Boryl Substituted Group 13 Metallylenes: Complexes with an Iron Carbonyl Fragment

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ELECTRONIC SUPPLEMENTARY INFORMATION

(11 pages)

Contents

1. Syntheses

General considerations. All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Pentane was distilled over Na/K alloy (25:75), while THF, hexane and toluene were distilled over molten potassium. ^{1}H, $^{13}C\{^{1}H\}$ and $^{11}B\{^{1}H\}$ NMR spectra were recorded on either Bruker AvanceIII 400 or Bruker DPX300 spectrometers and were referenced to the resonances of the solvent used, or external $[BF_3(OEt_2)]$. IR spectra were recorded for solid samples using an Agilent Cary 630 attenuated total reflectance (ATR) spectrometer. Mass spectra were recorded on an Agilent Techonlogies 5975D inert MSD with a solid state probe. Melting points were determined in sealed glass capillaries under dinitrogen, and are uncorrected. Microanalyses were carried out at the Science Centre, London Metropolitan University. $(THF)_2Li\{B(DAB)\}$[1] and $K_2[Fe(CO)_4]$[2] were prepared by literature procedures. All other reagents were used as received.

Synthesis of $AlBr_2(THF)\{B(DAB)\}$, 1. To a solution of $AlBr_3$ (0.15 g, 0.54 mmol) in toluene (5 mL) was added a solution of $(THF)_2Li\{B(DAB)\}$ (0.35 g, 0.65 mmol) in toluene (5 mL) at -78 °C. The resultant solution was warmed to room temperature over a period of 12 hrs whereupon volatiles were removed in *vacuo*. The colourless residue was extracted into pentane (20 mL) and the extract filtered. The filtrate was concentrated to *ca.* 5 mL and stored at -30 °C for 4 days to give colourless crystals of **1** (0.20 g, 57 %). M.p.: 116-120 °C; ^{1}H NMR (300 MHz, C_6D_6): δ = 0.84 (br. s, 4H, OCH_2CH_2), 1.22 (d, $^{3}J_{HH}$ = 6.9 Hz, 12H, $CH(CH_3)_2$), 1.42 (d, $^{3}J_{HH}$ = 6.9 Hz, 12H, $CH(CH_3)_2$), 3.39 (m, 8H, $CH(CH_3)_2$ and OCH_2), 6.36 (s, 2H, NCH), 7.14-7.23 (m, 6H, ArH); $^{13}C\{^{1}H\}$ NMR (75

MHz, C_6D_6): δ = 23.6 (CH(CH_3)$_2$), 24.5 (OCH$_2$$CH_2$), 25.9 (CH($CH_3$)$_2$), 28.6 ($CH$(CH$_3$)$_2$), 72.8 (O$CH_2$), 121.91 (N$CH$), 123.4, 127.6, 141.2, 146.5 (Ar-*C*); ^{11}B{^{1}H} NMR (C_6D_6, 128 MHz, 298 K): δ = 28.1 br.; IR *v*/cm^{-1} (ATR): 1589(w), 1256(s), 1111(w), 909(m), 803(s), 756(s); MS (EI) *m/z* (%): 387.4 [B(DAB)$^+$, 20]; anal. calc. for $C_{30}H_{44}AlBBr_2N_2O$: C 55.75%, H 6.86%, N 4.33%, found: C 55.66%, H 6.73%, N 4.4%.

Synthesis of GaCl$_2$(THF){B(DAB)}, 2. To a solution of $GaCl_3$ (0.15 g, 0.85 mmol) in toluene (10 mL) was added a solution of (THF)$_2$Li{B(DAB)} (0.48 g, 0.89 mmol) in toluene (5 mL) at -78 °C. The resultant solution was warmed to room temperature over a period of 12 hrs whereupon volatiles were removed in *vacuo*. The colourless residue was extracted into pentane (20 mL) and the extract filtered. The filtrate was concentrated to *ca.*5 mL and stored at -30 °C for 4 days to give colourless crystals of **2** (0.30 g, 59%). M.p.: 158-162 °C (dec); ^{1}H NMR (300 MHz, C_6D_6): δ = 0.94 (br. s, 4H, OCH$_2$CH_2), 1.19 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH_3)$_2$), 1.40 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH_3)$_2$), 3.29 (m, 8H, CH(CH$_3$)$_2$ and OCH_2), 6.31 (s, 2H, NCH), 7.11-7.18 (m, 6H, ArH); ^{13}C{^{1}H} NMR (75 MHz, C_6D_6): δ = 23.6 (CH(CH_3)$_2$), 24.5 (OCH$_2$$CH_2$), 25.6 (CH($CH_3$)$_2$), 28.7 ($CH$(CH$_3$)$_2$), 70.4 (O$CH_2$), 122.1 (N$CH$), 123.6, 128.1, 139.7, 146.3 (Ar-*C*); ^{11}B{^{1}H} NMR (C_6D_6, 128 MHz, 298 K): δ = 27.0 br.; IR *v*/cm^{-1} (ATR): 1615(s), 1259(m), 1157(m), 1033(s), 873(s), 747(s) 701(s); MS (EI) *m/z* (%): 387.4 [(B(DAB)$^+$, 90]; anal. calc. for $C_{30}H_{44}BCl_2GaN_2O$: C 60.04%, H 7.39%, N 4.67%, found: C 59.67%, H 7.16%, N 4.79%.

Synthesis of GaBr$_2$(THF){B(DAB)}, 3. To a solution of $GaBr_3$ (0.40 g, 1.29 mmol) in toluene (10 mL) was added a solution of (THF)$_2$Li{B(DAB)} (0.83 g, 1.55 mmol) in toluene (5 mL) at -78 °C. The resultant solution was warmed to room temperature over a period of 12 hrs whereupon volatiles were removed in *vacuo*. The colourless residue was extracted into pentane (20 mL) and filtered. The filtrate was concentrated to *ca.* 5 mL and stored at -30 °C for 4 days to give colourless crystals of **3** (0.65 g, 73%). M.p.: 167-170 °C (dec); ^{1}H NMR (300 MHz, C_6D_6): δ = 0.92 (bs, 4H, OCH$_2$CH_2), 1.19 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH_3)$_2$), 1.41 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH_3)$_2$), 3.32 (m, 8H, CH(CH$_3$)$_2$ and OCH_2), 6.31 (s, 2H, NCH), 7.12-7.22 (m, 6H, ArH); ^{13}C{^{1}H} NMR (75 MHz, C_6D_6): δ = 23.6 (CH(CH_3)$_2$), 24.6 (OCH$_2$$CH_2$), 25.8 (CH($CH_3$)$_2$), 28.7 ($CH$(CH$_3$)$_2$), 71.4 (O$CH_2$), 122.1 (N$CH$), 123.6, 128.1, 139.7, 146.3 (Ar-*C*); ^{11}B{^{1}H} NMR (C_6D_6, 128 MHz, 298 K): δ = 26.9 br.; IR *v*/cm^{-1} (ATR): 1588(w), 1256(s), 1118(s), 1111(m), 1059(m), 803(s), 756(s); MS (EI) *m/z* (%): 388.3 [HB(DAB)$^+$, 100]; anal. calc. for $C_{30}H_{44}BBr_2GaN_2O$: C 52.29%, H 6.44%, N 4.07%, found: C 52.36%, H 6.48%, N 4.17%.

Synthesis of [(DAB)B(THF)Al{Fe(CO)$_3$(μ-CO)}]$_2$, 4. A solution of **1** (0.30 g, 0.46 mmol) in THF (5 mL) was added to a suspension of $K_2[Fe(CO)_4]$ (0.12 g, 0.49 mmol) in THF (10 mL) at -78 °C. The resultant suspension was quickly warmed to room temperature and stirred over a period of 12 hrs, whereupon volatiles were removed in *vacuo*. The residue was extracted into toluene (3 mL) and the extract filtered. The filtrate was then layered with hexane in a Schlenk layering tube and the mixture stored at room temperature for 2 days to give colourless crystals of **4** (54 mg, 18%); M.p.: 230-234 °C (dec); ^{1}H NMR (300 MHz, C_6D_6): δ = 1.19 (m, 36H, CH(C*H*$_3$)$_2$), 1.42 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(C*H*$_3$)$_2$), 1.55 (br. s, 8H, OCH$_2$C*H*$_2$), 3.30 (sept., $^3J_{HH}$ = 6.9 Hz, 4H, C*H*(CH$_3$)$_2$), 3.39 (sept., $^3J_{HH}$ = 6.9 Hz, 4H, C*H*(CH$_3$)$_2$), 4.05 (m, 8H, OC*H*$_2$), 6.29 (s, 2H, NC*H*), 6.99-7.25 (m, 12H, Ar*H*); ^{13}C{^{1}H} NMR (75 MHz, C_6D_6): δ = 21.3, 22.9, 23.2, 26.3 (CH(*C*H$_3$)$_2$), 25.2 (OCH$_2$*C*H$_2$), 26.9, 28.6 (*C*H(CH$_3$)$_2$), 74.5 (O*C*H$_2$), 122.3 (N*C*H), 123.2, 123.9, 127.9, 128.5, 129.2, 141.2, 145.6, 145.8 (Ar-*C*); 215.8 (*C*O); ^{11}B{^{1}H} NMR (C_6D_6, 128 MHz, 298 K), δ = 30.5 br.; IR *ν*/cm^{-1} (ATR): 2005(CO, s), 1937(CO, s), 1902(CO, s), 1653(CO, vs), 1259(s), 1081(s), 800(s), 756(s); MS (EI) *m/z* (%): 387.4 [B(DAB)$^+$, 100]; N.B. A reproducible microanalysis could not be obtained for this compound due to difficulty in separating it from trace amounts of HB(DAB), despite repeated recrystallisations. The compound was, however, shown to have a purity of > 95% by ^{1}H NMR spectroscopy.

Synthesis of [(DAB)BGa{μ-Fe(CO)$_4$}]$_2$, 5. A solution of **2** (0.50 g, 0.83 mmol) in THF (5 mL) was added to a suspension of $K_2[Fe(CO)_4]$ (0.23 g, 0.91 mmol) in THF (10 mL) at -78 °C. The resultant suspension was quickly warmed to room temperature and stirred over a period of 12 hrs, whereupon volatiles were removed in *vacuo*. The residue was extracted into toluene (3 mL) and the extract filtered. The filtrate was then layered with hexane in a Schlenk layering tube. This was then stored at room temperature for 2 days to give colourless crystals of **5** (75 mg, 15.0%). M.p.: 253-257 °C (dec). ^{1}H NMR (300 MHz, C_6D_6): δ = 1.16 (d, $^3J_{HH}$ = 6.9 Hz, 24H, CH(C*H*$_3$)$_2$), 1.35 (d, $^3J_{HH}$ = 6.9 Hz, 24H, CH(C*H*$_3$)$_2$), 3.66 (m, $^3J_{HH}$ = 6.9 Hz, 8H, C*H*(CH$_3$)$_2$), 6.35 (s, 4H, NC*H*), 7.04-7.14 (m, 12H, Ar*H*); ^{13}C{^{1}H} NMR (75 MHz, C_6D_6): δ = 23.4 (CH(*C*H$_3$)$_2$), 26.5 (CH(*C*H$_3$)$_2$), 29.0 (*C*H(CH$_3$)$_2$), 123.8 (N*C*H), 127.5, 127.8, 128.2, 144.6 (Ar-*C*), CO resonances not observed; ^{11}B{^{1}H} NMR (C_6D_6, 128 MHz, 298 K): δ = 26.9 br.; IR *ν*/cm^{-1} (ATR): 2036(s), 1965(s) 1938(s), 1920(sh), 1259(m), 1118(s), 1034(s), 1056(m), 1016(s), 801(s); MS (EI) *m/z* (%): 387.4 [B(DAB)$^+$, 100]; anal. calc. for $C_{60}H_{72}B_2Fe_2Ga_2N_4O_8$: C 55.64%, H 5.80%, N 4.48%, found: C 57.83%, H 6.09%, N 4.67%.

N.B. An identical procedure, but using compound **3** as the starting material, gave a similar yield of **5**.

Synthesis of InBr{B(DAB)}$_2$. To a solution of $InBr_3$ (0.065 g, 0.18 mmol) in THF (10 mL) was added a solution of $(THF)_2Li\{B(DAB)\}$ (0.20 g, 0.37 mmol) in THF (5 mL) at -78 °C. The resultant solution was warmed to room temperature over a period of 12 hrs, whereupon volatiles were removed *in vacuo.* The residue was extracted into pentane (8 mL) and the extract filtered. The filtrate was concentrated to *ca.* 10 mL and stored at -30 ˚C overnight to give colorless crystals of the title compound. (0.154 g, 86%). M.p. = 184-186 °C (dec.); ^{1}H NMR (C_6D_6, 400 MHz, 296 K): δ = 0.99 (d, 24H, ^3J = 6.6 Hz, $CH(CH_3)_2$), 1.09 (d, 24H, ^3J = 6.9 Hz, $CH(CH_3)_2$), 3.20 (sept, 8H, ^3J = 6.6 Hz, $CH(CH_3)_2$), 6.19 (s, 4H, NC*H*), 7.02-7.16 (m, 12H, Ar*H*); ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz, 296 K): δ = 24.6 ($CH(CH_3)_2$), 25.4 ($CH(CH_3)_2$), 28.4 ($CH(CH_3)_2$), 122.2 (N*C*H), 123.7, 128.5, 129.9, 146.2 (Ar-*C*); ^{11}B{^{1}H} NMR (C_6D_6, 128 MHz, 296 K): δ = 37.1 (br.); IR (Nujol) ν/cm^{-1}: 1559(w), 1377(s), 1362(m), 1261(s), 1103(s), 1017(s), 933(w), 802(s), 757(s); MS EI: *m*/*z* (%): 969.4 [M^+, 12], 889.4 [M^+- Br, 95], 387.2 [$(DAB)B^+$, 18]; anal. calc. for $C_{52}H_{72}B_2BrInN_4$: C 64.42%, H 7.49%, N 5.78%; found C 64.36%, H 7.54%, N 5.86%.

2. X-Ray Crystallography

Crystals of **1**-**5** and $InBr\{B(DAB)\}_2$ **1S** suitable for X-ray structural determination were mounted in silicone oil. Crystallographic measurements were carried out with either a Bruker Apex X8 diffractometer using a graphite monochromator with Mo Kα radiation (λ = 0.71073 Å), or the MX1 beamline of the Australian Synchrotron (λ = 0.7109 Å). The software package Blu-Ice[3] was used for synchrotron data acquisition, while the program XDS[4] was employed for synchrotron data reduction. All structures were solved by direct methods and refined on F^2 by full matrix least squares (SHELX97[5]) using all unique data. Hydrogen atoms are included in calculated positions (riding model). The absolute structure parameter for the crystal structure of **2** is -0.003(9). Crystal data, details of data collections and refinements for all structures can be found in their CIF files and are summarized in Table S1.

Table S1. Crystal structure and refinement data for **1-5** and InBr{B(DAB)}$_2$ **1S**.

	1	**2**	**3**	**4**·(toluene)	**5**	**1S**
empirical form.	$C_{30}H_{44}AlBBr_2N_2O$	$C_{30}H_{44}BCl_2GaN_2O$	$C_{30}H_{44}BBr_2GaN_2O$	$C_{75}H_{96}Al_2B_2Fe_2N_4O_{10}$	$C_{60}H_{72}B_2Fe_2Ga_2N_4O_8$	$C_{52}H_{72}B_2BrInN_4$
formula wt	646.28	600.10	689.02	1400.84	1249.98	969.49
crystal syst.	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1$	$P2_1/c$	$P2_1/n$	$P2_1/n$	$P2_1/n$
a (Å)	14.1479(7)	10.2077(10)	14.1260(7)	12.057(2)	13.9550(11)	12.5003(4)
b (Å)	12.1971(7)	12.3372(11)	12.1475(6)	12.316(3)	11.3797(8)	21.3651(8)
c (Å)	19.3891(13)	13.3681(15)	19.3683(11)	25.080(5)	20.3233(16)	18.3157(7)
β (deg)	100.086(6)	106.068(11)	100.037(5)	91.93(3)	109.513(4)	19.6630(7)
vol (Å^3)	3294.1(3)	1617.7(3)	3272.6(3)	3722.1(13)	3042.1(4)	5243.3(3)
Z	4	2	4	2	2	4
ρ (calc) (g.cm^{-3})	1.303	1.232	1.398	1.250	1.365	1.228
μ (mm^{-1})	2.511	1.039	3.306	0.472	1.398	1.248
F(000)	1336	632	1408	1484	1296	2024
T (K)	123(2)	123(2)	123(2)	100(2)	123(2)	123(2)
reflns collect.	15151	13178	22256	26078	48391	20658
unique reflns	6455	5768	6093	6684	8293	10243
R_{int}	0.0387	0.0351	0.0355	0.0558	0.0422	0.0298
R1 [$I>2\sigma(I)$]	0.0379	0.0338	0.0314	0.0496	0.0306	0.0372
wR2 (all data)	0.0831	0.0830	0.0725	0.1284	0.0732	0.0887
CCDC No.	1510775	1510776	1510780	1510777	1510778	1510779

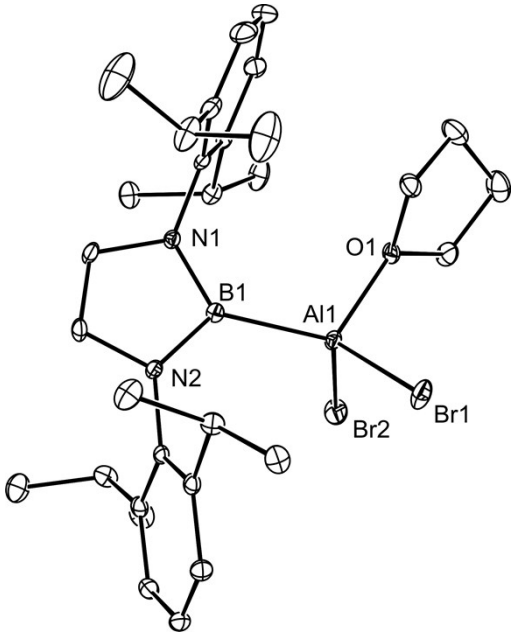

Fig. S1 Molecular structure of **1** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Br(1)-Al(1) 2.3199(9), Al(1)-O(1) 1.8798(19), Al(1)-B(1) 2.113(3), Al(1)-Br(2) 2.3168(9), O(1)-Al(1)-B(1) 113.79(10), Br(2)-Al(1)-Br(1) 110.57(3).

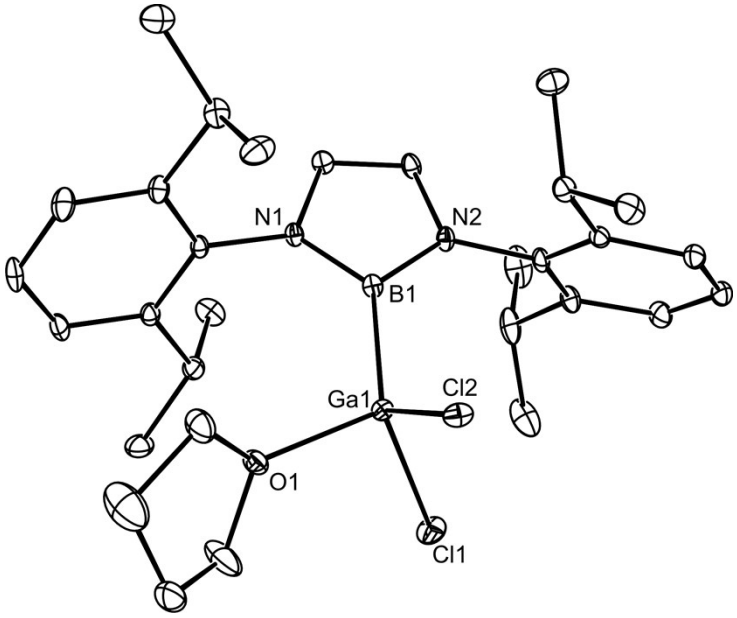

Fig. S2 Molecular structure of **2** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Ga(1)-O(1) 2.008(2), Ga(1)-B(1) 2.064(4), Ga(1)-Cl(1) 2.2078(8), Ga(1)-Cl(2) 2.2118(9), O(1)-Ga(1)-B(1) 113.44(12), Cl(1)-Ga(1)-Cl(2) 106.12(4).

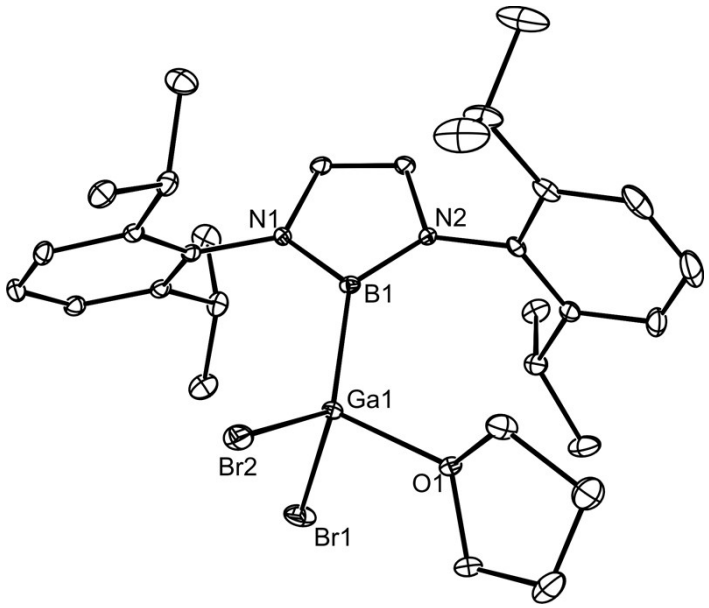

Fig. S3 Molecular structure of **3** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Ga(1)-O(1) 2.0081(16), Ga(1)-B(1) 2.061(3), Ga(1)-Br(2) 2.3412(4), Ga(1)-Br(1) 2.3445(4), O(1)-Ga(1)-B(1) 112.81(9), Br(2)-Ga(1)-Br(1) 109.274(16).

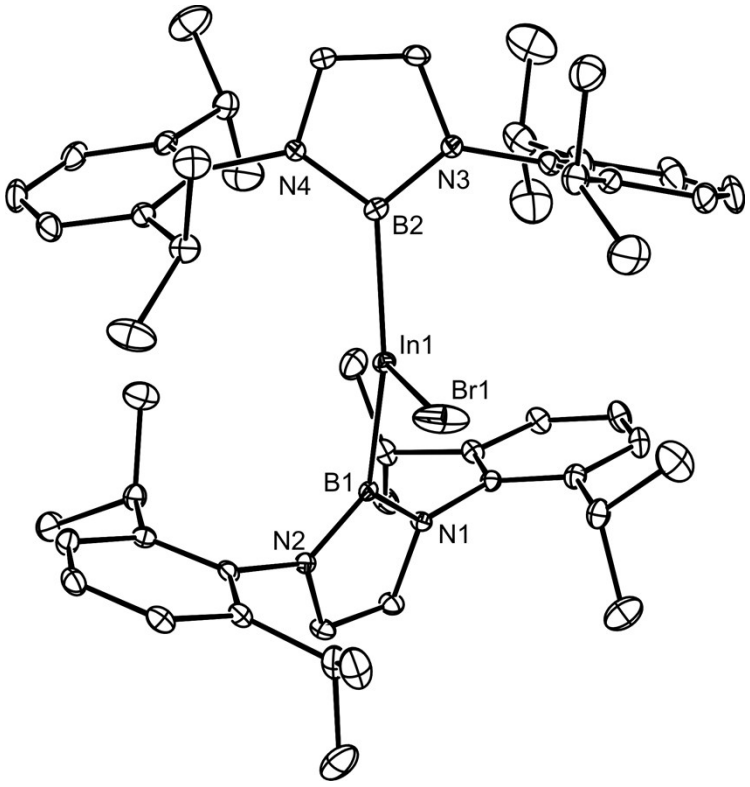

Fig. S4 Molecular structure of InBr{B(DAB)}$_2$ **1S** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): In(1)-B(2) 2.231(3), In(1)-B(1) 2.231(3), In(1)-Br(1) 2.5680(4),B(2)-In(1)-B(1) 154.94(11), B(2)-In(1)-Br(1) 101.78(8), B(1)-In(1)-Br(1) 103.23(8).

3. Computational Studies

Gas-phase structure optimisation of **5'** has been carried out with the ADF2016 program suite using the experimentally determined structure as input with BP86-functional[6] including Grimme dispersion correction with Becke-Johnson damping (BP-D3(BJ))[7,8] and TZP all-electron basis sets on all light elements (C,H,N,B,O) and TZ2P basis set on Ga and Fe.[9] Structure optimisation was followed by a single-point calculation with TZ2P basis set on all elements including a Bader analysis.[10]

Table S2. Cartesian coordinates of geometry optimized **5'**.

Ga	2.55034933	5.27973607	10.48146219
Fe	4.88173517	5.69289265	11.13852535
O	7.74095512	6.39227650	10.95032633
O	4.94694503	5.14002162	14.03986909
N	-0.16366605	5.53183726	12.00898568
O	5.09653847	2.86844570	10.28818476
O	3.80899571	8.43849011	11.38401266
N	0.34283759	3.35116337	11.56637033
C	1.01167277	2.13483745	11.19926269
C	-0.10741863	6.95845785	12.16326369
C	-0.87980303	7.78184474	11.31813646
C	0.76412617	7.50189862	13.13947042
C	0.58319328	1.41868085	10.06205881
C	4.98451606	3.98857700	10.59341985
C	2.11720838	1.70713964	11.97653016
C	1.28022732	0.25317959	9.71273567
H	0.96707767	-0.31367899	8.83534336
C	0.84914677	8.89602312	13.23403046
H	1.52141807	9.34457279	13.96317729
C	-0.76727382	9.17165905	11.46536335
H	-1.35178022	9.82682185	10.81835995
C	-0.60695127	1.86406246	9.22916246
H	-0.84276219	2.89757657	9.51312518
C	-0.94326380	3.41987426	12.12671588
H	-1.53625512	2.53091299	12.30976356
C	1.54725895	6.60558762	14.09315179
H	1.99806299	5.79683692	13.49391461
C	2.37498633	-0.17723478	10.45418610
H	2.91701807	-1.07667388	10.15841308
C	0.09219627	9.72583931	12.40753956
H	0.18030693	10.80953893	12.49764150
C	-1.83107941	7.20552603	10.28336804
H	-1.58251502	6.14408260	10.15789820
B	0.86537546	4.68479485	11.47757509
C	4.20757340	7.35073018	11.25039540
C	6.61258988	6.12128656	11.00108808
C	-1.24629360	4.72277540	12.39012253
H	-2.14359742	5.13812392	12.83498523
C	2.78763342	0.54647821	11.57272203
H	3.65031305	0.20110142	12.13943805
C	2.54275371	2.45344434	13.23712459
H	2.57309212	3.52856492	12.99139650

C	-1.84161019	0.99659873	9.53816365
H	-1.65477908	-0.05443825	9.27228905
H	-2.71198312	1.34514700	8.96403658
H	-2.09977343	1.02874983	10.60512408
C	-3.28763943	7.29375571	10.77796525
H	-3.41876947	6.78040363	11.73988816
H	-3.97142709	6.83592929	10.04885871
H	-3.58699837	8.34306608	10.91726099
C	-0.30131760	1.84613660	7.72285072
H	0.61078530	2.40959809	7.49136401
H	-1.13327797	2.29417112	7.16291062
H	-0.16365775	0.82122394	7.35017685
C	-1.68640937	7.88993993	8.91506422
H	-2.03368194	8.93248039	8.94573319
H	-2.28743921	7.36176963	8.16274253
H	-0.64257020	7.89635013	8.57832148
C	4.86681943	5.34616419	12.89960640
C	2.68169829	7.33212370	14.82276685
H	2.28944608	8.08386370	15.52328817
H	3.36320052	7.83711295	14.12591918
H	3.26616834	6.61165728	15.40750423
C	3.93252707	2.05439170	13.74418405
H	3.94460101	1.01419593	14.10145675
H	4.21532797	2.69439431	14.58858968
H	4.70070846	2.15772985	12.96685642
C	0.60334717	5.94474632	15.11740064
H	1.17443457	5.30066332	15.80085593
H	-0.15962828	5.32772795	14.62936678
H	0.09586682	6.71531746	15.71607244
C	1.50415399	2.27186384	14.36184050
H	0.51669703	2.64748424	14.07096712
H	1.82236198	2.81540649	15.26241806
H	1.40798154	1.20696588	14.61957843
Ga	4.61624723	6.09996392	8.67458392
Fe	2.28486139	5.68680735	8.01752076
O	-0.57435856	4.98742350	8.20571977
O	2.21965153	6.23967838	5.11617701
N	7.33026261	5.84786274	7.14706043
O	2.07005809	8.51125430	8.86786135
O	3.35760085	2.94120989	7.77203345
N	6.82375897	8.02853663	7.58967577
C	6.15492379	9.24486255	7.95678341
C	7.27401519	4.42124215	6.99278242
C	8.04639959	3.59785526	7.83790965
C	6.40247039	3.87780138	6.01657569
C	6.58340329	9.96101915	9.09398729
C	2.18208051	7.39112300	8.56262625
C	5.04938818	9.67256037	7.17951595
C	5.88636925	11.12652041	9.44331043
H	6.19951889	11.69337899	10.32070274
C	6.31744980	2.48367688	5.92201565
H	5.64517850	2.03512721	5.19286881
C	7.93387038	2.20804095	7.69068275
H	8.51837678	1.55287815	8.33768615
C	7.77354783	9.51563754	9.92688365

H	8.00935875	8.48212343	9.64292092
C	8.10986036	7.95982574	7.02933023
H	8.70285168	8.84878701	6.84628255
C	5.61933762	4.77411238	5.06289431
H	5.16853357	5.58286308	5.66213149
C	4.79161023	11.55693478	8.70186001
H	4.24957849	12.45637388	8.99763302
C	7.07440030	1.65386069	6.74850654
H	6.98628963	0.57016107	6.65840461
C	8.99767597	4.17417397	8.87267807
H	8.74911158	5.23561740	8.99814790
B	6.30122111	6.69490515	7.67847101
C	2.95902317	4.02896982	7.90565070
C	0.55400668	5.25841344	8.15495803
C	8.41289016	6.65692460	6.76592357
H	9.31019398	6.24157608	6.32106088
C	4.37896314	10.83322179	7.58332407
H	3.51628351	11.17859858	7.01660805
C	4.62384285	8.92625566	5.91892151
H	4.59350445	7.85113508	6.16464960
C	9.00820675	10.38310127	9.61788245
H	8.82137564	11.43413825	9.88375705
H	9.87857969	10.03455300	10.19200952
H	9.26636999	10.35095017	8.55092202
C	10.45423599	4.08594429	8.37808085
H	10.58536603	4.59929637	7.41615794
H	11.13802365	4.54377071	9.10718740
H	10.75359494	3.03663392	8.23878511
C	7.46791416	9.53356340	11.43319538
H	6.55581126	8.97010191	11.66468209
H	8.29987453	9.08552888	11.99313549
H	7.33025431	10.55847606	11.80586925
C	8.85300593	3.48976007	10.24098188
H	9.20027850	2.44721961	10.21031291
H	9.45403577	4.01793037	10.99330357
H	7.80916676	3.48334987	10.57772463
C	2.29977714	6.03353581	6.25643970
C	4.48489827	4.04757630	4.33327926
H	4.87715048	3.29583630	3.63275794
H	3.80339604	3.54258705	5.03012692
H	3.90042822	4.76804271	3.74854187
C	3.23406949	9.32530830	5.41186205
H	3.22199555	10.36550407	5.05458935
H	2.95126859	8.68530569	4.56745642
H	2.46588810	9.22197015	6.18918968
C	6.56324939	5.43495368	4.03864547
H	5.99216200	6.07903668	3.35519017
H	7.32622485	6.05197206	4.52667932
H	7.07072974	4.66438254	3.43997366
C	5.66244257	9.10783616	4.79420560
H	6.64989953	8.73221576	5.08507898
H	5.34423459	8.56429351	3.89362804
H	5.75861502	10.17273412	4.53646767

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