Table of Contents

1 General Considerations

RH, RK,[1] [(^{Mes}BDI)Mg]$_2$[2] were prepared according to literature protocols. AlI_3 was prepared by reaction of suspension of Al and I_2 in toluene by means of sonication.

Et_2O (Sigma-Aldrich), THF (Roth, 99%), n-hexane (Roth, 98%) and toluene (Roth, 99%) were dried over sodium and distilled prior to use. C_6D_6 (Eurisotop) was dried over sodium and distilled prior to use.

NMR spectra were acquired on a Bruker Avance 400 MHz spectrometer. Reported chemical shifts are referenced to the ^{1}H and ^{13}C NMR resonances of the deuterated solvent.[3] Coupling constants *J* are given in Hertz as positive values regardless of their real individual sign. ^{1}H, ^{11}B, ^{13}C, ^{15}N, ^{19}F, ^{29}Si NMR spectra were obtained at 400.1, 128.4, 100.6, 40.6, 376.5, 79.5 MHz, respectively.

IR spectra were recorded on a Bruker Alpha spectrometer using the attenuated total reflection (ATR) technique on powdered samples.

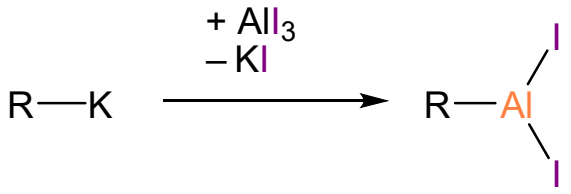
Elemental analyses were obtained with a Vario Micro Cube (Elementar Analysensysteme GmbH) in the institutional technical laboratories of the Karlsruhe Institute of Technology (KIT).

Melting points were determined with a ThermoFischer IA9300 melting point apparatus with a heating rate of 5 K/min. No corrections were applied.

Single crystals were mounted in perfluoropolyalkyl ether oil on a cryo loop and then brought into the cold nitrogen stream of a low-temperature device (Oxford Cryosystems Cryostream unit) so that the oil solidified. Diffraction data were collected using a Stoe IPDS II diffractometer and graphite-monochromated Mo-Kα (0.71073 Å) radiation or a Stoe STADIVARI diffractometer and Ga-Kα (1.34134 Å) radiation. The structures were solved by direct methods with SHELXS[4] or intrinsic phasing with SHELXT[5] followed by full-matrix least-squares refinement using SHELXL-2018/3[6] and the ShelXle GUI.[7] All non-hydrogen atoms were refined anisotropically. The contribution of the hydrogen atoms, in their calculated positions, was included in the refinement using a riding model.

2 Attempts of Reduction of [R–AlI$_2$]

2.1 Synthesis of [R–AlI$_2$]



To a solid mixture of R–H (483 mg, 0.736 mmol) and BzK (99 mg, 0.733 mmol), 5 ml of toluene were added. The suspension was stirred for 30 minutes, then AlI$_3$ (300 mg, 0.735 mmol) was added as a solid. The mixture was stirred overnight and then filtered. The filtrate was evaporated, leaving behind a dark green solid. After washing with n-hexane, an off-white crude product was obtained. Recrystallisation from hot toluene afforded colourless crystals of [R–AlI$_2$] (420 mg, 0.449 mmol, 61%).

^{1}H NMR (C_6D_6): 1.31 (s, 36 H, Ar-^{t}Bu), 1.38 (s, 18 H, Carb-^{t}Bu), 7.52 (d, J_{HH} = 1.8 Hz, 2 H, C^{2,7}*H*), 7.68 (d, J_{HH} = 1.8 Hz, 4 H, *o*-C*H*), 7.72 (d, J_{HH} = 1.8 Hz, 2 H, *p*-C*H*), 8.45 (d, J_{HH} = 1.8 Hz, 2 H, C^{4,5}*H*). **^{13}C NMR** (C_6D_6): 31.48 (s, Ar-C(CH_3)$_3$), 32.18 (s, Carb-C(CH_3)$_3$), 34.94 (s, Carb-*C*(CH_3)$_3$), 35.54 (s, Ar-*C*(CH_3)$_3$), 116.62 (s, *C*H), 124.87 (s, *C*H), 126.73 (s, *C*H), 127.41 (s, *C*H), 127.52 (s), 140.46 (s), 143.54 (s), 144.36 (s), 155.30 (s, Ar-*C*^{t}Bu). **^{15}N NMR** (C_6D_6): 132.8. **EA** found (calc. for $C_{48}H_{64}NAlI_2$): C 62.11 (61.61), H 7.12 (6.89), N 1.48 (1.50). **Mp**. (°C): 148 (dec.).

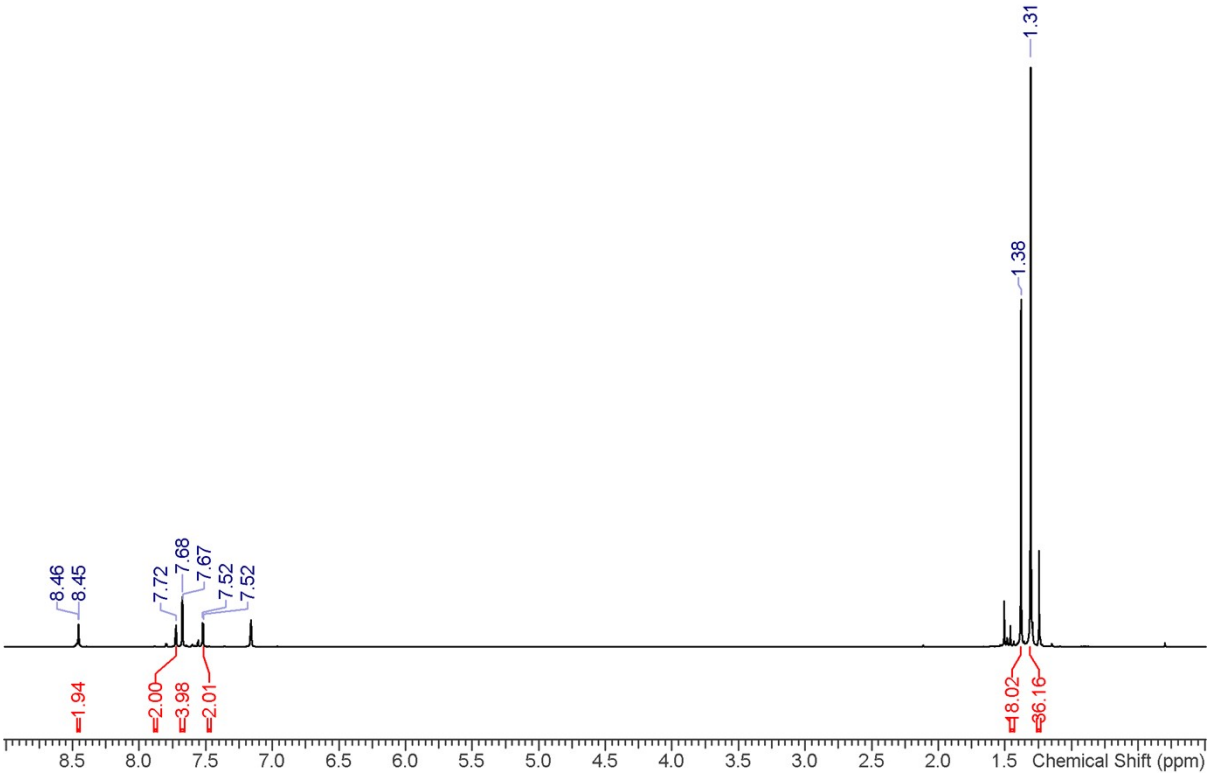


Figure S1: ^{1}H NMR spectrum of **[R–AlI$_2$]**.

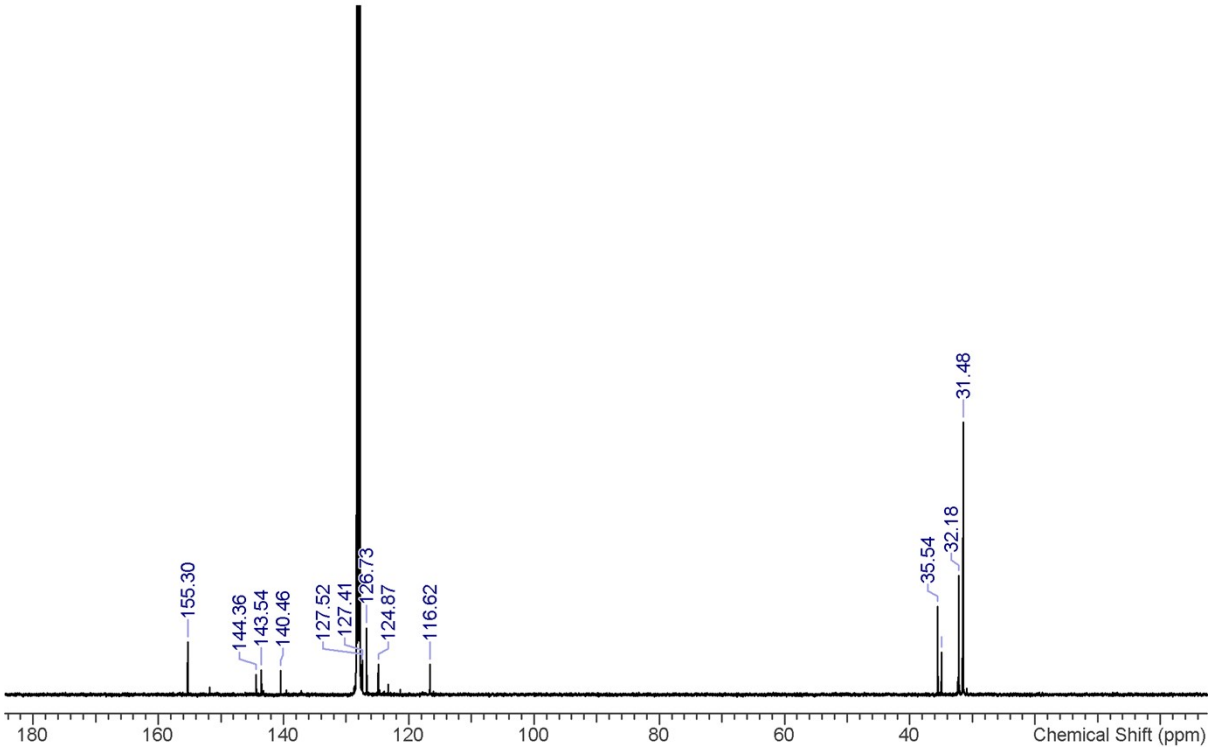


Figure S2: ^{13}C NMR spectrum of **[R–All$_2$]**.

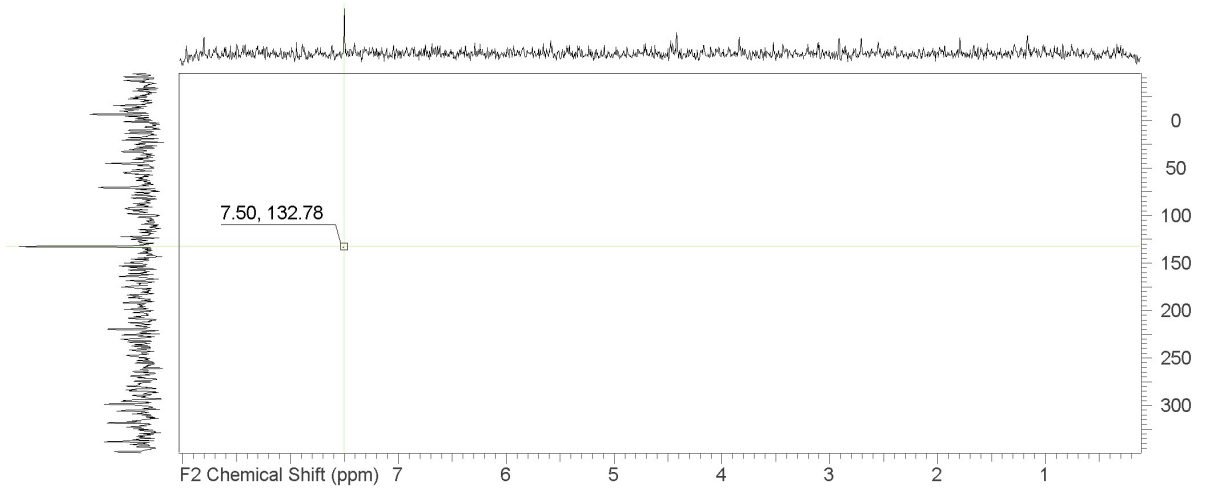


Figure S3: ^{1}H-^{15}N HMBC NMR spectrum of **[R–All$_2$]**.

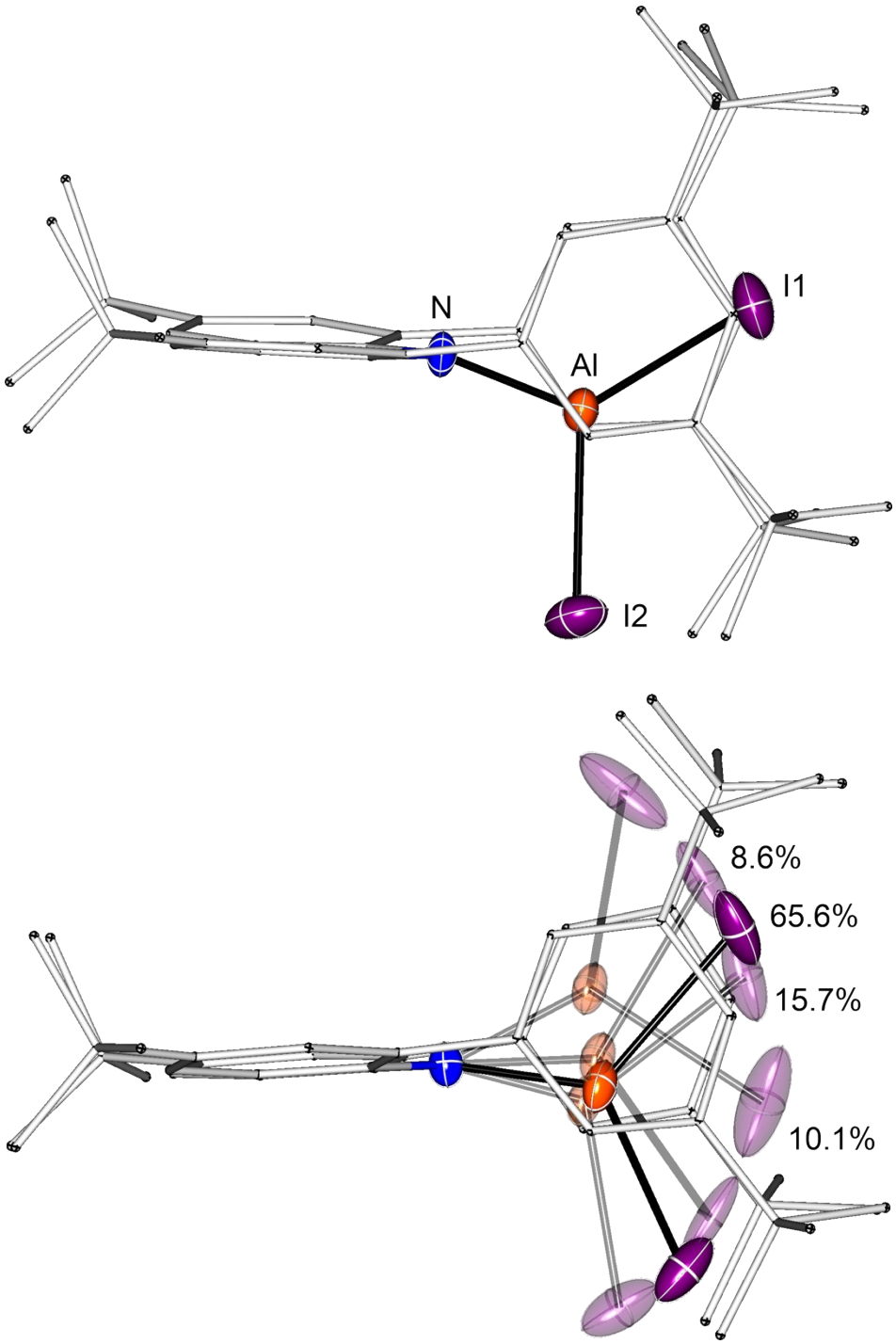
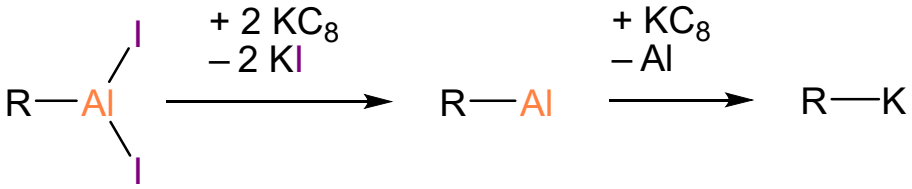


Figure S4: Molecular structure of **[R–AlI$_2$]** in solvent-free crystals and as benzene solvate.

The disordered positions were modelled with occupancies of 65.6%, 15.7%, 10.1% and 8.6%, respectively. The Al split position displacement parameters were constrained with EADP Al1 Al1B Al1C Al1D. All attached iodine atom displacement parameters were restrained with SIMU 0.01 0.02 3.5 Al1B I1B I2B Al1C I1C I2C Al1D I1D I2D and DELU 0.01 0.01 Al1B I1B I2B Al1C I1C I2C Al1D I1D I2D.

2.2 [R–AlI$_2$] with KC$_8$



A solution of [R–AlI$_2$] (210 mg, 0.224 mmol) in 15 ml of toluene was treated with KC$_8$ which was added in small portions of 5 mg (0.037 mmol) each. After addition, the suspension was stirred for approx. 12 hours at ambient temperature until KC$_8$ had reacted and then an NMR sample was taken. The mixture initially contained [R–AlI$_2$] and trace amounts of R–H. With progressing reduction, [R–Al] and then [R–K] were formed. The maximum spectroscopic yield of [R–Al] was 55% according to the ^{1}H NMR data. Characteristic ^{1}H NMR resonances of C^{4,5}*H*: R–H 8.45, [R–K] 8.57, [R–AlI$_2$] 8.44, [R–Al] 8.47 ppm.

^{1}H NMR (C$_6$D$_6$): 1.25 (s, 36 H, Ar-^{t}Bu), 1.50 (s, 36 H, Carb-^{t}Bu), 7.47 (d, 4 H, *o*-C*H*), 7.50 (t, 2 H, *p*-C*H*), 7.58 (d, 2 H, C^{2,7}*H*), 8.47 (d, J_{HH} = 1.8 Hz, 2 H, C^{4,5}*H*). **^{13}C NMR** (C$_6$D$_6$): 31.80 (s, Ar-C(*C*H$_3$)$_3$), 32.42 (s, Carb-C(*C*H$_3$)$_3$), 34.79 (s, Carb-*C*(CH$_3$)$_3$), 35.03 (s, Ar-*C*(CH$_3$)$_3$), 115.71 (s, *C*H), 122.70 (s, *C*H), 123.53 (s, *C*H), 124.62 (s, *C*H), 125.84 (s), 128.70 (s, *C*H), 135.79 (s), 142.40 (s), 143.24 (s), 150.01 (s). ^{13}C NMR assignment in the mixture is aggravated by overlap with resonances of RAlI$_2$, RH and RK. **^{15}N NMR** (C$_6$D$_6$): 183.0.

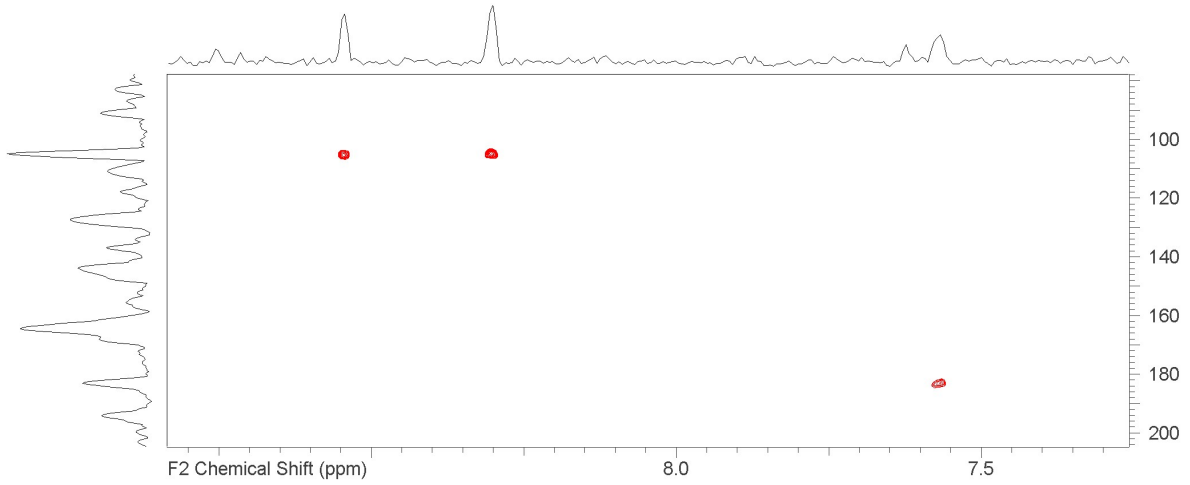


Figure S5: ^{1}H-^{15}N HMBC NMR spectrum oft the reaction mixture, showing resonances of **R-H** and **[R–AlI$_2$]**.

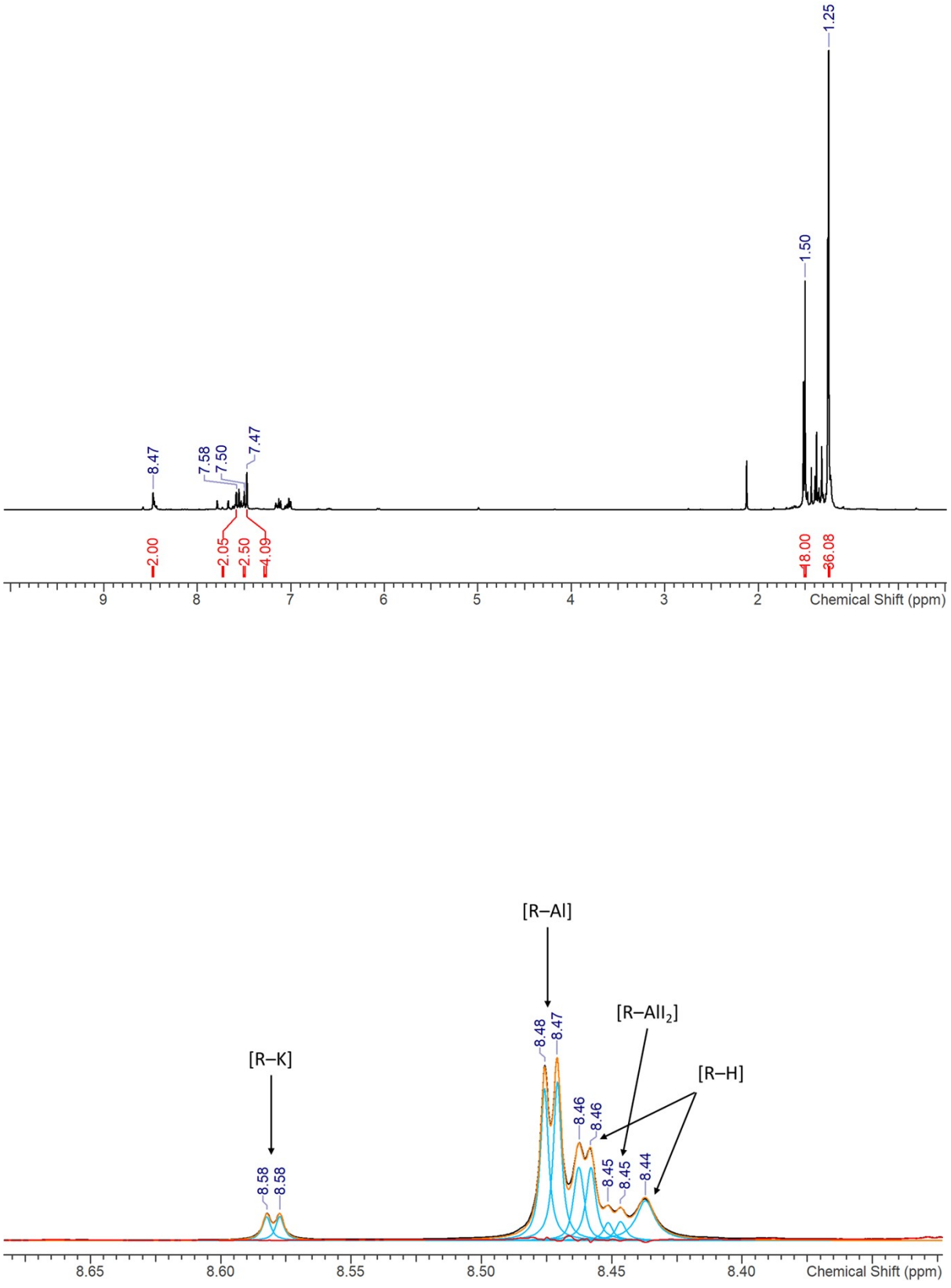


Figure S6: ^{1}H NMR spectrum oft the reaction mixture. Integral ratios by peak fitting for [R–Al] (**55%**), [R–All$_2$] (**7%**), [R–K] (**9%**) and [R–H] (**29%**).

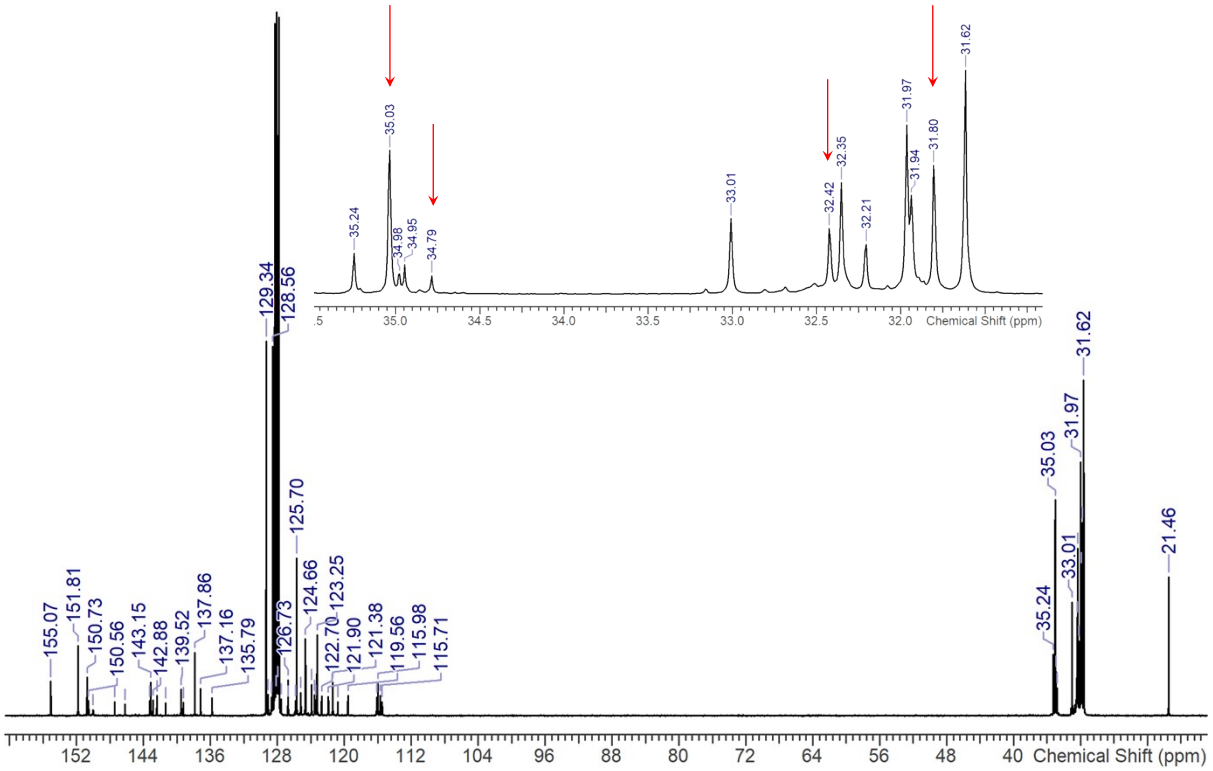
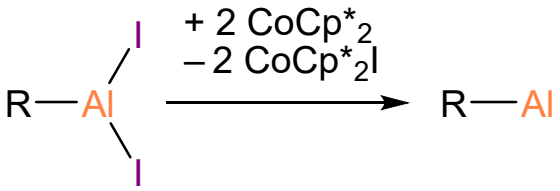


Figure S7: ^{13}C NMR spectrum oft the reaction mixture. Assignments of tBu resonances of [R–Al] are marked with arrows, all assignments given below.

(ppm)	Assignment
-1.19	grease
21.46	toluene
31.62	RH
31.80	**RAl**
31.94	$RAlI_2$
31.97	RK
32.21	$RAlI_2$
32.35	RH
32.42	**RAl**
33.01	RK
34.79	**RAl**
34.95	$RAlI_2$
34.98	RK
35.03	RH, RK, RAl
35.24	$RAlI_2$
115.48	$RAlI_2$
115.71	**RAl**
115.98	RH
116.12	RK
119.56	n.a.
120.77	n.a.
121.38	RK
121.90	RK
122.70	**RAl**
123.25	RH
123.46	$RAlI_2$
123.53	RAl
123.90	RH
124.62	**RAl**

(ppm)	Assignment
124.66	RH
125.20	RK
125.70	toluene
125.84	**RAl**
126.69	RK
126.73	RK
127.55	$RAlI_2$
128.56	toluene
128.70	**RAl**
129.09	$RAlI_2$
129.34	toluene
135.79	RK/**RAl**
137.16	RH
137.86	toluene
139.26	$RAlI_2$
139.52	RH
141.34	$RAlI_2$
142.40	RK/**RAl**
142.88	$RAlI_2$
143.15	RH
143.24	**RAl**
146.21	RK
147.43	$RAlI_2$
150.01	**RAl**
150.56	RK
150.73	RK
151.81	RH
155.07	$RAlI_2$

2.3 [R–AlI$_2$] with CoCp*$_2$



To a solution of [R–AlI$_2$] (90 mg, 0.096 mmol) in 3 ml toluene, 32 mg of CoCp*$_2$ were added at ambient temperature. The solution immediately turned dark brown and dark solid was deposited. The mixture was filtered, all volatiles removed and the residue washed with 1 ml of hexane. Then, the residue was treated with 5 ml of hexane, filtered, and the filtrate was concentrated to approx. 1.5 ml. Orange crystals formed overnight. The supernatant was removed via syringe and the crystals were dried in vacuo (8 mg, 0.012 mol, 12%).

EA found (calc. for $C_{48}H_{64}NAl$): C 81.73 (84.53), H 9.06 (9.46), N 1.90 (2.05).

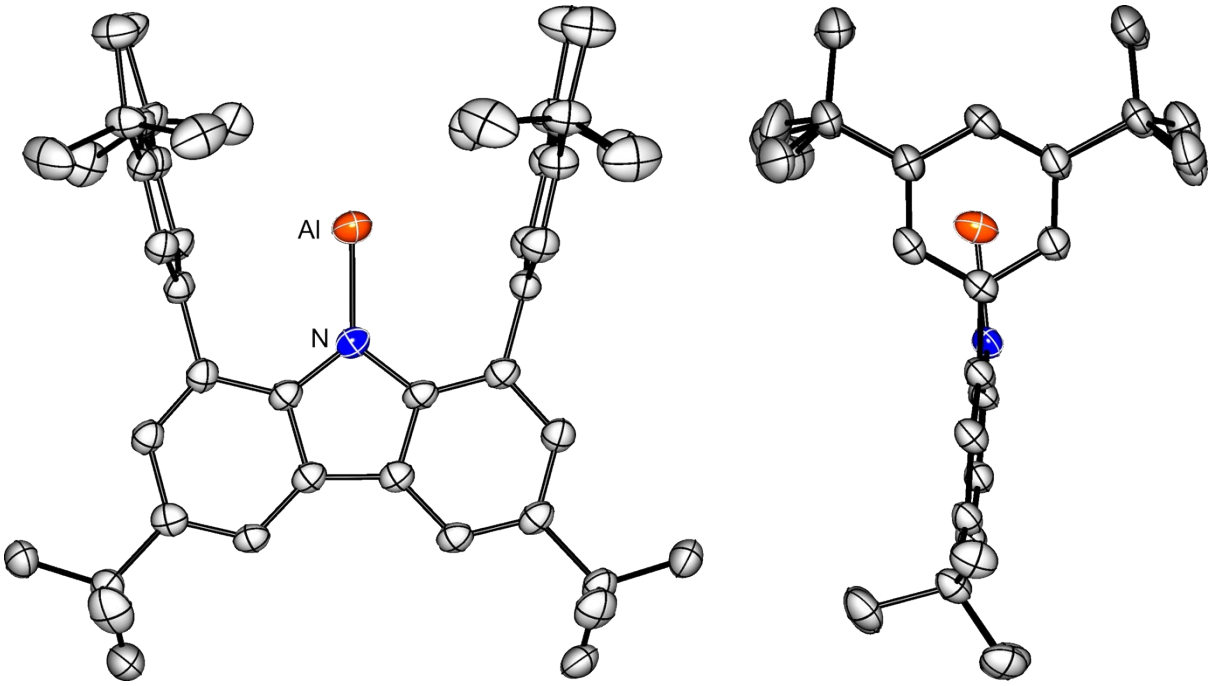


Figure S8: Molecular structure of **RAl**, data from major part: I1–Si1 2.4555(8); I2–Si1 2.4262(8); I3–Si1 2.4211(8); Si1–N1 1.770(2); C1–N1–C12 104.6(2); C1–N1–Si1 115.6(2); C12–N1–Si1 120.8(2); angle sum at N 341°.

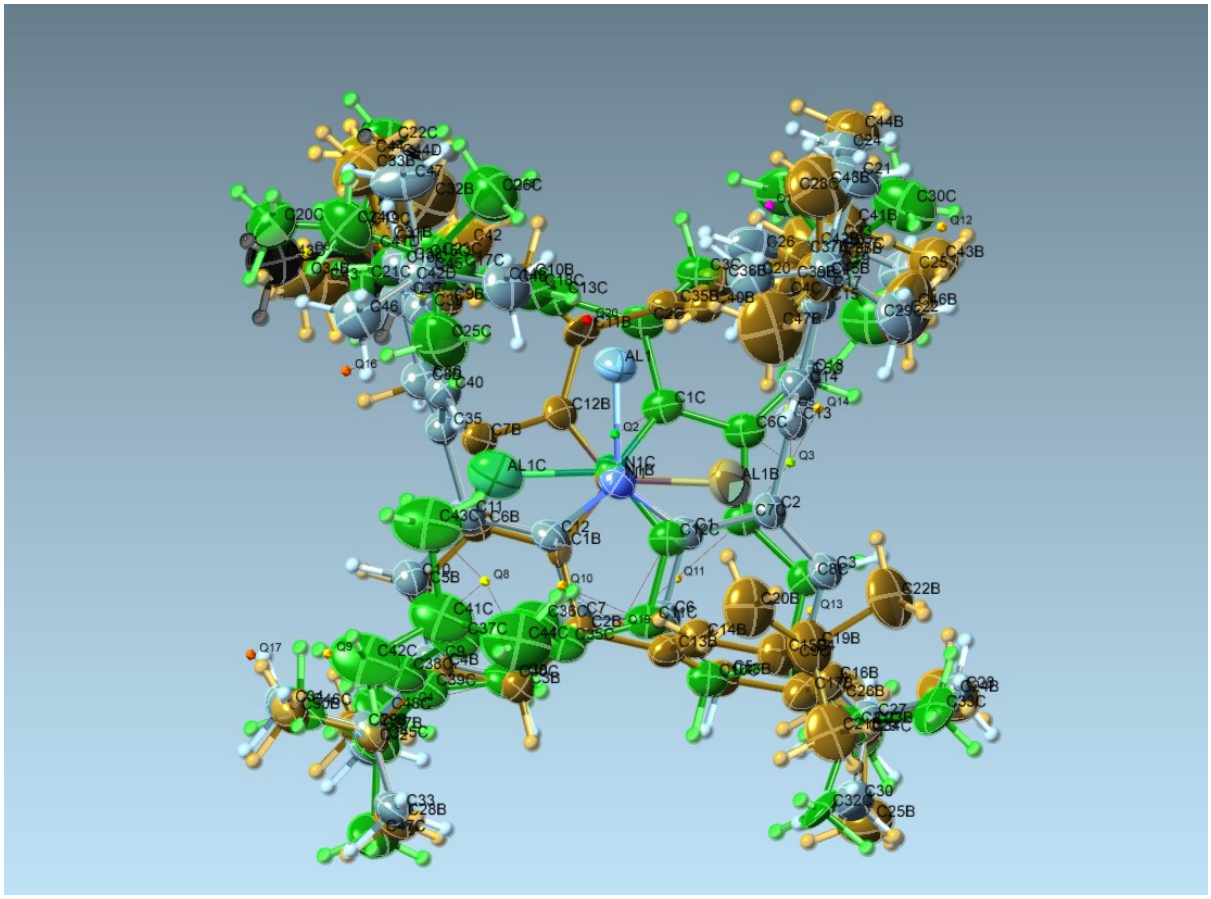
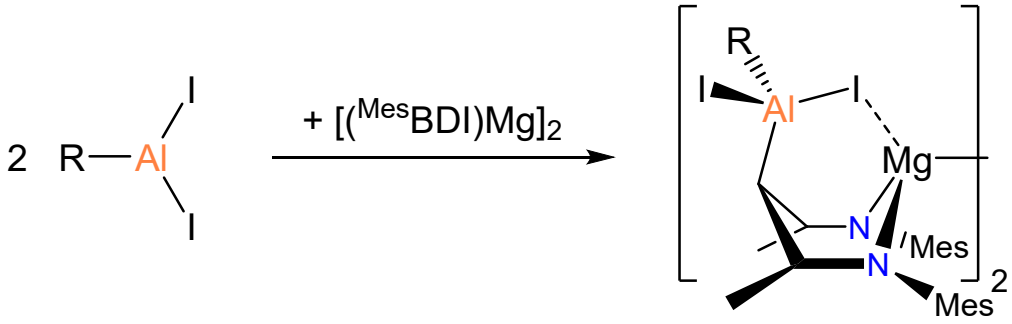


Figure S9: Modelled disorder of **RAl**.

The XRD data for [R–Al] showed its mono-ligated aluminium structural motif immediately after structure solution. However, significant residual electron densities remained. Eventually, the structure was modelled with three split positions where the two minor parts with occupancies of 16.5% and 5.0% originate from the major one by an approximate 90° rotation in which the position of the N atom remains nearly unchanged (see SI 2.4). To ensure stability of the refinement, the SAME command was used for the geometric parameters, and SIMU and DELU were used to restrain the thermal ellipsoids. The resulting refinement converged with R_1 = 4.39% and wR_2 = 12.11%. The origin of this problem is likely to be not disorder but twinning, but repeated measurements of different crystals did not allow indexing of multiple domains in the diffraction data.

2.4 [R–AlI$_2$] with Mg(I)



To a solid mixture of [R–AlI$_2$] (155 mg, 0.166 mmol) and [(^{Mes}BDI)Mg]$_2$ (59 mg, 0.082 mmol), 5 ml of toluene were added. The suspension was stirred at ambient temperature and quickly turned yellow. After 3 hours, the solution was filtered to remove turbidity and the clear solution was concentrated to incipient crystallisation (approx. 1 ml). After standing overnight without disturbance, yellow crystals deposited. The supernatant was removed via syringe and the crystals were dried in vacuo (110 mg, 0.037 mmol, 45%).

^{1}H NMR (C_6D_6): 0.77 (s, 3 H, BDI-CH_3), 1.12 (s, 3 H, Mes-*o*-CH_3), 1.22 (s, 9 H, ^{t}Bu), 1.31 (s, 3 H, Mes-*o*-CH_3), 1.35 (s, 9 H, ^{t}Bu), 1.46 (s, 9 H, ^{t}Bu), 1.53 (s, 3 H, Mes-*o*-CH_3), 1.55 (s, 9 H, ^{t}Bu), 1.57 (s, 3 H, BDI-CH_3), 1.61 (s, 18 H, ^{t}Bu), 1.91 (s, 3 H, Mes-*o*-CH_3), 2.14 (s, 3 H, Mes-*p*-CH_3), 2.20 (s, 3 H, Mes-*m*-C*H*), 4.56 (s, 1 H, BDI-C*H*), 6.43 (s, 1 H, Mes-*m*-C*H*), 6.61 (s, 1 H, Mes-*m*-C*H*), 6.63 (s, 1 H, Mes-*m*-C*H*), 6.75 (s, 1 H, Mes-*m*-C*H*), 7.48 (d, J_{HH} = 2.1 Hz, 1 H), 7.58 (t, J_{HH} = 1.8 Hz, 1 H), 7.68 (t, J_{HH} = 1.8 Hz, 1 H), 7.69 (d, J_{HH} = 2.1 Hz, 1 H), 7.81 (br s, 1 H), 8.00 (br s, 2 H), 8.13 (br s, 1 H), 8.19 (d, J_{HH} = 2.1 Hz, 1 H), 8.30 (d, J_{HH} = 2.1 Hz, 1 H). **^{13}C NMR** (C_6D_6): 18.13 (s, Mes-*o*-CH_3), 20.37 (s, Mes-*o*-CH_3), 20.72 (s, Mes-*p*-CH_3), 21.03 (s, Mes-*o*-CH_3), 21.21 (s, Mes-*p*-CH_3), 21.44 (s, Mes-*o*-CH_3), 22.27 (s, BDI-CH_3), 29.57 (s, BDI-CH_3), 31.59 (s, ^{t}Bu-CH_3), 31.77 (s, ^{t}Bu-CH_3), 31.84 (s, ^{t}Bu-CH_3), 31.87 (s, ^{t}Bu-CH_3), 32.06 (s, ^{t}Bu-CH_3), 32.24 (s, ^{t}Bu-CH_3), 32.31 (s, ^{t}Bu-CH_3), 34.45 (s, ^{t}Bu-*C*), 34.76 (s, ^{t}Bu-*C*), 34.90 (s, ^{t}Bu-*C*), 35.01 (s, ^{t}Bu-*C*), 35.28 (s, ^{t}Bu-*C*), 35.34 (s, ^{t}Bu-*C*), 59.99 (s, BDI-*C*H), 114.31 (s, *C*H), 115.33 (s, *C*H), 121.37 (s), 122.32 (s, *C*H), 124.09 (s, *C*H), 124.28 (s, *C*H), 126.59 (s, *C*H), 127.21 (s), 127.63 (s), 128.35 (s, *C*H), 128.74 (s, *C*H), 128.85 (s, *C*H), 128.96 (s, *C*H), 129.40 (s, *C*H), 129.92 (s, *C*H), 130.12 (s), 130.28 (s, *C*H), 131.26 (s), 131.57 (s), 132.43 (s), 133.46 (s), 134.30 (s), 134.37 (s), 142.34 (s), 142.52 (s), 142.87 (s), 142.98 (s), 143.89 (s), 144.13 (s), 145.66 (s), 146.70 (s), 149.87 (s), 150.95 (s), 151.58 (s), 151.82 (s), 169.49 (s), 178.42 (s), 179.81 (s). **^{15}N NMR** (C_6D_6): n.obs. (carb-N), 257.8 (N-BDI), 268.4 (N-BDI). **EA** found (calc. for $C_{170}H_{218}Al_2I_4Mg_2N_6$): C 68.07 (69.08), H 7.03 (7.43), N 2.66 (2.84). **Mp**. (°C): 161 (dec.).

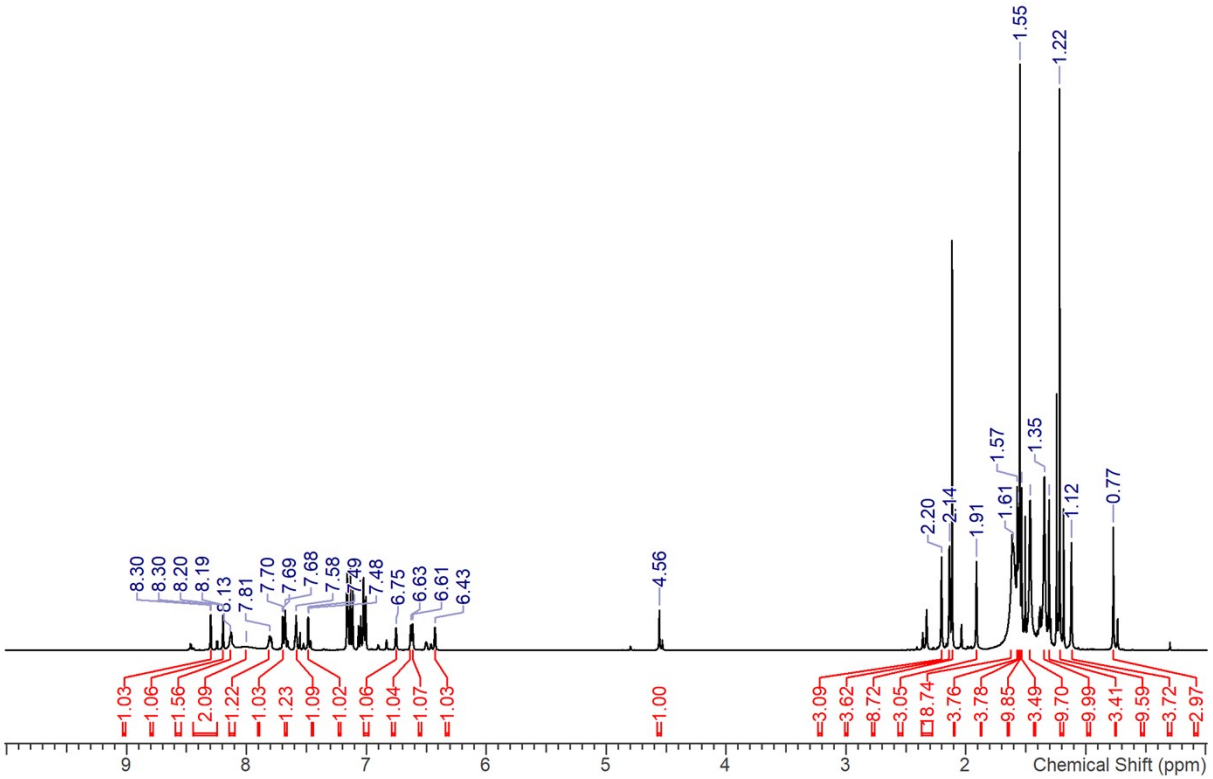


Figure S10: ^{1}H NMR spectrum of **[(RAlI$_2$)$_2${((^{Mes}BDI)Mg}$_2$]**.

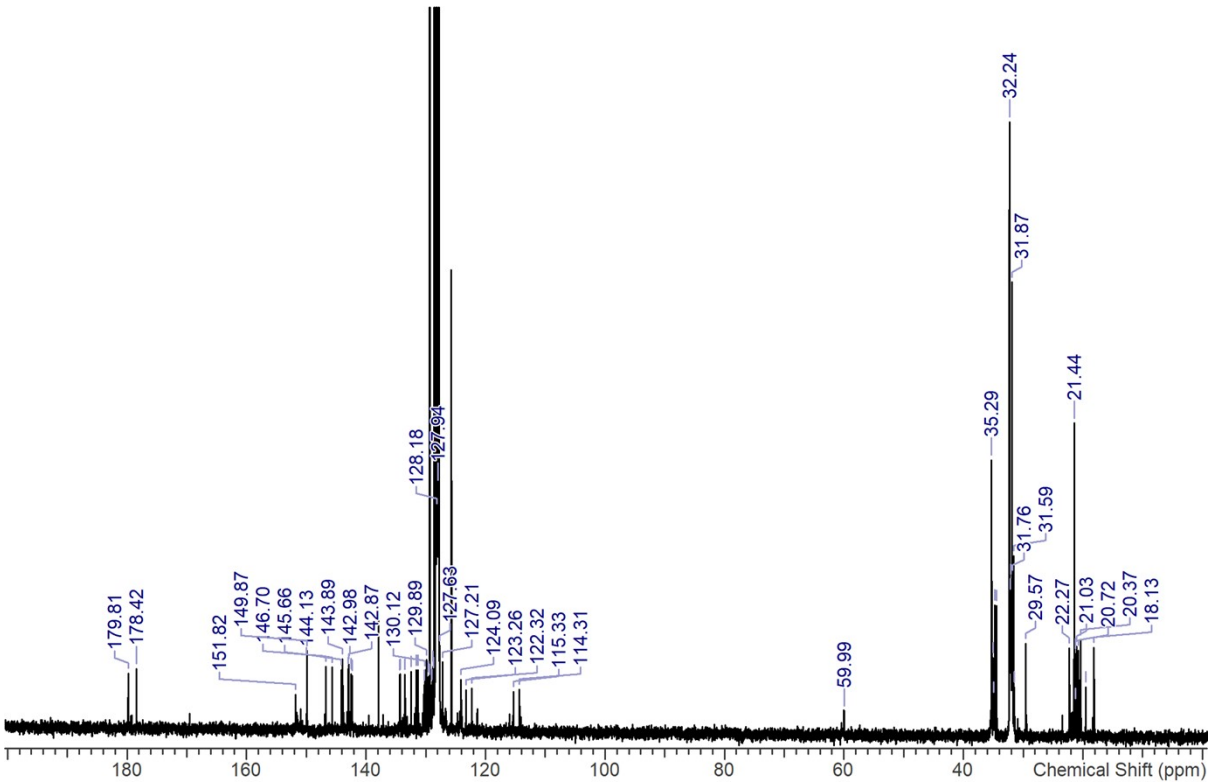


Figure S11: ^{13}C{^{1}H} NMR spectrum of **[(RAlI$_2$)$_2${((^{Mes}BDI)Mg}$_2$]**.

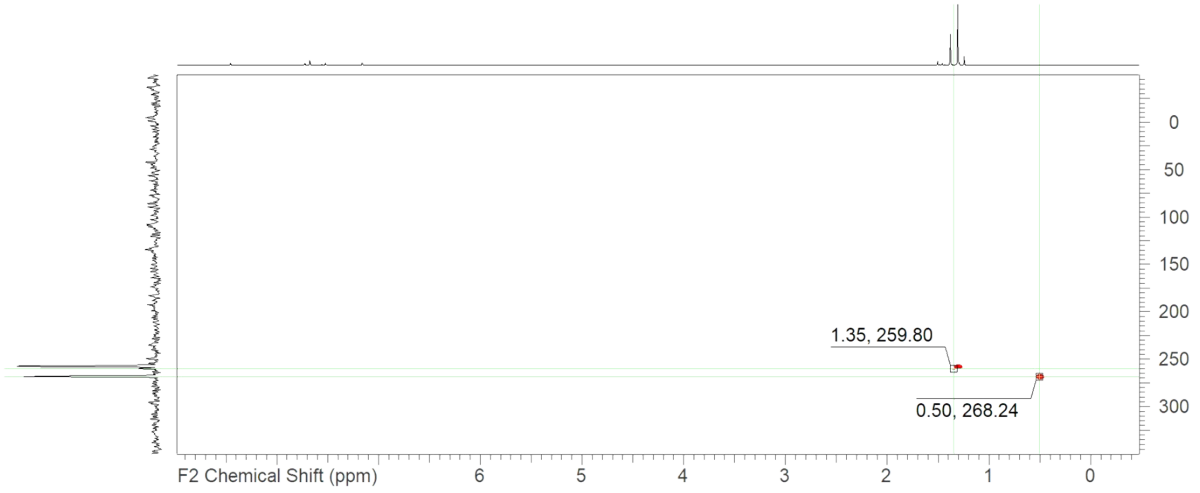


Figure S12: ^{1}H-^{15}N HMBC NMR spectrum of **[(RAlI$_2$)$_2${((^{Mes}BDI)Mg}$_2$]**.

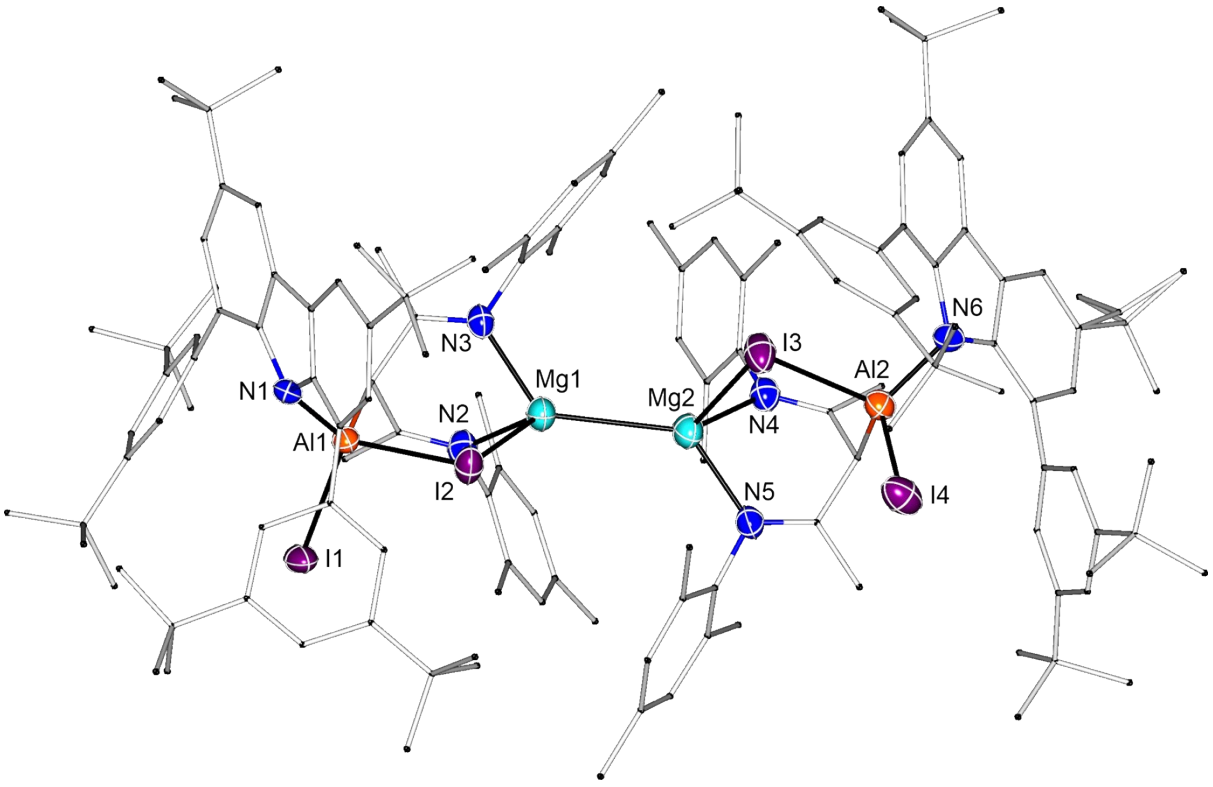


Figure S13: Molecular structure of **[(RAlI$_2$)$_2${((^{Mes}BDI)Mg}$_2$]**.

3 Crystallographic Details

Table S1: Crystallographic details for **[R–AlI$_2$]**.

	[R–AlI$_2$]	**[R–AlI$_2$]·C$_6$H$_6$**
CCDC #	*2108296*	*2108297*
Empirical formula	$C_{48}H_{64}NAlI_2$	$C_{54}H_{70}NAlI_2$
FW [g mol^{-1}]	935.78	1013.89
Wavelength [Å]	1.34143	0.71073
Temperature [K]	150(2)	200(2)
Crystal system	monoclinic	triclinic
Space group	$P2_1/n$	P-1
a [Å]	12.7908(5)	13.5538(7)
b [Å]	13.0762(7)	14.0871(7)
c [Å]	27.4839(15)	14.9705(9)
α [°]	90	89.785(4)
β [°]	99.379(4)	87.830(5)
γ [°]	90	63.479(4)
V [Å^3]	4535.4(4)	2555.5(3)
Z	4	2
ρ_{calc} (g·cm^{-3})	1.370	1.318
μ	7.568	1.281
F(000)	1912	1040
reflections collected	29337	13343
independent reflections	10707	7062
reflectionsGT (I > 2σ(I))	8503	6019
R_{int}	0.0214	0.0112
parameters	619	644
restraints	514	462
GooF	1.054	1.026
R1	0.0458	0.0467
R1 (all)	0.0588	0.0547
wR2	0.1132	0.1242
wR2 (all)	0.1176	0.1334
weight factors	0.0482 6.5512	0.0779 2.6889

Table S2: Crystallographic details for **[(RAlI$_2$)$_2${(^{Mes}BDI)Mg}$_2$]** and **RAl**.

	[(RAlI$_2$)$_2${(^{Mes}BDI)Mg}$_2$]·4Tol	**[R–Al]**
CCDC #	*2108298*	*2108299*
Empirical formula	$C_{170}H_{218}Al_2I_4Mg_2N_6$	$C_{48}H_{64}NAl$
FW [g mol^{-1}]	2955.67	681.98
Wavelength [Å]	1.34143	1.34143
Temperature [K]	110(2)	150(2)
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	P-1
a [Å]	30.510(3)	12.0243(9)
b [Å]	16.0909(13)	12.3868(15)
c [Å]	32.981(4)	14.3602(13)
α [°]	90	94.863(9)
β [°]	97.157(9)	95.352(7)
γ [°]	90	94.833(8)
V [Å^3]	16065(3)	2112.7(4)
Z	4	2
ρ_{calc} (g·cm^{-3})	1.222	1.072
μ	4.444	0.412
F(000)	6168	744
reflections collected	95988	24511
independent reflections	32730	8607
reflectionsGT (I > 2σ(I))	17863	5486
R_{int}	0.0761	0.0391
parameters	1586	1405
restraints	630	2067
GooF	0.924	0.972
R1	0.0672	0.0439
R1 (all)	0.1146	0.0756
wR2	0.1730	0.1111
wR2 (all)	0.1897	0.1211
weight factors	0.1086 0	0.0737 0

4 Computational Details

4.1 General Considerations

All computations wer performed using Gaussian16[8] utilizing the PBE1PBE level of theory, Def2SVP basis sets and empirical dispersion correction (GD3). No solvent corrections were applied. All optimized molecular structures where checked to be minima on the energy hypersurface and possess no imaginary vibrational frequencies. Natural Bond Orbital Theory was applied to study the electronic states.[9]

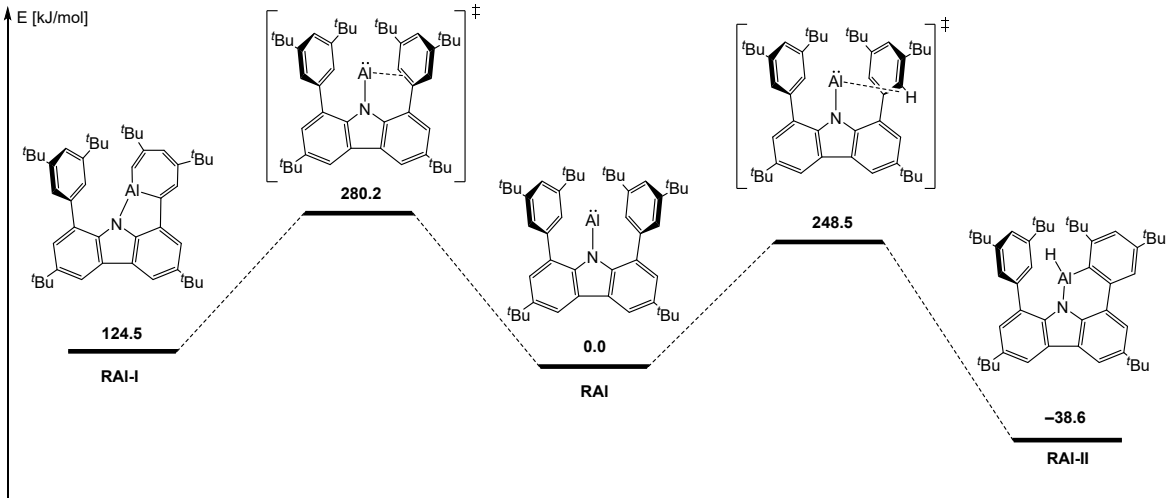


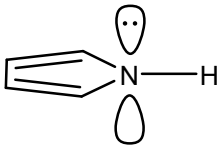
Figure S14: Computed energy profiles for the insertion of the Al atom into C-C and C-H bonds of [R–Al] (energy not to scale).

Table S3: Computed energies for the insertion of the terminal Al atom into C-C and C-H bonds of [R–Al].

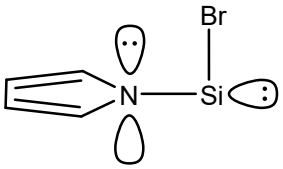
		G [a.u.]	ΔG [a.u.]	ΔG [kJ/mol]
[R–Al]		-2160.286661	0	0.0
	TS	-2160.192008	0.074327	248.5
[R–Al]-II	CH	-2160.301352	-0.008860	-38.6
	TS	-2160.179925	0.098392	280.2
[R–Al]-I	CC	-2160.239244	0.039040	124.5

4.2 ^{15}N NMR data

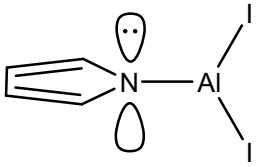
^{15}N NMR **obs.** (calc. isotropic, *anisotropy {YY}*)



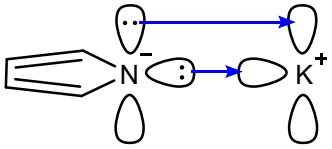
105 (125, *91 {102}*)



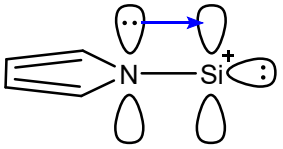
145 (161, *94 {98}*)



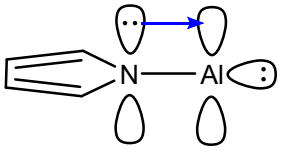
133 (154, *122 {92}*)



192 (201, *241 {-56}*)



206 (226, *177 {-130}*)



183 (206, *178 {-76}*)

[R-H] and [R-K]

[R-SiBr] and [R-Si]$^+$

[R-AlI$_2$] and [R-Al]

Figure S15: Observed computed ^{15}N NMR data for carbazolyl compounds (carbazole 5-membered ring shown only): observed isotropic chemical shift (bold), computed isotropic chemical shift, anisotropy and YY component of shielding tensor (italics) for [R–H], [R–K], [R–SiBr], [R–Si]$^+$, [R–AlI$_2$] and [R–Al].

Selected shielding tensor data for the above compounds:

RH

2 N Isotropic = 145.2609 Anisotropy = 90.6055
XX= 141.7566 YX= 0.0006 ZX= 5.7994
XY= 0.0027 YY= **101.6605** ZY= -0.0071
XZ= -64.1060 YZ= 0.0022 ZZ= 192.3654

RK

2 N Isotropic = 69.1736 Anisotropy = 240.6086
XX= 36.2460 YX= -17.5197 ZX= 0.2762
XY= -16.8927 YY= **-57.8532** ZY= 10.2072
XZ= -5.8525 YZ= 10.9759 ZZ= 229.1281

RSiBr

2 N Isotropic = 109.1257 Anisotropy = 93.6764
XX= 58.8325 YX= -11.3309 ZX= 3.2803
XY= -8.5827 YY= **98.3145** ZY= -0.9936
XZ= 3.7134 YZ= 20.5448 ZZ= 170.2300

RSi

2 N Isotropic = 43.3440 Anisotropy = 177.4823
XX= 106.3441 YX= -16.4283 ZX= -2.3960
XY= -15.1450 YY= **-129.8985** ZY= -27.2803
XZ= -3.7368 YZ= -69.7676 ZZ= 153.5863

RAlI2

2 N Isotropic = 116.1236 Anisotropy = 121.6936
XX= 58.9716 YX= 5.1822 ZX= 1.7873
XY= 3.2807 YY= **92.4365** ZY= -5.8251
XZ= -0.1540 YZ= -5.1521 ZZ= 196.9626

RAl

2 N Isotropic = 64.2198 Anisotropy = 177.8027
XX= 86.5038 YX= -33.0801 ZX= 1.6200
XY= -33.4026 YY= **-75.9555** ZY= 8.7979
XZ= 2.9284 YZ= 16.9317 ZZ= 182.1110

4.3 NBO and AIM data

NBO orbital composition

```
     1. (1.96662) BD ( 1) I   1 -Al   5
                ( 77.49%)   0.8803* I   1 s( 28.63%)p 2.48( 71.15%)d 0.01(  0.21%)
                                           0.0001  0.5351  0.0046 -0.0026  0.0001
                                           0.3355  0.0032  0.0005  0.0002  0.6854
                                           0.0127 -0.0003  0.0001  0.3590  0.0072
                                          -0.0002  0.0000  0.0251  0.0000  0.0129
                                           0.0000  0.0280 -0.0000 -0.0205  0.0000
                                          -0.0116
                ( 22.51%)   0.4745*Al   5 s( 28.32%)p 2.48( 70.30%)d 0.05(  1.38%)
                                          -0.0001  0.0005  0.5315  0.0261 -0.0001
                                          -0.4108 -0.0432 -0.0004 -0.6560 -0.0583
                                           0.0002 -0.3130 -0.0256  0.0592  0.0343
                                           0.0795 -0.0512 -0.0135
     2. (1.96312) BD ( 1) I   2 -Al   5
                ( 79.62%)   0.8923* I   2 s( 28.12%)p 2.55( 71.71%)d 0.01(  0.17%)
                                          -0.0002 -0.5302 -0.0094  0.0021  0.0002
                                           0.7514  0.0128  0.0002 -0.0001 -0.2717
                                           0.0026  0.0004  0.0000  0.2803  0.0026
                                          -0.0010  0.0000  0.0205 -0.0000 -0.0208
                                          -0.0000  0.0124 -0.0000 -0.0240  0.0000
                                           0.0113
                ( 20.38%)   0.4514*Al   5 s( 22.72%)p 3.34( 75.89%)d 0.06(  1.39%)
                                           0.0001 -0.0010 -0.4762  0.0206  0.0000
                                          -0.7194 -0.0291  0.0005  0.2722  0.0113
                                          -0.0004 -0.4066 -0.0291  0.0659 -0.0486
                                           0.0182 -0.0742  0.0371



     5. (1.76513) BD ( 1)Al   5 - C  65
                ( 13.63%)   0.3692*Al   5 s( 38.20%)p 1.59( 60.83%)d 0.03(  0.97%)
                                          -0.0003  0.0063 -0.6180  0.0062 -0.0010
                                          -0.0861 -0.0208 -0.0030 -0.6427 -0.0317
                                           0.0030  0.4305  0.0311 -0.0344  0.0363
                                           0.0759  0.0295 -0.0240
                ( 86.37%)   0.9293* C  65 s( 14.00%)p 6.14( 86.00%)d 0.00(  0.00%)
                                          -0.0005 -0.3696  0.0580  0.1849 -0.0085
                                           0.6185 -0.0492 -0.6630  0.0354 -0.0012
                                          -0.0000  0.0015  0.0040  0.0007
     6. (1.76359) BD ( 1)Al   6 - C  88
                ( 13.48%)   0.3671*Al   6 s( 35.99%)p 1.75( 63.01%)d 0.03(  1.00%)
                                           0.0003 -0.0062  0.5996 -0.0162 -0.0006
                                           0.0255 -0.0129 -0.0016 -0.1358 -0.0069
                                          -0.0042 -0.7805 -0.0399  0.0153  0.0331
                                           0.0512 -0.0046  0.0779
                ( 86.52%)   0.9302* C  88 s( 14.03%)p 6.13( 85.97%)d 0.00(  0.00%)
                                           0.0005  0.3706 -0.0543  0.0919  0.0002
                                           0.3252 -0.0149  0.8612 -0.0603  0.0007
                                          -0.0010 -0.0010 -0.0011  0.0026

     7. (1.88743) BD ( 1)Mg   7 -Mg   8
                ( 50.11%)   0.7079*Mg   7 s( 94.09%)p 0.06(  5.43%)d 0.01(  0.48%)
                                          -0.0001 -0.0021  0.9700  0.0034 -0.0004
                                           0.2245  0.0075  0.0002 -0.0373  0.0017
                                          -0.0001 -0.0446  0.0209 -0.0181 -0.0167
                                          -0.0046  0.0486 -0.0429
                ( 49.89%)   0.7063*Mg   8 s( 94.12%)p 0.06(  5.35%)d 0.01(  0.53%)
                                          -0.0001 -0.0021  0.9701  0.0037  0.0004
                                          -0.2301 -0.0034 -0.0002  0.0166  0.0106
                                          -0.0001 -0.0069  0.0116 -0.0131 -0.0134
                                          -0.0151  0.0635 -0.0267
```

```
 2794. (0.16791) BD*( 1)Mg   7 -Mg   8
               ( 49.89%)   0.7063*Mg   7 s( 94.09%)p 0.06(  5.43%)d 0.01(  0.48%)
                                          0.0001  0.0021 -0.9700 -0.0034  0.0004
                                         -0.2245 -0.0075 -0.0002  0.0373 -0.0017
                                          0.0001  0.0446 -0.0209  0.0181  0.0167
                                          0.0046 -0.0486  0.0429
               ( 50.11%)  -0.7079*Mg   8 s( 94.12%)p 0.06(  5.35%)d 0.01(  0.53%)
                                          0.0001  0.0021 -0.9701 -0.0037 -0.0004
                                          0.2301  0.0034  0.0002 -0.0166 -0.0106
                                          0.0001  0.0069 -0.0116  0.0131  0.0134
                                          0.0151 -0.0635  0.0267
```

Second Order Perturbation Theory Analysis

```
   2. BD (   1) I   2 -Al   5        /689. RY*(   2)Mg   7                    0.10    1.09    0.010
   2. BD (   1) I   2 -Al   5        /691. RY*(   4)Mg   7                    0.06    1.24    0.008
   2. BD (   1) I   2 -Al   5        /692. RY*(   5)Mg   7                    0.15    1.39    0.013
   2. BD (   1) I   2 -Al   5        /693. RY*(   6)Mg   7                    0.06    1.45    0.008
   2. BD (   1) I   2 -Al   5        /695. RY*(   8)Mg   7                    0.08    1.41    0.009
   2. BD (   1) I   2 -Al   5        /***. BD*(   1)Mg   7 -Mg   8            4.05    0.73    0.050
 401. CR (   1) I   2                /688. RY*(   1)Mg   7                    0.20    6.97    0.034
 401. CR (   1) I   2                /689. RY*(   2)Mg   7                    0.07    6.87    0.020
 401. CR (   1) I   2                /***. BD*(   1)Mg   7 -Mg   8            1.92    6.52    0.104
 402. CR (   2) I   2                /***. BD*(   1)Mg   7 -Mg   8            0.06    4.99    0.017
 404. CR (   4) I   2                /***. BD*(   1)Mg   7 -Mg   8            0.10    4.98    0.021

599. LP (   1) I   2                /688. RY*(   1)Mg   7                    0.49    1.37    0.023
 599. LP (   1) I   2                /689. RY*(   2)Mg   7                    0.07    1.27    0.009
 599. LP (   1) I   2                /697. RY*(  10)Mg   7                    0.05    1.48    0.008
 599. LP (   1) I   2                /***. BD*(   1)Mg   7 -Mg   8            3.91    0.92    0.055
 600. LP (   2) I   2                /694. RY*(   7)Mg   7                    0.10    1.00    0.009
 601. LP (   3) I   2                /688. RY*(   1)Mg   7                    4.02    0.92    0.055
 601. LP (   3) I   2                /689. RY*(   2)Mg   7                    0.06    0.82    0.006
 601. LP (   3) I   2                /691. RY*(   4)Mg   7                    0.10    0.97    0.009
 601. LP (   3) I   2                /695. RY*(   8)Mg   7                    0.10    1.14    0.010
 601. LP (   3) I   2                /698. RY*(  11)Mg   7                    0.23    1.09    0.015
 601. LP (   3) I   2                /***. BD*(   1)Mg   7 -Mg   8           12.10    0.46    0.068
```

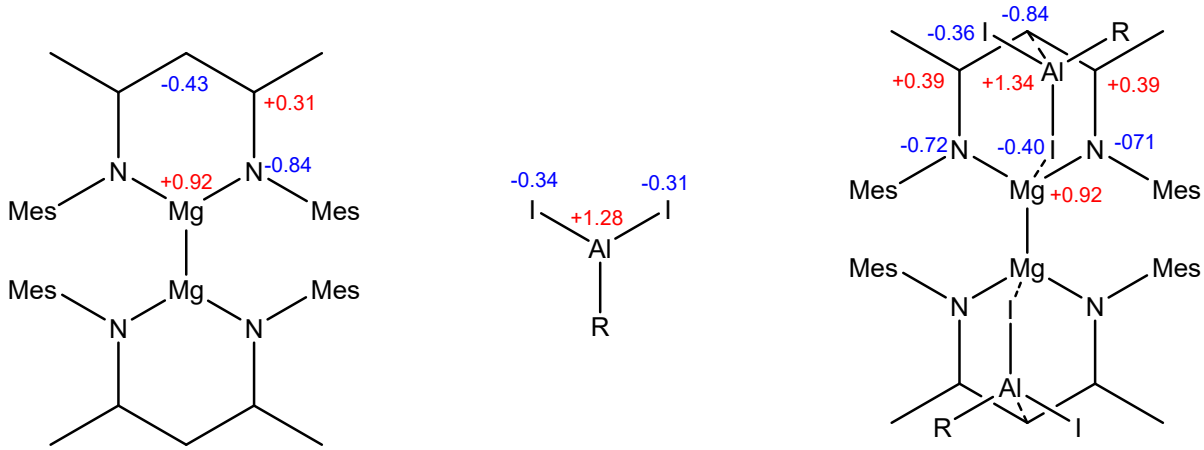


Figure S16: Computed NBO charges in [RAlI$_2$], [(^{Mes}BDI)Mg]$_2$] and [(RAlI$_2$)$_2${(^{Mes}BDI)Mg}$_2$].

Topological data at BCPs

1) Al–I bonds

```
Density of all electrons:  0.4414090133E-01
Density of Alpha electrons:  0.2207045066E-01
Density of Beta electrons:  0.2207045066E-01
Spin density of electrons:  0.0000000000E+00
Lagrangian kinetic energy G(r):  0.3426879314E-01
G(r) in X,Y,Z:  0.2294608382E-01  0.5590282195E-02  0.5732427120E-02
Hamiltonian kinetic energy K(r):  0.1192038283E-01
Potential energy density V(r): -0.4618917596E-01
Energy density E(r) or H(r): -0.1192038283E-01
Laplacian of electron density:  0.8939364198E-01
Electron localization function (ELF):  0.1757679266E+00

Density of all electrons:  0.4749223110E-01
Density of Alpha electrons:  0.2374611555E-01
Density of Beta electrons:  0.2374611555E-01
Spin density of electrons:  0.0000000000E+00
Lagrangian kinetic energy G(r):  0.3878383996E-01
G(r) in X,Y,Z:  0.2581148303E-01  0.7843989927E-02  0.5128367005E-02
Hamiltonian kinetic energy K(r):  0.1324654383E-01
Potential energy density V(r): -0.5203038380E-01
Energy density E(r) or H(r): -0.1324654383E-01
Laplacian of electron density:  0.1021491859E+00
Electron localization function (ELF):  0.1752559381E+00
```

2) Mg–I bonds

```
Density of all electrons:  0.1706395327E-01
Density of Alpha electrons:  0.8531976633E-02
Density of Beta electrons:  0.8531976633E-02
Spin density of electrons:  0.0000000000E+00
Lagrangian kinetic energy G(r):  0.1425856029E-01
G(r) in X,Y,Z:  0.3652958360E-02  0.3270401385E-02  0.7335200540E-02
Hamiltonian kinetic energy K(r): -0.6586736439E-03
Potential energy density V(r): -0.1359988664E-01
Energy density E(r) or H(r):  0.6586736439E-03
Laplacian of electron density:  0.5966893575E-01
Electron localization function (ELF):  0.4924667322E-01

Density of all electrons:  0.1716663401E-01
Density of Alpha electrons:  0.8583317007E-02
Density of Beta electrons:  0.8583317007E-02
Spin density of electrons:  0.0000000000E+00
Lagrangian kinetic energy G(r):  0.1425437815E-01
G(r) in X,Y,Z:  0.3274198070E-02  0.1882176874E-02  0.9098003202E-02
Hamiltonian kinetic energy K(r): -0.6270143408E-03
Potential energy density V(r): -0.1362736380E-01
Energy density E(r) or H(r):  0.6270143408E-03
Laplacian of electron density:  0.5952556998E-01
Electron localization function (ELF):  0.5021944670E-01
```

4.4 Optimised Geomietries

4.4.1 [$RAlI_2$]

```
0 1
 C                 -1.05432900    1.99267500    0.54212200
 N                  0.02729600    1.12138900    0.48826000
 C                 -1.61682400    4.34465200    0.60618900
 C                 -0.64726900    3.34128900    0.60186500
 C                  0.79996800    3.30583400    0.58492600
 C                  1.79102300    4.28733500    0.58589500
 C                  3.13998600    3.92985000    0.49236500
 C                  3.46106000    2.56091000    0.41303500
 C                  2.49724100    1.54992600    0.42664200
 C                  1.15826600    1.93688500    0.50705400
 C                 -2.74108700    0.18690800    0.44634100
 C                 -2.63356900   -0.54676600    1.64685400
 C                 -3.07862400   -1.86132900    1.72762200
 C                 -3.61512700   -2.44338000    0.56345400
 C                 -3.69877000   -1.77581500   -0.65582100
 C                 -3.24586300   -0.44334300   -0.70084600
 C                 -4.26662100   -2.42657400   -1.91928300
 C                 -3.05136900   -2.65964500    3.03397700
 C                 -4.02016800    5.14509000    0.51732900
 C                  4.21394900    5.02474900    0.48008300
 C                  2.86662600    0.11202500    0.39329000
 C                  3.29512100   -0.50015400   -0.78883200
 C                  3.69455100   -1.84287500   -0.80331700
 C                  3.64855700   -2.55108200    0.40178500
 C                  3.20547200   -1.97650300    1.60103200
 C                  2.81251500   -0.63735300    1.57418400
 C                  4.15178800   -2.48071600   -2.11875700
 C                  3.15981900   -2.75287700    2.92163800
 C                 -2.97752800    4.01955700    0.52587700
 C                 -3.34287700    2.66026000    0.45184500
 C                 -2.39759200    1.63360600    0.46537200
 C                 -3.89922100    5.96124700    1.81354900
 H                 -2.90133100    6.41195200    1.92104000
 H                 -4.63835500    6.77871800    1.82659100
 H                 -4.07508500    5.32527300    2.69495800
 C                 -3.76954400    6.06031200   -0.69140500
 H                 -4.50821300    6.87789500   -0.71728900
 H                 -2.76877000    6.51610400   -0.65899700
 H                 -3.84843300    5.49573700   -1.63327000
 C                 -5.45067200    4.60969700    0.42159800
 H                 -5.61148200    4.03476200   -0.50339500
 H                 -5.70501100    3.96504800    1.27705100
 H                 -6.16267800    5.44932700    0.41697500
 C                 -4.69319500   -3.87544500   -1.67638500
 H                 -5.48536000   -3.95090600   -0.91523600
 H                 -5.09044800   -4.30446400   -2.60866100
 H                 -3.84502500   -4.50159400   -1.35932700
 C                 -3.19329000   -2.41358500   -3.01729500
 H                 -2.88284100   -1.39230100   -3.28121400
 H                 -2.29198800   -2.95746400   -2.69513000
 H                 -3.57854700   -2.89241100   -3.93149800
 C                 -5.49413300   -1.62787400   -2.38491400
 H                 -5.91787300   -2.07765300   -3.29684700
 H                 -6.27745900   -1.61957500   -1.61097700
 H                 -5.23900500   -0.58343600   -2.61854500
 C                  3.97858100    5.95252500   -0.72207100
 H                  2.99094600    6.43544600   -0.67870300
 H                  4.73946000    6.74944800   -0.75067300
 H                  4.03386600    5.39046800   -1.66712500
 C                  5.62763300    4.44913200    0.36956100
 H                  5.87068800    3.79382400    1.22006900
 H                  5.76321200    3.87274100   -0.55847200
 H                  6.36335100    5.26814000    0.36149300
 C                  4.12678400    5.83780500    1.78093600
```

```
H                  4.88916900    6.63372900    1.79176800
H                  3.14297500    6.31622400    1.89859000
H                  4.29154700    5.19261800    2.65777000
C                  4.19881400   -2.15094400    3.88085100
H                  3.99508400   -1.08815000    4.08054300
H                  4.19016500   -2.68447800    4.84526500
H                  5.21240600   -2.22358900    3.45701800
C                  3.47446700   -4.23797000    2.72918600
H                  4.49270300   -4.39701100    2.34260200
H                  3.40479600   -4.76170700    3.69494200
H                  2.76431600   -4.71623100    2.03675800
C                 -4.50252300   -2.87509900    3.49339600
H                 -5.08480300   -3.43614500    2.74649800
H                 -4.52569200   -3.44507000    4.43601700
H                 -5.00964000   -1.91243500    3.66142900
C                 -2.37627700   -4.02149100    2.81571100
H                 -2.89313700   -4.62794700    2.05746400
H                 -1.33310900   -3.89577600    2.49138600
H                 -2.37784100   -4.59619700    3.75518100
C                 -2.28797500   -1.92176500    4.13610500
H                 -1.24781300   -1.71693000    3.83912400
H                 -2.76665900   -0.96754700    4.40347700
H                 -2.26005900   -2.54010800    5.04610300
C                  1.76040100   -2.63845600    3.54592800
H                  1.48727200   -1.59470200    3.76065500
H                  0.99505200   -3.05055300    2.87129800
H                  1.71924100   -3.19393800    4.49654000
C                  4.51851200   -3.95629400   -1.94832300
H                  4.83651600   -4.37357500   -2.91601400
H                  5.34950600   -4.09504800   -1.23938300
H                  3.66101500   -4.55069800   -1.59693400
C                  5.38748200   -1.72972700   -2.63835500
H                  6.21586700   -1.78644700   -1.91499100
H                  5.73135100   -2.16757200   -3.58933200
H                  5.17174200   -0.66622400   -2.81951900
C                  3.01638000   -2.38131600   -3.14894500
H                  2.11318100   -2.89860700   -2.79043300
H                  2.73516500   -1.33828100   -3.35513800
H                  3.32321300   -2.84060100   -4.10246100
H                 -4.39429300    2.37696700    0.39475500
H                 -1.30332000    5.39054600    0.65378300
H                  1.49921300    5.33885400    0.64656400
H                  4.50371500    2.24771100    0.35028800
H                  2.46859800   -0.13888700    2.48326400
H                  3.95262700   -3.59520800    0.40461500
H                  3.31796800    0.09813400   -1.70284900
H                 -3.32509700    0.14088100   -1.62064700
H                 -3.96991500   -3.47184900    0.62272500
H                 -2.22091300   -0.03426600    2.51562900
Al                -0.25580400   -0.36238200   -0.58228000
I                 -0.19130600    0.34233000   -2.97642400
I                  0.00008600   -2.78001100   -0.16647400
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4.4.2 [RAl]

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C                 -1.41128700    1.39561900   -0.06709800
N                 -0.79097100    0.15000700   -0.01059500
C                 -3.62329700    2.42130100   -0.11026300
C                 -2.82319800    1.27923300   -0.07518500
C                 -3.09877000   -0.13890000   -0.02877100
C                 -4.26813500   -0.89903800   -0.00785500
C                 -4.20638600   -2.29557600    0.04619300
C                 -2.93514500   -2.90259000    0.07238000
C                 -1.74689500   -2.17125100    0.04926400
C                 -1.83281300   -0.77405600    0.00418100
C                  0.67333500    2.75003700   -0.08706800
C                  1.40011600    2.49934200   -1.26405300
C                  2.79703800    2.49516000   -1.26141100
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C	3.45137500	2.74804100	-0.04500300
C	2.76598400	2.97546200	1.14820500
C	1.36203200	2.97672200	1.10494100
C	3.47814600	3.17343500	2.48833900
C	3.62390300	2.20268200	-2.51582700
C	-3.94285000	4.93594700	-0.16928100
C	-5.50529000	-3.11100200	0.07111800
C	-0.40493300	-2.80636000	0.05696100
C	0.23170900	-3.12167600	1.26242400
C	1.53789400	-3.62949200	1.28415700
C	2.18749300	-3.81738600	0.05903500
C	1.58677400	-3.50922400	-1.16797500
C	0.28307300	-2.99889400	-1.14751200
C	2.21235700	-3.91744200	2.62827900
C	2.29991800	-3.70129500	-2.50932300
C	-3.04327800	3.69406300	-0.13381800
C	-1.63710100	3.78204500	-0.12524600
C	-0.80828900	2.65937900	-0.09692900
C	-4.81720900	4.89563600	-1.43219300
H	-5.45640400	4.00048700	-1.45740800
H	-5.47561900	5.77861600	-1.47669300
H	-4.19363500	4.88588000	-2.33955400
C	-4.84254600	4.94915600	1.07632000
H	-5.50107500	5.83313100	1.06990100
H	-5.48291800	4.05593800	1.12682100
H	-4.23746900	4.97818400	1.99572700
C	-3.13594100	6.23620000	-0.18870700
H	-2.50394900	6.33879500	0.70688500
H	-2.48780400	6.30221800	-1.07611100
H	-3.81957500	7.09897900	-0.21258300
C	5.00090400	3.14907600	2.34323200
H	5.36159100	3.94766300	1.67653800
H	5.47023500	3.30169400	3.32708300
H	5.35853800	2.18404200	1.95259300
C	3.06363000	2.03597600	3.43657200
H	1.98064800	2.04015100	3.63056900
H	3.31973800	1.05510300	3.00601400
H	3.57816700	2.13674500	4.40575100
C	3.06889300	4.52606100	3.09057500
H	3.56416900	4.67804900	4.06290900
H	3.35692100	5.35550700	2.42620300
H	1.98334400	4.59027300	3.25646300
C	-6.32917300	-2.71847900	1.30738900
H	-6.58822900	-1.64919900	1.30241000
H	-7.27055800	-3.29081700	1.34405000
H	-5.76751300	-2.92128500	2.23241200
C	-5.24332900	-4.61766500	0.13099900
H	-4.67779600	-4.96971200	-0.74546100
H	-4.68471500	-4.90004600	1.03664900
H	-6.20024100	-5.16202300	0.14848900
C	-6.31689200	-2.81592400	-1.19983500
H	-7.25805400	-3.38980800	-1.20116400
H	-6.57567500	-1.74960400	-1.28035900
H	-5.74628600	-3.08968200	-2.10079100
C	1.52720700	-4.73816800	-3.33948400
H	0.49152500	-4.41845300	-3.52816700
H	2.01541700	-4.89060500	-4.31551100
H	1.48925700	-5.70804200	-2.81973800
C	3.73898100	-4.19083500	-2.33481900
H	3.78239500	-5.17018600	-1.83405200
H	4.21487900	-4.30389500	-3.32089500
H	4.34379800	-3.47792600	-1.75331400
C	4.40437400	3.46731700	-2.90515600
H	5.07242800	3.79597800	-2.09457200
H	5.02352900	3.27898800	-3.79708800
H	3.71860000	4.29807300	-3.13257500
C	4.60706200	1.05833100	-2.22105400
H	5.34311800	1.33263500	-1.45126900

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H                  4.07074900    0.16582800   -1.86334200
H                  5.16504600    0.78983800   -3.13214700
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H                  2.16189200    0.87793500   -3.46491900
H                  2.04306500    2.57904300   -3.99054500
H                  3.37511800    1.56033600   -4.56964900
C                  2.33713000   -2.36190700   -3.26169900
H                  1.32812400   -1.97602000   -3.46977200
H                  2.87210100   -1.59990700   -2.67491600
H                  2.85436500   -2.47784300   -4.22753100
C                  3.63040900   -4.46634900    2.45834800
H                  4.07242200   -4.66434400    3.44677500
H                  3.63907100   -5.41295100    1.89610900
H                  4.28646300   -3.75008900    1.94035200
C                  1.38144500   -4.95104500    3.40360900
H                  1.31064500   -5.89744900    2.84532300
H                  1.84694100   -5.16272900    4.37952900
H                  0.35771200   -4.59579600    3.59301000
C                  2.29373300   -2.60920100    3.43220200
H                  2.85959700   -1.84398200    2.87796400
H                  1.29589800   -2.19547000    3.64169400
H                  2.79391200   -2.78275500    4.39861000
H                 -1.15065400    4.75795000   -0.14691900
H                 -4.71076800    2.30920800   -0.11492800
H                 -5.23479700   -0.38900700   -0.03303900
H                 -2.84974600   -3.98928300    0.10687700
H                 -0.22693000   -2.73557800   -2.07722200
H                  3.20536400   -4.19965400    0.06062400
H                 -0.31368900   -2.94879100    2.19324800
H                  0.77790900    3.14039100    2.01355200
H                  4.54081500    2.73798200   -0.03372600
H                  0.83786800    2.30591100   -2.17829500
Al                 1.11455200   -0.21425800    0.19283100
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4.4.3 [RAl]-I

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C                  1.73132000   -1.50008100    0.00505500
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C                  3.12859100   -1.39079200   -0.05761900
C                  3.39597000    0.03786300   -0.01303700
C                  4.55119900    0.82749300   -0.07508200
C                  4.45441300    2.22022800   -0.03993400
C                  3.17353300    2.80910400    0.07995200
C                  2.00259100    2.06141800    0.16206100
C                  2.13059800    0.66831300    0.09170000
C                 -0.43170900   -2.50760100   -0.02243200
C                 -1.40499400   -3.44873300   -0.13694300
C                 -2.84614200   -3.26206800   -0.06970900
C                 -3.60760200   -2.13466000   -0.29175700
C                 -3.45861000   -0.73310600   -0.67983400
C                 -2.36432600    0.08094400   -0.54070700
C                  3.21881200   -3.81761800   -0.19047800
C                  1.80615300   -3.86686900   -0.14001000
C                  1.02083700   -2.71479600   -0.04947400
H                  1.30604000   -4.83831000   -0.17805800
H                  4.95909500   -2.52181000   -0.20432700
H                  5.52209000    0.33792100   -0.15818100
H                  3.08376400    3.89722900    0.13311200
H                 -2.49683400    1.12896700   -0.83214700
H                 -4.66324700   -2.36157300   -0.18732400
H                 -1.09111600   -4.49643700   -0.23497800
Al                -0.69069100   -0.59610100   -0.00371600
C                  0.64583100    2.63680600    0.33095200
C                 -0.10038200    2.29975100    1.46935600
C                  0.06330200    3.45097600   -0.64204400
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C	-1.40589000	2.76466000	1.65445200
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H	0.65081900	3.69441100	-1.53053100
C	-1.95843800	3.57049400	0.64999700
H	-2.97664200	3.93304200	0.77090800
C	-2.16241100	2.40472900	2.93829200
C	-1.85676700	4.79508100	-1.60770900
C	-2.23521100	0.87691200	3.08984300
H	-2.77987600	0.42264700	2.24753300
H	-1.23340000	0.42072200	3.13838000
H	-2.75800000	0.60789700	4.02148400
C	-3.59156100	2.95132300	2.94011100
H	-4.09850800	2.66270100	3.87355000
H	-3.61027400	4.05035200	2.88148100
H	-4.18197900	2.54948900	2.10308000
C	-1.41032400	3.00368800	4.13739900
H	-1.34254000	4.09912000	4.05041800
H	-1.93342300	2.76540500	5.07752500
H	-0.38582000	2.60999900	4.21371700
C	-3.31691400	5.15505300	-1.32410700
H	-3.42491600	5.73734700	-0.39625200
H	-3.71474900	5.76871000	-2.14671100
H	-3.95064000	4.25799000	-1.24370800
C	-1.04624900	6.09543500	-1.72187300
H	0.00823000	5.89702800	-1.96520200
H	-1.45903600	6.73859900	-2.51571300
H	-1.07217500	6.65814700	-0.77591000
C	-1.80191800	4.03644100	-2.94285000
H	-0.77144000	3.78630300	-3.23407800
H	-2.37024800	3.09532900	-2.88377100
H	-2.23814700	4.64694800	-3.74950000
C	5.68302900	3.13464100	-0.11508500
C	3.99365700	-5.13941600	-0.29063900
C	5.76921800	3.98239100	1.16383000
H	6.64718900	4.64787400	1.12851700
H	4.87786300	4.61323300	1.29817500
H	5.86087800	3.33986300	2.05318800
C	5.55646000	4.05922400	-1.33606800
H	4.65789100	4.69167600	-1.27935900
H	6.43034500	4.72706800	-1.40800500
H	5.49488500	3.47283000	-2.26593000
C	6.98409600	2.34088100	-0.25051000
H	7.14972000	1.67774500	0.61243100
H	6.99429300	1.72661300	-1.16401200
H	7.83910500	3.03231900	-0.30574600
C	5.50766500	-4.92194500	-0.33935000
H	5.80714700	-4.32528000	-1.21466900
H	5.87747600	-4.41605900	0.56576200
H	6.02147100	-5.89318100	-0.40937400
C	3.67615100	-6.01116800	0.93451800
H	2.60316600	-6.24434900	1.00443900
H	4.22280200	-6.96689300	0.88203200
H	3.96758400	-5.49928600	1.86471000
C	3.57717600	-5.88138800	-1.57041800
H	4.12301700	-6.83477800	-1.66033600
H	2.50132400	-6.11143800	-1.57931600
H	3.79585700	-5.27475700	-2.46281000
C	-3.59650100	-4.58022900	0.26756700
C	-4.74053700	-0.06322600	-1.27135000
C	-5.16496900	1.10843200	-0.37326900
H	-4.37179500	1.86547200	-0.28844400
H	-6.06124200	1.60274800	-0.78153100
H	-5.40361300	0.75777000	0.64335300
C	-4.40279900	0.45873400	-2.67736300
H	-5.28135500	0.94992800	-3.12587500
H	-3.58313700	1.19042500	-2.65572200
H	-4.09640300	-0.36622500	-3.33898600

C	-5.94650100	-0.99903700	-1.41702800
H	-5.71720100	-1.87638800	-2.04083200
H	-6.32795800	-1.35337300	-0.44697100
H	-6.76930500	-0.45302400	-1.90390200
C	-3.02012800	-5.17284700	1.56592700
H	-3.54202600	-6.10866600	1.82218600
H	-1.94814300	-5.40225900	1.48665200
H	-3.14788500	-4.46984500	2.40380000
C	-5.10225300	-4.40437000	0.48521300
H	-5.32114100	-3.69164900	1.29526800
H	-5.62327500	-4.06798900	-0.42391500
H	-5.54175100	-5.37256500	0.76954800
C	-3.41554600	-5.57840300	-0.88964200
H	-2.36049100	-5.82677300	-1.07452700
H	-3.93969700	-6.52093400	-0.66388000
H	-3.83264900	-5.17008800	-1.82319100

4.4.4 [RAl]-I TS

0 1

C	-0.62432900	1.98440400	0.21933300
N	-0.87504200	0.67367100	0.53807500
C	-1.66245500	4.07803500	-0.28603200
C	-1.80532300	2.72026800	0.04825500
C	-2.87892200	1.75214900	0.26265700
C	-4.27400200	1.74952000	0.19702600
C	-5.00185800	0.55907000	0.36531300
C	-4.30624200	-0.64885900	0.58221800
C	-2.91357900	-0.69462300	0.68114700
C	-2.22850600	0.51779000	0.54313800
C	1.72965900	1.42932900	0.30582300
C	3.09010000	1.75663700	0.56241100
C	4.15712500	0.89212300	0.47948300
C	4.08421500	-0.32960700	-0.28064900
C	3.07705400	-0.72038000	-1.14293100
C	1.72795100	-0.23922000	-1.06368800
C	-0.38301300	4.62689000	-0.44669600
C	0.77025000	3.81085300	-0.28539000
C	0.68733700	2.46135600	0.05351600
H	1.75932400	4.24968800	-0.44251100
H	-2.54977900	4.69584400	-0.42694600
H	-4.80200700	2.68487400	-0.00569000
H	-4.85664500	-1.58545700	0.68087000
H	1.20100800	-0.11319000	-2.02377600
H	5.02865900	-0.86649400	-0.37110700
H	3.28384000	2.79446400	0.85242400
C	-2.05778000	-1.90238600	0.72822400
C	-0.92743300	-1.93558300	1.57982000
C	-2.20904400	-2.93740700	-0.19161100
C	0.05606100	-2.93124800	1.47030800
H	-0.88675800	-1.19992000	2.39025800
C	-1.25625000	-3.96130600	-0.31992400
H	-3.06955700	-2.90173000	-0.86349800
C	-0.12537800	-3.92758100	0.50168000
H	0.63673000	-4.69373300	0.38476400
C	-0.17631000	6.10337300	-0.81567400
C	5.54176600	1.26635800	1.03343100
C	3.38013400	-1.67551000	-2.31808800
C	4.74428300	-2.35735500	-2.19399900
H	4.88063600	-3.06602300	-3.02592200
H	5.57359600	-1.63584000	-2.23718500
H	4.83081300	-2.92459900	-1.25358900
C	2.30987000	-2.77675900	-2.38850200
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H	1.30234000	-2.35549300	-2.51723800
H	2.50528500	-3.46214200	-3.22966300
C	3.36572800	-0.86102200	-3.62120500
H	4.14247200	-0.08168800	-3.59839100

H	3.55573400	-1.51481500	-4.48816900
H	2.39658900	-0.36611300	-3.78318600
C	5.53046000	2.60439000	1.77628000
H	6.52302300	2.79912500	2.21207600
H	5.29680400	3.44403400	1.10410100
H	4.79475400	2.60768700	2.59514600
C	6.57641000	1.36469900	-0.09943900
H	7.56638800	1.64129800	0.29922800
H	6.69099200	0.41367100	-0.64021600
H	6.27459400	2.12948100	-0.83167000
C	5.97707200	0.18091700	2.03228600
H	5.26621300	0.11995400	2.87224500
H	6.02877500	-0.81284300	1.56217500
H	6.97357300	0.40691300	2.44639200
C	0.64945800	6.79304400	0.28189900
H	0.81218300	7.85521300	0.03561600
H	0.13068600	6.74055900	1.25169800
H	1.63691300	6.32426800	0.40643000
C	-1.49981400	6.85848800	-0.95721500
H	-1.30304000	7.91039700	-1.21656300
H	-2.12980100	6.43348400	-1.75373700
H	-2.07706600	6.85012200	-0.01981700
C	0.57101800	6.19816700	-2.15535200
H	1.55668700	5.71174400	-2.11032500
H	-0.00428800	5.71149700	-2.95813800
H	0.73073800	7.25210900	-2.43651400
C	-6.96402500	1.15083700	-1.08293200
H	-6.57735600	2.16491600	-1.26252300
H	-6.59212400	0.50414800	-1.89276600
H	-8.06299800	1.19546000	-1.15550200
C	-6.53468900	0.60904100	0.28954800
C	-7.17156700	-0.77030900	0.47491400
H	-6.92439000	-1.20721200	1.45475200
H	-8.26773200	-0.68507700	0.41739300
H	-6.85401100	-1.47662700	-0.30780600
C	-7.06823000	1.53344100	1.39516500
H	-8.16859800	1.58828100	1.35836600
H	-6.77564500	1.16290200	2.38983500
H	-6.67869700	2.55731500	1.29348600
C	1.27296900	-2.89112500	2.40448000
C	-1.45922800	-5.04288600	-1.38428300
C	-1.52122700	-4.37791600	-2.76904500
H	-1.66328800	-5.14096300	-3.55061900
H	-2.35259000	-3.66207700	-2.84668300
H	-0.58820400	-3.83566900	-2.98531400
C	-0.32216500	-6.06678100	-1.39468400
H	-0.23287800	-6.59199000	-0.43111900
H	-0.51560200	-6.82592200	-2.16745500
H	0.64691200	-5.59934100	-1.62821300
C	-2.77808000	-5.77911900	-1.10219000
H	-2.94937500	-6.55793200	-1.86202300
H	-2.75567800	-6.26413900	-0.11401200
H	-3.64148100	-5.09774500	-1.12307700
C	2.33119600	-3.92918000	2.02777400
H	3.20122100	-3.83314700	2.69463900
H	1.94784100	-4.95495200	2.13076100
H	2.68592200	-3.78944900	0.99509400
C	1.92970900	-1.50574400	2.30450700
H	2.40720000	-1.34211500	1.30966400
H	1.24513600	-0.68138300	2.60220600
H	2.77512100	-1.38233000	2.99947900
C	0.80841100	-3.13822700	3.84682900
H	0.32481100	-4.12274900	3.93295900
H	1.66524300	-3.11450200	4.53841900
H	0.08361300	-2.37960900	4.17852800
Al	0.72559300	-0.21361200	0.53671100

4.4.5 [RAl]-II

```
0 1
 C                 -0.85409100    1.63558200   -0.16164900
 N                  0.24937000    0.79746300   -0.13783100
 C                 -1.39722800    4.01566200   -0.15733000
 C                 -0.45056800    2.99172400   -0.10619200
 C                  0.99420500    2.97532500   -0.00288300
 C                  1.98233200    3.95824300    0.08152000
 C                  3.33187100    3.59888300    0.17817600
 C                  3.66035100    2.22873900    0.22680100
 C                  2.69779500    1.21948300    0.16109100
 C                  1.36379200    1.61273800    0.00389300
 C                 -2.67992200   -0.15021500   -0.23045900
 C                 -4.00677200   -0.38253000    0.16499400
 C                 -4.59780400   -1.63912200    0.10353200
 C                 -3.82495100   -2.68882600   -0.40137700
 C                 -2.48613200   -2.52630800   -0.76813500
 C                 -1.86804600   -1.25302200   -0.63816200
 C                 -2.75054600    3.69284800   -0.27023300
 C                 -3.11318700    2.33289800   -0.30337700
 C                 -2.21024600    1.26263800   -0.22871200
 H                 -4.17153600    2.09581300   -0.41882500
 H                 -1.06319500    5.05312200   -0.11965300
 H                  1.69102400    5.01166000    0.07108500
 H                  4.69856700    1.91994300    0.35468000
 H                  1.20694100   -1.60446900   -1.59888200
 H                 -4.28401700   -3.66852900   -0.49649600
 H                 -4.58899500    0.45279800    0.55517100
 Al                 0.04951200   -0.90342800   -0.79389900
 C                  4.40020000    4.69748400    0.25461400
 C                 -3.85208200    4.75541600   -0.36588300
 C                 -3.28562300    6.17479400   -0.28958100
 H                 -2.75773000    6.35275300    0.66000200
 H                 -2.58755600    6.38055900   -1.11555100
 H                 -4.10396100    6.90820800   -0.35713700
 C                 -4.59247000    4.60412100   -1.70385200
 H                 -5.05887600    3.61245200   -1.80350600
 H                 -5.39047700    5.35928500   -1.79257700
 H                 -3.90075800    4.73379600   -2.55050900
 C                 -4.84475900    4.57304200    0.79301900
 H                 -5.64210400    5.33235100    0.74295400
 H                 -5.32641600    3.58389000    0.76822100
 H                 -4.33568800    4.67249500    1.76416700
 C                  4.32169900    5.56946500   -1.00826000
 H                  3.33669800    6.04805300   -1.11374100
 H                  5.08013600    6.36857500   -0.97481800
 H                  4.49801900    4.96617300   -1.91225500
 C                  4.14985900    5.56832500    1.49556600
 H                  4.19932000    4.96377000    2.41439900
 H                  4.90662600    6.36647700    1.56788400
 H                  3.16033500    6.04823600    1.46487600
 C                  5.81615000    4.12464200    0.35063900
 H                  5.95156600    3.51588400    1.25778700
 H                  6.06489000    3.50158100   -0.52228800
 H                  6.54814200    4.94603700    0.39143800
 C                  2.99455600   -0.22353800    0.31095000
 C                  3.83924900   -0.91229100   -0.55607900
 C                  2.32681700   -0.93436200    1.32160100
 C                  3.99462300   -2.30241700   -0.46290000
 H                  4.33741000   -0.35045700   -1.34957300
 C                  2.48372500   -2.31475000    1.47258000
 H                  1.70447200   -0.36873700    2.01789800
 C                  3.30728000   -2.97855000    0.55073200
 H                  3.42105300   -4.05715500    0.63373100
 C                 -1.72491200   -3.73680900   -1.35152200
 C                 -6.04411500   -1.82391600    0.57260600
 C                 -1.23887300   -3.39954100   -2.77071800
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 H                -0.53374900   -2.55701200   -2.78805800
 H                -0.72117000   -4.26462400   -3.21592900
 H                -2.08998000   -3.13658500   -3.41729900
 C                -0.54085500   -4.11855700   -0.45377200
 H                 0.20684100   -3.31753900   -0.33948800
 H                -0.89149300   -4.39688500    0.55118600
 H                 0.00589200   -4.97673100   -0.87724900
 C                -2.60649600   -4.98676200   -1.46717800
 H                -2.97310900   -5.32907500   -0.48744000
 H                -3.47448700   -4.81901200   -2.12244500
 H                -2.01854600   -5.80871900   -1.90345000
 C                -6.96625200   -0.90851800   -0.24797300
 H                -8.01321100   -1.02852100    0.07417300
 H                -6.70095500    0.15261200   -0.12938600
 H                -6.90724600   -1.15081200   -1.32034900
 C                -6.13900600   -1.44930900    2.05991700
 H                -5.84081300   -0.40545000    2.23826100
 H                -7.17289500   -1.56962500    2.42189700
 H                -5.48507800   -2.09247100    2.66893000
 C                -6.52757500   -3.26630800    0.40673200
 H                -6.50605900   -3.58713000   -0.64620000
 H                -5.91962200   -3.97177300    0.99380500
 H                -7.56722300   -3.35310700    0.75804500
 C                 4.86673300   -3.03182900   -1.48911100
 C                 1.84569900   -3.02876900    2.66881800
 C                 6.28852100   -2.45125900   -1.45664300
 H                 6.92701300   -2.95949500   -2.19686600
 H                 6.29931400   -1.37658300   -1.69085000
 H                 6.74437400   -2.58298600   -0.46307300
 C                 2.68787900   -2.69353000    3.91189800
 H                 2.70785000   -1.60888400    4.09750200
 H                 2.27177500   -3.18662300    4.80548900
 H                 3.72783500   -3.03175400    3.78488000
 C                 1.82499800   -4.54922100    2.48765100
 H                 2.83957200   -4.97320800    2.44764100
 H                 1.31125100   -5.01922100    3.34008900
 H                 1.29451900   -4.84348600    1.56996900
 C                 0.40671700   -2.54239600    2.89665400
 H                 0.36054800   -1.47157800    3.14123200
 H                -0.22594700   -2.71121200    2.01239900
 H                -0.04682600   -3.08534500    3.74044700
 C                 4.25627700   -2.83083800   -2.88567500
 H                 3.22957500   -3.22658400   -2.92414300
 H                 4.21128900   -1.76706300   -3.16201800
 H                 4.85805100   -3.35234700   -3.64745600
 C                 4.95400400   -4.53451800   -1.21406500
 H                 5.59570900   -5.01359300   -1.96924800
 H                 5.39037000   -4.74556900   -0.22547700
 H                 3.96656400   -5.01848300   -1.26604900
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4.4.6 [RAl]-II TS

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0 1
 C                -1.34961000    1.36185600    0.35106100
 N                -0.08392000    0.79415000    0.33959000
 C                -2.39363500    3.56849700    0.27653700
 C                -1.25431200    2.77154500    0.19815500
 C                 0.14807000    3.05858500   -0.00820400
 C                 0.87293300    4.21823200   -0.30317000
 C                 2.25133300    4.14886800   -0.51208700
 C                 2.88340300    2.88902400   -0.40461800
 C                 2.19888200    1.71947800   -0.08520600
 C                 0.81185000    1.81735300    0.10190500
 C                -2.76017000   -0.73136200    0.25623400
 C                -3.98096000   -1.22667600   -0.22991200
 C                -4.16013500   -2.56639600   -0.56599600
 C                -3.04615400   -3.41929600   -0.47777700
 C                -1.81280900   -2.97487200   -0.01966100
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C	-1.65824300	-1.62209300	0.39592700
C	-3.64475900	2.98211500	0.50185000
C	-3.71513600	1.58265000	0.57078600
C	-2.60531800	0.72771100	0.45656200
H	-4.69010000	1.11801700	0.70929400
H	-2.29481700	4.65278500	0.18015200
H	0.34271400	5.16823900	-0.38037000
H	3.96242800	2.81276800	-0.56216800
H	-1.13219700	-1.66602300	1.78661500
H	-3.15664000	-4.45600500	-0.79960900
H	-4.79893800	-0.52723900	-0.39303300
C	2.86161000	0.39986400	0.03814400
C	3.35846200	-0.26367600	-1.08272500
C	2.95344200	-0.22016200	1.30104700
C	3.95761200	-1.52738800	-0.97784900
H	3.25951100	0.22593400	-2.05426500
C	3.58982300	-1.46161600	1.45173000
H	2.62656500	0.34495000	2.17523900
C	4.06474200	-2.09490200	0.29641400
H	4.54197000	-3.06915200	0.40273100
C	-5.49637700	-3.12106400	-1.06516600
C	-0.60478400	-3.91687700	0.02061500
C	0.66965300	-3.11535400	-0.27954900
H	1.00973800	-2.50963300	0.60794200
H	1.54116400	-3.77265200	-0.42757700
H	0.56761400	-2.46818800	-1.16250800
C	-0.49871900	-4.56592200	1.41045200
H	-0.41288800	-3.80889100	2.20522400
H	-1.39314700	-5.17231900	1.61790500
H	0.38452400	-5.22265700	1.46988600
C	-0.70530400	-5.02340200	-1.03633200
H	-1.53523700	-5.71525000	-0.83056900
H	-0.85025000	-4.60484500	-2.04428200
H	0.21824500	-5.62347500	-1.04102100
C	-6.59407300	-2.05515700	-1.09071000
H	-7.53910800	-2.50245100	-1.43520400
H	-6.77225700	-1.62894500	-0.09144000
H	-6.34938900	-1.23067300	-1.77780700
C	-5.31943900	-3.66752500	-2.49090200
H	-4.99065700	-2.87195400	-3.17719900
H	-4.57320200	-4.47495600	-2.53144400
H	-6.27202300	-4.07395000	-2.86739300
C	-5.94723000	-4.25551900	-0.13120100
H	-6.07973800	-3.88707800	0.89776900
H	-6.90749400	-4.67501100	-0.47216700
H	-5.21575700	-5.07679100	-0.10126200
C	-4.88441700	3.87367600	0.64472800
C	3.10111800	5.37874300	-0.85124500
C	-5.06297000	4.70884600	-0.63254600
H	-5.19694200	4.05785000	-1.51034400
H	-5.94814900	5.36026400	-0.54875800
H	-4.19258100	5.35364200	-0.82520100
C	-6.16261100	3.06152600	0.86605900
H	-7.02261800	3.74122700	0.96873100
H	-6.37242500	2.38885100	0.01988700
H	-6.10831000	2.45503000	1.78324100
C	-4.69683800	4.81054500	1.84822700
H	-4.56826700	4.23336300	2.77692500
H	-3.81133500	5.45282200	1.72980100
H	-5.57369300	5.46740600	1.96972300
C	2.25843700	6.65296400	-0.93720500
H	1.48851600	6.58111700	-1.72079600
H	1.75824800	6.87659700	0.01762300
H	2.90287900	7.51122000	-1.18272500
C	3.78947800	5.16626300	-2.20866500
H	4.40737600	6.04063100	-2.47060100
H	4.44748600	4.28439300	-2.20046300
H	3.04452800	5.02077900	-3.00626800

C	4.16626800	5.58001100	0.23806900
H	3.69538700	5.73536500	1.22109100
H	4.83496100	4.71026800	0.32194000
H	4.78978000	6.46053400	0.01241100
C	4.47279000	-2.22583600	-2.23977700
C	3.77296600	-2.13222600	2.81673700
C	3.31350800	-2.40222800	-3.23337100
H	2.51623500	-3.02658800	-2.80151400
H	2.86642700	-1.43897500	-3.51969100
H	3.66923000	-2.89226600	-4.15374100
C	5.56931700	-1.35859800	-2.87807800
H	6.41096200	-1.21577200	-2.18286700
H	5.95601100	-1.83856700	-3.79137500
H	5.19200900	-0.36363500	-3.15714200
C	5.06033500	-3.60618400	-1.93918800
H	5.40834500	-4.07362200	-2.87287800
H	5.92312400	-3.54675600	-1.25818900
H	4.31323600	-4.27979000	-1.49083700
C	3.22347500	-1.27152600	3.95621200
H	3.36615500	-1.79131800	4.91590500
H	3.74240000	-0.30284700	4.02373800
H	2.14439900	-1.08492700	3.83474000
C	3.02550300	-3.47463400	2.82646400
H	3.38061300	-4.15041100	2.03339000
H	3.17032200	-3.98605400	3.79130200
H	1.94498400	-3.31752500	2.68769900
C	5.27066000	-2.37199400	3.06144600
H	5.42457400	-2.84300000	4.04544200
H	5.71227300	-3.03478000	2.30214900
H	5.82850100	-1.42293300	3.04517100
Al	0.13862900	-0.83080000	1.20666100

4.4.7 $[(RAlI_2)_2\{(^{Mes}BDI)Mg\}_2]$

0 1

I	6.13018700	-2.37529300	1.13543600
I	2.78921500	-1.15489000	-0.86321400
I	-2.64310700	0.70641900	-0.93315600
I	-5.22436900	-2.39065600	-1.72947400
Al	5.12788300	-0.35263900	0.00154500
Al	-4.93281100	-0.30945500	-0.32632100
Mg	1.37586400	0.13396700	1.34451800
Mg	-1.37036900	-0.17256400	1.54320500
N	6.16131900	0.35272900	-1.42151000
N	2.94904100	-0.07615100	2.77404400
N	2.36561100	1.92760400	0.75159500
N	-3.01852200	0.69055800	2.62354200
N	-2.43254700	-2.01686100	1.67141300
N	-6.35703800	0.94132900	-0.46079400
C	6.50386400	1.71508700	-1.47528000
C	7.19357400	2.53025100	-0.55346000
C	7.35849100	3.88337000	-0.90010800
C	6.86476300	4.47224300	-2.07110100
C	6.21604900	3.63736200	-2.98503800
C	6.06481400	2.28344900	-2.70364800
C	5.50615900	1.20546000	-3.48162200
C	4.89857100	1.16325900	-4.73492900
C	4.47711900	-0.05940500	-5.26315100
C	4.77096000	-1.22099800	-4.52876700
C	5.39672500	-1.21786300	-3.27566000
C	5.68370400	0.03623200	-2.70974400
C	7.74033200	2.09931400	0.75756000
C	8.45613800	0.90305900	0.92792900
C	9.03991200	0.58715500	2.15926500
C	8.82519500	1.45307500	3.24377400
C	8.10107300	2.63862100	3.12216900
C	7.58704400	2.94977700	1.86010200
C	9.95029000	-0.62771000	2.36402200

C	10.10877000	-1.43671900	1.07952300
C	9.36961300	-1.53799100	3.45650500
C	11.34159600	-0.13433400	2.79482500
C	7.89301200	3.61475300	4.28485800
C	8.36935200	3.03054200	5.61649000
C	8.69141800	4.89595100	3.99441800
C	6.40393500	3.96733600	4.42178700
C	7.01313200	5.96691800	-2.37040700
C	7.75725000	6.70989500	-1.25870500
C	7.78954500	6.15678900	-3.68202100
C	5.61167000	6.58330900	-2.50715300
C	3.74244800	-0.09955500	-6.60738200
C	4.59741900	0.57269200	-7.69158900
C	3.43477200	-1.52953500	-7.05704100
C	2.41052400	0.65276200	-6.45947600
C	5.82499900	-2.51392300	-2.69080400
C	4.91441000	-3.54662700	-2.47848000
C	5.32618100	-4.79819400	-2.00294900
C	6.69198200	-5.00109500	-1.81496900
C	7.64625400	-3.99983200	-2.05887900
C	7.19111000	-2.74740500	-2.46510200
C	4.27484000	-5.86108500	-1.67534900
C	3.41480500	-5.34759700	-0.51058700
C	3.38305200	-6.11072600	-2.90045000
C	4.90581500	-7.19154200	-1.26037900
C	9.13208500	-4.33370300	-1.89461700
C	10.02551600	-3.12761900	-2.18895100
C	9.39536500	-4.81047100	-0.45796100
C	9.50350100	-5.45441600	-2.87886400
C	4.15576200	0.35928000	2.60882900
C	5.22958200	0.16238100	3.63666900
C	4.55694900	1.10981900	1.39341100
C	3.63429500	2.14001900	0.83745800
C	4.22643900	3.44679400	0.40682500
C	2.50760000	-0.67492700	3.98402800
C	2.14425600	-2.04017100	3.95929400
C	1.60918300	-2.60972200	5.11305400
C	1.40449300	-1.87135400	6.28384900
C	1.76333600	-0.52550000	6.27391200
C	2.30705000	0.09693700	5.14338700
C	2.30223800	-2.85220300	2.71105600
C	0.77794100	-2.50936700	7.49037500
C	2.63095700	1.56295900	5.20786800
C	1.44623600	2.86456400	0.20788400
C	1.35475700	3.09066000	-1.17726100
C	0.29587000	3.88144300	-1.64438400
C	-0.65194500	4.44606000	-0.79427100
C	-0.49934700	4.24564600	0.58227000
C	0.53332500	3.46918400	1.10009100
C	2.35066900	2.54463400	-2.15855100
C	-1.81552700	5.22944100	-1.32497000
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