Electronic Supplementary Material (ESI) for ChemComm.

Supporting information for:

Synthesis of Cyclic Diborenes with Unprecedented *cis* Configuration

Philipp Bissinger, Holger Braunschweig, Mehmet Ali Celik, Christina Claes, Rian D. Dewhurst, Sebastian Endres, Hauke Kelch, Thomas Kramer, Ivo Krummenacher and Christoph Schneider*

Experimental Section

General considerations:

All reactions were accomplished under an atmosphere of dry argon using standard Schlenk line and glovebox techniques. Deuterated benzene was degassed by three freeze-pump-thaw cycles and dried over molecular sieves. Other solvents were dried by storage over, and distillation from, sodium (diethyl ether), potassium (benzene, thf) or Na/K alloy (all other solvents) under an argon atmosphere. The solvents were then stored under argon over activated 4 Å molecular sieves. NMR spectra were obtained from a Bruker Avance 500 NMR spectrometer (^{1}H: 500.13 MHz, ^{11}B: 160.46 MHz, ^{13}C{^{1}H}: 125.76 MHz, ^{31}P{^{1}H}: 202.5 MHz) at room temperature. Chemical shifts (δ) are given in ppm and internally referenced to the carbon nuclei (^{13}C{^{1}H}) or residual protons (^{1}H) of the solvent. ^{11}B and ^{31}P{^{1}H} NMR spectra were referenced to external standards [$BF_3 \cdot OEt_2$] or 85% H_3PO_4, respectively. Microanalyses (C, H, N) were performed on an Elementar vario MICRO cube elemental analyzer. UV-vis spectra were measured on a JASCO V-660 UV-vis spectrometer. $B_2Br_2Mes_2$ (**1**),[1] $B_2Br_2Mes_2(PMe_3)$ (**5**)[2] and PMe_3[3] were synthesized according to literature procedures. Potassium graphite (KC_8) was prepared by heating graphite (20.36 g, 1.695 mol; first heated to 180 °C under reduced pressure for ten hours) and freshly-cut potassium (8.35 g, 214 mmol) at 180 °C with stirring for two days, followed by filtering the powder through a tea strainer. Diphosphines dmpe and dppm were purchased from ABCR and used without further purification.

Preparation of *cis,cyclo*-[B_2Mes_2(dmpe)] 2:

A solution of **1** (198 mg, 472 μmol) in benzene (20 mL) was added dropwise to a suspension of dmpe (80.2 mg, 534 μmol) and KC_8 (336 mg, 2.49 mmol) in benzene (20 mL) at room temperature. The flask containing the diborane(4) was washed with benzene (2 mL) and the solution was added to the reaction mixture, which was filtered through celite after stirring overnight. The residue was washed with benzene (2×10 mL) and the filtrate was evaporated *in vacuo*. After three crystallisation cycles from a thf/pentane solution (1:1), **2** was obtained as pale yellow crystals (105 mg, 256 μmol, 54%).

^{1}H NMR (500.13 MHz, C_6D_6): δ = 6.96 (s, 4H, *m*-$C_{Mes}H$), 2.65 (s, 12H, *o*-$C_{Mes}CH_3$), 2.26 (s, 6H, *p*-$C_{Mes}CH_3$), 1.39 (m, 4H, PCH_2CH_2P), 0.78 (vt, N = $|^2J_{H-P}+^5J_{H-P}|$ = 9.55 Hz, 12H, PCH_3).

^{11}B NMR (160.46 MHz, C_6D_6): δ = 18.6 ppm

^{13}C{^{1}H} NMR (125.76 MHz, C_6D_6): δ = 145.43 (br s, *i*-C_{Mes}) 140.43 (vt, N = $|^3J_{C-P}+^4J_{C-P}|$ = 5.62 Hz, *o*-C_{Mes}), 132.70 (vt, N = $|^4J_{C-P}+^5J_{C-P}|$ = 4.30 Hz, *p*-C_{Mes}), 127.49 (m, *m*-$C_{Mes}H$), 24.94 (m, *o*-$C_{Mes}CH_3$), 21.37 (s, *p*-$C_{Mes}CH_3$), 20.86 (m, PCH_2CH_2P), 14.11 (m, PCH_3).

^{31}P{^{1}H} NMR (202.5 MHz, C_6D_6): δ = –21.4 (br s).

Elemental analysis: calculated for $C_{24}H_{38}B_2P_2$: C 70.29; H 9.34; found: C 70.08; H 9.28.

UV-vis: (thf solution): 285 (shoulder), 339 nm (maximum).

Preparation of *cis,cyclo*-[B_2Mes_2(dppm)] 3:

Benzene (50 mL) was added to a solid mixture of **1**(101 mg, 240 μmol), dppm (91.9 mg, 239 μmol) and KC_8 (162 mg, 1.19 mmol). After stirring for two days at room temperature the mixture was filtered through celite. The residue was washed with benzene (3×5 mL) and the volume of the filtrate was reduced by half and layered with hexane (25 mL). After three crystallisation cycles, **3** was obtained as red crystals (60.6 mg, 94.0 μmol, 40%).

^{1}H NMR (500.13 MHz, C_6D_6): δ = 7.45-7.41 (m, 8H, *m*-$C_{Ph}H$), 7.00-6.92 (m, 12H, *o/p*-$C_{Ph}H$), 6.87 (s, 4H, *m*-$C_{Mes}H$), 3.43 (t, $^2J_{H-P}$ = 4.78 Hz, 2H, PCH_2P), 2.44 (s, 12H, *o*-$C_{Mes}CH_3$), 2.19 (s, 6H, *p*-$C_{Mes}CH_3$).

^{11}B NMR (160.46 MHz, C_6D_6): δ = 29.0 (br s).

^{13}C{^{1}H} NMR (125.76 MHz, C_6D_6): δ = 143.63 (br s, *i*-C_{Mes}), 140.98 (vt, N = $|^1J_{C-P}+^3J_{C-P}|$ = 5.76 Hz, *o*-C_{Mes}), 136.11 (vt, N = $|^3J_{C-P}+^4J_{C-P}|$ = 49.69 Hz, *i*-C_{Ph}), 133.69 (m, *p*-C_{Mes}), 132.13 (vt, N = $|^2J_{C-P}+^4J_{C-P}|$ = 9.61 Hz, *m*-$C_{Ph}H$), 130.19 (s, $C_{Ph}H$), 128.79 (vt, N = $|^3J_{C-P}+^5J_{C-P}|$ = 9.62 Hz, $C_{Ph}H$), 128.59 (s, *m*-$C_{Mes}H$), 27.25 (t, $^1J_{C-P}$ = 44.59 Hz, PCH_2P), 24.74 (s, *o*-$C_{Mes}CH_3$), 21.30 (s, *p*-$C_{Mes}CH_3$).

^{31}P{^{1}H} NMR (202.5 MHz, C_6D_6): δ = 2.4 (br s).

Elemental analysis: calculated for $C_{43}H_{44}B_2P_2$: C 80.15; H 6.88; found: C 80.57; H 7.01.

UV-vis: (thf solution): 315 (shoulder), 443 nm (maximum).

Preparation of *trans*-[$B_2Mes_2(PMe_3)_2$] (4):

A solution of $B_2Br_2Mes_2(PMe_3)$ (**5**) (1.27 g, 2.56 mmol) and PMe_3 (0.32 mL, 235 mg, 3.09 mmol) in benzene (25 mL) was added dropwise to a suspension of KC_8 (1.125 g, 8.322 mmol) in benzene (15 mL) within 10 minutes at room temperature. The flask containing $B_2Br_2Mes_2(PMe_3)$ and phosphine was washed with benzene (2×5 mL) and each solution was added to the reaction mixture. After five hours at room temperature the yellow suspension was filtered through celite. The residue was washed with benzene (2×10 mL) and the filtrate was evaporated *in vacuo*. After six crystallization cycles from a benzene/pentane solution (2:1), **4** was obtained as yellow crystals (568 mg, 1.38 mmol, 54%).

^{1}H NMR (500.13 MHz, C_6D_6): δ = 7.12-7.10 (br s, 4H, *m*-$C_{Mes}H$), 2.74 (s, 12H, *o*-$C_{Mes}CH_3$), 2.37 (s, 6H, *p*-$C_{Mes}CH_3$), 0.71 (vt, N = $|^2J_{H-P}+^5J_{H-P}|$ = 9.75 Hz, 18H, PCH_3).

^{11}B NMR (160.46 MHz, C_6D_6): δ = 16.7 (s).

^{13}C{^{1}H} NMR (125.76 MHz, C_6D_6): δ = 149.42 (br s, *i*-C_{Mes}), 141.41 (m, *o*-C_{Mes}), 132.87 (m, *p*-C_{Mes}H), 127.35 (s, *m*-C_{Mes}), 26.32 (s, *o*-$C_{Mes}CH_3$), 21.49 (s, *p*-$C_{Mes}CH_3$), 14.12 (vt, N = $|^1J_{C-P}+^4J_{C-P}|$ = 35.14 Hz, PCH_3).

^{31}P{^{1}H} NMR (202.5 MHz, C_6D_6): δ = –24.4 (s).

Elemental analysis: calculated for $C_{24}H_{46}B_2P_2$: C 69.94; H 9.78; found: C 69.98; H 9.78.

UV-vis: (Et_2O solution): 290 (shoulder), 365 nm (maximum).

Crystal structure determination

The crystal data of *cis,cyclo*-[B_2Mes_2(dmpe)] (**2**) were collected on a Bruker D8-QUEST, *cis,cyclo*-[B_2Mes_2(dppm)] (**3**) and *trans*-[$B_2Mes_2(PMe_3)_2$] (**4**) on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structures were solved using direct methods, refined with the Shelx software package[4] and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned to idealised positions and were included in structure factor calculations.

Crystal data for **2**: $C_{24}H_{38}B_2P_2$, $M_r = 410.10$, colourless block, 0.151×0.119×0.069 mm^3, monoclinic space group $P2_1/c$, $a = 9.367(4)$ Å, $b = 15.172(3)$ Å, $c = 17.348(4)$ Å, $\beta = 96.96(2)°$, $V = 2447.3(12)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.113$ g·cm^{-3}, $\mu = 0.185$ mm^{-1}, $F(000) = 888$, $T = 100(2)$ K, $R_1 = 0.0500$, $wR^2 = 0.1089$, 5100 independent reflections [$2\theta \leq 53.5°$] and 263 parameters.

Crystal data for **3**: $C_{46}H_{47}B_2P_2$, $M_r = 683.40$, orange block, 0.32×0.28×0.21 mm^3, triclinic space group P-1, $a = 14.4599(13)$ Å, $b = 16.0807(15)$ Å, $c = 16.8670(16)$ Å, $\alpha = 79.939(3)°$, $\beta = 86.355(3)°$, $\gamma = 78.644(3)°$, $V = 3784.4(6)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.199$ g·cm^{-3}, $\mu = 0.147$ mm^{-1}, $F(000) = 1452$, $T = 100(2)$ K, $R_1 = 0.0536$, $wR^2 = 0.1044$, 15467 independent reflections [$2\theta \leq 52.74°$] and 913 parameters.

Crystal data for **4**: $C_{24}H_{40}B_2P_2$, $M_r = 412.12$, yellow block, 0.29×0.24×0.16 mm^3, monoclinic space group $P2_1/c$, $a = 9.4899(9)$ Å, $b = 13.6443(12)$ Å, $c = 9.7286(9)$ Å, $\beta = 99.393(3)°$, $V = 1242.8(2)$ Å^3, $Z = 2$, $\rho_{calcd} = 1.101$ g·cm^{-3}, $\mu = 0.183$ mm^{-1}, $F(000) = 448$, $T = 100(2)$ K, $R_1 = 0.0726$, $wR^2 = 0.1665$, 2533 independent reflections [$2\theta \leq 52.74°$] and 133 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication nos. CCDC-1418155 (**2**), CCDC-1418156 (**3**) and CCDC-1418157 (**4**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Cyclic Voltammetry Experiments

Cyclic voltammetry experiments were performed in an argon-filled glovebox using a Gamry Instruments Reference 600 potentiostat. A standard three-electrode cell configuration was employed using a platinum disk working electrode, a platinum wire counter electrode, and a silver wire, separated by a *Vycor* tip, serving as the reference electrode. Formal redox potentials are referenced to the ferrocene/ferrocenium (Fc/Fc^+) redox couple, either by using ferrocene or decamethylferrocene ($E_{1/2}$ = −427 mV vs. Fc/Fc^+) as internal standard. Tetra-*n*-butylammonium hexafluorophosphate ([*n*-Bu_4N][PF_6]) was employed as the supporting electrolyte. Compensation for resistive losses (*iR* drop) was employed for all measurements.

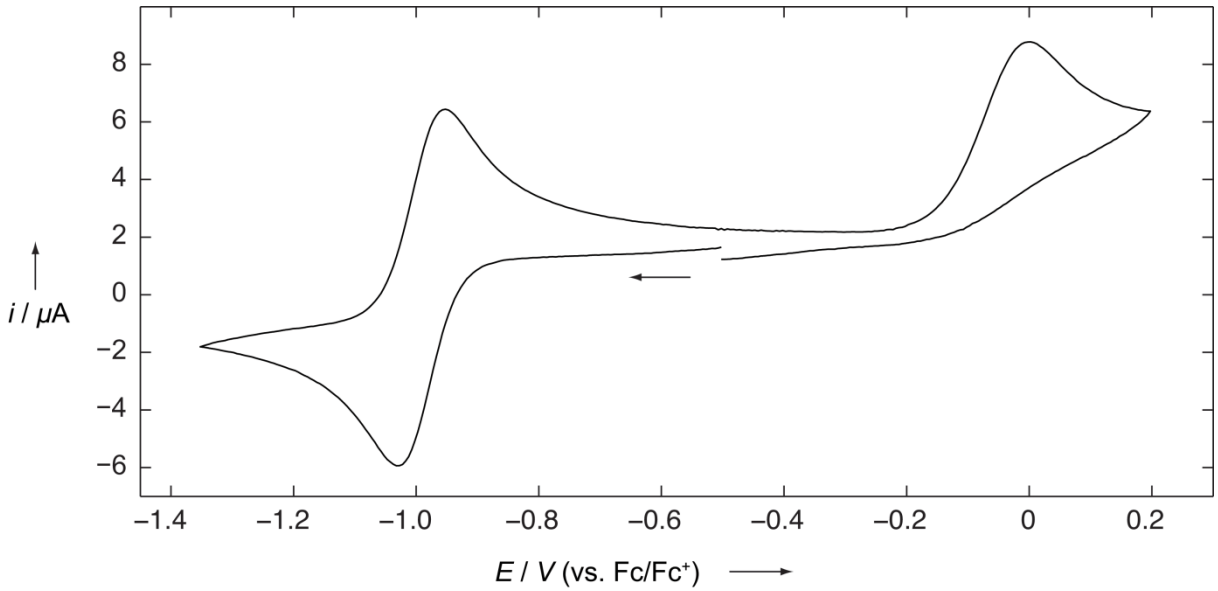


Figure S1. Cyclic voltammogram of **2** in THF with 0.1 M [*n*Bu_4N][PF_6] as the supporting electrolyte. Formal potentials: $E_{1/2}$ = −1.00 V, E_{pa} = 0.00 V.

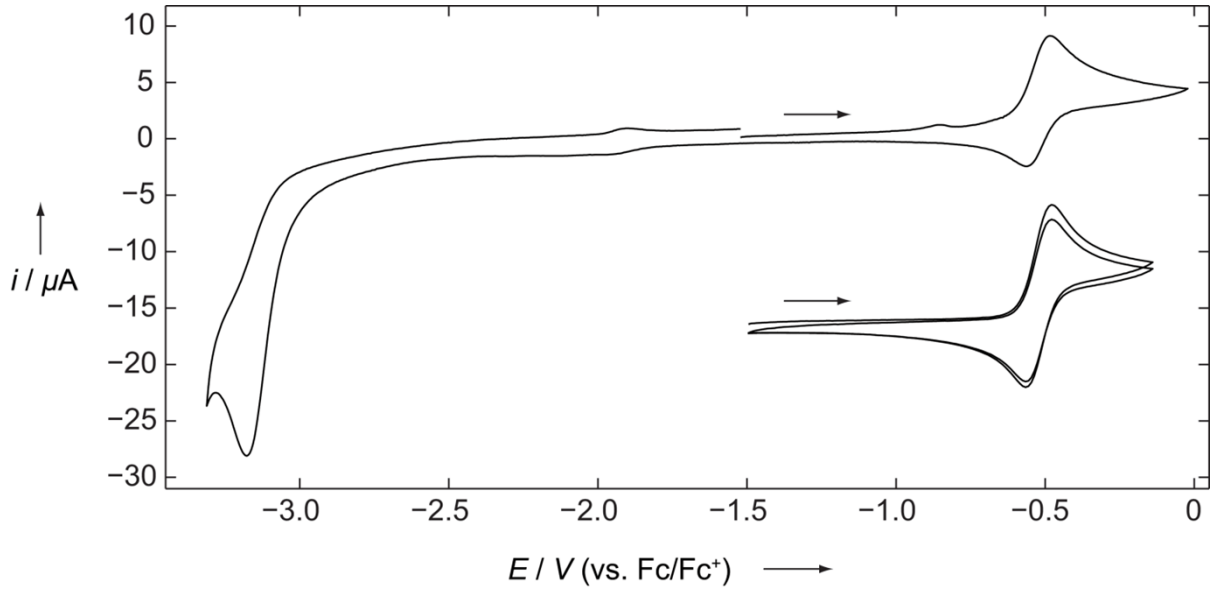


Figure S2. Cyclic voltammogram of **3** in THF with 0.1 M [nBu$_4$N][PF$_6$] as the supporting electrolyte. Formal potentials: $E_{1/2}$ = −0.51 V, E_{pc} = −3.17 V, E_{pa} = +0.33 V (not shown).

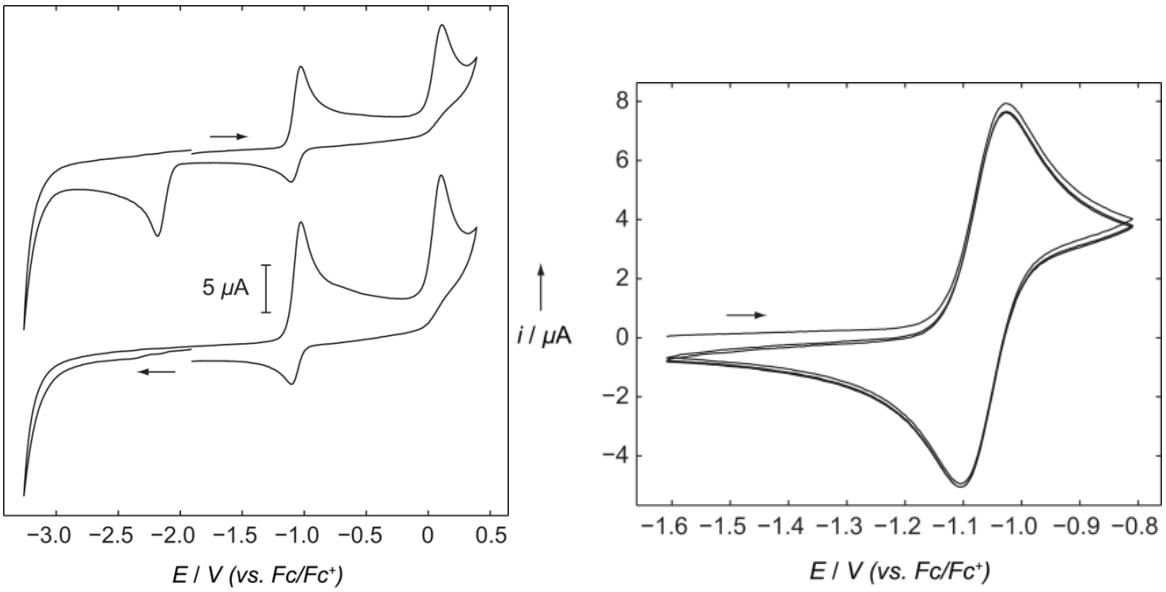
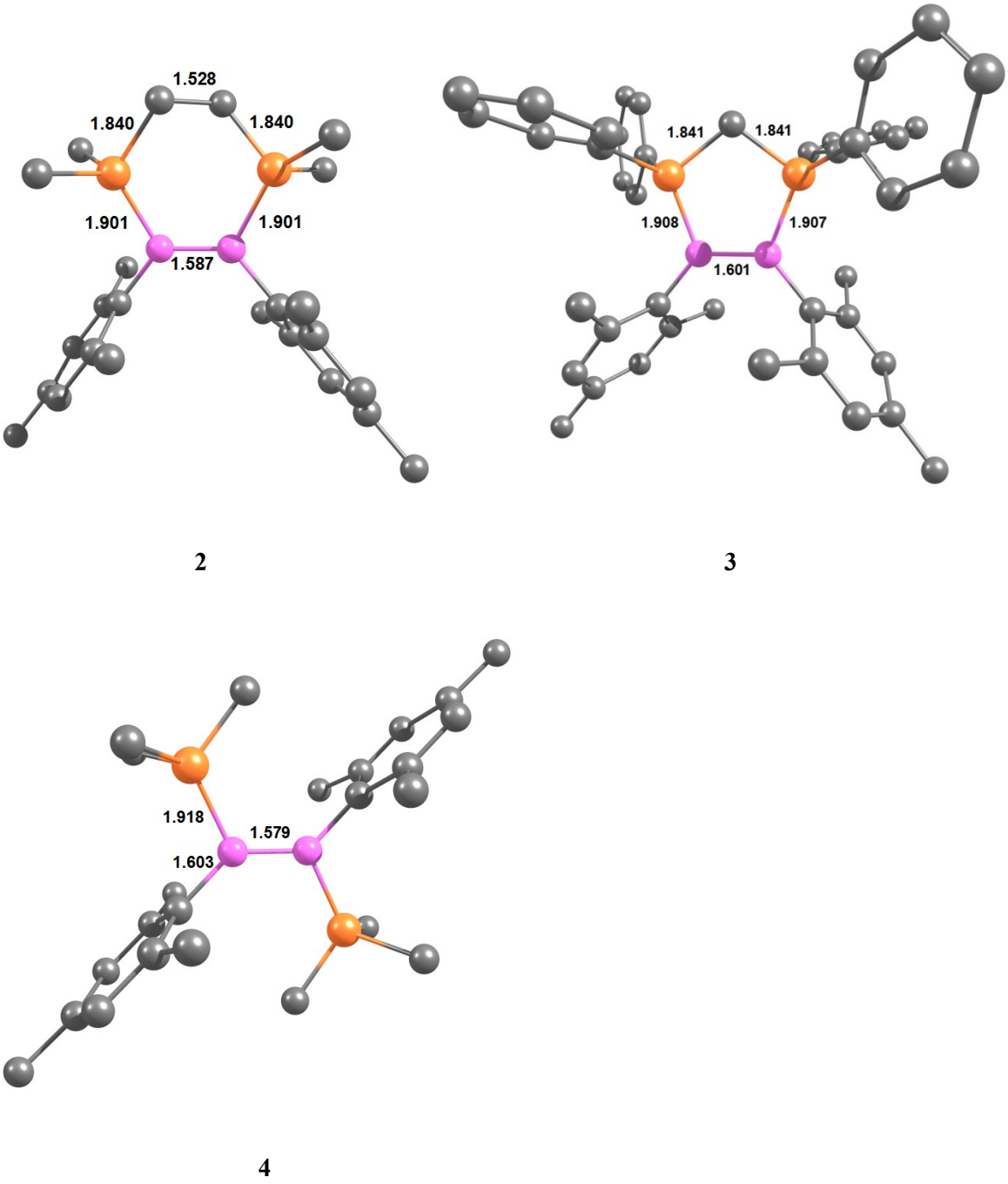


Figure S3. Cyclic voltammogram of **4** in THF with 0.1 M [nBu$_4$N][PF$_6$] as the supporting electrolyte. Formal potentials: $E_{1/2}$ = −1.06 V, E_{pa} = +0.11 V.

Computational Details

Geometry optimization of the structures was carried out at the *meta*-hybrid functional M05-2X[5] in conjunction with the def2-SVP[6] basis set including solvent effects by using the PCM[7] approach (THF for **2** and **3**, diethylether for **4**. The structures were characterized as minima by frequency calculation. All calculations were done using Gaussian 09, Revision D.01.[8]



2 **3**

4

Figure S4. Optimized geometry of the complexes at the PCM-M05-2X/def2-SVP level.

Table S1. Cartesian coordinates (Å) and energy (a.u) of **2-4** calculated at PCM-M05-2X/def2-SVP.

***cis,cyclo*-[B_2Mes_2(dmpe)]**

E = -1668.707577

P	-1.67019600	2.28494000	0.37557600
C	-0.53251100	3.72092800	0.54762800
H	-1.13543500	4.64018400	0.50862900
H	-0.07375300	3.66456600	1.54573200
B	-0.79329400	0.63616400	0.02181100
P	1.67020000	2.28493900	-0.37557400
C	0.53251700	3.72093000	-0.54762200
H	1.13544300	4.64018400	-0.50861800
H	0.07375900	3.66457200	-1.54572700
B	0.79329500	0.63616400	-0.02181100
C	-2.60130600	2.28174600	1.95745600
H	-1.89432100	2.14054200	2.78563700
H	-3.30804600	1.43960700	1.94348700
H	-3.15099200	3.22482900	2.09011400
C	-2.95701000	2.87026700	-0.80545400
H	-3.41215200	3.80443500	-0.44639400
H	-3.73124900	2.09505800	-0.88716600
H	-2.51026300	3.02804000	-1.79645200
C	2.60130600	2.28174400	-1.95745700
H	3.15099600	3.22482600	-2.09011500
H	1.89431800	2.14054500	-2.78563700
H	3.30804300	1.43960300	-1.94349200
C	2.95701800	2.87026200	0.80545300
H	3.41216500	3.80442500	0.44639000
H	3.73125200	2.09504800	0.88716900
H	2.51027100	3.02804100	1.79645100
C	-1.81482300	-0.60123300	0.02297300
C	-1.94201100	-1.44265500	1.16019900
C	-2.84021800	-2.51102900	1.16095100
H	-2.91446200	-3.14157500	2.05038700
C	-3.64266700	-2.80388900	0.05121900
C	-3.50533400	-1.99430600	-1.07189100
H	-4.10236900	-2.21021500	-1.96179400
C	-2.61331200	-0.91024300	-1.10019400

C	-1.08558000	-1.21460900	2.38318100
H	-0.02061800	-1.28922500	2.12172900
H	-1.31584200	-1.95325400	3.16478800
H	-1.23643000	-0.20694600	2.79724900
C	-4.61181200	-3.96071700	0.08252500
H	-4.10344400	-4.89565600	0.36188600
H	-5.08343200	-4.10655100	-0.89888400
H	-5.40998300	-3.78917800	0.82130800
C	-2.52406900	-0.12178500	-2.38997400
H	-1.69814900	0.60085000	-2.34909700
H	-3.45893300	0.42324200	-2.59468900
H	-2.35247200	-0.79835600	-3.24157800
C	1.81482200	-0.60123600	-0.02297300
C	2.61331200	-0.91024600	1.10019300
C	3.50533500	-1.99430800	1.07188900
H	4.10237300	-2.21021500	1.96179000
C	3.64266700	-2.80389100	-0.05122100
C	2.84022000	-2.51102800	-1.16095400
H	2.91446800	-3.14157100	-2.05039300
C	1.94201300	-1.44265500	-1.16020100
C	2.52407000	-0.12178800	2.38997300
H	3.45893700	0.42323300	2.59469000
H	2.35246800	-0.79835800	3.24157600
H	1.69815300	0.60085100	2.34909600
C	4.61178700	-3.96073900	-0.08251900
H	5.08363900	-4.10637800	0.89880600
H	5.40977900	-3.78937100	-0.82153300
H	4.10333600	-4.89573000	-0.36156000
C	1.08558400	-1.21460600	-2.38318500
H	1.23642900	-0.20693800	-2.79724400
H	0.02062200	-1.28923000	-2.12173600
H	1.31585300	-1.95324400	-3.16479600

***cis,cyclo*-[B_2Mes_2(dppm)]**

E=-2395.7304027

B	0.79211400	0.62027400	0.01820700

B	-0.80882200	0.61891600	0.01524200
P	-1.47877400	-1.16681700	0.03594800
C	-0.00816300	-2.26732100	0.16175400
H	0.00732500	-2.98759200	-0.66620100
H	-0.02826900	-2.82732800	1.10531600
P	1.46437100	-1.16391900	0.10051300
C	1.80572800	1.85085000	-0.08463300
C	2.65527000	2.23979400	0.97656000
C	3.52485100	3.32989200	0.83556200
H	4.15885300	3.61115800	1.68000000
C	3.59856800	4.06613500	-0.34484500
C	2.74159700	3.70025200	-1.38674000
H	2.75827600	4.27690300	-2.31450500
C	1.85145200	2.62870900	-1.27173900
C	2.64736700	1.52078700	2.30615300
H	2.83999400	2.22763400	3.12688000
H	3.42582500	0.74304200	2.34928500
H	1.68115300	1.02991300	2.48186700
C	4.57076200	5.20959500	-0.50130200
H	4.12993700	6.02731900	-1.08900000
H	5.48300600	4.88170800	-1.02478900
H	4.87314400	5.60781200	0.47708900
C	0.92071200	2.35026000	-2.42913800
H	1.19874000	2.95462200	-3.30458100
H	-0.11467200	2.59519300	-2.15038300
H	0.92343700	1.28792400	-2.71198200
C	-1.81985800	1.85491800	0.02091400
C	-1.87735200	2.70714000	1.15591100
C	-2.75802400	3.79086700	1.18775500
H	-2.78647600	4.42392000	2.07783600
C	-3.59489000	4.09654400	0.10942200
C	-3.51853900	3.27866900	-1.01484900
H	-4.14586900	3.50309600	-1.88084100
C	-2.65622000	2.17402300	-1.07189200
C	-0.97750300	2.48136400	2.34842400
H	-1.25695100	3.14765200	3.17724400
H	0.06984000	2.67970200	2.07803800

H	-1.01739200	1.43911300	2.69730400
C	-4.52543800	5.28338200	0.16493300
H	-5.15468200	5.33343600	-0.73402400
H	-3.96023600	6.22514300	0.23822100
H	-5.18495500	5.22855000	1.04399900
C	-2.64920200	1.35665400	-2.34325400
H	-2.85479100	1.99632600	-3.21427900
H	-3.41982800	0.57022300	-2.32068800
H	-1.67997700	0.86178900	-2.48838100
C	-2.59146300	-1.65133900	1.40684100
C	-2.81523400	-2.99968500	1.71708200
H	-2.33772800	-3.78693000	1.13083600
C	-3.66000200	-3.34346700	2.77040100
H	-3.82708700	-4.39293700	3.01162200
C	-4.29421900	-2.34314300	3.51165400
H	-4.95673300	-2.61309800	4.33383800
C	-4.08210500	-1.00089200	3.19917600
H	-4.57926500	-0.21968400	3.77343400
C	-3.22815200	-0.65272400	2.15049400
H	-3.05935700	0.39625100	1.90462400
C	-2.35851800	-1.81092900	-1.44791800
C	-1.62796300	-1.91968700	-2.63787100
H	-0.56508800	-1.66255600	-2.65161100
C	-2.25595800	-2.32496000	-3.81237900
H	-1.68054300	-2.40980000	-4.73387000
C	-3.62404200	-2.61078400	-3.80925600
H	-4.11823100	-2.92058900	-4.72985300
C	-4.35576700	-2.49771200	-2.62811800
H	-5.42300600	-2.71823100	-2.62249800
C	-3.72506200	-2.10108400	-1.44624300
H	-4.30508200	-2.01237200	-0.52789400
C	2.46143500	-1.68632000	1.55735500
C	3.83492200	-1.92894300	1.46981300
H	4.34036700	-1.88573700	0.50529700
C	4.56812100	-2.21964200	2.62273000
H	5.63971300	-2.40355600	2.54873800
C	3.93245600	-2.27492500	3.86217400

H	4.50617000	-2.50299200	4.76024000
C	2.55853200	-2.03581100	3.95227600
H	2.05797000	-2.07433500	4.91944300
C	1.82838300	-1.73512800	2.80569200
H	0.76186300	-1.51081900	2.88822700
C	2.47847000	-1.75780700	-1.30524800
C	3.04995700	-0.82181200	-2.17284000
H	2.89201000	0.24304900	-1.99954200
C	3.82751800	-1.25145100	-3.25039100
H	4.27413500	-0.51813400	-3.92120700
C	4.02801600	-2.61408700	-3.46778500
H	4.62978300	-2.94864400	-4.31260400
C	3.46096800	-3.55220200	-2.60133800
H	3.62063400	-4.61731300	-2.76729600
C	2.69381600	-3.12614700	-1.51906800
H	2.27228000	-3.86475600	-0.83487900

***trans*-[$B_2Mes_2(PMe_3)_2$]**

E=-1669.8978578

B	0.63186000	-0.47300500	0.00648200
P	0.26597500	-2.35546800	0.00083900
C	-1.48356900	-2.88813800	0.03825200
H	-1.51972300	-3.98720600	0.04113200
H	-2.01268400	-2.49622700	-0.83932800
H	-1.97294900	-2.49365900	0.93742800
C	1.01384700	-3.29841900	1.39541900
H	0.88803000	-4.37962500	1.23879800
H	0.52649700	-3.00534600	2.33525200
H	2.08467300	-3.05667000	1.45432700
C	0.94603800	-3.27874400	-1.44121500
H	0.80591100	-4.36099200	-1.30486700
H	2.01840100	-3.05539300	-1.53364300
H	0.43074600	-2.95495300	-2.35582000
C	2.21330400	-0.21302400	0.00324300
C	2.94132300	-0.09112200	1.21072000
C	4.32573100	0.11660800	1.19347900

H	4.86131900	0.21203700	2.14106000
C	5.03945000	0.21751300	-0.00247100
C	4.31923100	0.12748900	-1.19541500
H	4.84972700	0.23142400	-2.14495800
C	2.93472400	-0.07986400	-1.20701100
C	2.22919400	-0.09967300	2.54422900
H	2.94845300	-0.06835100	3.37548800
H	1.58851700	-0.98278900	2.66165500
H	1.55641000	0.76899000	2.62394300
C	6.53764100	0.40041400	-0.00567200
H	6.86718600	0.95357900	-0.89637200
H	7.05387500	-0.57292300	-0.01018100
H	6.87171400	0.94770000	0.88697600
C	2.21569000	-0.07541800	-2.53689100
H	2.93061200	-0.02754200	-3.37109200
H	1.53671500	0.78956300	-2.60089000
H	1.58113800	-0.96166500	-2.66396400
B	-0.63186000	0.47300700	0.00648300
P	-0.26597700	2.35546900	0.00084200
C	1.48356900	2.88813600	0.03825800
H	1.51972600	3.98720400	0.04114700
H	1.97294900	2.49364800	0.93742900
H	2.01268100	2.49623000	-0.83932700
C	-0.94603400	3.27874700	-1.44121300
H	-0.80591000	4.36099500	-1.30486200
H	-0.43073700	2.95495900	-2.35581500
H	-2.01839600	3.05539500	-1.53364700
C	-1.01385100	3.29841800	1.39542200
H	-0.88803200	4.37962400	1.23880300
H	-2.08467800	3.05666900	1.45432500
H	-0.52650400	3.00534200	2.33525500
C	-2.21330300	0.21302200	0.00324400
C	-2.93472300	0.07986500	-1.20701100
C	-4.31923100	-0.12748600	-1.19541500
H	-4.84972700	-0.23142000	-2.14495800
C	-5.03945000	-0.21751100	-0.00247100
C	-4.32573100	-0.11660900	1.19347900

H	-4.86131800	-0.21203900	2.14106000
C	-2.94132300	0.09111900	1.21072000
C	-2.21568900	0.07542000	-2.53689100
H	-2.93061100	0.02752600	-3.37109100
H	-1.58115400	0.96167900	-2.66397200
H	-1.53669900	-0.78954800	-2.60088400
C	-6.53764100	-0.40041000	-0.00567500
H	-6.87172300	-0.94764400	0.88700200
H	-7.05387400	0.57292700	-0.01024600
H	-6.86717900	-0.95362600	-0.89634600
C	-2.22919500	0.09966600	2.54423000
H	-2.94845500	0.06837500	3.37548900
H	-1.55643800	-0.76901700	2.62395600
H	-1.58849000	0.98276300	2.66164400

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