mo_{K\alpha}$, 0.71073
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/n$	$C2/c$
a [Å]	12.8350(12)	10.5785(15)	20.2695(12)
b [Å]	22.061(3)	11.7290(16)	13.5626(9)
c [Å]	9.0732(8)	17.244(3)	14.2131(8)
α [°]	90	90	90
β [°]	107.478(7)	104.849(12)	117.614(4)
γ [°]	90	90	90
V [Å^3]	2450.5(5)	2068.1(5)	3462.2(4)
Z	4	2	4
D_{calcd} [g cm^{-3}]	1.117	1.147	1.102
F(000)	880	772	1240
μ [mm^{-1}]	0.062	0.069	0.064
crystal size [mm^3]	0.25 × 0.23 × 0.17	0.36 × 0.31 × 0.30	0.37 × 0.36 × 0.33
rflns collected	16322	5231	18192
independent rflns (R_{int})	4331 (0.0948)	3656 (0.0622)	3242 (0.0836)
data/restraints/parameters	4331/0/296	3656/0/247	3242/0/202
GOF on F^2	0.913	1.101	1.046
R_1, wR_2 [$I > 2\sigma(I)$]	0.0717, 0.1390	0.0562, 0.1600	0.0448, 0.1184
R_1, wR_2 (all data)	0.1454, 0.1646	0.0833, 0.1682	0.0556, 0.1246
largest diff peak and hole [e Å^{-3}]	0.222, −0.251	0.568, −0.418	0.190, −0.226

Table S2. Crystallographic Data for *anti*-**2b**, **4a**, and *anti*-**4b**

	anti-**2b**	**4a**	*anti*-**4b**
formula	$C_{34}H_{26}B_2 \times 2\ C_6H_6$	$C_{32}H_{30}$	$C_{36}H_{26} \times 2\ C_6H_6$
M_r	612.38	414.56	614.78
colour, shape	yellow, block	colourless, plate	colourless, block
T [K]	173(2)	173(2)	173(2)
radiation, λ [Å]	$Mo_{K\alpha}$, 0.71073	$Mo_{K\alpha}$, 0.71073	$Mo_{K\alpha}$, 0.71073
crystal system	monoclinic	monoclinic	triclinic
space group	$P2_1/c$	$P2_1/c$	P-1
a [Å]	9.2654(6)	7.2622(4)	9.1166(17)
b [Å]	20.7217(10)	19.4203(12)	9.4240(18)
c [Å]	9.6220(6)	8.8976(5)	10.5376(18)
α [°]	90	90	87.558(15)
β [°]	109.597(5)	100.495(5)	81.861(14)
γ [°]	90	90	71.156(15)
V [Å^3]	1740.36(18)	1233.87(12)	848.2(3)
Z	2	2	1
D_{calcd} [g cm^{-3}]	1.169	1.116	1.204
F(000)	648	444	326
μ [mm^{-1}]	0.065	0.063	0.068
crystal size [mm^3]	0.36 × 0.33 × 0.24	0.55 × 0.55 × 0.20	0.23 × 0.22 × 0.19
rflns collected	28271	26584	7523
independent rflns (R_{int})	3276 (0.0596)	3144 (0.0692)	2969 (0.1172)
data/restraints/parameters	3276/0/219	3144/0/148	2969/0/218
GOF on F^2	1.027	1.115	1.134
R_1, wR_2 [$I > 2\sigma(I)$]	0.0435, 0.1075	0.0541, 0.1392	0.0988, 0.1984
R_1, wR_2 (all data)	0.0570, 0.1144	0.0619, 0.1442	0.1325, 0.2104
largest diff peak and hole [e Å^{-3}]	0.161, −0.153	0.284, −0.228	0.217, −0.259

Table S3. Crystallographic Data for *syn*-**4b**

	syn-**4b**
formula	$C_{36}H_{26} \times 2\ C_6H_6$
M_r	614.78
colour, shape	colourless, block
T [K]	173(2)
radiation, λ [Å]	$Mo_{K\alpha}$, 0.71073
crystal system	monoclinic
space group	$C2/c$
a [Å]	19.6910(15)
b [Å]	9.7696(5)
c [Å]	18.3312(14)
α [°]	90
β [°]	101.556(6)
γ [°]	90
V [Å^3]	3454.9(4)
Z	4
D_{calcd} [g cm^{-3}]	1.182
F(000)	1304
μ [mm^{-1}]	0.067
crystal size [mm^3]	0.50 × 0.48 × 0.38
rflns collected	23515
independent rflns (R_{int})	3235 (0.0548)
data/restraints/parameters	3235/0/218
GOF on F^2	1.143
R_1, wR_2 [$I > 2\sigma(I)$]	0.0486, 0.1281
R_1, wR_2 (all data)	0.0543, 0.1316
largest diff peak and hole [e Å^{-3}]	0.210, −0.185

3) Overlays of the UV/vis Absorption Spectra of 2a, Li[2a], Li_2[2a] and 2b, K[2b], K_2[2b]

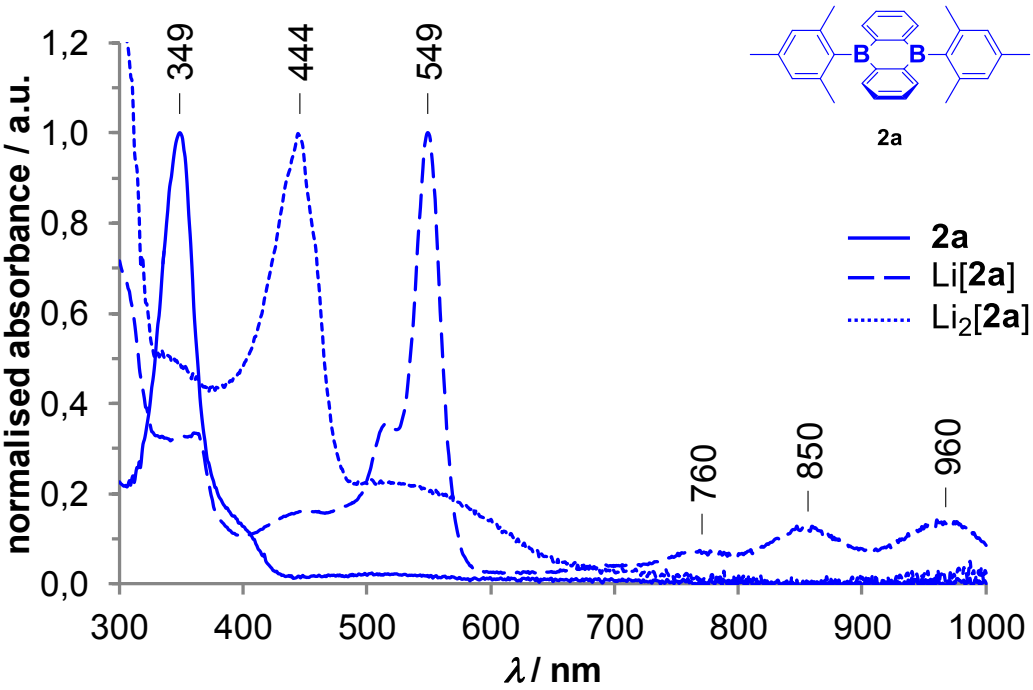


Figure S8: Normalised UV/vis absorption spectra of **2a**, Li[**2a**] and Li_2[**2a**] in THF.

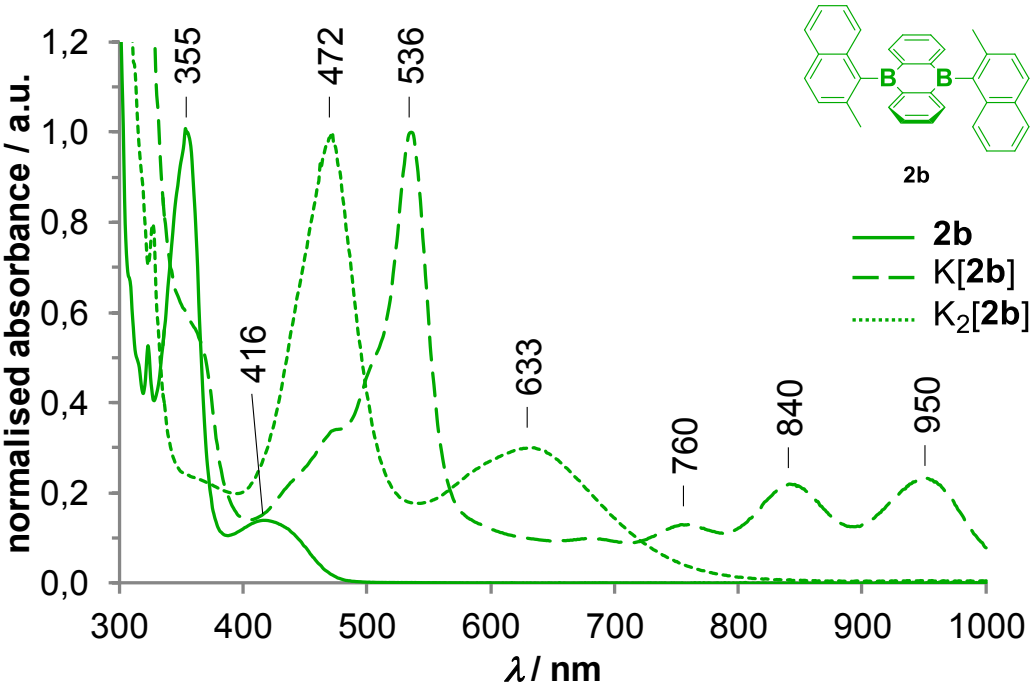


Figure S9: Normalised UV/vis absorption spectra of **2b**, K[**2b**] and K_2[**2b**] in THF.

4) Overlays of the CV-Plots of 2a-c and 4a-c; CVs of 4a-c with different switching potentials

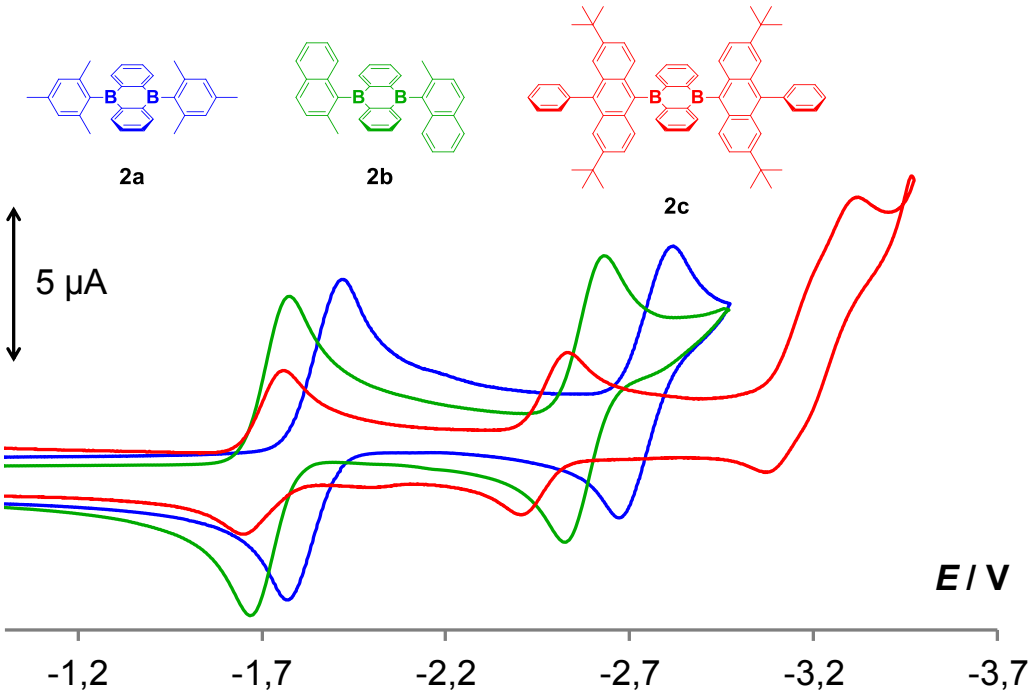


Figure S10: Overlay of the CV-plots of **2a** (blue), **2b** (green) and **2c** (red); solutions in THF, room temp., supporting electrolyte: [nBu$_4$N][PF$_6$] (0.1 M), scan rate: 200 mVs^{-1}, versus FcH/FcH$^+$.

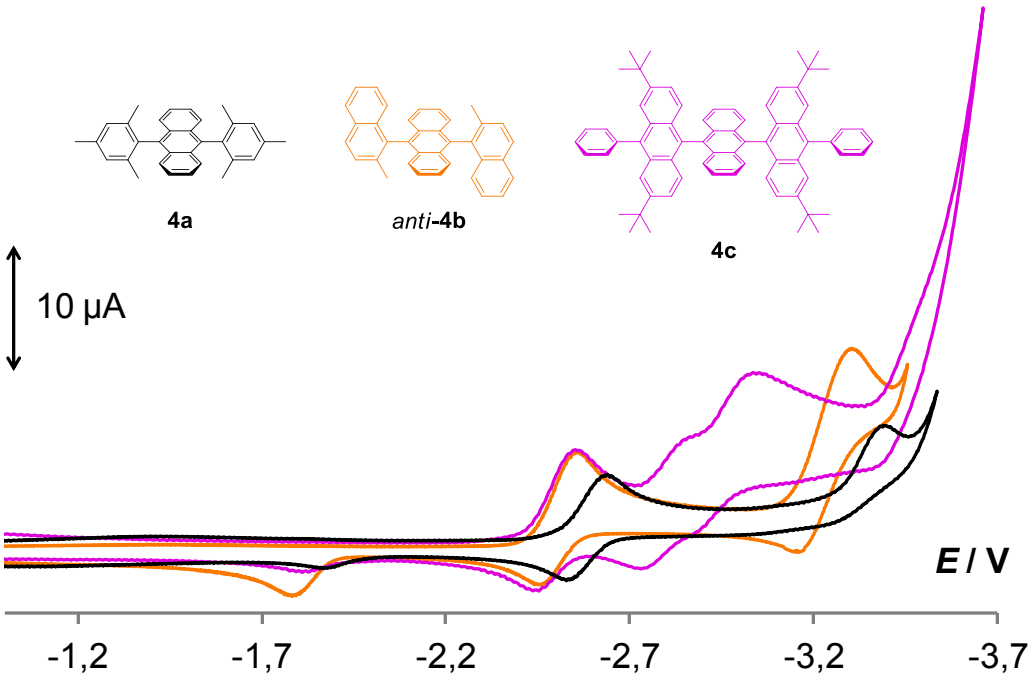


Figure S11: Overlay of the CV-plots of **4a** (black), anti-**4b** (orange) and **4c** (purple); solutions in THF, room temp., supporting electrolyte: [nBu$_4$N][PF$_6$] (0.1 M), scan rate: 200 mVs^{-1}, versus FcH/FcH$^+$.

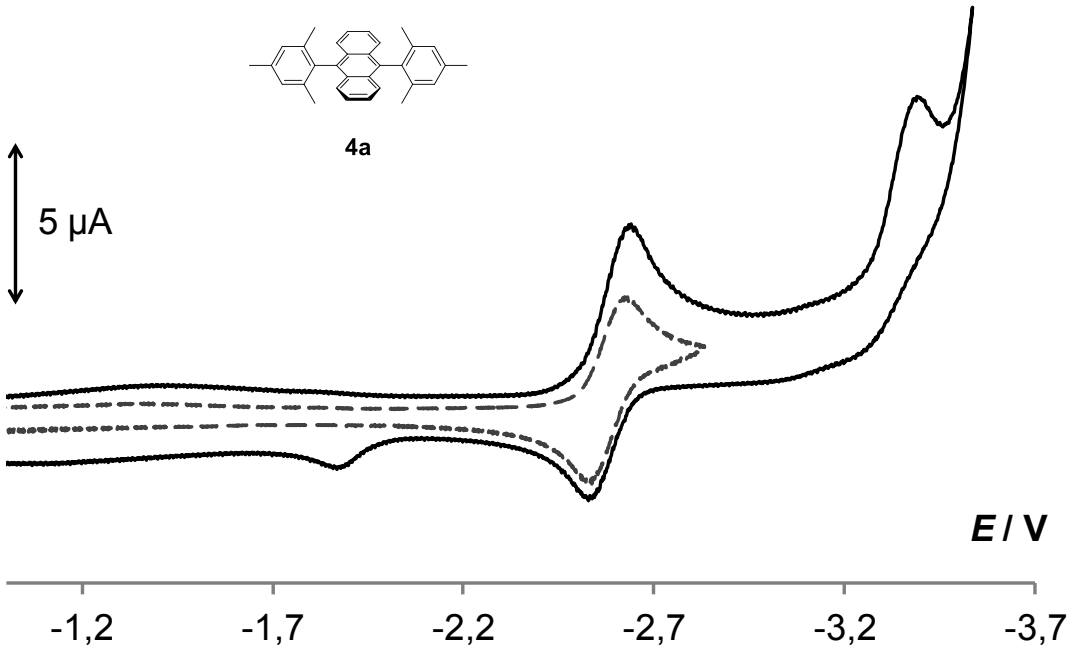


Figure S12: Cyclic voltammograms of **4a** with two different switching potentials (–2.83 V (dashed black line) and –3.54 V (solid black line)); solution in THF, room temp., supporting electrolyte: [nBu$_4$N][PF$_6$] (0.1 M), scan rate: 200 mVs^{-1}, versus FcH/FcH$^+$.

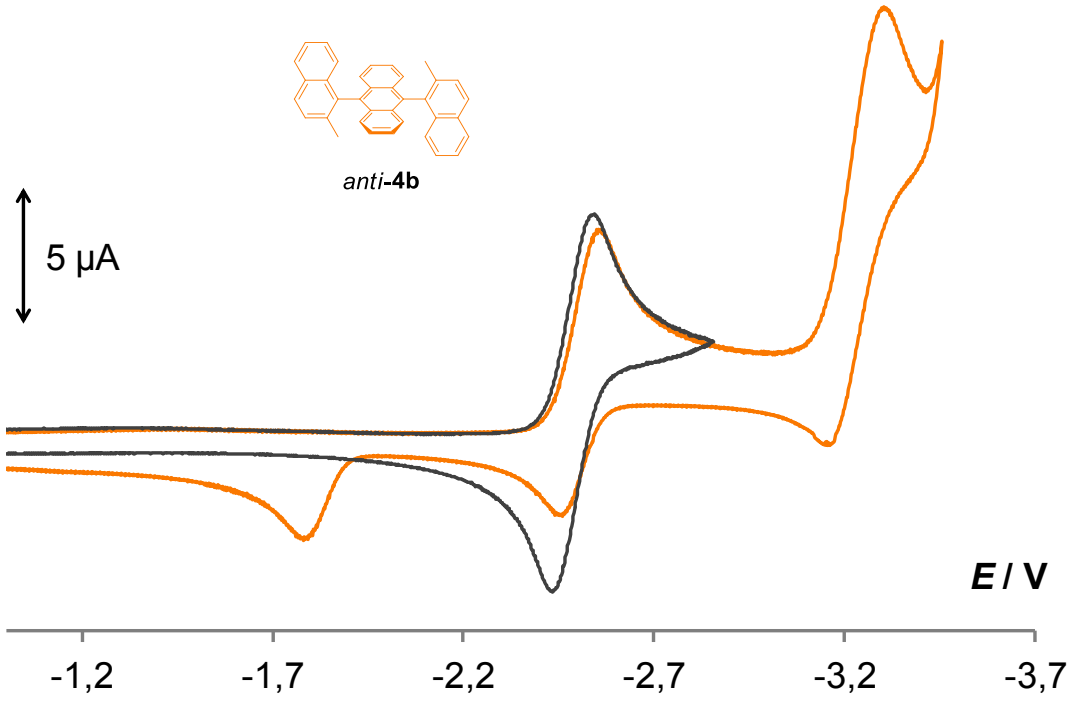


Figure S13: Cyclic voltammograms of *anti*-**4b** with two different switching potentials (–2.86 V (black) and –3.46 V (orange)); solution in THF, room temp., supporting electrolyte: [nBu$_4$N][PF$_6$] (0.1 M), scan rate: 200 mVs^{-1}, versus FcH/FcH$^+$.

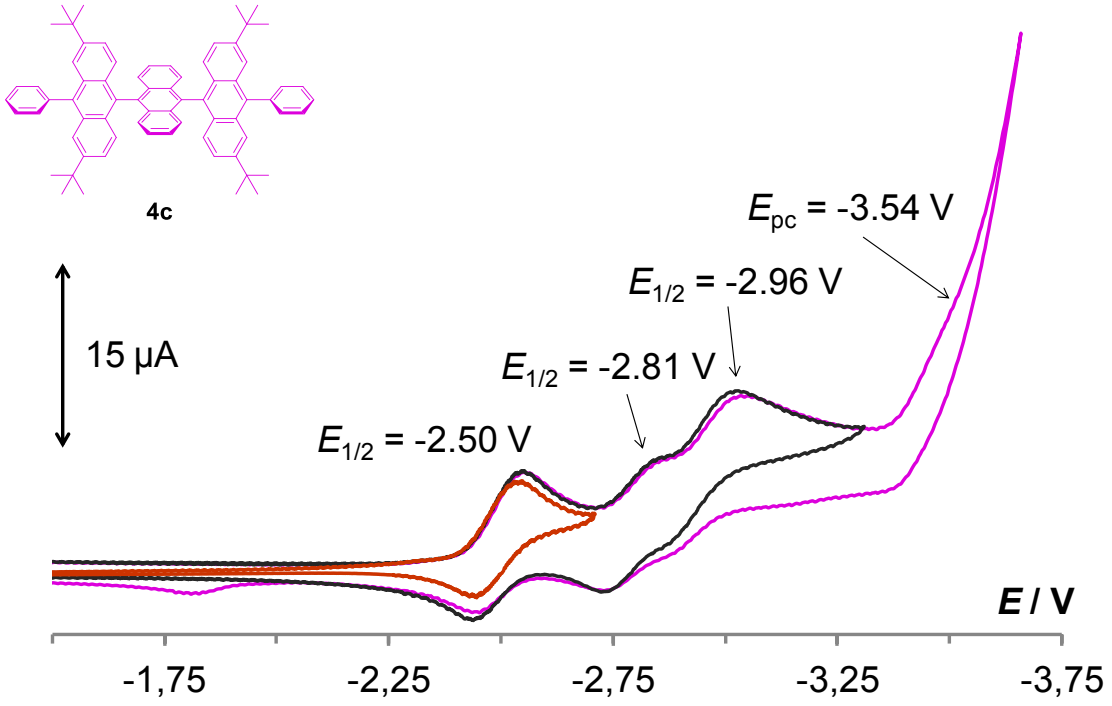


Figure S14: Cyclic voltammograms of **4c** with three different switching potentials (–2.71 V (brown), –3.31 V (black) and –3.66 V (purple)); solution in THF, room temp., supporting electrolyte: [nBu$_4$N][PF$_6$] (0.1 M), scan rate: 200 mVs^{-1}, versus FcH/FcH$^+$.

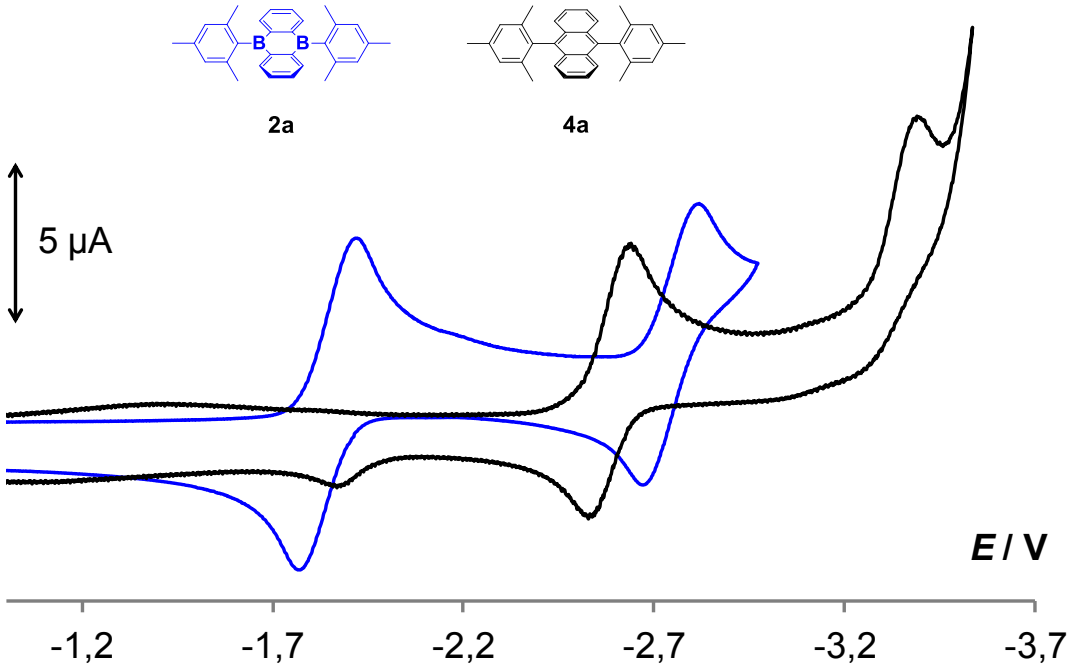


Figure S15: Overlay of the CV-plots of **2a** (blue) and **4a** (black); solutions in THF, room temp., supporting electrolyte: [nBu$_4$N][PF$_6$] (0.1 M), scan rate: 200 mVs^{-1}, versus FcH/FcH$^+$.

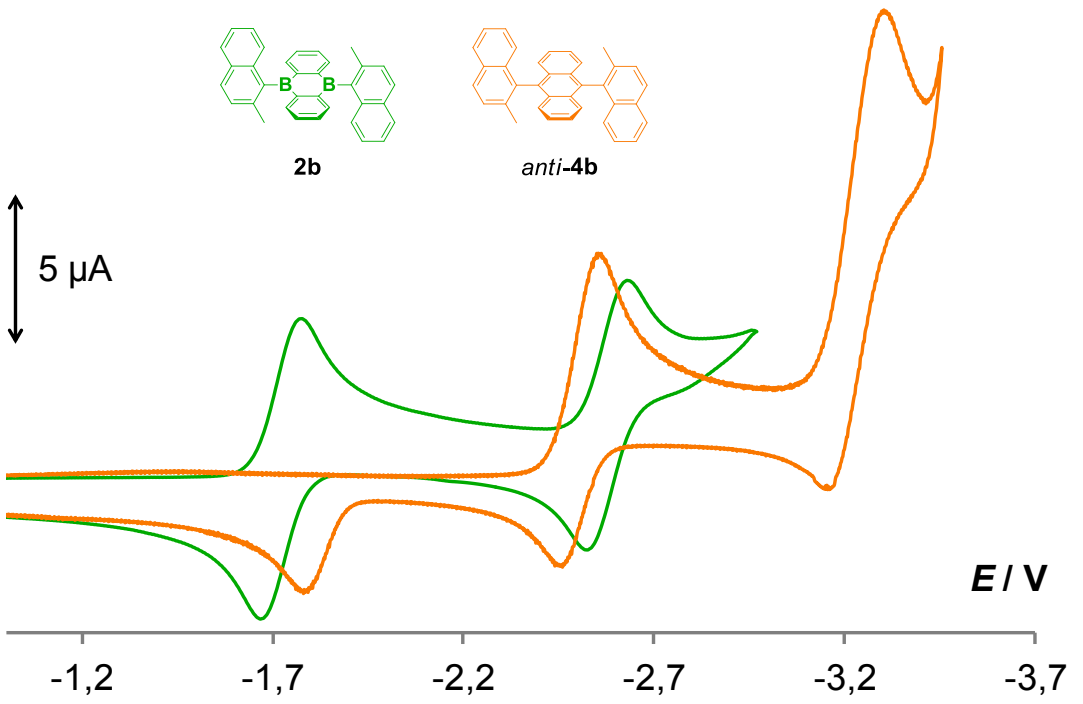


Figure S16: Overlay of the CV-plots of **2b** (green) and *anti*-**4b** (orange); solutions in THF, room temp., supporting electrolyte: [nBu$_4$N][PF$_6$] (0.1 M), scan rate: 200 mVs^{-1}, versus FcH/FcH$^+$.

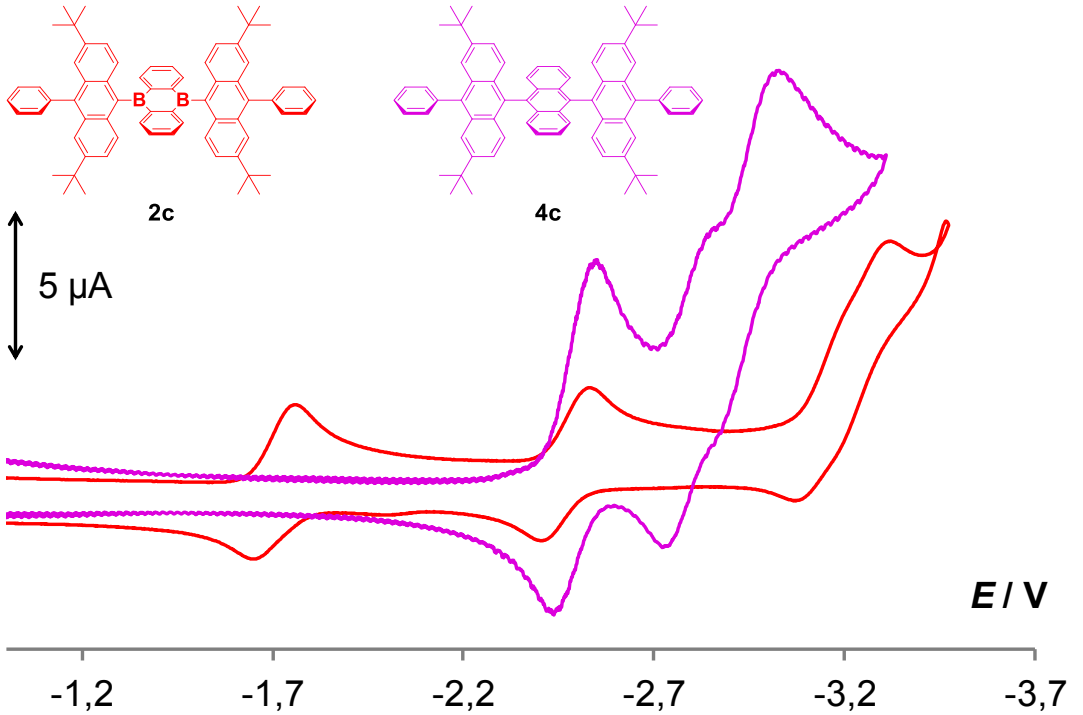


Figure S17: Overlay of the CV-plots of **2c** (red) and **4c** (purple); solutions in THF, room temp., supporting electrolyte: [nBu$_4$N][PF$_6$] (0.1 M), scan rate: 200 mVs^{-1}, versus FcH/FcH$^+$.

5) Overlays of the UV/vis Absorption and Fluorescence Spectra of 2a/4a, 2b/*anti*-4b and 2c/4c

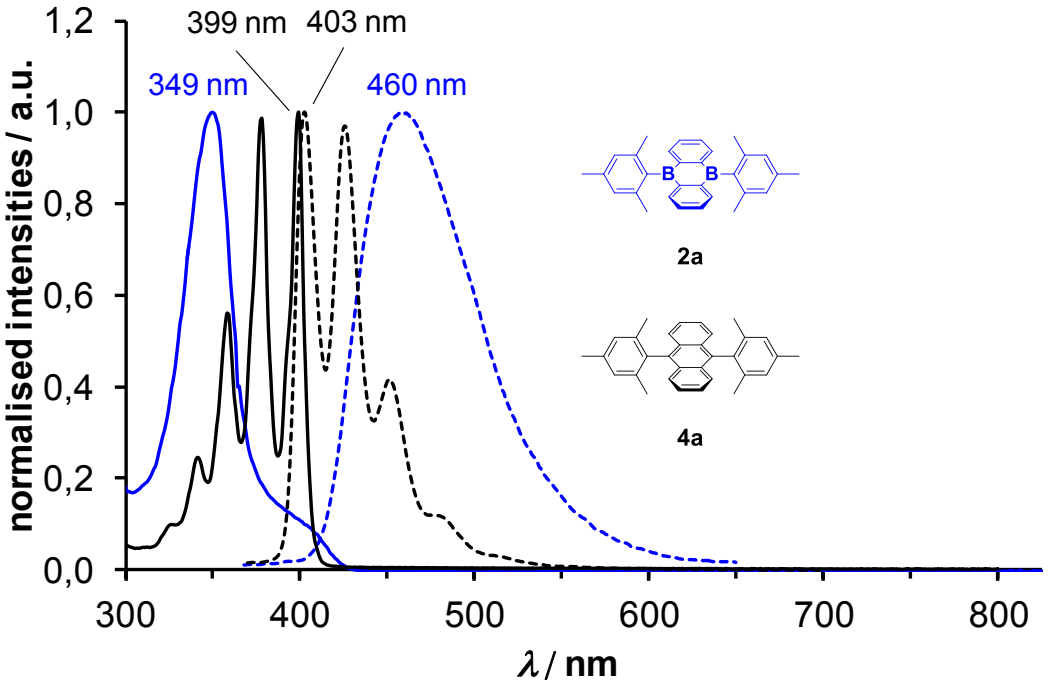


Figure S18: Overlay of the UV/vis absorption spectra of **2a** (blue) and **4a** (black) in C_6H_6.

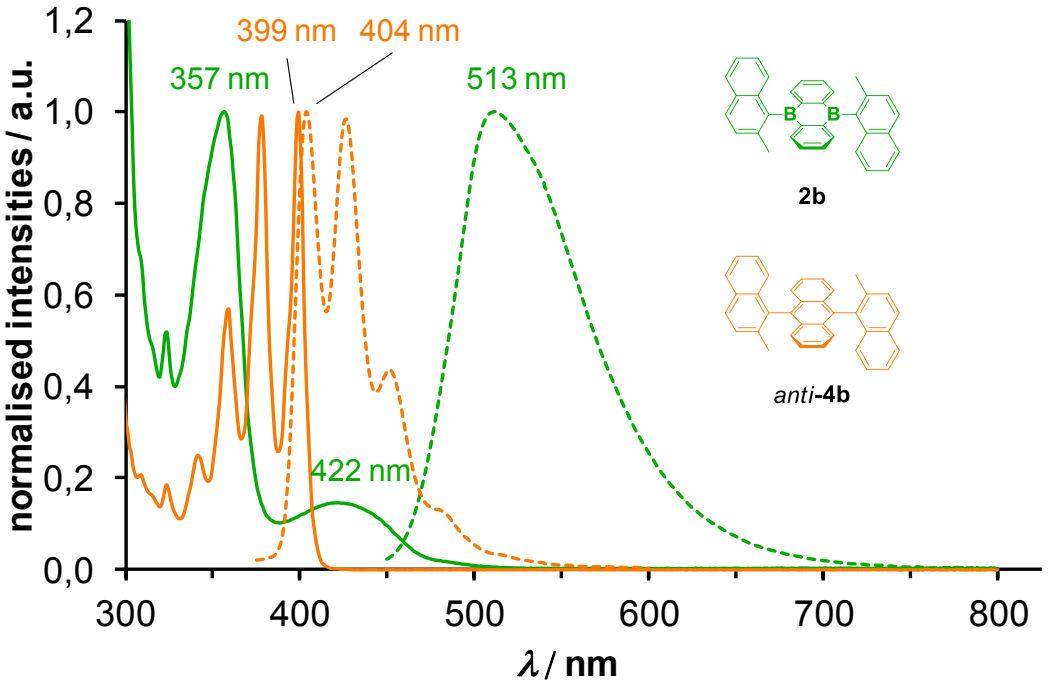


Figure S19: Overlay of the UV/vis absorption spectra of **2b** (green) and *anti*-**4b** (orange) in C_6H_6.

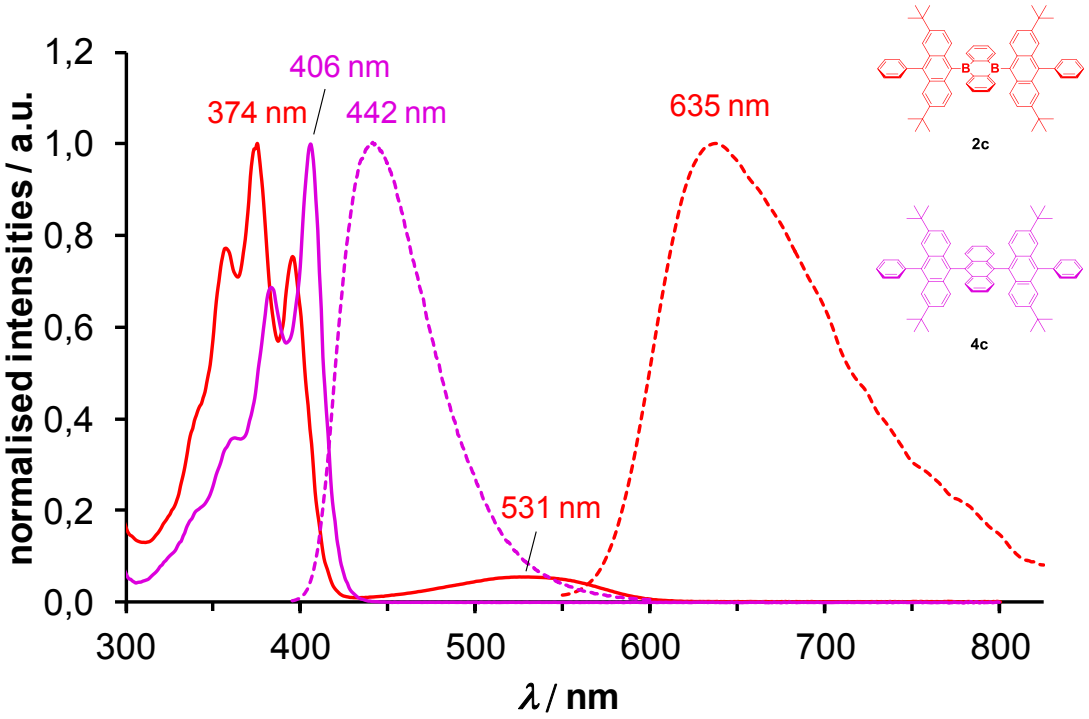


Figure S20: Overlay of the UV/vis absorption spectra of **2c** (red) and **4c** (purple) in C_6H_6.

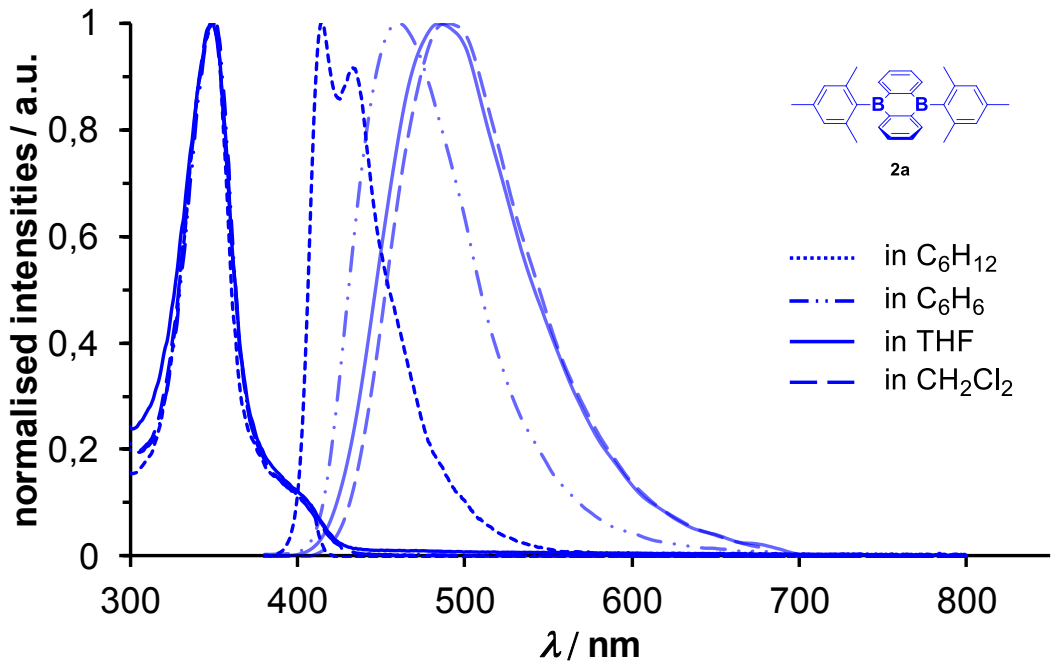


Figure S21: Solvatochromism of **2a** in solvents of different polarity (C_6H_{12}, C_6H_6, THF and CH_2Cl_2); UV/Vis absorption (left) and emission (right) spectra.

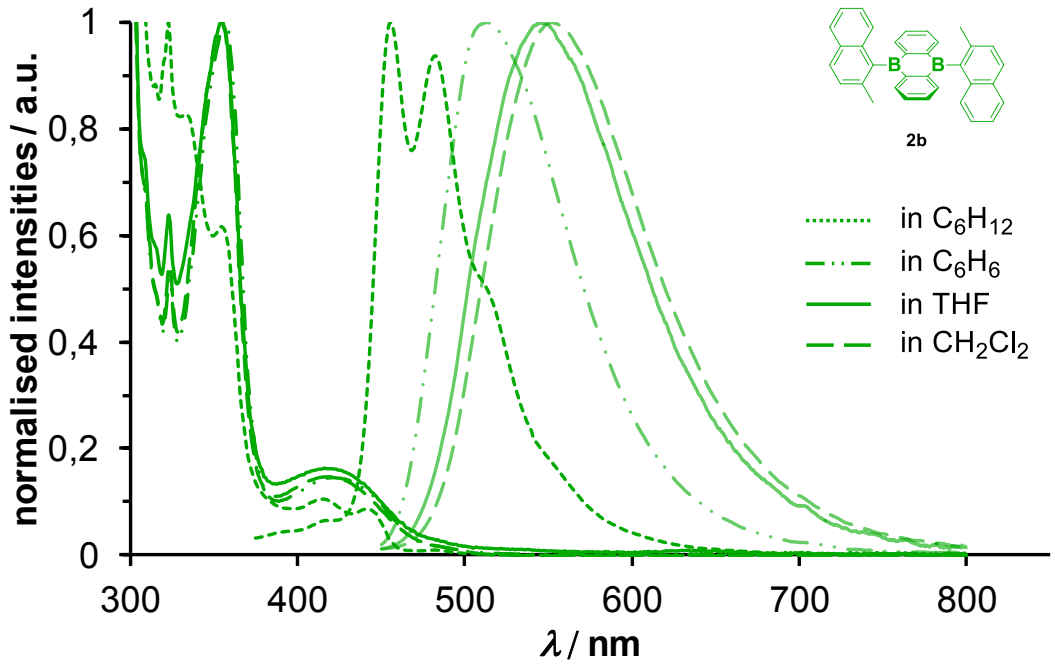


Figure S22: Solvatochromism of **2b** in solvents of different polarity (C_6H_{12}, C_6H_6, THF and CH_2Cl_2); UV/Vis absorption (left) and emission (right) spectra.

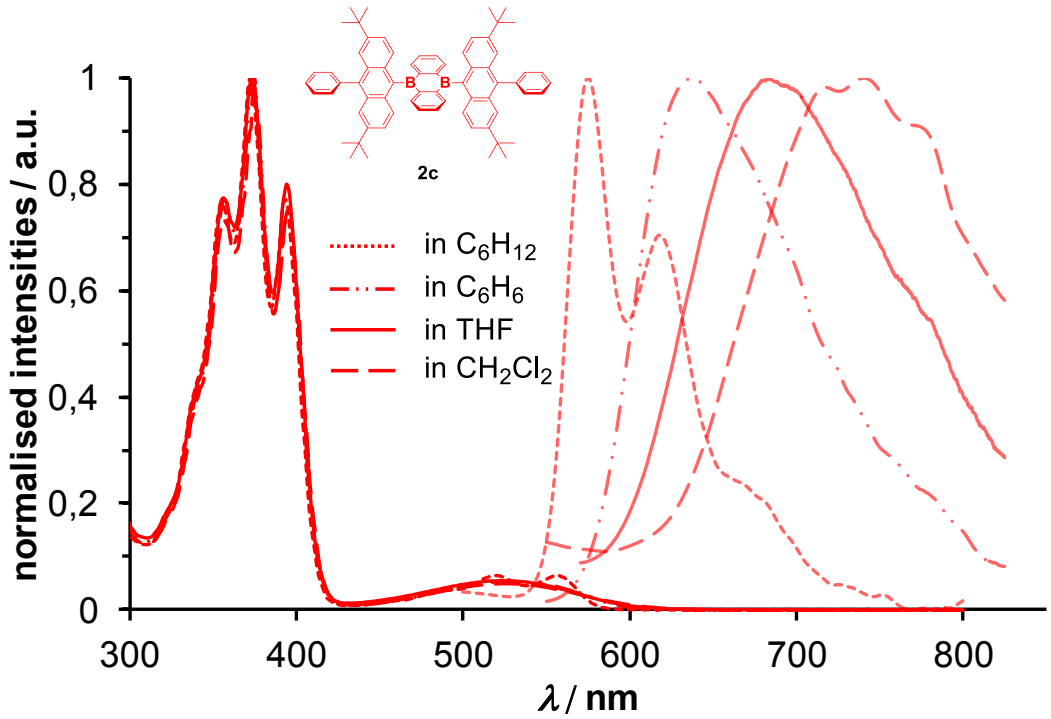


Figure S23: Solvatochromism of **2c** in solvents of different polarity (C_6H_{12}, C_6H_6, THF and CH_2Cl_2); UV/Vis absorption (left) and emission (right) spectra.

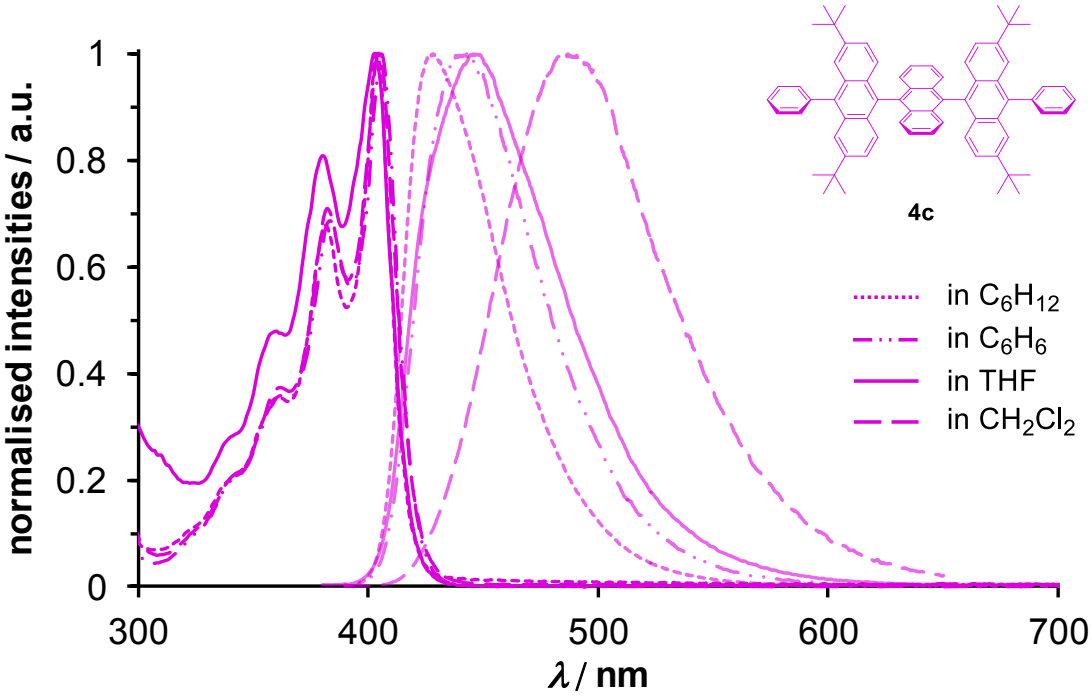


Figure S24: Solvatochromism of **4c** in solvents of different polarity (C_6H_{12}, C_6H_6, THF and CH_2Cl_2); UV/Vis absorption (left) and emission (right) spectra.

Table S4. Photophysical data of **2a-c** and **4a-c**

	solvent	λ_{max}(abs) [nm] (ε [$mol^{-1}dm^3cm^{-1}$])	λ_{max}(em) [nm] (λ_{ex} [nm])	Stokes Shift [cm^{-1}]	ϕ_F[a] (λ_{ex} [nm])
2a	C_6H_{12}	350 (9100)	415 (350)	4500	0.02
	C_6H_6	349 (10400)	460 (350)	6900	0.03
	THF	349 (9000)	485 (350)	8000	0.04
	DCM	349 (8000)	489 (350)	8200	0.04
2b	C_6H_{12}	355 (4200), 416 (500)	456 (420)	2100	0.04
	C_6H_6	357 (8600), 422 (1300)	513 (420)	4200	0.07
	THF	355 (6400), 416 (1200)	546 (420)	5700	0.09
	DCM	354 (7700), 418 (1100)	553 (420)	5800	0.12
2c	C_6H_{12}	373 (17800), 519 (1300)	575 (530)	1900	0.10
	C_6H_6	374 (28200), 531 (1500)	635 (530)	3100	0.05
	THF	374 (39700), 523 (2200)	684 (530)	4500	0.03
	DCM	374 (24700), 524 (1300)	740 (530)	5600	0.01
4a	C_6H_{12}	396 (23800)	401 (358)	300	0.77
	C_6H_6	399 (22300)	403 (358)	250	0.80
	THF	397 (14600)	402 (358)	300	0.80
	DCM	398 (14300)	404 (358)	375	0.85
4b	C_6H_{12}	396 (17500)	401 (358)	300	0.72
	C_6H_6	399 (17900)	404 (358)	300	0.77
	THF	397 (10100)	402 (358)	300	0.70
	DCM	398 (15400)	404 (358)	375	0.74
4c	C_6H_{12}	403 (10100)	425 (380)	1300	0.72
	C_6H_6	406 (47700)	442 (380)	2000	0.71
	THF	403 (24000)	445 (380)	2350	0.60
	DCM	404 (36000)	487 (380)	4200	0.27

[a] Quantum yields were determined using a calibrated integration sphere.

6 Computational Details

Natural population (NPA)[5] and Bader (AIM)[6,7] analyses, as well as NMR[8–10] shielding constants, σ, were computed under gas-phase conditions at the B97D/TZVP level of theory[11,12] with the Gaussian programme package.[13] The corresponding molecular geometries were optimised utilising the efficient density-fitting approach (B97D/TZVP/TZVPfit),[14,15] and employing tight convergence criteria.

Atomic partial charges, q, were obtained from the corresponding natural population (NPA) calculated within the NBO module as implemented in Gaussian, and from integration over the corresponding atomic basins resulting from an atoms-in-molecules (AIM) analysis of computed electron densities employing a locally modified version of AIMPAC.[16] NICS(0)/NICS(1) diagnostics[17–19] are determined at the positions of ring critical points as obtained from AIM analyses, and at a distance of 1 Å from the ring critical point above the ring plane (in the anthracene-derivatives, centroid A corresponds to the central, centroid B to the peripheral ring); the ring plane is defined through the three neighbouring atoms C-c/C-d/C-c′ (ring A), C-b/C-a/C-c (ring B), and $C^o/C^i/C^{o\prime}$ (Ph, Mes), respectively. The calculation of NICS indices requires the use of ghost atoms, which is partly incompatible with Gaussian's dispersion correction algorithm. NICS calculations were therefore performed separately.

Chemical shifts, δ(calc), were computed relative to the corresponding ^{1}H and ^{13}C shieldings of $SiMe_4$ obtained at the same level of theory, i.e., $\sigma(^1\mathrm{H}) = 31.7$ ppm, $\sigma(^{13}\mathrm{C}) = 183.3$ ppm. Experimental shifts, δ(exp), and NMR assignments are taken from the SDBS database,[20] if not presented in this work.

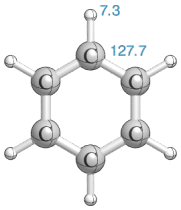
The HOMO and LUMO isosurfaces were plotted at an isovalue of $0.05\,a_0^{-3/2}$. The corresponding HOMO–LUMO energy gaps are taken as the orbital energy difference from B97D/TZVP single point calculations on the B97D/TZVP/TZVPfit geometries (1 a.u. = 27.2114 eV). The positive orbital energies for the bare dianionic species DBA^{2-}, $[\mathbf{2a}]^{2-}$, (see Table S6, marked in red), reflecting formally unbound electrons, are due to the lack of diffuse functions. For the calculations of compounds **4c**, **2c** and $[Li(THF)_2]_2$ [**2c**] the peripheral ^{t}Bu- and phenyl-groups of the anthryl substituent were omitted for the sake of computational efficacy (indicated by the subscript "model").

The optimised molecular geometries (B97D/TZVP/TZVPfit) are given in cartesian coordinates (Å) along with term symbols, point groups and the corresponding total electronic energies (a.u.), computed at the B97D/TZVP level of theory. Dihedral angles ϕ are defined between atoms C^o–C^i–$C^{i\prime}$–$C^{o\prime}$ (biphenyl), C-c–C-d–C^i–C^o (**4a**–**4c**) and C-c–B–C^i–C^o (**2a**–**2c** and derivatives), respectively. Graphical representations of molecular geometries and orbitals were produced with the MOLDEN[21,22] and POV-Ray[23] software.

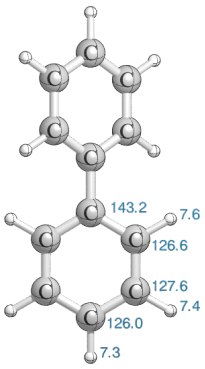
6.1 Atomic Partial Charges, NMR Shieldings, and NICS Diagnostics

Table S5: Atomic partial charges, q, derived from NPA and AIM analyses, NMR shieldings, σ, and shifts, δ (relative to TMS), in comparison with experiment. Signed deviations, Δ, are given as $\delta(\text{exp}) - \delta(\text{calc})$. The individual vaules of q listed in the Tables do not always sum up to the corresponding total charges due to rounding errors. Similarly, the individual figures, $\delta(\text{calc}) + \Delta$, do not always sum up to the corresponding experimental references, $\delta(\text{exp})$, due to rounding errors. All NMR-related data are given in ppm. The figures on the right-hand side show the molecular structures with the calculated NMR shifts of selected individual atoms.

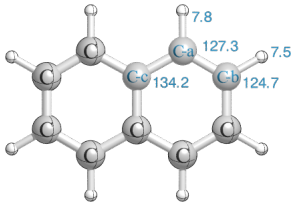
benzene (D_{6h})						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C	−0.21	−0.02	55.6	127.7	128.4	0.7
H	0.21	0.02	24.4	7.3	7.3	0.0
NICS(0)			−8.8			
NICS(1)			−10.0			



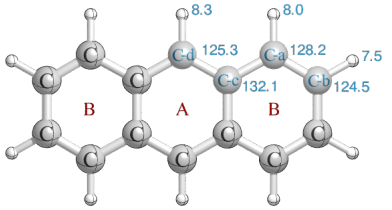
biphenyl (D_2)						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-i	−0.05	0.00	40.0	143.2	140.8	−2.4
C-o	−0.19	−0.02	56.6	126.6	126.8	0.2
C-m	−0.20	−0.01	55.7	127.6	128.3	0.8
C-p	−0.21	−0.01	57.2	126.0	126.8	0.8
H-o	0.21	0.02	24.2	7.6	7.6	0.0
H-m	0.21	0.02	24.3	7.4	7.4	0.1
H-p	0.21	0.02	24.4	7.3	7.3	0.1
NICS(0)			−7.9			
NICS(1)			−9.2			



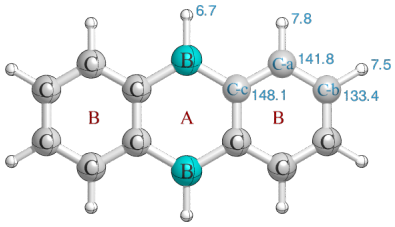
naphthalene (D_{2h})						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-a	−0.06	0.00	56.0	127.3	127.8	0.6
C-b	−0.18	−0.01	58.5	124.7	125.8	1.0
C-c	−0.21	−0.01	49.0	134.3	133.4	−0.8
H-a	0.21	0.02	23.9	7.8	7.8	0.0
H-b	0.21	0.02	24.3	7.5	7.5	0.0
NICS(0)			−9.1			
NICS(1)			−10.3			



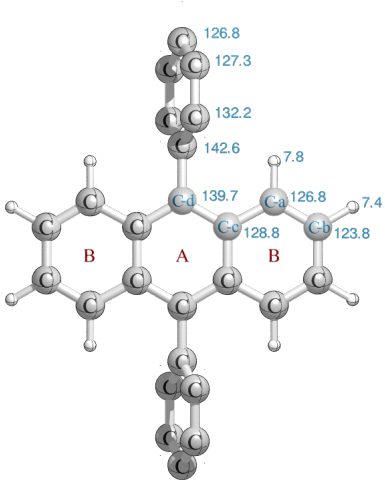
anthracene (D_{2h})						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-a	−0.18	−0.01	55.1	128.2	128.2	0.0
C-b	−0.21	−0.02	58.7	124.5	125.3	0.8
C-c	−0.06	0.00	51.2	132.1	131.7	−0.4
C-d	−0.15	−0.02	58.0	125.3	126.2	0.9
H-a	0.21	0.02	23.7	8.0	8.0	−0.1
H-b	0.21	0.02	24.2	7.5	7.4	−0.1
H-d	0.20	0.01	23.4	8.3	8.4	0.0
NICS(0)^{A}			−11.6			
NICS(0)^{B}			−8.1			
NICS(1)^{A}			−12.4			
NICS(1)^{B}			−9.5			



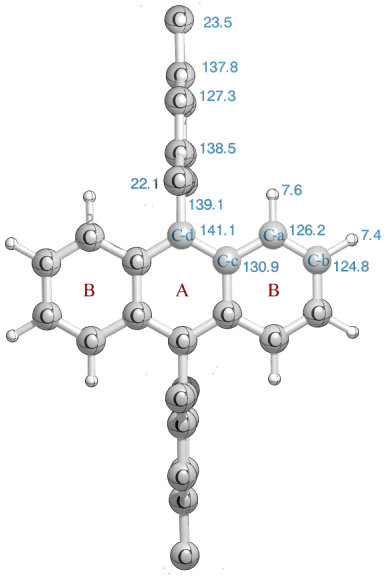
9,10-diboraanthracene (D_{2h})						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-a	−0.14	−0.02	41.5	141.8		
C-b	−0.19	−0.02	49.9	133.4		
C-c	−0.33	−0.63	35.2	148.1		
B	0.57	1.89				
H-a	0.21	0.02	23.9	7.8		
H-b	0.21	0.02	24.3	7.5		
H-c	−0.08	−0.63	25.0	6.7		
NICS(0)^{A}			10.6			
NICS(0)^{B}			−4.1			
NICS(1)^{A}			4.3			
NICS(1)^{B}			−7.2			



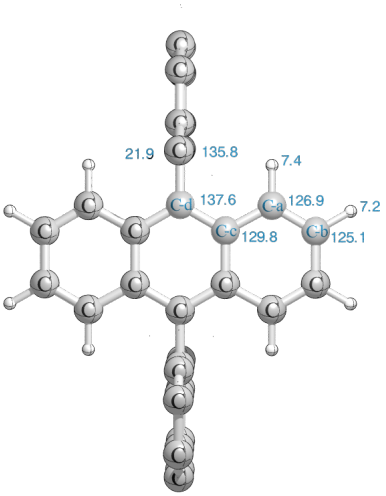
9,10-diphenylanthracene (C_{2h})						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-a	−0.19	−0.02	56.5	126.8	126.9	0.2
C-b	−0.20	−0.02	59.5	123.8	125.0	1.2
C-c	−0.04	−0.01	54.4	128.8	129.9	1.1
C-d	0.00	−0.01	43.6	139.7	137.1	−2.6
H-a	0.22	0.03	23.9	7.8	7.7	−0.1
H-b	0.21	0.02	24.3	7.4	7.3	−0.1
Ph-*i*	−0.04	−0.01	40.7	142.6	139.1	−3.5
Ph-*o*	−0.21	−0.02	51.0	132.2	128.4	−3.8
Ph-*m*	−0.20	−0.02	56.0	127.3	131.3	4.0
Ph-*p*	−0.20	−0.02	56.5	126.8	127.4	0.6
NICS(0)^{A}			−10.4			
NICS(0)^{B}			−7.8			
NICS(0)^{Ph}			−7.1			
NICS(1)^{A}			−11.3			
NICS(1)^{B}			−9.0			
NICS(1)^{Ph}			−8.4			



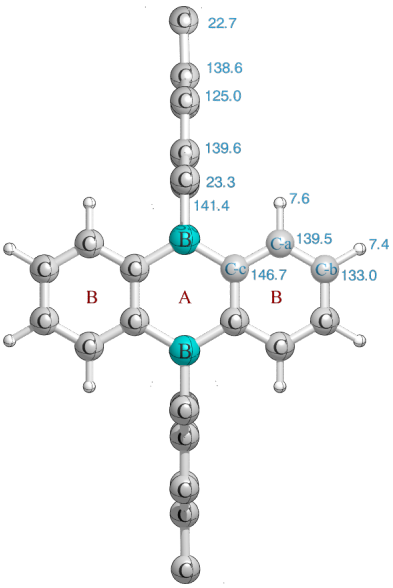
4a (C_i)						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-a	−0.19	−0.02	57.1	126.2	126.8	0.6
C-b	−0.20	−0.02	58.4	124.8	126.0	1.2
C-c	−0.05	−0.01	52.4	130.9	130.4	−0.5
C-d	0.02	−0.01	42.1	141.1	136.0	−5.1
H-a	0.22	0.04	24.1	7.6	7.8	0.2
H-b	0.21	0.02	24.4	7.4	7.1	−0.2
Mes-*i*	−0.06	−0.03	44.2	139.1	135.4	−3.7
Mes-*o*	−0.01	−0.01	44.7	138.5	137.8	−0.7
Mes-*m*	−0.21	−0.03	55.9	127.3	128.9	1.6
Mes-*p*	0.01	−0.01	45.5	137.8	137.2	−0.6
CH_3-*o*	−0.62	0.02	161.1	22.1	20.2	−1.9
NICS(0)^{A}			−9.9			
NICS(0)^{B}			−7.4			
NICS(0)^{Mes}			−6.8			
NICS(1)^{A}			−11.1			
NICS(1)^{B}			−9.1			
NICS(1)^{Mes}			−8.1			



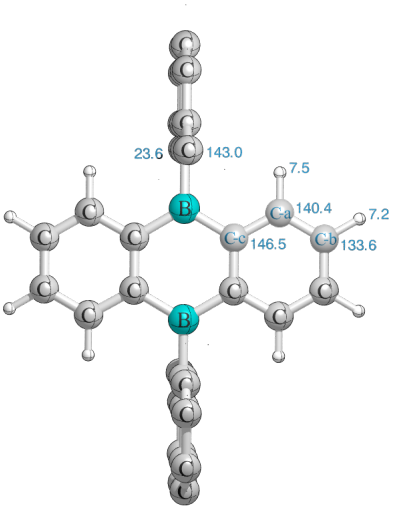
anti-**4b** (C_i)						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-a	−0.18	−0.02	56.4	126.9	127.2	0.3
C-b	−0.20	−0.02	58.2	125.1	126.2	1.1
C-c	−0.05	−0.01	53.4	129.8	131.1	1.3
C-d	0.01	−0.01	45.7	137.6	135.0	−2.6
H-a	0.22	0.03	24.3	7.4	7.6	0.2
H-b	0.21	0.02	24.5	7.2	6.9	−0.3
C-1	−0.02	−0.02	47.4	135.8	135.2	−0.6
C-2	0.00	−0.01	45.9	137.4	136.0	−1.4
C-3	−0.20	−0.02	55.8	127.5	129.2	1.7
C-4	−0.17	−0.02	55.8	127.4	128.6	1.2
C-4a	−0.06	−0.01	52.6	130.7	133.0	2.3
C-8a	−0.05	−0.01	49.6	133.6	134.6	1.0
C-5	−0.18	−0.02	55.8	127.5	128.6	1.1
C-6	−0.21	−0.02	59.3	123.9	125.5	1.6
C-7	−0.20	−0.02	58.4	124.9	126.8	1.9
C-8	−0.19	−0.02	57.4	125.8	126.9	1.1
CH_3	−0.62	0.02	161.4	21.9	20.6	−1.3



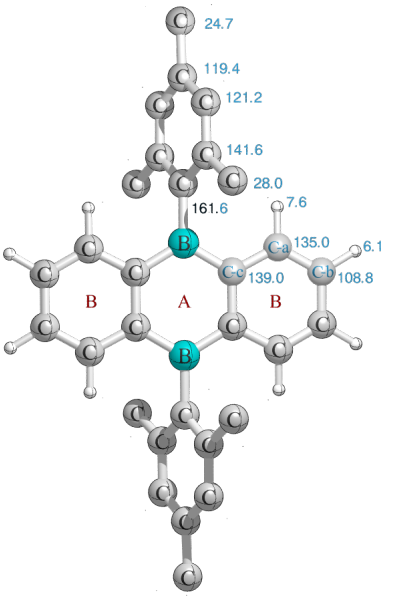
2a (C_{2h})						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-a	−0.15	−0.03	43.8	139.5	139.4	−0.1
C-b	−0.19	−0.02	50.2	133.0	134.0	1.0
C-c	−0.38	−0.62	36.6	146.7	145.8	−0.9
B	0.93	1.90				
H-a	0.22	0.03	24.1	7.6	7.8	0.2
H-b	0.21	0.02	24.4	7.4	7.1	−0.2
Mes-*i*	−0.40	−0.63	41.9	141.4	141.3	−0.1
Mes-*o*	−0.01	−0.01	43.7	139.6	138.1	−1.5
Mes-*m*	−0.22	−0.03	58.2	125.0	127.6	2.6
Mes-*p*	0.01	−0.02	44.7	138.6	137.0	−1.6
CH_3-*o*	−0.62	0.01	160.0	23.3	22.8	−0.5
NICS(0)^{A}			10.5			
NICS(0)^{B}			−4.0			
NICS(0)^{Mes}			−7.4			
NICS(1)^{A}			4.4			
NICS(1)^{B}			−7.2			
NICS(1)^{Mes}			−8.5			



anti-**2b** (C_i)						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-a	−0.15	−0.02	42.9	140.4	140.2	−0.2
C-b	−0.19	−0.02	49.7	133.6	134.3	0.7
C-c	−0.38	−0.63	36.8	146.5	146.0	−0.5
H-a	0.22	0.03	24.2	7.5	7.6	0.1
H-b	0.21	0.02	24.5	7.2	7.0	−0.3
C-1	−0.35	−0.61	40.3	143.0	142.1	−0.9
C-2	0.00	−0.02	46.2	137.1	135.9	−1.2
C-3	−0.20	−0.02	56.7	126.6	128.8	2.2
C-4	−0.18	−0.02	56.9	126.4	127.9	1.5
C-4a	−0.06	−0.01	53.6	129.6	132.1	2.5
C-8a	−0.04	−0.02	47.1	136.2	136.5	0.3
C-5	−0.18	−0.02	55.1	128.1	128.6	0.5
C-6	−0.21	−0.02	59.7	123.5	125.2	1.7
C-7	−0.21	−0.02	59.6	123.6	125.8	2.2
C-8	−0.19	−0.03	54.8	128.5	129.7	1.2
CH_3	−0.62	0.01	159.6	23.6	23.1	−0.5

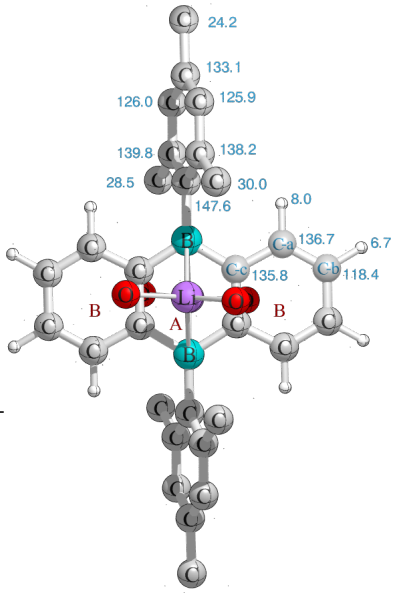


$[\mathbf{2a}]^{2-}$ (C_i)						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-a	−0.19	−0.06	48.3	135.0	137.5	2.5
C-b	−0.29	−0.09	74.5	108.8	118.8	10.0
C-c	−0.32	−0.67	44.2	139.0	134.9	−4.1
B	0.41	1.75				
H-a	0.18	−0.03	24.1	7.6	7.7	0.1
H-b	0.17	−0.06	25.6	6.1	6.6	0.4
Mes-*i*	−0.22	−0.50	21.6	161.6	148.3	−13.3
Mes-*o*	−0.08	−0.04	41.6	141.6	141.5	−0.1
Mes-*m*	−0.24	−0.06	62.1	121.2	127.7	6.5
Mes-*p*	−0.01	−0.03	63.8	119.4	133.3	13.9
CH_3-*o*	−0.62	0.01	155.2	28.0	25.1	−2.9
$NICS(0)^A$			−6.7			
$NICS(0)^B$			−4.4			
$NICS(0)^{Mes}$			−5.4			
$NICS(1)^A$			−9.3			
$NICS(1)^B$			−6.9			
$NICS(1)^{Mes}$			−6.9			
$NICS(-1)^A$			−9.3			
$NICS(-1)^B$			−6.4			
$NICS(-1)^{Mes}$			−6.7			



$[Li(THF)_2]_2$ [**2a**] (C_i)						
Atom	q(NPA)	q(AIM)	σ(calc)	δ(calc)	δ(exp)	Δ
C-a	−0.19	−0.05	46.5	136.7	137.5	0.8
C-b	−0.27	−0.06	64.9	118.4	118.8	0.4
C-c	−0.41	−0.82	47.5	135.8	134.9	−0.9
B	0.35	1.70				
Li	0.70	0.90	101.3	−8.0[a]	−7.2	0.8
H-a	0.21	0.01	23.7	8.0	7.7	−0.3
H-b	0.20	−0.01	25.0	6.7	6.6	−0.2
Mes-*i*	−0.25	−0.55	35.7	147.6	148.3	0.7
Mes-*o*	0.00	−0.03	43.5	139.8	141.5	1.7
Mes-*o*′	0.00	−0.03	45.0	138.2	141.5	3.3
Mes-*m*	−0.22	−0.04	57.2	126.0	127.7	1.7
Mes-*m*′	−0.22	−0.04	57.4	125.9	127.7	1.8
Mes-*p*	−0.03	−0.01	50.1	133.1	133.3	0.2
CH_3-*o*	−0.61	0.02	154.8	28.5	25.1	−3.4
CH_3-*o*′	−0.61	0.02	153.3	30.0	25.1	−4.9
CH_3-*p*	−0.61	0.03	159.0	24.2	21.4	−2.8
$NICS(0)^A$			−9.0			
$NICS(0)^B$			−4.8			
$NICS(0)^{Mes}$			−6.7			
$NICS(1)^A$			−13.1			
$NICS(1)^B$			−7.7			
$NICS(1)^{Mes}$			−8.1			
$NICS(-1)^A$			−13.1			
$NICS(-1)^B$			−7.2			
$NICS(-1)^{Mes}$			−7.9			

[a]NMR shift calculated relative to $Li(H_2O)_4^+$ ($\sigma(^7Li)$ = 93.3 ppm); for the bare Li^+ cation, $\sigma(^7Li)$ = 95.4 ppm, i.e., $\delta(^7Li)$ = −5.9 ppm. Taking η^5-LiCp as reference, $\sigma(^7Li)$ = 99.2 ppm, i.e., $\delta(^7Li)$ = −2.1 ppm.



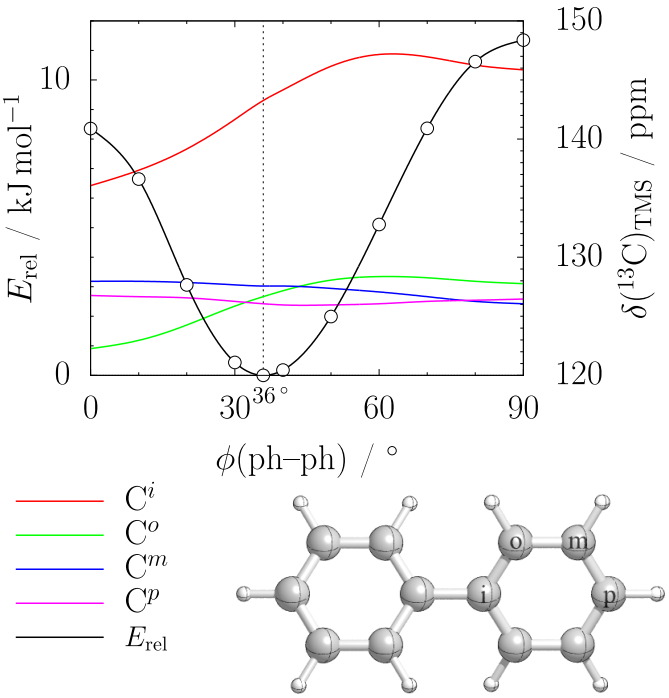


Figure S25: ^{13}C NMR shifts for biphenyl as a function of the torsional angle C^o–C^i–$C^{i'}$–$C^{o'}$ (relaxed potential-energy surface scan). Note the pronounced effect of the torsional angle on the ^{13}C NMR shifts of the *ortho*- and *meta*-carbon atoms.

6.2 HOMO–LUMO plots

Table S6: Orbital energies and energy gaps for the HOMO and LUMO of selected species.

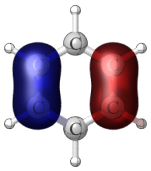
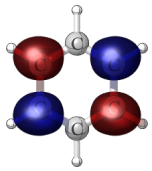
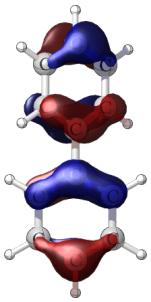
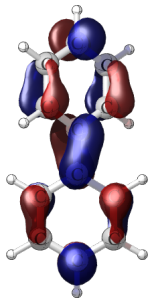
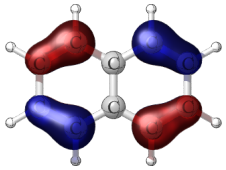
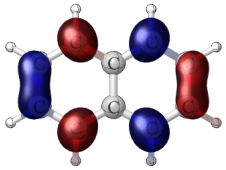
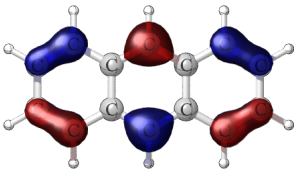
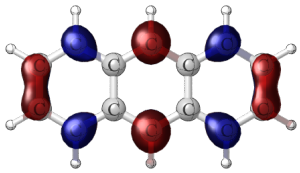
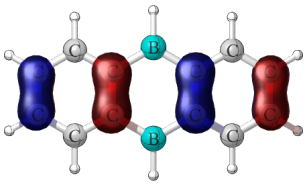
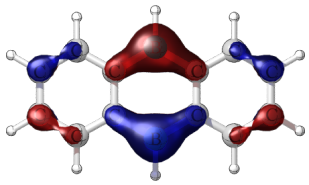
		E(HOMO)/a.u.	E(LUMO)/a.u.	E_{gap}/eV
benzene	D_{6h}	−0.227 114	−0.038 577	5.130
biphenyl	D_2	−0.204 415	−0.062 601	3.859
naphthalene	D_{2h}	−0.196 713	−0.071 066	3.419
anthracene	D_{2h}	−0.178 538	−0.091 918	2.357
9,10-diphenylanthracene	C_{2h}	−0.173 182	−0.090 887	2.239
DBA	D_{2h}	−0.224 986	−0.125 298	2.713
DBA^{2-}	D_{2h}	0.175 845	0.222 331	1.265
4a	C_i	−0.173 389	−0.090 754	2.249
anti-**4b**	C_i	−0.176 225	−0.093 300	2.257
$[\mathbf{4c}]_{model}$	C_{2h}	−0.176 106	−0.093 633	2.244
2a	C_{2h}	−0.194 809	−0.118 911	2.065
anti-**2b**	C_i	−0.185 797	−0.122 465	1.723
$[\mathbf{2c}]_{model}$	C_{2h}	−0.173 834	−0.123 303	1.375
$[\mathbf{2a}]^{2-}$	C_i	0.134 236	0.169 461	0.959
$[Li(THF)_2]_2$ [**2a**]	C_i	−0.111 137	−0.048 538	1.703
$[Li(THF)_2]_2$ [**2b**]	C_i	−0.113 892	−0.050 557	1.723
$[Li(THF)_2]_2$ $[\mathbf{2c}]_{model}$	C_i	−0.117 398	−0.076 099	1.124

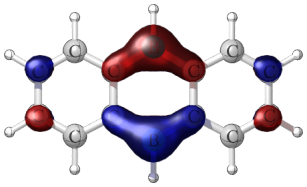
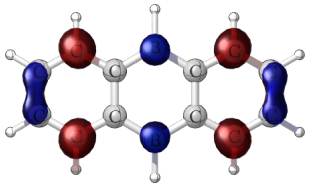
Table S7: Experimental band gaps, E_{gap}(exp), of **2a–c** and **4a–c**, naphthalene, anthracene and 9,10-diphenylanthracene, determined from the onset potential, λ, of the absorption spectrum, and compared to theory.

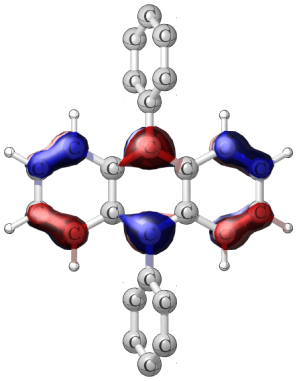
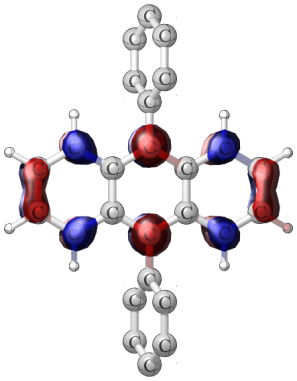
species	λ_{onset}/nm	E_{gap}(exp)/eV[a]	E_{gap}(calc)/eV	ΔE_{gap}(exp−calc)/eV
2a	428[b]	2.89	2.07	0.83
2b	477[b]	2.59	1.72	0.87
2c	599[b]	2.07	1.38[g]	0.70[g]
4a	406[b]	3.05	2.25	0.80
4b	407[b]	3.04	2.26	0.78
4c	420[b]	2.95	2.24[g]	0.71[g]
naphthalene	292[c,d]	4.25[e]	3.42	0.83
anthracene	385[b]	3.22[f]	2.34	0.86
9,10-diphenylanthracene	405[c,d]	3.06[f]	2.24	0.82

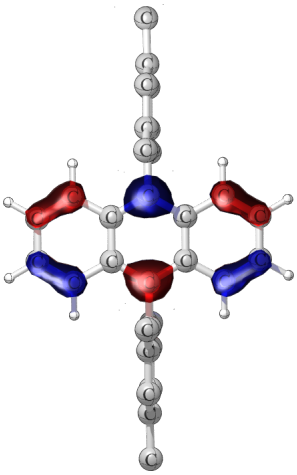
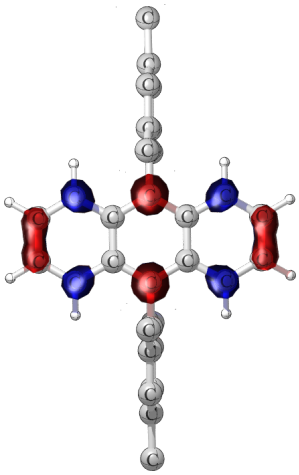
[a]Band gap vaules were calculated from the onset potential (λ) of the absorption spectrum.
[b]In C_6H_6.
[c]In C_6H_{12}.
[d]Spectra taken from `http://omlc.ogi.edu/spectra/PhotochemCAD/index.html`.
[e]Consistent with *Org. Electron.* 2009, **10**, 1396.
[f]Consistent with *J. Org. Chem.* 2007, **72**, 5567.
[g]Calculation for the model system; the additional ^{t}Bu and phenyl groups of the anthryl ligands in the full system are expected to lower E_{gap}(calc) by roughly 0.1 eV, i.e., E_{gap}(exp) = 2.18 eV according to λ_{onset} of the unsubstituted congener $DBA(ant)_2$.

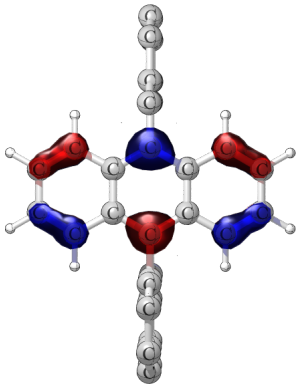
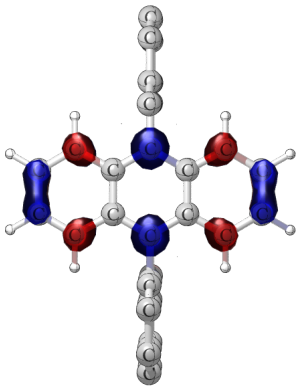
Table S8: Isosurface plots for the HOMO and LUMO (isovalue 0.05 $a_0^{-3/2}$) and calculated orbital energy differences. The H atoms of the mesityl, methylnaphthyl and anthryl substituents have been omitted for clarity.

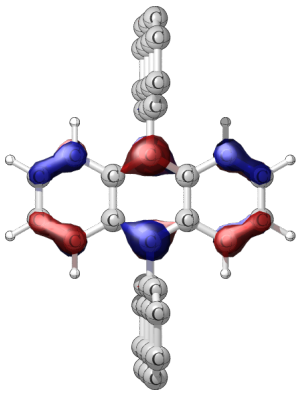
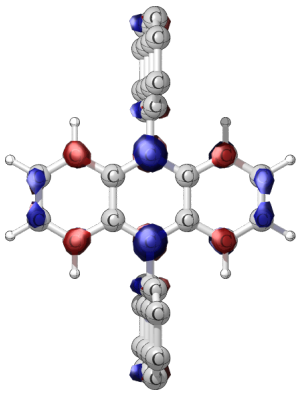
benzene (D_{6h})		
5.13 eV		
biphenyl (D_2)		
3.86 eV		
naphthalene (D_{2h})		
3.42 eV		
anthracene (D_{2h})		
2.36 eV		
9,10-diboraanthracene (D_{2h})		
2.71 eV		

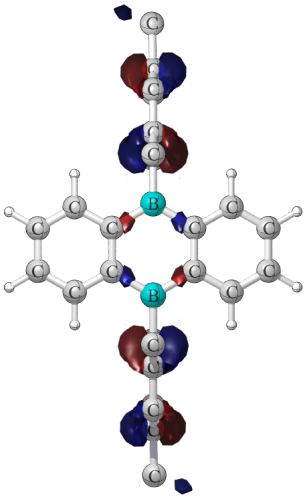
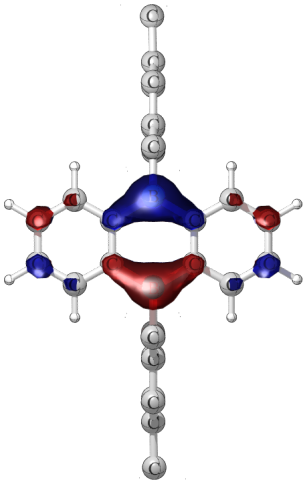
9,10-diboraanthracene^{2-} (D_{2h})		
1.27 eV		

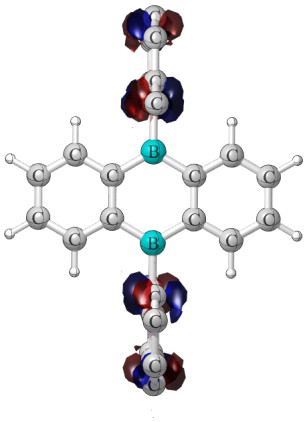
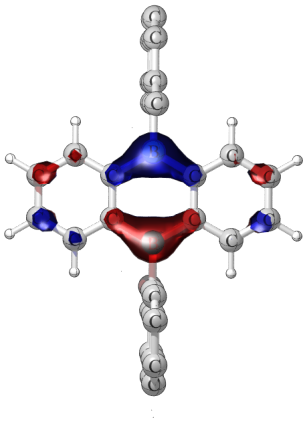
diphenylanthracene (C_{2h})		
2.34 eV		

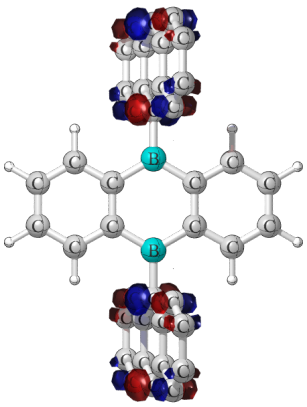
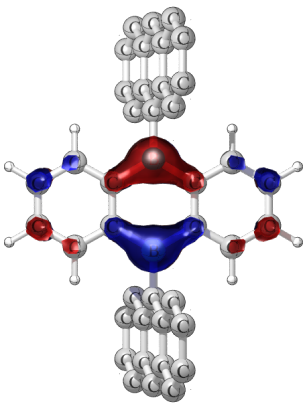
4a (C_i)		
2.25 eV		

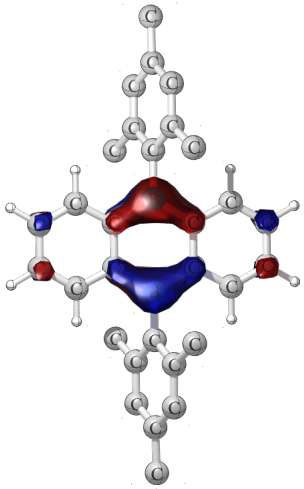
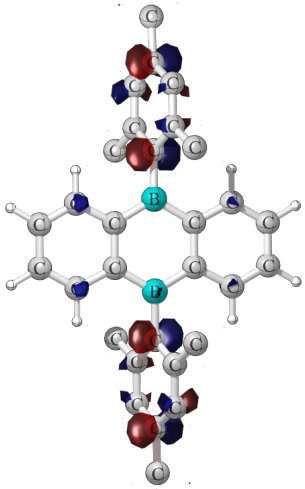
anti-**4b** (C_i)		
2.26 eV		

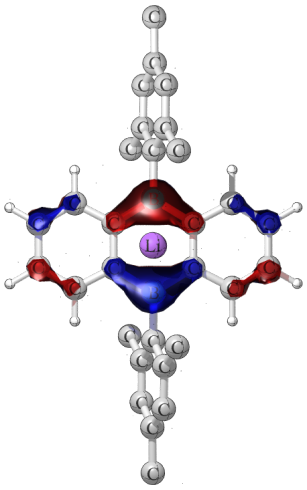
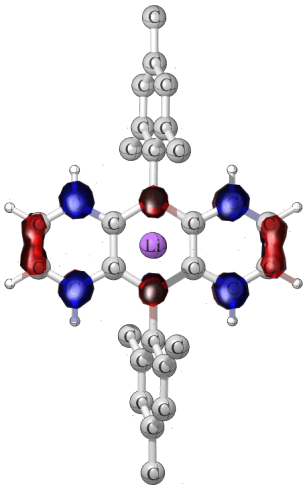
$[\mathbf{4c}]_\mathrm{model}$ (C_2h)		
2.24 eV		

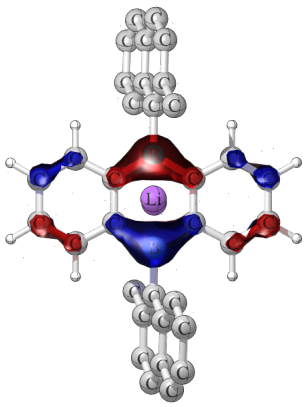
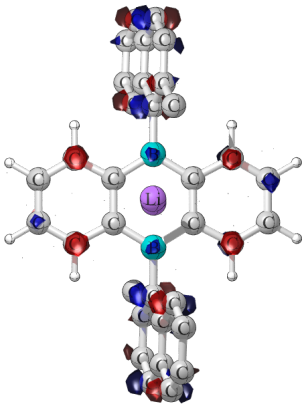
2a (C_2h)		
2.07 eV		

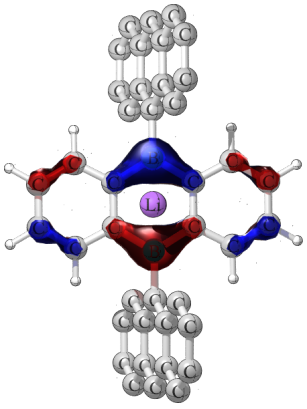
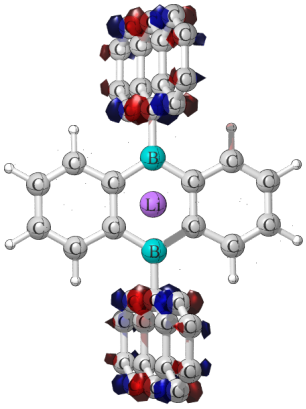
anti-**2b** (C_i)		
1.72 eV		

$[\mathbf{2c}]_\mathrm{model}$ (C_2h)		
1.38 eV		

$[\mathbf{2a}]^{2-}$ (C_i)		
0.96 eV		

$[Li(THF)_2]_2$ [**2a**] (C_i) THF molecules are omitted for clarity		
1.70 eV		

$[Li(THF)_2]_2$ [**2b**] (C_i) THF molecules are omitted for clarity		
1.72 eV		

$[Li(THF)_2]_2$ [**2c**]$_{model}$ (C_i) THF molecules are omitted for clarity		
1.12 eV		

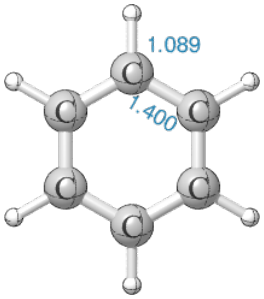
6.3 Molecular Geometries

Table S9: Term symbols, point groups and total electronic energies of the calculated systems (B97D/TZVP//B97D/TZVP/TZVPfit).

species			E_{tot}/a.u.
$^1\mathrm{A}_{1\mathrm{g}}$	benzene	$(D_{6\mathrm{h}})$	−232.144 766
$^1\mathrm{A}$	biphenyl	(D_2)	−463.094 206
$^1\mathrm{A}_{\mathrm{g}}$	naphthalene	$(D_{2\mathrm{h}})$	−385.713 724
$^1\mathrm{A}_{\mathrm{g}}$	anthracene	$(D_{2\mathrm{h}})$	−539.277 482
$^1\mathrm{A}_{\mathrm{g}}$	9,10-diboraanthracene	$(D_{2\mathrm{h}})$	−512.775 141
$^1\mathrm{A}_{\mathrm{g}}$	9,10-diboraanthracene^{2-}	$(D_{2\mathrm{h}})$	−512.721 455
$^1\mathrm{A}_{\mathrm{g}}$	diphenylanthracene	$(C_{2\mathrm{h}})$	−1001.170 371
$^1\mathrm{A}_{\mathrm{g}}$	**4a**	(C_{i})	−1236.990 402
$^1\mathrm{A}_{\mathrm{g}}$	*anti*-**4b**	(C_{i})	−1386.920 225
$^1\mathrm{A}_{\mathrm{g}}$	$[\mathbf{4c}]_{\mathrm{model}}$	$(C_{2\mathrm{h}})$	−1615.442 841
$^1\mathrm{A}_{\mathrm{g}}$	**2a**	$(C_{2\mathrm{h}})$	−1210.508 974
$^1\mathrm{A}_{\mathrm{g}}$	*anti*-**2b**	(C_{i})	−1360.440 262
$^1\mathrm{A}_{\mathrm{g}}$	$[\mathbf{2c}]_{\mathrm{model}}$	$(C_{2\mathrm{h}})$	−1588.964 630
$^1\mathrm{A}_{\mathrm{g}}$	$[\mathbf{2a}]^{2-}$	(C_{i})	−1210.487 731
$^1\mathrm{A}_{\mathrm{g}}$	$[\mathrm{Li(THF)_2}]_2\,[\mathbf{2a}]$	(C_{i})	−2155.317 385
$^1\mathrm{A}_{\mathrm{g}}$	$[\mathrm{Li(THF)_2}]_2\,[\mathbf{2b}]$	(C_{i})	−2305.256 259
$^1\mathrm{A}_{\mathrm{g}}$	$[\mathrm{Li(THF)_2}]_2\,[\mathbf{2c}]_{\mathrm{model}}$	(C_{i})	−2533.786 442
$^1\mathrm{S}$	Li^+	(K_{h})	−7.290 564
$^1\mathrm{A}$	$\mathrm{Li(H_2O)_4^+}$	(S_4)	−313.146 757
$^1\mathrm{A}_1$	η^5-LiCp	$(C_{5\mathrm{v}})$	−201.002 932
$^1\mathrm{A}_1$	$\mathrm{SiMe_4}$ (TMS)	(T_{d})	−449.129 441

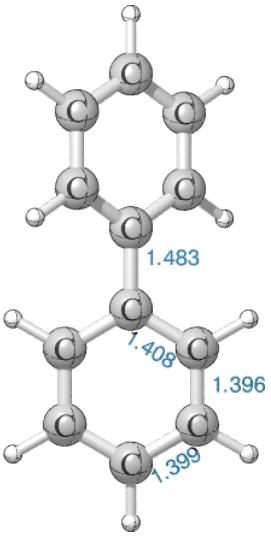
Table S10: Molecular geometries and cartesian coordinates computed at the B97D/TZVP/TZVPfit level of theory. The H atoms of the mesityl, methylnaphthyl and anthryl substituents have been omitted for clarity. For the same reason, in the di-lithiated compounds the THF ligands are represented by the corresponding O atoms only.

benzene (D_{6h})



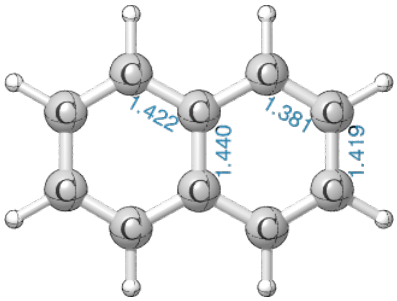
C	0.000000000000	1.399672535570	0.000000000000
C	1.212151972783	0.699836267785	0.000000000000
C	1.212151972783	-0.699836267785	0.000000000000
C	0.000000000000	-1.399672535570	0.000000000000
C	-1.212151972783	-0.699836267785	0.000000000000
C	-1.212151972783	0.699836267785	0.000000000000
H	0.000000000000	2.488276232061	0.000000000000
H	2.154910428598	1.244138116030	0.000000000000
H	2.154910428598	-1.244138116030	0.000000000000
H	0.000000000000	-2.488276232061	0.000000000000
H	-2.154910428598	-1.244138116030	0.000000000000
H	-2.154910428598	1.244138116030	0.000000000000

biphenyl (D_2), $\phi = 35.9°$



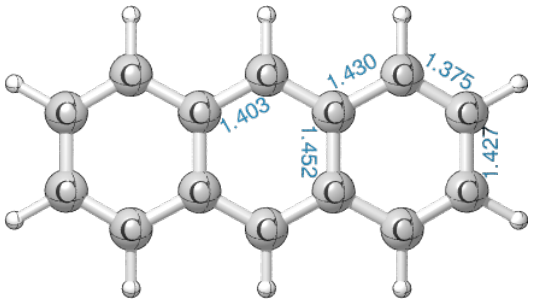
C	0.000000000000	0.000000000000	0.741502909477
C	0.000000000000	0.000000000000	-0.741502909477
C	-0.372295127200	1.149121993386	1.465163946496
C	-0.372295127200	-1.149121993386	-1.465163946496
C	0.372295127200	-1.149121993386	1.465163946496
C	0.372295127200	1.149121993386	-1.465163946496
C	-0.372500891867	1.149650413861	2.861590513626
C	-0.372500891867	-1.149650413861	-2.861590513626
C	0.372500891867	-1.149650413861	2.861590513626
C	0.372500891867	1.149650413861	-2.861590513626
C	0.000000000000	0.000000000000	3.566887503532
C	0.000000000000	0.000000000000	-3.566887503532
H	-0.685989105414	2.039566599524	0.924482248766
H	-0.685989105414	-2.039566599524	-0.924482248766
H	0.685989105414	-2.039566599524	0.924482248766
H	0.685989105414	2.039566599524	-0.924482248766
H	-0.672379216694	2.046767330938	3.400372806567
H	-0.672379216694	-2.046767330938	-3.400372806567
H	0.672379216694	-2.046767330938	3.400372806567
H	0.672379216694	2.046767330938	-3.400372806567
H	0.000000000000	0.000000000000	4.655151226833
H	0.000000000000	0.000000000000	-4.655151226833

naphthalene (D_{2h})



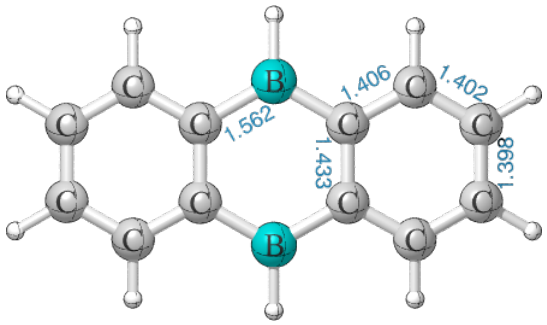
C	0.000000000000	0.000000000000	0.741502909477
C	0.000000000000	0.000000000000	-0.741502909477
C	-0.372295127200	1.149121993386	1.465163946496
C	-0.372295127200	-1.149121993386	-1.465163946496
C	0.372295127200	-1.149121993386	1.465163946496
C	0.372295127200	1.149121993386	-1.465163946496
C	-0.372500891867	1.149650413861	2.861590513626
C	-0.372500891867	-1.149650413861	-2.861590513626
C	0.372500891867	-1.149650413861	2.861590513626
C	0.372500891867	1.149650413861	-2.861590513626
C	0.000000000000	0.000000000000	3.566887503532
C	0.000000000000	0.000000000000	-3.566887503532
H	-0.685989105414	2.039566599524	0.924482248766
H	-0.685989105414	-2.039566599524	-0.924482248766
H	0.685989105414	-2.039566599524	0.924482248766
H	0.685989105414	2.039566599524	-0.924482248766
H	-0.672379216694	2.046767330938	3.400372806567
H	-0.672379216694	-2.046767330938	-3.400372806567
H	0.672379216694	-2.046767330938	3.400372806567
H	0.672379216694	2.046767330938	-3.400372806567
H	0.000000000000	0.000000000000	4.655151226833
H	0.000000000000	0.000000000000	-4.655151226833

anthracene (D_{2h})



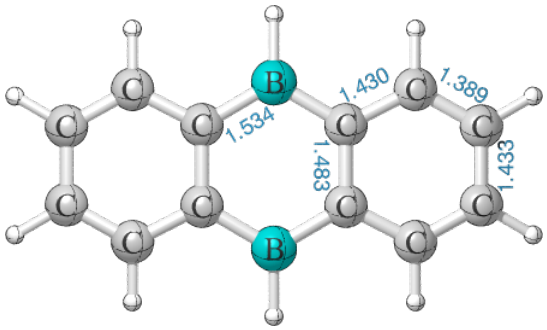
C	0.000000000000	0.000000000000	1.408986871219
C	0.000000000000	1.225092816667	0.725779042614
C	0.000000000000	1.225092816667	-0.725779042614
C	0.000000000000	0.000000000000	-1.408986871219
C	0.000000000000	-1.225092816667	-0.725779042614
C	0.000000000000	-1.225092816667	0.725779042614
C	0.000000000000	-2.480355336822	1.410458467239
C	0.000000000000	-3.665320235685	0.713512349627
C	0.000000000000	-3.665320235685	-0.713512349627
C	0.000000000000	-2.480355336822	-1.410458467239
C	0.000000000000	2.480355336822	1.410458467239
C	0.000000000000	3.665320235685	0.713512349627
C	0.000000000000	3.665320235685	-0.713512349627
C	0.000000000000	2.480355336822	-1.410458467239
H	0.000000000000	0.000000000000	2.498981827565
H	0.000000000000	0.000000000000	-2.498981827565
H	0.000000000000	-2.477686717204	2.499672961453
H	0.000000000000	-4.613192377126	1.248336243606
H	0.000000000000	-4.613192377126	-1.248336243606
H	0.000000000000	-2.477686717204	-2.499672961453
H	0.000000000000	2.477686717204	2.499672961453
H	0.000000000000	4.613192377126	1.248336243606
H	0.000000000000	4.613192377126	-1.248336243606
H	0.000000000000	2.477686717204	-2.499672961453

9,10-diboraanthracene (D_{2h})



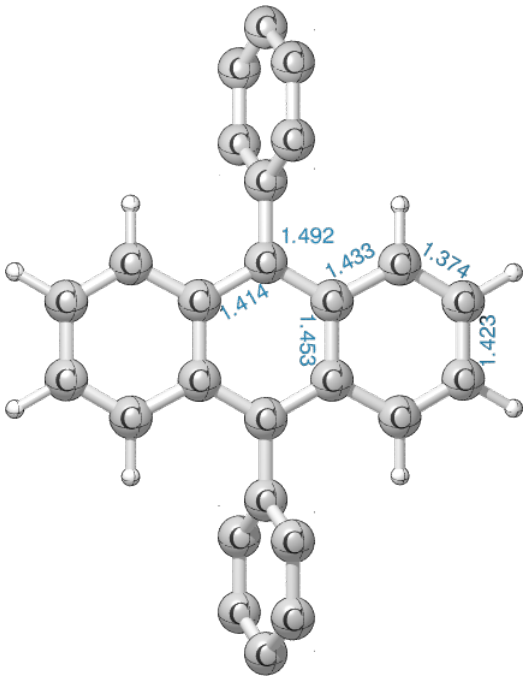
B	0.000000000000	0.000000000000	1.496207454905
C	0.000000000000	1.353573511759	0.716705566937
C	0.000000000000	1.353573511759	-0.716705566937
B	0.000000000000	0.000000000000	-1.496207454905
C	0.000000000000	-1.353573511759	-0.716705566937
C	0.000000000000	-1.353573511759	0.716705566937
C	0.000000000000	-2.584167245640	1.396724113810
C	0.000000000000	-3.800699720697	0.698833150680
C	0.000000000000	-3.800699720697	-0.698833150680
C	0.000000000000	-2.584167245640	-1.396724113810
C	0.000000000000	2.584167245640	1.396724113810
C	0.000000000000	3.800699720697	0.698833150680
C	0.000000000000	3.800699720697	-0.698833150680
C	0.000000000000	2.584167245640	-1.396724113810
H	0.000000000000	0.000000000000	2.703421702096
H	0.000000000000	0.000000000000	-2.703421702096
H	0.000000000000	-2.588601846253	2.486514595320
H	0.000000000000	-4.743895969402	1.243230458125
H	0.000000000000	-4.743895969402	-1.243230458125
H	0.000000000000	-2.588601846253	-2.486514595320
H	0.000000000000	2.588601846253	2.486514595320
H	0.000000000000	4.743895969402	1.243230458125
H	0.000000000000	4.743895969402	-1.243230458125
H	0.000000000000	2.588601846253	-2.486514595320

9,10-diboraanthracene^{2-} (D_{2h})



B	0.000000000000	0.000000000000	1.519037807845
C	0.000000000000	1.322010028474	0.741444842880
C	0.000000000000	1.322010028474	-0.741444842880
B	0.000000000000	0.000000000000	-1.519037807845
C	0.000000000000	-1.322010028474	-0.741444842880
C	0.000000000000	-1.322010028474	0.741444842880
C	0.000000000000	-2.594916509708	1.393521501405
C	0.000000000000	-3.807677227370	0.716596496616
C	0.000000000000	-3.807677227370	-0.716596496616
C	0.000000000000	-2.594916509708	-1.393521501405
C	0.000000000000	2.594916509708	1.393521501405
C	0.000000000000	3.807677227370	0.716596496616
C	0.000000000000	3.807677227370	-0.716596496616
C	0.000000000000	2.594916509708	-1.393521501405
H	0.000000000000	0.000000000000	2.756001824510
H	0.000000000000	0.000000000000	-2.756001824510
H	0.000000000000	-2.598979589374	2.490620954588
H	0.000000000000	-4.755223832309	1.267150603819
H	0.000000000000	-4.755223832309	-1.267150603819
H	0.000000000000	-2.598979589374	-2.490620954588
H	0.000000000000	2.598979589374	2.490620954588
H	0.000000000000	4.755223832309	1.267150603819
H	0.000000000000	4.755223832309	-1.267150603819
H	0.000000000000	2.598979589374	-2.490620954588

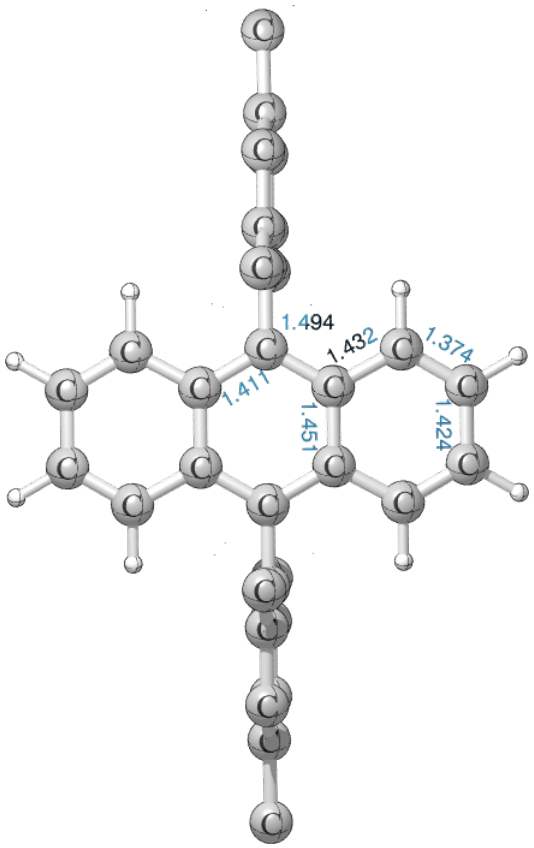
diphenylanthracene (C_{2h}), $\phi = 73.0°$



C	0.000000000000	0.000000000000	1.432115032225
C	-1.172150248105	0.357775793634	0.726280746284
C	-1.172150248105	0.357775793634	-0.726280746284
C	0.000000000000	0.000000000000	-1.432115032225
C	1.172150248105	-0.357775793634	-0.726280746284
C	1.172150248105	-0.357775793634	0.726280746284
C	2.388455710765	-0.696644265811	1.404620317242
C	3.528624537294	-1.023669515669	0.711349139923
C	3.528624537294	-1.023669515669	-0.711349139923
C	2.388455710765	-0.696644265811	-1.404620317242
C	-2.388455710765	0.696644265811	1.404620317242
C	-3.528624537294	1.023669515669	0.711349139923
C	-3.528624537294	1.023669515669	-0.711349139923
C	-2.388455710765	0.696644265811	-1.404620317242
H	2.398804187471	-0.685495848375	2.490556908479
H	4.439754946379	-1.273500774813	1.251870625347
H	4.439754946379	-1.273500774813	-1.251870625347
H	2.398804187471	-0.685495848375	-2.490556908479
H	-2.398804187471	0.685495848375	2.490556908479
H	-4.439754946379	1.273500774813	1.251870625347
H	-4.439754946379	1.273500774813	-1.251870625347
H	-2.398804187471	0.685495848375	-2.490556908479
C	0.000000000000	0.000000000000	2.924236344259
C	-0.001036136627	1.208632443513	3.638320661004
C	0.000000000000	1.209655597483	5.036370638139
C	0.000000000000	0.000000000000	5.739443609197
C	0.000000000000	-1.209655597483	5.036370638139

C	0.001036136627	-1.208632443513	3.638320661004
H	-0.001022959246	2.147961871000	3.088820122836
H	0.002953514442	2.154848415021	5.576429953226
H	0.000000000000	0.000000000000	6.827827342560
H	-0.002953514442	-2.154848415021	5.576429953226
H	0.001022959246	-2.147961871000	3.088820122836
C	0.000000000000	0.000000000000	-2.924236344259
C	0.001036136627	-1.208632443513	-3.638320661004
C	0.000000000000	-1.209655597483	-5.036370638139
C	0.000000000000	0.000000000000	-5.739443609197
C	0.000000000000	1.209655597483	-5.036370638139
C	-0.001036136627	1.208632443513	-3.638320661004
H	0.001022959246	-2.147961871000	-3.088820122836
H	-0.002953514442	-2.154848415021	-5.576429953226
H	0.000000000000	0.000000000000	-6.827827342560
H	0.002953514442	2.154848415021	-5.576429953226
H	-0.001022959246	2.147961871000	-3.088820122836

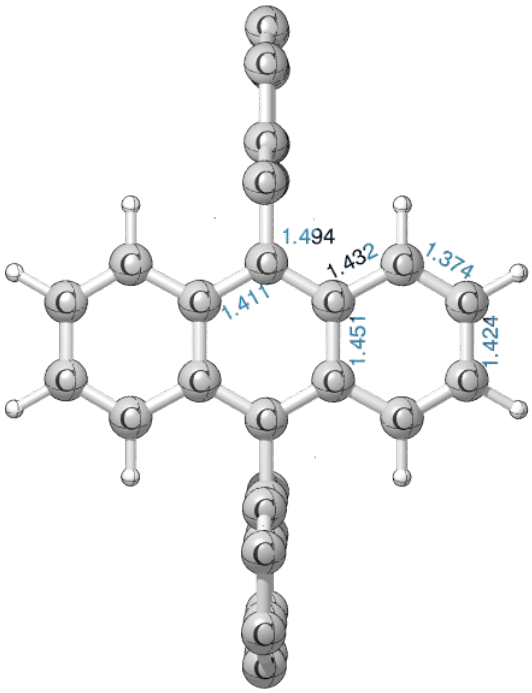
4a (C_i), $\phi = 89.2°$



C	1.414503389980	-0.166156142844	-0.141892502157
C	0.543579539254	-1.230142743749	-0.459372243523
C	-0.890111363704	-1.061820673858	-0.315420392290
C	-1.414503389980	0.166156142844	0.141892502157
C	-0.543579539254	1.230142743749	0.459372243523
C	0.890111363704	1.061820673858	0.315420392290
C	1.741670617211	2.164480918270	0.646260159827
C	1.224086941108	3.357167989622	1.091555495507
C	-0.183407705631	3.522230261317	1.233462882202
C	-1.037794772388	2.490579490616	0.926218122828
C	1.037794772388	-2.490579490616	-0.926218122828
C	0.183407705631	-3.522230261317	-1.233462882202
C	-1.224086941108	-3.357167989622	-1.091555495507
C	-1.741670617211	-2.164480918270	-0.646260159827
H	2.815918481733	2.038148035496	0.537242079480
H	1.891149244816	4.181413336015	1.337547981287
H	-0.581908693614	4.471502766906	1.586940736899
H	-2.112328888543	2.616416896646	1.033831179557
H	2.112328888543	-2.616416896646	-1.033831179557
H	0.581908693614	-4.471502766906	-1.586940736899
H	-1.891149244816	-4.181413336015	-1.337547981287
H	-2.815918481733	-2.038148035496	-0.537242079480

C	2.891054971378	-0.337885687533	-0.290194313020
C	3.658846513737	-0.791200547714	0.800288798627
C	5.043463396846	-0.936931569950	0.643782103664
C	5.681751348154	-0.644756811171	-0.567073088411
C	4.898813318333	-0.192201639638	-1.636561427294
C	3.512575009773	-0.034605062334	-1.518292102725
C	2.999745115590	-1.109794663650	2.122609176844
H	5.636210353126	-1.284335957498	1.490263163532
C	7.172731081402	-0.837953155138	-0.726908104116
H	5.377575026945	0.048536657948	-2.586129916132
C	2.693809037304	0.459129488210	-2.688852516351
H	3.739066761681	-1.455916162609	2.854453633562
H	2.491082959438	-0.225448466129	2.529983813832
H	2.234554848783	-1.888723274502	2.002484711986
H	7.395621009174	-1.819106474615	-1.172688555438
H	7.684733379061	-0.790625930953	0.242357865711
H	7.603378622755	-0.073090448045	-1.386036813863
H	3.332640512459	0.654861742538	-3.558085723635
H	2.158642130731	1.383233987361	-2.431131831523
H	1.932044016064	-0.279554007311	-2.973041441757
C	-2.891054971378	0.337885687533	0.290194313020
C	-3.658846513737	0.791200547714	-0.800288798627
C	-5.043463396846	0.936931569950	-0.643782103664
C	-5.681751348154	0.644756811171	0.567073088411
C	-4.898813318333	0.192201639638	1.636561427294
C	-3.512575009773	0.034605062334	1.518292102725
C	-2.999745115590	1.109794663650	-2.122609176844
H	-5.636210353126	1.284335957498	-1.490263163532
C	-7.172731081402	0.837953155138	0.726908104116
H	-5.377575026945	-0.048536657948	2.586129916132
C	-2.693809037304	-0.459129488210	2.688852516351
H	-3.739066761681	1.455916162609	-2.854453633562
H	-2.491082959438	0.225448466129	-2.529983813832
H	-2.234554848783	1.888723274502	-2.002484711986
H	-7.395621009174	1.819106474615	1.172688555438
H	-7.684733379061	0.790625930953	-0.242357865711
H	-7.603378622755	0.073090448045	1.386036813863
H	-3.332640512459	-0.654861742538	3.558085723635
H	-2.158642130731	-1.383233987361	2.431131831523
H	-1.932044016064	0.279554007311	2.973041441757

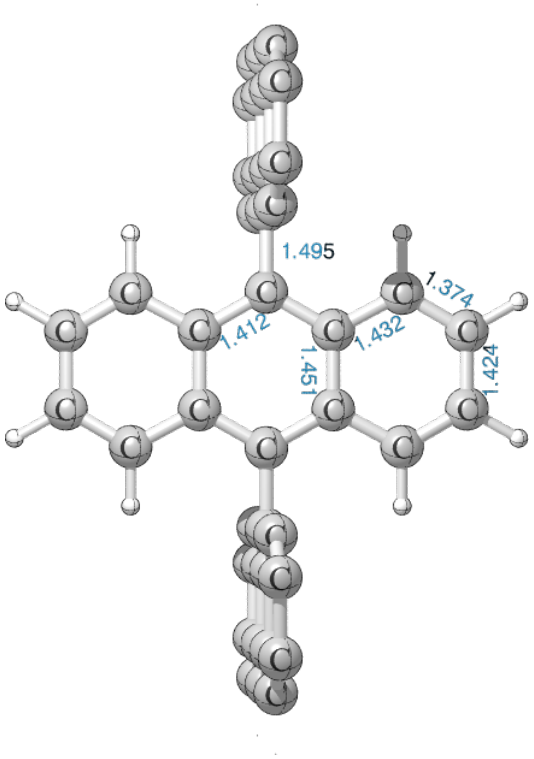
anti-**4b** (C_i), $\phi = 89.6°$



C	1.021930944926	0.994044751522	0.101212922680
C	0.591417376949	0.554014543700	-1.168604661089
C	-0.448444396526	-0.452432209308	-1.271374443707
C	-1.021930944926	-0.994044751522	-0.101212922680
C	-0.591417376949	-0.554014543700	1.168604661089
C	0.448444396526	0.452432209308	1.271374443707
C	0.864029363797	0.871821060154	2.575928291703
C	0.296339503066	0.341468337689	3.709187333725
C	-0.725882626835	-0.644971429180	3.608243460732
C	-1.154976496590	-1.077133786780	2.376514099058
C	1.154976496590	1.077133786780	-2.376514099058
C	0.725882626835	0.644971429180	-3.608243460732
C	-0.296339503066	-0.341468337689	-3.709187333725
C	-0.864029363797	-0.871821060154	-2.575928291703
H	1.645980184676	1.622572824434	2.654205686997
H	0.629009119554	0.674477226407	4.690543221649
H	-1.169818978994	-1.055744264990	4.513124809467
H	-1.937955987942	-1.827219927064	2.300708451918
H	1.937955987942	1.827219927064	-2.300708451918
H	1.169818978994	1.055744264990	-4.513124809467
H	-0.629009119554	-0.674477226407	-4.690543221649
H	-1.645980184676	-1.622572824434	-2.654205686997
C	2.078922096729	2.044845608942	0.207782446765
C	1.714199506664	3.387982160733	0.240791024512
C	2.725559397761	4.380553128100	0.341981646029

C	4.060779976581	4.044696568620	0.407649681707
C	4.464899881734	2.684967841769	0.376392466171
C	3.455304786113	1.663878634192	0.275152739980
C	3.870499944931	0.302235460834	0.244477893310
C	5.208137598765	-0.033051037237	0.309918033693
C	6.200631814173	0.974581962342	0.409552447380
C	5.833442783420	2.304429796325	0.441877244215
C	0.261282915887	3.798681105469	0.169257328867
H	0.159998789644	4.889111297639	0.218205936008
H	-0.312292093410	3.356342893470	0.994931256812
H	-0.200000211614	3.446154795935	-0.763269575140
H	2.425711788452	5.427398948017	0.366595969839
H	4.823074788370	4.818985692619	0.484440660339
H	3.113836411154	-0.474541877308	0.167827604513
H	5.505276212111	-1.079892850417	0.284871868962
H	7.251299597320	0.695166796275	0.460293887231
H	6.588136044893	3.086328033889	0.518143465401
C	-2.078922096729	-2.044845608942	-0.207782446765
C	-1.714199506664	-3.387982160733	-0.240791024512
C	-2.725559397761	-4.380553128100	-0.341981646029
C	-4.060779976581	-4.044696568620	-0.407649681707
C	-4.464899881734	-2.684967841769	-0.376392466171
C	-3.455304786113	-1.663878634192	-0.275152739980
C	-3.870499944931	-0.302235460834	-0.244477893310
C	-5.208137598765	0.033051037237	-0.309918033693
C	-6.200631814173	-0.974581962342	-0.409552447380
C	-5.833442783420	-2.304429796325	-0.441877244215
C	-0.261282915887	-3.798681105469	-0.169257328867
H	-0.159998789644	-4.889111297639	-0.218205936008
H	0.312292093410	-3.356342893470	-0.994931256812
H	0.200000211614	-3.446154795935	0.763269575140
H	-2.425711788452	-5.427398948017	-0.366595969839
H	-4.823074788370	-4.818985692619	-0.484440660339
H	-3.113836411154	0.474541877308	-0.167827604513
H	-5.505276212111	1.079892850417	-0.284871868962
H	-7.251299597320	-0.695166796275	-0.460293887231
H	-6.588136044893	-3.086328033889	-0.518143465401

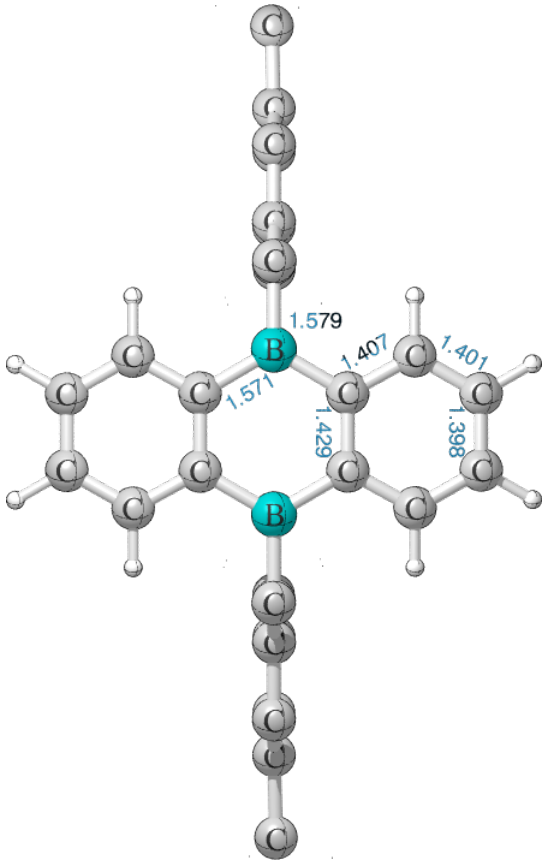
$[\mathbf{4c}]_{\mathrm{model}}$ (C_{2h}), $\phi = 85.6°$



C	0.000000000000	0.000000000000	1.428489819438
C	-0.183318934052	1.210129693490	0.725358722178
C	-0.183318934052	1.210129693490	-0.725358722178
C	0.000000000000	0.000000000000	-1.428489819438
C	0.183318934052	-1.210129693490	-0.725358722178
C	0.183318934052	-1.210129693490	0.725358722178
C	0.367769519956	-2.455967091893	1.406705822518
C	0.543317312008	-3.627977912380	0.712024115877
C	0.543317312008	-3.627977912380	-0.712024115877
C	0.367769519956	-2.455967091893	-1.406705822518
C	-0.367769519956	2.455967091893	1.406705822518
C	-0.543317312008	3.627977912380	0.712024115877
C	-0.543317312008	3.627977912380	-0.712024115877
C	-0.367769519956	2.455967091893	-1.406705822518
H	0.367380509134	-2.457867813863	2.493260862983
H	0.682251198144	-4.563222461713	1.251041439466
H	0.682251198144	-4.563222461713	-1.251041439466
H	0.367380509134	-2.457867813863	-2.493260862983
H	-0.367380509134	2.457867813863	2.493260862983
H	-0.682251198144	4.563222461713	1.251041439466
H	-0.682251198144	4.563222461713	-1.251041439466
H	-0.367380509134	2.457867813863	-2.493260862983
C	0.000000000000	0.000000000000	2.923098329407
C	-1.223282950901	-0.089722505802	3.625108019092
C	-1.219089257438	-0.087794631699	5.076047555477

C	0.000000000000	0.000000000000	5.760061716776
C	1.219089257438	0.087794631699	5.076047555477
C	1.223282950901	0.089722505802	3.625108019092
C	2.484430995027	0.186624621534	2.955178374490
C	3.659782302083	0.272347306284	3.662941183996
C	3.653060504593	0.267327648201	5.088583777911
C	2.464948370288	0.177954966718	5.772458750359
C	-2.484430995027	-0.186624621534	2.955178374490
C	-3.659782302083	-0.272347306284	3.662941183996
C	-3.653060504593	-0.267327648201	5.088583777911
C	-2.464948370288	-0.177954966718	5.772458750359
H	0.000000000000	0.000000000000	6.849999788346
H	2.497889915533	0.190238627681	1.868498398631
H	4.607229556106	0.345692559063	3.132355015779
H	4.593946637486	0.335963121202	5.631234651229
H	2.449158626623	0.174718353219	6.861577130419
H	-2.497889915533	-0.190238627681	1.868498398631
H	-4.607229556106	-0.345692559063	3.132355015779
H	-4.593946637486	-0.335963121202	5.631234651229
H	-2.449158626623	-0.174718353219	6.861577130419
C	0.000000000000	0.000000000000	-2.923098329407
C	1.223282950901	0.089722505802	-3.625108019092
C	1.219089257438	0.087794631699	-5.076047555477
C	0.000000000000	0.000000000000	-5.760061716776
C	-1.219089257438	-0.087794631699	-5.076047555477
C	-1.223282950901	-0.089722505802	-3.625108019092
C	-2.484430995027	-0.186624621534	-2.955178374490
C	-3.659782302083	-0.272347306284	-3.662941183996
C	-3.653060504593	-0.267327648201	-5.088583777911
C	-2.464948370288	-0.177954966718	-5.772458750359
C	2.484430995027	0.186624621534	-2.955178374490
C	3.659782302083	0.272347306284	-3.662941183996
C	3.653060504593	0.267327648201	-5.088583777911
C	2.464948370288	0.177954966718	-5.772458750359
H	0.000000000000	0.000000000000	-6.849999788346
H	-2.497889915533	-0.190238627681	-1.868498398631
H	-4.607229556106	-0.345692559063	-3.132355015779
H	-4.593946637486	-0.335963121202	-5.631234651229
H	-2.449158626623	-0.174718353219	-6.861577130419
H	2.497889915533	0.190238627681	-1.868498398631
H	4.607229556106	0.345692559063	-3.132355015779
H	4.593946637486	0.335963121202	-5.631234651229
H	2.449158626623	0.174718353219	-6.861577130419

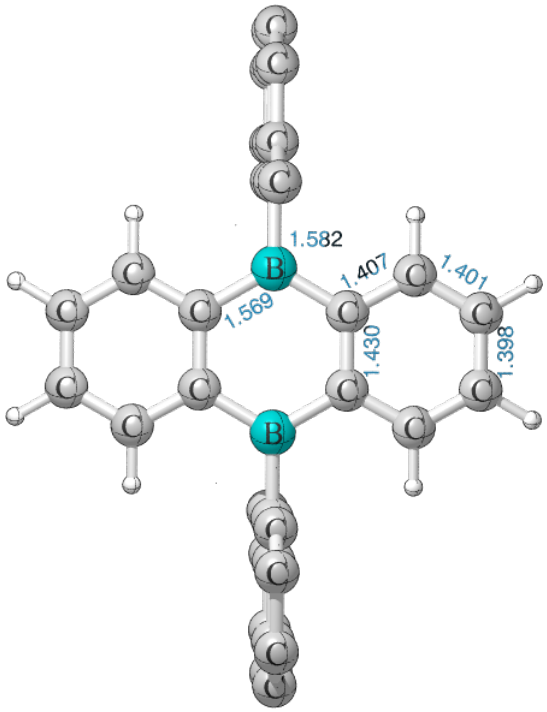
2a (C_{2h}), $\phi = 89.8°$



B	0.001632337069	1.510586773128	0.000000000000
C	1.355165038026	0.713146773121	0.000000000000
C	1.353566375917	-0.716085321147	0.000000000000
B	-0.001632337069	-1.510586773128	0.000000000000
C	-1.355165038026	-0.713146773121	0.000000000000
C	-1.353566375917	0.716085321147	0.000000000000
C	-2.583936397806	1.398250091833	0.000000000000
C	-3.800011024774	0.703463235195	0.000000000000
C	-3.801567236271	-0.695005581401	0.000000000000
C	-2.587062423071	-1.392539485167	0.000000000000
C	2.587062423071	1.392539485167	0.000000000000
C	3.801567236271	0.695005581401	0.000000000000
C	3.800011024774	-0.703463235195	0.000000000000
C	2.583936397806	-1.398250091833	0.000000000000
H	-2.582163564246	2.487825450289	0.000000000000
H	-4.742171901387	1.249904210705	0.000000000000
H	-4.744962930720	-1.239317561990	0.000000000000
H	-2.587679024476	-2.482098307294	0.000000000000
H	2.587679024476	2.482098307294	0.000000000000
H	4.744962930720	1.239317561990	0.000000000000
H	4.742171901387	-1.249904210705	0.000000000000
H	2.582163564246	-2.487825450289	0.000000000000

C	0.003407290667	3.089748434736	0.000000000000
C	0.000976317674	3.807207800424	1.216570130338
C	-0.000976317674	5.207646878076	1.201105396980
C	0.001368571373	5.927535398517	0.000000000000
C	-0.000976317674	5.207646878076	-1.201105396980
C	0.000976317674	3.807207800424	-1.216570130338
C	-0.005643046898	3.057051513197	2.532415778464
H	-0.006907322974	5.748460232873	2.148452345496
C	0.036677303063	7.439223457531	0.000000000000
H	-0.006907322974	5.748460232873	-2.148452345496
C	-0.005643046898	3.057051513197	-2.532415778464
H	0.005267102284	3.745213973601	3.386274330766
H	-0.897355040175	2.418754848305	2.615363569283
H	0.869510112096	2.395749671276	2.611027790320
H	1.073775715655	7.807840763181	0.000000000000
H	-0.457710781991	7.847690201466	0.890771216155
H	-0.457710781991	7.847690201466	-0.890771216155
H	0.005267102284	3.745213973601	-3.386274330766
H	-0.897355040175	2.418754848305	-2.615363569283
H	0.869510112096	2.395749671276	-2.611027790320
C	-0.003407290667	-3.089748434736	0.000000000000
C	-0.000976317674	-3.807207800424	-1.216570130338
C	0.000976317674	-5.207646878076	-1.201105396980
C	-0.001368571373	-5.927535398517	0.000000000000
C	0.000976317674	-5.207646878076	1.201105396980
C	-0.000976317674	-3.807207800424	1.216570130338
C	0.005643046898	-3.057051513197	-2.532415778464
H	0.006907322974	-5.748460232873	-2.148452345496
C	-0.036677303063	-7.439223457531	0.000000000000
H	0.006907322974	-5.748460232873	2.148452345496
C	0.005643046898	-3.057051513197	2.532415778464
H	-0.005267102284	-3.745213973601	-3.386274330766
H	0.897355040175	-2.418754848305	-2.615363569283
H	-0.869510112096	-2.395749671276	-2.611027790320
H	-1.073775715655	-7.807840763181	0.000000000000
H	0.457710781991	-7.847690201466	-0.890771216155
H	0.457710781991	-7.847690201466	0.890771216155
H	-0.005267102284	-3.745213973601	3.386274330766
H	0.897355040175	-2.418754848305	2.615363569283
H	-0.869510112096	-2.395749671276	2.611027790320

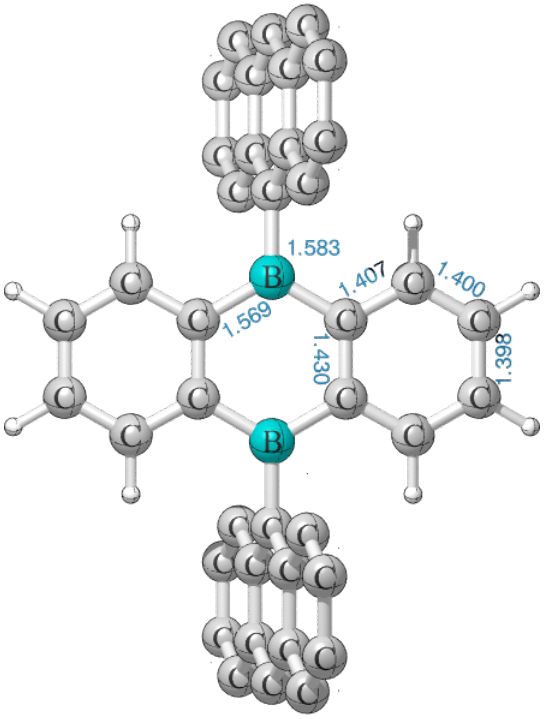
anti-**2b** (C_i), $\phi = 83.9°$



B	1.091706144813	1.033552968090	0.116319341193
C	0.659495067522	0.492166319076	-1.291555054388
C	-0.380805213144	-0.482709739377	-1.402016686813
B	-1.091706144813	-1.033552968090	-0.116319341193
C	-0.659495067522	-0.492166319076	1.291555054388
C	0.380805213144	0.482709739377	1.402016686813
C	0.758182014926	0.933036506846	2.679951921772
C	0.131974700632	0.448724860448	3.835277016323
C	-0.888579542889	-0.501010676143	3.726839936645
C	-1.276479204289	-0.965576266907	2.463770019283
C	1.276479204289	0.965576266907	-2.463770019283
C	0.888579542889	0.501010676143	-3.726839936645
C	-0.131974700632	-0.448724860448	-3.835277016323
C	-0.758182014926	-0.933036506846	-2.679951921772
H	1.553651298724	1.672117217280	2.765153871997
H	0.438710671601	0.810336918989	4.815690313932
H	-1.379655991196	-0.878825736705	4.622437724937
H	-2.071086336442	-1.705654960598	2.380577638100
H	2.071086336442	1.705654960598	-2.380577638100
H	1.379655991196	0.878825736705	-4.622437724937
H	-0.438710671601	-0.810336918989	-4.815690313932
H	-1.553651298724	-1.672117217280	-2.765153871997
C	2.215312793080	2.140462852603	0.239313139575
C	1.859943184328	3.487373855935	0.327849964497

C	2.866649569492	4.484152018522	0.433623706470
C	4.205254958630	4.154565533995	0.459089591531
C	4.612257056788	2.797640174457	0.376891452555
C	3.600814158919	1.778818825299	0.263143449723
C	4.023989841685	0.419866917641	0.181968648699
C	5.362527329930	0.082904311040	0.210172107244
C	6.353290316761	1.091198089849	0.321397405986
C	5.982597028967	2.418408268348	0.402233877563
C	0.401286053280	3.898814752301	0.319989745090
H	0.293794251686	4.985991935288	0.223983815115
H	-0.098877909335	3.586030133078	1.247998622626
H	-0.140147750512	3.425564519748	-0.511580011122
H	2.562834026560	5.529067792455	0.492781753087
H	4.966196579707	4.929829416916	0.540506035569
H	3.272585392453	-0.364425775107	0.095019035085
H	5.661415990857	-0.961815181053	0.146544206784
H	7.405686546655	0.814244290993	0.342884768419
H	6.737600185543	3.199321785469	0.488061108048
C	-2.215312793080	-2.140462852603	-0.239313139575
C	-1.859943184328	-3.487373855935	-0.327849964497
C	-2.866649569492	-4.484152018522	-0.433623706470
C	-4.205254958630	-4.154565533995	-0.459089591531
C	-4.612257056788	-2.797640174457	-0.376891452555
C	-3.600814158919	-1.778818825299	-0.263143449723
C	-4.023989841685	-0.419866917641	-0.181968648699
C	-5.362527329930	-0.082904311040	-0.210172107244
C	-6.353290316761	-1.091198089849	-0.321397405986
C	-5.982597028967	-2.418408268348	-0.402233877563
C	-0.401286053280	-3.898814752301	-0.319989745090
H	-0.293794251686	-4.985991935288	-0.223983815115
H	0.098877909335	-3.586030133078	-1.247998622626
H	0.140147750512	-3.425564519748	0.511580011122
H	-2.562834026560	-5.529067792455	-0.492781753087
H	-4.966196579707	-4.929829416916	-0.540506035569
H	-3.272585392453	0.364425775107	-0.095019035085
H	-5.661415990857	0.961815181053	-0.146544206784
H	-7.405686546655	-0.814244290993	-0.342884768419
H	-6.737600185543	-3.199321785469	-0.488061108048

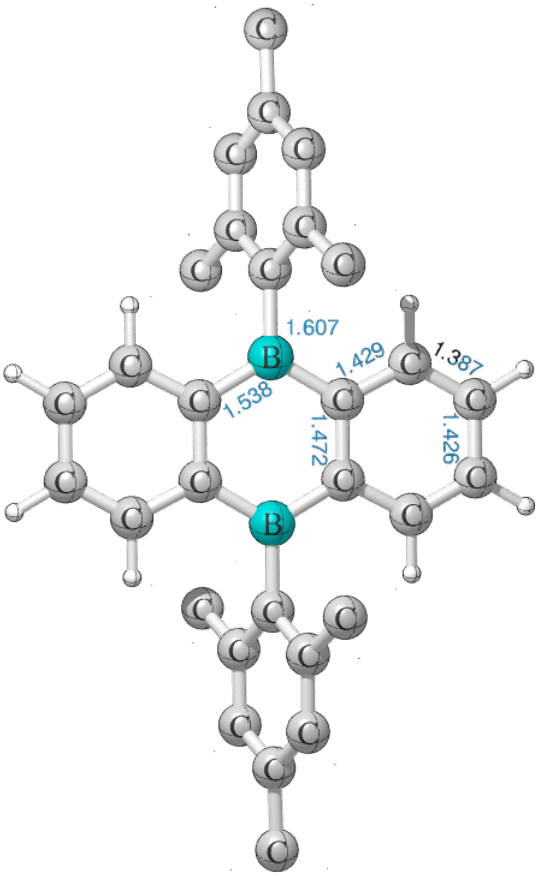
$[\mathbf{2c}]_{\mathrm{model}}$ (C_{2h}), $\phi = 74.1°$



B	0.000000000000	0.000000000000	1.507589632244
C	0.651792074683	1.186789187728	0.715092770454
C	0.651792074683	1.186789187728	-0.715092770454
B	0.000000000000	0.000000000000	-1.507589632244
C	-0.651792074683	-1.186789187728	-0.715092770454
C	-0.651792074683	-1.186789187728	0.715092770454
C	-1.210212448766	-2.285076371954	1.394985944399
C	-1.766968220063	-3.364481315556	0.699190782641
C	-1.766968220063	-3.364481315556	-0.699190782641
C	-1.210212448766	-2.285076371954	-1.394985944399
C	1.210212448766	2.285076371954	1.394985944399
C	1.766968220063	3.364481315556	0.699190782641
C	1.766968220063	3.364481315556	-0.699190782641
C	1.210212448766	2.285076371954	-1.394985944399
H	-1.209149387051	-2.288182061173	2.483539987076
H	-2.196655794201	-4.202987094740	1.245264902166
H	-2.196655794201	-4.202987094740	-1.245264902166
H	-1.209149387051	-2.288182061173	-2.483539987076
H	1.209149387051	2.288182061173	2.483539987076
H	2.196655794201	4.202987094740	1.245264902166
H	2.196655794201	4.202987094740	-1.245264902166
H	1.209149387051	2.288182061173	-2.483539987076
C	0.000000000000	0.000000000000	3.091067778021
C	-1.191105630268	0.273094502261	3.809864614565

C	-1.189809469848	0.276953133731	5.261473867307
C	0.000000000000	0.000000000000	5.946748466786
C	1.189809469848	-0.276953133731	5.261473867307
C	1.191105630268	-0.273094502261	3.809864614565
C	2.424277868315	-0.575353474129	3.145065038881
C	3.573163858642	-0.845969774770	3.850062364697
C	3.565534557848	-0.840691878676	5.275451388004
C	2.405261024005	-0.565199698139	5.958051951062
C	-2.424277868315	0.575353474129	3.145065038881
C	-3.573163858642	0.845969774770	3.850062364697
C	-3.565534557848	0.840691878676	5.275451388004
C	-2.405261024005	0.565199698139	5.958051951062
H	0.000000000000	0.000000000000	7.036830403259
H	2.446232959544	-0.584690329188	2.056758056829
H	4.496845161071	-1.068263560176	3.319051172661
H	4.482882701939	-1.058695123907	5.819112760393
H	2.389329582669	-0.563453033581	7.047359553297
H	-2.446232959544	0.584690329188	2.056758056829
H	-4.496845161071	1.068263560176	3.319051172661
H	-4.482882701939	1.058695123907	5.819112760393
H	-2.389329582669	0.563453033581	7.047359553297
C	0.000000000000	0.000000000000	-3.091067778021
C	1.191105630268	-0.273094502261	-3.809864614565
C	1.189809469848	-0.276953133731	-5.261473867307
C	0.000000000000	0.000000000000	-5.946748466786
C	-1.189809469848	0.276953133731	-5.261473867307
C	-1.191105630268	0.273094502261	-3.809864614565
C	-2.424277868315	0.575353474129	-3.145065038881
C	-3.573163858642	0.845969774770	-3.850062364697
C	-3.565534557848	0.840691878676	-5.275451388004
C	-2.405261024005	0.565199698139	-5.958051951062
C	2.424277868315	-0.575353474129	-3.145065038881
C	3.573163858642	-0.845969774770	-3.850062364697
C	3.565534557848	-0.840691878676	-5.275451388004
C	2.405261024005	-0.565199698139	-5.958051951062
H	0.000000000000	0.000000000000	-7.036830403259
H	-2.446232959544	0.584690329188	-2.056758056829
H	-4.496845161071	1.068263560176	-3.319051172661
H	-4.482882701939	1.058695123907	-5.819112760393
H	-2.389329582669	0.563453033581	-7.047359553297
H	2.446232959544	-0.584690329188	-2.056758056829
H	4.496845161071	-1.068263560176	-3.319051172661
H	4.482882701939	-1.058695123907	-5.819112760393
H	2.389329582669	-0.563453033581	-7.047359553297

$[\mathbf{2a}]^{2-}$ (C_{i}), $\phi = 66.3°$



B	1.507813284648	-0.171852231060	-0.149076208216
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C	-1.185849727968	-3.647724569724	-0.484892885396
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H	2.787058089083	2.262189281555	0.171445393834
H	1.851689360510	4.509730067977	0.586631013773
H	-0.648647354908	4.795954842697	0.829274609092
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H	-1.851689360510	-4.509730067977	-0.586631013773

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C	3.873158428319	-1.066654596698	0.651119989045
C	5.260076082908	-1.213749914047	0.504751542167
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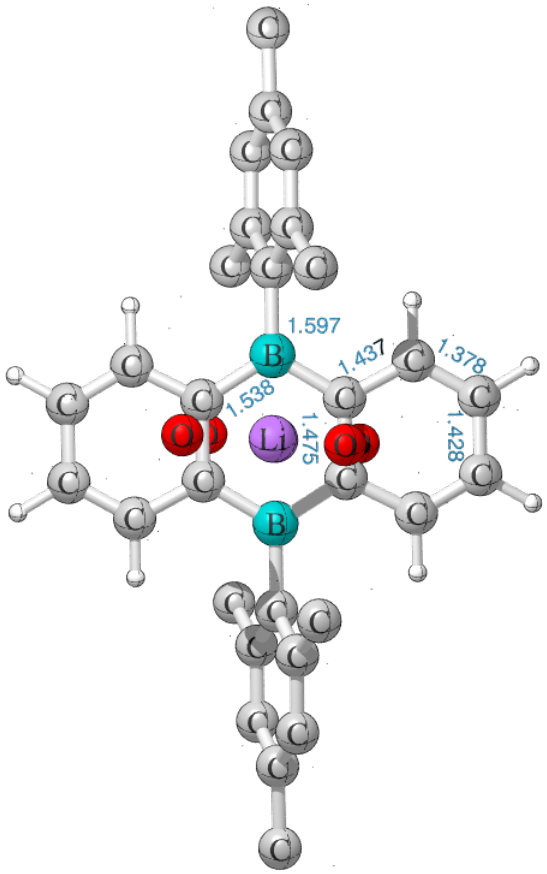
$[\mathrm{Li(THF)_2}]_2\,[\mathbf{2a}]$ (C_i), $\phi = 72.5°$



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C	-1.465715993924	1.085530561793	2.302733562073
C	-0.952521918955	1.033597492252	3.580220919093
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C	1.012944244228	-0.127412423547	2.756985627692
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C	-0.313074522695	-0.413919323441	-3.811884944789
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H	-1.979369645355	0.598920344229	-2.937391164940
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C	-2.915778977362	-3.056055010124	3.648017075686
H	-3.749208567524	-2.389802802933	3.392040769000
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C	-3.022633082022	-4.378194041524	2.867057676869

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H	-3.283165327656	-3.628778945754	0.824452805164
H	-1.938269441299	-4.792240169306	0.981610881791
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H	1.533054903576	1.399673940371	-3.145922738197
O	-1.393206828430	-3.086910747940	-1.181400092376
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O	1.393206828430	3.086910747940	1.181400092376
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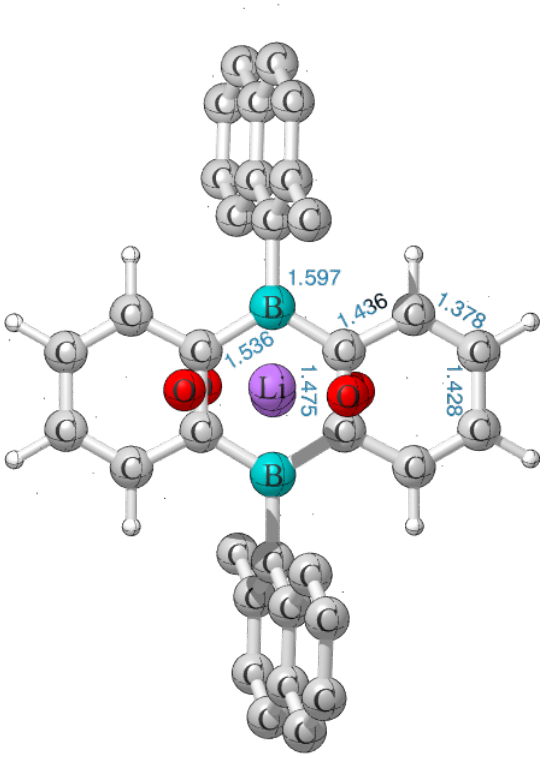
$[\mathrm{Li(THF)_2}]_2\,[\mathbf{2b}]$ (C_i), $\phi = 72.6°$



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C	1.215924860121	-0.939976914549	-2.506592538481
C	-1.215924860121	0.939976914549	2.506592538481
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H	2.750855608559	4.185895987516	-3.233166531232
H	3.918168350200	3.116456664944	-4.056681759942
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H	-1.657833849848	-2.000313434525	2.951080395191
O	2.134919407357	2.289574434932	1.754508006169
C	1.472686686248	3.236462797182	2.632511302113
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H	0.475843253781	2.847684955074	2.877380438351
C	2.361159057262	3.325522990844	3.875649316452
H	3.172858450373	4.048486168809	3.719046488302
H	1.793681393607	3.619931055700	4.765536332360
C	2.921211556510	1.893799513550	3.967087056075
H	3.853002124709	1.831161188083	4.540245834292
H	2.177119397195	1.224719433999	4.412102385515
C	3.124002343599	1.524157307318	2.495965613531
H	4.122105312590	1.812659074932	2.132649122076
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O	-2.134919407357	-2.289574434932	-1.754508006169
C	-1.472686686248	-3.236462797182	-2.632511302113
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H	-3.172858450373	-4.048486168809	-3.719046488302
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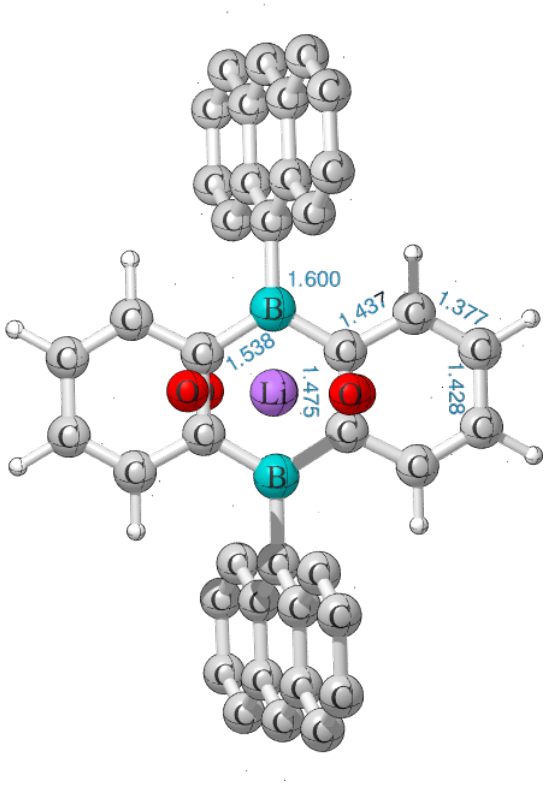
H	-3.853002124709	-1.831161188083	-4.540245834292
C	-3.124002343599	-1.524157307318	-2.495965613531
H	-2.956001799399	-0.462873015799	-2.288529112473
H	-4.122105312590	-1.812659074932	-2.132649122076

$[\mathrm{Li(THF)_2}]_2\,[\mathbf{2c}]_{\mathrm{model}}$ (C_i), $\phi = 72.0°$



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C	-1.059720239870	0.478589835676	3.666083459894
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H	0.763786208911	1.086350625939	4.705299895615
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H	-2.676592656899	-0.096691982372	2.394063136466
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C	4.046528526153	-0.303018019017	0.104108489408

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Li	0.405464633709	-1.776780783132	0.404317185535
Li	-0.405464633709	1.776780783132	-0.404317185535
O	0.837808467546	-3.540597413787	-0.590684412853
C	0.864458944492	-3.702988587352	-2.031213673876
H	0.832762395146	-2.706374782278	-2.468346549694
H	-0.023512454038	-4.273571467190	-2.346764200730

C	2.152015724791	-4.474889490399	-2.301773569079
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C	2.177633467976	-5.458769385275	-1.115559465518
H	3.187707986261	-5.804621756915	-0.867683675808
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C	1.555401646112	-4.640273831353	0.033174263003
H	2.314134347743	-4.203009565151	0.690281785688
H	0.853652127464	-5.223686599816	0.642423621841
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O	0.608029791734	-2.759123414954	2.175087868135
C	1.739442506868	-2.585061580733	3.067764590271
H	2.607522751535	-3.074489294754	2.609329069553
H	1.939176709865	-1.511480609937	3.169041177181
C	1.305179263957	-3.207635883645	4.396452835227
H	1.495071542422	-4.289406957126	4.396561317680
H	1.826412781014	-2.758784062912	5.249272603324
C	-0.208792177163	-2.924284293176	4.401047551015
H	-0.771297540266	-3.594615044604	5.060630141862
H	-0.397678612768	-1.885655510914	4.693243259651
C	-0.582081613907	-3.113934129982	2.929026998115
H	-0.835531311654	-4.160177838184	2.699348464396
H	-1.397086310357	-2.459448526414	2.601323762675
O	-0.608029791734	2.759123414954	-2.175087868135
C	-1.739442506868	2.585061580733	-3.067764590271
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H	1.397086310357	2.459448526414	-2.601323762675
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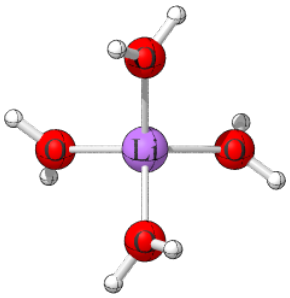
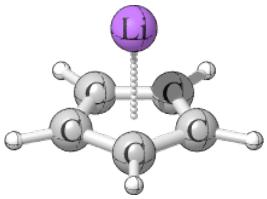
$Li(H_2O)_4^+$ (S_4)



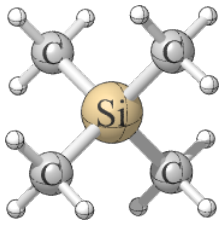
Li	0.000000000000	0.000000000000	0.000000000000
O	0.000000000000	1.656730447055	1.229842671767
O	1.656730447055	0.000000000000	-1.229842671767
O	0.000000000000	-1.656730447055	1.229842671767
O	-1.656730447055	0.000000000000	-1.229842671767
H	0.572033247188	2.429316439883	1.135850795016
H	-0.503322347182	1.794714706337	2.042389244840
H	2.429316439883	-0.572033247188	-1.135850795016
H	1.794714706337	0.503322347182	-2.042389244840
H	-0.572033247188	-2.429316439883	1.135850795016
H	0.503322347182	-1.794714706337	2.042389244840
H	-2.429316439883	0.572033247188	-1.135850795016
H	-1.794714706337	-0.503322347182	-2.042389244840

η^5-LiCp (C_{5v})



Li	0.000000000000	0.000000000000	1.753550607100
C	0.000000000000	1.212069244758	-0.146011351554
C	1.152746353428	0.374549994989	-0.146011351554
C	0.712436426826	-0.980584617368	-0.146011351554
C	-0.712436426826	-0.980584617368	-0.146011351554
C	-1.152746353428	0.374549994989	-0.146011351554
H	0.000000000000	2.297640767726	-0.176062254935
H	2.185186224251	0.710010044196	-0.176062254935
H	1.350519358335	-1.858830428059	-0.176062254935
H	-1.350519358335	-1.858830428059	-0.176062254935
H	-2.185186224251	0.710010044196	-0.176062254935

$SiMe_4$ (TMS) (T_d)



Si	0.000000000000	0.000000000000	0.000000000000
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C	-1.102067661113	-1.102067661113	1.102067661113
C	-1.102067661113	1.102067661113	-1.102067661113
C	1.102067661113	-1.102067661113	-1.102067661113
H	1.749543723816	1.749543723816	0.493569731323
H	1.749543723816	0.493569731323	1.749543723816
H	0.493569731323	1.749543723816	1.749543723816
H	-0.493569731323	-1.749543723816	1.749543723816
H	-1.749543723816	-1.749543723816	0.493569731323
H	-1.749543723816	-0.493569731323	1.749543723816
H	-1.749543723816	1.749543723816	-0.493569731323
H	-1.749543723816	0.493569731323	-1.749543723816
H	-0.493569731323	1.749543723816	-1.749543723816
H	0.493569731323	-1.749543723816	-1.749543723816
H	1.749543723816	-1.749543723816	-0.493569731323
H	1.749543723816	-0.493569731323	-1.749543723816

References

1 E. Januszewski, A. Lorbach, R. Grewal, M. Bolte, J. W. Bats, H.-W. Lerner, M. Wagner, *Chem. Eur. J.* 2011, **17**, 12 696–12 705.

2 C. Hoffend, F. Schödel, M. Bolte, H.-W. Lerner, M. Wagner, *Chem. Eur. J.* 2012, **18**, 15 394–15 405.

3 G. M. Sheldrick, *Acta Cryst. A* 1990, **46**, 467–473.

4 *SHELXL-97. A program for the Refinement of Crystal Structures*, G. M. Sheldrick (Universität Göttingen, Göttingen, Germany), 1997.

5 E. D. Glendening, C. R. Landis, F. Weinhold, *WIREs Comput. Mol. Sci.* 2012, **2**, 1–42.

6 R. F. W. Bader, *Atoms in Molecules: A Quantum Theory*, International Series of Monographs on Chemistry (Clarendon Press, Oxford, UK), 2003 reprinted edn., 1994.

7 C. F. Matta, R. J. Boyd (eds.), *The Quantum Theory of Atoms in Molecules* (Wiley-VCH, Weinheim), 2007.

8 R. Ditchfield, *Mol. Phys.* 1974, **27**, 789–807.

9 K. Wolinski, J. F. Hinton, P. Pulay, *J. Am. Chem. Soc.* 1990, **112**, 8251–8260.

10 J. R. Cheeseman, G. W. Trucks, T. A. Keith, M. J. Frisch, *J. Chem. Phys.* 1996, **104**, 5497–5509.

11 S. Grimme, *J. Comput. Chem.* 2006, **27**, 1787–1799.

12 A. Schäfer, C. Huber, R. Ahlrichs, *J. Chem. Phys.* 1994, **100**, 5829–5835.

13 *Gaussian 09, Revision C.01*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox (Gaussian, Inc., Wallingford, CT), 2010, see `http://www.gaussian.com`.

14 B. I. Dunlap, *J. Mol. Struct. (THEOCHEM)* 2000, **529**, 37–40.

15 K. Eichkorn, F. Weigend, O. Treutler, R. Ahlrichs, *Theor. Chem. Acc.* 1997, **97**, 119–124.

16 *AIMPAC*, R. F. W. Bader and coworkers (Department of Chemistry, McMaster University, Hamilton, Ont., Canada), 1995, see `http://www.chemistry.mcmaster.ca/aimpac/`.

17 P. von Ragué Schleyer, C. Maerker, A. Dransfeld, H. Jiao, N. J. R. van Eikema Hommes, *J. Am. Chem. Soc.* 1996, **118**, 6317–6318.

18 P. von Ragué Schleyer, H. Jiao, N. J. R. van Eikema Hommes, V. G. Malkin, O. L. Malkina, *J. Am. Chem. Soc.* 1997, **119**, 12 669–12 670.

19 Z. Chen, C. S. Wannere, C. Corminboeuf, R. Puchta, P. von Ragué Schleyer, *Chem. Rev.* 2005, **105**, 3842–3888.

20 *Spectral Database for Organic Compounds (SDBS)*, (National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan), Jan. 2013, see `http://riodb01.ibase.aist.go.jp/sdbs/`.

21 *Molden version 5.0*, G. Schaftenaar (Centre for Molecular and Biomolecular Informatics (CMBI), Radboud Universiteit Nijmegen, Nijmegen, NL), 1996-2010, see `http://www.cmbi.ru.nl/molden/molden.html`.

22 G. Schaftenaar, J. H. Noordik, *J. Comput.-Aided Mol. Design* 2000, **14**, 123–134.

23 *Persistence of Vision Raytracer Version 3.6*, (Persistence of Vision Pty. Ltd., Williamstown, Victoria, Australia), 2004, see `http://www.povray.org`.