Supplementary Material (ESI) for Chemical Communications

Supporting Information for:

Tuning the $[L_2Rh\cdots H_3B{\cdot}NR_3]^+$ Interaction using Phosphine Bite Angle. Demonstration by the Catalytic Formation of Polyaminoboranes

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Experimental

All manipulations, unless otherwise stated, were performed under an atmosphere of argon, using standard Schlenk and glove-box techniques. Glassware was oven dried at 130°C overnight and flamed under vacuum prior to use. MeCN, THF, hexane and pentane were dried using a Grubbs type solvent purification system (MBraun SPS-800) and degassed by successive freeze-pump-thaw cycles.[1] CD_2Cl_2, C_6H_5F and 1,2-$C_6H_4F_2$ were distilled under vacuum from CaH_2 and stored over 3 Å molecular sieves, 1,2-$C_6H_4F_2$ was stirred over alumina for two hours prior to drying. $H_3B{\cdot}NMe_3$ and $H_3B{\cdot}NMe_2H$ were purchased from Aldrich and sublimed before use (5×10^{-2} Torr, 298 K). $H_3B{\cdot}NMeH_2$ [2] and $[Rh(NBD)(Ph_2P(CH_2)_nPPh_2)][BAr^F_4]$ (n=2-5)[3] were prepared as previously described. NMR spectra were recorded on Varian Unity Plus 500 MHz or Varian Venus 300 MHz spectrometers at room temperature unless otherwise stated. In C_6H_5F, ^1H NMR spectra were referenced to the centre of the downfield solvent multiplet ($\delta = 7.11$). ^{31}P spectra were referenced against 85% H_3PO_4 (external). ^{11}B NMR spectra were referenced against $BF_3{\cdot}OEt_2$ (external). Chemical shifts are quoted in ppm and coupling constants in Hz. ESI-MS were recorded on a Bruker MicrOTOF instrument. Microanalyses were performed by Elemental Microanalysis Ltd and London Metropolitan University. GPC data were obtained in THF solutions at 0.5 mg/ml, containing 0.1 % $[nBu_4]NBr$ and use polystyrene standards for column calibration. Both the instrumentation and method are described in detail elsewhere.[4]

Synthesis of new complexes

Preparation of $[Rh(Ph_2P(CH_2)_2PPh_2)(C_6H_5F)][BAr^F_4]$ (1a)

A suspension of $[Rh(Ph_2P(CH_2)_2PPh_2)Cl)]_2$ (80.0 mg, 0.0745 mmol) and $Na[BAr^F_4]$ (132.1 mg, 0.149 mmol) in C_6H_5F (10 mL) was stirred at room temperature for 2 hours. Pentane (8 mL) was added to the flask to encourage the full precipitation of NaCl (which is partially soluble in C_6H_5F) and then filtered. The product was isolated by first concentrating the filtrate (~ 5 mL) and then adding the solution dropwise to pentane (30 mL) with rigorous stirring causing **1a** to precipitate as a red solid. Yield 80 mg, 37 %.

^1H NMR (500 MHz, C_6H_5F): δ 8.37 (s, 8H, BAr^F_4), 7.63 (s, 4H, BAr^F_4), 1.83 (apparent d, *J* = 20, 4H, CH_2). The co-ordinated C_6H_5F signals were not unambiguously located and the phenyl signals not assigned as they were obscured by C_6H_5F solvent δ 7.31 – 6.70.

^{31}P {^1H} NMR (121 MHz, C_6H_5F): δ 73.48 [d, *J*(RhP) 203].

ESI-MS (C_6H_5F, 60°C, 4.5kV) positive ion: m/z, 597.1083 $[M]^+$, (calc. 597.0778).

Anal. Calcd for $C_{64}H_{41}B_1F_{25}P_2Rh_1$ (1460.6344 $gmol^{-1}$): C, 52.63; H, 2.83. Found: C, 52.17; H, 3.25.

Preparation of [Rh($Ph_2P(CH_2)_nPPh_2$)(C_6H_5F)][$BAr^F{}_4$] n = 3 (1b), 4 (1c), 5 (1d).

In a typical experiment, [Rh($Ph_2P(CH_2)_nPPh_2$)(NBD)][$BAr^F{}_4$] (100 mg) was stirred in C_6H_5F (5 mL) in a Young's flask until fully dissolved. The flask was placed under hydrogen (4 atm) and then left to stir at room temperature for 20 minutes. The solution was then concentrated *in vacuo* (~2 mL) and then added dropwise to pentane (30 mL) with rigorous stirring resulting in the precipitation of **1b-d** as a red/orange solid. Diffusion of pentane into a solution of the isolated solid in C_6H_5F (3 mL) gave **1b** as red crystals. Yield: 74 mg, 74 % **(1b)**, 72 mg, 72 % **(1c)**, 78 mg, 78 % **(1d)**.

1b

^{1}H NMR (500 MHz, C_6H_5F): δ 8.37 (s, 8H, $BAr^F{}_4$), 7.65 (s, 4H, $BAr^F{}_4$), 5.66 (m, 4H, *o&m*-C_6H_5F), 5.08 (m, 1H, *p*-C_6H_5F), 2.06 (m, 4H, CH_2), 1.57 (m, 2H, CH_2). The phenyl signals were not assigned as they were obscured by C_6H_5F solvent δ 7.31 – 6.70.

^{31}P {^{1}H} NMR (202 MHz, C_6H_5F): δ 25.50 [d, *J*(RhP) 196].

ESI-MS (C_6H_5F, 60°C, 4.5kV) positive ion: m/z, 611.1351 $[M]^+$ (calc. 611.0935).

Anal. Calcd for $C_{65}H_{43}B_1F_{25}P_2Rh_1$ (1474.6610 $gmol^{-1}$): C, 52.94; H, 2.94. Found: C, 52.85; H, 2.47.

1c

^{1}H NMR (500 MHz, C_6H_5F): δ 8.37 (s, 8H, $BAr^F{}_4$), 7.65 (s, 4H, $BAr^F{}_4$), 5.50 (m, 2H, *o/m*-C_6H_5F), 5.44 (m, 2H, *o/m*-C_6H_5F), 5.10 (m, 1H, *p*-C_6H_5F), 1.99 (m, 4H, CH_2), 1.24 (m, 4H, CH_2). The phenyl signals were not assigned as they were obscured by C_6H_5F solvent δ 7.31 – 6.70.

^{31}P {^{1}H} NMR (121 MHz, C_6H_5F): δ 38.39 [d, *J*(RhP) 199].

ESI-MS (C_6H_5F, 60°C, 4.5kV) positive ion: m/z, 625.1256 $[M]^+$ (calc. 625.1091).

Anal. Calcd for $C_{66}H_{45}B_1F_{25}P_2Rh_1$ (1488.6876 $gmol^{-1}$): C, 53.25; H, 3.05. Found: C, 53.28; H, 3.38.

1d

^{1}H NMR (500 MHz, C_6H_5F): δ 8.37 (s, 8H, $BAr^F{}_4$), 7.65 (s, 4H, $BAr^F{}_4$), 5.54 (m, 2H, *o/m*-C_6H_5F), 5.49 (m, 2H, *o/m*-C_6H_5F,) 5.26 (m, 1H, *p*-C_6H_5F), 2.11 (m, 2H, CH_2), 1.95 (m, 4H, CH_2), 1.59 (m, 4H, CH_2). The phenyl signals were not assigned as they were obscured by C_6H_5F solvent δ 7.31 – 6.70.

^{31}P {^{1}H} NMR (202 MHz, C_6H_5F): δ 27.01 [d, *J*(RhP) 207].

ESI-MS (C_6H_5F, 60°C, 4.5kV) positive ion: m/z, 639.1730 $[M]^+$ (calc. 639.1248).

Anal. Calcd for $C_{67}H_{47}B_1F_{25}P_2Rh_1$ (1502.7142 $gmol^{-1}$): C, 53.55; H, 3.15. Found: C, 53.56; H, 3.37.

Preparation of [Rh($Ph_2P(CH_2)_3PPh_2$)($H_3B·NMe_3$)][BAr^F_4] (2b).

$H_3B·NMe_3$ (1.2 mg, 0.016 mmol) was added to a solution of **1b** (24 mg, 0.016 mmol) in 1,2-$C_6H_4F_2$ (3 mL). Diffusion of pentane at -35°C yielded **2b** as red crystals. Yield: 14 mg, 59 %.

^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.74 (m, 8H, BAr^F_4), 7.68 – 7.60 (m, 8H, Ph), 7.49 – 7.35 (m, 12H, Ph), 2.59 (s, 9H, NMe), 2.40 (m, 4H, CH_2), 2.01 (m, 2H, CH_2), -1.30 (br, 3H, BH_3).

^{31}P {^{1}H} NMR (202 MHz, 1,2-$C_6H_4F_2$): δ 34.02 [d, *J*(RhP) 167].

^{11}B NMR (121 MHz, CD_2Cl_2): δ 16.40 (v br).

ESI-MS (1,2-$C_6H_4F_2$, 60°C, 4.5kV) positive ion: m/z, 629.1168 [M-$H_3B·NMe_3$+$C_6H_4F_2$]$^+$ (100 %, calc. 629.0840), 515.0861 [M-$H_3B·NMe_3$]$^+$ (40 %, calc. 515.0559).

Preparation of [Rh($Ph_2P(CH_2)_4PPh_2$)($H_3B·NMe_3$)][BAr^F_4] (2c).

$H_3B·NMe_3$ (1.2 mg, 0.016 mmol) was added to a solution of **1c** (24 mg, 0.016 mmol) dissolved in 1,2-$C_6H_4F_2$ (3 mL). Diffusion of pentane at -35°C yielded **2c** as purple crystals. Yield: 19 mg, 80 %.

^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.74 (m, 8H, BAr^F_4), 7.69 – 7.61 (m, 8H, Ph), 7.54 – 7.41 (m, 12H, Ph), 2.51 (s, 9H, NMe), 2.47 (m, 4H, CH_2), 1.84 (m, 4H, CH_2), -1.66 (br, 3H, BH_3).

^{31}P {^{1}H} NMR (121 MHz, 1,2-$C_6H_4F_2$): δ 47.12 [d, *J*(RhP) 170].

^{11}B NMR (121 MHz, CD_2Cl_2): δ 18.26 (br).

ESI-MS (1,2-$C_6H_4F_2$, 60°C, 4.5kV) positive ion: m/z, 643.1342 [M-$H_3B·NMe_3$+$C_6H_4F_2$]$^+$ (100 %, calc. 643.0997), 602.2105 [M]$^+$ (10 %, calc. 602.1784).

Preparation of [Rh($Ph_2P(CH_2)_5PPh_2$)($H_3B·NMe_3$)][BAr^F_4] (2d).

$H_3B·NMe_3$ (1.2 mg, 0.016 mmol) was added to a solution of **1d** (24 mg, 0.016 mmol) dissolved in 1,2-$C_6H_4F_2$ (3 mL). Diffusion of pentane at -35°C yielded **2d** as purple crystals. Yield: 21 mg, 89 %.

^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.74 (m, 8H, BAr^F_4), 7.57 (m, 8H, Ph), 7.55 – 7.30 (m, 12H, Ph), 2.55 (s, 9H, NMe), 2.66 (m, 2H, CH_2), 2.39 (m, 4H, CH_2), 1.75 (m, 4H, CH_2), -1.99 (br, 3H, BH_3).

^{31}P {^{1}H} NMR (202 MHz, 1,2-$C_6H_4F_2$): δ 34.89 [d, *J*(RhP) 176].

^{11}B NMR (121 MHz, CD_2Cl_2): 20.34 (br).

ESI-MS (1,2-$C_6H_4F_2$, 60°C, 4.5kV) positive ion: m/z, 657.0915 [M-$H_3B·NMe_3$+$C_6H_4F_2$]$^+$ (100 %, calc. 657.1153), 616.1779 [M]$^+$ (75 % calc. 616.1941).

Dehydrocoupling methodology

$H_3B{\cdot}NMe_2H$ dehydrocoupling experiments for dehydrocoupling plots

A stock solution of $H_3B{\cdot}NMe_2H$ in 1,2-$C_6H_4F_2$ (0.07 M) was added to a Schlenk flask under argon containing the catalyst (**1b-d**) which was itself attached to an external mineral oil bubbler.100 µL aliquots were taken over time; these were quenched immediately in an NMR tube by addition of MeCN (250 µL) and frozen to 77 K until analysis by ^{11}B NMR Spectroscopy. ^{11}B NMR spectra were processed using back linear prediction. Peaks which never reach > 10 % total integration value were not included in the analysis but are detailed in the footnotes of each plot.

$H_3B{\cdot}NMeH_2$ polymerisation

To a Schlenk flask charged with catalyst (**1b-d**) and $H_3B{\cdot}NMeH_2$ (100 mg, 2.2 mmol) was added 1,2-$C_6H_4F_2$ (5 mL) and the resulting solution stirred open to argon for 2 hours. The reaction was subsequently quenched by addition of hexane (30 mL). After the precipitation of the polymer (*ca.* 10 minutes), the solvent was removed by decantation and the resulting solid redissolved in THF (3 mL). This solution was filtered into a new Schlenk containing hexane (30 mL). After decanting all solvent the resulting solid was dried overnight *in vacuo*. These polymerisations were essentially quantitative by ^{11}B NMR spectroscopy, even though isolated yields are lower.

Isolated yields:
0.2 mol % **1b**: 57 mg, 60 %
0.2 mol % **1c**: 48 mg, 50 %
0.2 mol % **1d**: 14 mg, 15 %
1 mol % **1b**: 72 mg, 75 %

Selected ^{11}B NMR spectra

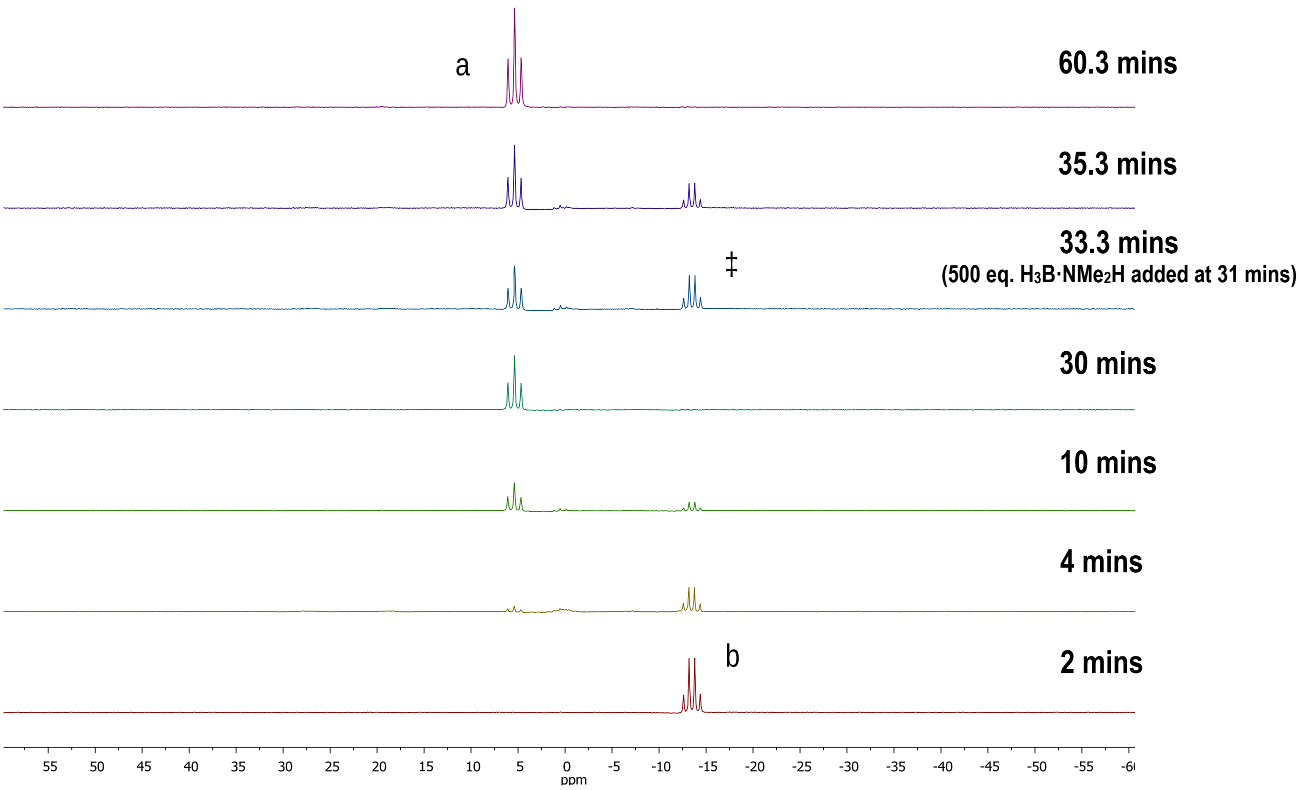

Figure S-1: Representative ^{11}B NMR spectra during catalyst recycling experiment. 500 eq. $H_3B·NMe_2H$ in 1,2-$C_6H_4F_2$ (5 mL) added to **1b** at t = 0 minutes. ‡ A further 500 eq. $H_3B·NMe_2H$ (based on amount **1b** remaining after 30 minutes of sampling) in 600 μL 1,2-$C_6H_4F_2$ added at 31 minutes. a = $[H_2BNMe_2]_2$, b = $H_3B·NMe_2H$.

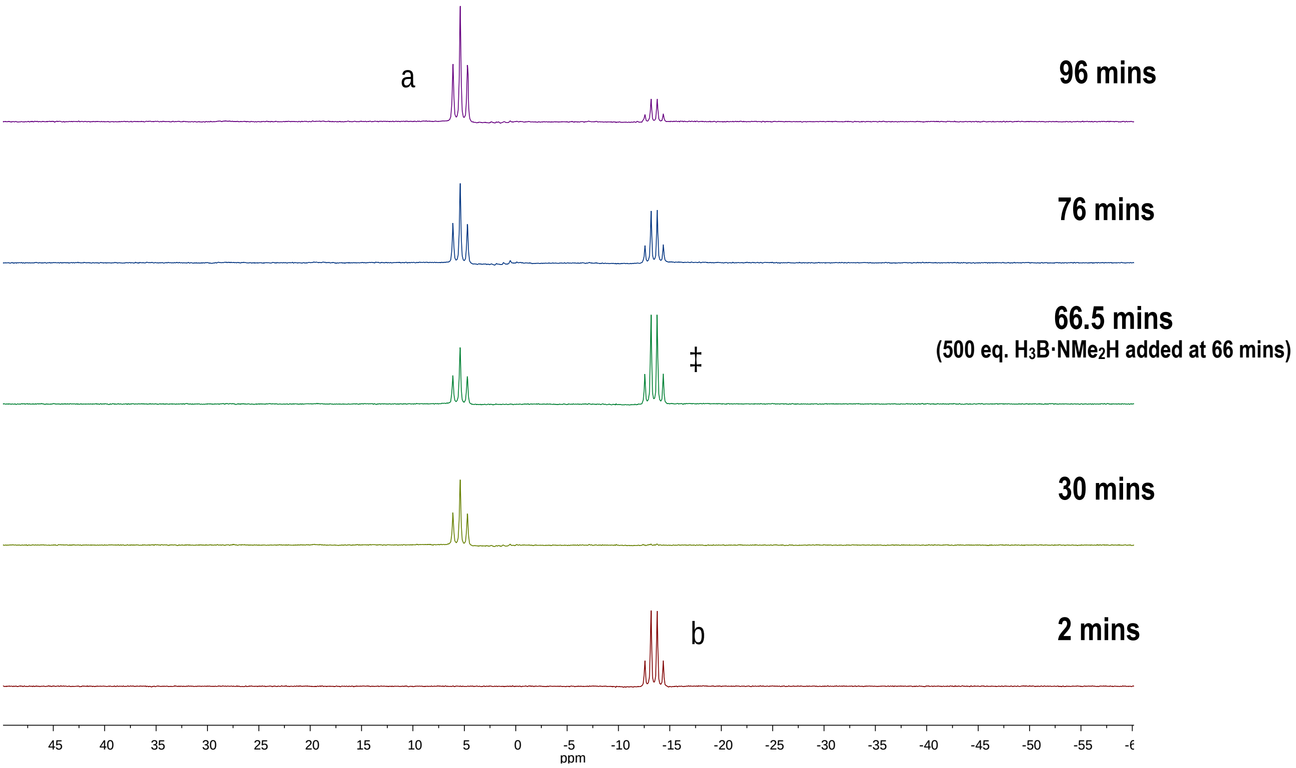

Figure S-2: Representative ^{11}B NMR spectra during catalyst filtration experiment to test for heterogeneous catalysis. Catalysis solution taken into glove box and filtered between 30 minutes and 66 minutes. ‡ 500 eq. $H_3B·NMe_2H$ (based on amount of catalyst remaining after 30 minutes of sampling) in 600 μL 1,2-$C_6H_4F_2$ added at 66 minutes. a = $[H_2BNMe_2]_2$, b = $H_3B·NMe_2H$.

$H_3B{\cdot}NMe_2H$ Dehydrocoupling plots

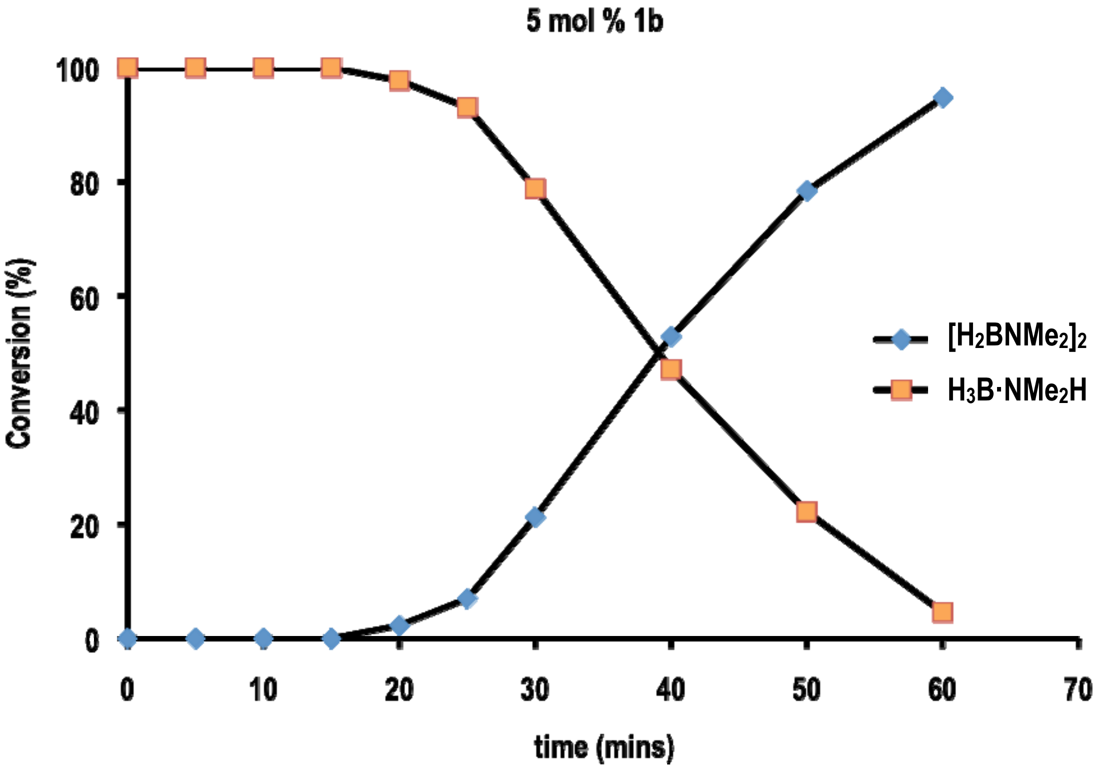

Figure S-3: Representative plot of the catalytic dehydrocoupling of $H_3B{\cdot}NMe_2H$ (5 mol % **1b**). Minor species observed by ^{11}B NMR Spectroscopy but not included in the above plot are: $[HB(NMe_2)_2]$ δ 28.6 (br d, *J* = 130) observed from 5 – 60 minutes, trace quantity remains at 60 minutes; $H_3BNMe_2BH_2NMe_2H$ δ 2.5 (t, *J* = 108) -12.9 (q, *J* = 95) observed from 40 minutes, trace quantity remains at 60 minutes.

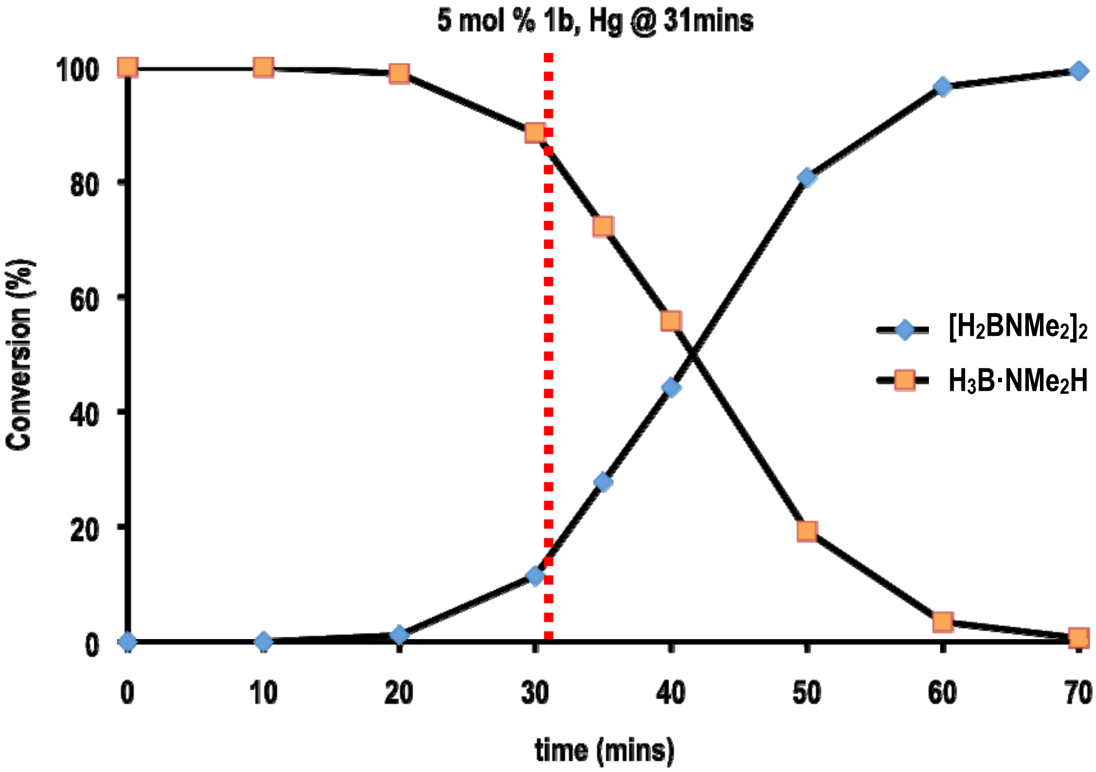

Figure S-4: Representative plot of the catalytic dehydrocoupling of $H_3B{\cdot}NMe_2H$ (5 mol % **1b**). 100 µL Hg added by syringe to the catalytic mixture at 31 minutes (dotted line). Minor species observed by ^{11}B NMR Spectroscopy but not included in the above plot are: $[HB(NMe_2)_2]$ δ 28.6 (br d, *J* = 130) observed 10 - 70 minutes, trace quantity remains at 70 minutes; $H_3BNMe_2BH_2NMe_2H$ δ 2.5 (t, *J* = 108) -12.9 (q, *J* = 95) observed from 35 minutes, trace quantity remains at 70 minutes.

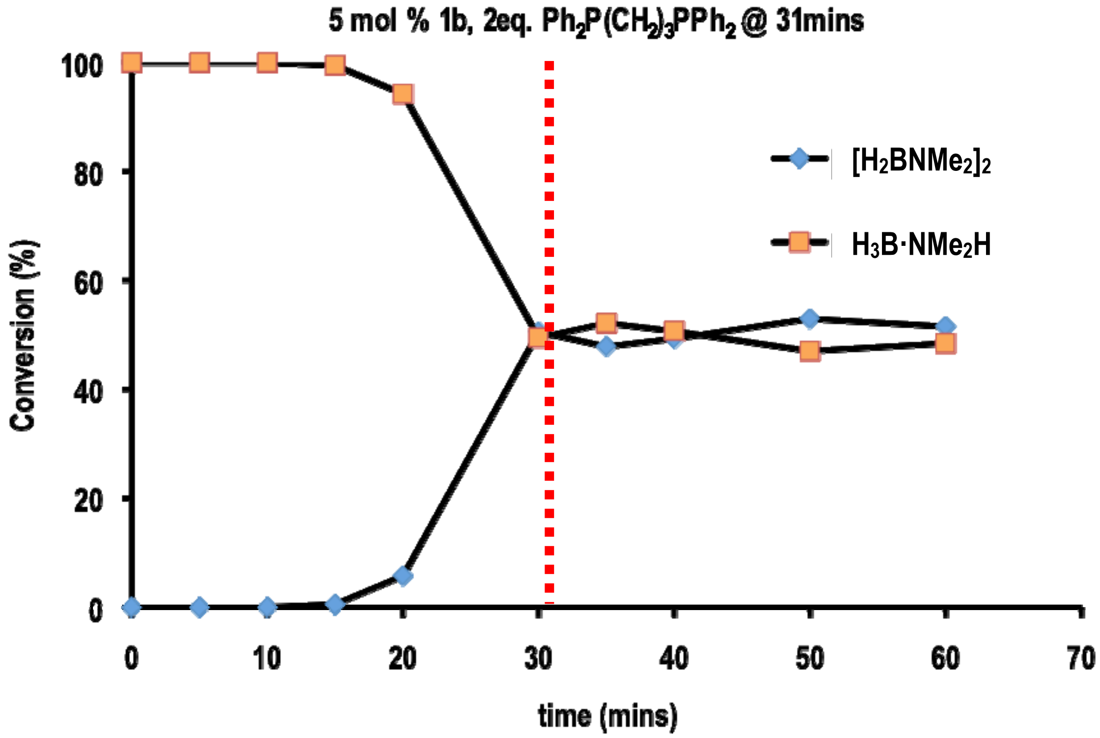

Figure S-5: Representative plot of the catalytic dehydrocoupling of $H_3B·NMe_2H$ (5 mol % **1b**). 2 eq. $Ph_2P(CH_2)_3PPh_2$ in 600 µL 1,2-$C_6H_4F_2$ added by syringe to the catalytic mixture at 31 minutes (dotted line). Minor species observed by ^{11}B NMR Spectroscopy but not included in the above plot are: $[HB(NMe_2)_2]$ δ 28.6 (br d, *J* = 130) observed 5 – 60 minutes, trace amount remains at 60 minutes; $H_3BNMe_2BH_2NMe_2H$ δ 2.5 (t, *J* = 108) -12.9 (q, *J* = 95) observed from 35 minutes, < 5% remains at 60 minutes.

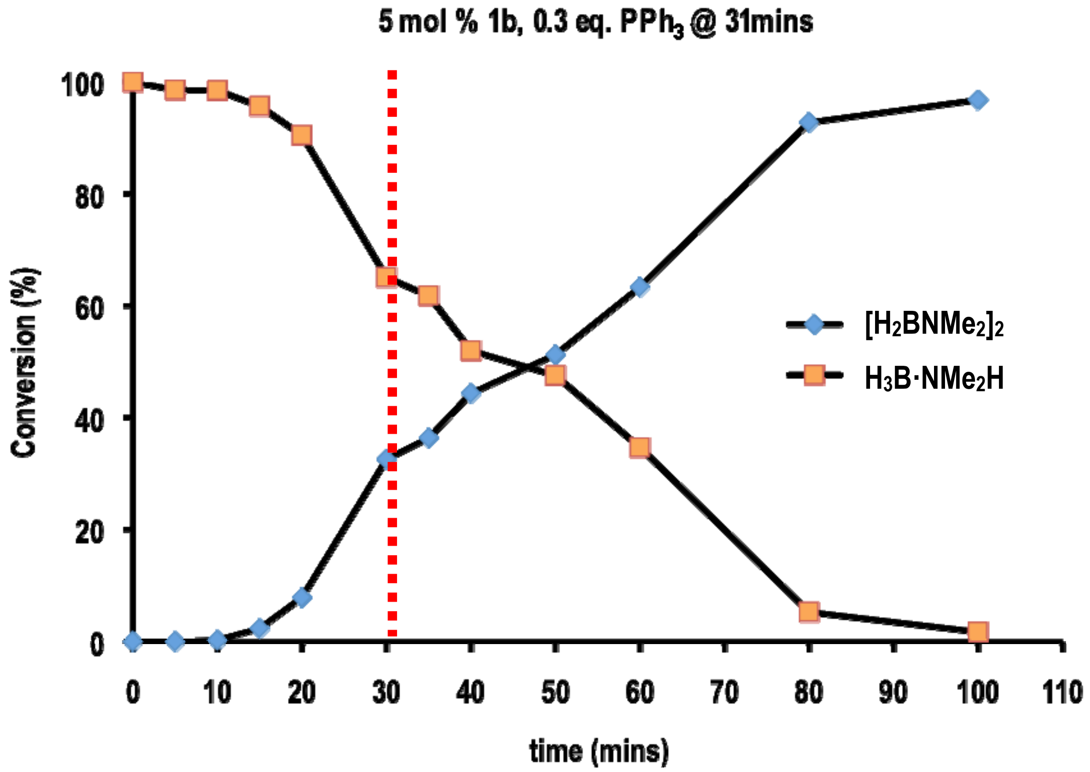

Figure S-6: Representative plot of the catalytic dehydrocoupling of $H_3B·NMe_2H$ (5 mol % **1b**). 0.3 eq. PPh_3 in 600 µL 1,2-$C_6H_4F_2$ added by syringe to the catalytic mixture at 31 minutes (dotted line). Minor species observed by ^{11}B NMR Spectroscopy but not included in the above plot are: [HB(NMe$_2$)$_2$] δ 28.6 (br d, *J* = 130) observed 5 - 80 minutes; $H_3BNMe_2BH_2NMe_2H$ δ 2.5 (t, *J* = 108) -12.9 (q, *J* = 95) observed from 35 minutes, < 5% remains at 60 minutes.

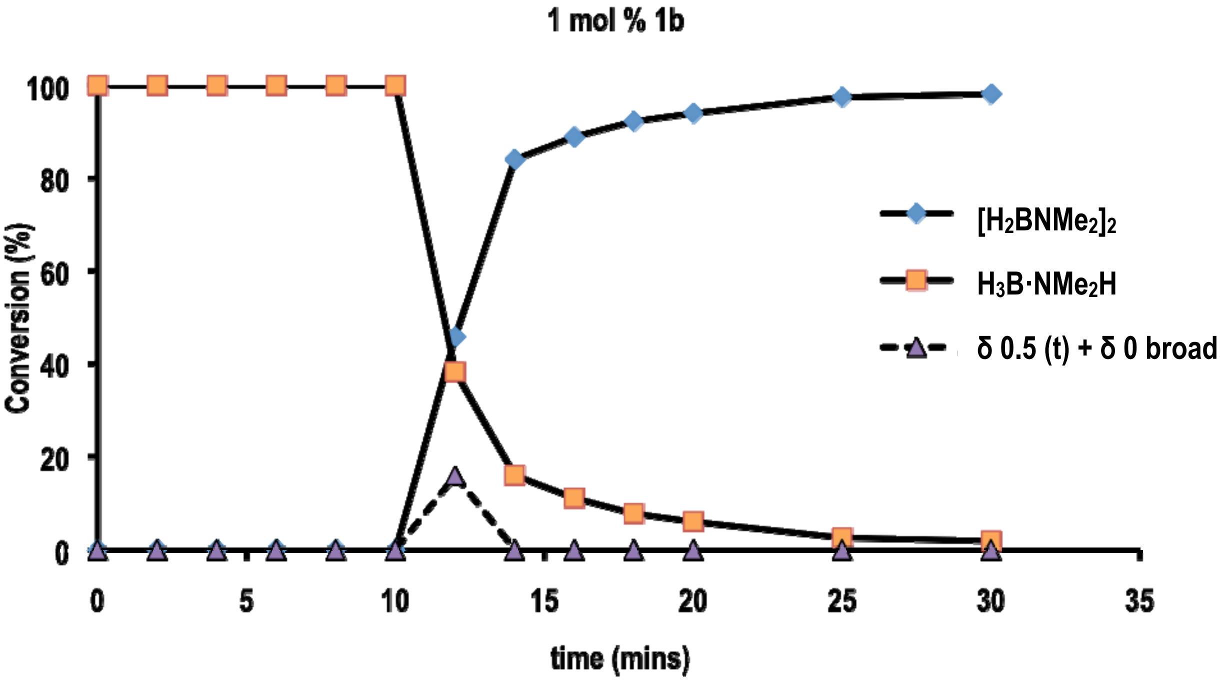

Figure S-7: Representative plot of the catalytic dehydrocoupling of $H_3B{\cdot}NMe_2H$ (1 mol % **1b**). Minor species observed by ^{11}B NMR Spectroscopy but not included in the above plot are: [HB(NMe$_2$)$_2$] δ 28.6 (br d, *J* = 130) observed from 12 – 30 minutes, trace quantity remains at 30 minutes. Dotted lines indicate the reduction of signals closer to the baseline resulting in reliable integration not being possible. Species at δ 0.5 (t, *J* = 103) and δ 0 (br) are observed from 12 - 20 minutes.

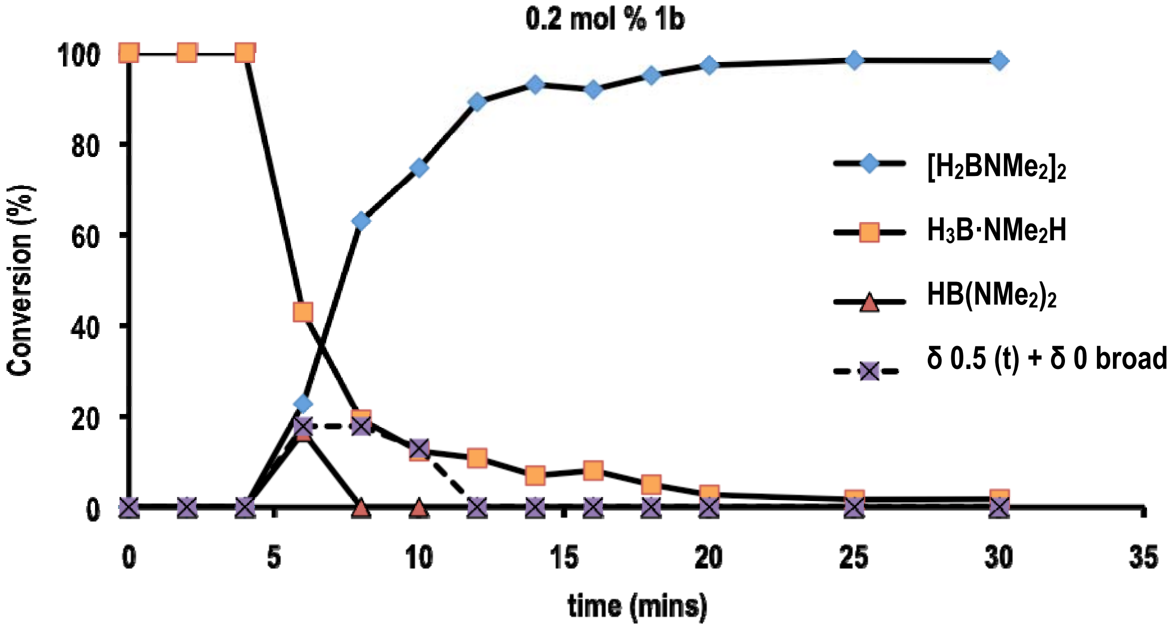

Figure S-8: Representative plot of the catalytic dehydrocoupling of $H_3B{\cdot}NMe_2H$ (0.2 mol % **1b**). Minor species observed by ^{11}B NMR Spectroscopy but not included in the above plot are: δ 19.4 (br) observed at 8 minutes and δ 3.5 (t, *J* = 117) observed from 10 -30 minutes, < 5% remains at 30 minutes. Dotted lines indicate the reduction of signals closer to the baseline resulting in reliable integration not being possible. Species at δ 0.5 (t, *J* = 103) and δ 0 (br) are observed from 2 - 25 minutes.

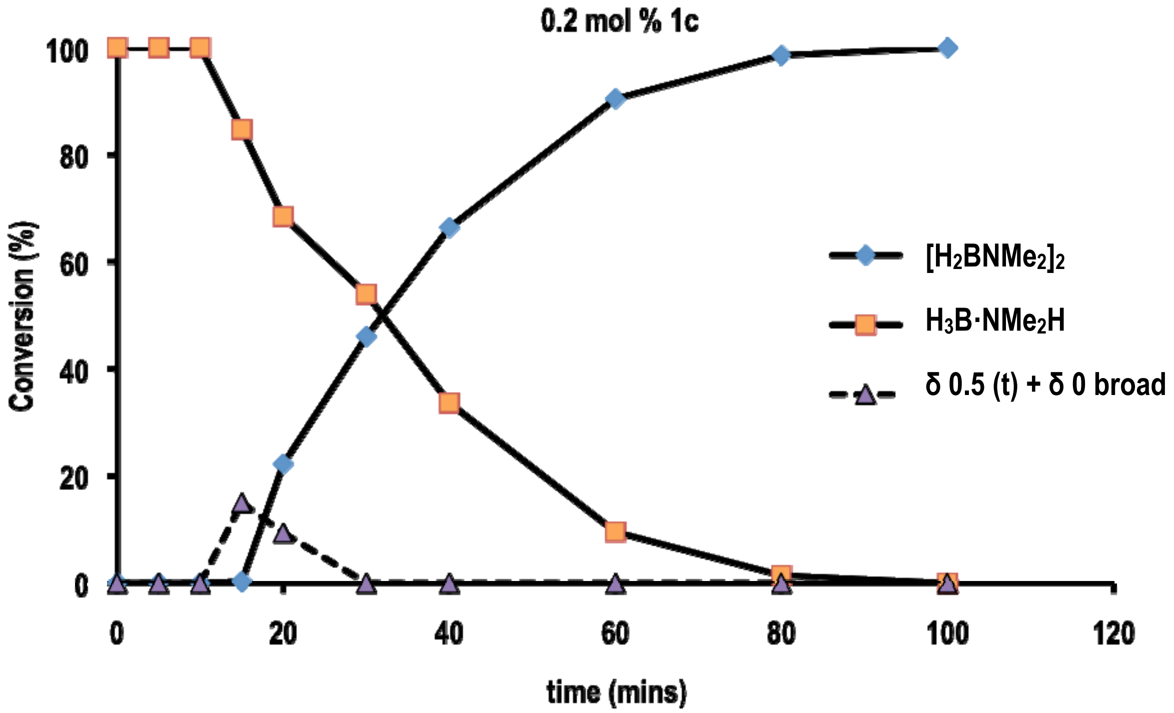

Figure S-9: Representative plot of the catalytic dehydrocoupling of $H_3B{\cdot}NMe_2H$ (0.2 mol % **1c**). Minor species observed by ^{11}B NMR Spectroscopy but not included in the above plot are: δ 19.4 (br) observed at from 5 – 100 minutes, trace quantity remains at 100 minutes; δ 3.5 (t, *J* = 117) observed from 20 -100 minutes, < 5 % remains at 100 minutes. Dotted lines indicate the reduction of signals closer to the baseline resulting in reliable integration not being possible. Species at δ 0.5 (t, *J* = 103) and δ 0 (br) are observed from 5 - 80 minutes.

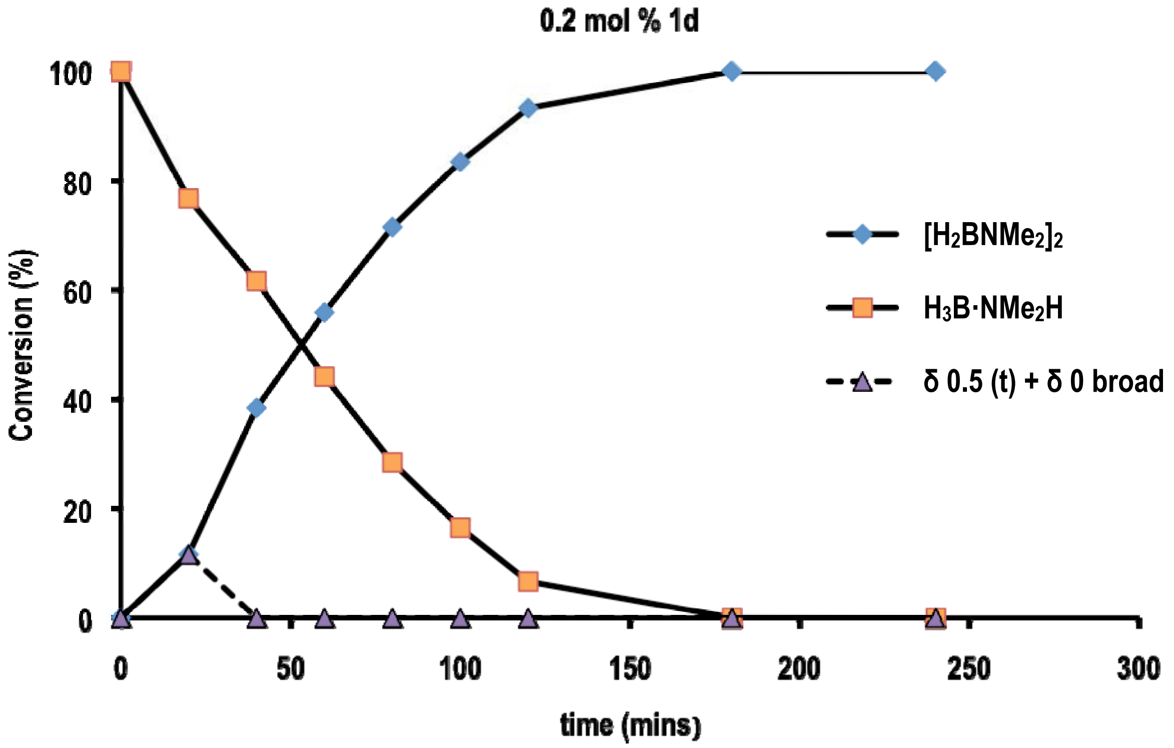

Figure S-10: Representative plot of the catalytic dehydrocoupling of $H_3B{\cdot}NMe_2H$ (0.2 mol % **1d**). Minor species observed by ^{11}B NMR Spectroscopy but not included in the above plot are: δ 19.4 (br) observed from 20 - 240 minutes, < 5 % remains at 240 minutes and δ 3.5 (t, *J* = 117) observed from 20 - 240 minutes, < 5 % remains at 240 minutes. Dotted lines indicate the reduction of signals closer to the baseline resulting in reliable integration not being possible. Species at δ 0.5 (t, *J* = 103) and δ 0 (br) are observed from 20 - 240 minutes, trace quantity remains at 240 minutes.

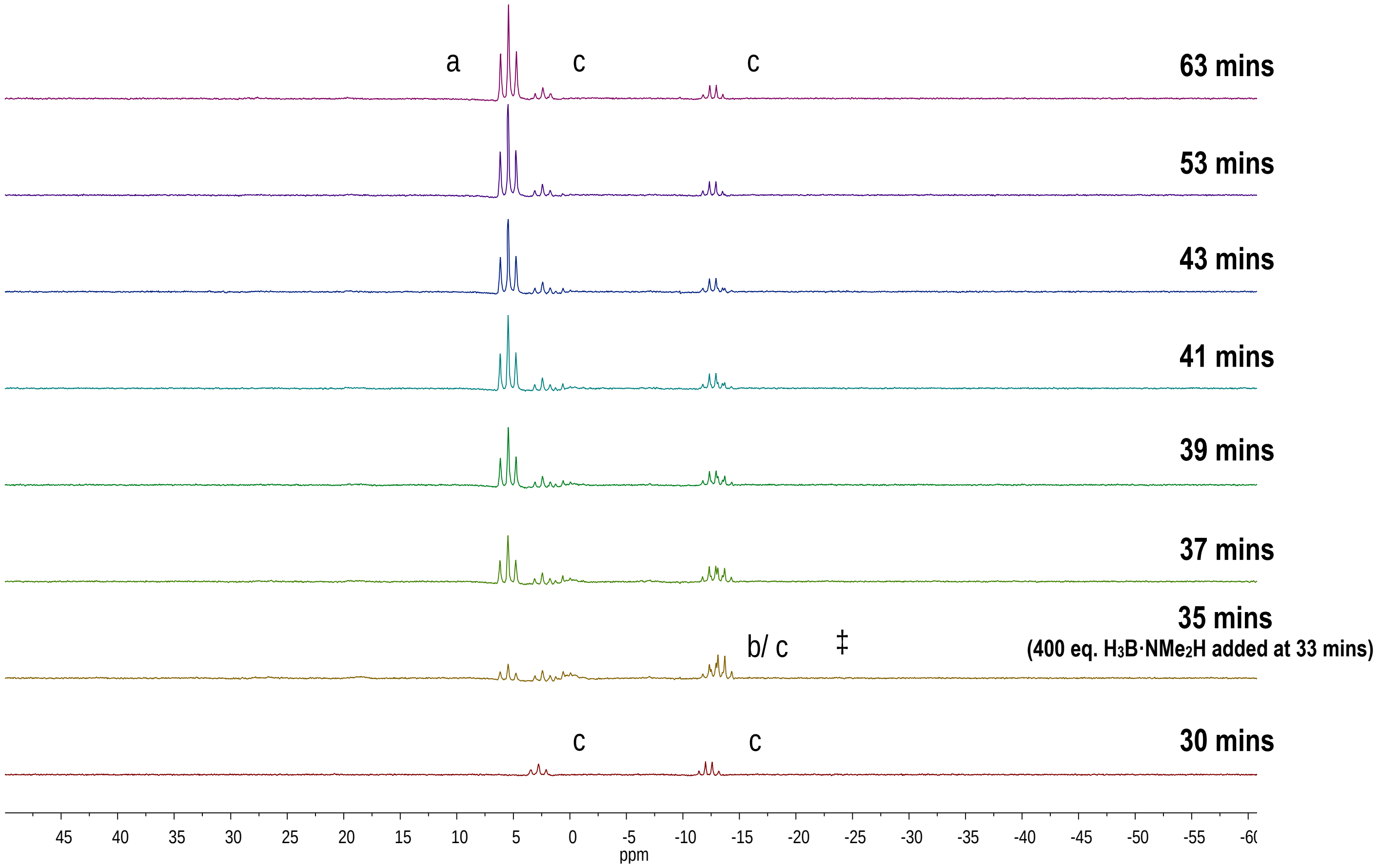

Figure S-11: Representative ^{11}B NMR spectra during $H_3B{\cdot}NMe_2BH_2{\cdot}NMe_2H$ + $H_3B{\cdot}NMe_2H$ experiment. 50 eq. $H_3B{\cdot}NMe_2BH_2{\cdot}NMe_2H$ in 1,2-$C_6H_4F_2$ (5 mL) added to **1b** at t = 0 minutes. ‡ 400 eq. $H_3B{\cdot}NMe_2H$ added to the reaction mixture at 33 minutes. a = $[H_2BNMe_2]_2$, b = $H_3B{\cdot}NMe_2H$, c = $H_3B{\cdot}NMe_2BH_2{\cdot}NMe_2H$.

Crystallography

Relevant details about the structure refinements are given in Table 1. Data were collected on an Enraf Nonius Kappa CCD diffractometer using graphite monochromated Mo Kα radiation (λ = 0.71073 Å) and a low-temperature device;[5] data were collected using COLLECT, reduction and cell refinement was performed using DENZO/SCALEPACK.[6] The structures were solved by direct methods using SIR2004 (**1b**, **2d**)[7] or by Patterson interpretation using SHELXS-86 (**2b**)[8] and refined full-matrix least squares on F^2 using SHELXL-97.[8] All non-hydrogen atoms were refined anisotropically. H1A, H1B, H1C in **2d** were located on the Fourier difference map; their isotropic displacement parameters were fixed to ride on the parent atoms. The following restraints were applied: B1-H1A = B1-H1B; H1A-H1C = H1B-H1C. H1A, H1B, H1C, H11A, H11B and H11C in **2b** were placed in calculated positions, with the B-H distance free to refine (the restraint B1-H1A = B1-H1B = B1-H1C = B11-H11A = B11-H11B = B11-H11C was applied). All other hydrogen atoms were placed in calculated positions using the riding model. Disorder of the fluorobenzene ligand in **1b** was treated by modelling the fluorine atom over three sites and restraining the 1,2- and 1,3- C-F distances. A planarity restraint was also applied about each disordered fluorine atom. Disorder of the amine-borane ligand in **2b** was treated by modelling it over two sites and restraining its geometry. Problematic solvent disorder in the structure of **2b** was treated using the SQUEEZE algorithm.[9] Further details of disorder modelling are documented in the crystallographic information files under the heading _refine_special_details. Restraints to thermal parameters were applied where necessary in order to maintain sensible values.

Table 1: Crystallographic data for **1b**, **2b** and **2d**.

	1b	**2b.$^{5}/_{4}$($C_6H_4F_2$)**	**2d.(C_5H_{12})**
CCDC number	801544	801541	801542
Formula	$C_{65}H_{43}BF_{25}P_2Rh$	$C_{69.5}H_{55}B_2F_{26.5}NP_2Rh$	$C_{69}H_{66}B_2F_{24}NP_2Rh$
M	1474.65	1594.11	1551.70
Crystal System	Triclinic	Triclinic	Monoclinic
Space group	P-1	P-1	$P2_1/c$
T [K]	150(2)	150(2)	150(2)
a [Å]	12.5134(2)	12.9731(2)	14.94180(10)
b [Å]	13.5513(2)	17.4492(2)	19.2670(2)
c [Å]	19.5061(4)	18.3033(3)	25.1468(2)
α [deg]	105.8393(7)	110.1373(6)	90
β [deg]	94.3128(7)	95.3780(7)	91.2143(3)
γ [deg]	94.6952(9)	99.4374(7)	90
V [Å^3]	3154.98(9)	3786.61(9)	7237.73(11)
Z	2	2	4
Density [gcm^{-3}]	1.552	1.398	1.424
μ (mm^{-1})	0.436	0.372	0.382
θ range [deg]	$5.14 \leq \theta \leq 26.37$	$5.50 \leq \theta \leq 26.37$	$5.11 \leq \theta \leq 26.37$
Reflns collected	19313	26357	28480
R_{int}	0.0246	0.0216	0.0224
Completeness	96.0 %	98.3 %	99.2 %
No. of data/restr/ param	12382 / 654 / 1005	15201 / 1688 / 1196	14685 / 542 / 1018
R_1 [$I > 2\sigma(I)$]	0.0458	0.0529	0.0427
wR_2 [all data]	0.1145	0.1541	0.1072
GoF	1.020	1.046	1.025
Largest diff. pk and hole [eÅ^{-3}]	0.622, -0.545	0.840, -0.604	0.663, -0.405

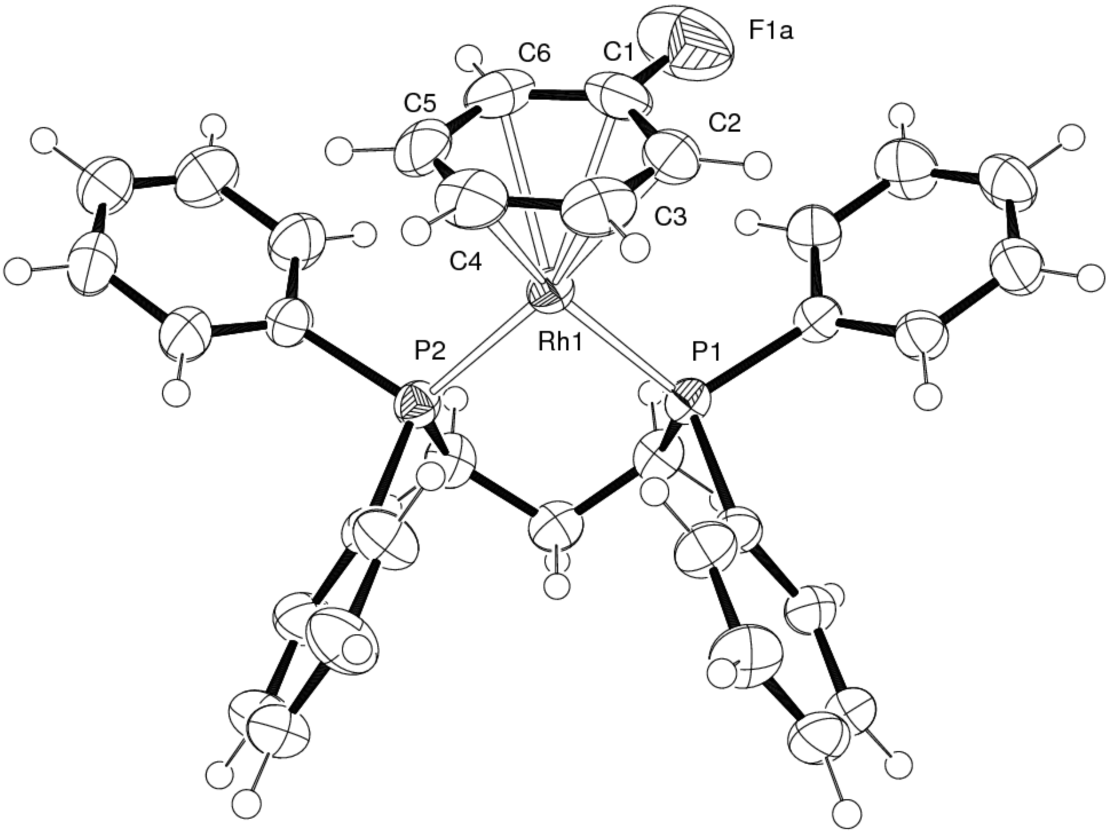

Figure S-12 Solid state structure of **1b**; ellipsoids drawn are depicted at the 50% probability level. Anion and minor disordered components omitted for clarity. Selected bond lengths (Å) and angles (°): Rh1-P1, 2.2266(9); Rh1-P2 2.2343(9); Rh1-C_{arene}, 2.292(4) – 2.377(4), P1-Rh1-P2 90.07(3).

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