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Supporting Information

Magnesocenophane-Catalyzed Amine Borane Dehydrocoupling

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SUPPORTING INFORMATION

Experimental Procedures

All manipulations were carried out under an argon inert gas atmosphere (argon 5.0), using either Schlenk line techniques or a glovebox. $Me_2NH{\cdot}BH_3$ was purchased from ABCR and used as received. Me_2NH_2Cl was purchased from Alfa Aesar and used as received. 2,2-dicyclopentadienylpropane,[1] magnesocene and magnesocenophanes, **1b**-**d**,[2] di*iso*propylamine borane, **2b**,[3] and methylamine borane, **2c**,[4] linear diborazane, **3b**,[5] and N-deuterated derivative of dimethylamine borane, **2aND**[6] were synthesized according to literature known procedures.
NMR spectra were recorded on Bruker Avance III 300 and Bruker Avance III 400 spectrometers. ^{1}H and ^{13}C NMR spectra were referenced using the solvent signals.[7] ^{11}B NMR spectra were referenced using an external standard ($\delta^{11}B(BF_3{\cdot}OEt_2) = 0$). Mass spectrometry was performed on a Bruker SolariX FT-ICR MS 7 Tesla spectrometer. Single crystal X-ray diffraction analysis were carried out at low temperatures on a Bruker AXS X8 Apex CCD diffractometer and on a Bruker AXS D8 Venture diffractometer operating with graphite monochromated Mo Kα radiation. Structure solution and refinement were performed using SHELX.[8]

Synthesis of C[1]magnesocenophane 1a:
This compound had been described before,[9] and was synthesized by a modified procedure:
To a solution of 24.0 g (139 mmol) 2,2-dicyclopentadienylpropane in hexane was added 199 mL of a solution of *n*-butyl-*sec*-butylmagnesium (139 mmol, 0.7 M in hexane) at 273 K. The mixture was allowed to warm to room temperature and subsequently stirred over night at 333 K. After filtration, the precipitate was washed with small portions of cold hexane and dried *in vacuo*.
Yield: 16.9 g / 56%.
δ^1H (400.13 MHz, C_6D_6/dme) = 2.35 (s, 6 H, C$\underline{H}_3$), 6.02 (t, $^3J_{HH}$ = 2.5 Hz, 4 H, Cp-$\underline{H}$), 6.08 (t, $^3J_{HH}$ = 2.5 Hz, 4 H, Cp-$\underline{H}$);
δ^1H (400.13 MHz, C_6D_6/thf) = 1.39 (THF), 2.27 (s, 6 H, C$\underline{H}_3$), 3.51 (THF), 6.07 (t, $^3J_{HH}$ = 2 Hz, 4 H, Cp-$\underline{H}$), 6.15 (t, $^3J_{HH}$ = 2 Hz, 4 H, Cp-$\underline{H}$);
δ^1H (400.13 MHz, thf-D8) = 1.71 (s, 6 H, C$\underline{H}_3$), 5.60 (t, $^3J_{HH}$ = 2 Hz, 4 H, Cp-$\underline{H}$), 5.76 (t, $^3J_{HH}$ = 2 Hz, 4 H, Cp-$\underline{H}$);
$\delta^{13}C\{^1H\}$ (100.62 MHz, C_6D_6/dme) = 27.6 (C$\underline{H}_3$), 38.5 (C-$\underline{C}$-CH_3), 96.0 (Cp), 107.1 (Cp);
$\delta^{13}C\{^1H\}$ (100.62 MHz, C_6D_6/thf) = 25.7 (THF), 29.1 (C$\underline{H}_3$), 37.8 (C-$\underline{C}$-CH_3), 68.1 (THF), 95.7 (Cp), 108.1 (Cp), 141.3 (Cp);
$\delta^{13}C\{^1H\}$ (100.62 MHz, thf-D8) = 29.2 (C$\underline{H}_3$), 37.8 (C-$\underline{C}$-CH_3), 95.6 (Cp), 108.2 (Cp), 141.3 (Cp).

Synthesis of 2aBD:
Note: $Me_2NH{\cdot}BD_3$, **2aBD**, cannot be synthesized by treatment of Me_2NH_2Cl with $NaBD_4$.[6]
Dimethylammoniumchlorid was N-deuterated by repeatedly stirring it in D_2O. Full N-deuteration was confirmed by ^{1}H NMR spectroscopy. 1.50 g (18.0 mmol) of N-deuterated dimethylammoniumchlorid and 0.75 g (17.9 mmol) of sodium borodeuteride were added to a Schlenk flask and cooled to 273 K. 75 mL of precooled thf were added and the solution was stirred for 1 h at 273 K and subsequently allowed to warm to room temperature and stirred over night. The mixture was filtered, all volatiles were removed *in vacuo* and the crude was stirred in water for 5 h to allow for N-D/H exchange. The product was subsequently extracted with dichloromethane and dried *in vacuo*.
Yield: 0.44 g / 40%.
δ^1H (400.13 MHz, C_6D_6) = 1.78 (d, 6 H, C$\underline{H}_3$), 2.82 (br s, 1 H, N$\underline{H}$);
$\delta^{13}C\{^1H\}$ (100.62 MHz, C_6D_6) = 43.8 (C$\underline{H}_3$);
δ^{11}B (128.38 MHz, C_6D_6) = -13.4 (m, $\underline{B}D_3$).

Synthesis of 2aNDBD:
Dimethylammoniumchlorid was N-deuterated by repeatedly stirring it in D_2O. Full N-deuteration was confirmed by ^{1}H NMR spectroscopy. 2.0 g (23.9 mmol) of N-deuterated dimethylammoniumchlorid and 1.0 g (23.9 mmol) of sodium borodeuteride were added to a Schlenk flask and cooled to 273 K. 100 mL of precooled thf were added and the solution was stirred for 1 h at 273 K and subsequently allowed to warm to room temperature and stirred over night. All volatiles were removed *in vacuo* and the product was sublimed from the crude *in vacuo* at 313 K.
Yield: 0.22 g / 15%.
δ^1H (400.13 MHz, C_6D_6) = 1.70 (s, 6 H, C$\underline{H}_3$);
$\delta^{13}C\{^1H\}$ (100.62 MHz, C_6D_6) = 43.7 (C$\underline{H}_3$);
δ^{11}B (128.38 MHz, C_6D_6) = -13.2 (m, $\underline{B}D_3$).

Synthesis of magnesium complex 5:

The thf derivative of this compound had been described before.[10] Complex **5** was synthesized by following the corresponding procedure, but using toluene/dme 10:1 as solvent.

δ^{1}H (400.13 MHz, C_6D_6) = 1.35 - 2.01 (m, 20 H, B<u>H</u>), 2.17 (s, 24 H, N-C<u>H</u>$_3$), 2.21 (s, 24 H, N-C<u>H</u>$_3$), 3.15 (s, 6 H, O-C<u>H</u>$_3$), 3.36 (s, 4 H, O-C<u>H</u>$_2$);

δ^{13}C{^{1}H} (100.62 MHz, C_6D_6) = 52.0 (<u>C</u>H$_3$), 59.6 (dme-<u>C</u>H$_3$), 72.0 (dme-<u>C</u>H$_2$);

δ^{11}B (128.38 MHz, C_6D_6) = -16.6 (t, $^{1}J_{BH}$ = 86 Hz, <u>B</u>H$_2$), 2.9 (q, $^{1}J_{BH}$ = 106 Hz, <u>B</u>H$_3$);

δ^{11}B (128.38 MHz, dme) = -15.4 (q, $^{1}J_{BH}$ = 89 Hz), 3.7 (t, $^{1}J_{BH}$ = 102 Hz).

Elemental analysis for $C_{20}H_{78}B_8Mg_2N_8O_2$: calculated: C: 40.17%, H: 13.15%, N: 18.74%; found: C: 40.10%, H: 12.81%, N: 18.59%.

Catalytic dehydrocoupling:

In a typical run, the reaction was performed in a glovebox using a 5 mL volume vial. Magnesocenophane **1a** (5 mol%: 8.0 mg, 0.04 mmol) was added to a solution of the corresponding amine borane (**2a**: 50 mg, 0.85 mmol; **2b**: 95 mg, 0.83 mmol; **2c**: 37 mg, 0.82 mmol) in 1 mL dme and the mixture was stirred at ambient conditions for a given amount of time.

For NMR measurements, a sample of approximately 0.3 mL was added to a NMR tube, diluted with approximately 0.3 mL of C_6D_6, and analyzed by ^{11}B NMR spectroscopy.

For discontinuous monitoring of the reaction, the reaction was performed at approximately three times the scale, and aliquots were taken at the corresponding points in time and analyzed by ^{11}B NMR spectroscopy.

The following signals were observed for the different species in dme: δ^{11}B (128 MHz, dme) = -21.0 (**2b** (*i*Pr$_2$NH·BH$_3$), q, $^{1}J_{BH}$ = 98.0 Hz); -18.0 (**2c** (MeNH$_2$·BH$_3$), q, $^{1}J_{BH}$ = 96.0 Hz); -13.3 (**2a** (Me$_2$NH·BH$_3$), q, $^{1}J_{BH}$ = 98.0 Hz); -5.3 ([MeNHBH$_2$]$_3$), t, $^{1}J_{BH}$ = 106 Hz); 5.4 (**3a** ([Me$_2$NBH$_2$]$_2$), t, $^{1}J_{BH}$ = 114 Hz); 28.8 ([Me$_2$N]$_2$BH, d, $^{1}J_{BH}$ = 132 Hz); 35.1 (**4b** (*i*Pr$_2$N=BH$_2$), t, $^{1}J_{BH}$ = 127 Hz); 37.7 (**4a** (Me$_2$N=BH)$_2$, t, $^{1}J_{BH}$ = 128 Hz).

Reaction Monitoring

For continuous monitoring of the reaction at elevated temperatures by ^{11}B NMR spectroscopy, dme solutions of **2a** and 5 mol% of **1a** were charged into NMR tubes and analyzed by *in-situ* ^{11}B NMR spectroscopy at 323 K and 333 K (spectrometer temperature), with ^{11}B NMR spectra being recorded at regular intervals of 3 min. In all cases, conversions were determined by integration of **2a** *vs* **3a**. In some cases, a slight deviation from a linear fit for ln c/T is observed for the first few data points. This might arise from the sample warming up in the preheated spectrometer.

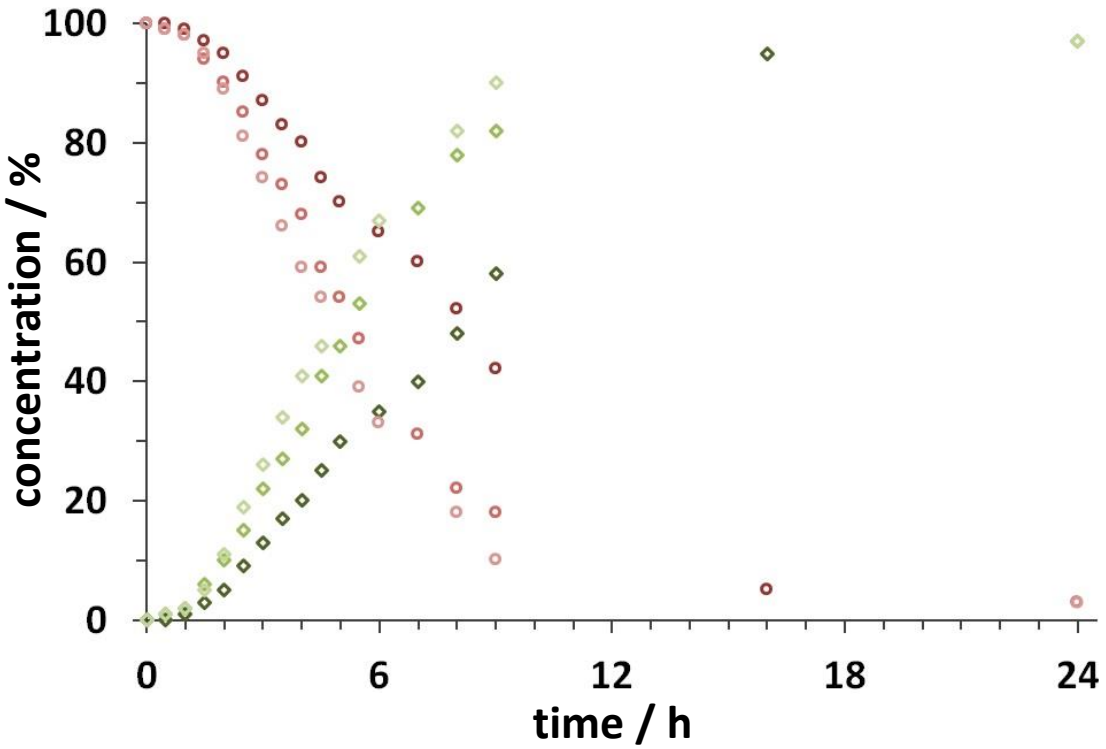


Figure S1. Relative concentration of **2a** (○) (c_0 = 850 mM) and **3a** (◇) *vs* time, for reactions catalyzed by 5 mol% (■■), 7.5 mol% (■■) and 10 mol% (■■) of **1a** in dme at r.t., as determined by discontinuous ^{11}B NMR measurements.

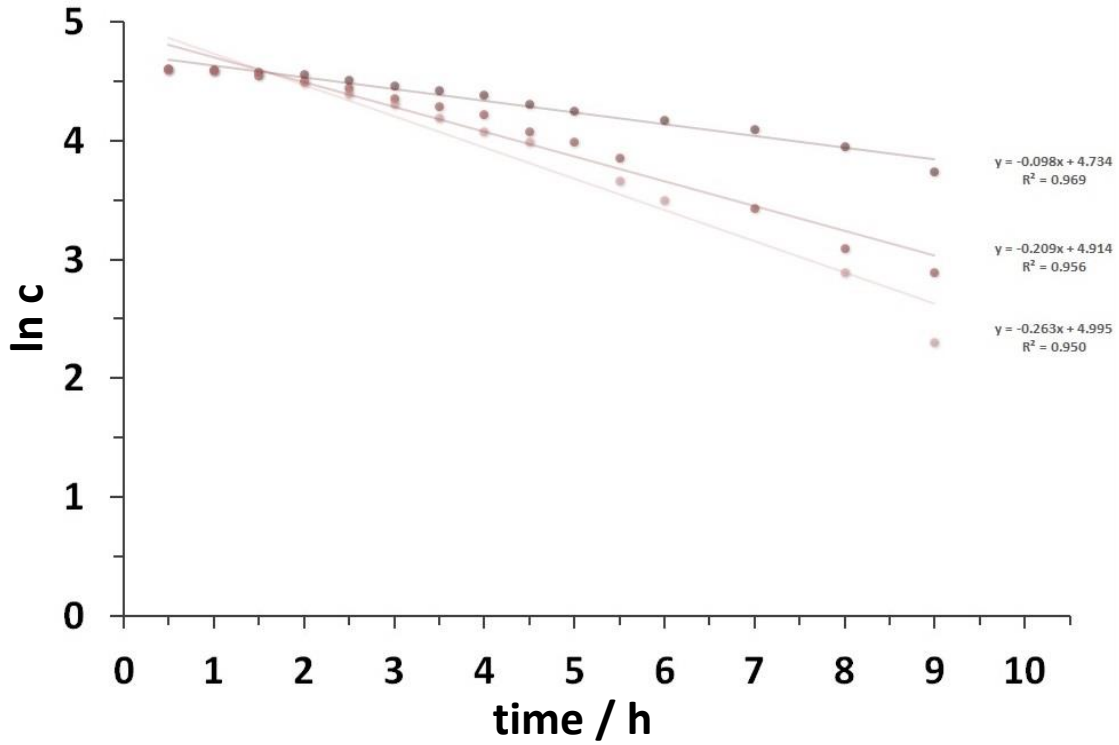


Figure S2. Plots of ln[**2a**] (for relative concentrations in %, c_0 = 850 mM) *vs* time, for reactions catalyzed by 5 mol% (■), 7.5 mol% (■) and 10 mol% (■) of **1a** in dme at r. t., as determined by discontinuous ^{11}B NMR measurements.

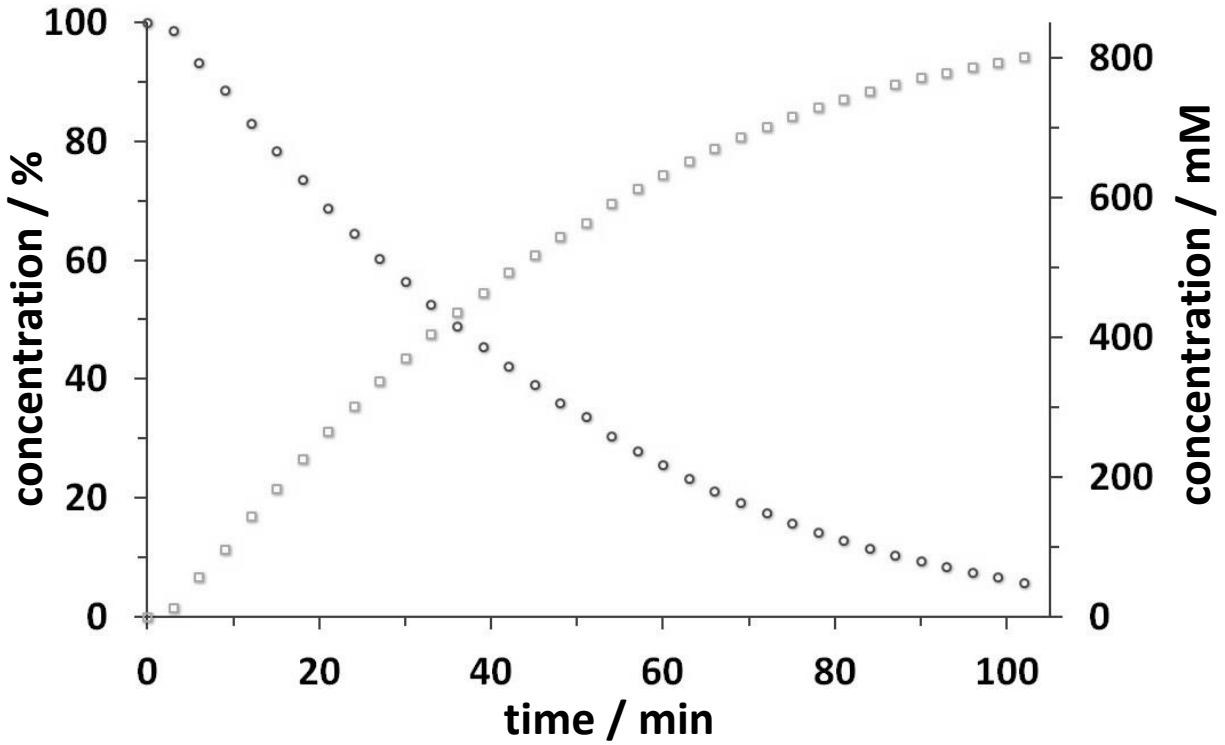


Figure S3. Plot of concentration of **2a** (○) (c_0 = 850 mM) and **3a** (□) *vs* time, for reactions catalyzed by 5 mol% of **1a** in dme at 333 K, as determined by *in-situ* ^{11}B NMR measurements.

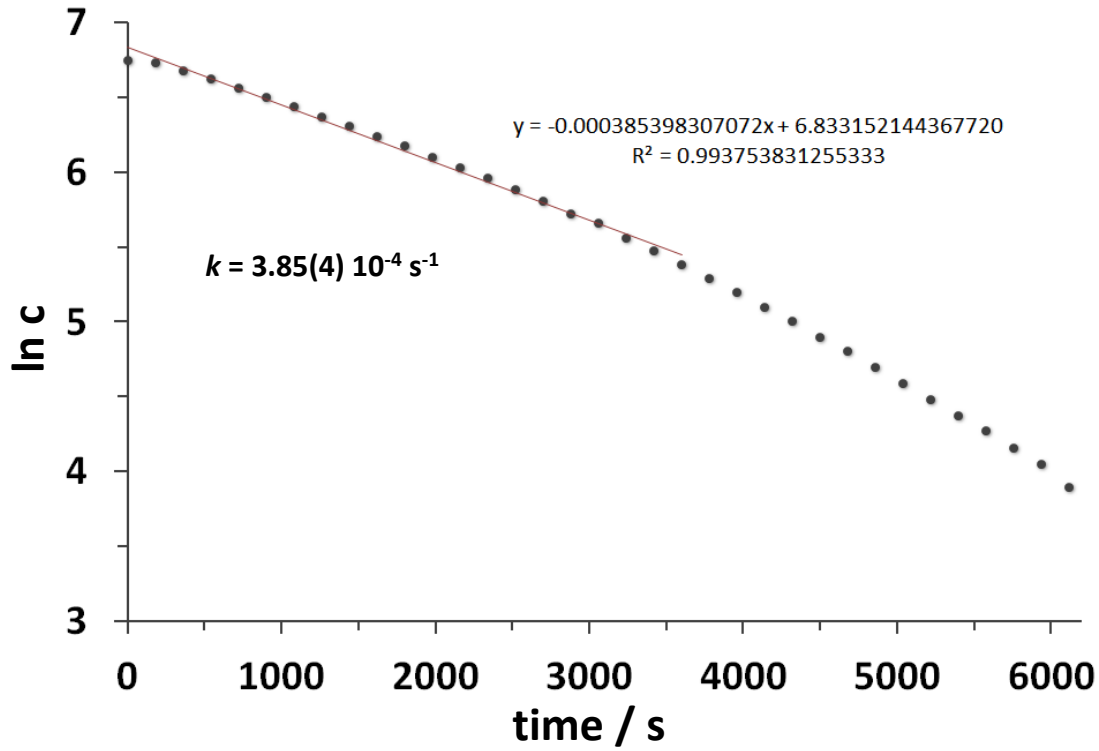


Figure S4. Plot of ln[**2a**] (for concentrations in mmol L^{-1} estimated from the known starting concentrations of c_0 = 850 mM for **2a**) *vs* time, for reactions catalyzed by 5 mol% of **1a** in dme at 333 K, as determined by *in-situ* ^{11}B NMR measurements. Rate constant *k*(**2a**) was determined by a linear fitting for 0 - 60 min (error of the rate constant was estimated from R^2).

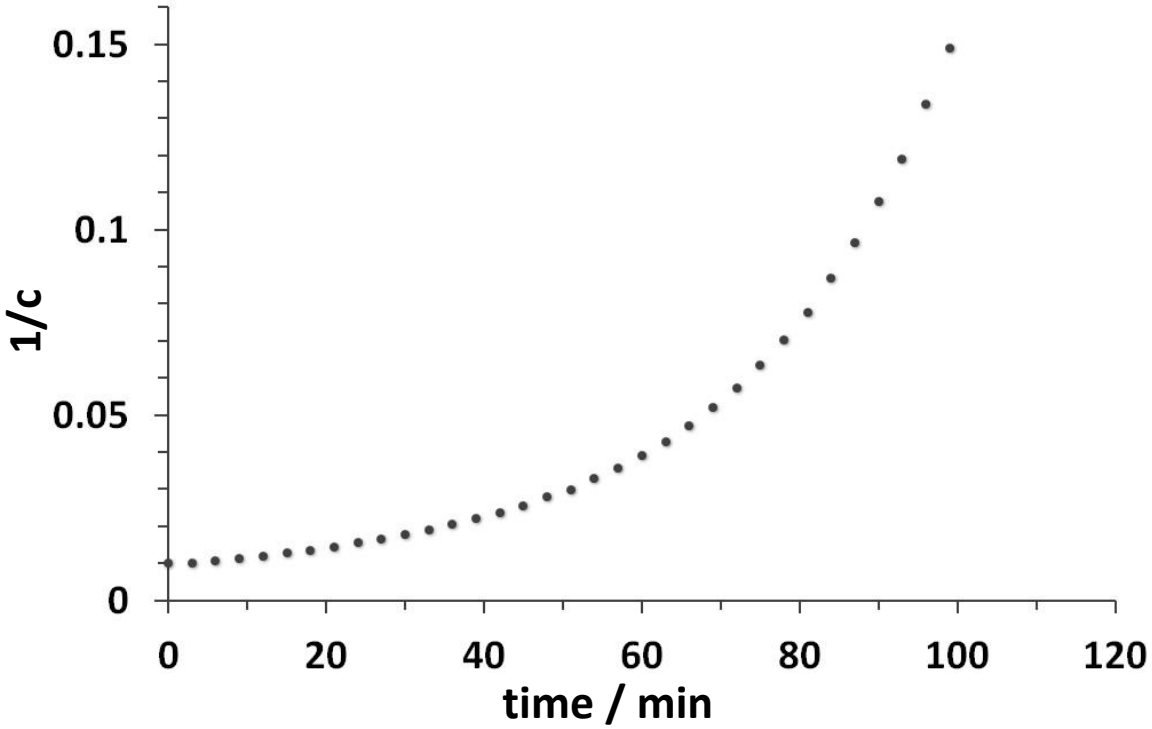


Figure S5. Plot of 1/[**2a**] (for relative concentrations in %, c_0 = 850 mM) *vs* time, for reactions catalyzed by 5 mol% of **1a** in dme at 333 K, as determined by *in-situ* ^{11}B NMR measurements.

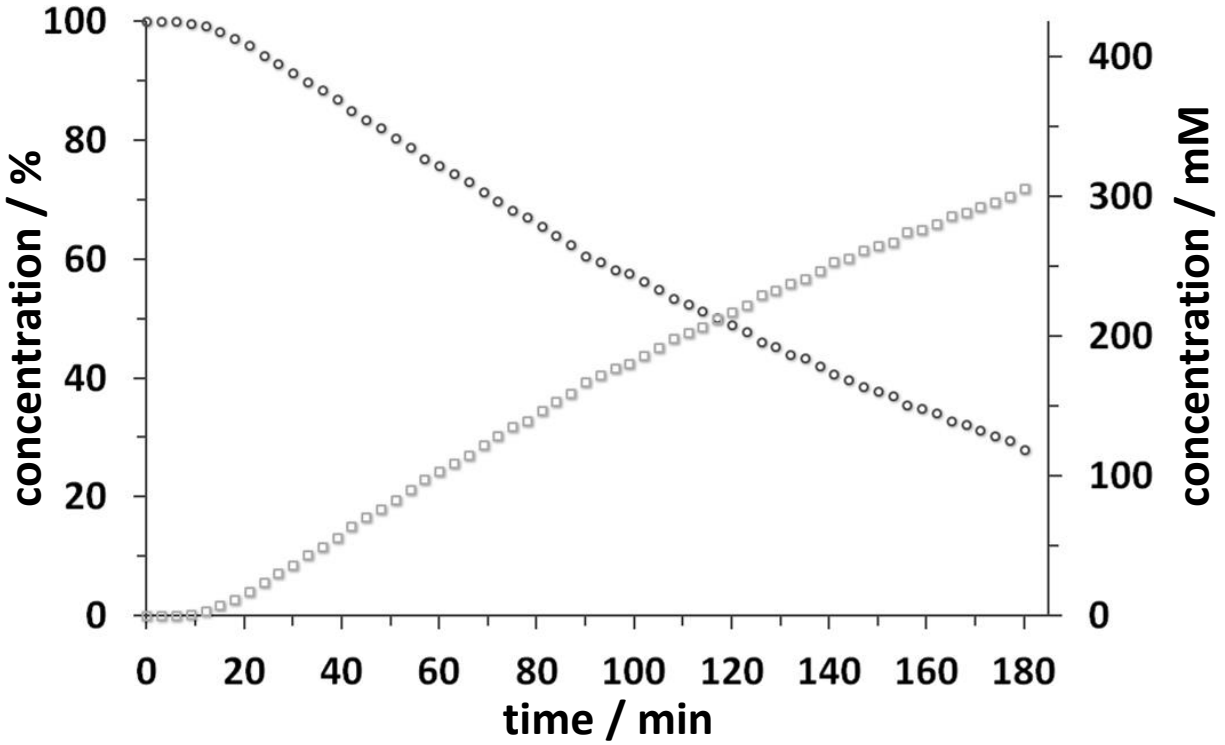


Figure S6. Plot of concentration of **2a** (○) (c_0 = 425 mM) and **3a** (□) *vs* time, for reactions catalyzed by 5 mol% of **1a** in dme at 323 K, as determined by *in-situ* ^{11}B NMR measurements.

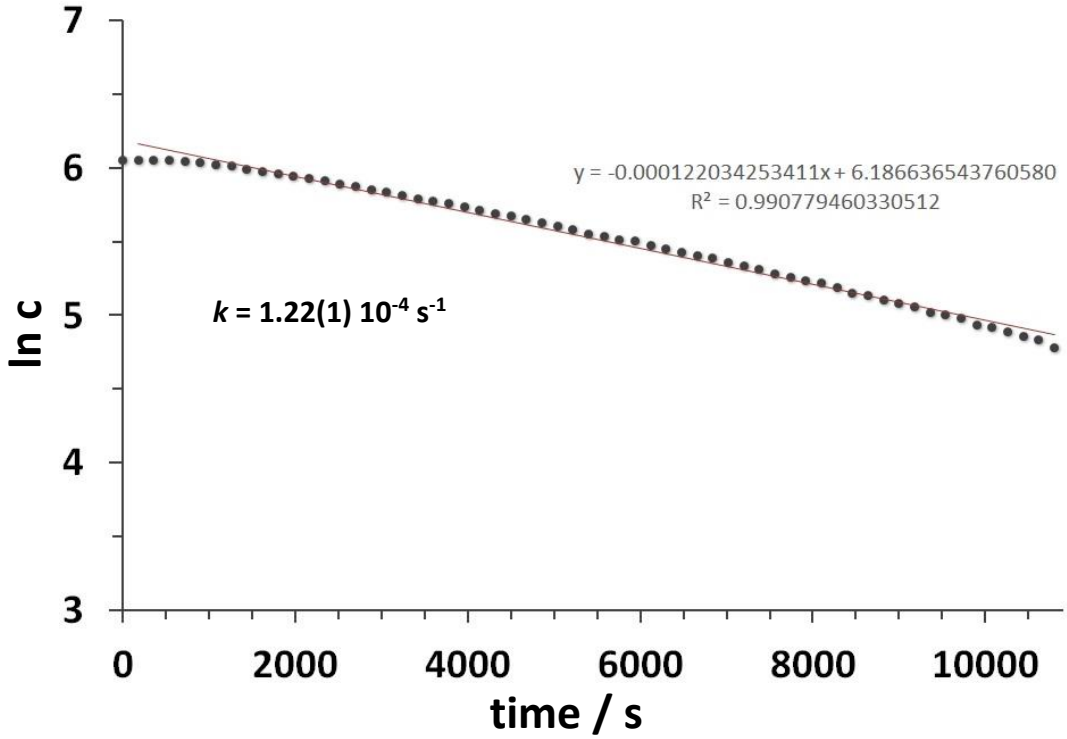


Figure S7. Plot of ln[**2a**] (for concentrations in mmol L^{-1} estimated from the known starting concentrations of c_0 = 425 mM for **2a**) *vs* time, for reactions catalyzed by 5 mol% of **1a** in dme at 323 K, as determined by *in-situ* ^{11}B NMR measurements. Rate constant *k*(**2a**) was determined by a linear fitting for 3-180 min (error of the rate constant was estimated from R^2).

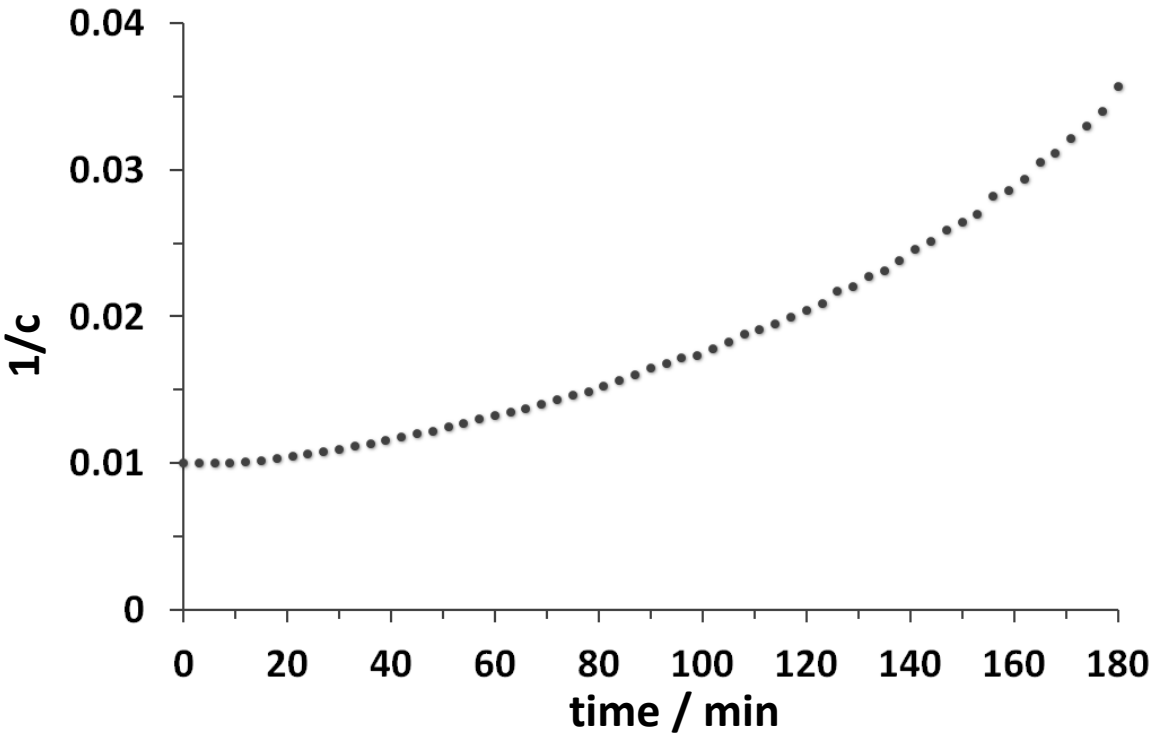


Figure S8. Plot of 1/[**2a**] (for relative concentrations in %, c_0 = 425 mM) *vs* time, for reactions catalyzed by 5 mol% of **1a** in dme at 323 K, as determined by *in-situ* ^{11}B NMR measurements.

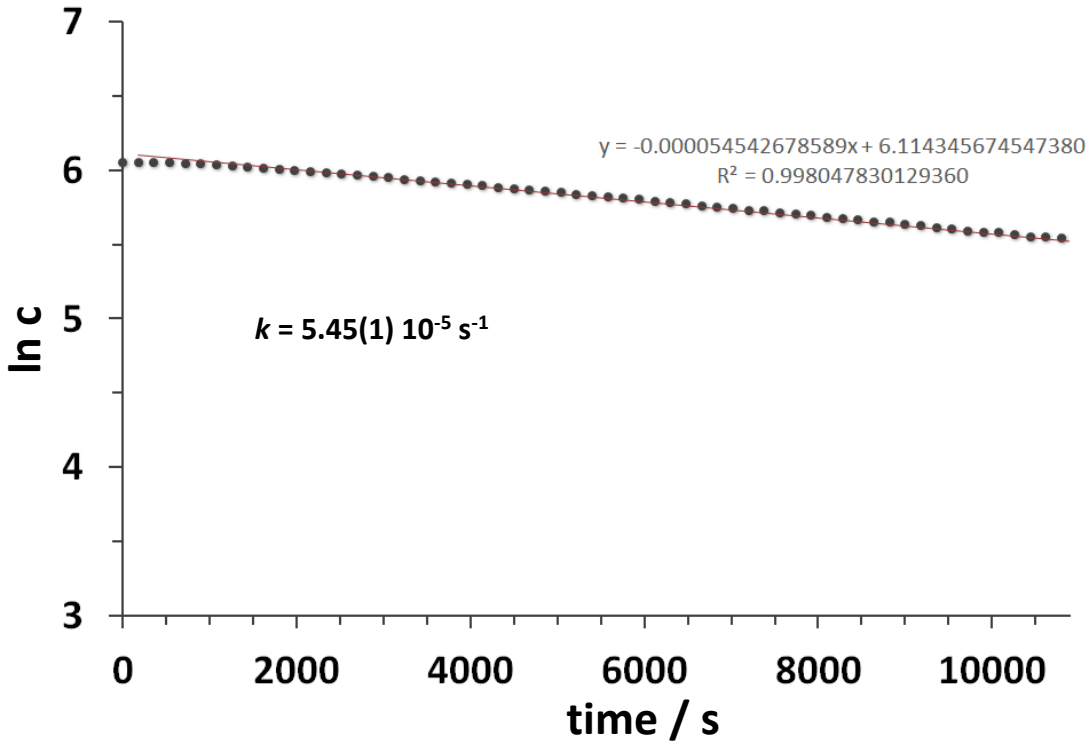


Figure S9. Plot of ln[**2aND**] (for concentrations in mmol L^{-1} estimated from the known starting concentrations of c_0 = 425 mM for **2aND**) *vs* time, for reactions catalyzed by 5 mol% of **1a** in dme at 323 K, as determined by *in-situ* ^{11}B NMR measurements. Rate constant *k*(**2aND**) was determined by a linear fitting for 3-309 min (error of the rate constant was estimated from R^2).

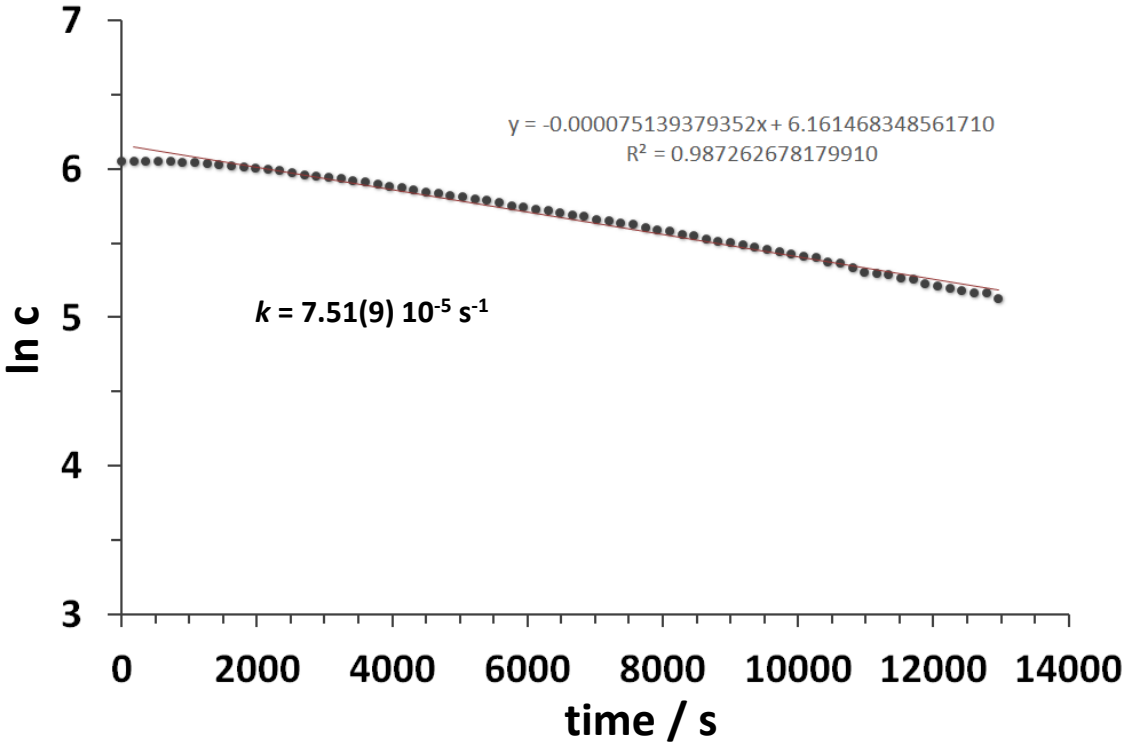


Figure S10. Plot of ln[**2aBD**] (for concentrations in mmol L^{-1} estimated from the known starting concentrations of c_0 = 425 mM for **2aBD**) *vs* time, for reactions catalyzed by 5 mol% of **1a** in dme at 323 K, as determined by *in-situ* ^{11}B NMR measurements. Rate constant *k*(**2aBD**) was determined by a linear fitting for 3-216 min (error of the rate constant was estimated from R^2).

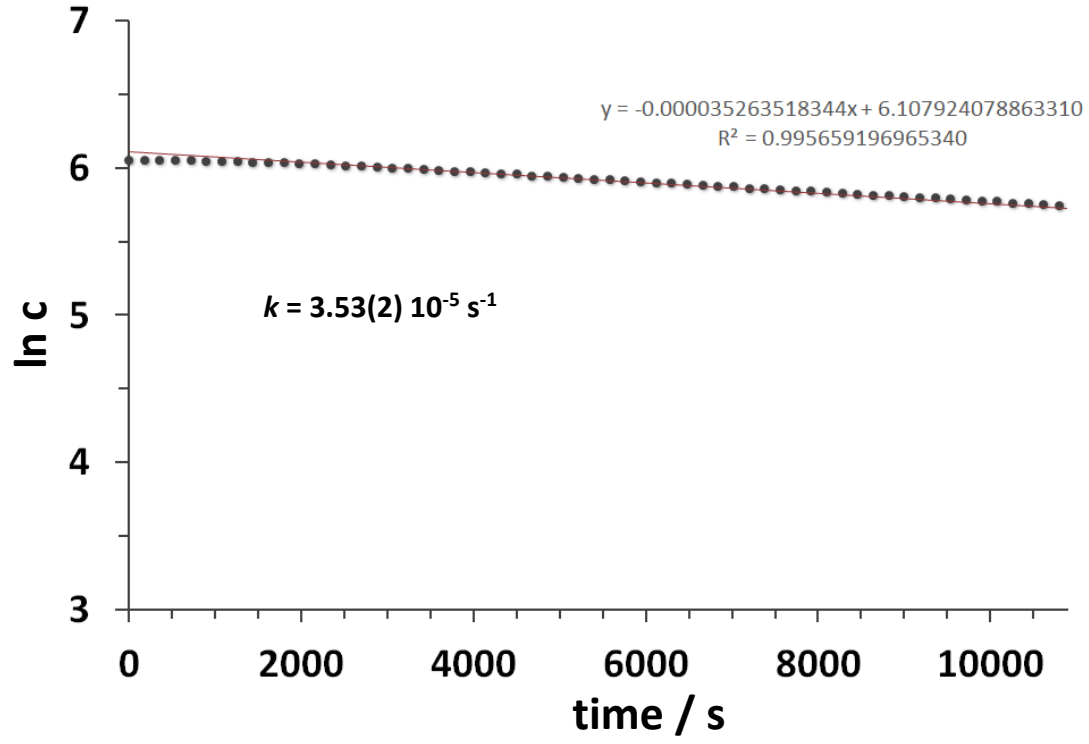


Figure S11. Plot of ln[**2aNDBD**] (for concentrations in mmol L^{-1} estimated from the known starting concentrations of c_0 = 425 mM for **2aBD**) *vs* time, for reactions catalyzed by 5 mol% of **1a** in dme at 323 K, as determined by *in-situ* ^{11}B NMR measurements. Rate constant *k*(**2aBD**) was determined by a linear fitting for 3-360 min (error of the rate constant was estimated from R^2).

NMR spectra

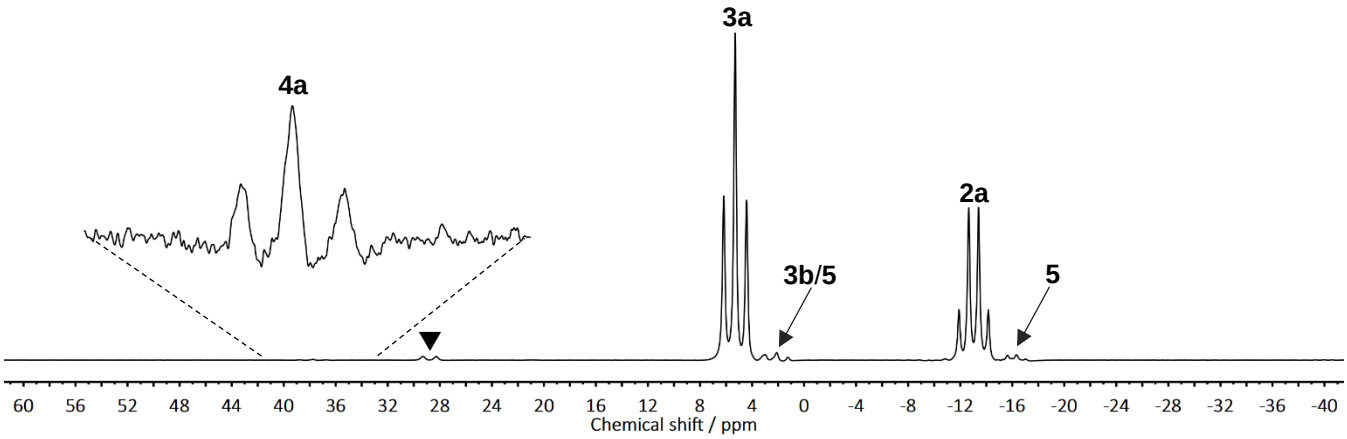


Figure S12. ^{11}B NMR spectrum (128.38 MHz, 293 K, C_6D_6/dme) of the reaction mixture of **2a** with 3 mol% of **1a** at r.t. after 24 h (▼$[Me_2N]_2BH$).

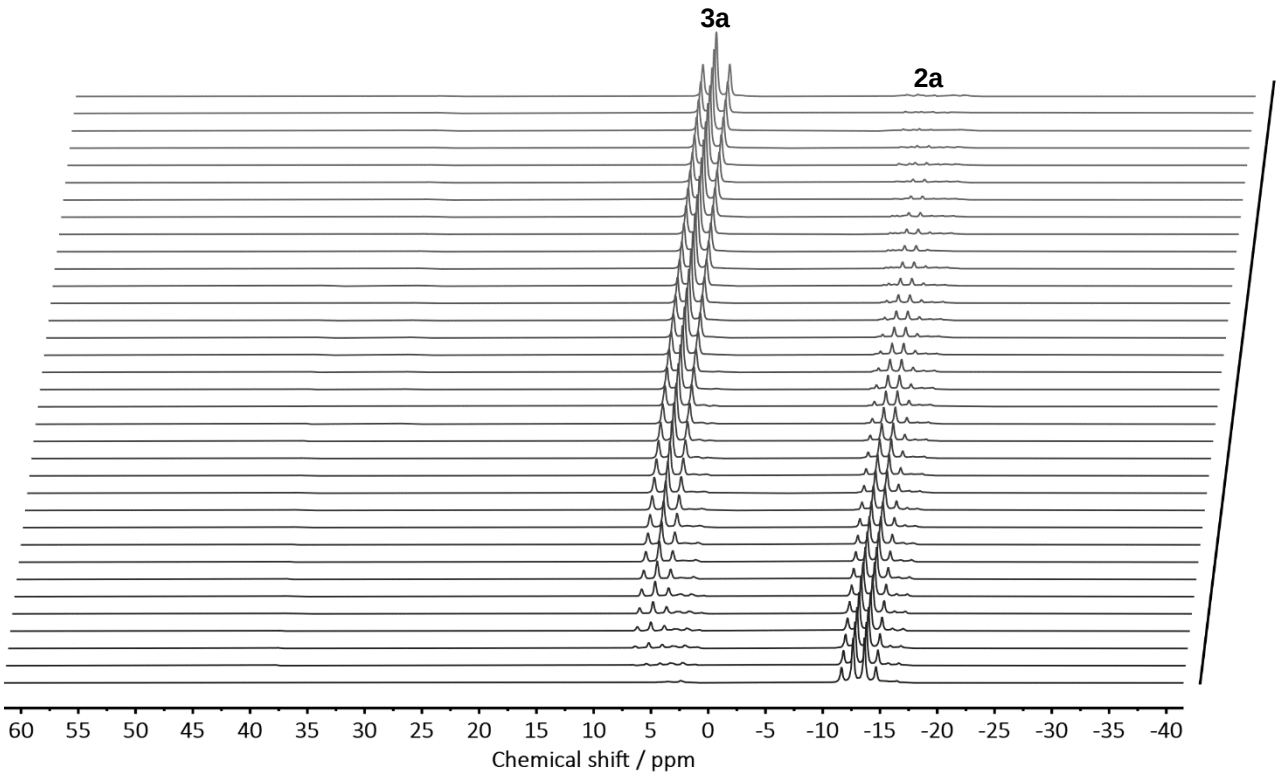


Figure S13. ^{11}B NMR spectra (96.29 MHz, 333 K, dme) of *in-situ* NMR monitoring of the reaction mixture of **2a** with 5 mol% of **1a** at 333 K in interval of 3 min (▼$[Me_2N]_2BH$).

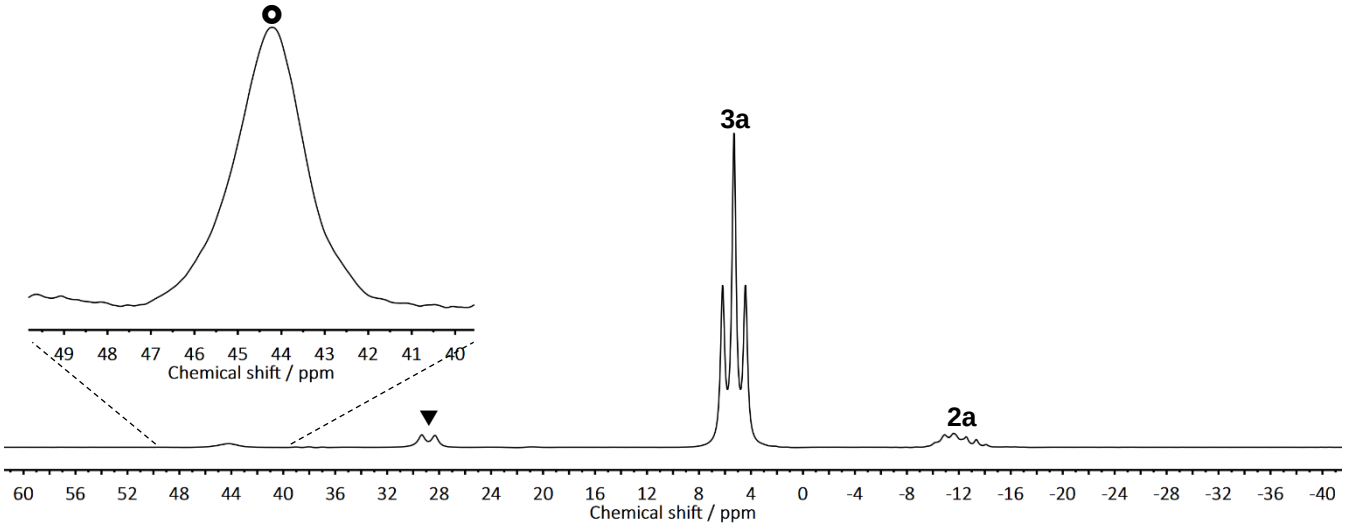


Figure S14. ^{11}B NMR spectrum (128.38 MHz, 293 K, C_6D_6/thf) of the reaction mixture of **2a** with 5 mol% of **1a** at r.t. after 24 h in the presence of cyclohexene (O $Me_2N{=}BCy_2$; ▼$[Me_2N]_2BH$).

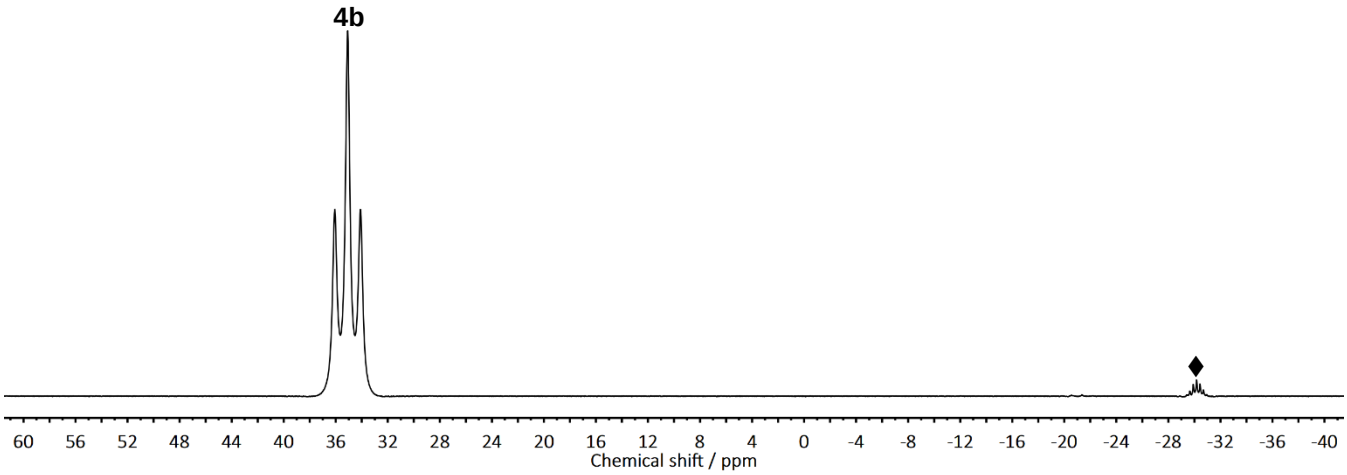


Figure S15. ^{11}B NMR spectrum (128.38 MHz, 293 K, C_6D_6/dme) of the reaction mixture of **2b** with 5 mol% of **1a** at r.t. after 24 h (♦BH_4^-).

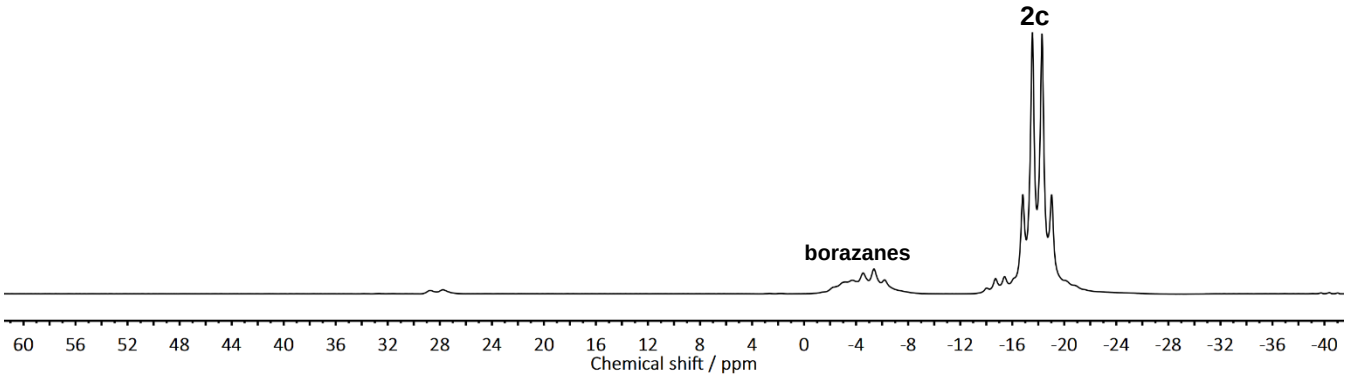


Figure S16. ^{11}B NMR spectrum (128.38 MHz, 293 K, C_6D_6/dme) of the reaction mixture of **2c** with 5 mol% of **1a** at r.t. after 24 h.

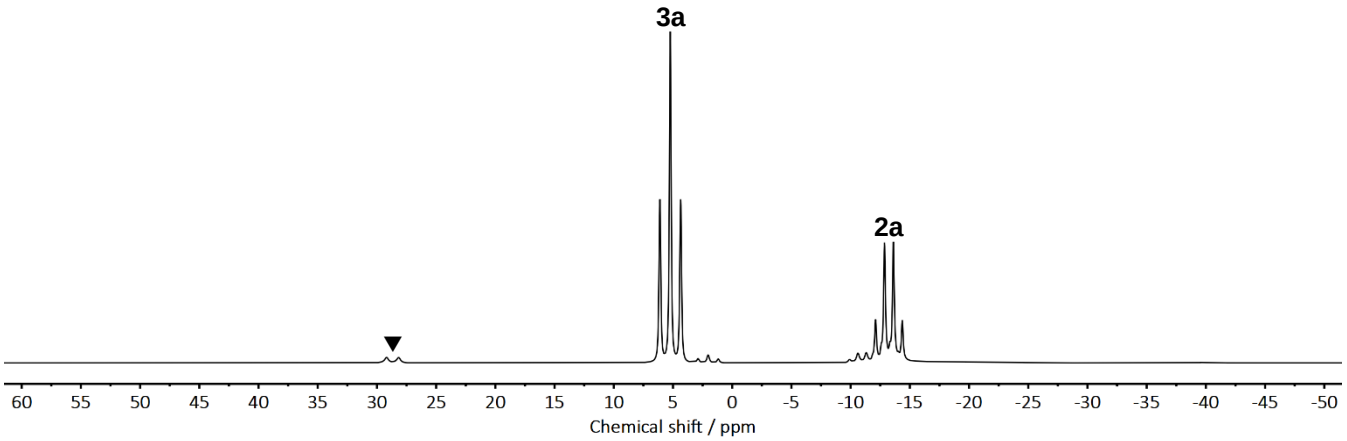


Figure S17. ^{11}B NMR spectrum (128.38 MHz, 294 K, C_6D_6/dme) of the reaction mixture of **3b** with 5 mol% of **1a** at r.t. after 16 h (▼$[Me_2N]_2BH$).

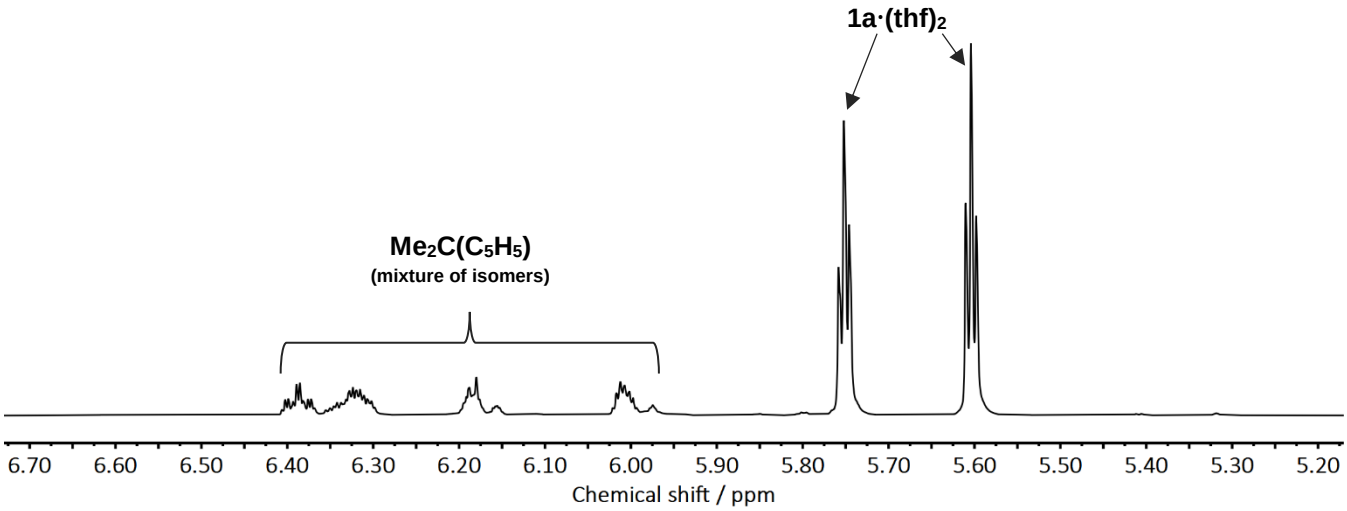


Figure S18. Part of the ^{1}H NMR spectrum (400.13 MHz, 293 K, thf-D8) of the reaction mixture of 1 eq **1a** with 1 eq **2a** at r.t. after 48 h.

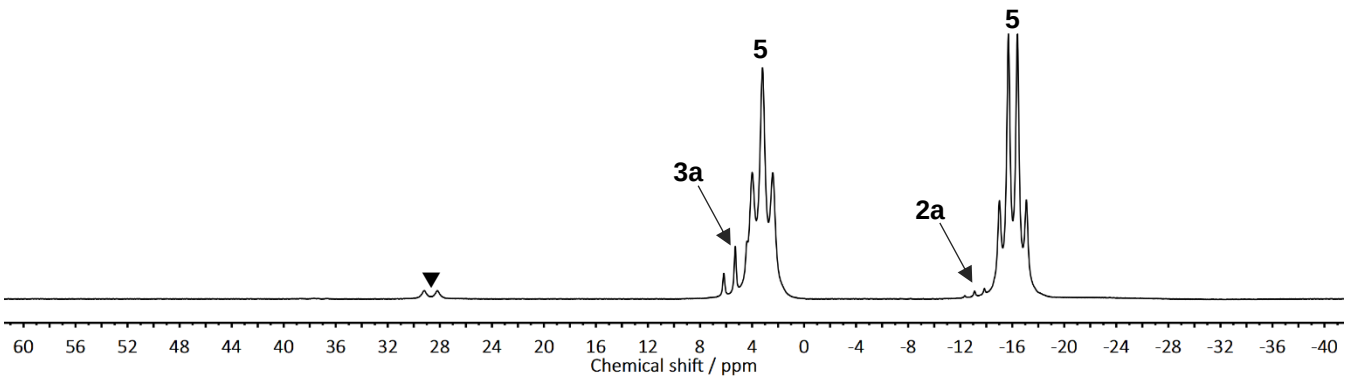


Figure S19. ^{11}B NMR spectrum (128.38 MHz, 293 K, thf-D8) of the reaction mixture of 1 eq **1a** with 1 eq **2a** at r.t. after 48 h (▼$[Me_2N]_2BH$).

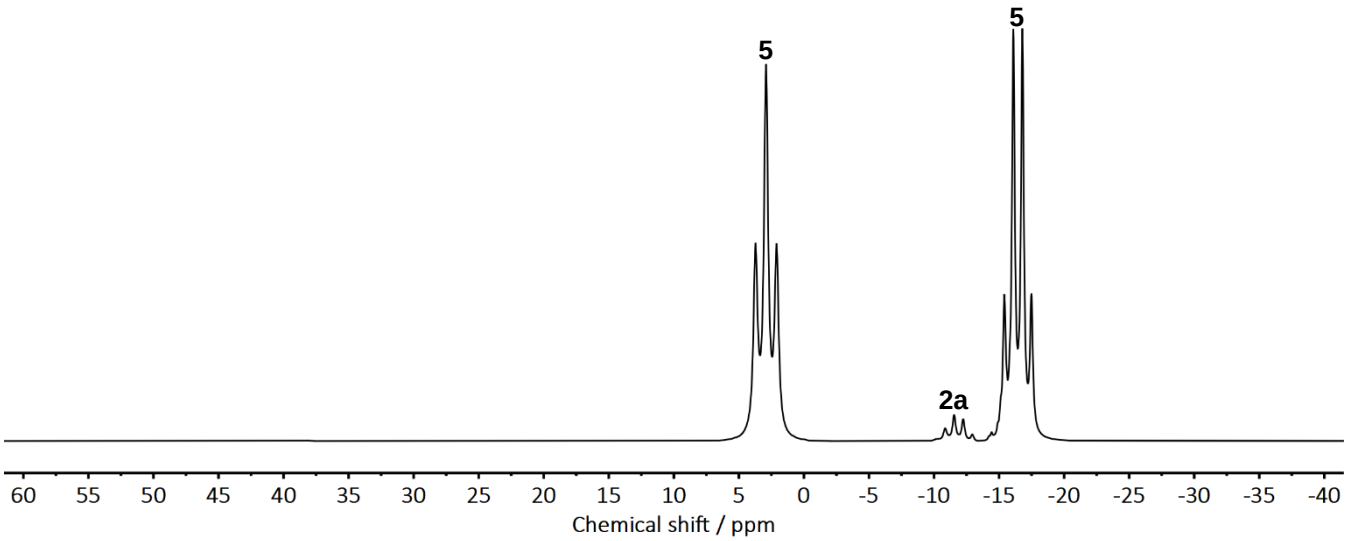


Figure S20. ^{11}B NMR spectrum (128.38 MHz, 293 K, C_6D_6) of magnesium complex **5**.

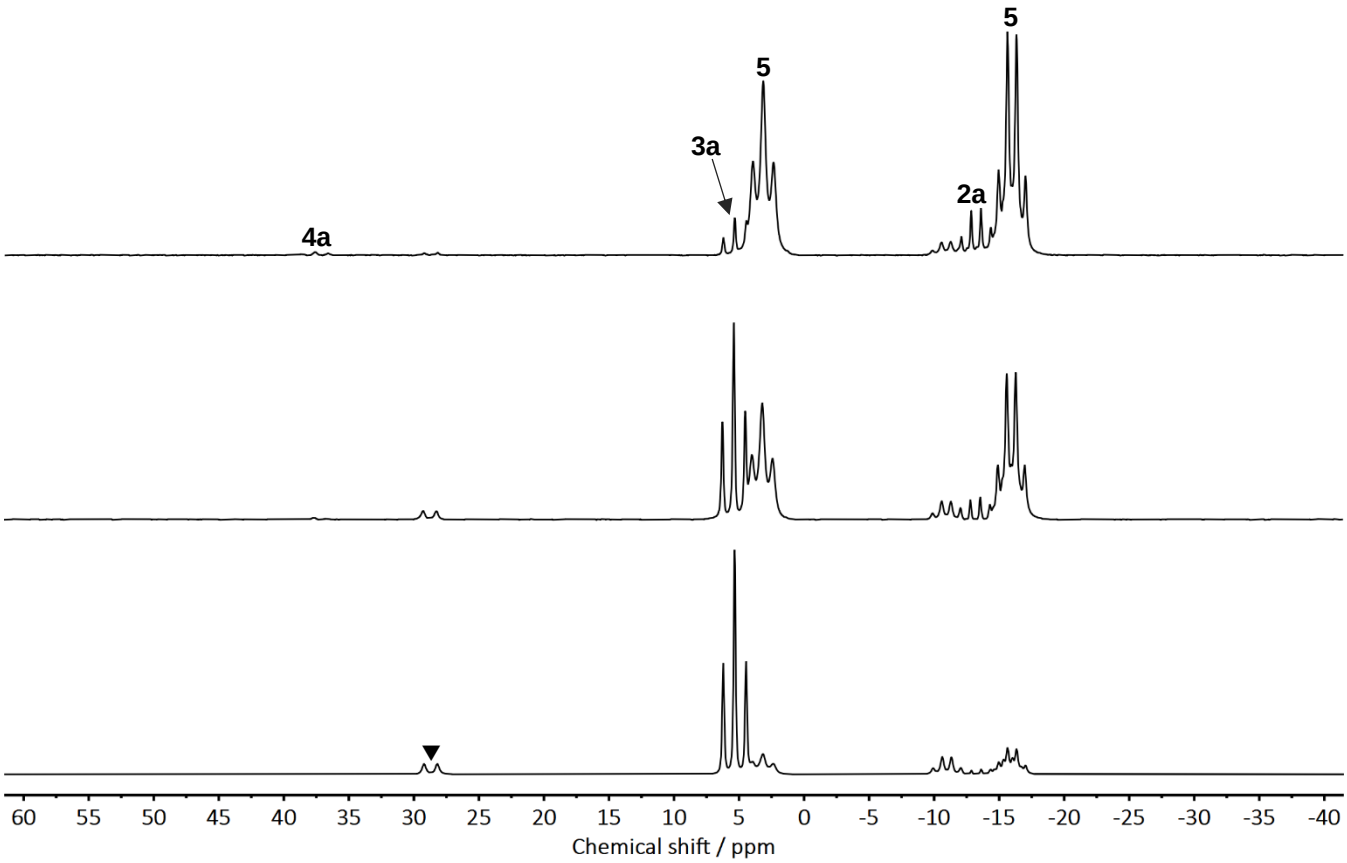


Figure S21. ^{11}B NMR spectra (128.38 MHz, 293 K, dme) of a mixture of magnesium complex **5** and 2,2-dicyclopentadienylpropane at r.t. after 1 h (top), 24 h (center) and 96 h (bottom) (▼$[Me_2N]_2BH$).

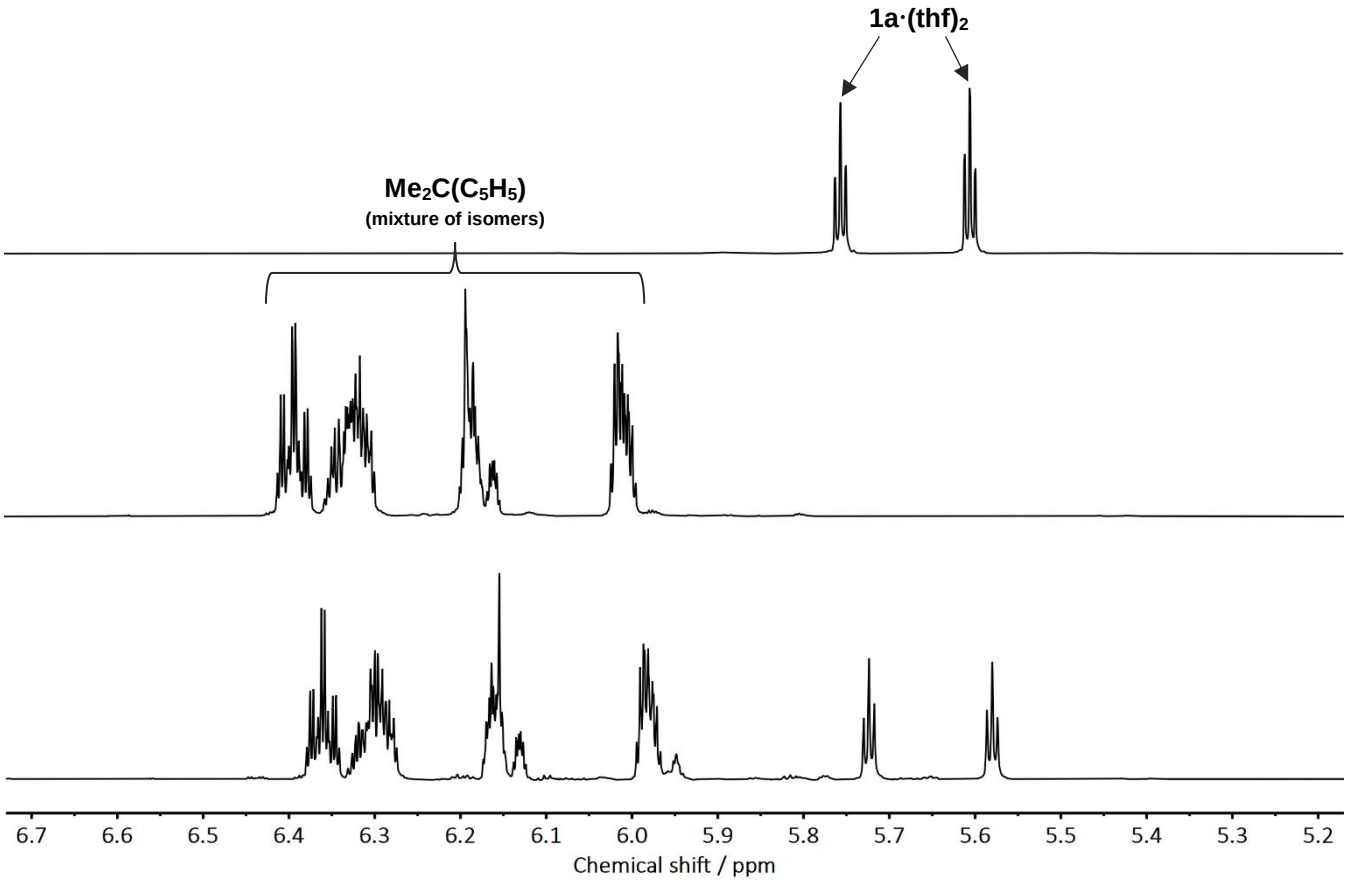


Figure S22. Part of the ^{1}H NMR spectra (400.13 MHz, 294 K, thf-D8) of 2,2-dicyclopentadienylpropane (top), C[1]magnesocenophane·bis(thf), **1a**·(thf)$_2$, (center), and of a mixture of magnesium complex **5** and 2,2-dicyclopentadienylpropane (bottom) at r.t. after 2 h.

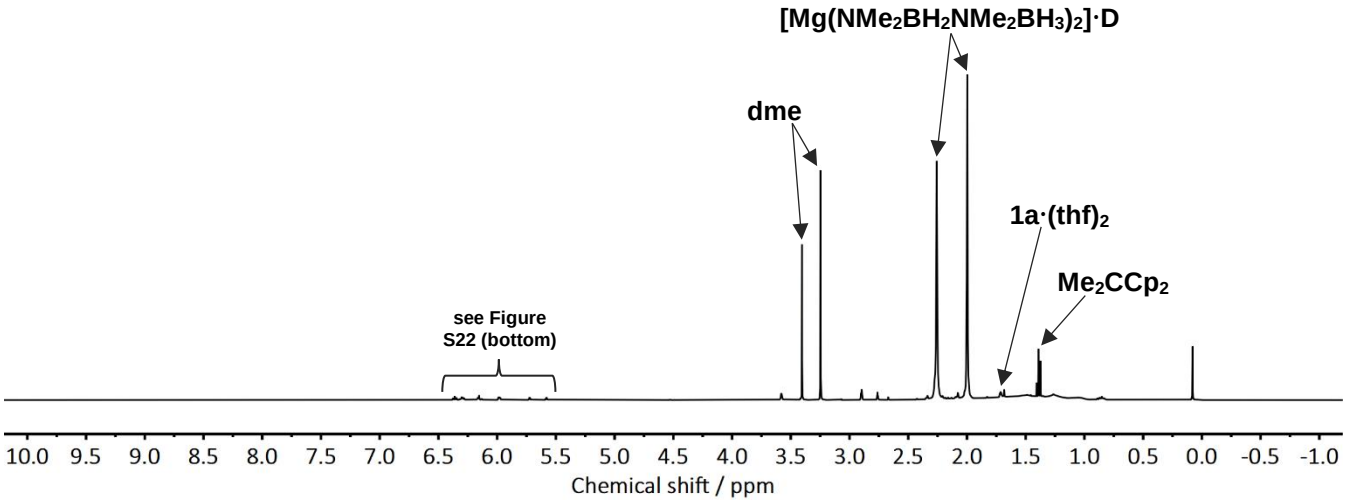


Figure S23. ^{1}H NMR spectrum (400.13 MHz, 294 K, thf-D8) of a mixture of magnesium complex **5** and 2,2-dicyclopentadienylpropane at r.t. after 2 h.

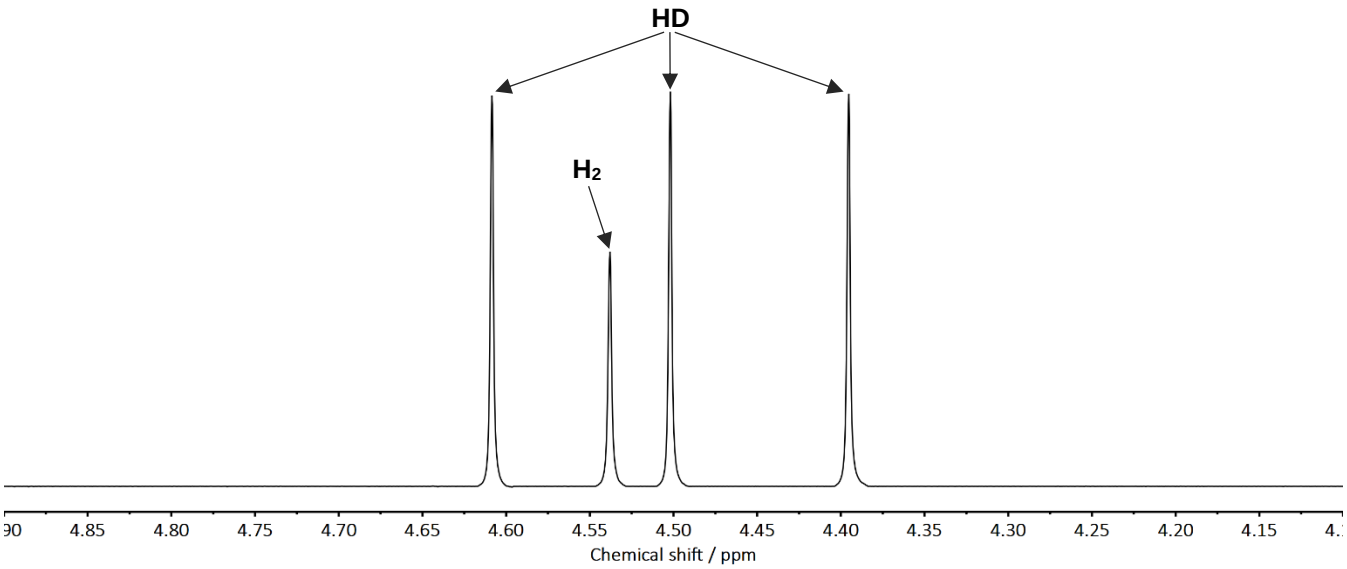


Figure S24. Part of the ^{1}H NMR spectrum (400.13 MHz, 294 K, thf-D8) of the reaction mixture of **2aNDBD** with 10 mol% of **1a** at r.t. after 96 h.

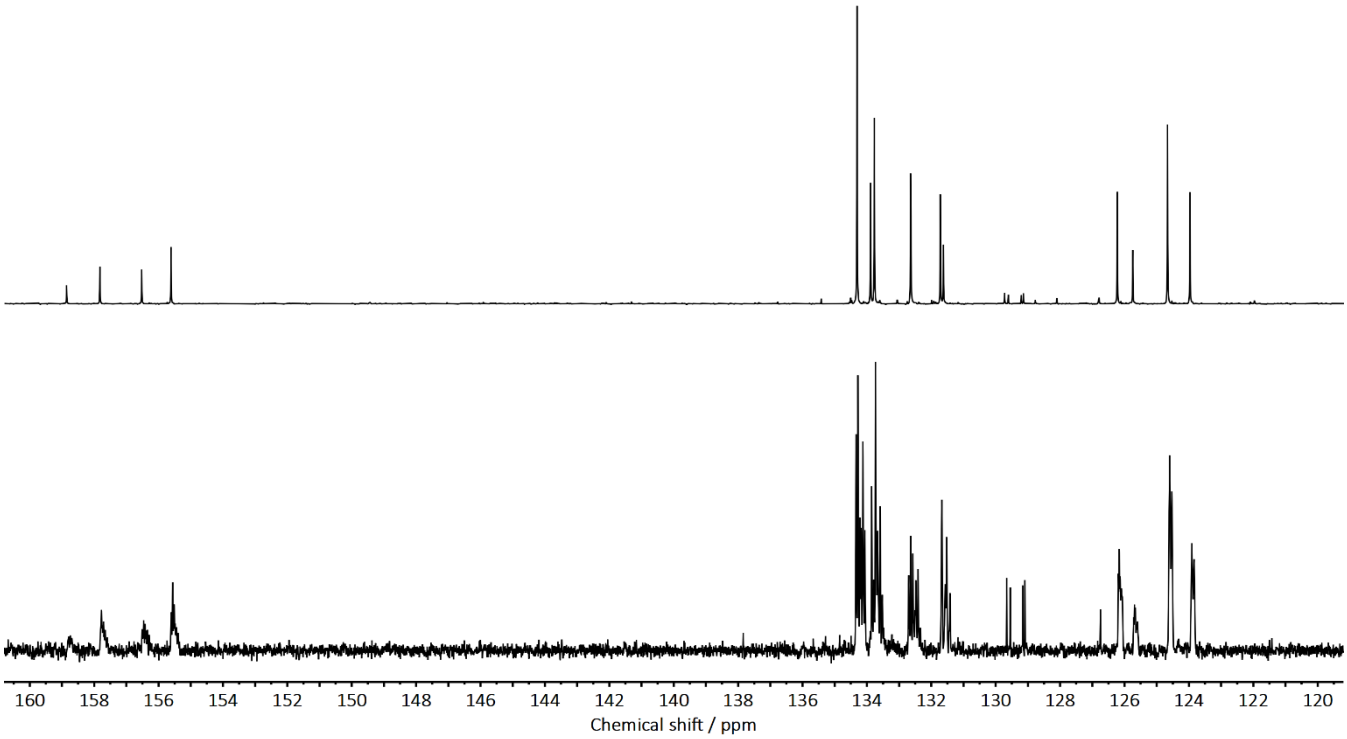


Figure S25. Part of the ^{13}C NMR spectra (100.62 MHz, 293 K, thf-D8) of 2,2-dicyclopentadienylpropane (top), and of the reaction mixture of **2aNDBD** with 10 mol% of **1a** at r.t. after 96 h (bottom).

MS spectra

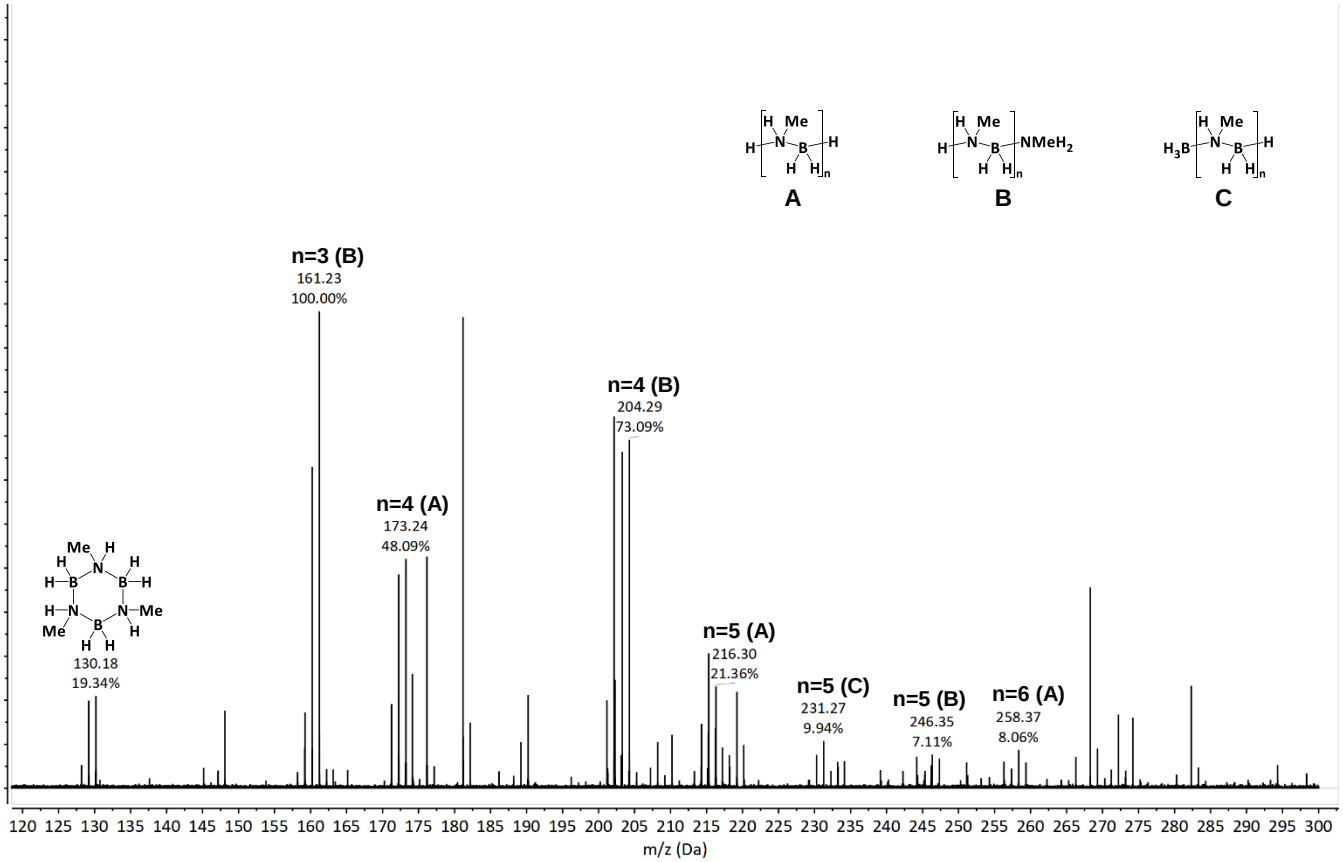


Figure S26. MS spectrum (ESI) of the reaction mixture of **2c** with 10 mol% of **1a** after 72 h

XRD data

Crystal structure data has been deposited with the Cambridge Crystallographic Data Centre (CCDC) and is available free of charge from the Cambridge Structural Database.

crystal structure data of 1a·dme
(this compound was crystallized in two different modification)

CCDC code:	1921397		1971379	
empirical formula	$C_{17}H_{24}MgO_2$		$C_{17}H_{24}MgO_2$	
formula weight	284.67		189.78	
temperature	212(2) K		132(2) K	
wavelength	0.71073 Å		0.71073 Å	
crystal system	monoclinic		orthorhombic	
space group	*C*2/c		*Pbca*	
unit cell dimensions	a = 9.5539(9) Å	α = 90°	a = 14.3619(4) Å	α= 90°
	b = 13.3525(9) Å	β = 97.564(3)°	b = 14.5325(5) Å	β= 90°
	c = 12.4343(8) Å	γ = 90°	c = 15.0215(5) Å	γ = 90°
volume	1572.4(2) $Å^3$		3135.20(17) $Å^3$	
Z	4		12	
density (calculated)	1.202 mg m^{-3}		1.206 Mg/m^3	
absorption coefficient	0.112 mm^{-3}		0.112 mm^{-1}	
F(000)	616		1232	
crystal size	0.273 x 0.184 x 0.174 mm^3		0.382 x 0.376 x 0.344 mm^3	
theta range for data collection	2.637 to 32.665°		2.411 to 30.396°	
index ranges	-11 ≤ h ≤ 14, -19 ≤ k ≤ 20, -18 ≤ l ≤ 18		-20<=h<=20, -15<=k<=20, -21<=l<=21	
reflections collected	16705		31413	
independent reflections	2888 [R(int) = 0.0358]		4684 [R(int) = 0.0236]	
completeness to theta = 25.242°	100.0%		99.8%	
absorption correction	semi-empirical from equivalents		semi-empirical from equivalents	
max. and min. transmission	0.7464 and 0.7216		0.7460 and 0.7152	
refinement method	full-matrix least-squares on F^2		full-matrix least-squares on F^2	
data / restraints / parameters	2888 / 0 / 140		4684 / 0 / 185	
goodness-of-fit on F^2	1.034		1.051	
final R indices [I>2sigma(I)]	R1 = 0.0532, wR2 = 0.1404		R1 = 0.0346, wR2 = 0.0840	
R indices (all data)	R1 = 0.0780, wR2 = 0.1602		R1 = 0.0487, wR2 = 0.0915	
extinction coefficient	n/a		n/a	
largest diff. peak and hole	0.238 and -0.551 e.$Å^{-3}$		0.362 and -0.221 e.$Å^{-3}$	

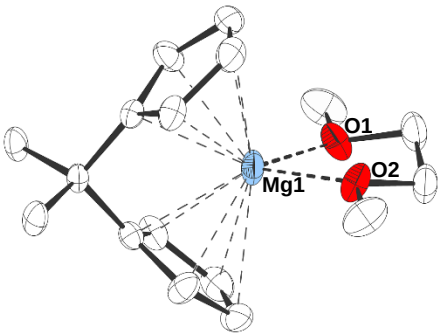


Figure S27. Molecular structure of 1a**·dme** in the crystal (thermal ellipsoids at 30% probability level; hydrogen atoms omitted for clarity; selected bond length and angles: Mg1-O1/O2: 205.3 pm, Mg1-$Cp^{centroid}$: 230.4 pm, α = 80.1°).

crystal structure data of 5

CCDC code:	1971378	
empirical formula	$C_{20}H_{78}B_8Mg_2N_8O_2$	
formula weight	598.00	
temperature	173(2) K	
wavelength	0.71073 Å	
crystal system	monoclinic	
space group	$P2_1/c$	
unit cell dimensions	a = 8.6472(4) Å	α = 90°
	b = 9.4595(6) Å	β = 93.600(2)°
	c = 23.9567(16) Å	γ = 90°
volume	1955.7(2) $Å^3$	
Z	2	
density (calculated)	1.015 mg m^{-3}	
absorption coefficient	0.090 mm^{-1}	
F(000)	668	
crystal size	0.318 x 0.201 x 0.138 mm^3	
theta range for data collection	2.315 to 33.271°	
index ranges	-13 ≤ h ≤ 12, -11 ≤ k ≤ 14, -34 ≤ l ≤ 36	
reflections collected	24493	
independent reflections	7446 [R(int) = 0.0362]	
completeness to theta = 25.242°	99.9%	
absorption correction	semi-empirical from equivalents	
max. and min. transmission	0.7465 and 0.7035	
refinement method	full-matrix least-squares on F^2	
data / restraints / parameters	7446 / 0 / 336	
goodness-of-fit on F^2	1.027	
final R indices [I>2sigma(I)]	R1 = 0.0452, wR2 = 0.1026	
R indices (all data)	R1 = 0.0701, wR2 = 0.1140	
extinction coefficient	n/a	
largest diff. peak and hole	0.262 and -0.234 e.$Å^{-3}$	

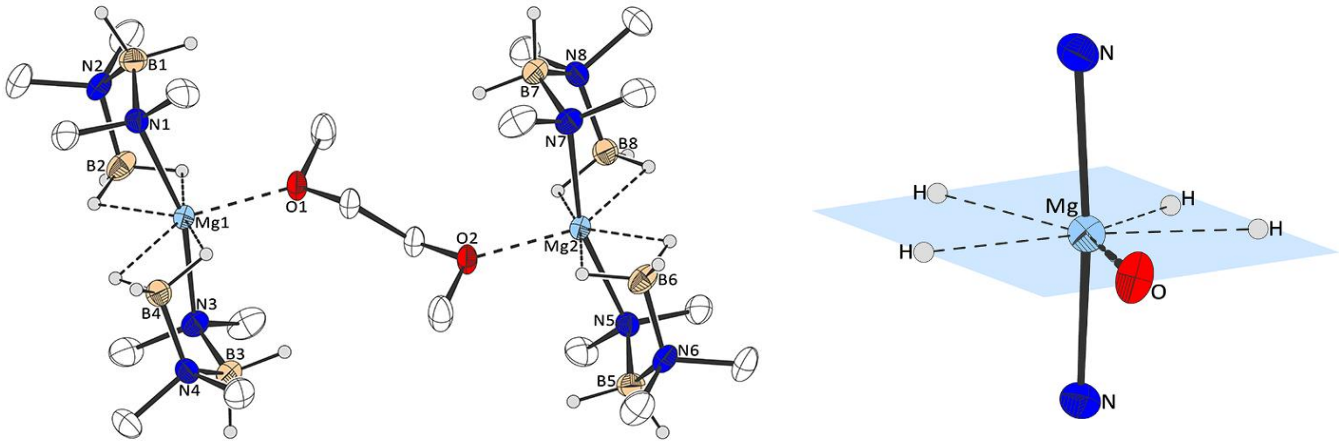


Figure S28. Molecular structure of magnesium complex **5** (left) and of coordination environment of magnesium in **5** (right) in the crystal (thermal ellipsoids at 50% probability level; hydrogen atoms except for (B)-H omitted for clarity; selected bond length: Mg1/2-O1/2: 218.1 pm, Mg1/2-N1/3/5/7: 216.1 pm / 215.9 pm).

Computational Details

All calculations were performed using the Gaussian 09, Revision D.01 package of programs.[11] All geometry optimizations have been carried out at the B3LYP-D3[12]/def2-TZVP[13] level of theory. Every optimized structure was confirmed to be either a minimum or a maximum on the potential energy surface by a subsequent frequency analysis (all positive eigenvalues for minima, one negative eigenvalue for maxima (transition state)) All transition states very verified to be connected to the corresponding minima by calculations along the intrinsic reaction coordinate.

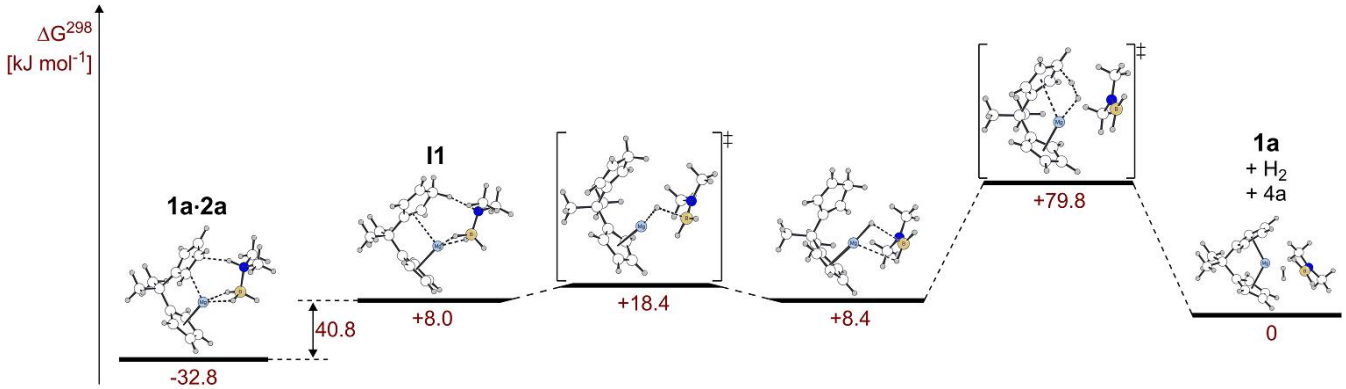
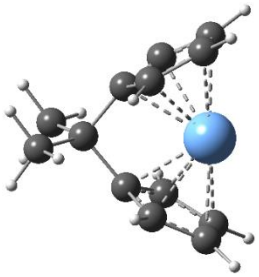


Figure S29. Calculated reaction pathway for the dehydrogenation reaction of dimethylamine borane, **2a**, with magnesocenophane, **1a**, without solvent coordination.

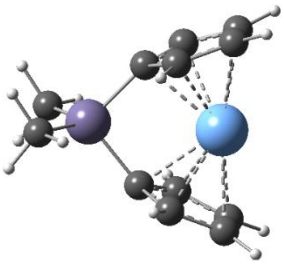
optimized geometry of 1a

Mg	0.00000000	1.39696500	0.00000000
C	0.00000000	-1.54543800	0.00000000
C	1.20375100	-0.57238400	0.00000400
C	-1.20375100	-0.57238400	-0.00000400
C	1.62587400	0.16403700	-1.13915500
C	-1.62587400	0.16403700	1.13915500
C	2.24721400	1.36448900	-0.71281100
C	-2.24721400	1.36448900	0.71281100
C	-1.62587700	0.16404400	-1.13915900
C	1.62587700	0.16404300	1.13915900
C	-2.24721400	1.36449500	-0.71280800
C	2.24721400	1.36449500	0.71280800
H	1.43358900	-0.09937400	-2.16689100
H	-1.43358900	-0.09937400	2.16689100
C	0.00000300	-2.43862400	-1.24534700
C	-0.00000300	-2.43862400	1.24534700
H	2.72675900	2.09524200	-1.34546600
H	-2.72675900	2.09524200	1.34546600
H	-1.43358800	-0.09935100	-2.16689800
H	1.43358800	-0.09935100	2.16689800
H	-2.72675500	2.09525300	-1.34545900
H	2.72675500	2.09525300	1.34545900
H	-0.88609200	-3.07573100	-1.25256500
H	0.88608200	-3.07575600	-1.25254500
H	0.00002000	-1.86210100	-2.16950400
H	0.88609200	-3.07573100	1.25256500
H	-0.88608200	-3.07575600	1.25254500
H	-0.00002000	-1.86210100	2.16950400



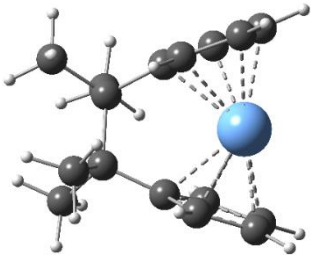
optimized geometry of 1b

Mg	1.45066400	-0.00000800	0.00000000
C	1.66313100	-2.23195100	-0.71283000
C	1.66313100	-2.23195500	0.71282900
C	0.40191000	-1.74897900	-1.13855300
H	2.45344100	-2.60614600	-1.34565800
C	0.40191200	-1.74898700	1.13855700
H	2.45344200	-2.60615300	1.34565400
C	-0.39469600	-1.42146100	0.00000300
H	0.11425400	-1.59657000	-2.16846100
H	0.11425700	-1.59658500	2.16846600
C	0.40192900	1.74898500	-1.13855800
C	-0.39468100	1.42146400	-0.00000300
C	1.66315400	2.23194000	-0.71282900
H	0.11427200	1.59659300	-2.16846800
C	0.40192900	1.74897500	1.13855400
C	1.66315400	2.23193500	0.71282900
H	2.45346700	2.60613300	-1.34565400
H	0.11427100	1.59657600	2.16846200



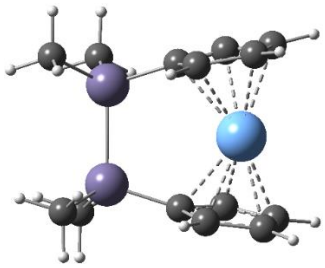
H	2.45346700	2.60612200	1.34565700
C	-2.68176100	0.00002200	1.55568100
H	-3.32031900	0.88508000	1.59655800
H	-3.32030900	-0.88504300	1.59657700
H	-2.05573000	0.00003600	2.45059500
C	-2.68176300	-0.00000100	-1.55568000
H	-3.32035100	-0.88504000	-1.59653200
H	-3.32028300	0.88508400	-1.59660000
H	-2.05573300	-0.00006100	-2.45059400
Si	-1.63787200	0.00001000	0.00000000

optimized geometry of 1c



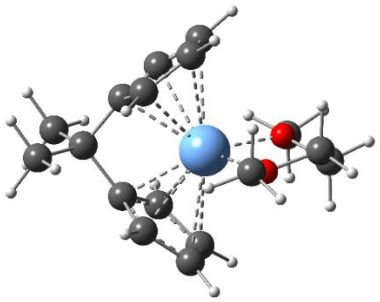
C	0.08349600	-1.44526900	-0.03551700
C	1.78859900	-0.85720400	-1.75453400
C	2.51381900	-1.59843300	0.48416100
C	0.08292100	1.44539400	0.03532200
C	1.78823100	0.85768700	1.75450600
C	2.51336000	1.59925000	-0.48410100
Mg	-1.73881900	-0.00025700	0.00066000
C	-0.56839800	-1.65880100	1.20772000
C	-0.84365900	-1.82207600	-1.04637600
H	1.12767100	-0.25370600	-2.37429000
H	2.81089100	-0.53128400	-1.93755100
H	1.71062600	-1.89045700	-2.09507500
H	3.49996800	-1.13763200	0.39570200
H	2.57123600	-2.59589700	0.04500300
H	2.28698200	-1.72251400	1.54133100
C	-0.84421600	1.82240400	1.04614700
C	-0.56920700	1.65819200	-1.20790800
H	1.12740300	0.25398000	2.37416800
H	2.81059200	0.53200000	1.93755700
H	1.70999700	1.89088900	2.09513400
H	3.49967200	1.13884100	-0.39539800
H	2.57030100	2.59678900	-0.04505400
H	2.28665500	1.72310400	-1.54132600
H	-0.15084300	-1.46405800	2.18168600
C	-1.88458300	-2.12324800	0.97215400
H	-2.60476200	-2.40166100	1.72571200
C	-2.06096600	-2.22717700	-0.43474100
C	-2.06179000	2.22672500	0.43445700
H	-2.92869300	2.62017000	0.94206900
C	-1.88551200	2.12222600	-0.97239900
H	-2.60591400	2.39995600	-1.72599700
H	-0.15170900	1.46313600	-2.18183100
H	-0.67475300	-1.78350900	-2.10975400
H	-0.67514500	1.78444700	2.10952200
H	-2.92781400	-2.62064400	-0.94243200
C	1.43854300	-0.77791900	-0.25691800
C	1.43827500	0.77844000	0.25684500

optimized geometry of 1d



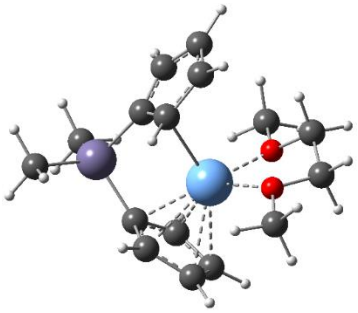
Si	1.49585900	1.19319100	0.10085200
Si	1.49589000	-1.19318900	-0.10062700
C	-0.28687300	1.75530900	-0.04402700
C	2.15382800	1.70788300	1.79351000
C	2.52547900	1.98847800	-1.26609400
C	-0.28686000	-1.75528000	0.04400700
C	2.15402400	-1.70766800	-1.79328900
C	2.52539800	-1.98862100	1.26631200
Mg	-1.83886300	-0.00001000	-0.00010100
C	-1.06743100	1.81686400	-1.23787200
C	-1.19579400	1.97950900	1.03361600
H	1.56905600	1.25759700	2.59884900
H	3.19025200	1.38870600	1.92336400
H	2.11374800	2.79303600	1.91512800
H	3.56278800	1.64763100	-1.22757800
H	2.52006000	3.07696000	-1.17090000
H	2.13158600	1.73629800	-2.25310800
C	-1.19564500	-1.97951000	-1.03374500
C	-1.06755900	-1.81688000	1.23776000
H	1.56929000	-1.25731900	-2.59862100
H	3.19043300	-1.38839000	-1.92301200
H	2.11403200	-2.79280800	-1.91504700
H	3.56267600	-1.64765900	1.22799900
H	2.52010100	-3.07708600	1.17090200
H	2.13133800	-1.73667900	2.25331800
H	-0.69223800	1.68093300	-2.24142000
C	-2.41953800	2.06801400	-0.90127700
H	-3.23661000	2.19728800	-1.59438800
C	-2.50050500	2.16818800	0.51459400
C	-2.50041200	-2.16822600	-0.51488100
H	-3.38834400	-2.39200200	-1.08602100
C	-2.41961800	-2.06806200	0.90100000
H	-3.23676900	-2.19736500	1.59401200
H	-0.69249400	-1.68098000	2.24136100
H	-0.93488200	1.99552500	2.08101900
H	-0.93460500	-1.99552900	-2.08111600
H	-3.38851100	2.39195300	1.08562600

optimized geometry of 1a·dme



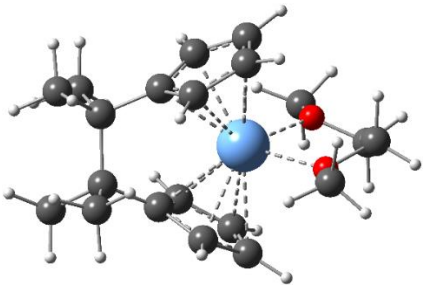
Mg	0.32566600	0.00000000	0.00000000
O	1.99565000	0.57042600	1.18448500
O	1.99564800	-0.57042500	-1.18448500
C	-2.59748200	0.00000000	0.00000100
C	-1.65150300	1.05711700	-0.58813900
C	-1.65150200	-1.05711700	0.58814000
C	-0.96485400	2.04853700	0.16122300
C	-0.96485400	-2.04853700	-0.16122300
C	0.10205600	2.55494100	-0.62428800
C	0.10205600	-2.55494200	0.62428700
C	-0.97470900	-0.94870200	1.83338200
C	-0.97471000	0.94870100	-1.83338200
C	0.09222300	-1.87756300	1.85517600
C	0.09222200	1.87756300	-1.85517600
C	3.21406400	0.61080400	0.44489000
C	3.21406200	-0.61080700	-0.44488900
C	1.87434800	1.56424100	2.20375300
C	1.87434600	-1.56423900	-2.20375500
H	-1.21967200	2.37528500	1.15744400
H	-1.21967300	-2.37528500	-1.15744400
H	0.90039600	1.41455300	2.66190700
H	0.90039300	-1.41454900	-2.66190900
C	-3.49641700	0.60671700	1.08584600
C	-3.49641800	-0.60671700	-1.08584400
H	0.76932500	3.35747900	-0.34518600
H	0.76932500	-3.35747900	0.34518500
H	-1.23809500	-0.27909500	2.63741800
H	-1.23809700	0.27909400	-2.63741800
H	0.76907000	-2.04353200	2.67981700
H	0.76906800	2.04353200	-2.67981800
H	3.24711500	1.52722800	-0.15370500
H	4.07119700	0.58530800	1.12451300
H	3.24711100	-1.52723100	0.15370500
H	4.07119600	-0.58531300	-1.12451300
H	2.66348900	1.42895200	2.94723300
H	1.92411100	2.56511700	1.77029600
H	2.66348700	-1.42894800	-2.94723500
H	1.92410900	-2.56511600	-1.77030000
H	-4.13336000	-0.16387200	1.52442900
H	-4.13139800	1.38467300	0.65777200
H	-2.92014500	1.05791400	1.89255100
H	-4.13336100	0.16387200	-1.52442700
H	-4.13139900	-1.38467200	-0.65777000
H	-2.92014700	-1.05791400	-1.89255000

optimized geometry of 1b·dme



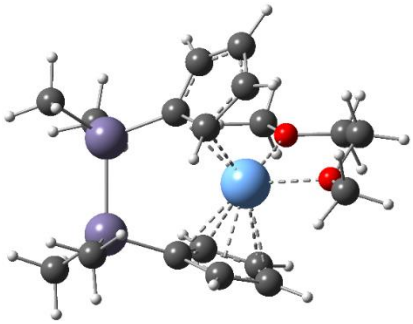
Mg	-0.54055000	-0.41486900	-0.03170900
O	-2.51850000	-0.53057600	-0.82866700
O	-1.66611500	0.73687500	1.31019100
C	1.32304100	1.17555600	-0.63982400
C	-0.48463400	2.13274900	-1.73861400
C	0.31378200	0.96414800	-1.65926400
H	0.35795200	0.19903800	-2.42882900
C	1.07340700	2.45818700	-0.11116200
H	1.62552800	2.91187700	0.70123300
C	-0.02285000	3.04127400	-0.78086000
C	1.47424700	-1.52185700	0.40130900
C	0.72059900	-1.57021200	1.61228700
H	0.97083900	-1.05063000	2.52605300
C	-0.40645400	-2.40447500	1.43046100
C	-0.37141300	-2.88966900	0.10385100
C	0.77427600	-2.34891200	-0.52600400
H	1.06751900	-2.52617400	-1.55066700
C	-2.88144600	1.21654600	0.72555700
H	-2.63915600	2.02058900	0.02626300
C	-3.51635500	0.04205600	0.01787100
C	-2.98930100	-1.57595000	-1.67903500
H	-2.13492500	-1.92177900	-2.25461400
C	-1.09658700	1.61333200	2.29328700
H	-0.13959400	1.18273800	2.57234100
C	3.53620200	0.55741900	1.39438500
C	3.74768700	-0.59525500	-1.46787000
H	-1.29066400	2.29671100	-2.44084100
H	-0.43518600	4.02266900	-0.58671700
H	-1.14250300	-2.65444800	2.17986900
H	-1.07220600	-3.58424400	-0.33479300
H	-3.55399300	1.58495200	1.50558600
H	-4.36876000	0.37982300	-0.57946400
H	-3.85465900	-0.71223000	0.73676500
H	-3.38612100	-2.40463600	-1.08701200
H	-3.75971500	-1.19004300	-2.35087200
H	-1.75817400	1.66163600	3.16188600
H	-0.93201600	2.60029300	1.86278700
H	4.25233100	-0.18601700	1.75111100
H	4.08759500	1.46402600	1.13511000
H	2.86638500	0.80223300	2.22175500
H	3.19163600	-0.99299800	-2.31999400
H	4.32189500	0.26397900	-1.82188500
H	4.44765000	-1.36495900	-1.13391000
Si	2.57690400	-0.08885600	-0.08722100

optimized geometry of 1c·dme



C	-1.18832700	1.40380200	-0.29017100
C	-2.85304100	0.46950300	-1.89571200
C	-3.62803300	1.65069700	0.12287300
C	-1.18834300	-1.40380200	0.29018800
C	-2.85308300	-0.46949300	1.89569400
C	-3.62804400	-1.65067700	-0.12290600
Mg	0.73949200	-0.00000800	0.00001100
C	-0.58525200	1.91384000	0.88809200
C	-0.28500800	1.68026400	-1.35457100
H	-2.16177600	-0.22497600	-2.36913900
H	-3.86297700	0.08387100	-2.02671300
H	-2.79333500	1.41627300	-2.43388000
H	-4.61101900	1.17348300	0.11471600
H	-3.67954500	2.53325800	-0.51725600
H	-3.42236100	1.99702700	1.13371900
C	-0.28503800	-1.68025300	1.35460300
C	-0.58525300	-1.91384900	-0.88806300
H	-2.16182400	0.22498400	2.36913500
H	-3.86302000	-0.08385800	2.02667400
H	-2.79338900	-1.41626400	2.43386100
H	-4.61102400	-1.17345300	-0.11476300
H	-3.67957300	-2.53323800	0.51722100
H	-3.42235900	-1.99700700	-1.13374900
H	-1.00962900	1.89161900	1.87834100
C	0.64928000	2.51641300	0.54697800
H	1.31866700	3.01429300	1.23197200
C	0.83408300	2.37629600	-0.83690400
C	0.83406000	-2.37629000	0.83695700
H	1.68109700	-2.72149300	1.40913300
C	0.64927600	-2.51641900	-0.54692700
H	1.31867300	-3.01430600	-1.23190700
H	-1.00961600	-1.89163700	-1.87831700
O	2.48948800	0.09170200	1.31305100
O	2.48945800	-0.09172200	-1.31307500
C	3.70595100	0.39814500	0.64248200
C	3.70594500	-0.39813800	-0.64253700
C	2.41347100	0.54689800	2.66134800
H	1.42563800	0.27502000	3.02432200
C	2.41341300	-0.54691700	-2.66137000
H	1.42558000	-0.27502300	-3.02432900
H	-0.44484300	1.45074800	-2.39563600
H	-0.44488600	-1.45072700	2.39566300
H	1.68112700	2.72150500	-1.40906700
H	3.74812800	1.47236600	0.43350900
H	4.56367400	0.11337700	1.26030200
H	3.74815600	-1.47235800	-0.43356700
H	4.56364500	-0.11334800	-1.26037800
H	3.18010600	0.05328100	3.26455000
H	2.53471500	1.63108700	2.71337400
H	3.18004600	-0.05331200	-3.26458400
H	2.53464200	-1.63110800	-2.71339700
C	-2.53288400	-0.69944000	0.40615200
C	-2.53287000	0.69945000	-0.40616400

optimized geometry of 1d·dme

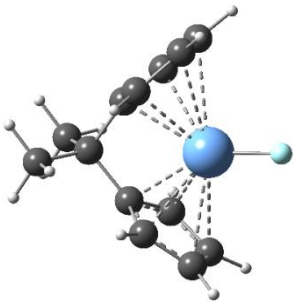


Si	2.16096100	1.30493500	0.12679900
Si	2.64376600	-0.98008300	-0.21886100
C	0.39925200	1.58910900	-0.41320300
C	2.30839400	1.69676400	1.97648100
C	3.33513000	2.45911900	-0.80489400
C	1.03104600	-1.83220500	0.17663000
C	3.11146300	-1.36195300	-2.00900900
C	4.01553500	-1.59630400	0.92544000
Mg	-0.92900200	-0.45249900	-0.03845600
C	-0.21879900	1.10677000	-1.63295600
C	-0.41629700	2.66551300	0.02592900
H	1.76012300	0.97190400	2.58254500
H	3.35159600	1.67213100	2.29984000
H	1.91482900	2.69203700	2.19911700
H	4.37515300	2.29851100	-0.50814400
H	3.08107500	3.50383700	-0.60815900
H	3.26120700	2.29647700	-1.88217800
C	0.15632500	-2.50088600	-0.72888300
C	0.36638200	-1.83006300	1.43829400
H	2.34253300	-1.01943200	-2.70457700
H	4.04645100	-0.86770400	-2.28200200
H	3.24312800	-2.43737600	-2.15433500
H	4.95187000	-1.06176800	0.74644700
H	4.19718700	-2.66296400	0.77129700
H	3.74339500	-1.45168700	1.97318400
H	0.24277800	0.42313000	-2.33572400
C	-1.35276300	1.90321400	-1.89954600
H	-1.99701300	1.81409000	-2.76309100
C	-1.47363500	2.85377400	-0.87275300
C	-0.99894400	-2.91836000	-0.03129900
H	-1.83966500	-3.44984600	-0.44995600
C	-0.87193000	-2.49973100	1.30998900
H	-1.59194900	-2.66548100	2.09771100
H	0.76151100	-1.41494000	2.35406300
O	-2.95424700	-0.74326000	-0.76357500
O	-2.15865900	0.47878900	1.39503400
C	-3.87961200	0.17887400	-0.18557900
C	-3.55818300	0.23640400	1.28934000
C	-3.21752800	-1.07178400	-2.12727800
H	-2.40983700	-1.72472000	-2.44933200
C	-1.70270100	0.84444500	2.69588800

H	-0.63673400	1.03227700	2.61063400
H	-0.24882600	3.24670500	0.92251400
H	0.35877100	-2.67934800	-1.77472000
H	-2.25797300	3.59358500	-0.78479000
H	-3.74093100	1.15999600	-0.64754300
H	-4.90628300	-0.16940900	-0.33577700
H	-3.80254400	-0.70929600	1.78517100
H	-4.11825800	1.04884400	1.76175800
H	-4.17234500	-1.59806100	-2.20543000
H	-3.23078400	-0.17191800	-2.74430200
H	-2.20638100	1.75725300	3.02136000
H	-1.88578600	0.03478700	3.40753200

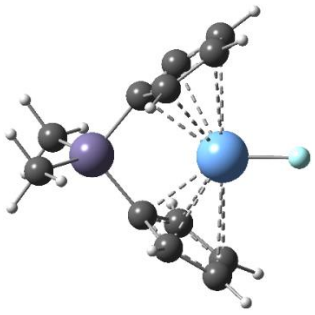
optimized geometry of 1a·F$^-$

Mg	0.00000300	1.25931500	-0.00000300
C	-2.60874200	0.92982400	0.70124200
C	-2.60874200	0.92982000	-0.70124800
C	-1.74300300	-0.10129100	1.13928600
H	-3.14417200	1.61786200	1.33845800
C	-1.74300300	-0.10129700	-1.13928600
H	-3.14417200	1.61785500	-1.33846700
C	-1.21430300	-0.76617100	0.00000200
H	-1.52244700	-0.33915300	2.16900900
H	-1.52244600	-0.33916500	-2.16900700
C	1.74300400	-0.10129200	1.13928600
C	1.21430600	-0.76617400	0.00000200
C	2.60873900	0.92982600	0.70124300
H	1.52244800	-0.33915400	2.16900900
C	1.74300400	-0.10129800	-1.13928500
C	2.60873900	0.92982300	-0.70124700
H	3.14416700	1.61786600	1.33845800
H	1.52244800	-0.33916600	-2.16900700
H	3.14416700	1.61785900	-1.33846700
C	0.00000100	-1.70145500	0.00000500
C	0.00000000	-2.60450800	-1.24215600
H	0.88909200	-3.24017600	-1.24826000
H	-0.88909500	-3.24017400	-1.24826000
H	0.00000000	-2.02628800	-2.16516300
C	-0.00000100	-2.60450200	1.24217100
H	-0.88909500	-3.24016700	1.24827800
H	0.88909200	-3.24016900	1.24827800
H	0.00000000	-2.02627600	2.16517400
F	-0.00000200	3.06209400	-0.00000800



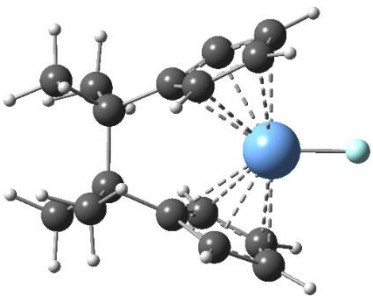
optimized geometry of 1b·F$^-$

Mg	1.31279000	-0.00014100	0.00000000
C	1.22664600	-2.69924400	-0.70286600
C	1.22664900	-2.69924100	0.70286500
C	0.13590300	-1.91953000	-1.13996100
H	1.96436500	-3.16946700	-1.33654800
C	0.13590200	-1.91953200	1.13996000
H	1.96436900	-3.16946200	1.33654700
C	-0.58325700	-1.44089400	0.00000000
H	-0.12672800	-1.72472100	-2.17099500
H	-0.12672900	-1.72472400	2.17099400
C	0.13624900	1.91950100	-1.13996100
C	-0.58300200	1.44100200	0.00000000
C	1.22714200	2.69900200	-0.70286500
H	-0.12642300	1.72474400	-2.17099400
C	0.13625000	1.91949900	1.13996100
C	1.22714200	2.69900200	0.70286600
H	1.96496100	3.16907000	-1.33654600
H	-0.12642100	1.72474200	2.17099500
H	1.96496100	3.16907000	1.33654600
C	-2.83448800	0.00025300	1.54564800
H	-3.47128600	0.88788800	1.58010800
H	-3.47138400	-0.88731000	1.58015200
H	-2.21327600	0.00024200	2.44442300
C	-2.83448700	0.00025300	-1.54564900
H	-3.47138300	-0.88731000	-1.58015400
H	-3.47128700	0.88788700	-1.58010700
H	-2.21327500	0.00024500	-2.44442400
Si	-1.75203500	0.00016000	0.00000000
F	3.11496100	-0.00020900	0.00000000



optimized geometry of 1c·F$^-$

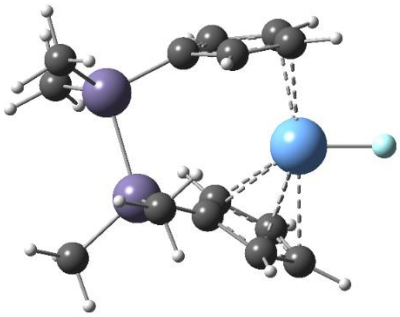
Mg	1.76315900	0.00002300	0.00000500
C	-0.33720800	1.42682400	-0.07243900
C	0.25230200	1.77581400	1.16639000
C	0.59127500	1.80686600	-1.08206100
C	1.51347600	2.36783500	0.92537600
H	-0.17865900	1.61775400	2.14266000
C	1.71981100	2.39884800	-0.46510200
H	0.45839500	1.68802500	-2.14583700
H	2.21445900	2.69709300	1.67734100
H	2.61110500	2.73869300	-0.96826800
C	0.25236100	-1.77582900	-1.16643200
C	1.51355100	-2.36781300	-0.92541600
C	-0.33715800	-1.42684400	0.07239600
H	-0.17859500	-1.61777800	-2.14270300
C	1.71987900	-2.39883200	0.46506100
H	2.21454100	-2.69705400	-1.67738200
C	0.59132600	-1.80687800	1.08201800
H	2.61117600	-2.73866300	0.96823100
H	0.45843700	-1.68804900	2.14579500
C	-1.68295800	-0.75512600	0.29105300



C	-1.68299200	0.75508000	-0.29108500
C	-2.00747100	-0.75885700	1.79835400
H	-3.02486600	-0.41380800	1.98708400
H	-1.92691400	-1.77601700	2.18508600
H	-1.32421300	-0.13331300	2.36886200
C	-2.77986500	-1.61204200	-0.37900700
H	-2.82890600	-2.58424200	0.11645900
H	-3.76554500	-1.14306400	-0.29903600
H	-2.57086400	-1.79742400	-1.43091900
C	-2.77985600	1.61192100	0.37912700
H	-2.82893200	2.58417300	-0.11623400
H	-3.76553700	1.14294200	0.29917700
H	-2.57078200	1.79718600	1.43104900
C	-2.00761300	0.75892000	-1.79836900
H	-3.02498800	0.41380100	-1.98706400
H	-1.92718400	1.77612600	-2.18500500
H	-1.32433600	0.13350600	-2.36899300
F	3.58679300	0.00005800	0.00005000

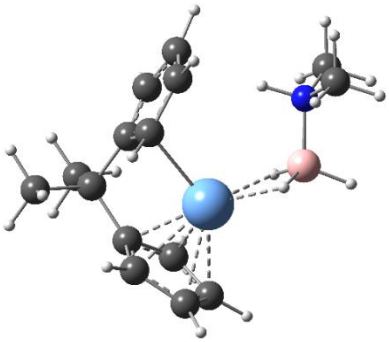
optimized geometry of 1d·F$^-$

Mg	-2.15432600	0.34547800	-0.13671200
C	-0.52603400	-1.43622200	0.19336000
C	-1.03892200	-1.05335800	1.47039900
C	-1.61875000	-2.04811400	-0.49920100
C	-2.39819700	-1.42683100	1.55135200
H	-0.47778900	-0.55082300	2.24334300
C	-2.75217500	-2.04649000	0.33158500
H	-1.58059200	-2.43435600	-1.50749500
H	-3.06204200	-1.23540400	2.38166500
H	-3.74494000	-2.35961600	0.04894700
C	-0.02296300	1.96101400	-1.23172500
C	-1.32391300	2.43356700	-0.98795300
C	0.67249500	1.84379200	0.00508800
H	0.37175800	1.70333500	-2.20570000
C	-1.46094100	2.60711900	0.42430800
H	-2.07658400	2.67402000	-1.72444500
C	-0.23203100	2.25260400	1.01498700
H	-2.32396900	3.02754300	0.92198800
H	-0.03427700	2.23807000	2.07821600
C	2.70732300	0.77499500	2.05816300
H	3.55744900	0.10533300	2.21244800
H	3.01166000	1.78570100	2.34502400
H	1.90796700	0.46134500	2.73265600
C	3.60338600	1.19940700	-0.84311700
H	3.99570800	2.18233800	-0.56674600
H	4.41408800	0.46982700	-0.75770400
H	3.30141800	1.24433100	-1.89216000
C	2.21100600	-2.84273000	0.38358200
H	1.76226300	-3.79138100	0.07498300
H	3.25729800	-2.83860100	0.06301500
H	2.19240400	-2.80503000	1.47532100
C	1.30470800	-1.57504900	-2.23877100
H	2.33277000	-1.59385500	-2.60948700
H	0.81963500	-2.50770200	-2.54064400
H	0.78067900	-0.75088800	-2.72646700
Si	2.12240100	0.73918100	0.25419300
Si	1.25147500	-1.37301500	-0.35229000
F	-3.83746700	0.64905900	-0.75835600



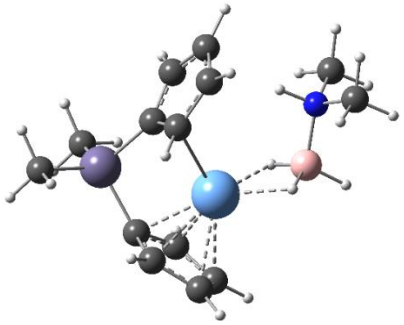
optimized geometry of 1a·2a

Mg	0.04881800	1.04287000	0.31390000
C	-1.23624100	-1.67144500	1.27488300
C	-1.33507300	-2.32808300	0.04568600
C	0.03574100	-1.02389100	1.32662800
H	-1.94952800	-1.70822400	2.08743600
C	-0.12964700	-2.12146700	-0.67021900
H	-2.17738600	-2.91273600	-0.30008900
C	0.74540000	-1.36325100	0.11552500
H	0.50748500	-0.69971300	2.24713900
H	0.07867700	-2.50009100	-1.65911200
C	2.24700000	1.37291300	1.01184400
C	2.22122000	0.58491000	-0.16680500
C	1.76017400	2.67135400	0.70573100
H	2.54264400	1.03489900	1.99203600
C	1.74206000	1.42349300	-1.21162600
C	1.45485500	2.70255000	-0.67540900
H	1.70087800	3.50524100	1.38795000
H	1.58255400	1.12859600	-2.23654700
H	1.10243700	3.55898200	-1.22869700
C	2.19256800	-0.94466900	-0.20212900
C	2.62104900	-1.46186400	-1.58094800
H	3.63263900	-1.12249600	-1.80910900
H	2.60983100	-2.55291800	-1.60039000
H	1.95935500	-1.10972800	-2.37238900
C	3.14275300	-1.53853600	0.85377600
H	3.09410100	-2.62850300	0.82724400
H	4.17222800	-1.22807700	0.66186600
H	2.87411000	-1.22380400	1.86149600
H	-1.76325100	1.80593500	0.80046000
H	-1.36547400	1.22253200	-1.11305100
B	-2.22729500	1.55196800	-0.31088400
H	-2.82824600	2.50408500	-0.71854400
N	-3.18423100	0.29299800	-0.14612300
H	-2.58038100	-0.49160300	0.17403000
C	-3.77365800	-0.12294200	-1.44174500
H	-4.39255900	-1.00945800	-1.30368400
H	-4.37600700	0.69274000	-1.83816400
H	-2.96704700	-0.35170900	-2.13368200



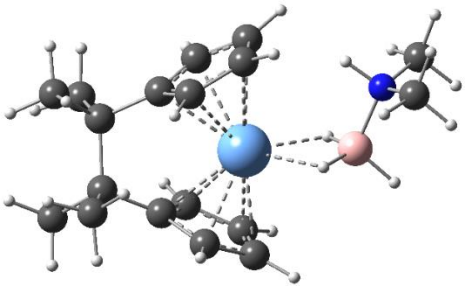
C	-4.22177100	0.50199800	0.88967100
H	-4.84313700	1.35003600	0.60634900
H	-4.83867000	-0.39118600	0.99098400
H	-3.73355700	0.71551000	1.83776800

optimized geometry of 1b·2a



Mg	0.06445500	1.01384900	-0.25400600
C	1.41074100	-1.67700000	-1.49594100
C	1.56713900	-2.36680600	-0.27974600
C	0.16244700	-1.01429100	-1.46333200
H	2.09413600	-1.69085900	-2.33407600
C	0.42198800	-2.13960800	0.50667000
H	2.41153600	-2.98557100	-0.00444400
C	-0.49070000	-1.33041400	-0.20881300
H	-0.32544300	-0.58961100	-2.33392700
H	0.25543800	-2.53291100	1.49966200
C	-2.01450800	1.68753500	-1.09926200
C	-2.20477500	0.99396200	0.13367200
C	-1.32214000	2.89818700	-0.85288700
H	-2.32336100	1.33390500	-2.07207500
C	-1.62001500	1.82228900	1.14200100
C	-1.08350100	2.98290300	0.54075700
H	-1.06576200	3.64807400	-1.58580100
H	-1.56754800	1.58410900	2.19433700
H	-0.59693100	3.79973500	1.05139100
C	-2.63059600	-1.44984700	1.99237500
H	-3.63852400	-1.15281000	2.29012300
H	-2.56335100	-2.53772400	2.06402700
H	-1.92834600	-1.02372500	2.71196600
C	-3.47791900	-1.59608200	-0.98115400
H	-3.42013500	-2.68675500	-0.98829900
H	-4.50193700	-1.30558800	-0.73473200
H	-3.26382000	-1.24695000	-1.99357900
H	1.90622500	1.73774900	-0.68515000
H	1.46373700	1.09844900	1.20021900
B	2.34280700	1.44871600	0.42572100
H	2.94053900	2.38276700	0.87834300
N	3.29931400	0.19183600	0.23771900
H	2.71090100	-0.57763200	-0.13381600
C	3.85037300	-0.27974400	1.53100000
H	4.47003100	-1.16271700	1.37463500
H	4.44376500	0.51664400	1.97687000
H	3.02340200	-0.53229100	2.18979000
C	4.36720600	0.44207300	-0.75790400
H	4.98425900	1.27235300	-0.41819400
H	4.98205500	-0.44947900	-0.88287800
H	3.90634000	0.70157700	-1.70806900
Si	-2.25673800	-0.87087900	0.24675000

optimized geometry of 1c·2a

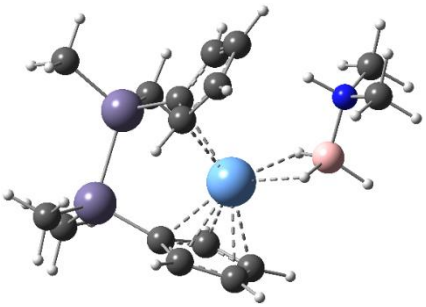


C	-0.45396400	-1.31638000	-0.11931000
C	-1.90380700	-1.35265600	1.91989400
C	-2.63421300	-2.48626800	-0.15170100
C	-1.77203300	1.32587600	-0.01829900
C	-3.25030500	-0.03529200	-1.50816800
C	-3.90839000	0.38537600	0.82361900
Mg	0.48879100	0.84153500	-0.15158600
C	0.03791800	-1.06691500	-1.45155800
C	0.60208600	-1.97808900	0.55992600
H	-1.36799700	-0.53425000	2.39783300
H	-2.91621100	-1.38175300	2.31730800
H	-1.42334800	-2.28251700	2.22114600
H	-3.68850300	-2.49339500	0.13526000
H	-2.16626900	-3.37903500	0.26566200
H	-2.56942700	-2.56245300	-1.23547100
C	-1.25182000	2.05200400	-1.12124600
C	-1.16761600	1.87471600	1.14718800
H	-2.50030700	-0.32830900	-2.23892100
H	-4.04590800	-0.77850800	-1.53730500
H	-3.67845600	0.91457000	-1.83055200
H	-4.57171600	-0.48054800	0.87952200
H	-4.47902900	1.21630000	0.40548600
H	-3.62417300	0.66636200	1.83549600
H	-0.53136400	-0.66911300	-2.27536700
C	1.33913200	-1.60096700	-1.56456300
H	1.94467300	-1.58446700	-2.45948600
C	1.68161200	-2.17250300	-0.32576300
C	-0.33267900	3.02125100	-0.64379800
H	0.21548400	3.72720400	-1.24785900
C	-0.28533300	2.91353700	0.76127900
H	0.31274200	3.51555700	1.42714300
H	-1.35890600	1.57438900	2.16386900
H	0.57585400	-2.32476700	1.58023200
H	-1.49465400	1.88763800	-2.15819900
H	2.57706300	-2.74024000	-0.10419900
B	2.83867100	1.22283000	0.33463100
H	2.01052500	0.91254300	1.17933300
H	3.43916800	2.19906700	0.68192300
H	2.34541400	1.40085500	-0.77071400
N	3.81102100	-0.02929100	0.19352900
H	3.18393700	-0.80600000	-0.07878900
C	4.43797800	-0.39957100	1.48326000
H	3.65183900	-0.61049700	2.20457600
H	5.06675800	-1.28188600	1.35949100
H	5.03935400	0.43520800	1.83924700
C	4.81287800	0.15067500	-0.88170800
H	5.43597500	-0.73954900	-0.97288700
H	4.29135200	0.32947200	-1.81910300

H	5.43424900	1.01319800	-0.64649700
C	-2.68558700	0.11110100	-0.07991300
C	-1.90654200	-1.22966400	0.38302800

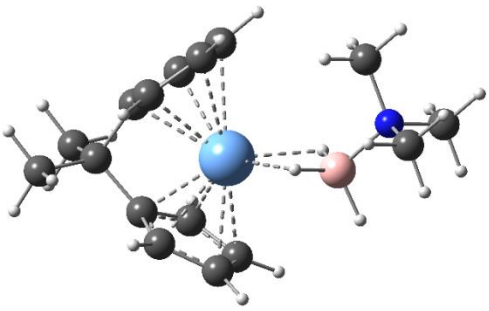
optimized geometry of 1d·2a

C	-0.16916200	-1.32076100	0.33235100
C	1.29380600	-1.71563900	-2.31481700
C	2.24953500	-3.21904700	0.18747400
C	1.65146000	1.70286800	0.01283500
C	3.62307000	0.17574200	1.79109000
C	4.22926100	0.53205500	-1.21709600
Mg	-0.60457700	0.99935700	0.16025400
C	-0.44955600	-0.83883800	1.67124700
C	-1.31989800	-2.07314500	-0.04312800
H	0.89994100	-0.78334000	-2.72609200
H	2.24145800	-1.92870100	-2.81437700
H	0.59499400	-2.51629300	-2.57079100
H	3.23140900	-3.41250500	-0.25265000
H	1.59279100	-4.05623300	-0.06193700
H	2.36455300	-3.19682800	1.27320900
C	1.06592300	2.37324200	1.12491200
C	0.95980800	2.17781100	-1.14502600
H	2.85722100	0.01376300	2.55236100
H	4.32907100	-0.65542000	1.85295200
H	4.15856900	1.09497600	2.04135600
H	4.91057700	-0.32189500	-1.24373100
H	4.81411300	1.42732700	-0.99181800
H	3.80572900	0.65239200	-2.21650400
H	0.26391600	-0.34955900	2.32238000
C	-1.71677100	-1.29226100	2.06358500
H	-2.19012600	-1.09860500	3.01534000
C	-2.24684300	-2.06865400	1.01064400
C	0.05073300	3.24349900	0.66060800
H	-0.56115700	3.89100900	1.26959400
C	-0.00892200	3.12717100	-0.74751600
H	-0.68530600	3.65816300	-1.39901700
H	1.15586900	1.87385500	-2.16293800
H	-1.44021000	-2.59437300	-0.98288000
H	1.35133100	2.23991800	2.15756300
H	-3.18299400	-2.61345700	1.03762600
B	-2.93556900	1.29267500	-0.53348300
H	-2.05258600	0.92561800	-1.29396700
H	-3.50419000	2.24621900	-0.98553300
H	-2.52131900	1.54237100	0.59022700
N	-3.93047600	0.06043700	-0.37495700
H	-3.35871900	-0.69969000	0.03308600
C	-4.44074000	-0.41930800	-1.67959100
H	-3.59503800	-0.69502000	-2.30512700
H	-5.08829700	-1.28522200	-1.53800900
H	-4.99765700	0.38314200	-2.16059600
C	-5.02641700	0.34348100	0.58000300
H	-5.66571900	-0.53266700	0.69246800
H	-4.59093400	0.60202000	1.54229700
H	-5.61247700	1.18362800	0.21115800
Si	1.52268600	-1.59061300	-0.44016000
Si	2.86656900	0.28757000	0.06572800



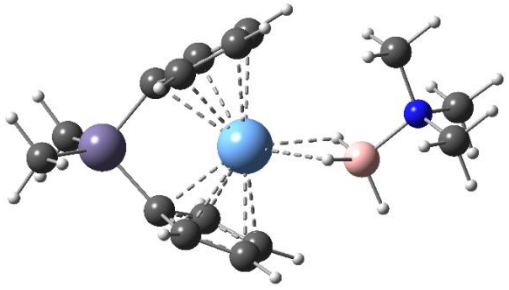
optimized geometry of 1a·(Me_3NBH_3)

Mg	0.06770200	0.21927400	0.00580800
C	3.01969300	-0.23202100	-0.00903600
C	2.24755600	1.09676800	-0.00131600
C	1.88833100	-1.27266100	-0.00189700
C	1.60034600	1.65491600	-1.13549400
C	1.12740800	-1.62971000	1.14167200
C	0.57298500	2.52291200	-0.69528700
C	-0.10261700	-2.18630200	0.71940100
C	1.10987600	-1.62721500	-1.13485300
C	1.61071400	1.64679900	1.14258600
C	-0.11365400	-2.18467600	-0.69464200
C	0.57915100	2.51766500	0.71798400
H	1.81985200	1.42435300	-2.16601500
H	1.41637600	-1.46922900	2.16817000
C	3.89764000	-0.36629200	-1.25950800
C	3.91647100	-0.36963800	1.22766700
H	-0.07320600	3.11478400	-1.32452300
H	-0.85398300	-2.61033700	1.36824100
H	1.38393500	-1.46659600	-2.16546300
H	1.83912600	1.40815000	2.16931700
H	-0.87539200	-2.60725100	-1.33168100
H	-0.06107800	3.10525600	1.35729800
H	4.39419100	-1.33863000	-1.27113100
H	4.65992900	0.41503000	-1.26958400
H	3.32235400	-0.27752600	-2.18004600
H	4.67904100	0.41145900	1.22782200
H	4.41276100	-1.34218400	1.22950200
H	3.35533200	-0.28267100	2.15705700
H	-1.76931700	0.56773200	-1.02108400
H	-1.75828800	0.53129700	1.00544300
B	-2.36380600	0.86648700	0.00057500
H	-2.63507700	2.03223200	0.02628800
N	-3.75409400	0.03266600	-0.00371900
C	-3.51085800	-1.43427700	-0.07276300
H	-2.97310400	-1.65991800	-0.98841900
H	-2.89244900	-1.72945300	0.76910100
H	-4.46122300	-1.97005300	-0.05219200
C	-4.56085700	0.45127700	-1.18388700
H	-5.51062000	-0.08597500	-1.19629700
H	-4.73954500	1.52210100	-1.12866300



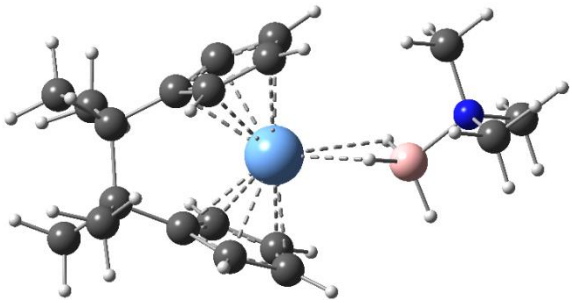
H	-4.00004200	0.23066600	-2.08889400
C	-4.50659800	0.34694200	1.24282300
H	-4.66629100	1.42086000	1.29784600
H	-5.46542500	-0.17405100	1.24143300
H	-3.91610900	0.03064200	2.09923300

optimized geometry of 1b·(Me_3NBH_3)



Mg	-0.04767800	0.20447400	-0.00922500
C	2.07089800	1.36528000	-0.00117500
C	1.71105900	-1.43129900	0.00225100
C	1.34905900	1.80857700	-1.14858800
C	0.88187700	-1.70413500	1.12927000
C	0.19947200	2.51657300	-0.73343000
C	-0.38280600	-2.14879300	0.68318500
C	0.91595800	-1.71584900	-1.14547500
C	1.32784500	1.82035900	1.12790300
C	-0.36037500	-2.15714000	-0.73338700
C	0.18595200	2.52406000	0.68362100
H	1.62044100	1.61019900	-2.17546300
H	1.16528400	-1.57185800	2.16328500
C	4.17771600	-0.33419500	-1.52172700
C	4.14050100	-0.32403300	1.57936400
H	-0.52776900	2.99042700	-1.37410700
H	-1.19390500	-2.47689100	1.31396400
H	1.22852100	-1.58918000	-2.17169900
H	1.58060100	1.63443500	2.16186000
H	-1.15151700	-2.49080900	-1.38842500
H	-0.55225100	3.00540200	1.30559100
H	4.69411000	-1.29636300	-1.54938800
H	4.92870100	0.45846200	-1.55272400
H	3.57288400	-0.25428400	-2.42763300
H	4.88907500	0.47022000	1.62451300
H	4.65781800	-1.28504500	1.62456700
H	3.51373800	-0.24070100	2.46992300
H	-1.93178300	0.40318400	-0.87472700
H	-2.08899400	0.60302100	1.13582500
B	-2.60145400	0.82167100	0.05791000
H	-2.86748700	1.98014800	-0.09845700
N	-4.00134800	-0.00574600	0.00950800
C	-3.79006900	-1.44983900	0.29775700
H	-3.07484000	-1.85114000	-0.41272200
H	-3.38118400	-1.55199500	1.29860600
H	-4.73708100	-1.98750900	0.22526000
C	-4.60622200	0.14163500	-1.34298000
H	-5.57425500	-0.36114700	-1.37794100
H	-4.72803300	1.19979300	-1.56075800
H	-3.93560700	-0.29739900	-2.07759800
C	-4.92647800	0.56433800	1.02740400
H	-5.09657900	1.61411900	0.80299700
H	-5.87355600	0.02174900	1.01783900
H	-4.46355600	0.48204600	2.00783600
Si	3.11069700	-0.18528200	0.01572900

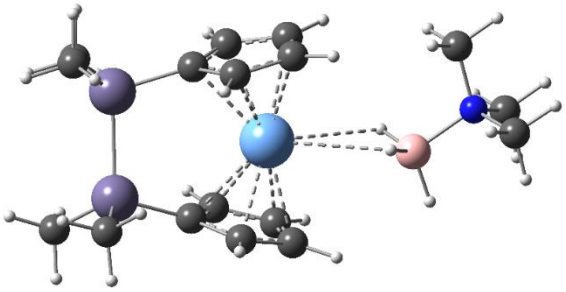
optimized geometry of 1c·(Me_3NBH_3)



C	1.70045100	1.41309900	0.03500100
C	3.24413300	0.63664200	1.83000000
C	4.15908800	1.33002300	-0.35227500
C	1.39655700	-1.41773600	-0.06232400
C	3.22299900	-1.00967500	-1.70864000
C	3.77223500	-1.86056200	0.53772200
Mg	-0.38091300	0.22003300	-0.06664700
C	1.13359400	1.70188900	-1.23175200
C	0.80409100	1.93885100	1.00655300
H	2.48181200	0.11078500	2.40192500
H	4.21044200	0.19176900	2.06322900
H	3.26844600	1.66867200	2.18207700
H	5.08761800	0.76759500	-0.22546300
H	4.29554200	2.30907500	0.11048600
H	3.99970900	1.49501100	-1.41619200
C	0.48451100	-1.70912500	-1.11092300
C	0.68832500	-1.60923700	1.15087400
H	2.65517300	-0.33089600	-2.34175800
H	4.28119000	-0.79356600	-1.84631600
H	3.04737500	-2.02455700	-2.06804000
H	4.80606300	-1.50952100	0.49632600
H	3.73735000	-2.85078900	0.07962500
H	3.49180800	-1.97729400	1.58281400
H	1.55210700	1.44057500	-2.18933000
C	-0.09398500	2.38309600	-1.04637600
H	-0.74692800	2.74083800	-1.82677400
C	-0.29355900	2.54021300	0.34353700
C	-0.76492300	-2.07082500	-0.55041900
H	-1.63180400	-2.38407900	-1.10824800
C	-0.63683300	-2.00634900	0.85651300
H	-1.39394800	-2.24885500	1.58679700
H	1.08238100	-1.46976500	2.14391400
H	0.92968200	1.89655100	2.07595200
H	0.69373900	-1.66383300	-2.16681000
H	-1.12846400	3.03235200	0.81460400
C	2.96603600	0.61321200	0.31490900
C	2.82438000	-0.91050300	-0.22393600
H	-2.32458600	0.44768100	0.69351000
H	-2.67791900	0.55441400	-1.29913400
B	-3.08020900	0.82221500	-0.19027100
H	-3.35181700	1.98367300	-0.05244100
N	-4.45824600	-0.02015700	0.03909500
C	-5.48003500	0.46350700	-0.92861300
H	-6.41293000	-0.08807500	-0.79689400

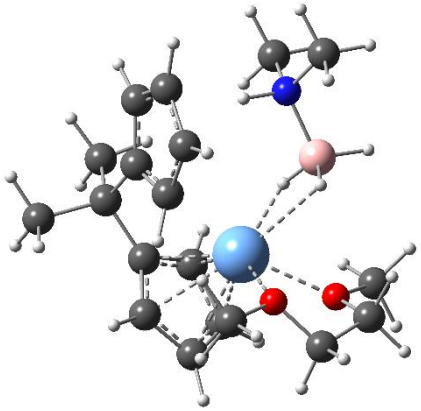
H	-5.64854900	1.52452000	-0.76324000
H	-5.10364400	0.31841900	-1.93831400
C	-4.23334400	-1.47472800	-0.17295600
H	-3.89208000	-1.63067700	-1.19247500
H	-3.46273400	-1.81718700	0.51099800
H	-5.15928600	-2.02725600	-0.00255600
C	-4.94804700	0.20429600	1.42608200
H	-5.08723300	1.27117200	1.58217500
H	-5.89176300	-0.32174600	1.58299700
H	-4.20106900	-0.16191500	2.12615200

optimized geometry of 1d·(Me_3NBH_3)



C	1.37601500	1.74487600	-0.09171200
C	3.56421400	1.41174800	2.00492100
C	4.33769000	1.83681900	-0.95520600
C	1.07054900	-1.68077000	0.03543500
C	3.44049700	-1.75574300	-1.88623300
C	3.88816300	-2.28336900	1.12355300
Mg	-0.45808000	0.18999000	-0.06625400
C	0.69185000	1.82069900	-1.34025600
C	0.43389900	2.14766800	0.90091300
H	2.86217500	0.95206100	2.70440500
H	4.55882900	1.02051600	2.23019000
H	3.57129900	2.48785600	2.19577000
H	5.33109400	1.40165700	-0.82064800
H	4.40943900	2.91305900	-0.78001800
H	4.04758600	1.68612000	-1.99727500
C	0.14279900	-1.89835300	-1.02338800
C	0.30210800	-1.65033100	1.23554900
H	2.86891300	-1.20759500	-2.63857400
H	4.49601500	-1.51926300	-2.03817500
H	3.30078700	-2.82387100	-2.07078400
H	4.95358100	-2.04863800	1.05943900
H	3.76455600	-3.35672500	0.95982200
H	3.56040400	-2.05965300	2.14110900
H	1.11238200	1.57175900	-2.30364100
C	-0.63302300	2.26661100	-1.11985100
H	-1.38819900	2.43262300	-1.87164300
C	-0.79288500	2.47257800	0.27543400
C	-1.16138100	-2.00566100	-0.48631300
H	-2.06365500	-2.18551100	-1.04718500
C	-1.06181100	-1.85239600	0.92135300
H	-1.87523100	-1.89049100	1.62845400
H	0.69328400	-1.49119700	2.22962500
H	0.62671100	2.20117700	1.96188200
H	0.39230400	-1.96644400	-2.07144100
H	-1.69071300	2.81687000	0.76169500
H	-3.07167300	0.49619900	0.94356500
H	-3.15675300	0.41503700	-1.06704400
B	-3.69841100	0.79185200	-0.05085100
H	-3.98627400	1.96319300	-0.08318900
N	-5.11697800	-0.02852700	0.04544100
C	-5.96712600	0.31956100	-1.12261100
H	-6.91554300	-0.22047900	-1.07676300
H	-6.14926100	1.39124200	-1.11780000
H	-5.43527400	0.05695400	-2.03386600
C	-4.86215700	-1.49202800	0.04882100
H	-4.36807800	-1.76431300	-0.87962500
H	-4.20565900	-1.73493700	0.87984100
H	-5.80134000	-2.04153500	0.14233100
C	-5.82014200	0.35176400	1.29838200
H	-5.98332600	1.42667700	1.29713900
H	-6.77676400	-0.17043100	1.37095100
H	-5.19118500	0.09201700	2.14629500
Si	3.08133700	1.04854900	0.21462900
Si	2.89165400	-1.29179400	-0.13865500

optimized geometry of 1a·dme·2a

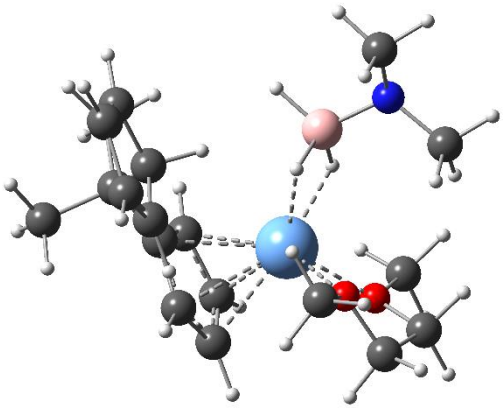


Mg	0.78760000	-0.22378500	-0.06599600
C	-1.57060100	0.86167700	2.23095600
C	-2.81729400	1.18820600	1.70240000
C	-1.07549900	-0.26784500	1.51319100
H	-1.07076200	1.36473100	3.04720500
C	-3.12307600	0.25551900	0.66519700
H	-3.44787400	2.01000300	2.01618400
C	-2.07387300	-0.65726500	0.56192200
H	-0.37963600	-0.97918200	1.93490900
H	-4.01906400	0.26747900	0.06154900
C	0.49101700	-2.65714400	0.14129300
C	-0.52275300	-2.12757600	-0.69583100
C	1.73898500	-2.53588500	-0.51686800
H	0.33788800	-3.09558000	1.11492400
C	0.12180700	-1.67496500	-1.87841200
C	1.50714100	-1.94183300	-1.77067200
H	2.69110600	-2.88137500	-0.14163100
H	-0.36409000	-1.23234700	-2.73308000
H	2.25308700	-1.73410900	-2.52152100
C	-1.98087300	-1.90333200	-0.31540300
C	-2.84370300	-1.74497300	-1.57706500
H	-2.73890600	-2.61737800	-2.22476600
H	-3.89692500	-1.64225600	-1.31125700
H	-2.55876600	-0.85958800	-2.14732700
C	-2.51454400	-3.11709600	0.47813800
H	-3.56000000	-2.95505800	0.74710200
H	-2.43795600	-4.03251200	-0.11371600
H	-1.95561700	-3.25859100	1.40304500
H	0.74722100	2.17457300	0.22512400
H	0.06780400	1.14341900	-1.38475200

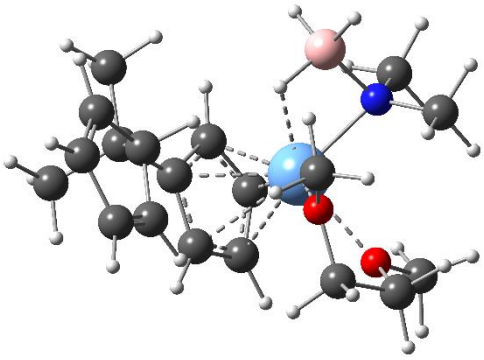
B	0.14897400	2.22791600	-0.82645400
H	0.64922800	3.02146700	-1.58660800
N	-1.34409600	2.67292200	-0.51541000
H	-1.74242000	2.00169900	0.16467900
C	-2.20989600	2.63243200	-1.71507500
H	-3.23301000	2.89720800	-1.44790100
H	-1.82461600	3.33091000	-2.45702900
H	-2.19756900	1.62415100	-2.11927900
C	-1.39470900	3.99628800	0.14516800
H	-0.96838700	4.74463800	-0.52153700
H	-2.42518300	4.25667300	0.38823000
H	-0.81102100	3.94862500	1.06105200
O	2.16965600	0.13795100	1.65739900
C	2.02118200	-0.54969300	2.90550200
H	0.99650000	-0.41034400	3.23198000
H	2.23200100	-1.61481600	2.77971200
H	2.69951200	-0.11999300	3.64632400
C	3.53715800	0.26658200	1.26197200
H	4.12423100	0.68925400	2.08320900
H	3.93416400	-0.72021700	1.00173300
C	3.58167900	1.18464000	0.06847500
H	3.25301300	2.19486100	0.33536400
H	4.60412800	1.22937200	-0.32147400
O	2.70264300	0.63379200	-0.89923400
C	2.88250600	1.14598600	-2.21893500
H	2.79432500	2.23374200	-2.22444500
H	3.85960700	0.84045000	-2.60377300
H	2.09427800	0.71920300	-2.83117300

optimized geometry of I1·dme

Mg	1.02058500	-0.53633300	-0.23198000
C	-3.72591600	1.08504700	2.00947900
C	-4.39985400	1.72328100	0.87928600
C	-2.70776100	0.33896300	1.54980400
H	-4.01182000	1.20542500	3.04565000
C	-3.79167000	1.35152600	-0.25918600
H	-5.23947000	2.39931700	0.96367500
C	-2.62429800	0.44845400	0.04937200
H	-2.04247600	-0.25593600	2.15106700
H	-4.04266300	1.68980200	-1.25196900
C	-0.64434000	-2.08086400	0.66467900
C	-1.17940600	-1.58314100	-0.55573700
C	0.54804100	-2.79045500	0.39092900
H	-1.09971400	-2.00061100	1.63742000
C	-0.28326700	-1.98986300	-1.58005300
C	0.77256300	-2.73551500	-1.00199500
H	1.16439700	-3.29784500	1.11738600
H	-0.37969300	-1.76852300	-2.62946600
H	1.59531200	-3.18719200	-1.53440400
C	-2.52704900	-0.89515400	-0.76105200
C	-2.72671500	-0.57929900	-2.25218900
H	-2.62046100	-1.48533600	-2.84955200
H	-3.72858500	-0.19061700	-2.43054800
H	-2.00156400	0.15485200	-2.60639500
C	-3.64934300	-1.85144300	-0.31272900
H	-4.62425400	-1.36734300	-0.40572100
H	-3.64620400	-2.74977800	-0.93284100
H	-3.52016200	-2.15846700	0.72442500
H	0.30264600	1.20131300	-0.37464600
H	-0.04649300	1.47229600	-2.29962000
B	0.85825900	1.48291300	-1.50316300
H	1.63408500	0.54365000	-1.77335600
N	1.60236400	2.78033100	-1.40483800
H	-1.71700800	1.01506600	-0.20319100
C	0.75081900	3.93388100	-1.20441000
H	0.28522300	3.95784600	-0.19849100
H	1.31675800	4.86544200	-1.32196200
H	-0.05695200	3.93153000	-1.93730600
C	2.73833900	2.80140900	-0.51962700
H	3.28919700	3.74524600	-0.60276400
H	2.46811700	2.67452700	0.55015600
H	3.42750000	1.99389100	-0.77993400
O	1.66682400	0.19449700	1.67221000
C	0.75255500	0.64670700	2.67353900
H	-0.06791600	1.13001500	2.15071500
H	0.37446400	-0.19626200	3.25720800
H	1.24797300	1.36670100	3.32861600
C	2.84119000	-0.44902300	2.16417000
H	3.23912100	0.09237000	3.02675100
H	2.59733200	-1.47382700	2.46184200
C	3.84624000	-0.42827500	1.03504000
H	4.19117900	0.59307000	0.85048500
H	4.70525800	-1.06224100	1.27847500
O	3.17759400	-0.92312800	-0.12174000
C	3.99742100	-1.00547300	-1.28864800
H	4.38410800	-0.02024400	-1.55892200
H	4.82329900	-1.70041100	-1.11639900
H	3.36396800	-1.37414300	-2.09073800

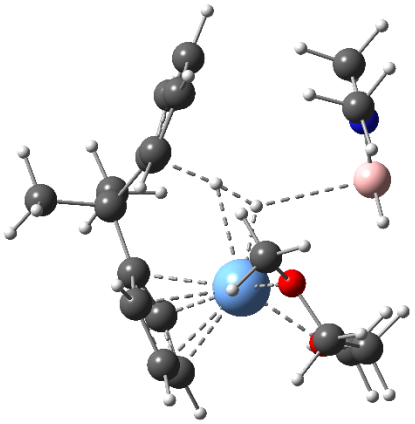


optimized geometry of I2·dme



Mg	-1.03154100	-0.32797500	0.01519000
C	3.62058000	2.13564100	-0.35561300
C	4.43943600	1.58110900	0.72303400
C	2.55171800	1.34450900	-0.54735500
H	3.84996200	3.04186300	-0.89999700
C	3.86313200	0.45464100	1.17380900
H	5.35258400	2.02501700	1.09485900
C	2.58189700	0.19323700	0.42255400
H	1.76534800	1.50152200	-1.26462800
H	4.22424500	-0.16358500	1.98036300
C	0.46628300	-0.75780700	-1.90643500
C	0.99776800	-1.43056900	-0.76879200
C	-0.78685500	-1.32102000	-2.22636700
H	0.96691100	0.00071800	-2.48555200
C	0.03436100	-2.40063800	-0.39042500
C	-1.06569600	-2.32888200	-1.28105700
H	-1.42498700	-1.01242900	-3.03944800
H	0.10393900	-3.06684400	0.45203700
H	-1.94471500	-2.95446900	-1.24776700
C	2.38769500	-1.25373800	-0.16524000
C	2.58582100	-2.26319300	0.97728800
H	2.42358000	-3.27852700	0.61424000
H	3.60244300	-2.21508500	1.36627400
H	1.88998300	-2.07979200	1.79783300
C	3.44723200	-1.51997600	-1.25050400
H	4.45453700	-1.39497600	-0.84707200
H	3.34690100	-2.53955700	-1.62635900
H	3.33204500	-0.83874300	-2.09290900
H	-0.72325600	-1.87833900	2.73435000
H	-0.09458000	-0.24905600	1.82512700
B	-1.01992500	-0.73075900	2.50740000
H	-1.11960300	-0.05707000	3.51216100
N	-2.34355800	-0.65981700	1.61464000
H	1.75951500	0.32290500	1.13986500
C	-3.18381300	0.48175400	1.97377100
H	-4.04326500	0.56839000	1.30028400
H	-3.56174700	0.39646500	3.00071700
H	-2.60825000	1.40457100	1.91287100
C	-3.13550600	-1.88988700	1.66460000
H	-3.49967200	-2.09612900	2.68008700
H	-4.00424700	-1.82149000	0.99968000
H	-2.52542800	-2.73269300	1.34731500
O	-0.63088100	1.78127700	0.22538800
C	-0.04385100	2.52843600	1.30301800
H	0.11745700	1.82500300	2.11333500
H	0.90442200	2.96157500	0.98183000
H	-0.73491500	3.30878600	1.63111000
C	-1.08361300	2.55314000	-0.89085700
H	-0.96546900	3.62012900	-0.69781700
H	-0.48139100	2.27868900	-1.75947900
C	-2.53712700	2.20691700	-1.13029100
H	-3.17225700	2.58176500	-0.31964200
H	-2.87953600	2.63410700	-2.07972400
O	-2.59337700	0.78833300	-1.16945700
C	-3.83794100	0.23743800	-1.58121700
H	-4.64548900	0.56138300	-0.91883300
H	-4.06484000	0.53371800	-2.60937000
H	-3.73226700	-0.84316000	-1.52848400

optimized geometry of TS1

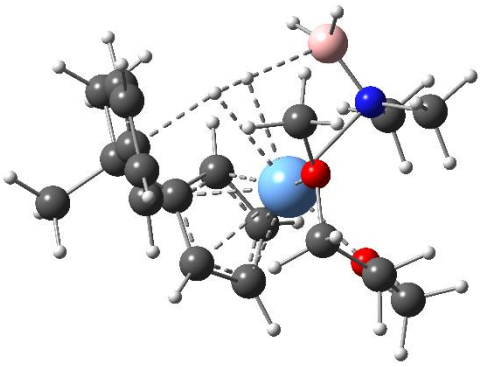


Mg	1.05305400	-0.65453500	-0.11395800
C	-2.78830800	1.05138900	1.83040200
C	-3.38162900	1.53703600	0.62777900
C	-2.15759300	-0.14551300	1.55193600
H	-2.83637300	1.53509800	2.79682800
C	-3.11880500	0.63182300	-0.38212400
H	-3.92870700	2.46351900	0.52405000
C	-2.28103300	-0.42404600	0.13957100
H	-1.67654000	-0.78518900	2.27478400
H	-3.40954400	0.74081500	-1.41589900
C	0.04064900	-2.52709900	0.89844400
C	-0.63772900	-2.29005900	-0.32517700
C	1.38612800	-2.88948900	0.62026900
H	-0.39893500	-2.48428100	1.88074500
C	0.31386700	-2.50275500	-1.36044000
C	1.55174800	-2.88180900	-0.77988900
H	2.13204300	-3.16651000	1.35018800
H	0.12526200	-2.41241700	-2.41780700
H	2.45879100	-3.11653100	-1.31514900
C	-2.08526500	-1.81921400	-0.48600100
C	-2.44852900	-1.77064000	-1.97727300
H	-2.27058700	-2.73842500	-2.44925600
H	-3.50304200	-1.52453800	-2.10114500
H	-1.86387700	-1.01630800	-2.50789500
C	-3.02214800	-2.83193300	0.20519400
H	-4.05891900	-2.50083100	0.11712000
H	-2.92551800	-3.82177500	-0.24956400
H	-2.78862600	-2.92020600	1.26579300
H	-0.16865000	0.59825600	-0.67769600
H	0.84399000	2.56788600	-2.59420500
B	0.84256900	2.80409300	-1.42250300
H	1.77206600	2.49968000	-0.73739700
N	-0.20211300	3.50889100	-0.85118100
H	-1.03348500	0.25754700	-0.33629200
C	-1.39653100	3.90531400	-1.58355900
H	-2.26374200	3.34940900	-1.21668800

H	-1.59066700	4.97505500	-1.45159500
H	-1.26766800	3.70025400	-2.64410700
C	-0.31683800	3.73268900	0.58117800
H	-0.53028400	4.78542400	0.79407600
H	-1.12948200	3.12440200	0.99372800
H	0.61319200	3.45591000	1.07477400
O	1.83271700	0.42270800	1.51616700
C	1.19402000	0.47135000	2.80040200
H	0.13227300	0.60676300	2.60628200
H	1.36203000	-0.46044400	3.34612800
H	1.58420300	1.31754600	3.36973600
C	3.25799400	0.31509400	1.54454200
H	3.67544900	1.00297600	2.28445700
H	3.53821100	-0.71057100	1.80607100
C	3.74995300	0.68428600	0.16200900
H	3.60193100	1.74989100	-0.02856200
H	4.81061600	0.43542000	0.05732000
O	2.97600600	-0.07351500	-0.76932700
C	3.30243700	0.15162900	-2.14545500
H	3.12286100	1.19456500	-2.41060000
H	4.34481000	-0.11896700	-2.32854600
H	2.64809500	-0.49357600	-2.72697600

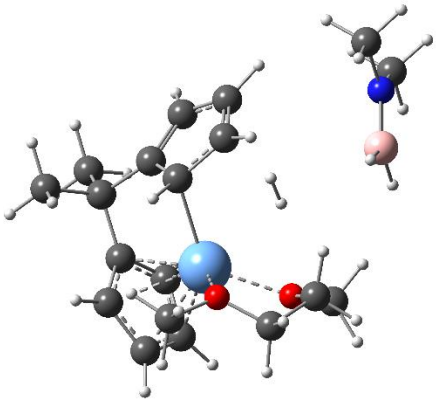
optimized geometry of TS2

Mg	-0.81956700	-0.29819400	-0.04817900
C	2.98953000	2.36661500	-0.61739500
C	3.48924900	2.24201100	0.69801400
C	2.44961000	1.13002500	-1.00140400
H	3.02092300	3.26016500	-1.22707800
C	3.27694300	0.92323700	1.11632700
H	3.94585400	3.02677000	1.28448600
C	2.62373900	0.20666700	0.06559000
H	2.06733100	0.89682100	-1.98381200
H	3.57466300	0.51144600	2.06907000
C	0.47010700	-1.39696800	-1.76434400
C	1.04435800	-1.68770100	-0.49480600
C	-0.80880600	-1.98783700	-1.83601800
H	0.95577200	-0.86633900	-2.56535100
C	0.07253000	-2.43072100	0.22542400
C	-1.07315300	-2.61186900	-0.60215600
H	-1.47003600	-1.94995000	-2.68770600
H	0.19621200	-2.83059700	1.21823700
H	-1.95234600	-3.18374400	-0.35095100
C	2.45308100	-1.31088800	-0.04099800
C	2.77353800	-1.99556000	1.29719800
H	2.66193100	-3.07781800	1.20708400
H	3.80303000	-1.78482400	1.58617000
H	2.12524900	-1.65366400	2.10458000
C	3.45849700	-1.85337300	-1.08662900
H	4.47622000	-1.60459100	-0.78035300
H	3.37189600	-2.93941700	-1.18449100
H	3.28692900	-1.40433000	-2.06388300
H	-0.62661500	-1.19623800	3.27420500
H	0.51284700	0.13152100	1.85721400
B	-1.10655300	-0.18199400	2.88530900
H	-0.88324500	0.86256100	3.40714800
N	-2.18652000	-0.26003600	1.91673000
H	1.17397800	0.32950100	1.41997400
C	-3.08931800	0.90037400	1.82164800
H	-3.66812300	0.85456400	0.89849900
H	-3.78724000	0.91848400	2.66453200
H	-2.51201600	1.81917200	1.81969000
C	-2.95104700	-1.52194000	1.87903900
H	-3.66165800	-1.56317100	2.71096000
H	-3.51062800	-1.60296200	0.94625000
H	-2.27310500	-2.36601300	1.94857100
O	-0.71102000	1.81587900	0.04539800
C	0.04412400	2.70558200	0.90646000
H	-0.01223400	2.29331200	1.90679100
H	1.08160400	2.75517200	0.57630600
H	-0.43183900	3.68890800	0.88577900
C	-0.93066800	2.31222900	-1.27963000
H	-0.86867500	3.40112900	-1.29740000
H	-0.16050600	1.90980000	-1.94131500
C	-2.31827300	1.85802800	-1.67171300
H	-3.08646700	2.41487300	-1.12439500
H	-2.47850700	1.98456700	-2.74676300
O	-2.40732300	0.47381400	-1.32206700
C	-3.58023000	-0.17867100	-1.80195200
H	-4.47541600	0.30538700	-1.40038400
H	-3.60842400	-0.15508400	-2.89405500
H	-3.53027800	-1.20986000	-1.46568900



optimized geometry of 1a·dme + 4a + H_2

Mg	-0.96478200	0.67129300	0.15063400
C	1.25465200	-1.02694000	-1.28271700
C	1.62774200	-2.13045100	-0.53750500
C	-0.17779700	-0.91293800	-1.21904500
H	1.91048700	-0.37857300	-1.84663400
C	0.45087200	-2.74897900	-0.01906500
H	2.63826300	-2.46259800	-0.35034700
C	-0.65905200	-2.03962800	-0.44754400
H	-0.75353600	-0.47099700	-2.03033300
H	0.44119100	-3.60007600	0.64608000
C	-3.27452400	0.10945200	-0.14876800
C	-2.62875100	-0.95236900	0.52883700
C	-3.26712900	1.25956000	0.68366500
H	-3.70305700	0.05623000	-1.13688200
C	-2.22556900	-0.44758500	1.79336200
C	-2.62163300	0.91083800	1.88925300
H	-3.72290700	2.21222100	0.45949600
H	-1.68860500	-1.00116100	2.54715500
H	-2.49304500	1.55280700	2.74777000
C	-2.13010900	-2.25808700	-0.09017200
C	-2.29702700	-3.41432800	0.90620300
H	-3.35018800	-3.53967300	1.16470900
H	-1.93343400	-4.34860600	0.47396300
H	-1.74042300	-3.23391500	1.82565700
C	-2.92895400	-2.59944900	-1.36250500
H	-2.56979200	-3.54149900	-1.77977600
H	-3.99526600	-2.69696500	-1.14335300
H	-2.80583500	-1.83552500	-2.13096900
H	0.94441400	-0.46234000	2.11858800
H	3.61493800	1.31043800	1.07783200
B	4.03097100	0.86578700	0.04937100
H	3.88137400	1.45548300	-0.98004500
N	4.71995700	-0.33226500	0.05830800
H	1.15759000	-0.84653300	1.51235600
C	4.91632700	-1.13229600	1.25830500
H	4.39801300	-2.09193400	1.17076900
H	5.98045400	-1.33408800	1.41878500
H	4.52247900	-0.60661200	2.12492200
C	5.23580200	-0.96748800	-1.14616900
H	6.31009500	-1.15729100	-1.05291900
H	4.73604100	-1.92453400	-1.32192800
H	5.06509200	-0.32576200	-2.00714800
O	-0.77539800	2.21184900	-1.39027300
C	-1.78505700	2.42303100	-2.37726200
H	-2.21166500	1.44955300	-2.60078000
H	-2.56879000	3.07983800	-1.99062200
H	-1.34261200	2.85369700	-3.27881800
C	-0.11804400	3.39941500	-0.95591800
H	0.34524000	3.91108400	-1.80579800
H	-0.84676400	4.06828300	-0.48398300
C	0.93463900	2.96952900	0.03790300
H	1.72441000	2.38981800	-0.44188200
H	1.37423200	3.84368500	0.52267100
O	0.26890200	2.14672700	1.00765300
C	0.77238000	2.22844900	2.34437700
H	1.80442700	1.87968500	2.38638800
H	0.70299400	3.25930400	2.69980400
H	0.13637800	1.59094800	2.95220600



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