On The Nature and Limits of Alkaline Earth–Triel Bonding

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Contents

Experimental Details

General Considerations

Health warning: *beryllium and its compounds are extremely toxic and can cause irreversible health effects through inhalation or skin contact. The work with beryllium-containing materials described herein was carried out by trained operators, with strict adherence to local and national rules/regulations.*[1]

All manipulations were carried out using Schlenk line or glovebox techniques under an atmosphere of argon or dinitrogen. Solvents were dried by passage through activated alumina towers, dried with NaK_2 and degassed before use. Solvents were stored over NaK_2. NMR spectra were measured in C_6D_6 which was dried over NaK_2, with the solvent being distilled under reduced pressure, degassed by three freeze-pump-thaw-cycles and stored under argon in a Teflon valve ampoule. NMR samples were prepared under argon in 5 mm Wilmad 507-PP tubes fitted with J. Young Teflon valves. NMR spectra were measured on a Bruker Avance III HD Nanobay 400 MHz NMR spectrometer equipped with a 9.4 T magnet, Bruker Avance III 500 MHz NMR spectrometer equipped with a 11.75 T magnet, or a Bruker Avance III NMR 500 MHz NMR spectrometer equipped with a 11.75 T magnet and a ^{13}C detect cryoprobe. ^{1}H and ^{13}C NMR spectra were referenced internally to residual protio-solvent (^{1}H) or solvent (^{13}C) resonances and are reported relative to tetramethylsilane (δ = 0 ppm). ^{9}Be NMR spectra were referenced to a 0.43 M solution of $BeSO_4{\cdot}4H_2O$ in D_2O (δ = 0 ppm). Chemical shifts are quoted in δ (ppm) and coupling constants in Hz. Elemental analyses were carried out by London Metropolitan University. The compounds $[K\{Al(NON)\}]_2$ (**1**),[2] $[K\{Ga(NON)\}]_2$ (**2**),[2] $K_2(NON)$, NaCp,[3] and $BeCp_2$ [4] were prepared as described previously. *N,N′*-diisopropylcarbodiimide (CDI) was dried over 3 Å molecular sieves, degassed, distilled, and stored over 3 Å molecular sieves. InCp was purchased and sublimed *in vacuo* before use. $MgCp_2$ (magnesocene) was prepared via a novel synthetic method (see below).

Synthetic Methods

Synthesis of $MgCp_2$

MgI_2 (1.6 g, 5.7 mmol) and NaCp (1.0 g, 11.4 mmol) were combined in a Schlenk flask equipped with a Teflon coated stirrer bar. Toluene (150 mL) was added to the Schlenk flask and the reaction mixture was stirred at 100 °C for a week. The resulting suspension was filtered and the volatiles were removed *in vacuo*. The filtrate was purified by sublimation at 100 °C under reduced pressure to give $MgCp_2$ as a white solid (600 mg, 68%). All data match that reported previously for this compound. ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 6.01 (s, 10H, $C_5\mathit{H}_5$).[5]

Synthesis of (NON)Al(MgCp) (AlMg)

Compound **1** (900 mg, 0.608 mmol) and $MgCp_2$ (188 mg, 1.22 mmol) were combined in a Schlenk flask equipped with a Teflon coated stirrer bar. Toluene (100 mL) was added to the flask and the reaction mixture was stirred overnight at room temperature, leading to the formation of an off-white precipitate. The reaction mixture was filtered and volatiles from the filtrate were removed in vacuo. The resulting waxy off-white solid was dried in vacuo for a further 2 h to remove unreacted $MgCp_2$. The solid was extracted into hot hexane (20 mL) and volatiles were removed *in vacuo* to give (NON)AlMgCp as an off-white powder (0.644 g, 67%). Single crystals suitable for X-ray diffraction experiments were obtained by slow concentration of a hexane solution in a sealed glass λ-type tube. Anal. Calcd for $C_{52}H_{67}AlMgN_2O$: C, 79.32; H, 8.58; N, 3.56. Found: C, 79.14; H, 8.31; N, 3.29. ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 1.14 (d, $^3J_{HH}$ = 6.8 Hz, 12 H, CH(CH_3)$_2$), 1.21 (s, 18 H, C(CH_3)$_3$), 1.25 (d, $^3J_{HH}$ = 6.8 Hz, 12 H, CH(CH_3)$_2$), 1.59 (s, 6H, XA-C(CH_3)$_2$), 3.39 (sept., $^3J_{HH}$ = 6.8 Hz, 4H, C*H*(CH$_3$)$_2$), 5.80 (s, 5H, C_5H_5), 6.38 (d, $^4J_{HH}$ = 2.0 Hz, 2H, XA-*o*-C*H*), 6.76 (d, $^4J_{HH}$ = 2.0 Hz, 2H, XA-*p*-C*H*), 7.27 (s, 6H, ArH). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 23.0, 25.0 (CH(*C*H$_3$)$_2$), 25.7 (XA-*C*(CH$_3$)$_2$), 29.0 (*C*H(CH$_3$)$_2$), 31.8 (C(*C*H$_3$)$_3$), 35.2 (*C*(CH$_3$)$_3$), 36.9 (XA-C(*C*H$_3$)$_2$), 105.7 (C_5H_5), 107.6, 110.2, 124.3, 124.9, 126.7, 126.9, 141.9, 147.1, 148.2, 149.0 (Ar-*C*).

Synthesis of (NON)In(BeCp) (InBe)

Procedure conducted in the absence of light. A solid mixture of K_2(NON) (30 mg, 0.040 mmol) and InCp (7.2 mg, 0.04 mmol) was added to an ampoule fitted with a Teflon valve and equipped with a glass-coated stirrer bar. Benzene (1 mL) was condensed into the vessel *in vacuo* at –196 °C. The mixture was allowed to warm to room temperature and stirred for 10 minutes. Subsequently, $BeCp_2$ (5.6 mg, 0.040 mmol) in benzene (1 mL) was added to the reaction flask. The bright-yellow solution and metallic precipitate was stirred for one hour. Subsequently, volatiles were removed *in vacuo*, and soluble material was dissolved in hexane (0.5 mL). The suspension was filtered and volatiles were removed *in vacuo*, leaving a bright yellow powder. Yield: 15 mg, 43%. Single crystals suitable for X-ray diffraction experiments were obtained by slow concentration of a hexane solution in a sealed glass λ-type tube. Complex **InBe** is sensitive to light and degrades in solution over the course of 48 hours. Anal. Calcd for $C_{52}H_{67}BeInN_2O$: C, 72.63; H, 7.85; N, 3.26. Found: C, 72.86; H, 7.99; N, 3.29. ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 1.09 (d, $^3J_{HH}$= 7.0 Hz, 12H, CH(CH_3)$_2$), 1.22 (d, $^3J_{HH}$= 6.9 Hz, 12H, CH(CH_3)$_2$), 1.31 (s, 18H, C(CH_3)$_3$), 1.67 (s, 6H, C(CH_3)$_2$), 3.45 (sept, $^3J_{HH}$= 6.5 Hz, 4H, C*H*(CH$_3$)$_2$), 5.15 (s, 5H, C_5H_5), 6.38 (d, $^4J_{HH}$= 2.5 Hz 2H, XA-*o*-C*H*), 6.78 (d, $^4J_{HH}$= 2.5 Hz 2H, XA-*p*-C*H*), 7.23 (m, 6H, Ar*H*); ^{9}Be NMR (42 MHz, C_6D_6): δ = –25.6 ($w_{1/2}$ = 21.7 Hz) ^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ = 24.2, 24.4 (CH(*C*H$_3$)$_2$), 24.9 (*C*(CH$_3$)$_2$), 28.4 (*C*H(CH$_3$)$_2$), 28.5 (C(*C*H$_3$)$_3$), 31.3 (*C*(CH$_3$)$_3$), 31.7 (C(*C*H$_3$)$_2$), 102.8 (C_5H_5), 107.7, 109.1, 123.9, 125.8, 129.7, 142.4, 145.7, 146.0, 147.4, 149.8 (Ar-*C*).

Synthesis of (NON)Ga(η¹-Cp)

A solid mixture of **2** (80 mg, 0.051 mmol) and $MgCp_2$ (16 mg, 0.10 mmol) was added to an ampoule fitted with a Teflon valve and equipped with a Teflon-coated stirrer bar. Benzene (1 mL) was condensed into the vessel *in vacuo* at –196 °C. The mixture was allowed to warm to room temperature and stirred for 10 minutes. Subsequently, volatiles were removed *in vacuo*, and soluble material was dissolved in hexane (0.5 mL). The suspension was filtered and the resulting yellow solution was slowly concentrated to 0.2 mL, forming colourless crystals of (NON)Ga(η¹-Cp). Yield: 5.8 mg, 7%. Single crystals suitable for X-ray diffraction experiments were obtained by slow concentration of a hexane solution in a sealed glass λ-type tube. Anal. calcd for $C_{52}H_{67}GaN_2O$: C, 77.51; H, 8.38; N, 3.48. Found: C, 77.42; H, 8.24; N, 3.22. ^{1}H NMR (400 MHz, C_6D_6, 298 K): 1.14 (d, $^3J_{HH}$ = 7.0 Hz, 12 H, CH(CH_3)$_2$), 1.17 (d, $^3J_{HH}$ = 7.0 Hz, 12 H, CH(CH_3)$_2$), 1.24 (s, 18 H, C(CH_3)$_3$), 1.68 (s, 6H, XA-C(CH_3)$_2$), 3.47 (sept., $^3J_{HH}$ = 7.0 Hz, 4H, C*H*(CH$_3$)$_2$), 5.93 (s, 5H, C_5H_5), 6.52 (d, $^4J_{HH}$ = 2.2 Hz, 2H, XA-*o*-C*H*), 6.99 (d, $^4J_{HH}$ = 2.2 Hz, 2H, XA-*p*-C*H*), 7.23 (s, 2H, Ar*H*), 7.25 (s, 2H, Ar*H*). As the product was not isolable from the reaction mixture in bulk quantities, satisfactory ^{13}C{^{1}H} NMR data could not be obtained.

Synthesis of (NON)Al{(N^{i}Pr)$_2$C(NH^{i}Pr)} (4)

Compound **AlMg** (40 mg, 0.051 mmol) was added to a Schlenk flask equipped with a Teflon-coated stirrer bar. Benzene (1 mL) and *N,N'*-diisopropylcarbodiimide (0.1 mL) was condensed into the vessel *in vacuo* at –196 °C. The mixture was allowed to warm to room temperature and stirred overnight, forming a brown solution. Subsequently, volatiles were removed *in vacuo*, and soluble material was dissolved in hexane (0.5 mL). The brown solution was filtered and slowly concentrated to 0.2 mL, forming colourless crystals of **4**. Yield: 30 mg, 61%. Anal. calcd. for $C_{63}H_{98}AlN_5O$: C, 78.13; H, 10.20; N, 7.23. Found: C, 78.06; H, 9.84; N, 7.17. ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 0.06 (d, $^3J_{HH}$ = 6.5 Hz, 3H, NCH(CH_3)$_2$), 0.81 (d, $^3J_{HH}$ = 6.5 Hz, 3H, NCH(CH_3)$_2$), 1.11 (d, $^3J_{HH}$ = 6.5 Hz, 6H, NCH(CH_3)$_2$), 1.23 (m, 24H, ArCH(CH_3)$_2$), 1.27 (s, 18H, C(CH_3)$_3$), 1.31 (d, $^3J_{HH}$ = 6.5 Hz, 6H, NCH(CH_3)$_2$), 1.68 (s, 3H, C(CH_3)$_2$), 1.87 (s, 3H, C(CH_3)$_2$), 2.41 (sept., $^3J_{HH}$ = 6.5 Hz, 1H, NC*H*(CH$_3$)$_2$), 3.60 (sept., $^3J_{HH}$ = 6.8 Hz, 2H, ArC*H*(CH$_3$)$_2$), 3.81 (sept., $^3J_{HH}$ = 6.5 Hz, 1H, NC*H*(CH$_3$)$_2$), 3.95 (sept., $^3J_{HH}$ = 6.8 Hz, 2H, ArC*H*(CH$_3$)$_2$), 4.12 (sept., $^3J_{HH}$ = 6.5 Hz, 1H, NC*H*(CH$_3$)$_2$), 6.17 (d, $^4J_{HH}$ = 2.0 Hz, 2H, XA-*o*-C*H*), 6.76 (d, $^4J_{HH}$ = 2.0 Hz, 2H, XA-*p*-C*H*), 7.26-7.36 (m, 6H, Ar*H*). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 23.1 (NCH(*C*H$_3$)$_2$), 25.0, 25.1, 25.2, 25.9 (CH(*C*H$_3$)$_2$), 26.2, 26.5 (*C*H(CH$_3$)$_2$), 27.5, 29.0 (NCH(*C*H$_3$)$_2$), 31.9 (C(*C*H$_3$)$_3$), 32.0 (*C*(CH$_3$)$_3$), 35.2 (C(*C*H$_3$)$_2$), 37.0 (*C*(CH$_3$)$_2$), 43.9, 44.1, 45.1 (N*C*H(CH$_3$)$_2$), 106.1, 111.2, 124.3, 124.4, 125.9, 131.7, 139.3, 144.7, 145.1, 147.3, 147.6, 148.4 (Ar-*C*), 160.0 (N*C*N).

Spectroscopic Data

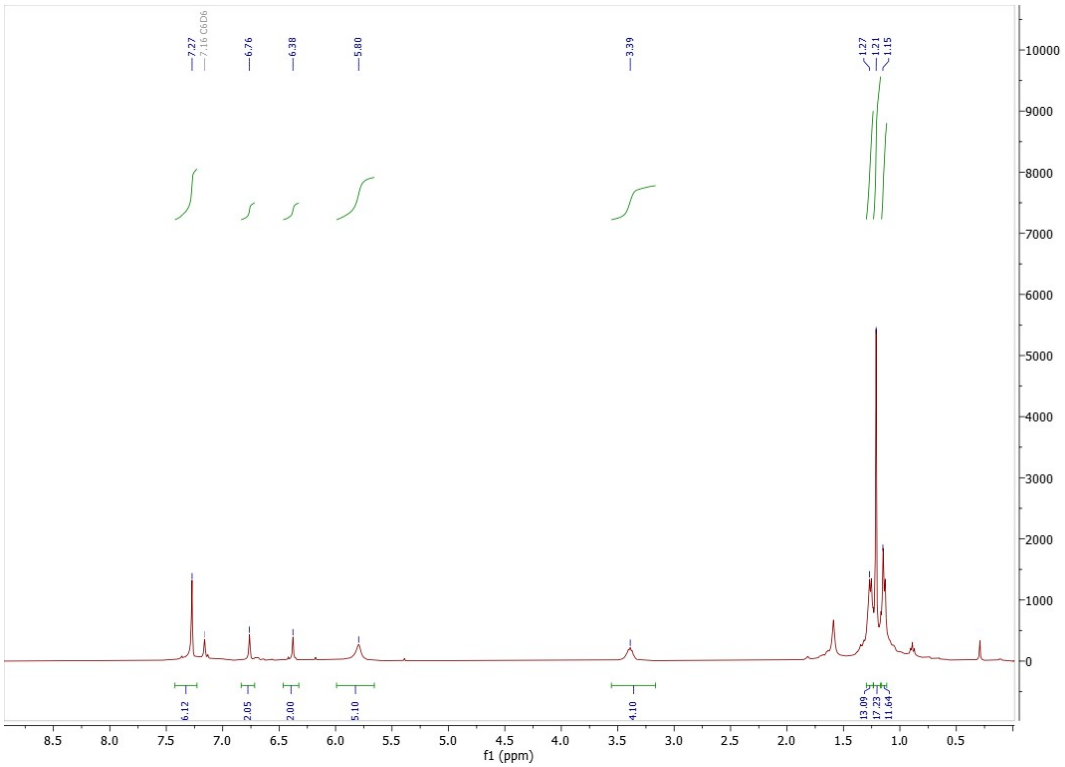

Figure S1: ^{1}H NMR spectrum of compound **AlMg** in C_6D_6.

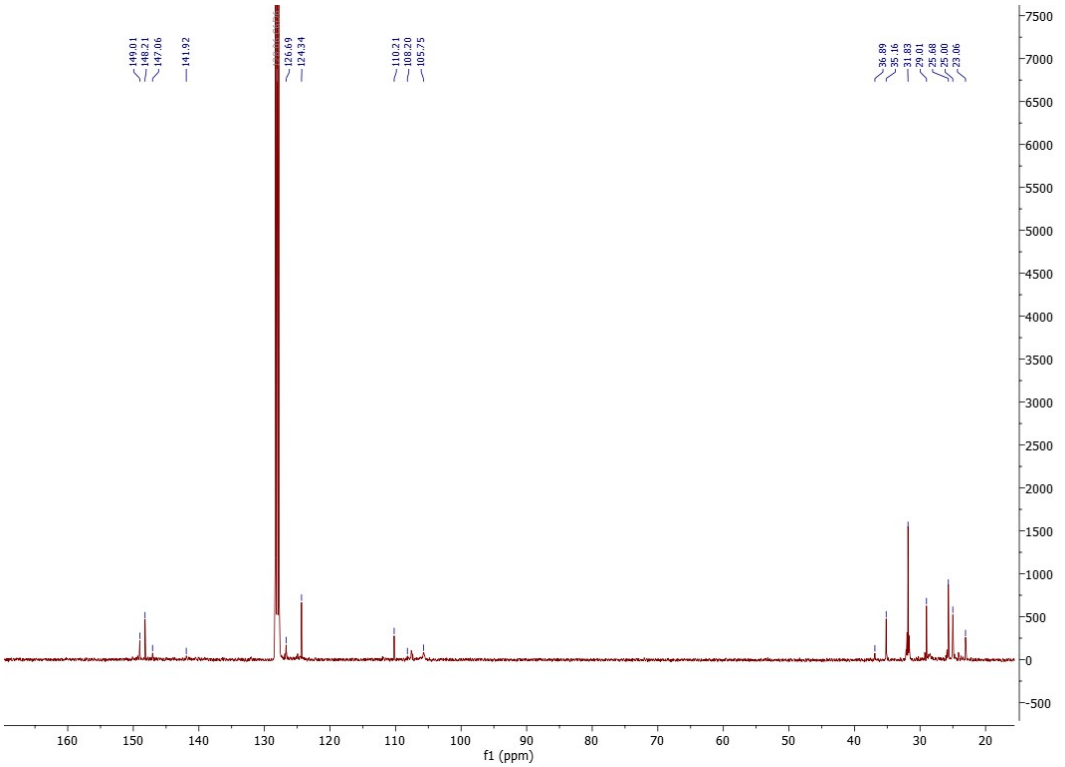

Figure S2: ^{13}C {^{1}H} NMR spectrum of compound **AlMg** in C_6D_6.

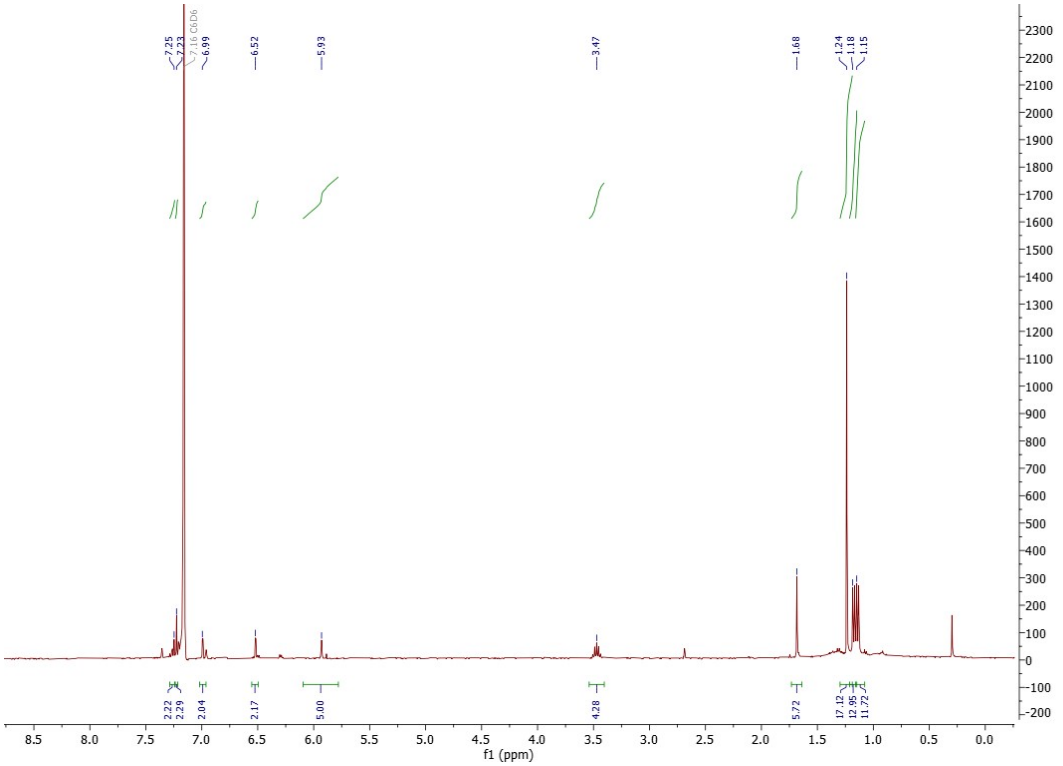

Figure S3: ^{1}H NMR spectrum of (NON)Ga(η^1-Cp) in C_6D_6.

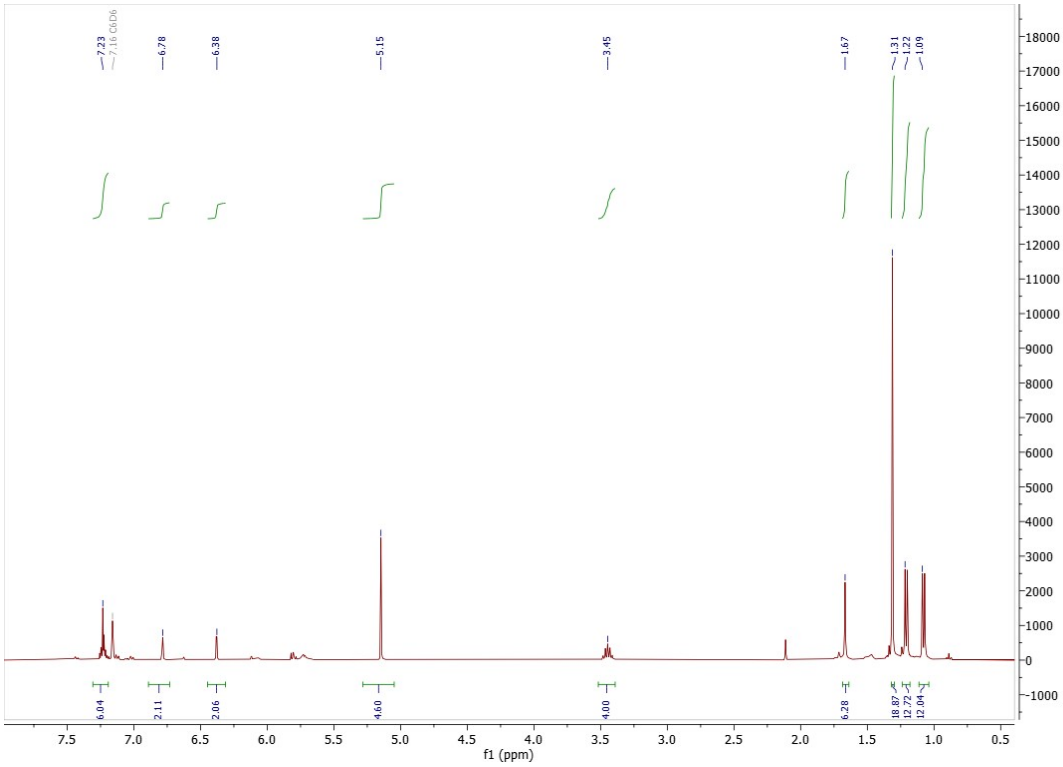

Figure S4: ^{1}H NMR spectrum of compound **InBe** in C_6D_6.

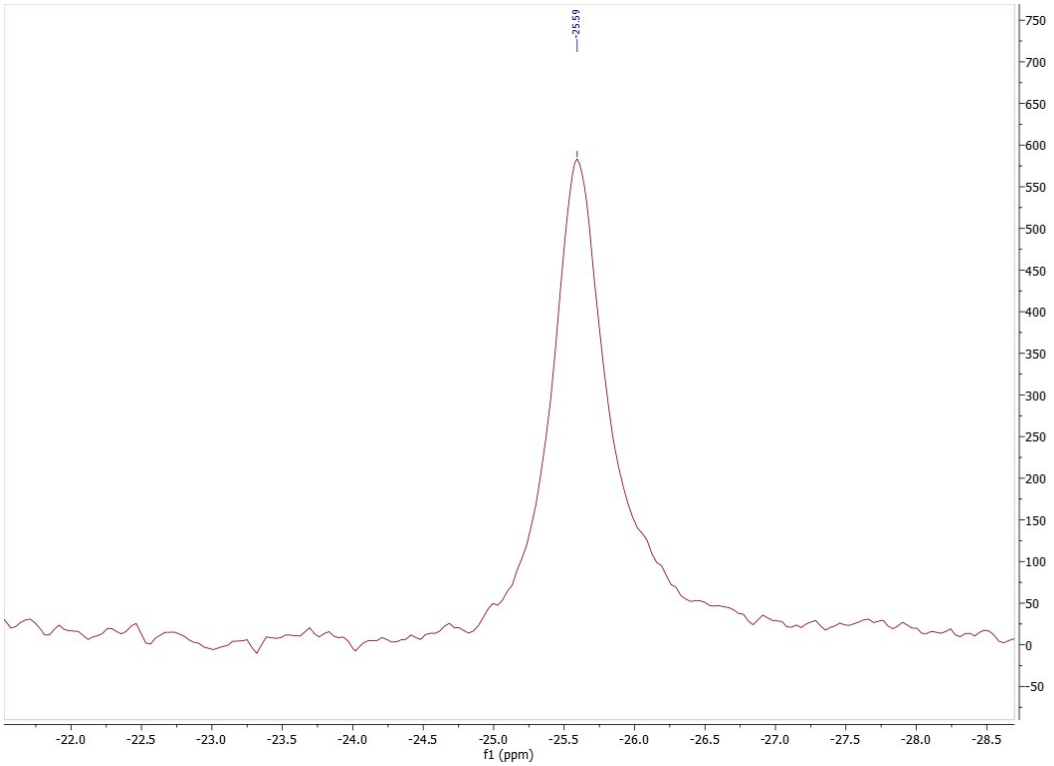

Figure S5: ^{9}Be NMR spectrum of compound **InBe** in C_6D_6.

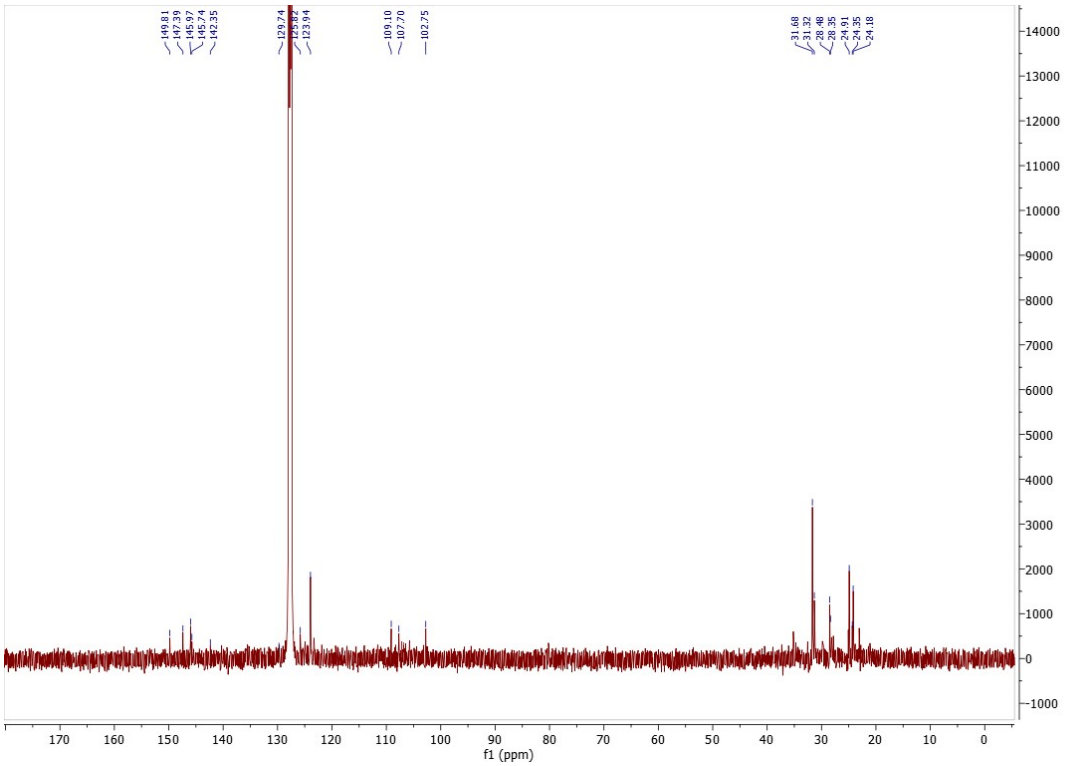

Figure S6: ^{13}C {^{1}H} NMR spectrum of compound **InBe** in C_6D_6.

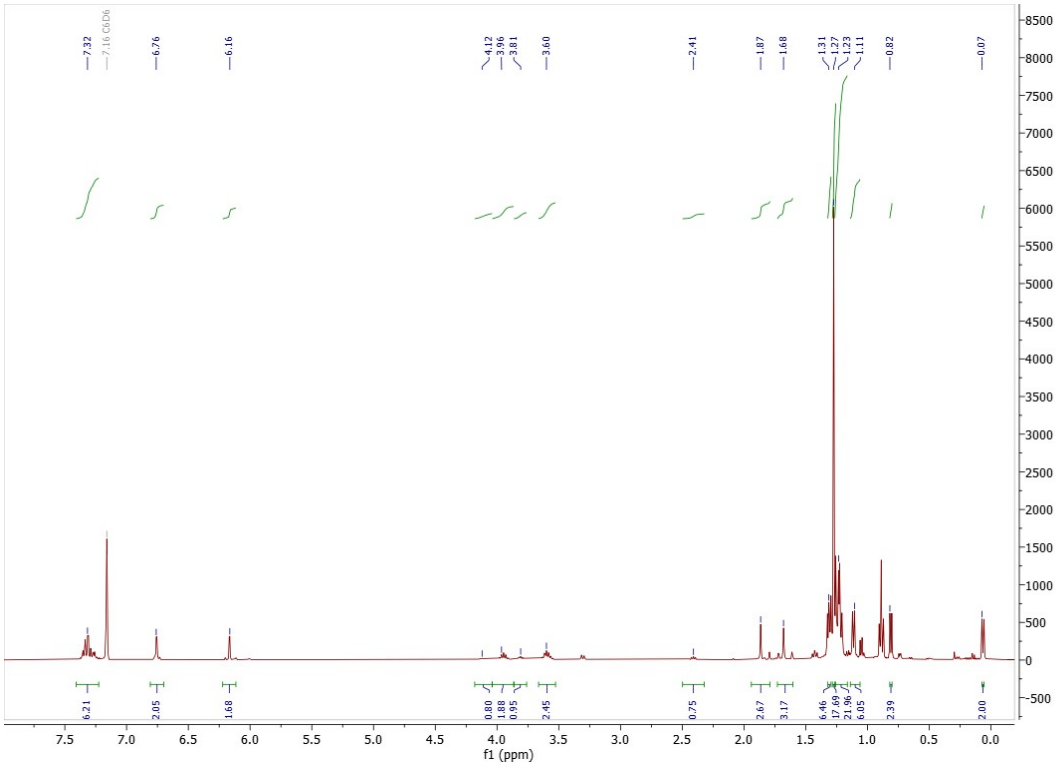

Figure S7: ^{1}H NMR spectrum of compound **4** in C_6D_6.

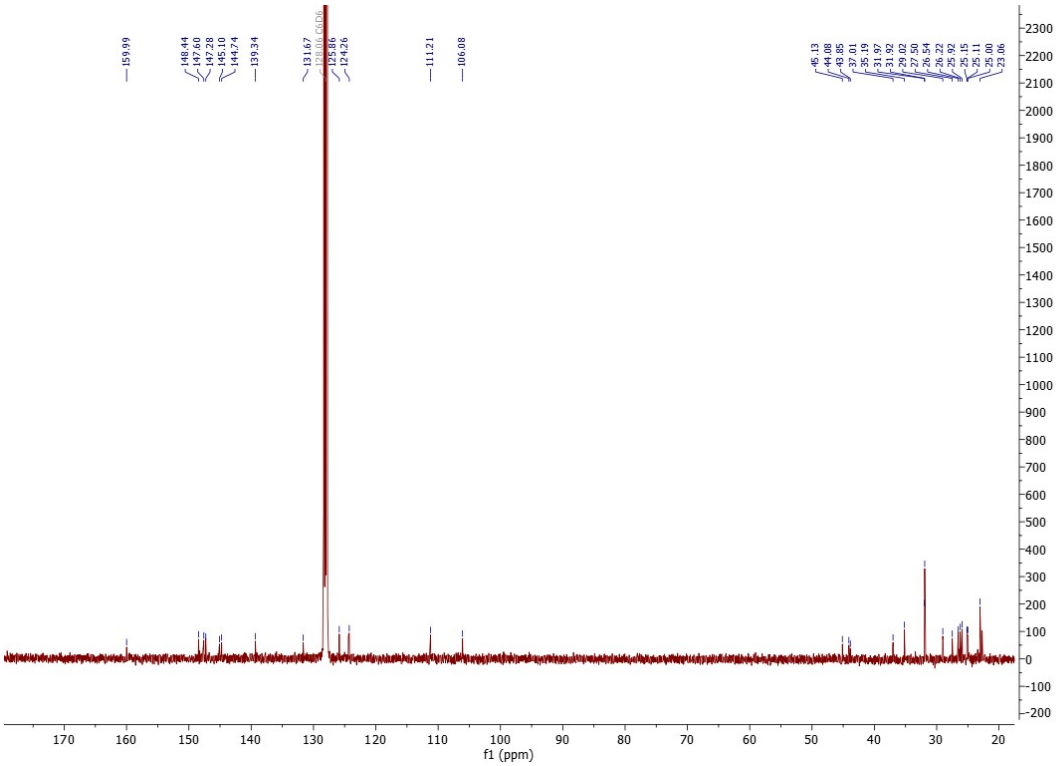

Figure S8: ^{13}C {^{1}H} NMR spectrum of compound **4** in C_6D_6.

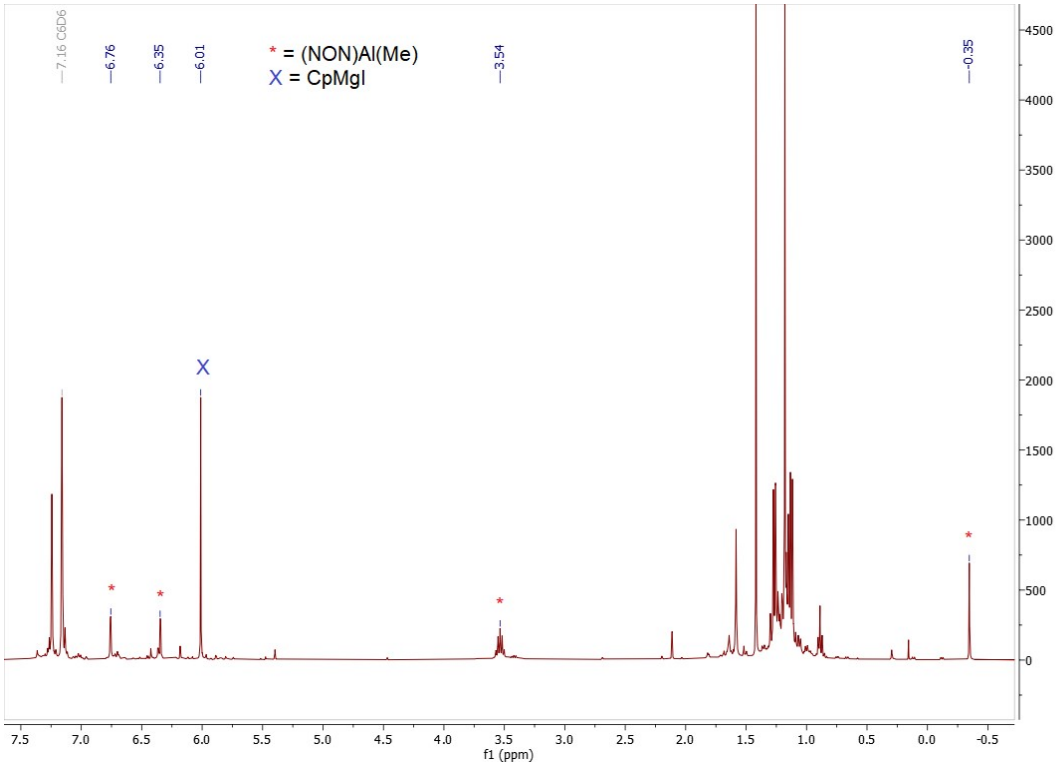

Figure S9: ^{1}H NMR spectrum of reaction of **AlMg** with MeI in C_6D_6.

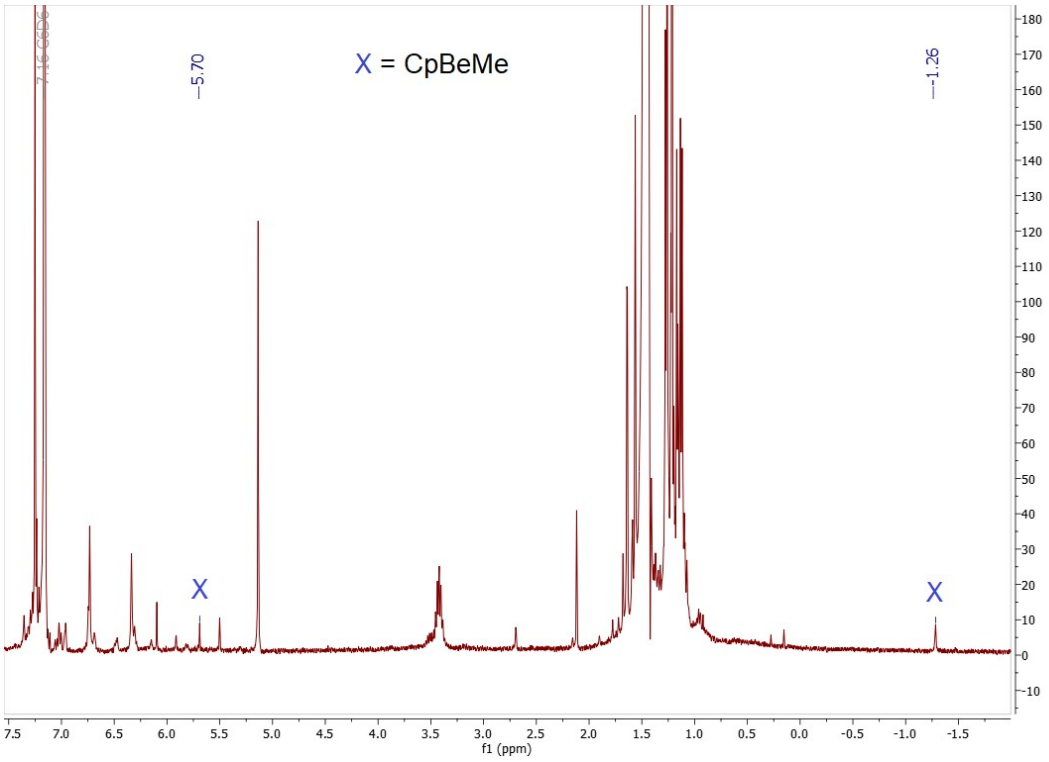

Figure S10: ^{1}H NMR spectrum of reaction of **InBe** with MeI in C_6D_6.

Crystallographic Data

Crystallographic data for **AlMg**, (NON)Ga(η^1-Cp), **InBe**, and **4** were collected using an Oxford Diffraction/Agilent SuperNova or Rigaku XtaLAB Synergy-R. Crystals were selected under Paratone-N or perfluorinated oil, mounted on MiTeGen Micromount loops and quench-cooled using an Oxford Cryosystems open flow N_2 cooling device.[6] Selected details of data collection are given in Table 1. Data collected were processed using the CrysAlisPro package, including unit cell parameter refinement and inter-frame scaling (which was carried out using SCALE3 ABSPACK within CrysAlisPro).[7] Equivalent reflections were merged and diffraction patterns processed with the CrysAlisPro suite. Structures were solved *ab initio* from the integrated intensities using SHELXT and refined on F2 using SHELXL with the graphical interface OLEX2.[8–10] Crystallographic data is given in the supplementary deposited CIF files (CCDC 2346890-2346893) and can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* http://www.ccdc.cam.ac.uk/data_request/cif.

Table S1: Selected X-ray data collection and refinement parameters

	AlMg	**(NON)Ga(Cp)**	**InBe**	**4**
Formula	C52 H67 Al Mg N2 O	C52 H67 Ga N2 O	C52 H67 Be In N2 O	C63 H98 Al N5 O
Fw (g mol^{-1})	787.36	805.79	859.90	968.44
Cell setting	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	C2/c	$P2_1/c$	$P2_1/c$
a (Å)	13.6415(2)	19.3033(2)	13.9427(2)	13.87645(13)
b (Å)	19.3339(3)	17.3028(2)	19.1025(3)	21.59607(19)
c (Å)	18.9730(3)	27.4999(4)	18.6052(3)	20.08526(15)
α (°)	90	90	90	90
β (°)	109.1377(17)	103.2039(12)	108.451(2)	102.7343(8)
γ (°)	90	90	90	90
V (Å^{-3})	4727.45(13)	8942.17(19)	4700.59(14)	5871.03(9)
Z	4	8	4	4
ρ_{calc} (g cm^{-3})	1.106	0.085	1.215	1.096
Radiation, λ (Å)	1.54184	0.71073	1.54184	1.54184
μ (mm^{-1})	0.778	0.654	4.288	0.621
$R_{(int)}$	0.0908	0.0747	0.0401	0.0383
Parameters	530	556	530	813
R_1 (all data/I >2σ(I))	0.0661	0.0607	0.0313	0.0585
ωR_2 (all data/I >2σ(I))	0.2016	0.1667	0.0806	0.1800
GooF	1.044	1.163	1.038	1.017
T (K)	100.0(2)	100.0(2)	150.0(2)	150.0(2)
CCDC Deposition No.	2346890	2346893	2346892	2346891

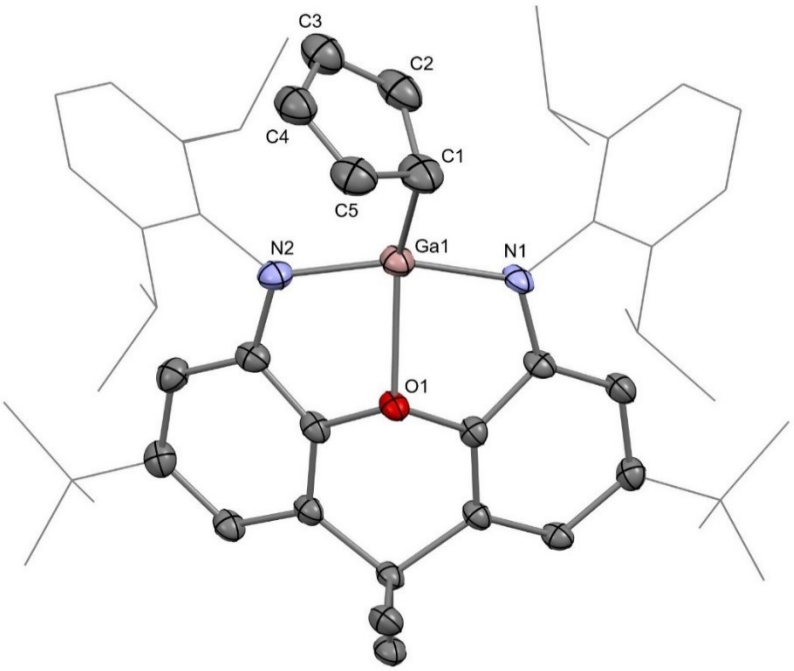

Figure S11: Molecular structure of (NON)Ga(η^1-Cp) in the solid state as determined by X-ray crystallography. Thermal ellipsoids set at 50% probability; hydrogen atoms omitted and selected substituents shown in wireframe format for clarity.

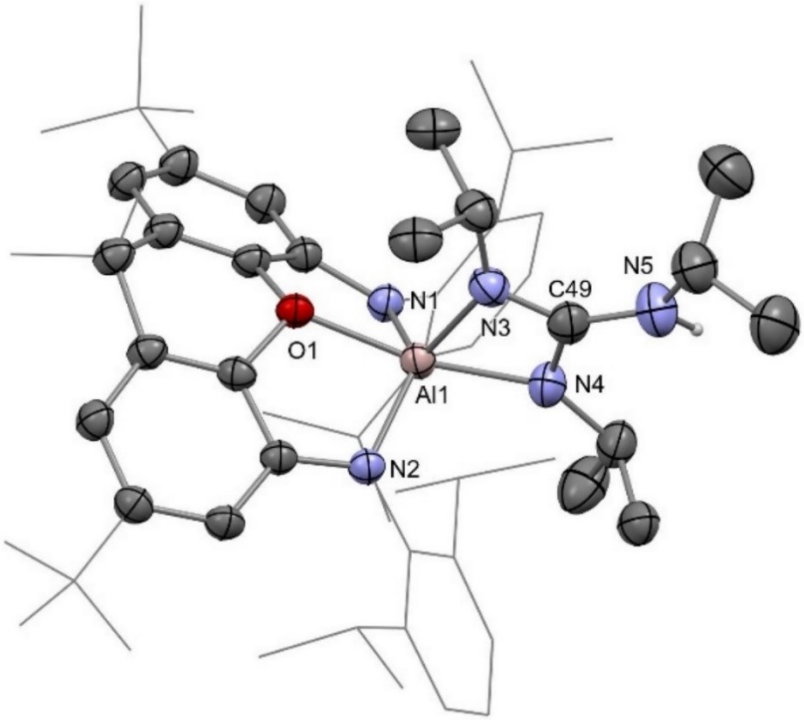

Figure S12: Molecular structure of compound **4** in the solid state as determined by X-ray crystallography. Thermal ellipsoids set at 50% probability; residual solvent and selected hydrogen atoms omitted for clarity. Selected substituents shown in wireframe format for clarity.

^{9}Be NMR Chemical Shifts – CpBeR Complexes

^{9}Be NMR chemical shift is very sensitive to the degree of electron density at a particular beryllium centre.[11,12] Of relevance here is the ^{9}Be NMR chemical shift of a cyclopentadienyl-coordinated beryllium centre. Increasingly upfield ^{9}Be NMR signals correspond to beryllium centres which are more electron-rich/reduced.[13]

Table S2: ^{9}Be NMR chemical shifts (in C_6D_6) for a range of CpBeR species and the Pauling electronegativity of the atom from each group which is bonded to beryllium.[11]

R-Group (CpBeR)	$\delta_{^{9}Be}$ / ppm	Pauling Electroneg. of Donor Atom
[(NON)Al]	–28.8	1.61
(^{Dipp}Nacnac)Zn	–27.7	1.65
Me_3Si	–27.7	1.90
CpBe	–27.6	1.57
[$Me_2(SiMe_3)Si$]	–27.2	1.90
[(NON)Ga]	–26.9	1.81
[(NON)In]	–25.6	1.78
[{NON}Al{($N^{i}Pr)_2C$}]	–24.6	2.55
Me	–20.5	2.55
Cl	–19.5	3.16
Br	–19.5	2.96

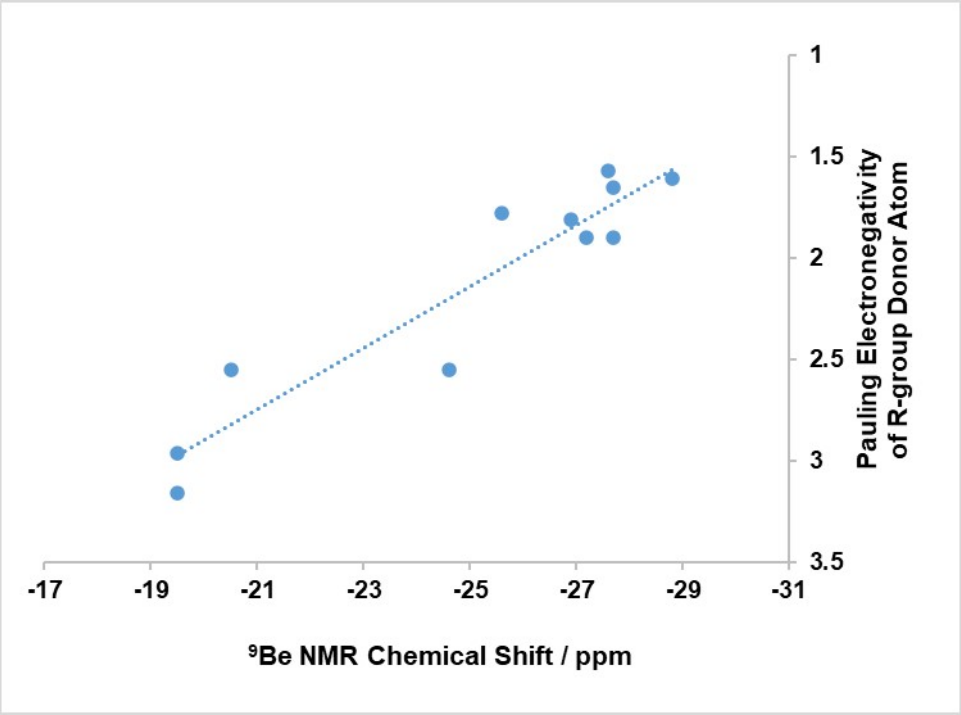

Figure S13: Plot of ^{9}Be NMR chemical shifts for a range of CpBeR species *vs* the Pauling electronegativity of the atom from each group which is bonded to beryllium.

Computational Details

The structures of complexes **AlBe**, **GaBe**, **InBe**, **AlMg**, **GaMg**, **InMg**, and **AlLi** were optimised using ORCA (Revision 5.0.4).[14,15] Specifically, R2-SCAN was used,[16,17] in conjunction with the Def2-TZVPPm basis set with the D4 dispersion correction,[18] employing the geometrical counterpoise correction gCP (together known as the R2SCAN-3c method).[19,20] Subsequently, a single point calculation was performed on this optimised structure with the ωB97X range-separated hybrid functional,[21,22] in conjunction with the Def2-QZVPP basis set [23,24] and the D4 dispersion correction.[18] The nature of the stationary points (minima) was confirmed by full frequency calculations, and are characterized by zero imaginary frequencies. Natural bond orbital was performed on the ORCA wavefunction using NBO 7.0.[25] Quantum Theory of Atoms in Molecules calculations were performed using the ORCA wavefunctions for the respective complexes, and were generated using Multiwfn 3.8.[26] EDA-NOCV was performed using Multiwfn 3.8 and ORCA (Revision 5.0.4) at the M062x-def2-TZVP level for comparisons with our previous work.

Relevant Molecular Orbitals

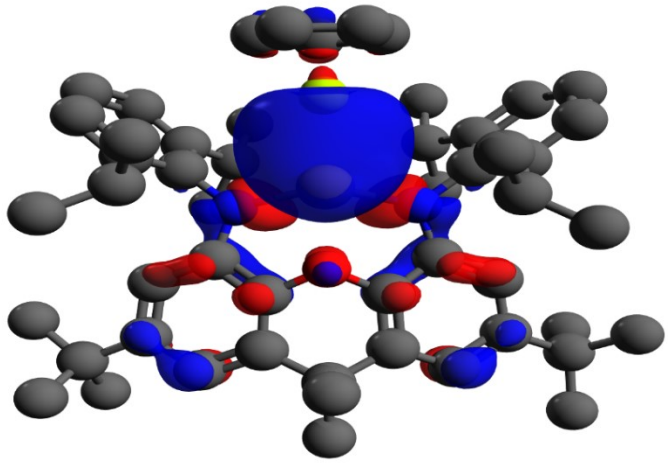

Figure S14: Principal Al–Be bonding orbital (HOMO–2) of **AlBe** (0.03 a.u.).

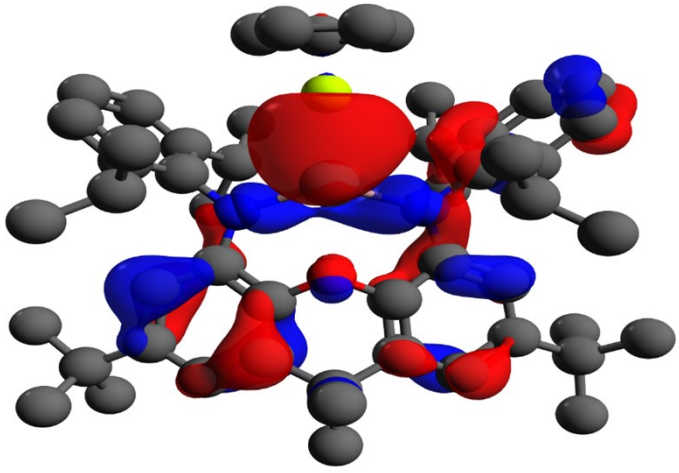

Figure S15: Principal Ga–Be bonding orbital (HOMO–4) of **GaBe** (0.03 a.u.).

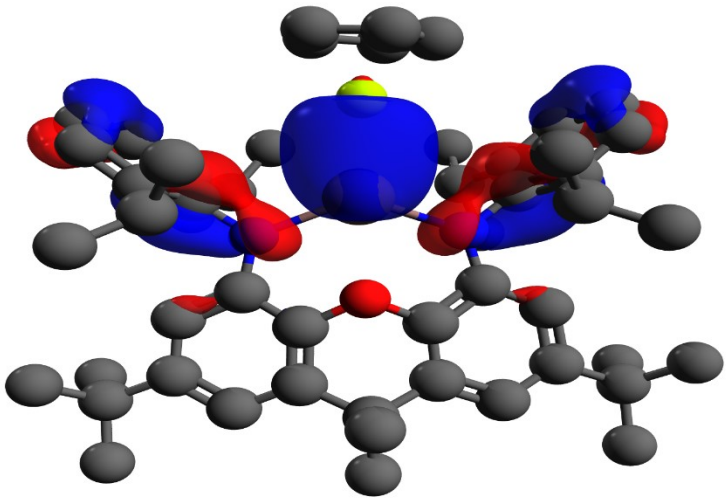

Figure S16: Principal In–Be bonding orbital (HOMO–8) of **InBe** (0.03 a.u.).

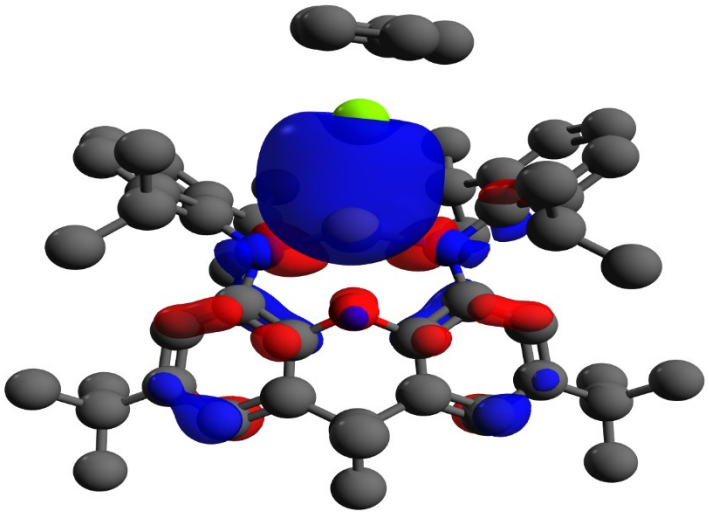

Figure S17: Principal Al–Mg bonding orbital (HOMO–2) of **AlMg** (0.03 a.u.).

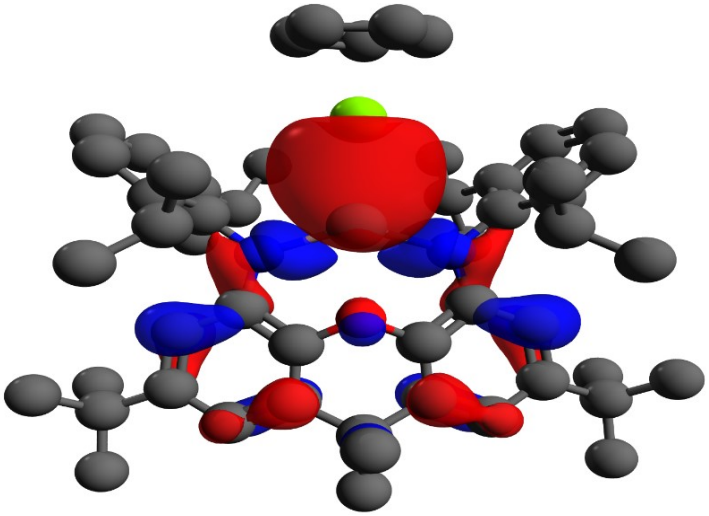

Figure S18: Principal Ga–Mg bonding orbital (HOMO–3) of **GaMg** (0.03 a.u.).

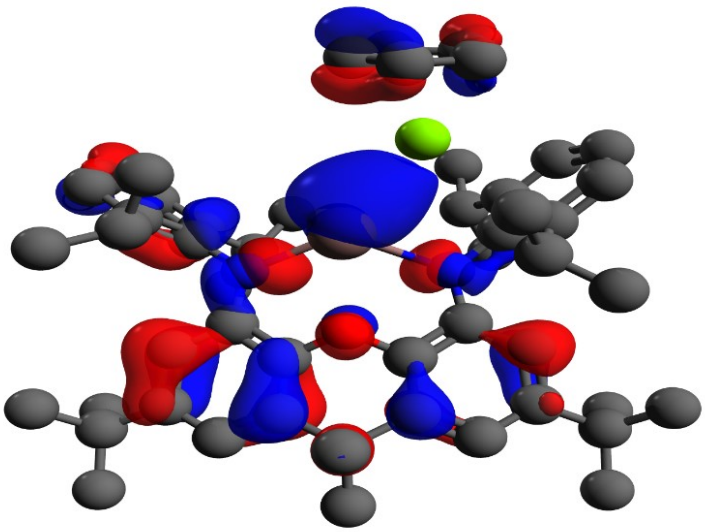

Figure S19: Principal In–Mg bonding orbital (HOMO–3) of **InMg** (0.03 a.u.).

Quantum Theory of Atoms in Molecules Calculations

Table S3: Charge distribution (Bader) calculated for complexes examined in this study.

	Tr	**Ae**	**NNA**
AlBe	2.056106	1.401902	-0.960639
GaBe	0.568247	1.494281	-
InBe	0.599657	1.443632	-
AlMg	1.143892	1.434668	-
GaMg	0.59264	1.524848	-
InMg	0.586081	1.605489	-

Table S4: Summary of QTAIM data generated for **AlBe, GaBe, and InBe**. All values in a.u., unless explicitly stated.

	AlBe			**GaBe**	**InBe**
Critical Point	**Be-NNA**	**Al-NNA**	**NNA**	**Ga-Be**	**In-Be**
ρ_{bcp} / e⁻ Bohr⁻³	0.062	0.063	0.063	0.061	0.055
Lag. E_k G(r)	0.023	0.014	0.0030	0.034	0.024
Hamilt. E_k K(r)	0.036	0.031	0.027	0.032	0.030
Pot. E Density V	-0.058	-0.045	-0.030	-0.066	-0.054
Energy Density E_b	-0.036	-0.031	-0.027	-0.032	-0.030
$\nabla^2\rho_{bcp}$ / e⁻ Bohr⁻⁵	-0.053	-0.069	-0.095	0.0092	-0.021
ELF	0.599	0.808	0.989	0.385	0.467
LOL	0.550	0.672	0.906	0.442	0.484

Table S5: Summary of QTAIM data generated for **AlMg**, **GaMg**, **InMg**, and **AlLi**. All values in a.u., unless explicitly stated.

	AlMg	**GaMg**	**InMg**	**AlLi**
Critical Point	**Al-Mg**	**Ga-Mg**	**In-Mg**	**Al-Li**
ρ_{bcp} / e⁻ Bohr^{-3}	0.034	0.036	0.027	0.018
Lag. E_k G(r)	0.018	0.024	0.016	0.011
Hamilt. E_k K(r)	0.0059	0.0045	0.0026	-0.00046
Pot. E Density V	-0.024	-0.029	-0.019	-0.011
Energy Density E_b	-0.0059	-0.0045	-0.0026	0.00046
$\nabla^2\rho_{bcp}$ / e⁻ Bohr^{-5}	0.047	0.078	0.054	0.046
ELF	0.257	0.180	0.157	0.0972
LOL	0.371	0.319	0.301	0.247

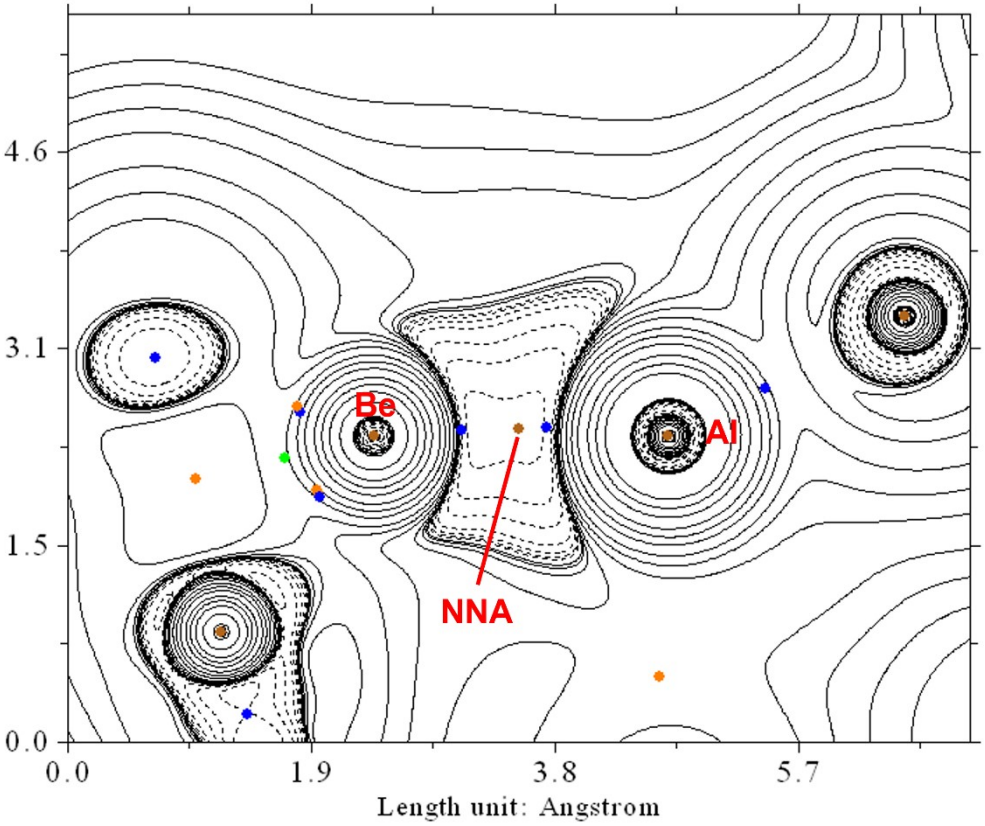

Figure S20: Laplacian of electron density contour plot for **AlBe**. Blue dots are (3, –1) points (BCP), brown dots are (3, –3) points (nucleus/NNA).

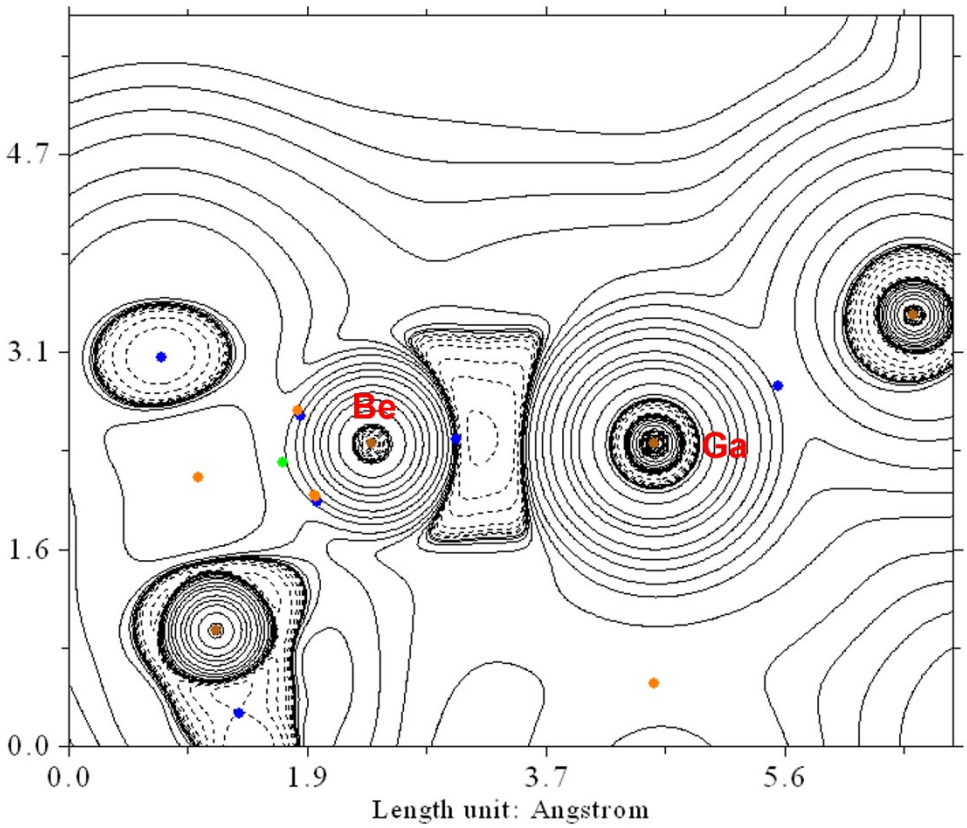

Figure S21: Laplacian of electron density contour plot for **GaBe**. Blue dots are (3, –1) points (BCP), brown dots are (3, –3) points (nucleus/NNA).

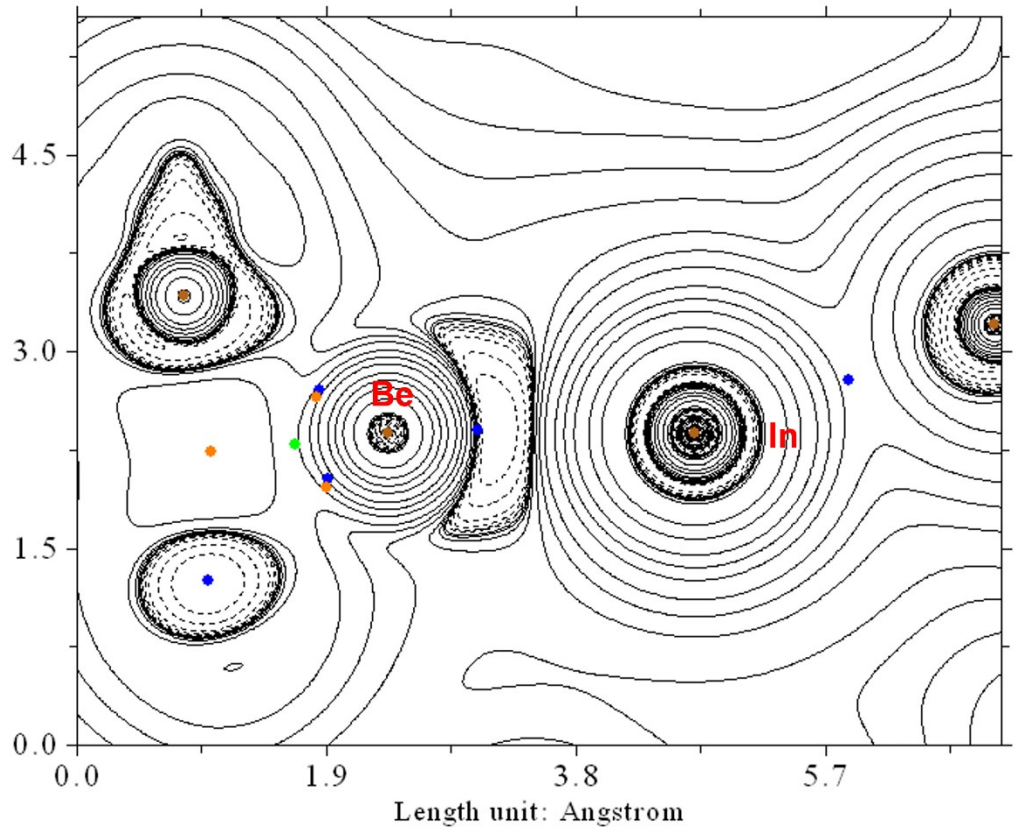

Figure S22: Laplacian of electron density contour plot for **InBe**. Blue dots are (3, –1) points (BCP), brown dots are (3, –3) points (nucleus/NNA).

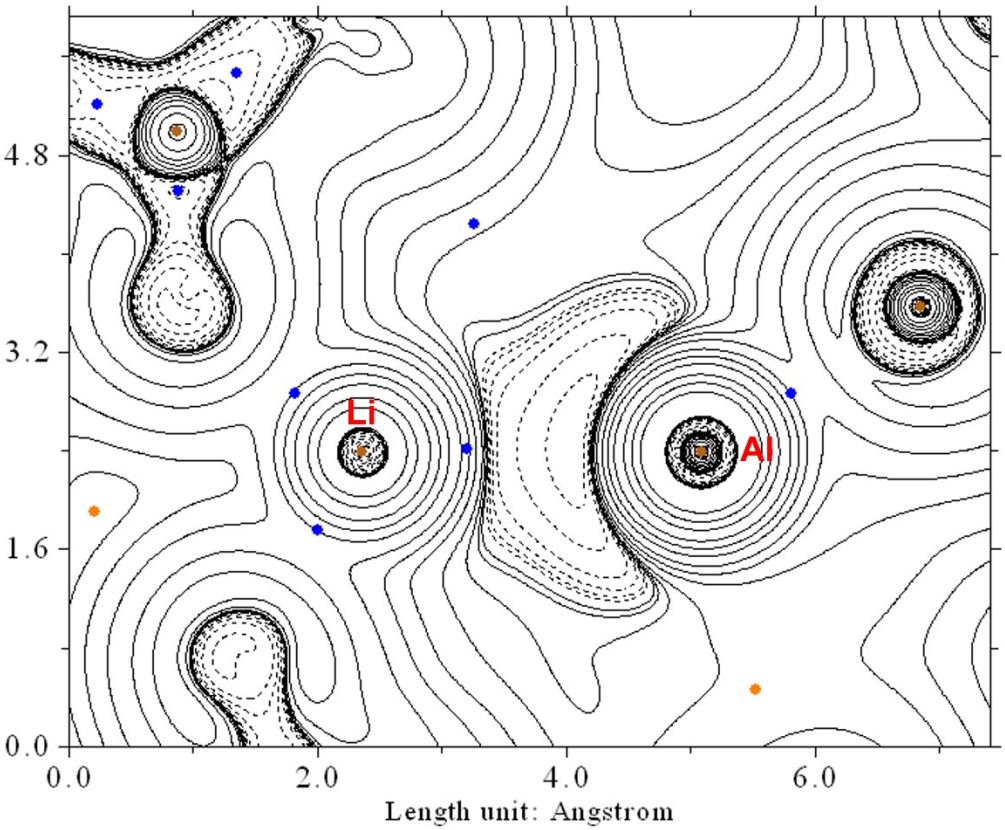

Figure S23: Laplacian of electron density contour plot for **AlLi**. Blue dots are (3, –1) points (BCP), brown dots are (3, –3) points (nucleus/NNA).

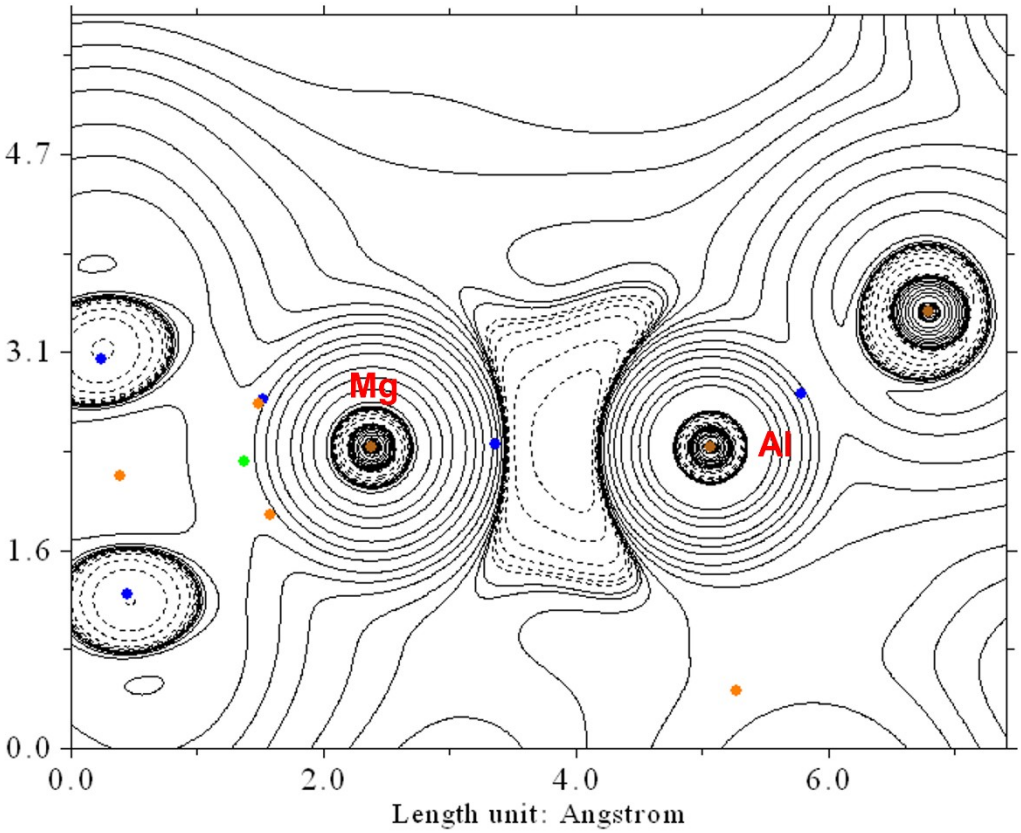

Figure S24: Laplacian of electron density contour plot for **AlMg**. Blue dots are (3, –1) points (BCP), brown dots are (3, –3) points (nucleus/NNA).

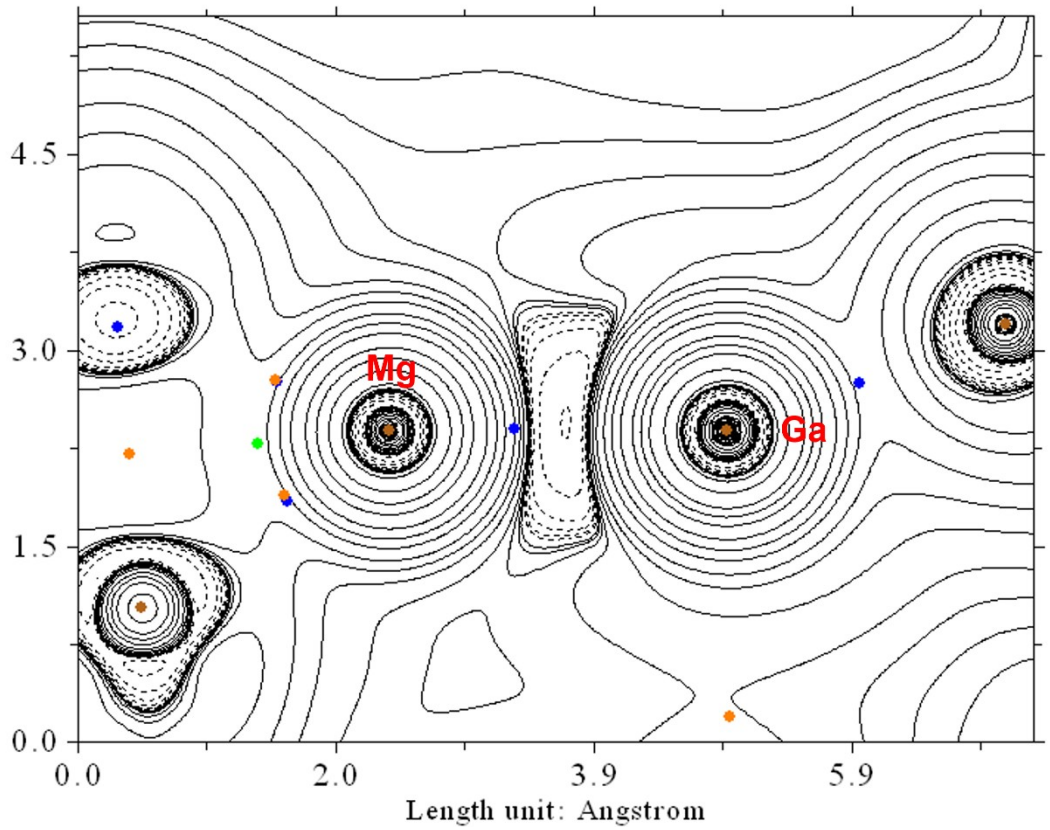

Figure S25: Laplacian of electron density contour plot for **GaMg**. Blue dots are (3, –1) points (BCP), brown dots are (3, –3) points (nucleus/NNA).

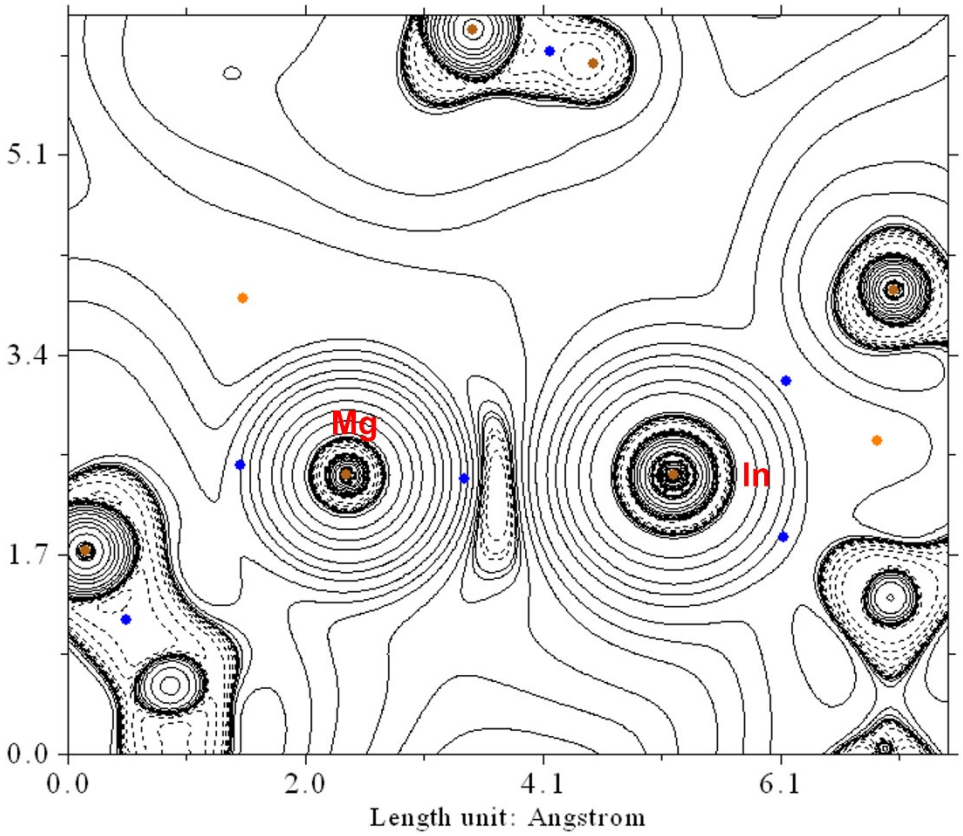

Figure S26: Laplacian of electron density contour plot for **InMg**. Blue dots are (3, –1) points (BCP), brown dots are (3, –3) points (nucleus/NNA).

Energy Decomposition Analysis with Natural Orbitals for Chemical Valence

Table S6: EDA-NOCV data for complexes and their respective fragments – homolytic cleavage of metal-metal bond. Shaded boxes represent smallest $|E_{orb}|$.

		Pair α_1			**Pair β_1**		
	E_{orb} / kcal mol^{-1}	**Energy** / kcal mol^{-1}	**Eigenvalue**	**% of total**	**Energy** / kcal mol^{-1}	**Eigenvalue**	**% of total**
AlBe	-79.95	-29.84	0.32061	45.6	-43.12	0.38232	54.4
GaBe	-88.07	-26.15	0.2912	40.4	-53.4	0.42909	59.6
InBe	-98.77	-24.65	0.29595	39.6	-65.78	0.45097	60.4
AlMg	-74.94	-23.55	0.31964	40.2	-47.59	0.47472	59.8
GaMg	-81.43	-19.67	0.29049	35.9	-57.14	0.5195	64.1
InMg	-125.44	-17.24	0.28499	29.7	-92.94	0.67384	70.3
AlLi	-86.65	-9.95	0.1968	25.1	-66.9	0.58592	74.9

Table S7: EDA-NOCV data for complexes and their respective fragments – donor-acceptor fragmentation of metal-metal bond. Shaded boxes represent smallest $|E_{orb}|$.

	M→Tr			**Tr→M**		
	E_{orb} / kcal mol^{-1}	**Pair 1**	**Pair 2**	**E_{orb}** / kcal mol^{-1}	**Pair 1**	**Pair 2**
AlBe	-162.72	-131.004	-6.986	-96.86	-72.524	-1.983
GaBe	-192.45	-158.724	-9.454	-90.18	-65.34	-2.496
InBe	-221.74	-188.347	-11.843	-82.77	-61.458	-2.422
AlMg	-125.90	-107.679	-3.458	-75.38	-50.688	-2.134
GaMg	-147.65	-129.448	-3.985	-71.04	-45.074	-3.156
InMg	-203.80	-185.361	-4.848	-76.67	-40.518	-8.868
AlLi	-212.87	-188.287	-3.386	-31.03	-14.866	-0.88

Singlet-Triplet Gap Calculations

Table S8: Calculated S-T gaps for complexes relevant to this study.

	ΔG / kcal mol^{-1}	**ΔE /** kcal mol^{-1}
AlBe	-52.0755	-54.7354
GaBe	-50.5548	-53.8934
InBe	-38.3601	-40.5165
AlMg	-50.6708	-51.7464
GaMg	-45.5822	-48.2929
InMg	-34.3381	-35.8057

Miscellaneous Charge Distribution Data

Table S9: Calculated charges for Tr and Ae atoms of complexes relevant to this study, as assessed by various computational techniques.

	Tr			Ae		
	CHELPG	**VDD**	**ADCH**	**CHELPG**	**VDD**	**ADCH**
AlBe	0.0281	0.2442	0.188704	0.1205	-0.0652	-0.14287
GaBe	0.1811	0.2422	0.224769	0.1009	-0.0177	-0.10394
InBe	0.4159	0.2514	0.297786	0.0176	-0.0059	-0.10023
AlMg	-0.0719	0.1682	0.000945	0.2563	0.2504	0.202162
GaMg	0.1020	0.1608	0.069526	0.2803	0.3182	0.25552
InMg	0.1686	0.1366	0.093475	0.2256	0.3693	0.308523

Coordinates of Optimised Structures

Table S10: xyz-Coordinates of selected optimized structures

AlBe

Al	5.27577	5.11221	8.36417
O	5.85138	6.86350	9.28479
N	4.13913	5.10884	9.90275
N	7.16566	5.03953	8.10861
Be	4.26948	3.92151	6.68119
C	5.21144	7.09564	10.51355
C	7.24432	7.01185	9.37814
C	2.99963	4.26065	9.97304
C	4.25274	6.13749	10.81774
C	7.74531	4.31636	7.02521
C	7.94768	6.01598	8.70523
C	2.79587	3.60212	5.48565
C	2.79950	2.67652	6.55980
C	4.05082	2.00746	6.54979
C	4.82092	2.51646	5.47144
C	4.04613	3.50403	4.81402
C	5.63705	8.10809	11.34279
C	7.78745	8.01170	10.14668
C	3.16038	2.91264	10.36245
C	1.73291	4.75180	9.59502
C	3.54888	6.32851	12.01800
C	7.99907	2.93239	7.14690
C	8.01100	4.98582	5.81078
C	9.34150	6.12712	8.73243
H	2.00524	4.30112	5.25274
H	2.03552	2.57833	7.32039
H	4.39138	1.30137	7.29429
H	5.85393	2.27678	5.25582
H	4.37406	4.11768	3.98686
C	4.94194	8.24395	12.54708
C	6.82166	8.95660	10.86994
C	9.18808	8.06792	10.18074
C	2.04805	2.07071	10.33879
C	4.50307	2.41673	10.86798
C	0.64570	3.87556	9.59899
C	1.51824	6.19185	9.16173
H	2.77000	5.61962	12.27378
C	3.88443	7.37889	12.87710
C	8.55237	2.25395	6.05965
C	7.67510	2.20087	8.43688
C	8.56129	4.26445	4.74995
C	7.68211	6.45427	5.60084
H	9.92937	5.38563	8.19927
C	9.96490	7.14808	9.46588
H	5.22957	9.02533	13.24057
C	6.30580	10.00428	9.85392
C	7.49856	9.68226	12.03166
H	9.66722	8.83212	10.77763
H	2.15206	1.02915	10.62576
C	0.79793	2.54431	9.95812

AlMg

Al	2.58107	9.44032	12.81795
O	3.13988	8.42727	11.14485
N	4.25913	8.77094	13.39028
N	0.91590	8.65703	12.34184
C	4.36426	7.75033	11.28121
C	0.90785	7.75361	11.28974
C	4.97822	7.98181	12.50977
C	4.77361	6.85185	10.32802
C	2.12683	7.59674	10.63480
C	2.41120	6.67912	9.65432
C	-0.14459	6.96157	10.82135
H	-1.11815	7.06344	11.29180
C	5.99814	6.21305	10.57098
H	6.36812	5.49627	9.85063
C	3.84995	6.62520	9.12637
C	4.14659	5.30203	8.42202
H	5.17167	5.29338	8.04029
H	3.48420	5.17380	7.56098
H	4.01588	4.44929	9.09566
C	1.33764	5.88239	9.23161
H	1.50875	5.13904	8.46488
C	-0.32390	9.23597	12.73720
C	-1.00187	10.10666	11.85459
C	6.21568	7.35781	12.69958
H	6.74594	7.52999	13.63143
C	4.92551	9.22107	14.56739
C	6.73130	6.48173	11.73323
C	0.06353	6.02804	9.79429
C	-0.43934	10.50032	10.49923
H	0.53306	10.01395	10.37353
C	5.79949	10.32668	14.49365
C	6.06030	11.06490	13.19326
H	5.35649	10.68305	12.44518
C	-1.11814	5.15727	9.35056
C	4.04709	7.78612	8.12167
H	3.83987	8.75291	8.58946
H	3.36931	7.66247	7.27013
H	5.07976	7.79450	7.75671
C	8.07886	5.80600	12.01376
C	-0.83620	8.98911	14.03120
C	-2.22004	10.65627	12.25857
H	-2.75620	11.31763	11.58262
C	4.69136	8.56810	15.79636
C	-0.09344	8.07603	14.99161
H	0.97301	8.34370	14.93135
C	-1.34182	10.03572	9.34848
H	-2.32280	10.52269	9.39265
H	-1.49434	8.95371	9.38321
H	-0.88718	10.28588	8.38332
C	6.45152	10.74209	15.65624

H	5.28468	2.90824	10.27440
C	4.69870	0.90642	10.73666
C	4.71560	2.85116	12.32733
H	-0.33501	4.24000	9.30330
H	2.46406	6.72900	9.27464
C	1.12878	6.26959	7.67994
C	0.47984	6.89924	10.04233
C	3.13133	7.60349	14.19391
H	8.75881	1.19154	6.13401
C	8.83886	2.91163	4.86980
H	6.68648	2.55582	8.76301
C	7.58065	0.68292	8.27405
C	8.67859	2.54935	9.54665
H	8.76736	4.77093	3.81040
H	7.31539	6.86528	6.54531
C	6.55542	6.61667	4.57094
C	8.92034	7.26653	5.20153
C	11.49748	7.19763	9.48670
H	5.58711	10.67307	10.33969
H	5.80892	9.52289	9.00649
H	7.14265	10.59822	9.47081
H	8.32762	10.29626	11.66781
H	7.88354	8.97827	12.77610
H	6.79222	10.35901	12.52140
H	-0.05711	1.87410	9.94648
H	5.72690	0.64427	11.00575
H	4.51318	0.55716	9.71504
H	4.03928	0.35060	11.41251
H	3.93670	2.41867	12.96679
H	4.67737	3.93865	12.42912
H	5.69057	2.50778	12.69203
H	1.91377	5.82689	7.05931
H	0.99378	7.31311	7.37298
H	0.19173	5.73550	7.48319
H	-0.51318	6.44853	9.93470
H	0.39989	7.95491	9.76032
H	0.76448	6.85038	11.09807
C	2.04017	6.55281	14.43152
C	2.46158	8.99080	14.15947
C	4.11892	7.53895	15.37450
H	9.27022	2.36496	4.03591
H	8.55732	0.23909	8.05014
H	6.88660	0.39889	7.47509
H	7.22966	0.23033	9.20587
H	8.40868	2.04202	10.48058
H	8.71080	3.62444	9.73868
H	9.68502	2.22175	9.25995
H	6.84570	6.21397	3.59370
H	6.30652	7.67601	4.43970
H	5.65543	6.08982	4.90540
H	9.31079	6.95280	4.22683
H	9.71692	7.15090	5.94266
H	8.66944	8.33087	5.13289
C	12.04017	5.89320	10.10164
C	12.02399	7.34184	8.04646
C	12.03802	8.37335	10.30964
H	1.53418	6.75980	15.38051
H	2.45680	5.54132	14.48929
H	1.28161	6.57029	13.64152
H	1.90264	9.16730	15.08612
H	1.76449	9.05983	13.31708
H	3.19923	9.79187	14.05107
H	4.88926	8.31256	15.30526
H	4.62084	6.56585	15.40478
H	3.58533	7.68185	16.32148
H	11.74169	5.01706	9.51816
H	11.66271	5.76165	11.12153
H	13.13570	5.91762	10.13843
H	13.11892	7.39817	8.04630
H	11.63196	8.25333	7.58184
H	11.73314	6.49212	7.42123
H	13.13270	8.36425	10.27930
H	11.73635	8.30729	11.36063
H	11.70218	9.33647	9.90976

GaBe

Ga	5.22916	4.98815	8.27956
O	5.84365	6.94505	9.26553
N	4.12647	5.12504	9.90434
N	7.18150	5.05038	8.10554
Be	4.26908	3.78138	6.68592
C	5.21215	7.13015	10.49397
C	7.22839	7.04909	9.36715
C	2.98500	4.28709	9.96960
C	4.25973	6.16300	10.80097
C	7.75792	4.33520	7.02214
C	7.93384	6.04390	8.70521
C	2.78714	3.49481	5.51940
C	2.80405	2.55643	6.58319
H	7.13357	11.58733	15.61425
C	8.52698	4.88975	10.86869
H	7.82505	4.06369	10.71105
H	9.50131	4.45348	11.11268
H	8.63471	5.44124	9.92830
C	-0.20276	12.01577	10.42208
H	0.26535	12.28080	9.46742
H	0.45384	12.35334	11.23172
H	-1.14237	12.57325	10.50176
C	-2.04721	9.57919	14.39564
H	-2.45731	9.40179	15.38380
C	6.24093	10.09683	16.86532
H	6.75701	10.43321	17.76022
C	-0.75043	4.20922	8.20257
H	-0.41305	4.75788	7.31628
H	-1.63162	3.62508	7.91714
H	0.03354	3.50242	8.49518
C	-2.74612	10.39298	13.51329
H	-3.69290	10.83344	13.81315
C	5.36261	9.02354	16.93219
H	5.19911	8.53279	17.88656
C	-2.27370	6.05721	8.87475
H	-2.63754	6.70800	9.67549
H	-3.11592	5.44372	8.53397
H	-1.95243	6.69285	8.04223
C	3.77196	7.36217	15.88116
H	3.01564	7.46690	15.09277
C	5.81431	12.57266	13.33509
H	4.82086	12.77588	13.75073
H	5.88412	13.06318	12.35783
H	6.55234	13.04262	13.99437
C	-1.59185	4.30402	10.54316
H	-0.77801	3.66840	10.90832
H	-2.42551	3.65890	10.24146
H	-1.93168	4.92657	11.37664
C	7.96450	4.95475	13.29335
H	7.72079	5.56787	14.16633
H	8.91316	4.44350	13.49513
H	7.18010	4.19770	13.18496
C	9.15932	6.88556	12.21435
H	9.24789	7.51498	11.32201
H	10.13209	6.41723	12.40472
H	8.92863	7.53548	13.06387
C	7.48204	10.79864	12.67662
H	8.23024	11.15573	13.39404
H	7.64906	11.31904	11.72664
H	7.64718	9.72992	12.51328
C	-0.51963	8.24526	16.45031
H	-0.45283	9.28979	16.77301
H	0.12740	7.64717	17.09766
H	-1.54678	7.89957	16.61292
C	-0.22357	6.60483	14.56919
H	-1.27552	6.29710	14.60106
H	0.34084	5.95895	15.25197
H	0.14991	6.44012	13.55541
C	4.53972	6.06096	15.59660
H	5.35328	5.93396	16.32132
H	4.97309	6.06019	14.59299
H	3.86992	5.19723	15.67939
C	3.04059	7.25661	17.22189
H	2.28129	6.46931	17.16744
H	2.54754	8.19734	17.48883
H	3.72169	6.98616	18.03638
Mg	1.88601	11.77256	13.94252
C	0.68813	12.63515	15.77852
H	0.28342	11.98531	16.54384
C	1.97443	13.23750	15.78965
H	2.72343	13.12847	16.56388
C	2.09939	14.02211	14.61312
H	2.95220	14.63148	14.34165
C	0.01709	13.04663	14.59794
H	-0.97938	12.74761	14.29684
C	0.88889	13.90395	13.87672
H	0.66047	14.40429	12.94416

GaMg

Ga	2.50204	9.47030	12.93000
O	3.15818	8.33444	11.07030
N	4.28826	8.79306	13.32870
N	0.88166	8.60769	12.24196
C	4.34514	7.64295	11.27466
C	0.90085	7.74217	11.16561
C	4.96851	7.93429	12.49020
C	4.76386	6.69543	10.37098
C	2.14095	7.54117	10.55602
C	2.41637	6.58932	9.60205
C	-0.16829	7.00761	10.64141
H	-1.15466	7.15488	11.07166
C	5.97454	6.04938	10.65909

C	4.05487	1.88542	6.54794
C	4.81168	2.40670	5.46506
C	4.02878	3.40359	4.82946
C	5.63720	8.12962	11.34378
C	7.78721	8.03682	10.14565
C	3.13877	2.93515	10.35493
C	1.72293	4.77926	9.57405
C	3.56302	6.34236	12.00906
C	8.00604	2.94829	7.14141
C	8.01079	5.00140	5.80219
C	9.32943	6.14696	8.74187
H	1.99477	4.19874	5.30825
H	2.05101	2.45342	7.35426
H	4.40628	1.17216	7.28028
H	5.84168	2.16893	5.23292
H	4.34773	4.02818	4.00693
C	4.95569	8.24910	12.55630
C	6.82287	8.98042	10.87441
C	9.18659	8.08137	10.19409
C	2.02436	2.09651	10.31955
C	4.47719	2.43412	10.86768
C	0.63388	3.90565	9.56597
C	1.52018	6.21986	9.13801
H	2.78816	5.62780	12.26191
C	3.89975	7.38057	12.88093
C	8.54810	2.26808	6.04973
C	7.69704	2.21935	8.43732
C	8.55358	4.27878	4.73868
C	7.67001	6.46687	5.59419
H	9.91414	5.39928	8.21354
C	9.96003	7.15963	9.47849
H	5.25191	9.01765	13.26069
C	6.30788	10.03571	9.86560
C	7.50125	9.69921	12.03940
H	9.66806	8.83617	10.80130
H	2.12287	1.05433	10.60672
C	0.77881	2.57395	9.92778
H	5.26335	2.92490	10.27964
C	4.66937	0.92331	10.73538
C	4.68451	2.86696	12.32809
H	-0.34286	4.27250	9.25992
H	2.47046	6.74877	9.25179
C	1.13164	6.30046	7.65582
C	0.48625	6.93537	10.01725
C	3.15538	7.58440	14.20605
H	8.75366	1.20525	6.12299
C	8.82926	2.92513	4.85784
H	6.71199	2.57100	8.77800
C	7.60457	0.70053	8.28089
C	8.71210	2.57407	9.53459
H	8.75388	4.78412	3.79713
H	7.28833	6.86942	6.53627
C	6.55369	6.62241	4.55152
C	8.90489	7.29186	5.21142
C	11.49289	7.19651	9.50370
H	5.59082	10.70243	10.35685
H	5.80987	9.56075	9.01551
H	7.14561	10.63125	9.48658
H	8.33050	10.31489	11.67844
H	7.88668	8.99095	12.77969
H	6.79552	10.37342	12.53380
H	-0.07822	1.90637	9.90895
H	5.69681	0.65851	11.00490
H	4.48423	0.57462	9.71341
H	4.00787	0.36813	11.40979
H	3.90009	2.43863	12.96364
H	4.65242	3.95464	12.42878
H	5.65584	2.51810	12.69716
H	1.91167	5.85282	7.03181
H	1.00516	7.34495	7.34897
H	0.19046	5.77416	7.45795
H	-0.50937	6.48987	9.91094
H	0.41278	7.99114	9.73404
H	0.77200	6.88621	11.07259
C	2.05872	6.53640	14.42976
C	2.49461	8.97633	14.20436
C	4.14993	7.49028	15.37890
H	9.25488	2.37723	4.02178
H	8.58042	0.25764	8.05163
H	6.90583	0.41089	7.48795
H	7.26085	0.25147	9.21726
H	8.45788	2.06280	10.47067
H	8.73711	3.64899	9.72790
H	9.71720	2.25509	9.23390
H	6.86410	6.24210	3.57156
H	6.28444	7.67823	4.43398
H	5.65858	6.07238	4.86219
H	9.31404	6.97752	4.24451
H	9.68979	7.18731	5.96648
H	8.64398	8.35323	5.13490
H	6.34227	5.29387	9.97788
C	3.87453	6.45520	9.14448
C	4.14393	5.09335	8.50491
H	5.18191	5.02726	8.16593
H	3.51174	4.95488	7.62309
H	3.95097	4.27553	9.20650
C	1.32838	5.83829	9.13595
H	1.49864	5.07465	8.38897
C	-0.34736	9.17494	12.66620
C	-0.97379	10.16108	11.87171
C	6.19317	7.30090	12.72363
H	6.72414	7.52659	13.64413
C	4.97925	9.41193	14.40313
C	6.70341	6.36521	11.81169
C	0.03677	6.05928	9.62880
C	-0.38469	10.63309	10.55470
H	0.55213	10.09370	10.38359
C	5.79706	10.53624	14.14667
C	6.01624	11.06087	12.73979
H	5.38413	10.47813	12.06164
C	-1.16828	5.25076	9.13388
C	4.16408	7.56675	8.10652
H	3.97828	8.55732	8.53176
H	3.51776	7.43941	7.23121
H	5.21086	7.51890	7.78693
C	8.04294	5.69182	12.13299
C	-0.88670	8.82046	13.92597
C	-2.15920	10.73982	12.32857
H	-2.65335	11.49378	11.72095
C	4.78659	8.95496	15.72307
C	-0.22293	7.75206	14.78093
H	0.86228	7.93496	14.75736
C	-1.31696	10.32274	9.37593
H	-2.26513	10.86532	9.46492
H	-1.53802	9.25246	9.32580
H	-0.84826	10.61899	8.43089
C	6.41548	11.17506	15.22132
H	7.04769	12.04021	15.03800
C	8.48063	4.70217	11.04647
H	7.76813	3.87732	10.93621
H	9.44881	4.26912	11.31915
H	8.59755	5.19371	10.07447
C	-0.04683	12.13026	10.60594
H	0.43584	12.44495	9.67397
H	0.63559	12.35184	11.43520
H	-0.94569	12.74180	10.74150
C	-2.06608	9.43965	14.34480
H	-2.49757	9.18284	15.30612
C	6.23368	10.72849	16.52370
H	6.72364	11.23858	17.34839
C	-0.80321	4.29256	7.99355
H	-0.40029	4.83060	7.12840
H	-1.70074	3.75729	7.66591
H	-0.06964	3.54381	8.31124
C	-2.70603	10.38338	13.55138
H	-3.62684	10.84719	13.89411
C	5.42469	9.62846	16.76744
H	5.29122	9.28142	17.78876
C	-2.25987	6.20864	8.62137
H	-2.62140	6.87138	9.41318
H	-3.11742	5.63826	8.24556
H	-1.87649	6.83261	7.80652
C	3.95123	7.72602	16.02562
H	3.43191	7.44221	15.10284
C	5.59800	12.53168	12.61094
H	4.55681	12.67380	12.92354
H	5.69066	12.86425	11.57115
H	6.22456	13.18583	13.22707
C	-1.72970	4.41581	10.30155
H	-0.96179	3.74214	10.69699
H	-2.57975	3.81108	9.96361
H	-2.07356	5.05135	11.12374
C	7.92327	4.92059	13.46186
H	7.69892	5.59011	14.29785
H	8.86392	4.40491	13.68860
H	7.12383	4.17401	13.40425
C	9.13519	6.77002	12.26740
H	9.23223	7.34023	11.33695
H	10.10281	6.30559	12.49123
H	8.90672	7.47510	13.07236
C	7.47321	10.86453	12.29720
H	8.15877	11.44018	12.92996
H	7.60726	11.19891	11.26233
H	7.75839	9.80951	12.35473
C	-0.66292	7.77848	16.24501
H	-0.53160	8.76832	16.69597
H	-0.07033	7.06220	16.82106
H	-1.71374	7.48761	16.35467
C	-0.45807	6.35225	14.19084
H	-1.53215	6.13288	14.15974

C	12.02497	5.88616	10.11527
C	12.02412	7.34173	8.06524
C	12.04007	8.36541	10.33194
H	1.55686	6.73025	15.38380
H	2.46962	5.52165	14.46933
H	1.29810	6.57127	13.64220
H	1.94254	9.13781	15.13795
H	1.79307	9.06774	13.36780
H	3.23711	9.77438	14.10763
H	4.92513	8.25968	15.31789
H	4.64526	6.51336	15.38658
H	3.62420	7.61887	16.33245
H	11.72127	5.01431	9.52798
H	11.64374	5.75386	11.13367
H	13.12066	5.90207	10.15490
H	13.11961	7.38844	8.06708
H	11.64081	8.25846	7.60363
H	11.72653	6.49706	7.43621
H	13.13480	8.34929	10.30372
H	11.73560	8.29748	11.38199
H	11.71079	9.33204	9.93514
H	0.02759	5.59038	14.81131
H	-0.06246	6.26889	13.17630
C	4.85016	6.54699	16.42586
H	5.40506	6.77018	17.34474
H	5.57450	6.32477	15.63612
H	4.24945	5.64730	16.60044
C	2.89497	7.99666	17.10162
H	2.27040	7.10968	17.25000
H	2.24346	8.83159	16.81771
H	3.35179	8.24154	18.06664
Mg	1.85001	11.46663	14.42914
C	0.92304	12.05345	16.49300
H	0.57925	11.31313	17.20418
C	2.23046	12.60803	16.43398
H	3.06245	12.35314	17.07870
C	2.25487	13.55758	15.37909
H	3.10342	14.16669	15.09377
C	0.13872	12.65976	15.47555
H	-0.90050	12.44508	15.25925
C	0.96158	13.58964	14.78588
H	0.65048	14.22848	13.96882

InBe

In	5.21378	9.61583	4.73999
O	4.57896	8.21774	6.63833
N	3.24949	8.78748	4.45213
N	6.94498	8.60243	5.56835
C	6.34628	13.32868	3.57753
H	6.41432	13.92894	4.47412
C	5.18541	13.15905	2.77262
H	4.21465	13.59955	2.95209
C	5.49183	12.21827	1.75492
H	4.78793	11.81178	1.04125
C	6.84148	11.80866	1.93089
H	7.35262	11.03975	1.36884
C	7.36995	12.49193	3.05726
H	8.34279	12.31878	3.49968
C	2.76396	6.66593	1.06512
H	2.34015	6.97635	0.10321
H	1.94011	6.34107	1.70842
H	3.41518	5.80374	0.88295
C	3.55438	7.80528	1.72309
H	3.97854	7.41586	2.65604
C	4.71310	8.25527	0.82458
H	5.37130	7.41159	0.59101
H	5.31315	9.03190	1.31441
H	4.34576	8.66529	-0.12344
C	2.64774	8.96553	2.08595
C	1.95175	9.63683	1.07761
H	2.08330	9.33164	0.04214
C	2.46918	9.37119	3.42487
C	1.57390	10.41959	3.73694
C	0.89439	11.05652	2.69919
H	0.20893	11.86895	2.92842
C	1.08275	10.67651	1.37567
H	0.54586	11.18525	0.57982
C	1.36835	10.88779	5.16567
H	1.92932	10.21712	5.82342
C	-0.10504	10.81269	5.58414
H	-0.72797	11.49590	4.99588
H	-0.21491	11.08564	6.63959
H	-0.49237	9.79758	5.45283
C	1.92802	12.30431	5.36189
H	2.99121	12.34332	5.09627
H	1.82313	12.62001	6.40624
H	1.39711	13.03009	4.73459
C	8.19060	9.10729	5.13349
C	8.68821	8.73619	3.85977
C	7.97578	7.67532	3.03674
H	6.89497	7.87519	3.09957
C	8.35962	7.67330	1.55686
H	8.23176	8.65745	1.09268
H	7.73107	6.96085	1.01421
H	9.39966	7.36025	1.41129
C	8.20694	6.27774	3.63478
H	9.27611	6.03442	3.61567
H	7.67317	5.51856	3.05157
H	7.86205	6.21998	4.66936
C	9.86485	9.32939	3.39989
H	10.26137	9.05823	2.42688
C	10.55129	10.26129	4.16994
H	11.46979	10.70538	3.79627
C	10.05812	10.62012	5.41603
H	10.59314	11.35715	6.01019
C	8.87740	10.06494	5.91224
C	8.33259	10.54878	7.24331
H	7.45593	9.94454	7.49385
C	7.86789	12.00879	7.13276
H	8.70603	12.67425	6.89435

InMg

In	2.60749	9.68782	13.22697
O	3.13033	8.31103	11.25805
N	4.56821	8.84812	13.40683
N	0.78288	8.55939	12.43086
C	4.36300	7.67151	11.34257
C	0.84980	7.71389	11.34778
C	5.11095	7.97863	12.48871
C	4.74553	6.76469	10.37868
C	2.10394	7.52344	10.74875
C	2.36135	6.60790	9.75044
C	-0.20687	6.95099	10.82890
H	-1.18946	7.07452	11.27689
C	5.99391	6.14716	10.53440
H	6.32014	5.42855	9.79525
C	3.78967	6.54105	9.20495
C	4.06457	5.22112	8.48437
H	5.08181	5.20821	8.08285
H	3.38767	5.10272	7.63333
H	3.94075	4.36371	9.15363
C	1.28310	5.84347	9.28599
H	1.45926	5.10803	8.51307
C	-0.38390	9.22900	12.75833
C	-1.02560	10.12485	11.84855
C	6.36263	7.35526	12.59397
H	6.97151	7.57985	13.46452
C	5.33603	9.17982	14.55397
C	6.81147	6.44822	11.62735
C	-0.00244	6.01387	9.80958
C	-0.44676	10.41823	10.47550
H	0.47075	9.83404	10.36403
C	6.26424	10.24064	14.48922
C	6.47345	11.02047	13.20531
H	5.98652	10.46443	12.39762
C	-1.18861	5.16267	9.34000
C	3.97513	7.70529	8.20017
H	3.78389	8.66988	8.67982
H	3.27923	7.59119	7.36160
H	5.00095	7.70905	7.81564
C	8.18683	5.79855	11.81802
C	-0.86318	9.15560	14.10594
C	-2.19969	10.76681	12.24245
H	-2.70498	11.42189	11.53665
C	5.14405	8.46747	15.75565
C	-0.22493	8.17743	15.08147
H	0.86618	8.23556	14.95568
C	-1.40036	10.00699	9.34788
H	-2.32815	10.59022	9.37577
H	-1.65566	8.94696	9.42254
H	-0.92896	10.17395	8.37337
C	6.96890	10.58692	15.64171
H	7.67781	11.41028	15.61009
C	8.56092	4.86593	10.65986
H	7.85805	4.03083	10.56640
H	9.55510	4.44301	10.83949
H	8.59406	5.40122	9.70450
C	-0.06462	11.90136	10.35490
H	0.39073	12.09845	9.37821
H	0.65839	12.19066	11.12763
H	-0.93943	12.55337	10.45771
C	-2.03098	9.85036	14.45018
H	-2.41350	9.77659	15.46303
C	6.77987	9.89612	16.83221
H	7.33953	10.17745	17.71990
C	-0.81635	4.22758	8.18292
H	-0.45888	4.78634	7.31096
H	-1.69966	3.65753	7.87578

H	7.42545	12.34624	8.07709
H	7.11559	12.11605	6.34272
C	9.34656	10.37767	8.38067
H	9.67084	9.33552	8.45783
H	8.89587	10.66531	9.33697
H	10.23386	11.00280	8.22978
C	2.67811	7.86774	5.29893
C	1.45205	7.21679	5.11038
H	0.87441	7.46740	4.22501
C	0.99649	6.24602	6.01116
C	-0.34294	5.55652	5.72664
C	-1.45799	6.61565	5.63767
H	-1.53039	7.17996	6.57403
H	-2.42506	6.13493	5.44794
H	-1.27371	7.32832	4.82815
C	-0.25112	4.80083	4.38672
H	-0.04791	5.48248	3.55512
H	-1.19365	4.28161	4.17553
H	0.55412	4.05895	4.41810
C	-0.73030	4.54993	6.81670
H	-0.00224	3.73527	6.89649
H	-1.70041	4.10429	6.57205
H	-0.82189	5.03136	7.79651
C	1.77852	5.91630	7.12218
H	1.44631	5.15017	7.80926
C	2.99687	6.56653	7.36582
C	3.90194	6.33101	8.57872
C	3.66087	4.96094	9.21350
H	3.86718	4.15023	8.50746
H	2.62613	4.87277	9.55681
H	4.29808	4.83063	10.09273
C	3.59664	7.42940	9.62707
H	4.25008	7.30806	10.49812
H	2.55213	7.36075	9.95073
H	3.76313	8.42579	9.20673
C	3.38535	7.53010	6.46262
C	5.61461	7.45948	7.17060
C	5.35442	6.49848	8.12197
C	6.87800	7.71668	6.61621
C	6.44884	5.77703	8.61914
H	6.27803	5.01008	9.36205
C	7.94951	7.00439	7.17458
H	8.94394	7.18921	6.77831
C	7.74582	6.03595	8.16507
C	8.95723	5.24945	8.67945
C	9.54633	4.42151	7.52032
H	10.40344	3.83248	7.86868
H	9.88695	5.06278	6.70106
H	8.79474	3.73383	7.11761
C	10.02946	6.22247	9.20361
H	9.62576	6.84894	10.00662
H	10.39784	6.88198	8.41248
H	10.88660	5.66384	9.59776
C	8.59161	4.28801	9.81698
H	9.49292	3.76880	10.16013
H	7.87570	3.52618	9.49043
H	8.16567	4.82190	10.67365
Be	5.79757	11.51757	3.49663
H	-0.04430	3.50817	8.47597
C	-2.71704	10.62238	13.52354
H	-3.62651	11.14114	13.81092
C	5.87648	8.84419	16.88333
H	5.73963	8.30291	17.81625
C	-2.33446	6.07484	8.86529
H	-2.70619	6.71270	9.67296
H	-3.17554	5.47081	8.50493
H	-2.00108	6.72283	8.04715
C	4.18755	7.29293	15.83940
H	3.65575	7.22837	14.88265
C	5.79948	12.39767	13.30032
H	4.73016	12.29849	13.52247
H	5.90584	12.94816	12.35837
H	6.25120	12.99749	14.09920
C	-1.68101	4.29729	10.51644
H	-0.87506	3.65154	10.88117
H	-2.51716	3.66200	10.20020
H	-2.02241	4.91362	11.35421
C	8.18359	4.97276	13.11902
H	7.99954	5.60362	13.99418
H	9.15156	4.47685	13.25911
H	7.40278	4.20510	13.08576
C	9.26427	6.89568	11.91592
H	9.26567	7.51867	11.01473
H	10.25730	6.44413	12.02683
H	9.09542	7.54919	12.77698
C	7.95542	11.15802	12.83759
H	8.50149	11.77481	13.55997
H	8.05714	11.63360	11.85591
H	8.43891	10.17688	12.79258
C	-0.53539	8.47543	16.54814
H	-0.30444	9.51432	16.81527
H	0.06319	7.82361	17.19137
H	-1.58790	8.28803	16.78823
C	-0.63440	6.74166	14.71616
H	-1.72188	6.62747	14.79592
H	-0.16248	6.02559	15.39820
H	-0.33098	6.49599	13.69492
C	4.94844	5.97262	16.02603
H	5.50911	5.97101	16.96807
H	5.65650	5.81272	15.20692
H	4.25142	5.12708	16.04470
C	3.14302	7.48535	16.94608
H	2.40448	6.67566	16.91634
H	2.61573	8.43949	16.83186
H	3.60274	7.47824	17.94056
Mg	0.65371	11.44485	14.13743
C	-0.61837	12.87802	15.44814
H	-1.52933	12.53062	15.91727
C	0.67916	12.87943	16.03021
H	0.93064	12.52862	17.02330
C	1.57707	13.45608	15.09772
H	2.64208	13.58765	15.24063
C	-0.51508	13.44490	14.14871
H	-1.33305	13.60252	13.45751
C	0.84576	13.80302	13.93716
H	1.24603	14.27400	13.04806

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