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# Bronsted acid catalyzed skeletal rearrangements in polycyclic conjugated boracycles: a thermal route to a ladder diborole

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## Supporting Information

## Contents

## 1. Experimental Procedures

***General Details***. Toluene, hexane and tetrahydrofuran (THF) solvents were dried and purified using the Grubbs/Dow purification system[1] and stored in 500 mL thick-walled glass vessels under vacuum over sodium/benzophenone ketal. Pentanes were dried over $CH_2Cl_2$ and stored over sodium/benzophenone ketal in thick-walled glass vessels under vacuum. Dichloromethane were dried over $CH_2Cl_2$ and stored over molecular sieves (4A) in thick-walled glass vessels under vacuum. Unless otherwise noted, solvents were introduced into the reaction vessels *via* vacuum distillation with condensation at -78 ºC. Silica gel column chromatography was carried out on Silia-P Flash Silica Gel (particle size 40 – 63 μm) from Silicycle. Bis(pentamethylcyclopentadienyl) cobalt(II), silver trifluoromethanesulfonate, 4-methoxyphenol, Bis(trifluoromethane)sulfonamide, 2,6-dimethylphenol, *t*-butanol and bis(triphenylphosphoranylidene)ammonium chloride were purchased from Sigma-Aldrich. Nuclear magnetic resonance spectroscopy ($^1$H, $^{11}$B, $^{13}$C{$^1$H}, HSQC, HMBC, and COSY experiments) was performed on Bruker 400 MHz ($^1$H: 400 MHz; $^{11}$B: 128 MHz, $^{13}$C: 100 MHz) or Bruker 600 MHz ($^1$H: 600 MHz; $^{11}$B: 192 MHz, $^{13}$C: 150 MHz) spectrometers. All 2D NMR experiments were performed using Bruker 400 MHz or Bruker 600 MHz spectrometers. All $^1$H NMR spectra were referenced to $SiMe_4$ through residual $^1$H resonance(s) of the employed solvent: $CD_2Cl_2$ (5.32 ppm) or THF-*d8* (3.58 ppm). $^{11}$B NMR spectra were referenced to an external standard of boron trifluoride diethyl etherate (0.0 ppm) in $C_6D_6$ prior to spectrum acquisition. $^{13}$C{$^1$H} NMR spectra were referenced relative to $SiMe_4$ through the resonance(s) of the employed solvent: $CD_2Cl_2$ (54.0 ppm) or THF-*d8* (25.31 ppm). High-resolution mass spectra were obtained on a Kratos MS-80 spectrometer operating in electron impact (EI) mode or using a Bruker Esquire 3000 spectrometer operating in electrospray ionization (ESI) mode. UV-visible spectra were obtained on a Varian Cary 5000 UV-vis-NIR spectrophotometer operating in single-beam mode. EPR measurements were made on a Bruker EMX10/12, equipped with VT capabilities. X-ray crystallographic analyses were performed on suitable crystals coated in Paratone oil and mounted on a Nonius Kappa CCD diffractometer. Supplementary crystallographic data for CCDC-997324 (**2Co**), CCDC-997321 (**1K$_2$**), CCDC-997322 (**2K$_2$**), CCDC-997323 (**3**), and CCDC-885085 (**IV**) can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, UK, CB21EZ; fax: (+44) 1223-336-03; or deposit@ccdc.cam.ac.uk).

### Synthesis of 1K$_2$

A mixture of potassium metal (12.9 mg, 0.33 mmol) and naphthalene (133 mg, 0.36 mmol) in THF (8 mL) was stirred at room temperature under argon for 4 h. The produced solution of potassium naphthalenide was added to a solution of **1** (100 mg, 0.165 mmol) in THF (30 mL) at -78 °C and the solution was stirred for 2 h

at room temperature. After this period of time, the solution turned brown. Solvent and naphthalene were removed in vacuo. The brown solid was dissolved in THF (6 mL), layered with hexanes (6 mL) and allowed to crystallize for 6 days at -35 ºC. Compound **1K$_2$** (0.081 g) was isolated as a dark brown solid in 61 % yield. $^1$H NMR (400 MHz, THF-d8) δ 6.77 (s, 4H), 5.47 (s, 2H), 5.29 (s, 5.7 Hz, 2H), 5.09 (s, 2H), 4.21 (s, 2H), 3.59 (4H buried under the proteo THF signal), 2.76 (s, 2H), 1.19 (s, 36H) all the signals in the $^1$H NMR spectrum are broad. $^{13}$C{$^1$H} NMR (101 MHz, THF-d8) δ 176.66, 167.45 (small and broad), 152.17, 145.42, 143.42 (small and broad), 129.36 (small and broad), 125.94, 120.72, 119.29, 113.32, 101.04, 35.59, 34.06, 26.55, 24.96. $^{11}$B NMR (128 MHz, THF-d8): δ 38.7. HRMS: Calcd for $C_{44}H_{54}B_2$ [[M]$^+$-(K+THF)]: 604.4431, Observed: 604.4423. Anal. Calcd. for $C_{52}H_{70}B_2K_2O_2$: C, 75.53; H, 8.53. Found: C, 75.89; H, 8.51.

**Synthesis of 2K$_2$ from 1K$_2$ (acid promoted isomerization)**

In a 25 mL round-bottomed flask compound **1K$_2$** (70 mg, 0.085 mmol) was dissolved in THF (15 mL). A solution of *t*-butanol (1.1 mL, 0.093 mmol, 87.7 mM) in THF was slowly added to the solution of **1K$_2$** while stirring at 0 ºC. The cold bath was removed and the solution was stirred for 1 h at room temperature. The solution slowly changed from dark brown to dark red and the solvent was removed under vacuum. The dark red solid was dissolved in 1 mL of THF and layered with 1 mL of hexanes and stored at -35 ºC for 3 days. Removal of the mother liquor yielded compound **2K$_2$** as red crystals (62 mg, 89 %). $^1$H NMR (600 MHz, THF-d8) δ 6.94 (s, 4H), 6.80 – 6.62 (m, 4H), 6.32 – 6.22 (m, 2H), 6.09 (td, J = 7.0, 1.2 Hz, 2H), 3.41 (hept, J = 7.0 Hz, 4H), 2.87 (hept, J = 6.9 Hz, 2H), 1.30 (d, J = 6.9 Hz, 12H), 1.14 (d, J = 7.0 Hz, 12H), 1.12 (d, J = 6.9 Hz, 12H). $^{13}$C{$^1$H} NMR (151 MHz, THF) δ 155.13 (small and broad), 154.20, 151.27, 146.77 (small and broad), 145.06, 137.90 (small and broad), 129.86, 123.51, 120.63, 119.42, 118.26, 35.53, 34.57, 26.55, 25.03. $^{11}$B NMR (128 MHz, THF-d8): δ 32.0. HRMS: Calcd for $C_{44}H_{54}B_2$ [[M]$^+$-(K+THF)]: 604.4431, Observed: 604.4413. Anal. Calcd. for $C_{52}H_{70}B_2K_2O_2$: C, 75.53; H, 8.53. Found: C, 75.60; H, 8.63.

**Synthesis of 2K$_2$**

A mixture of potassium metal (3.0 mg, 0.051 mmol) and naphthalene (6.4 mg, 0.050 mmol) in THF (3 mL) was stirred at room temperature under argon for 4 h. The produced solution of potassium naphthalenide was added to a solution of **2** (15 mg, 0.0248 mmol) in THF (5 mL) at -78 °C and the solution was stirred for 2 h at room temperature. After this period of time, the solution turned red. Solvent and naphthalene were removed in vacuo. The red solid was dissolved in THF (1 mL), layered with hexanes (1 mL) and allowed to

crystallize for 6 days at -35 ºC. Compound **2K$_2$** (12.0 mg) was isolated as a red solid in 55 % yield. Spectroscopic data are identical to **2K$_2$** prepared by isomerization of **1K$_2$**.

### Synthesis of 3

In a 25 mL round-bottomed flask compound **1K$_2$** (55 mg, 0.066 mmol) was dissolved in THF (5 mL). 4-methoxyphenol (17 mg, 0.137 mmol) was dissolved in THF (1 mL) and added dropwise to the solution of **1K$_2$** while stirring. After the addition was complete the solution turned colorless. Solvent was removed under vacuum. The crude white solid was dissolved in boiling hexanes (6 mL) and filtered through a fine frit to remove the potassium 4-methoxyphenoxide produced. After removal of the solvent, the crude white solid was dissolved in boiling hexanes (3 mL) and stored at -35 ºC for 3 days. Removal of the mother liquor yielded compound **3** as a white solid (29 mg, 72 %). $^{1}$H NMR (600 MHz, $CD_2Cl_2$) δ 7.52 (ddd, *J* = 7.4, 1.3, 0.8 Hz, 2H), 7.38 (ddd, *J* = 7.8, 7.2, 1.4 Hz, 2H), 7.16 – 7.10 (m, 4H), 7.10 (d, *J* = 1.5 Hz, 2H), 6.86 (d, *J* = 1.6 Hz, 1H), 4.16 (s, 2H), 2.93 (hept, *J* = 7.1 Hz, 2H), 2.70 – 2.60 (m, *J* = 6.8 Hz, 2H), 1.41 (d, *J* = 6.7 Hz, 6H), 1.31 (d, *J* = 2.8 Hz, 6H), 1.30 (d, *J* = 2.8 Hz, 6H), 1.28 (hept, *J* = 6.9 Hz, 2H), 1.21 (d, *J* = 6.8 Hz, 6H), 0.77 (d, *J* = 6.7 Hz, 6H), 0.33 (d, *J* = 6.7 Hz, 6H). $^{13}$C{$^{1}$H} NMR (151 MHz, $CD_2Cl_2$) δ 163.54, 149.64, 148.97, 148.91, 145.05 (small and broad), 136.47 (small and broad), 135.15, 134.89, 125.62, 125.46, 120.17, 120.09, 57.86, 53.84, 36.52, 35.93, 34.72, 25.60, 24.86, 24.68, 24.32, 24.25, 22.37. $^{11}$B NMR (193 MHz, $CD_2Cl_2$) δ 77.0. HRMS: Calcd for $C_{44}H_{56}B_2$ ([M]$^+$): 606.4568, Observed: 606.4573.

### Synthesis of 2 from 2K$_2$

In a 25 mL round-bottomed flask compound **2K$_2$** (80 mg, 0.0967 mmol) and $AgSO_3CF_3$ (49.7 mg, 0.193 mmol) were dissolved in THF (15 mL) at -78 ºC. The solution was stirred for 10 minutes at room temperature. After this period of time the solution turned brown-greenish. Solvent was removed in vacuo. In the glove box the greenish solid was dissolved in dichloromethane (4 mL) and filtered through a sintered glass filter to remove the potassium triflate produced in the reaction. Solvent was removed in vacuo and the solid was re-dissolved in dichloromethane (2 mL), layered with hexanes (2 mL) and left in the fridge at -35 ºC for 2 days. Compound **2** (0.035 g) was isolated as green crystals in 60 % yield. The spectroscopic data are consistent with previously published data.[2]

### Generation of 1K

In a 20 mL scintillation vial compound **1** (27 mg, 0.0447 mmol) was dissolved in THF (8 mL). $KC_8$ (6.2 mg, 0.0459 mmol) was added to the solution of **1**. After the addition was complete the solution turned violet. The

solution was filtered through a sintered glass filter to remove the graphite and the solvent was removed under vacuum. The crude brown-violet solid was dissolved THF (1 mL) and the solution was layered with hexanes (1.5 mL). The solution was stored at -35 ºC for 21 days. Removal of the mother liquor yielded compound **1K** (25 mg) as very sensitive violet crystals. Due to the high sensitivity of the crystals elemental analysis could not be determined.

### Generation of 2K

In a 20 mL scintillation vial compound **2** (10 mg, 0.0165 mmol) was dissolved in THF (3 mL). $KC_8$ (2.2 mg, 0.0163 mmol) was added to the solution of **2**. After the addition was complete the solution turned blue. The solution was filtered through a sintered glass filter to remove the graphite and the solvent was removed under vacuum. The crude blue solid was dissolved THF (0.5 mL) and the solution was layered with hexanes (1 mL). The solution was stored at -35 ºC for 5 days. After removal of the mother liquor the blue crystals were dried under vacuum, yielding 9.5 mg of compound **1K**. Due to the high sensitivity of the crystals elemental analysis could not be determined.

### Synthesis of 2Co

In a 3 mL vial compound **2** (4.0 mg, 0.006 mmol) was dissolved in dichloromethane (1 mL) and added into another vial containing decamethylcobaltocene. After the addition was complete the solution turned blue. The solution was layered with hexanes (1 mL) and allowed to crystallize for 6 days at -35 ºC. After removal of the mother liquor the blue crystals were dried under vacuum, yielding 2.1 mg of compound **1K** (34% yield). Due to the high sensitivity of the crystals elemental analysis could not be determined.

## 2. EPR Spectroscopy

The structure of compounds **1K** and **2K** were modeled by DFT using the UB3PW91 functional with the 6-31+G(d) basis set (compounds were modeled as anionic species without the counter cation). The hyperfine coupling constants (hfcc) were calculated using the basis set EPR-II, which is optimized for their computation. The hyperfine coupling constants were used as the initial values for the simulations and they were modified by hand until the correlation between the simulated and the experimental spectrum was higher than 97%. Subsequently, the program algorithm was utilized, which allowed reaching a correlation of 99.6% for **1K** and 99.9% for **2K**

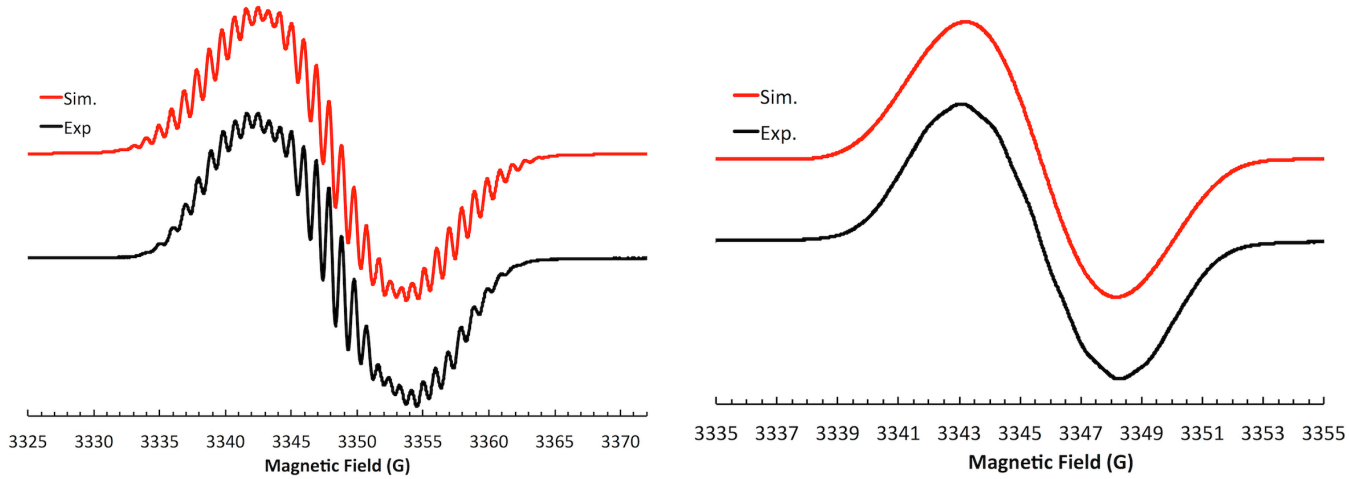



**Figure S1**. Experimental (black) and simulated (red) EPR spectrum of **1K** (left). Experimental (black) and simulated (red) EPR spectrum of **2K** (right)

Titration Experiment

Compound $\mathbf{1K_2}$ was dissolved in THF in an EPR tube and the spectrum was measured (Figure S2, series "1"). Approximately 1 mg of compound **1** was dissolved in 1 mL of THF and a couple of drops were added into the EPR tube and the spectrum was measured again (Figure S2, series "2"). This procedure was repeated two more times (Figure S2, series "3" and "4" respectively). Along with the augmentation of the EPR signal there is also a change in color of the solution from dark brown to violet. Since compound $\mathbf{1K_2}$ is capable of reducing compound **1**, this experiments generates the radical **1K** *in situ* upon subsequent additions of **1** to the EPR tube containing $\mathbf{1K_2}$.

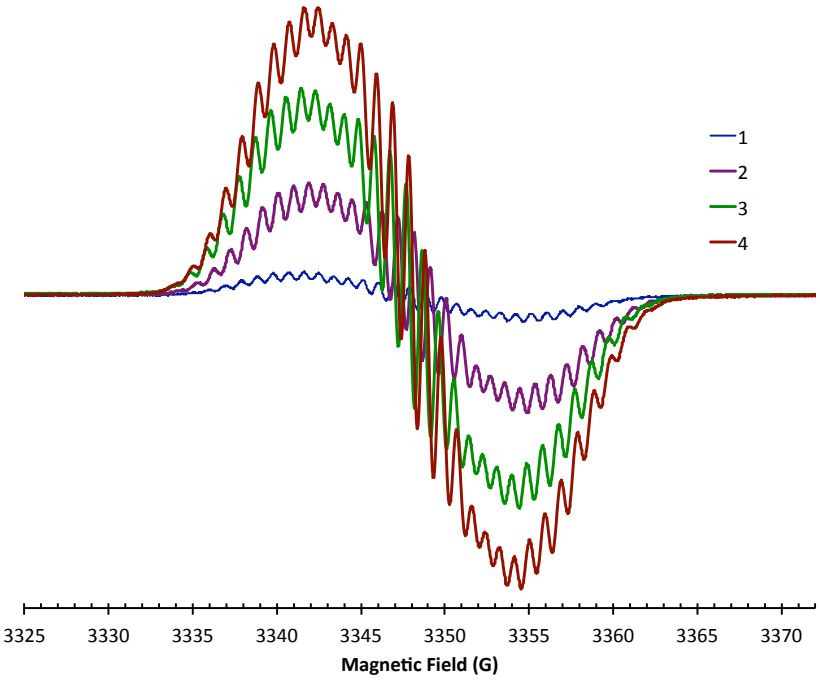



**Figure S2**. Qualitative titration of compound $\mathbf{1K_2}$. The increment in the series numbers indicate a qualitative increment in the amount of compound **1** added to the EPR tube containing $\mathbf{1K_2}$.

## 3. UV-Vis spectroscopy

Compound **1K$_2$** is dark brown in the solid state and in solution (THF). Contrasting to **1**, **1K$_2$** is not emissive under UV-light and its absorption spectrum is considerably red-shifted (Figure S3), with the longest absorption maximum at 802 nm ($\varepsilon$ = 9640 $M^{-1}$ $cm^{-1}$). According to TD-DFT calculations (B3LYP/6-311G(d)) this energy transition can be attributed to a transition from HOMO to LUMO (calcd: 805 nm, f = 0.1468) and is mainly $\pi \rightarrow \pi^*$ in character.

**2K$_2$** exhibits a magenta colour in solution (THF) and displays purplish pink emission under UV light ($\lambda_{max}$ = 620 nm). In contrast, the precursor **2** is non-fluorescent under UV light. Compound **2K$_2$** shows major peaks at 531 nm, 352 nm, 337 nm and a shoulder at 507 nm in the absorption spectrum (Figure S3). Based on TD-DFT calculations (B3LYP/6-311G(d)) the longest absorption band is manly comprised of the HOMO-LUMO transition (calcd: 485 nm, f = 0.2530) and is mainly $\pi \rightarrow \pi^*$ in character. Compound **2K$_2$** is isoelectronic to dibenzopentalene. However, the former is non-emissive under UV-light and the longest absorption maximum is around 450 nm. This clearly shows that the exchange of carbon for the more electropositive boron atom causes a significant change in the electronic and photophysical properties.

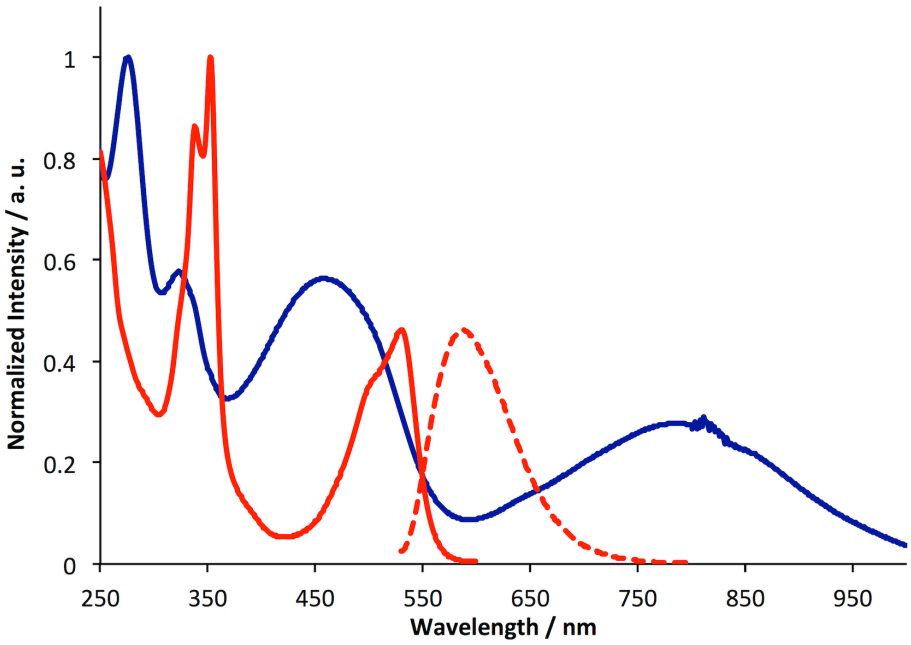



**Figure S3**. Absorption and emission spectrum of compounds **1K$_2$** and **2K$_2$** in THF. Blue line: **1K$_2$** absorption; red line: **2K$_2$** absorption; dotted red line: **2K$_2$** emission.

## 4. NMR Spectroscopy

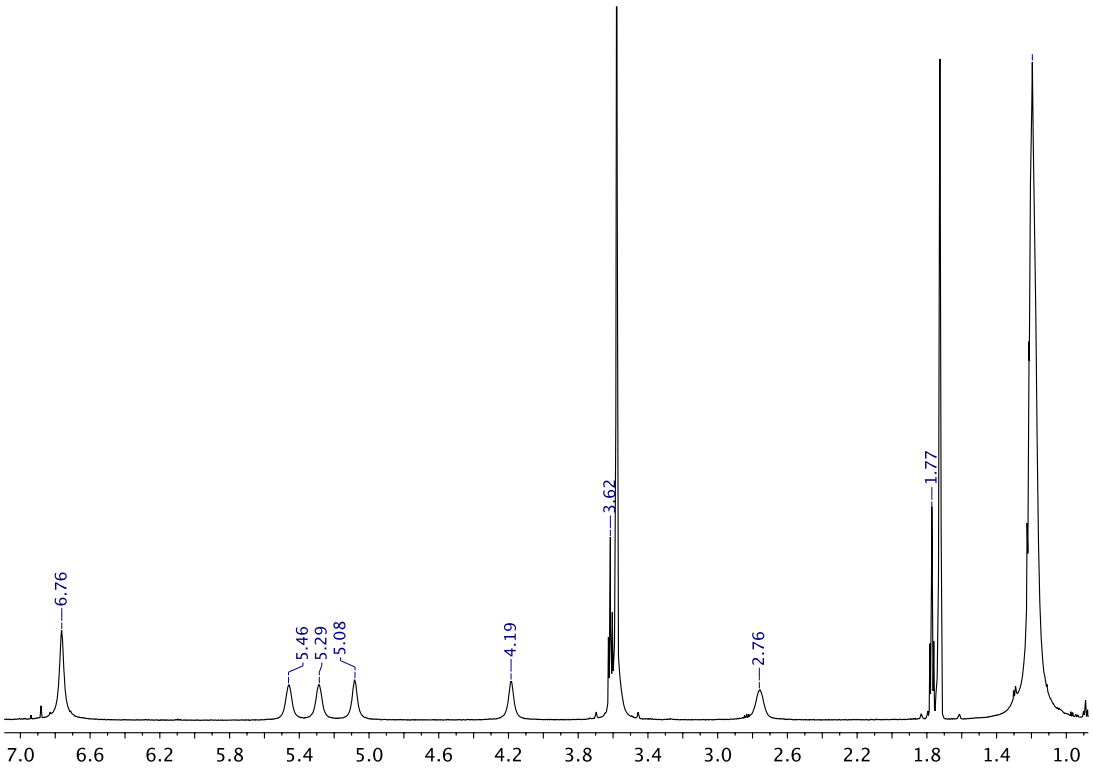
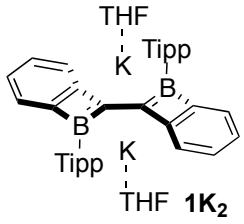



**Figure S4**. $^{1}$H NMR spectrum of **1K$_2$** in THF-d$_8$.



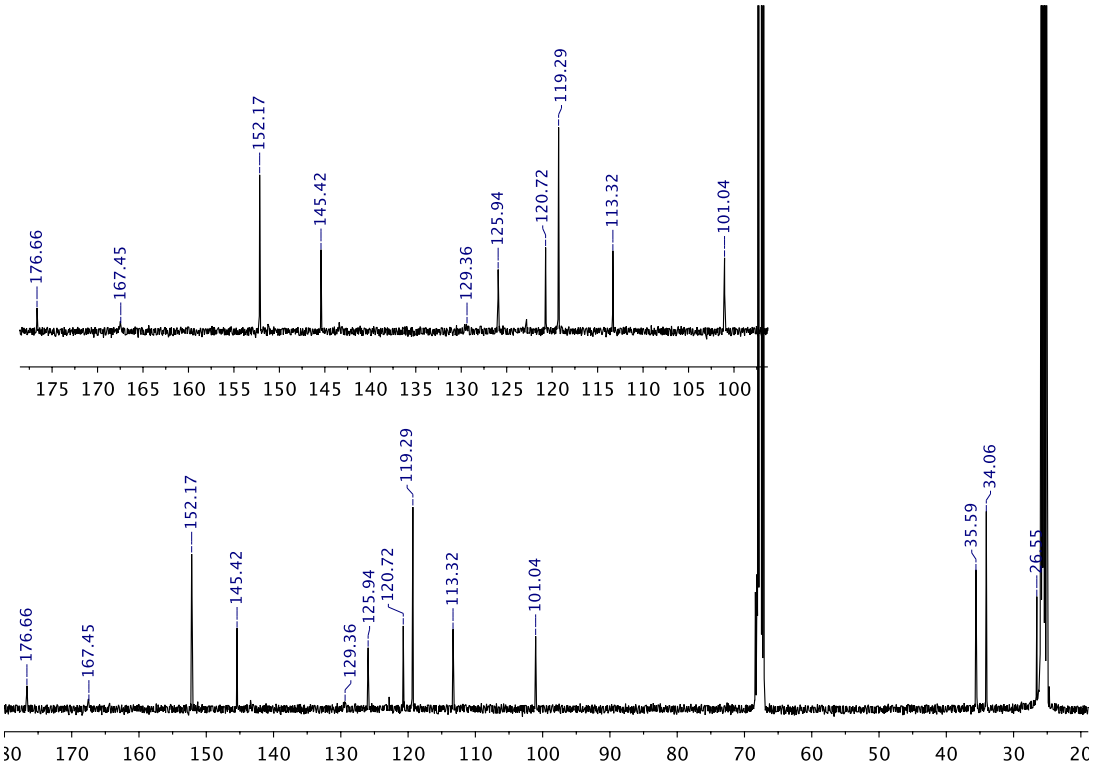




**Figure S5**. $^{13}$C{$^{1}$H} spectrum of **1K$_2$** in THF-d$_8$.

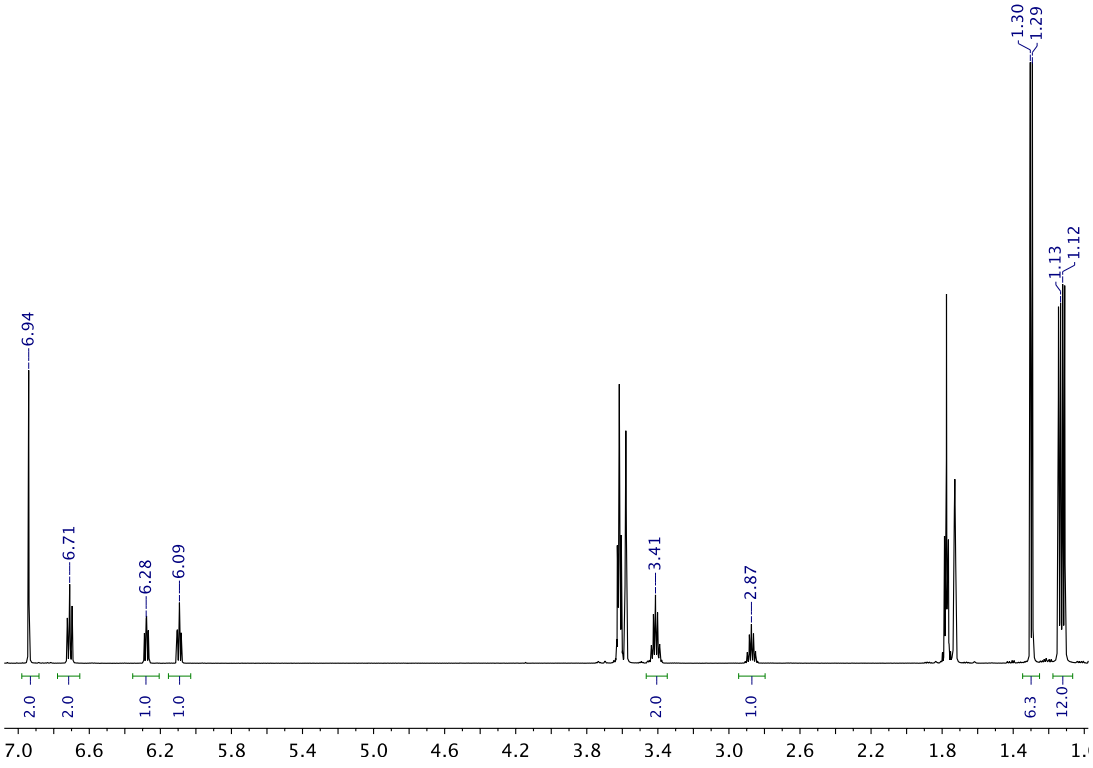
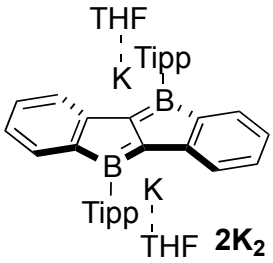



**Figure S6**. $^{1}$H NMR spectrum of **2K$_2$** in THF-d$_8$.



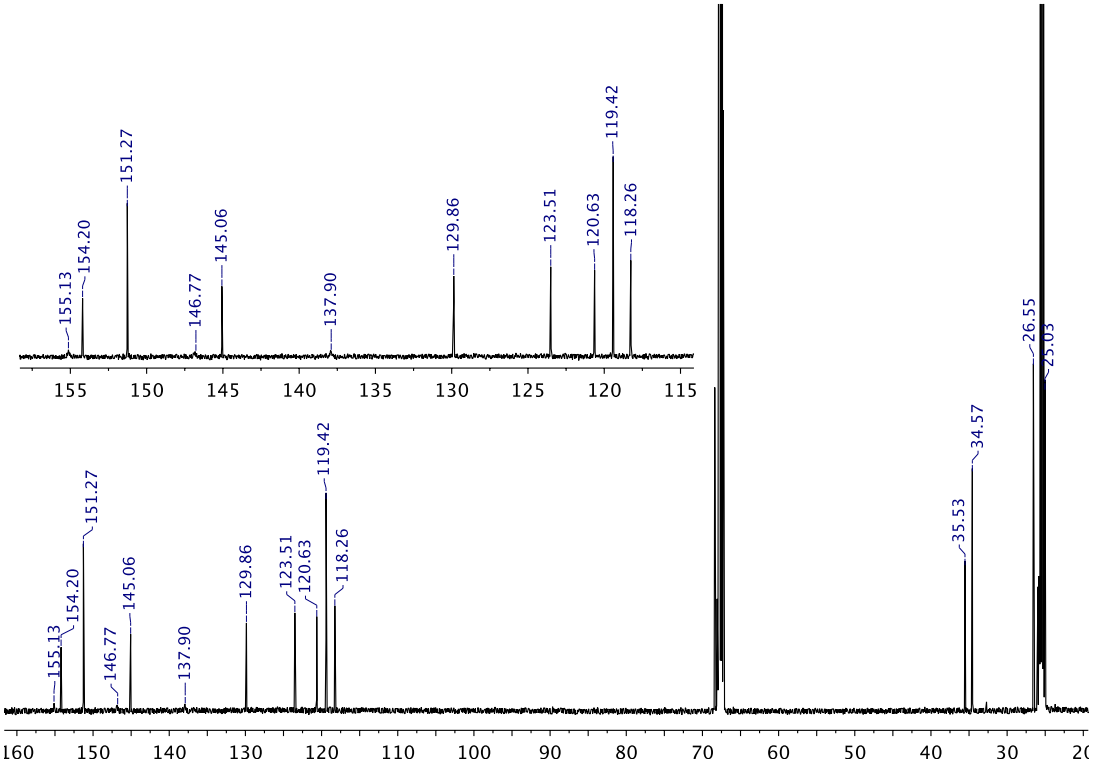




**Figure S7**. $^{13}$C{$^{1}$H} NMR spectrum of **2K$_2$** in THF-d$_8$.

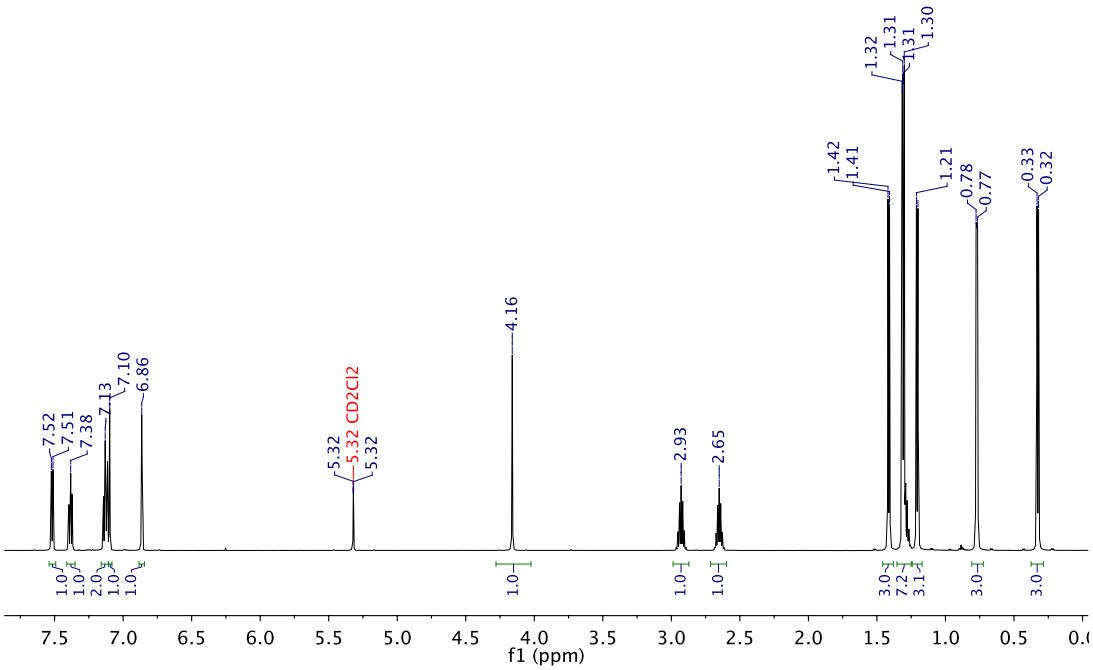
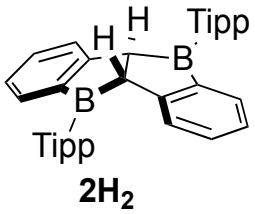



**Figure S8**. $^{1}H$ NMR spectrum of **3** in $CD_2Cl_2$.




**2H$_2$**

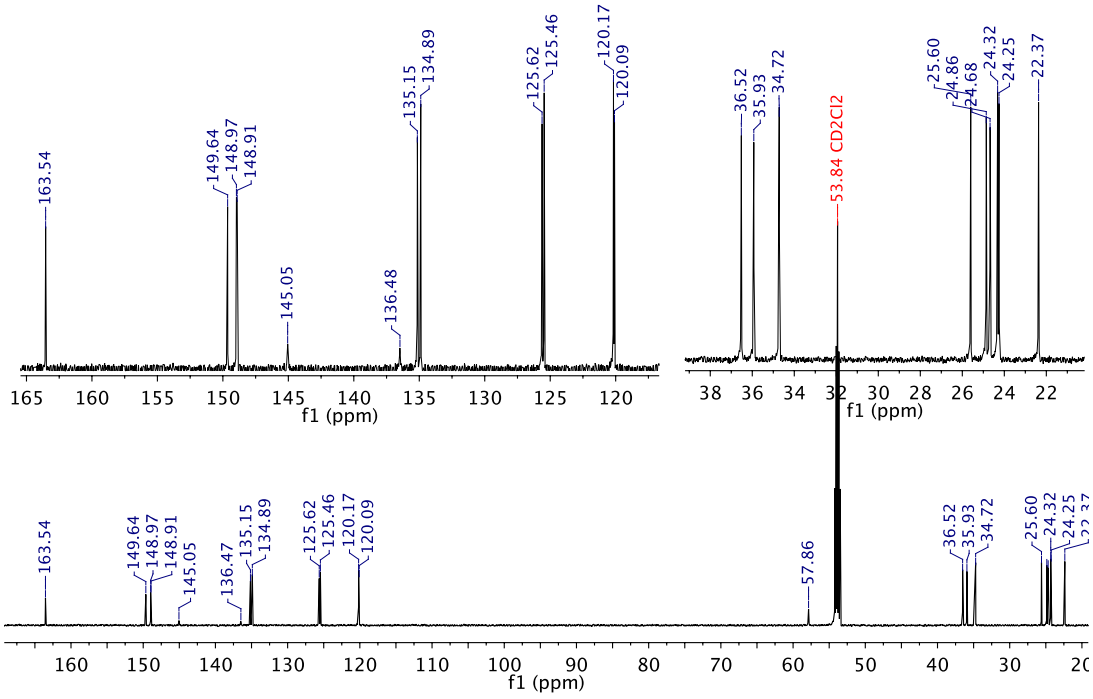



**Figure S9**. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in $CD_2Cl_2$.

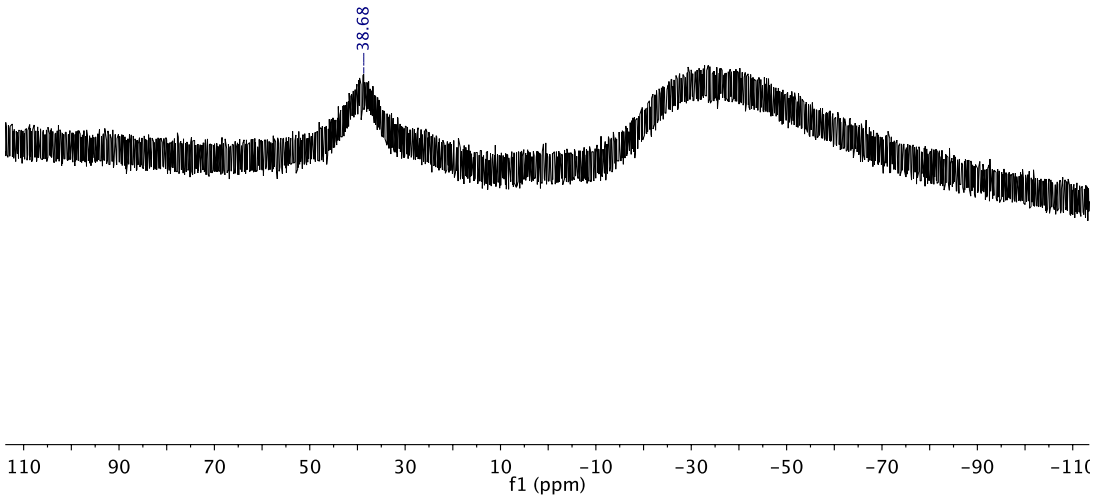



**Figure S10**. $^{11}$B NMR spectrum of **1K$_2$** in THF-d$_8$.

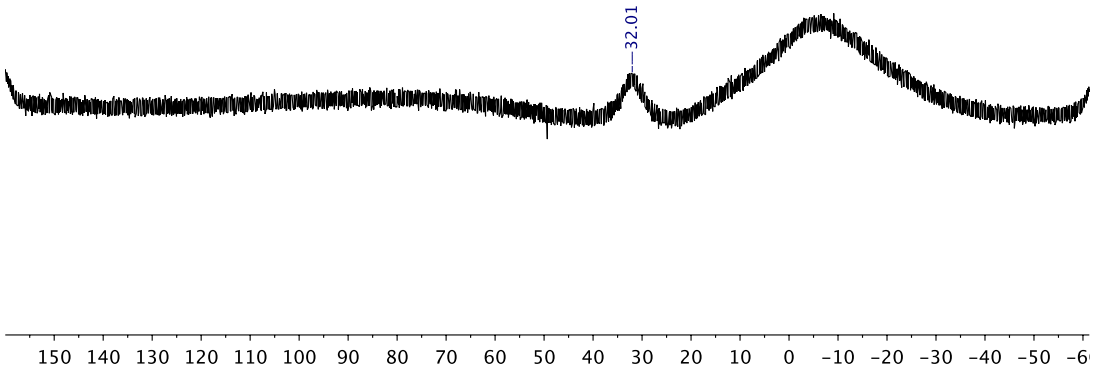



**Figure S11**. $^{11}$B NMR spectrum of **2K$_2$** in THF-d$_8$.

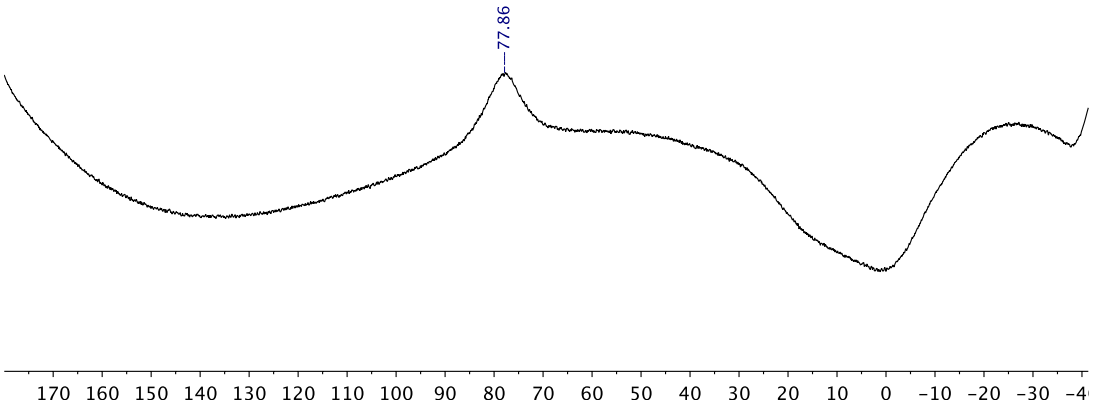



**Figure S12**. $^{11}$B NMR spectrum of **3** in $CD_2Cl_2$.

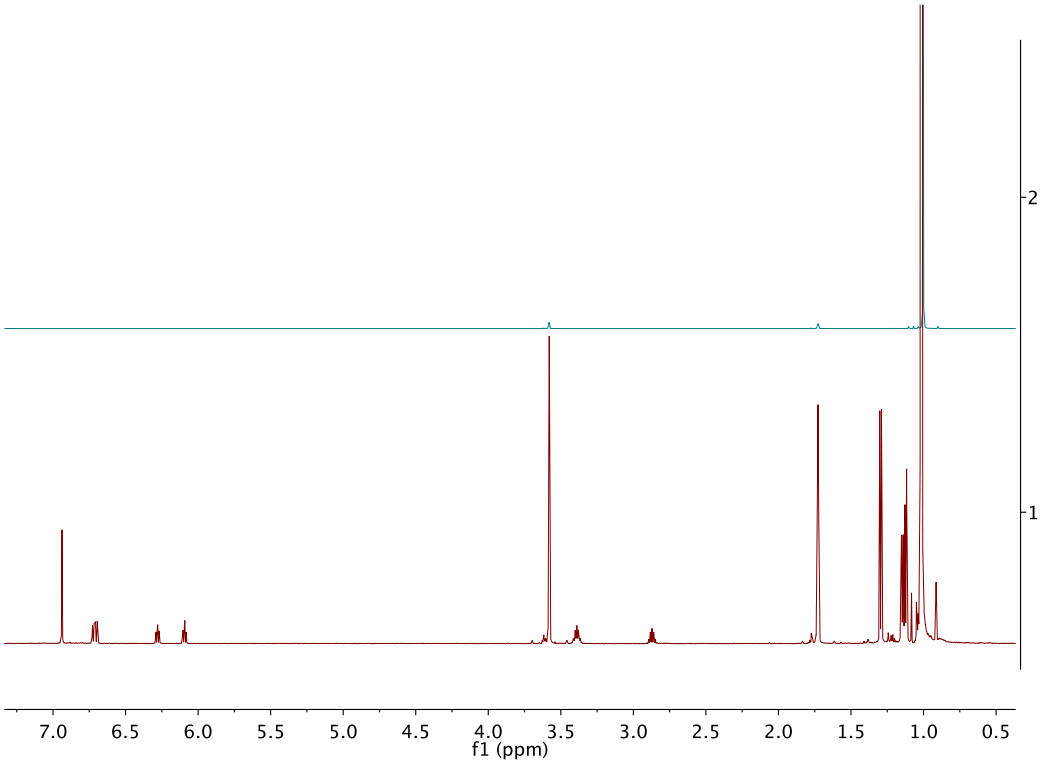



**Figure S13**. $^1$H NMR spectrum of KO$^t$Bu in THF-$d_8$ (top) and $^1$H NMR spectrum of KO$^t$Bu after addition of **3** (bottom) showing the immediate formation of **2K$_2$**.

## 5. X-ray crystallography

**Table S1**: Data Collection and Structure Refinement Details for **$1K_2$**, **$2K_2$**, **2Co**, and **3**

| | **$1K_2$** | **$2K_2$** | **2Co** | **3** |
|---|---|---|---|---|
| Empirical formula | $C_{76}H_{118}B_2K_2O_8$ | $C_{60}H_{86}B_2K_2O_4$ | $C_{66}H_{88}B_2Cl_4Co$ | $C_{44}H_{56}B_2$ |
| Crystal system | Orthorhombic | Monoclinic | Triclinic | Triclinic |
| *Fw* | 1259.52 | 485.55 | 1103.71 | 606.51 |
| *F*(000) | 2744 | 1052 | 589 | 660 |
| *T* (K) | 173(2) | 123(2) | 173(2) | 173(2) |
| Wavelength (Å) | 1.54178 | 0.71073 | 1.54178 | 0.71073 |
| Space group | Pbca | P21/c | P-1 | P-1 |
| *a* (Å) | 16.1537(3) | 10.3128(2) | 11.5296(9) | 11.3370(7) |
| *b* (Å) | 19.9550(4) | 14.6667(2) | 13.487(2) | 11.9746(7) |
| *c* (Å) | 22.8279(5) | 19.3119(4) | 14.651(1) | 13.9071(6) |
| α (deg) | 90 | 90 | 112.337(6) | 83.312(3) |
| β (deg) | 90 | 102.005(1) | 111.343(4) | 85.920(3) |
| γ (deg) | 90 | 90 | 95.399(6) | 88.345(2) |
| *Z* | 4 | 4 | 1 | 2 |
| *V* (Å$^3$) | 7358.5(3) | 2857.13(9) | 1890.0(3) | 1870.0(2) |
| $\rho_{calcd}$ (g·cm$^{-3}$) | 1.137 | 1.129 | 0.97 | 1.077 |
| μ (mm$^{-1}$) | 1.534 | 0.209 | 3.303 | 0.059 |
| θ range (deg) | 3.87 − 72.96 | 2.45 − 27.57 | 3.62 − 68.19 | 2.13 − 27.29 |
| Completeness | 0.987 | 0.99 | 0.964 | 0.983 |
| Data/Restraints/Param | 5969 / 15 / 415 | 5625 / 0 / 313 | 5395 / 6 / 356 | 4895 / 0 / 427 |
| Collected reflections; $R_\sigma$ | 77463; 0.0115 | 23720; 0.0247 | 24504; 0.0419 | 15376; 0.1145 |
| Unique reflections; $R_{int}$ | 7247; 0.0243 | 6559; 0.0356 | 6666; 0.0398 | 8259; 0.0946 |
| $R_1$; $wR_2$ [I > 2σ(I)] | 0.0701; 0.2082 | 0.0682; 0.1642 | 0.0586; 0.1638 | 0.1478; 0.2176 |
| $R_1$; $wR_2$ [all data] | 0.0805; 0.2222 | 0.0791; 0.1742 | 0.0665; 0.1699 | 0.2218; 0.2406 |
| GOF | 1.001 | 1.022 | 1.108 | 1.495 |
| largest diff peak and hole | 0.684 and -0.549 | 1.137 and -0.345 | 0.462 and -0.346 | 0.297 and -0.274 |

## 6. Cyclic voltammetry

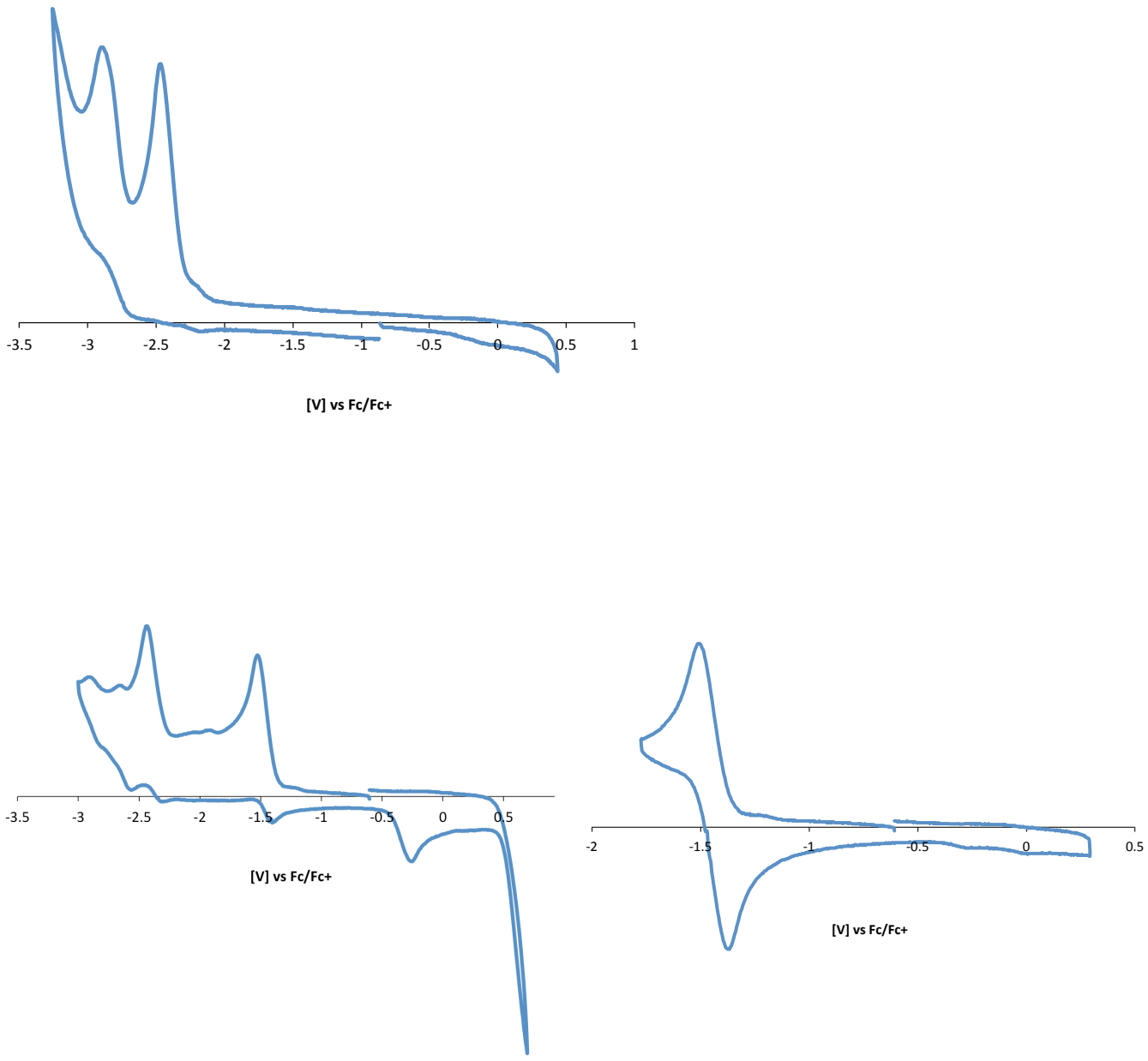



**Figure S15**. Cyclic voltammetry traces for **1** (top) and **2** (bottom). Cyclic voltammetry was carried out at a scan rate of 100 mV/s in THF with 1mM substrate and 0.1M $[NBu_4][PF_6]$ as the supporting electrolyte. Ferrocene was added as an internal standard and set to 0 V. Cyclic voltammogram on bottom right shows reversibility of this potential when the scan does not exceed –1.75 V. **2**: $E_{pc}$ = -2.47 V, -2.89 V; **3**: $E_{pc}$ = -1.52 V, 2.44 V, $E_{1/2}$ = -1.45 V.

## 7. Quantum Chemical Calculations

### XYZ-coordinates of optimized structures

**1K'**

| | | | |
|---|---|---|---|
| B | -1.748856 | 1.215171 | 0.112532 |
| C | -0.331427 | 0.602230 | 0.073202 |
| C | 0.203182 | 1.979008 | 0.284465 |
| C | 1.399460 | 2.671985 | 0.419843 |
| H | 2.367694 | 2.178022 | 0.379032 |
| C | 1.306220 | 4.071330 | 0.616539 |
| H | 2.221437 | 4.652529 | 0.728199 |
| C | 0.077777 | 4.725289 | 0.671204 |
| H | 0.053388 | 5.803876 | 0.824270 |
| C | -1.135854 | 4.006886 | 0.530302 |
| H | -2.088848 | 4.534713 | 0.575292 |
| C | -1.061329 | 2.636344 | 0.337682 |
| C | -3.242828 | 0.719241 | -0.012579 |
| C | -3.968229 | 0.305228 | 1.128470 |
| C | -5.292815 | -0.124041 | 1.001877 |
| H | -5.833102 | -0.441891 | 1.893790 |
| C | -5.940214 | -0.158747 | -0.236959 |
| C | -5.219266 | 0.256517 | -1.357985 |
| H | -5.710721 | 0.233008 | -2.331566 |
| C | -3.893095 | 0.695112 | -1.265528 |
| C | -3.315104 | 0.338240 | 2.504267 |
| H | -2.275253 | 0.661939 | 2.356879 |
| C | -3.264824 | -1.047531 | 3.161036 |
| H | -4.272652 | -1.437300 | 3.357077 |
| H | -2.734368 | -0.999038 | 4.121290 |
| H | -2.742659 | -1.766706 | 2.520968 |
| C | -3.986989 | 1.364178 | 3.428030 |
| H | -3.987133 | 2.361115 | 2.972996 |
| H | -3.456091 | 1.427598 | 4.387197 |
| H | -5.029330 | 1.090024 | 3.639599 |
| C | -7.378036 | -0.632335 | -0.372509 |
| H | -7.639919 | -0.557976 | -1.438481 |
| C | -8.356439 | 0.262604 | 0.402122 |
| H | -9.394409 | -0.057813 | 0.238609 |
| H | -8.266068 | 1.309046 | 0.088632 |
| H | -8.160520 | 0.221867 | 1.480780 |
| C | -7.542315 | -2.102710 | 0.038238 |
| H | -7.306736 | -2.245216 | 1.100066 |
| H | -6.872219 | -2.750003 | -0.538696 |
| H | -8.574336 | -2.442286 | -0.124416 |
| C | -3.157048 | 1.140699 | -2.522289 |
| H | -2.160735 | 1.480481 | -2.206448 |
| C | -2.945886 | -0.019136 | -3.505228 |
| H | -2.398184 | -0.840178 | -3.030544 |

| | | | |
|---|---|---|---|
| H | -2.369727 | 0.314971 | -4.378455 |
| H | -3.904238 | -0.415063 | -3.867421 |
| C | -3.847423 | 2.327533 | -3.208364 |
| H | -4.839530 | 2.051784 | -3.590039 |
| H | -3.250149 | 2.680304 | -4.059501 |
| H | -3.975718 | 3.164685 | -2.512730 |
| B | 1.748752 | -1.215196 | -0.112324 |
| C | 0.331327 | -0.602251 | -0.072912 |
| C | -0.203298 | -1.979026 | -0.284163 |
| C | -1.399586 | -2.672000 | -0.419467 |
| H | -2.367817 | -2.178041 | -0.378565 |
| C | -1.306359 | -4.071340 | -0.616215 |
| H | -2.221585 | -4.652535 | -0.727822 |
| C | -0.077921 | -4.725294 | -0.671001 |
| H | -0.053542 | -5.803876 | -0.824107 |
| C | 1.135720 | -4.006894 | -0.530169 |
| H | 2.088712 | -4.534719 | -0.575251 |
| C | 1.061208 | -2.636359 | -0.337490 |
| C | 3.242756 | -0.719327 | 0.012651 |
| C | 3.968087 | -0.305419 | -1.128481 |
| C | 5.292737 | 0.123698 | -1.002033 |
| H | 5.832964 | 0.441478 | -1.894007 |
| C | 5.940273 | 0.158336 | 0.236733 |
| C | 5.219391 | -0.256812 | 1.357843 |
| H | 5.710958 | -0.233358 | 2.331370 |
| C | 3.893149 | -0.695226 | 1.265535 |
| C | 3.314808 | -0.338351 | -2.504205 |
| H | 2.274956 | -0.662003 | -2.356714 |
| C | 3.264524 | 1.047455 | -3.160903 |
| H | 4.272351 | 1.437183 | -3.357027 |
| H | 2.733965 | 0.999036 | -4.121106 |
| H | 2.742460 | 1.766625 | -2.520746 |
| C | 3.986533 | -1.364279 | -3.428092 |
| H | 3.986687 | -2.361236 | -2.973102 |
| H | 3.455513 | -1.427634 | -4.387197 |
| H | 5.028862 | -1.090164 | -3.639781 |
| C | 7.378171 | 0.631745 | 0.372122 |
| H | 7.640162 | 0.557360 | 1.438065 |
| C | 8.356379 | -0.263320 | -0.402610 |
| H | 9.394408 | 0.056959 | -0.239200 |
| H | 8.265902 | -1.309752 | -0.089114 |
| H | 8.160357 | -0.222554 | -1.481249 |
| C | 7.542585 | 2.102096 | -0.038653 |
| H | 7.306906 | 2.244623 | -1.100455 |
| H | 6.872633 | 2.749477 | 0.538352 |
| H | 8.574666 | 2.441548 | 0.123883 |
| C | 3.157214 | -1.140785 | 2.522372 |
| H | 2.160538 | -1.479699 | 2.206743 |
| C | 2.947253 | 0.018729 | 3.505941 |

| | | | |
|---|---|---|---|
| H | 2.400084 | 0.840448 | 3.031812 |
| H | 2.371048 | -0.315357 | 4.379146 |
| H | 3.906004 | 0.413706 | 3.868112 |
| C | 3.847008 | -2.328436 | 3.207621 |
| H | 4.839528 | -2.053586 | 3.588879 |
| H | 3.249898 | -2.681102 | 4.058918 |
| H | 3.974303 | -3.165395 | 2.511572 |

**2K'**

| | | | |
|---|---|---|---|
| C | -0.609339 | -0.261099 | 0.252324 |
| C | -0.329296 | -1.354395 | 1.186597 |
| C | 1.085401 | -1.556306 | 1.300017 |
| C | 1.560830 | -2.557368 | 2.143926 |
| H | 2.634733 | -2.723235 | 2.241400 |
| C | 0.668417 | -3.361628 | 2.874693 |
| H | 1.047577 | -4.143529 | 3.531556 |
| C | -0.707039 | -3.155480 | 2.756154 |
| H | -1.397954 | -3.778842 | 3.323156 |
| C | -1.212608 | -2.152371 | 1.913726 |
| H | -2.287659 | -1.999899 | 1.829688 |
| C | -3.351006 | 0.328161 | -0.135220 |
| C | -4.102614 | -0.572777 | -0.925678 |
| C | -5.478725 | -0.713731 | -0.720561 |
| H | -6.037310 | -1.413439 | -1.342932 |
| C | -6.155799 | 0.016609 | 0.260662 |
| C | -5.409558 | 0.906090 | 1.035393 |
| H | -5.922499 | 1.483033 | 1.806268 |
| C | -4.031634 | 1.073685 | 0.852490 |
| C | -3.419232 | -1.391389 | -2.014441 |
| H | -2.347315 | -1.154844 | -1.969005 |
| C | -3.912461 | -1.003164 | -3.415472 |
| H | -4.981425 | -1.223135 | -3.539215 |
| H | -3.364154 | -1.559770 | -4.187159 |
| H | -3.764881 | 0.066740 | -3.599841 |
| C | -3.555835 | -2.902061 | -1.780605 |
| H | -2.995717 | -3.461713 | -2.541386 |
| H | -4.604125 | -3.225283 | -1.834042 |
| H | -3.163929 | -3.183679 | -0.797285 |
| C | -7.650689 | -0.140104 | 0.484364 |
| H | -7.921320 | 0.526362 | 1.316911 |
| C | -8.027213 | -1.569213 | 0.901220 |
| H | -9.101328 | -1.644362 | 1.119302 |
| H | -7.472355 | -1.877609 | 1.794669 |
| H | -7.797201 | -2.287677 | 0.104714 |
| C | -8.465534 | 0.303072 | -0.739631 |
| H | -9.543684 | 0.240276 | -0.537858 |
| H | -8.249986 | -0.331880 | -1.607976 |
| H | -8.226941 | 1.336035 | -1.017954 |

| | | | |
|---|---|---|---|
| C | -3.271191 | 2.054861 | 1.735795 |
| H | -2.227702 | 2.054529 | 1.392285 |
| C | -3.262225 | 1.611820 | 3.205672 |
| H | -4.278079 | 1.592463 | 3.623068 |
| H | -2.662333 | 2.301447 | 3.814448 |
| H | -2.834139 | 0.609025 | 3.309708 |
| C | -3.794841 | 3.490676 | 1.596238 |
| H | -3.182140 | 4.183689 | 2.187875 |
| H | -4.831330 | 3.578693 | 1.948638 |
| H | -3.764995 | 3.819621 | 0.551376 |
| B | -1.790021 | 0.499899 | -0.354971 |
| C | 0.609376 | 0.261054 | -0.252403 |
| C | 0.329337 | 1.354411 | -1.186606 |
| C | -1.085359 | 1.556337 | -1.300009 |
| C | -1.560783 | 2.557481 | -2.143822 |
| H | -2.634686 | 2.723359 | -2.241284 |
| C | -0.668367 | 3.361796 | -2.874526 |
| H | -1.047524 | 4.143755 | -3.531321 |
| C | 0.707087 | 3.155625 | -2.756012 |
| H | 1.398005 | 3.779032 | -3.322962 |
| C | 1.212652 | 2.152443 | -1.913669 |
| H | 2.287703 | 1.999963 | -1.829639 |
| C | 3.351049 | -0.328102 | 0.135256 |
| C | 4.102494 | 0.572922 | 0.925770 |
| C | 5.478612 | 0.714003 | 0.720787 |
| H | 6.037070 | 1.413776 | 1.343199 |
| C | 6.155851 | -0.016294 | -0.260354 |
| C | 5.409771 | -0.905862 | -1.035140 |
| H | 5.922842 | -1.482772 | -1.805953 |
| C | 4.031844 | -1.073583 | -0.852372 |
| C | 3.418922 | 1.391487 | 2.014448 |
| H | 2.347031 | 1.154846 | 1.968898 |
| C | 3.912033 | 1.003322 | 3.415537 |
| H | 4.980965 | 1.223385 | 3.539391 |
| H | 3.363596 | 1.559890 | 4.187159 |
| H | 3.764526 | -0.066593 | 3.599903 |
| C | 3.555414 | 2.902169 | 1.780610 |
| H | 2.995153 | 3.461777 | 2.541319 |
| H | 4.603667 | 3.225491 | 1.834168 |
| H | 3.163597 | 3.183739 | 0.797241 |
| C | 7.650748 | 0.140561 | -0.483914 |
| H | 7.921530 | -0.525922 | -1.316399 |
| C | 8.027161 | 1.569688 | -0.900811 |
| H | 9.101289 | 1.644943 | -1.118787 |
| H | 7.472360 | 1.877975 | -1.794333 |
| H | 7.796987 | 2.288169 | -0.104367 |
| C | 8.465520 | -0.302463 | 0.740184 |
| H | 9.543683 | -0.239567 | 0.538509 |
| H | 8.249825 | 0.332515 | 1.608473 |

| | | | |
|---|---|---|---|
| H | 8.227007 | -1.335435 | 1.018541 |
| C | 3.271583 | -2.054846 | -1.735737 |
| H | 2.228060 | -2.054610 | -1.392332 |
| C | 3.262722 | -1.611827 | -3.205622 |
| H | 4.278615 | -1.592379 | -3.622918 |
| H | 2.662956 | -2.301520 | -3.814447 |
| H | 2.834550 | -0.609075 | -3.309715 |
| C | 3.795359 | -3.490607 | -1.596108 |
| H | 3.182784 | -4.183689 | -2.187795 |
| H | 4.831892 | -3.578529 | -1.948406 |
| H | 3.765443 | -3.819541 | -0.551245 |
| B | 1.790057 | -0.499976 | 0.354855 |

**3-*cis***

| | | | |
|---|---|---|---|
| C | -0.303127 | 0.448755 | 1.295504 |
| H | -0.688985 | 1.042399 | 2.141601 |
| C | 0.023153 | 1.352192 | 0.060463 |
| H | 0.035276 | 2.421288 | 0.332620 |
| C | -1.067591 | 1.098992 | -0.953208 |
| C | -1.938669 | 0.047967 | -0.572253 |
| C | -3.007038 | -0.307398 | -1.416735 |
| H | -3.680729 | -1.109946 | -1.123930 |
| C | -3.210934 | 0.376290 | -2.611043 |
| H | -4.039493 | 0.113082 | -3.263195 |
| C | -2.343241 | 1.419054 | -2.972500 |
| H | -2.509839 | 1.953446 | -3.905068 |
| C | -1.271852 | 1.784163 | -2.155805 |
| H | -0.606414 | 2.589946 | -2.454616 |
| C | 0.994208 | -0.214996 | 1.692784 |
| C | 2.044506 | 0.039493 | 0.776345 |
| C | 3.318297 | -0.511307 | 1.010618 |
| H | 4.128021 | -0.310584 | 0.312323 |
| C | 3.545079 | -1.291948 | 2.139545 |
| H | 4.528664 | -1.712463 | 2.331418 |
| C | 2.496624 | -1.530436 | 3.042144 |
| H | 2.680480 | -2.136867 | 3.926154 |
| C | 1.223000 | -1.001291 | 2.827276 |
| H | 0.421606 | -1.201661 | 3.533786 |
| C | -2.160944 | -1.689948 | 1.609206 |
| C | -1.790708 | -3.029083 | 1.335085 |
| C | -2.376469 | -4.073219 | 2.057015 |
| H | -2.082788 | -5.096984 | 1.836626 |
| C | -3.330556 | -3.839735 | 3.053673 |
| C | -3.696251 | -2.516201 | 3.306646 |
| H | -4.445126 | -2.319811 | 4.071951 |
| C | -3.134206 | -1.443582 | 2.603747 |
| C | -0.778616 | -3.350898 | 0.233934 |
| H | -0.341462 | -2.401083 | -0.105785 |

| | | | |
|---|---|---|---|
| C | 0.389862 | -4.224018 | 0.726144 |
| H | 1.124378 | -4.363553 | -0.076026 |
| H | 0.047597 | -5.218814 | 1.034898 |
| H | 0.899431 | -3.760579 | 1.576367 |
| C | -1.466081 | -3.991589 | -0.987493 |
| H | -0.738264 | -4.185693 | -1.785038 |
| H | -2.246556 | -3.338266 | -1.391536 |
| H | -1.933072 | -4.946882 | -0.719191 |
| C | -3.957967 | -4.983757 | 3.840032 |
| H | -4.677845 | -4.536356 | 4.539400 |
| C | -2.913509 | -5.743131 | 4.680169 |
| H | -3.393518 | -6.523204 | 5.283600 |
| H | -2.382540 | -5.065498 | 5.357765 |
| H | -2.165838 | -6.228807 | 4.041769 |
| C | -4.741470 | -5.948958 | 2.930532 |
| H | -5.234683 | -6.727335 | 3.525338 |
| H | -4.078457 | -6.448684 | 2.214335 |
| H | -5.509954 | -5.417647 | 2.358447 |
| C | -3.601595 | -0.020565 | 2.912120 |
| H | -3.061170 | 0.664066 | 2.244021 |
| C | -5.100490 | 0.169989 | 2.611197 |
| H | -5.401631 | 1.209794 | 2.787250 |
| H | -5.720690 | -0.469564 | 3.249935 |
| H | -5.326549 | -0.078668 | 1.568652 |
| C | -3.268360 | 0.400324 | 4.355766 |
| H | -3.566209 | 1.440372 | 4.536347 |
| H | -2.194726 | 0.312810 | 4.557733 |
| H | -3.794046 | -0.227603 | 5.084634 |
| C | 2.337248 | 1.477207 | -1.603387 |
| C | 2.457851 | 0.672012 | -2.761963 |
| C | 3.179901 | 1.142770 | -3.862800 |
| H | 3.265498 | 0.512968 | -4.745524 |
| C | 3.795906 | 2.399244 | -3.861434 |
| C | 3.679240 | 3.179579 | -2.709290 |
| H | 4.161531 | 4.155256 | -2.690107 |
| C | 2.969592 | 2.741130 | -1.584938 |
| C | 1.830437 | -0.722122 | -2.814278 |
| H | 1.201904 | -0.840057 | -1.920016 |
| C | 0.908822 | -0.920124 | -4.031473 |
| H | 0.425214 | -1.903304 | -3.987038 |
| H | 1.468811 | -0.871698 | -4.972808 |
| H | 0.125073 | -0.157156 | -4.062537 |
| C | 2.906875 | -1.823596 | -2.756061 |
| H | 2.444910 | -2.818605 | -2.759395 |
| H | 3.516688 | -1.735008 | -1.850829 |
| H | 3.578197 | -1.762362 | -3.620986 |
| C | 4.571645 | 2.908141 | -5.069714 |
| H | 4.959330 | 3.902359 | -4.807493 |
| C | 3.664477 | 3.079345 | -6.302993 |

| | | | |
|---|---|---|---|
| H | 4.227699 | 3.503215 | -7.143294 |
| H | 2.822484 | 3.745456 | -6.084938 |
| H | 3.252324 | 2.117272 | -6.629960 |
| C | 5.783191 | 2.014742 | -5.396486 |
| H | 6.360905 | 2.434482 | -6.228934 |
| H | 5.467210 | 1.005774 | -5.687081 |
| H | 6.449135 | 1.919286 | -4.531907 |
| C | 2.902158 | 3.634827 | -0.346017 |
| H | 2.364468 | 3.082831 | 0.437256 |
| C | 2.113743 | 4.930935 | -0.612862 |
| H | 2.039362 | 5.536902 | 0.298390 |
| H | 1.097830 | 4.714045 | -0.962334 |
| H | 2.603941 | 5.541094 | -1.380638 |
| C | 4.299328 | 3.944605 | 0.224422 |
| H | 4.217389 | 4.531528 | 1.147196 |
| H | 4.903698 | 4.522492 | -0.484305 |
| H | 4.844031 | 3.022467 | 0.454130 |
| B | -1.514975 | -0.497108 | 0.811280 |
| B | 1.534285 | 0.969380 | -0.348282 |

**3-*trans***

| | | | |
|---|---|---|---|
| C | -0.666749 | -0.565743 | -0.152445 |
| C | 0.370214 | 0.565889 | 0.132982 |
| H | -0.086198 | 1.145290 | 0.968496 |
| C | 0.271443 | 1.475015 | -1.064583 |
| C | -0.991640 | 1.307171 | -1.703336 |
| C | -1.325016 | 2.137345 | -2.783095 |
| H | -2.291076 | 2.028244 | -3.271983 |
| C | -0.416721 | 3.095059 | -3.238544 |
| H | -0.669777 | 3.733219 | -4.081264 |
| C | 0.825738 | 3.234640 | -2.609969 |
| H | 1.527866 | 3.982486 | -2.971198 |
| C | 1.176507 | 2.432244 | -1.517510 |
| H | 2.138377 | 2.559962 | -1.027558 |
| C | -0.567769 | -1.474981 | 1.045031 |
| C | 0.695987 | -1.307926 | 1.682756 |
| C | 1.029997 | -2.138976 | 2.761632 |
| H | 1.996635 | -2.030743 | 3.249558 |
| C | 0.121637 | -3.096441 | 3.217526 |
| H | 0.375252 | -3.735207 | 4.059617 |
| C | -1.121581 | -3.234917 | 2.590258 |
| H | -1.823795 | -3.982486 | 2.951881 |
| C | -1.472983 | -2.431796 | 1.498511 |
| H | -2.435491 | -2.558688 | 1.009575 |
| C | -3.279628 | -0.293460 | -1.277924 |
| C | -3.658060 | -1.115016 | -2.365139 |
| C | -5.000610 | -1.472221 | -2.526819 |
| H | -5.279749 | -2.113591 | -3.359776 |
| C | -5.995428 | -1.030108 | -1.647591 |

| | | | |
|---|---|---|---|
| C | -5.608665 | -0.213386 | -0.582058 |
| H | -6.372704 | 0.143605 | 0.106092 |
| C | -4.274002 | 0.155075 | -0.380748 |
| C | -2.609652 | -1.651623 | -3.339916 |
| H | -1.659929 | -1.144506 | -3.119768 |
| C | -2.377143 | -3.162124 | -3.138657 |
| H | -1.585491 | -3.527462 | -3.804265 |
| H | -3.288321 | -3.732050 | -3.356489 |
| H | -2.085650 | -3.385373 | -2.106188 |
| C | -2.943236 | -1.336279 | -4.809508 |
| H | -2.134530 | -1.675455 | -5.467837 |
| H | -3.077967 | -0.259971 | -4.962912 |
| H | -3.862926 | -1.837622 | -5.132411 |
| C | -7.456027 | -1.418994 | -1.839139 |
| H | -8.022703 | -0.954009 | -1.020599 |
| C | -7.665336 | -2.941607 | -1.735099 |
| H | -8.729513 | -3.193416 | -1.818547 |
| H | -7.297020 | -3.326867 | -0.777973 |
| H | -7.134431 | -3.472296 | -2.534450 |
| C | -8.027208 | -0.872279 | -3.161307 |
| H | -9.093927 | -1.111031 | -3.251101 |
| H | -7.514697 | -1.308522 | -4.027013 |
| H | -7.914083 | 0.215725 | -3.220845 |
| C | -3.901469 | 1.073177 | 0.783131 |
| H | -2.802233 | 1.136740 | 0.817219 |
| C | -4.424120 | 2.505409 | 0.558866 |
| H | -4.110109 | 3.167448 | 1.375015 |
| H | -5.519648 | 2.520859 | 0.515967 |
| H | -4.046251 | 2.919690 | -0.382096 |
| C | -4.353145 | 0.521082 | 2.147184 |
| H | -4.017412 | 1.178197 | 2.958310 |
| H | -3.939945 | -0.477289 | 2.325279 |
| H | -5.445250 | 0.451664 | 2.209707 |
| C | 2.984264 | 0.292707 | 1.253094 |
| C | 3.974962 | -0.143667 | 0.342187 |
| C | 5.308792 | 0.225603 | 0.533762 |
| H | 6.061990 | -0.125511 | -0.168214 |
| C | 5.700943 | 1.034133 | 1.607139 |
| C | 4.713101 | 1.460749 | 2.497582 |
| H | 5.005287 | 2.092862 | 3.333998 |
| C | 3.367903 | 1.101865 | 2.344870 |
| C | 3.593615 | -1.055034 | -0.824601 |
| H | 2.493894 | -1.109224 | -0.857774 |
| C | 4.047825 | -0.505070 | -2.188509 |
| H | 3.702241 | -1.156689 | -2.999895 |
| H | 5.140443 | -0.448264 | -2.254824 |
| H | 3.645542 | 0.498268 | -2.363496 |
| C | 4.104191 | -2.492149 | -0.603156 |
| H | 3.784317 | -3.150244 | -1.420236 |

| | | | |
|---|---|---|---|
| H | 3.723343 | -2.904806 | 0.337317 |
| H | 5.199597 | -2.516590 | -0.560539 |
| C | 7.155584 | 1.440553 | 1.806951 |
| H | 7.193412 | 2.069277 | 2.707300 |
| C | 7.682773 | 2.287190 | 0.632907 |
| H | 8.711014 | 2.617469 | 0.823935 |
| H | 7.062034 | 3.176141 | 0.475917 |
| H | 7.685987 | 1.713445 | -0.301551 |
| C | 8.063780 | 0.222176 | 2.059110 |
| H | 9.093926 | 0.541029 | 2.259174 |
| H | 8.085226 | -0.444659 | 1.188918 |
| H | 7.713861 | -0.361502 | 2.917580 |
| C | 2.328449 | 1.625698 | 3.335534 |
| H | 1.375906 | 1.124072 | 3.115046 |
| C | 2.097715 | 3.139697 | 3.159871 |
| H | 1.311925 | 3.495841 | 3.837296 |
| H | 1.798588 | 3.379888 | 2.133387 |
| H | 3.011567 | 3.704512 | 3.379753 |
| C | 2.674080 | 1.287251 | 4.797240 |
| H | 1.872148 | 1.618393 | 5.467837 |
| H | 3.598037 | 1.781403 | 5.119038 |
| H | 2.807346 | 0.208411 | 4.933247 |
| B | -1.787206 | 0.130213 | -1.032673 |
| B | 1.491356 | -0.131022 | 1.011673 |
| H | -0.209606 | -1.145274 | -0.987498 |

**$2K_2$'**

| | | | |
|---|---|---|---|
| C | 0.638873 | -0.261763 | -0.255340 |
| C | 0.352571 | -1.319382 | -1.200855 |
| C | -1.081123 | -1.515545 | -1.321038 |
| C | -1.551108 | -2.503061 | -2.193265 |
| H | -2.626344 | -2.662875 | -2.297317 |
| C | -0.670928 | -3.297280 | -2.942656 |
| H | -1.057212 | -4.062870 | -3.616013 |
| C | 0.710782 | -3.100248 | -2.822124 |
| H | 1.398350 | -3.713565 | -3.405604 |
| C | 1.218909 | -2.121051 | -1.961736 |
| H | 2.295520 | -1.977099 | -1.883819 |
| C | 3.359719 | 0.326371 | 0.162290 |
| C | 4.110047 | -0.662347 | 0.849786 |
| C | 5.490184 | -0.780870 | 0.655733 |
| H | 6.034643 | -1.551829 | 1.199506 |
| C | 6.187218 | 0.056863 | -0.217030 |
| C | 5.454194 | 1.033918 | -0.891130 |
| H | 5.981240 | 1.692158 | -1.581186 |
| C | 4.074914 | 1.184200 | -0.711043 |
| C | 3.416195 | -1.606961 | 1.829963 |
| H | 2.349547 | -1.369520 | 1.781181 |
| C | 3.880008 | -1.369297 | 3.277387 |

| | | | |
|---|---|---|---|
| H | 4.948555 | -1.584281 | 3.404338 |
| H | 3.326733 | -2.010692 | 3.973981 |
| H | 3.708271 | -0.330769 | 3.571456 |
| C | 3.565757 | -3.084317 | 1.431457 |
| H | 3.011841 | -3.728893 | 2.124284 |
| H | 4.613411 | -3.410700 | 1.442064 |
| H | 3.165994 | -3.255265 | 0.429552 |
| C | 7.686643 | -0.082628 | -0.442830 |
| H | 7.977364 | 0.705971 | -1.149863 |
| C | 8.055628 | -1.430215 | -1.089661 |
| H | 9.130258 | -1.489891 | -1.305866 |
| H | 7.509880 | -1.574837 | -2.025560 |
| H | 7.800784 | -2.266600 | -0.431792 |
| C | 8.499858 | 0.141831 | 0.844783 |
| H | 9.578984 | 0.099639 | 0.648468 |
| H | 8.269115 | -0.619284 | 1.596336 |
| H | 8.270540 | 1.115654 | 1.285554 |
| C | 3.325809 | 2.252527 | -1.505315 |
| H | 2.342341 | 2.350988 | -1.037754 |
| C | 3.088134 | 1.796933 | -2.955500 |
| H | 4.036076 | 1.636373 | -3.484618 |
| H | 2.513043 | 2.546517 | -3.512934 |
| H | 2.523860 | 0.862362 | -2.972603 |
| C | 3.996861 | 3.634547 | -1.458185 |
| H | 3.364358 | 4.382481 | -1.950102 |
| H | 4.968705 | 3.646402 | -1.966584 |
| H | 4.154661 | 3.958436 | -0.425589 |
| B | 1.779987 | 0.475675 | 0.363238 |
| C | -0.638869 | 0.262026 | 0.255071 |
| C | -0.352566 | 1.319611 | 1.200624 |
| C | 1.081128 | 1.515770 | 1.320812 |
| C | 1.551114 | 2.503236 | 2.193095 |
| H | 2.626350 | 2.663044 | 2.297155 |
| C | 0.670935 | 3.297424 | 2.942520 |
| H | 1.057219 | 4.062983 | 3.615912 |
| C | -0.710776 | 3.100408 | 2.821971 |
| H | -1.398343 | 3.713702 | 3.405475 |
| C | -1.218904 | 2.121251 | 1.961536 |
| H | -2.295516 | 1.977308 | 1.883609 |
| C | -3.359715 | -0.326107 | -0.162562 |
| C | -4.110055 | 0.662679 | -0.849945 |
| C | -5.490189 | 0.781179 | -0.655858 |
| H | -6.034657 | 1.552201 | -1.199533 |
| C | -6.187210 | -0.056657 | 0.216817 |
| C | -5.454176 | -1.033787 | 0.890795 |
| H | -5.981212 | -1.692115 | 1.580776 |
| C | -4.074896 | -1.184038 | 0.710680 |
| C | -3.416214 | 1.607414 | -1.830012 |
| H | -2.349565 | 1.369978 | -1.781263 |

| | | | |
|---|---|---|---|
| C | -3.880029 | 1.369918 | -3.277464 |
| H | -4.948582 | 1.584893 | -3.404384 |
| H | -3.326772 | 2.011410 | -3.973981 |
| H | -3.708269 | 0.331429 | -3.571662 |
| C | -3.565791 | 3.084721 | -1.431331 |
| H | -3.011880 | 3.729385 | -2.124079 |
| H | -4.613449 | 3.411094 | -1.441901 |
| H | -3.166033 | 3.255551 | -0.429404 |
| C | -7.686632 | 0.082806 | 0.442653 |
| H | -7.977347 | -0.705888 | 1.149583 |
| C | -8.055607 | 1.430306 | 1.089670 |
| H | -9.130236 | 1.489961 | 1.305883 |
| H | -7.509858 | 1.574796 | 2.025590 |
| H | -7.800755 | 2.266780 | 0.431917 |
| C | -8.499861 | -0.141476 | -0.844981 |
| H | -9.578985 | -0.099305 | -0.648648 |
| H | -8.269124 | 0.619737 | -1.596435 |
| H | -8.270554 | -1.115242 | -1.285885 |
| C | -3.325780 | -2.252469 | 1.504802 |
| H | -2.342318 | -2.350867 | 1.037214 |
| C | -3.088085 | -1.797067 | 2.955043 |
| H | -4.036020 | -1.636569 | 3.484193 |
| H | -2.512994 | -2.546728 | 3.512374 |
| H | -2.523803 | -0.862502 | 2.972264 |
| C | -3.996833 | -3.634484 | 1.457498 |
| H | -3.364328 | -4.382481 | 1.949317 |
| H | -4.968674 | -3.646402 | 1.965900 |
| H | -4.154638 | -3.958241 | 0.424861 |
| B | -1.779984 | -0.475379 | -0.363543 |

**C**

| | | | |
|---|---|---|---|
| C | 0.172157 | -0.511511 | 0.492812 |
| C | 1.632243 | -0.569473 | 0.570764 |
| C | 2.118094 | 0.381648 | -0.373798 |
| C | 3.481550 | 0.601455 | -0.508185 |
| C | 4.371845 | -0.138330 | 0.283028 |
| C | 3.898283 | -1.068590 | 1.202304 |
| C | 2.521794 | -1.288054 | 1.356221 |
| C | -1.080700 | -2.108194 | 2.046494 |
| C | -0.344914 | -3.297929 | 1.930195 |
| C | -0.454770 | -4.300886 | 2.888343 |
| C | -1.297593 | -4.133710 | 3.986002 |
| C | -2.034086 | -2.957605 | 4.114775 |
| C | -1.933529 | -1.957713 | 3.152023 |
| C | -0.963042 | -1.049801 | 1.031792 |
| C | -0.172157 | 0.511511 | -0.492812 |
| C | -1.632243 | 0.569473 | -0.570764 |
| C | -2.118094 | -0.381648 | 0.373798 |

| | | | |
|---|---|---|---|
| C | -3.481550 | -0.601455 | 0.508185 |
| C | -4.371845 | 0.138330 | -0.283028 |
| C | -3.898283 | 1.068590 | -1.202304 |
| C | -2.521794 | 1.288054 | -1.356221 |
| C | 1.080700 | 2.108194 | -2.046494 |
| C | 0.344914 | 3.297929 | -1.930195 |
| C | 0.454770 | 4.300886 | -2.888343 |
| C | 1.297593 | 4.133710 | -3.986002 |
| C | 2.034086 | 2.957605 | -4.114775 |
| C | 1.933529 | 1.957713 | -3.152023 |
| C | 0.963042 | 1.049801 | -1.031792 |
| H | 3.860024 | 1.344654 | -1.201512 |
| H | 5.440015 | 0.025058 | 0.182035 |
| H | 4.599617 | -1.627229 | 1.813849 |
| H | 2.164838 | -2.002136 | 2.089657 |
| H | 0.297066 | -3.440490 | 1.067695 |
| H | 0.115224 | -5.217616 | 2.774543 |
| H | -1.381763 | -4.915341 | 4.734098 |
| H | -2.688506 | -2.816545 | 4.969180 |
| H | -2.497342 | -1.038661 | 3.269672 |
| H | -3.860024 | -1.344654 | 1.201512 |
| H | -5.440015 | -0.025058 | -0.182035 |
| H | -4.599617 | 1.627229 | -1.813849 |
| H | -2.164838 | 2.002136 | -2.089657 |
| H | -0.297066 | 3.440490 | -1.067695 |
| H | -0.115224 | 5.217616 | -2.774543 |
| H | 1.381763 | 4.915341 | -4.734098 |
| H | 2.688506 | 2.816545 | -4.969180 |
| H | 2.497342 | 1.038661 | -3.269672 |

**$1K_2$**

| | | | |
|---|---|---|---|
| K | 0.597814 | 2.861744 | -0.035602 |
| O | 0.777740 | 4.514110 | -2.254842 |
| O | -1.223264 | 4.123754 | 1.631931 |
| O | 2.948429 | 4.266844 | 0.487679 |
| B | -1.738002 | 0.452772 | -1.122863 |
| C | -0.676671 | 0.044877 | -0.100400 |
| C | -1.781655 | -0.210905 | 0.885661 |
| C | -1.998451 | -0.669148 | 2.173509 |
| H | -1.187835 | -0.938282 | 2.843498 |
| C | -3.356008 | -0.728833 | 2.627032 |
| H | -3.560676 | -1.060869 | 3.642470 |
| C | -4.401240 | -0.362414 | 1.807699 |
| H | -5.421612 | -0.412624 | 2.180124 |
| C | -4.159013 | 0.085741 | 0.467190 |
| H | -5.005009 | 0.361136 | -0.158342 |
| C | -2.858534 | 0.155541 | 0.019198 |
| C | -1.893057 | 0.941355 | -2.630053 |

| | | | |
|---|---|---|---|
| C | -1.381059 | 0.199226 | -3.737440 |
| C | -1.576999 | 0.645198 | -5.045804 |
| H | -1.181571 | 0.058415 | -5.867695 |
| C | -2.284835 | 1.812772 | -5.340980 |
| C | -2.809310 | 2.523867 | -4.267129 |
| H | -3.381016 | 3.425950 | -4.473392 |
| C | -2.635381 | 2.114008 | -2.939766 |
| C | -0.716090 | -1.160843 | -3.520158 |
| H | -0.164811 | -1.104833 | -2.579114 |
| C | 0.282768 | -1.572347 | -4.610078 |
| H | -0.203231 | -1.767228 | -5.570974 |
| H | 0.784286 | -2.499233 | -4.320193 |
| H | 1.052449 | -0.813069 | -4.765566 |
| C | -1.792838 | -2.252386 | -3.365194 |
| H | -2.483405 | -2.019544 | -2.551774 |
| H | -1.330008 | -3.224292 | -3.158604 |
| H | -2.381214 | -2.350353 | -4.283535 |
| C | -2.511765 | 2.272701 | -6.774195 |
| H | -3.043289 | 3.231250 | -6.721751 |
| C | -3.412316 | 1.295374 | -7.551317 |
| H | -3.618805 | 1.669517 | -8.559477 |
| H | -4.367853 | 1.149510 | -7.041231 |
| H | -2.939040 | 0.314111 | -7.652636 |
| C | -1.195744 | 2.521495 | -7.531067 |
| H | -0.614736 | 1.601196 | -7.640776 |
| H | -0.567717 | 3.246954 | -7.007088 |
| H | -1.391141 | 2.908664 | -8.536329 |
| C | -3.297344 | 2.961562 | -1.854387 |
| H | -3.013069 | 2.535555 | -0.890547 |
| C | -2.832291 | 4.429212 | -1.867915 |
| H | -1.744657 | 4.512587 | -1.810134 |
| H | -3.260716 | 4.975471 | -1.020916 |
| H | -3.153387 | 4.946514 | -2.777745 |
| C | -4.832432 | 2.888457 | -1.949908 |
| H | -5.197016 | 3.354099 | -2.871256 |
| H | -5.303217 | 3.406839 | -1.107906 |
| H | -5.179643 | 1.853612 | -1.944023 |
| C | 0.775448 | 4.041649 | -3.612626 |
| H | 0.008206 | 3.273556 | -3.694390 |
| H | 1.752774 | 3.595843 | -3.835828 |
| C | 0.513627 | 5.286908 | -4.480429 |
| H | 1.106782 | 5.263517 | -5.396939 |
| H | -0.536602 | 5.341695 | -4.770629 |
| C | 0.896937 | 6.475663 | -3.558082 |
| H | 0.020260 | 7.086146 | -3.331517 |
| H | 1.648040 | 7.131821 | -4.003368 |
| C | 1.421293 | 5.789672 | -2.287174 |
| H | 2.509980 | 5.650485 | -2.330631 |
| H | 1.176997 | 6.310196 | -1.360654 |

| | | | |
|---|---|---|---|
| C | -2.457064 | 3.505724 | 2.086757 |
| H | -2.244092 | 2.913606 | 2.980327 |
| H | -2.810650 | 2.829378 | 1.309892 |
| C | -3.406063 | 4.661426 | 2.392019 |
| H | -4.157901 | 4.393930 | 3.136963 |
| H | -3.928431 | 4.982497 | 1.485979 |
| C | -2.437989 | 5.752419 | 2.871190 |
| H | -2.842411 | 6.762974 | 2.781530 |
| H | -2.169675 | 5.589417 | 3.919455 |
| C | -1.225328 | 5.525091 | 1.964702 |
| H | -1.304801 | 6.107061 | 1.038515 |
| H | -0.275836 | 5.771627 | 2.448321 |
| C | 4.112079 | 3.796179 | -0.214405 |
| H | 3.857850 | 2.860282 | -0.709095 |
| H | 4.393958 | 4.537198 | -0.976153 |
| C | 5.201681 | 3.659915 | 0.858402 |
| H | 6.191644 | 3.886797 | 0.457422 |
| H | 5.226284 | 2.638506 | 1.240086 |
| C | 4.761846 | 4.656891 | 1.963974 |
| H | 5.492772 | 5.451879 | 2.127622 |
| H | 4.617477 | 4.141654 | 2.914908 |
| C | 3.428244 | 5.220583 | 1.438280 |
| H | 2.662988 | 5.339707 | 2.206557 |
| H | 3.576832 | 6.189290 | 0.939594 |
| B | 1.767307 | -0.532180 | 1.171157 |
| C | 0.724226 | -0.116413 | 0.134251 |
| C | 1.847260 | 0.154533 | -0.827410 |
| C | 2.093248 | 0.639536 | -2.100411 |
| H | 1.298733 | 0.923980 | -2.783576 |
| C | 3.460094 | 0.704219 | -2.524178 |
| H | 3.686279 | 1.054309 | -3.528934 |
| C | 4.488044 | 0.323394 | -1.689901 |
| H | 5.515838 | 0.378790 | -2.040307 |
| C | 4.217241 | -0.145677 | -0.362168 |
| H | 5.049281 | -0.427288 | 0.279347 |
| C | 2.907684 | -0.225516 | 0.054746 |
| C | 1.886292 | -1.022801 | 2.681263 |
| C | 1.427954 | -0.234813 | 3.778715 |
| C | 1.578258 | -0.685993 | 5.091210 |
| H | 1.222604 | -0.065665 | 5.906861 |
| C | 2.191166 | -1.903641 | 5.396938 |
| C | 2.669559 | -2.658751 | 4.331483 |
| H | 3.172425 | -3.598627 | 4.547684 |
| C | 2.537814 | -2.243546 | 3.000743 |
| C | 0.880078 | 1.172342 | 3.540899 |
| H | 0.322329 | 1.145504 | 2.601705 |
| C | -0.076545 | 1.689636 | 4.622910 |
| H | 0.425340 | 1.855897 | 5.581116 |
| H | -0.491667 | 2.652898 | 4.314653 |

| | | | |
|---|---|---|---|
| H | -0.910415 | 1.003674 | 4.789939 |
| C | 2.049818 | 2.160216 | 3.363201 |
| H | 2.709983 | 1.853979 | 2.548925 |
| H | 1.679550 | 3.168186 | 3.144543 |
| H | 2.650618 | 2.215379 | 4.277115 |
| C | 2.370855 | -2.371924 | 6.834100 |
| H | 2.830015 | -3.367609 | 6.790989 |
| C | 3.334869 | -1.460372 | 7.614969 |
| H | 3.506550 | -1.845456 | 8.625555 |
| H | 4.301949 | -1.386321 | 7.111234 |
| H | 2.934066 | -0.446771 | 7.710496 |
| C | 1.033006 | -2.517692 | 7.579625 |
| H | 0.522715 | -1.555329 | 7.679904 |
| H | 0.356451 | -3.195962 | 7.052699 |
| H | 1.189390 | -2.913636 | 8.588249 |
| C | 3.157386 | -3.128429 | 1.920293 |
| H | 2.866695 | -2.709857 | 0.953968 |
| C | 2.659412 | -4.584221 | 1.963900 |
| H | 1.569529 | -4.645356 | 1.924890 |
| H | 3.061562 | -5.152178 | 1.118383 |
| H | 2.985012 | -5.096270 | 2.874950 |
| C | 4.695086 | -3.089632 | 1.991263 |
| H | 5.059997 | -3.542517 | 2.918885 |
| H | 5.141568 | -3.638787 | 1.155446 |
| H | 5.066149 | -2.064044 | 1.955423 |
| K | -0.628726 | -2.924311 | 0.053637 |
| O | -0.924838 | -4.584155 | 2.261190 |
| O | 1.233686 | -4.223497 | -1.548833 |
| O | -3.019389 | -4.233225 | -0.530633 |
| C | -0.970786 | -4.103022 | 3.615701 |
| H | -0.175713 | -3.368224 | 3.731851 |
| H | -1.936687 | -3.612080 | 3.785511 |
| C | -0.807865 | -5.351529 | 4.503872 |
| H | -1.459918 | -5.302373 | 5.378414 |
| H | 0.217888 | -5.440568 | 4.864872 |
| C | -1.169911 | -6.532705 | 3.563598 |
| H | -0.295904 | -7.161584 | 3.380925 |
| H | -1.956128 | -7.172500 | 3.970400 |
| C | -1.612889 | -5.836721 | 2.268249 |
| H | -2.696990 | -5.660504 | 2.261582 |
| H | -1.344543 | -6.370129 | 1.355714 |
| C | 2.486714 | -3.640947 | -1.996123 |
| H | 2.302565 | -3.067470 | -2.908251 |
| H | 2.839601 | -2.951835 | -1.230095 |
| C | 3.418187 | -4.821510 | -2.256669 |
| H | 4.189198 | -4.586150 | -2.992847 |
| H | 3.916821 | -5.131785 | -1.333713 |
| C | 2.437091 | -5.903480 | -2.729823 |
| H | 2.819043 | -6.919686 | -2.610694 |

| | | | |
|---|---|---|---|
| H | 2.191230 | -5.758112 | -3.786148 |
| C | 1.212832 | -5.631797 | -1.851674 |
| H | 1.262689 | -6.194198 | -0.911569 |
| H | 0.267631 | -5.869501 | -2.347970 |
| C | -4.186373 | -3.758773 | 0.162633 |
| H | -3.919144 | -2.849982 | 0.699059 |
| H | -4.508333 | -4.521332 | 0.886532 |
| C | -5.241044 | -3.548844 | -0.930981 |
| H | -6.251400 | -3.732997 | -0.559985 |
| H | -5.202982 | -2.519781 | -1.290750 |
| C | -4.821529 | -4.543929 | -2.045601 |
| H | -5.568544 | -5.323067 | -2.212893 |
| H | -4.670569 | -4.025223 | -2.993652 |
| C | -3.498793 | -5.141390 | -1.525857 |
| H | -2.725742 | -5.235827 | -2.289460 |
| H | -3.662502 | -6.127995 | -1.069152 |

**$2K_2$**

| | | | |
|---|---|---|---|
| K | 0.593638 | -0.113455 | -2.769916 |
| O | -0.356287 | 1.102771 | -4.994590 |
| O | 2.709095 | -1.715792 | -3.410409 |
| C | -0.672637 | -0.242846 | -0.196504 |
| C | -1.438789 | 0.905129 | -0.654753 |
| C | -0.644887 | 2.113122 | -0.559691 |
| C | -1.222484 | 3.324810 | -0.963248 |
| H | -0.642422 | 4.244119 | -0.899073 |
| C | -2.536209 | 3.378636 | -1.442462 |
| H | -2.971956 | 4.328654 | -1.740893 |
| C | -3.294954 | 2.202775 | -1.532903 |
| H | -4.316186 | 2.247957 | -1.903785 |
| C | -2.753169 | 0.973684 | -1.149235 |
| H | -3.352250 | 0.069288 | -1.224776 |
| C | -1.954672 | -2.770562 | -0.350577 |
| C | -3.130000 | -2.868394 | 0.444032 |
| C | -4.118104 | -3.809771 | 0.150278 |
| H | -5.000127 | -3.865563 | 0.781016 |
| C | -4.011781 | -4.684228 | -0.933086 |
| C | -2.870132 | -4.583428 | -1.720664 |
| H | -2.773306 | -5.246709 | -2.577181 |
| C | -1.854281 | -3.659492 | -1.448518 |
| C | -3.303856 | -1.975850 | 1.672001 |
| H | -2.748345 | -1.057881 | 1.456074 |
| C | -2.679178 | -2.640303 | 2.914321 |
| H | -3.195714 | -3.575571 | 3.151295 |
| H | -2.756800 | -1.992885 | 3.797260 |
| H | -1.626182 | -2.884627 | 2.750579 |
| C | -4.752644 | -1.557845 | 1.962973 |
| H | -4.774013 | -0.802022 | 2.754716 |

| | | | |
|---|---|---|---|
| H | -5.369014 | -2.394188 | 2.305973 |
| H | -5.230632 | -1.130727 | 1.077863 |
| C | -5.094384 | -5.706476 | -1.248416 |
| H | -4.766797 | -6.253695 | -2.141262 |
| C | -6.439818 | -5.042097 | -1.589194 |
| H | -7.185072 | -5.791226 | -1.875975 |
| H | -6.333070 | -4.336628 | -2.417334 |
| H | -6.840255 | -4.488772 | -0.734593 |
| C | -5.260572 | -6.737748 | -0.118469 |
| H | -5.996803 | -7.501527 | -0.389498 |
| H | -5.601788 | -6.264047 | 0.806913 |
| H | -4.314635 | -7.240740 | 0.098489 |
| C | -0.664253 | -3.603148 | -2.404574 |
| H | 0.076021 | -2.935554 | -1.954113 |
| C | -1.073824 | -3.009009 | -3.765597 |
| H | -1.777316 | -3.662313 | -4.290209 |
| H | -0.202992 | -2.874747 | -4.417878 |
| H | -1.573560 | -2.042396 | -3.645185 |
| C | 0.030110 | -4.961456 | -2.593015 |
| H | 0.914296 | -4.854924 | -3.230066 |
| H | -0.625703 | -5.697388 | -3.067360 |
| H | 0.354018 | -5.372979 | -1.634288 |
| C | -1.698019 | 1.626986 | -4.997249 |
| H | -2.078981 | 1.577952 | -3.977966 |
| H | -2.322429 | 0.997439 | -5.644796 |
| C | -1.581642 | 3.059894 | -5.548346 |
| H | -2.414575 | 3.296703 | -6.213508 |
| H | -1.592611 | 3.785203 | -4.734069 |
| C | -0.215826 | 3.069544 | -6.286722 |
| H | 0.487862 | 3.737226 | -5.786088 |
| H | -0.297611 | 3.394234 | -7.326155 |
| C | 0.260775 | 1.613860 | -6.180411 |
| H | -0.066145 | 1.021764 | -7.046892 |
| H | 1.340650 | 1.504263 | -6.070616 |
| C | 3.510103 | -2.322388 | -2.373466 |
| H | 2.891500 | -2.411856 | -1.482727 |
| H | 4.353955 | -1.660612 | -2.146988 |
| C | 3.991993 | -3.665495 | -2.953547 |
| H | 3.402563 | -4.494736 | -2.560773 |
| H | 5.034842 | -3.853694 | -2.690962 |
| C | 3.790742 | -3.513608 | -4.484984 |
| H | 4.696687 | -3.728459 | -5.055595 |
| H | 3.009982 | -4.189159 | -4.840948 |
| C | 3.347472 | -2.052936 | -4.645398 |
| H | 4.210601 | -1.391628 | -4.806855 |
| H | 2.628038 | -1.889610 | -5.449625 |
| B | -0.778572 | -1.731777 | -0.026639 |
| C | 0.672620 | 0.242865 | 0.196534 |
| C | 1.438772 | -0.905111 | 0.654781 |

| | | | |
|---|---|---|---|
| C | 0.644871 | -2.113102 | 0.559719 |
| C | 1.222471 | -3.324795 | 0.963273 |
| H | 0.642408 | -4.244100 | 0.899097 |
| C | 2.536196 | -3.378618 | 1.442485 |
| H | 2.971945 | -4.328636 | 1.740913 |
| C | 3.294940 | -2.202756 | 1.532926 |
| H | 4.316172 | -2.247940 | 1.903805 |
| C | 2.753152 | -0.973665 | 1.149260 |
| H | 3.352235 | -0.069269 | 1.224802 |
| C | 1.954660 | 2.770576 | 0.350599 |
| C | 3.129987 | 2.868405 | -0.444014 |
| C | 4.118094 | 3.809783 | -0.150260 |
| H | 5.000113 | 3.865578 | -0.781001 |
| C | 4.011775 | 4.684238 | 0.933107 |
| C | 2.870129 | 4.583435 | 1.720689 |
| H | 2.773308 | 5.246717 | 2.577207 |
| C | 1.854273 | 3.659502 | 1.448543 |
| C | 3.303830 | 1.975862 | -1.671984 |
| H | 2.748329 | 1.057892 | -1.456049 |
| C | 2.679135 | 2.640308 | -2.914298 |
| H | 3.195671 | 3.575572 | -3.151291 |
| H | 2.756736 | 1.992884 | -3.797236 |
| H | 1.626143 | 2.884642 | -2.750539 |
| C | 4.752613 | 1.557850 | -1.962979 |
| H | 4.773966 | 0.802009 | -2.754707 |
| H | 5.368973 | 2.394185 | -2.306015 |
| H | 5.230623 | 1.130752 | -1.077872 |
| C | 5.094378 | 5.706483 | 1.248434 |
| H | 4.766794 | 6.253703 | 2.141279 |
| C | 6.439812 | 5.042102 | 1.589210 |
| H | 7.185071 | 5.791232 | 1.875989 |
| H | 6.333068 | 4.336632 | 2.417350 |
| H | 6.840247 | 4.488775 | 0.734608 |
| C | 5.260570 | 6.737756 | 0.118487 |
| H | 5.996799 | 7.501530 | 0.389516 |
| H | 5.601784 | 6.264055 | -0.806895 |
| H | 4.314633 | 7.240752 | -0.098471 |
| C | 0.664251 | 3.603159 | 2.404604 |
| H | -0.076027 | 2.935569 | 1.954140 |
| C | 1.073826 | 3.009006 | 3.765622 |
| H | 1.777322 | 3.662302 | 4.290232 |
| H | 0.202997 | 2.874742 | 4.417906 |
| H | 1.573556 | 2.042391 | 3.645199 |
| C | -0.030105 | 4.961466 | 2.593058 |
| H | -0.914293 | 4.854933 | 3.230109 |
| H | 0.625712 | 5.697392 | 3.067406 |
| H | -0.354015 | 5.372999 | 1.634336 |
| B | 0.778557 | 1.731795 | 0.026666 |
| K | -0.593669 | 0.113485 | 2.769944 |

| | | | |
|---|---|---|---|
| O | 0.356237 | -1.102786 | 4.994607 |
| O | -2.709121 | 1.715833 | 3.410429 |
| C | 1.697966 | -1.627010 | 4.997253 |
| H | 2.078927 | -1.577958 | 3.977971 |
| H | 2.322379 | -0.997479 | 5.644812 |
| C | 1.581582 | -3.059932 | 5.548320 |
| H | 2.414497 | -3.296746 | 6.213499 |
| H | 1.592577 | -3.785224 | 4.734030 |
| C | 0.215748 | -3.069606 | 6.286660 |
| H | -0.487933 | -3.737257 | 5.785974 |
| H | 0.297503 | -3.394345 | 7.326079 |
| C | -0.260839 | -1.613912 | 6.180402 |
| H | 0.066086 | -1.021854 | 7.046910 |
| H | -1.340711 | -1.504299 | 6.070606 |
| C | -3.510110 | 2.322442 | 2.373482 |
| H | -2.891509 | 2.411881 | 1.482740 |
| H | -4.353985 | 1.660691 | 2.147012 |
| C | -3.991955 | 3.665569 | 2.953550 |
| H | -3.402461 | 4.494778 | 2.560805 |
| H | -5.034782 | 3.853828 | 2.690924 |
| C | -3.790767 | 3.513663 | 4.484996 |
| H | -4.696738 | 3.728506 | 5.055570 |
| H | -3.010027 | 4.189213 | 4.841000 |
| C | -3.347505 | 2.052987 | 4.645412 |
| H | -4.210638 | 1.391685 | 4.806869 |
| H | -2.628077 | 1.889662 | 5.449647 |

**TD-DFT calculations, td=(nstates=20) B3LYP/6-311G(d)**

Excitation energies and oscillator strengths (**1K$_2$**):

Excited State 1: Singlet-A 1.5396 eV 805.32 nm f=0.1468 <S**2>=0.000
303 -> 304 0.70192
Excited State 2: Singlet-A 1.6856 eV 735.54 nm f=0.0017 <S**2>=0.000
303 -> 305 0.70436
Excited State 3: Singlet-A 1.7014 eV 728.70 nm f=0.0000 <S**2>=0.000
303 -> 306 0.70047
Excited State 4: Singlet-A 1.7950 eV 690.73 nm f=0.0000 <S**2>=0.000
303 -> 307 0.65455
303 -> 309 0.20526
303 -> 315 0.11832
Excited State 5: Singlet-A 2.1039 eV 589.32 nm f=0.0058 <S**2>=0.000
303 -> 308 0.70452
Excited State 6: Singlet-A 2.1432 eV 578.50 nm f=0.0001 <S**2>=0.000
303 -> 307 -0.22267
303 -> 309 0.65681
Excited State 7: Singlet-A 2.2229 eV 557.76 nm f=0.0001 <S**2>=0.000

303 -> 309 -0.10418
303 -> 310 0.67701
303 -> 312 -0.12764
Excited State 8: Singlet-A 2.2447 eV 552.35 nm f=0.0047 <S**2>=0.000
303 -> 311 0.67336
303 -> 312 -0.12219
303 -> 313 -0.15560
Excited State 9: Singlet-A 2.3248 eV 533.32 nm f=0.0007 <S**2>=0.000
303 -> 310 0.14485
303 -> 312 0.51792
303 -> 313 -0.44674
Excited State 10: Singlet-A 2.3270 eV 532.81 nm f=0.0014 <S**2>=0.000
303 -> 311 0.19529
303 -> 312 0.43118
303 -> 313 0.51156
303 -> 314 0.10448
Excited State 11: Singlet-A 2.4034 eV 515.87 nm f=0.0110 <S**2>=0.000
303 -> 314 0.32212
303 -> 315 0.59624
303 -> 316 -0.11344
Excited State 12: Singlet-A 2.4353 eV 509.12 nm f=0.0943 <S**2>=0.000
303 -> 314 0.59905
303 -> 315 -0.31807
303 -> 318 -0.10917
Excited State 13: Singlet-A 2.6176 eV 473.65 nm f=0.0001 <S**2>=0.000
303 -> 315 0.13202
303 -> 316 0.68743
Excited State 14: Singlet-A 2.7137 eV 456.88 nm f=0.0388 <S**2>=0.000
303 -> 317 0.69702
Excited State 15: Singlet-A 3.0412 eV 407.68 nm f=0.1661 <S**2>=0.000
303 -> 314 0.10489
303 -> 318 0.68496
Excited State 16: Singlet-A 3.1299 eV 396.13 nm f=0.0001 <S**2>=0.000
303 -> 319 -0.22025
303 -> 320 0.63910
303 -> 321 0.10613
303 -> 322 -0.11359
Excited State 17: Singlet-A 3.2062 eV 386.70 nm f=0.0055 <S**2>=0.000
303 -> 319 -0.45360
303 -> 320 -0.23899
303 -> 321 0.46068
Excited State 18: Singlet-A 3.2102 eV 386.22 nm f=0.0045 <S**2>=0.000
303 -> 319 0.47981
303 -> 321 0.49153
Excited State 19: Singlet-A 3.2390 eV 382.78 nm f=0.0005 <S**2>=0.000
302 -> 304 0.69242
Excited State 20: Singlet-A 3.3039 eV 375.26 nm f=0.0000 <S**2>=0.000
303 -> 320 0.10484
303 -> 322 0.67594

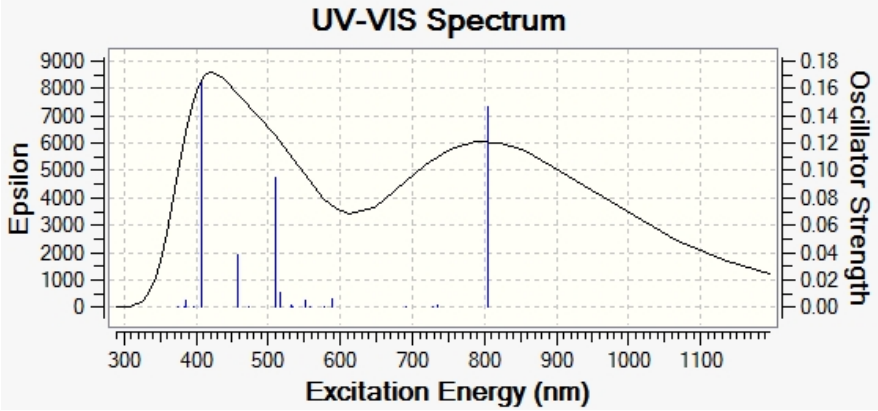



**Figure S16**. Calculated TD-DFT UV-VIS spectrum **1K$_2$**.

Excitation energies and oscillator strengths (**2K$_2$**):

Excited State 1: Singlet-A 2.5559 eV 485.10 nm f=0.2530 <S**2>=0.000
262 -> 267 0.16027
263 -> 264 0.68195
Excited State 2: Singlet-A 2.5784 eV 480.86 nm f=0.0000 <S**2>=0.000
263 -> 266 0.70130
Excited State 3: Singlet-A 2.6021 eV 476.48 nm f=0.0007 <S**2>=0.000
263 -> 265 0.70494
Excited State 4: Singlet-A 2.7211 eV 455.64 nm f=0.0000 <S**2>=0.000
262 -> 264 0.69069
263 -> 267 -0.12457
Excited State 5: Singlet-A 2.8825 eV 430.13 nm f=0.0000 <S**2>=0.000
262 -> 264 0.13523
263 -> 267 0.65684
263 -> 271 0.20192
Excited State 6: Singlet-A 3.0940 eV 400.72 nm f=0.0041 <S**2>=0.000
263 -> 268 0.70277
Excited State 7: Singlet-A 3.1286 eV 396.29 nm f=0.0048 <S**2>=0.000
263 -> 270 0.70075
Excited State 8: Singlet-A 3.1509 eV 393.49 nm f=0.0000 <S**2>=0.000
263 -> 269 0.70114
Excited State 9: Singlet-A 3.2303 eV 383.82 nm f=0.0000 <S**2>=0.000
263 -> 267 -0.20276
263 -> 271 0.64716
263 -> 273 0.18142
Excited State 10: Singlet-A 3.2714 eV 379.00 nm f=0.0020 <S**2>=0.000
262 -> 266 0.69572
Excited State 11: Singlet-A 3.2941 eV 376.38 nm f=0.0000 <S**2>=0.000
262 -> 265 0.69837
Excited State 12: Singlet-A 3.3001 eV 375.70 nm f=0.0096 <S**2>=0.000
263 -> 272 0.62874
263 -> 274 -0.30847
Excited State 13: Singlet-A 3.3237 eV 373.03 nm f=0.0000 <S**2>=0.000

263 -> 271 -0.18005
263 -> 273 0.67670
Excited State 14: Singlet-A 3.3263 eV 372.73 nm f=0.0255 <S**2>=0.000
263 -> 272 0.30825
263 -> 274 0.61672
Excited State 15: Singlet-A 3.3939 eV 365.31 nm f=0.0000 <S**2>=0.000
263 -> 275 0.60796
263 -> 276 0.34968
Excited State 16: Singlet-A 3.5031 eV 353.93 nm f=0.0000 <S**2>=0.000
263 -> 275 -0.34907
263 -> 276 0.60343
Excited State 17: Singlet-A 3.5744 eV 346.87 nm f=0.0032 <S**2>=0.000
263 -> 277 0.67980
263 -> 279 0.16190
Excited State 18: Singlet-A 3.7733 eV 328.58 nm f=0.0000 <S**2>=0.000
262 -> 268 0.68309
262 -> 270 -0.16242
Excited State 19: Singlet-A 3.8142 eV 325.06 nm f=0.0000 <S**2>=0.000
262 -> 268 0.16253
262 -> 270 0.68517
Excited State 20: Singlet-A 3.8275 eV 323.93 nm f=0.2266 <S**2>=0.000
262 -> 267 0.56201
262 -> 269 -0.34932
263 -> 264 -0.12034

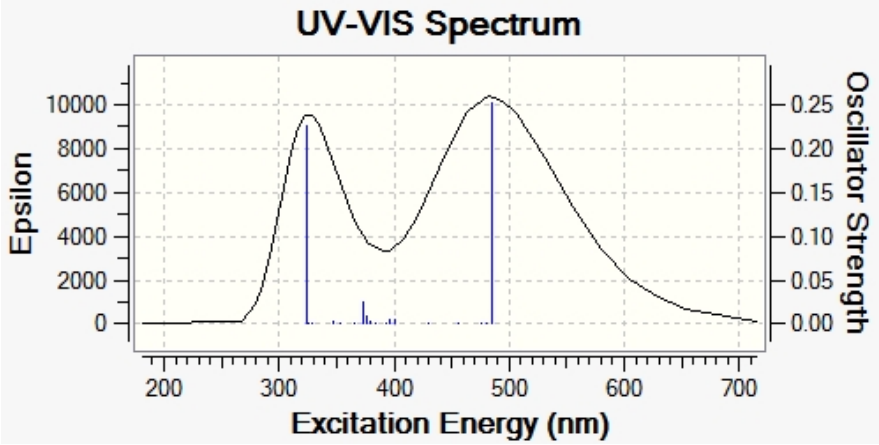



**Figure S17**. Calculated TD-DFT UV-VIS spectrum **2K$_2$**.

## 8. Full citation for reference 32

All calculations were carried out using Gaussian 09, Revision **A.1**, 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, 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.

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## 9. References

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