Supporting Information

Synthesis, structural studies and ligand influence on the stability of Aryl-NHC stabilized trimethylaluminium complexes.

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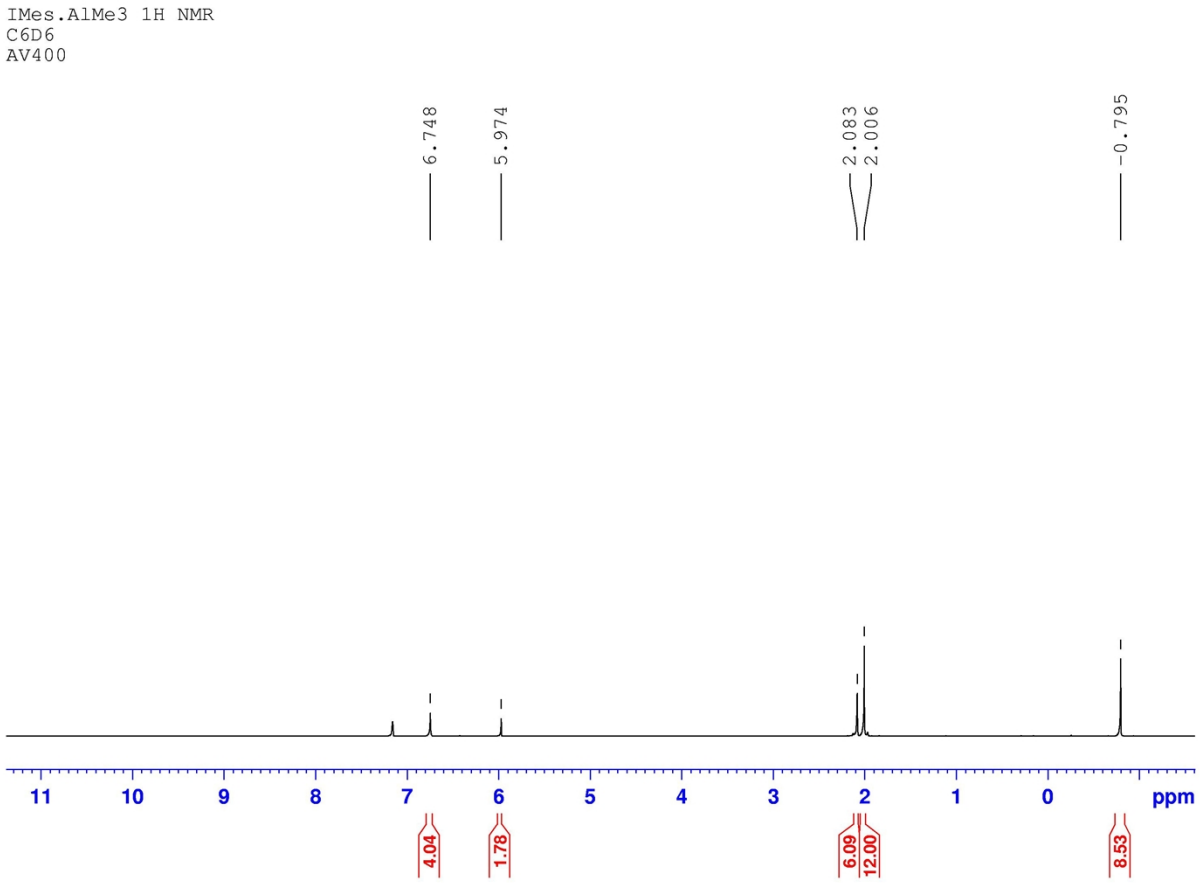
Contents

^{1}H and ^{13}C NMR of 1-4



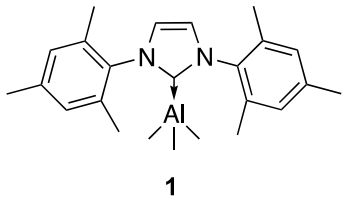


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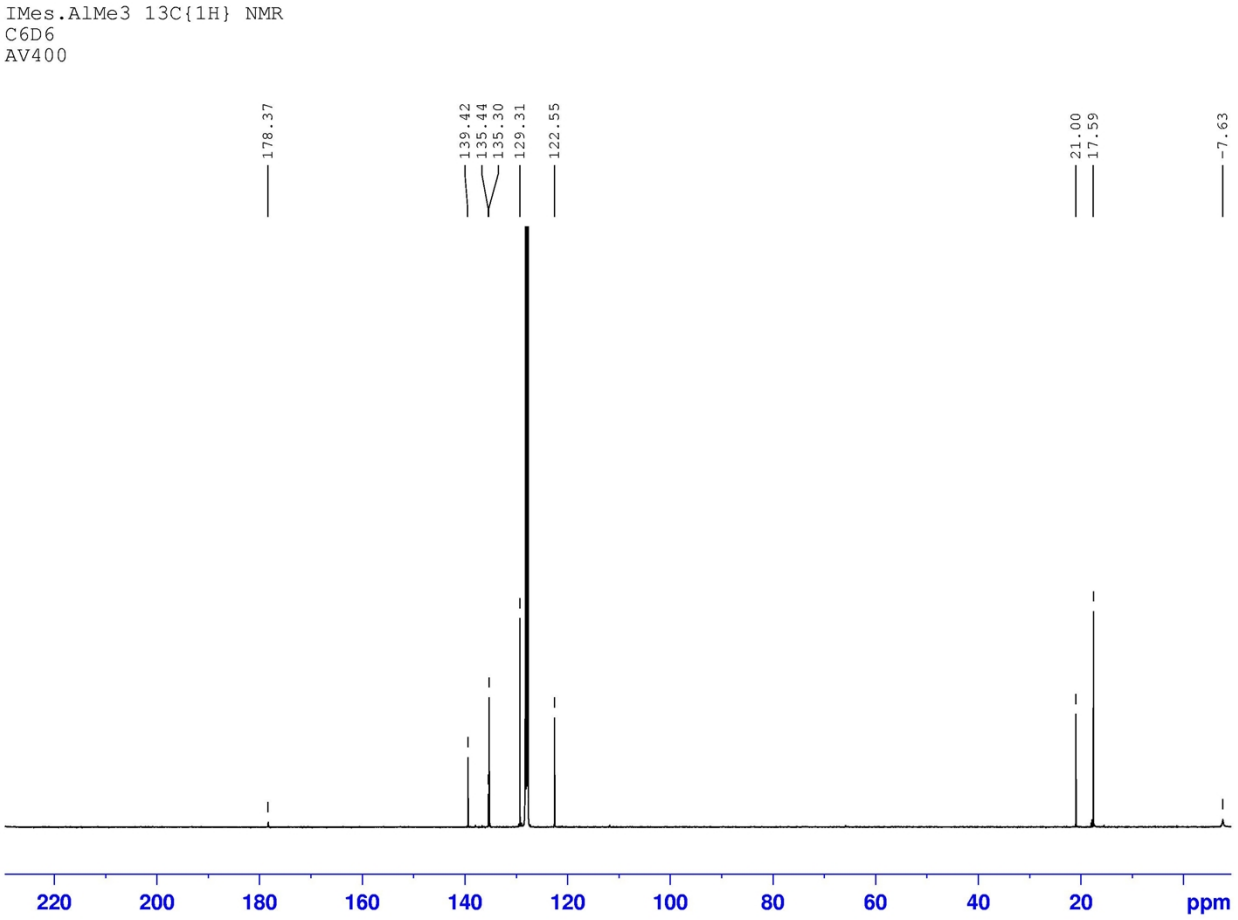
Figure S1. IMes•$AlMe_3$ (1) ^{1}H NMR spectrum.



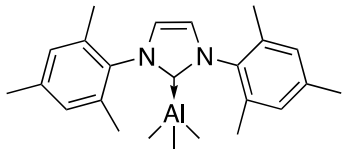


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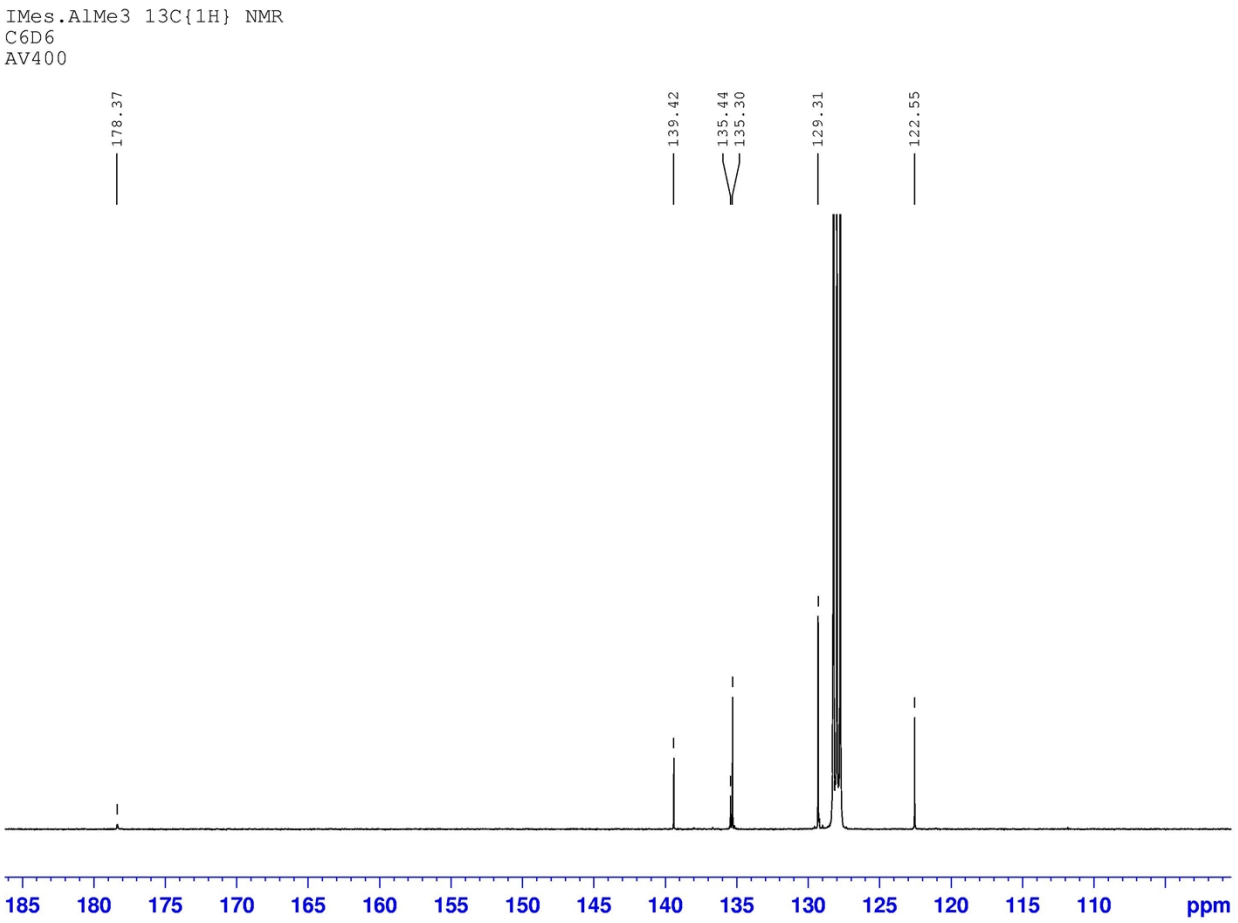
Figure S2. IMes•$AlMe_3$ (1) $^{13}C\{^1H\}$ NMR spectrum.



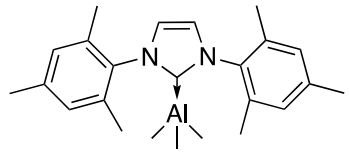


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Figure S3. IMes•$AlMe_3$ (1) $^{13}C\{^1H\}$ NMR spectrum (expanded).

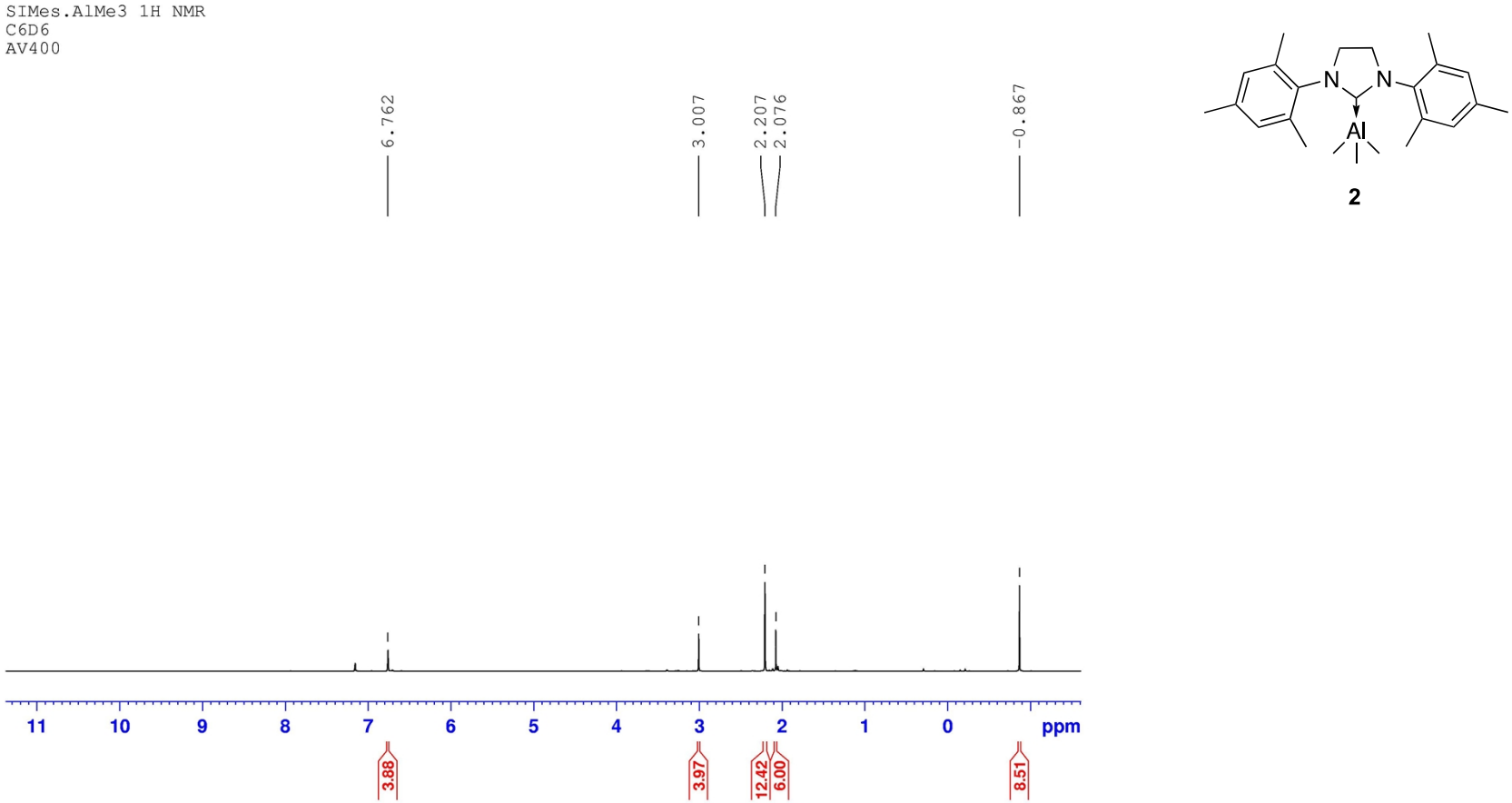


Figure S4. SIMes•$AlMe_3$ (2) ^1H NMR spectrum.

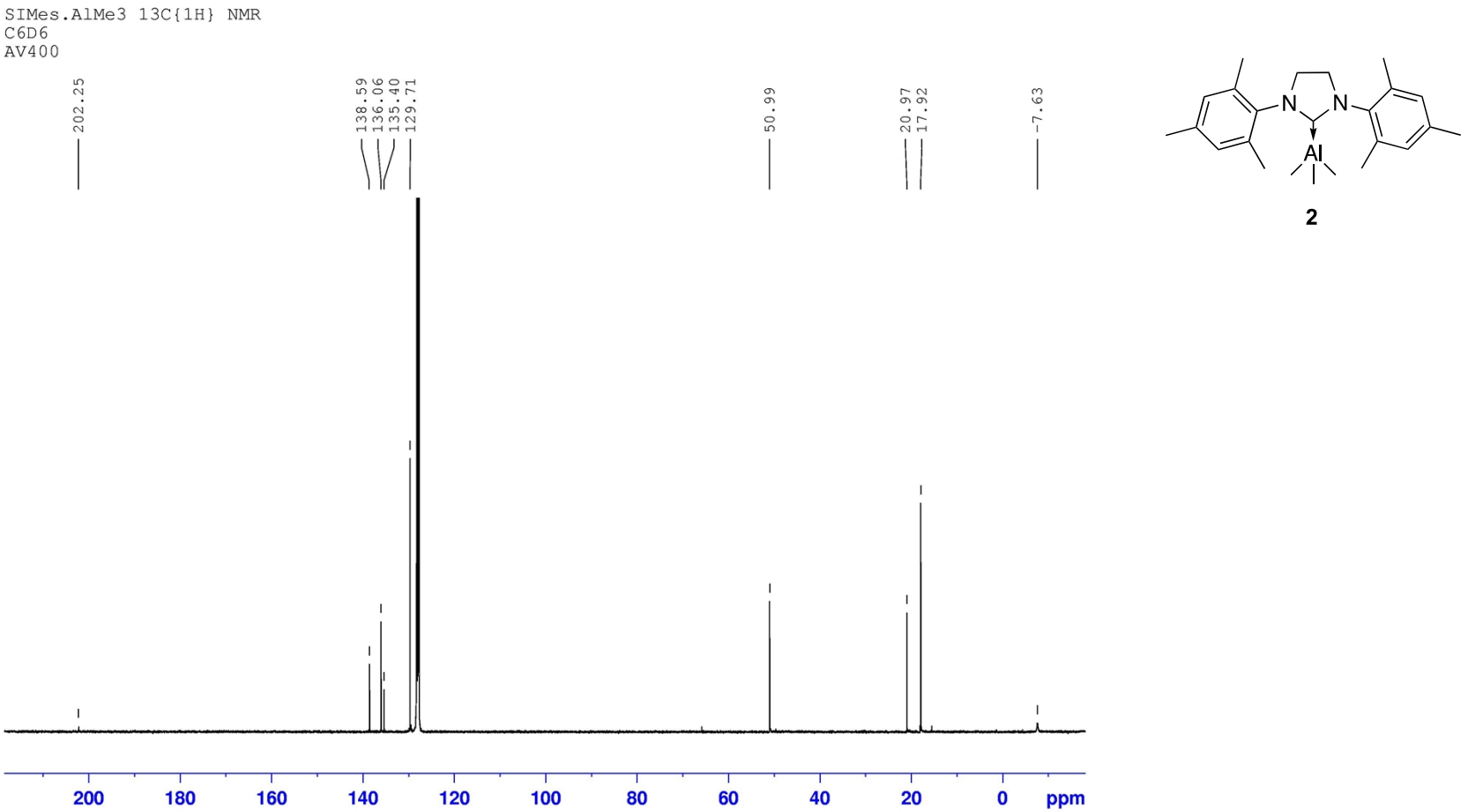
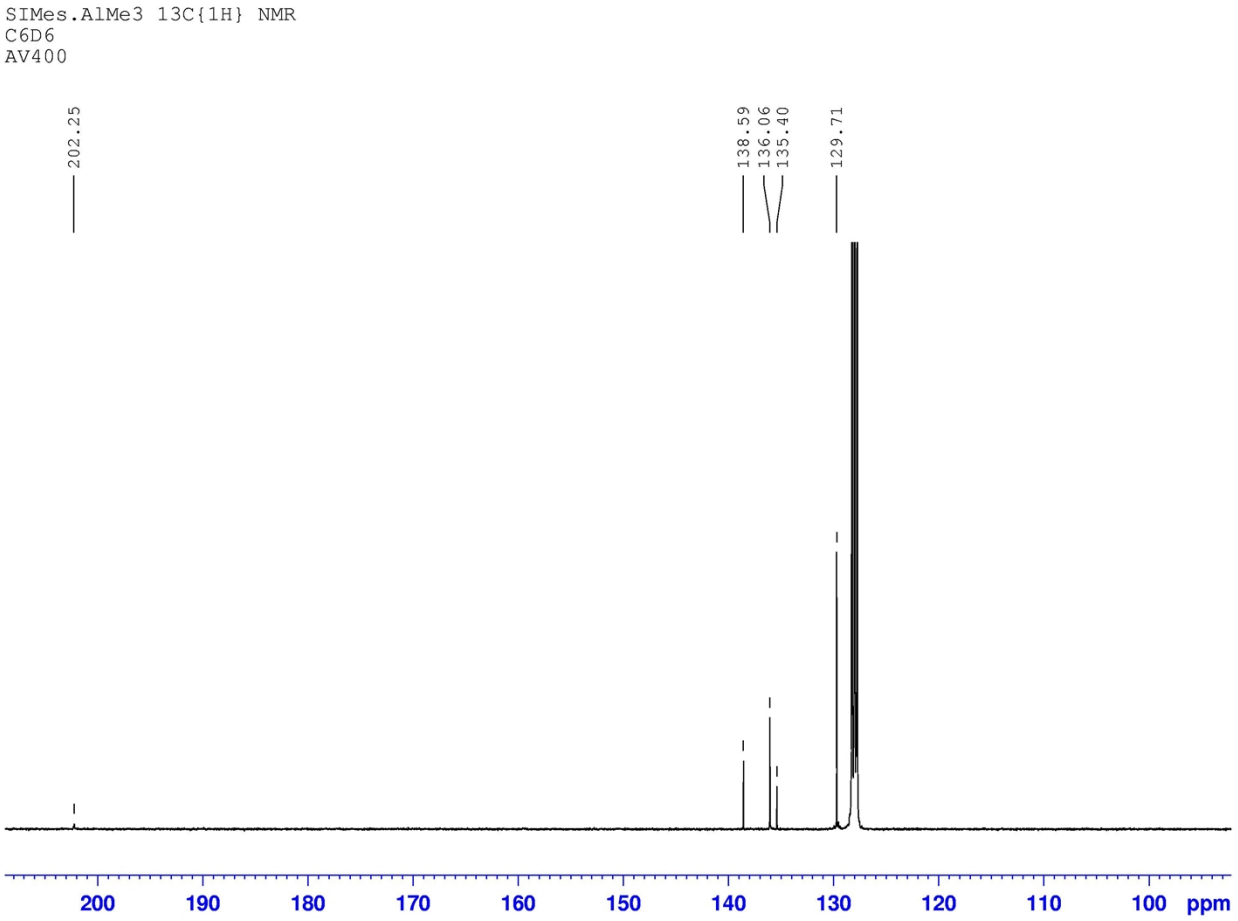
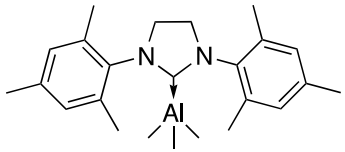


Figure S5. SIMes•$AlMe_3$ (2) $^{13}C\{^1H\}$ NMR spectrum.





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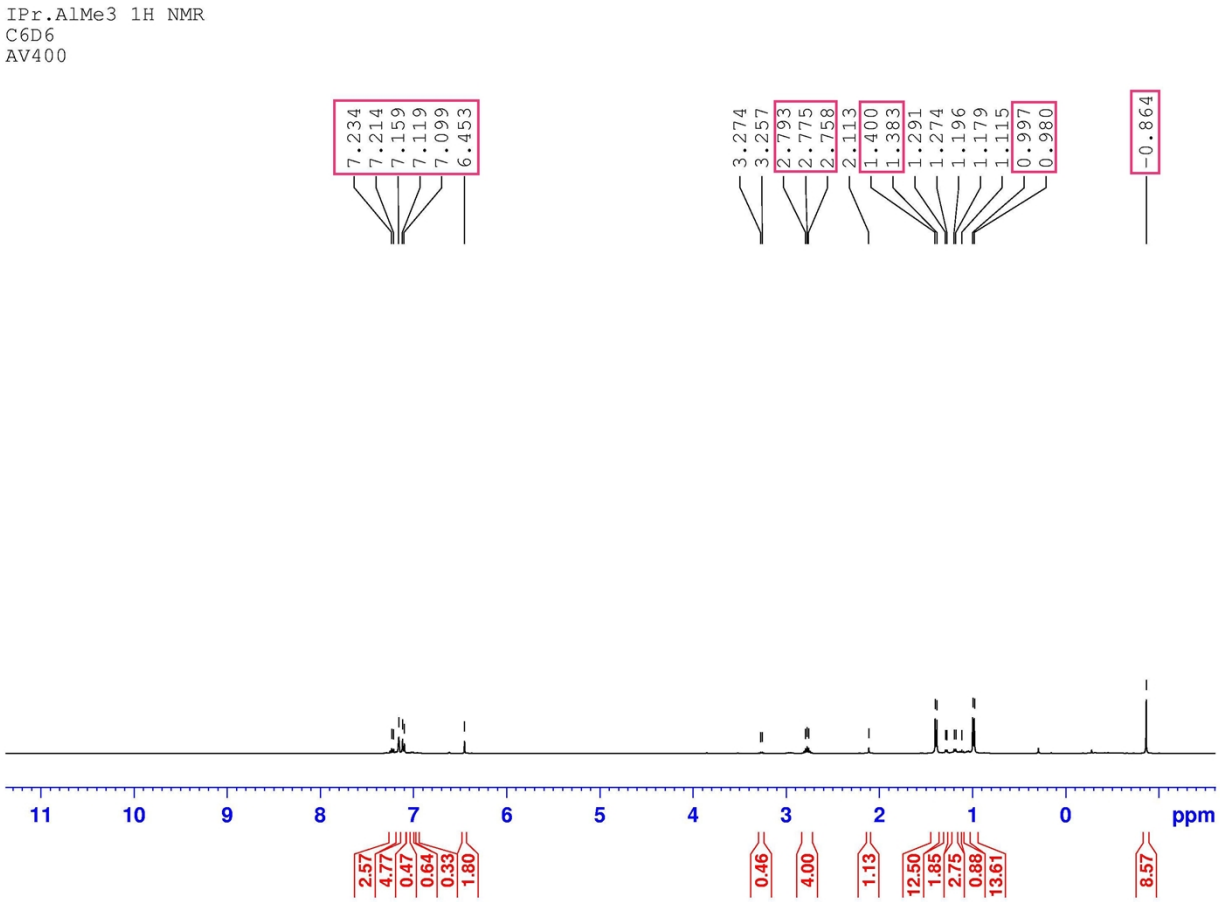
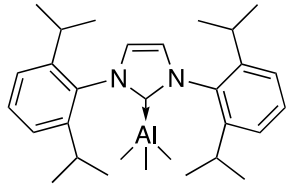




3

Red – Compound

- 7.21-7.24 (m, 2H, *p*-C_6H_3)
- 7.10-7.12 (m, 4H, *m*-C_6H_3)
- 6.45 (s, 4H, NCH_2)
- 2.76-2.79 (p, 4H, $J_{H\text{-}H}$ = 6.8 Hz, $CH(CH_3)_2$)
- 1.38-1.40 (d, 12H, $J_{H\text{-}H}$ = 6.8 Hz, $CH(CH_3)_2$)
- 0.98-1.00 (d, 12H, $J_{H\text{-}H}$ = 6.8 Hz, $CH(CH_3)_2$)
- -0.86 (s, 9H, $AlCH_3$)

Other

- IPr - 2.97 – 3.01 & 1.18 -1.29
- Ether – 1.12 & 3.26 – 3.27
- Toluene – 2.11

Figure S7. IPr•$AlMe_3$ (3) ^{1}H NMR spectrum.

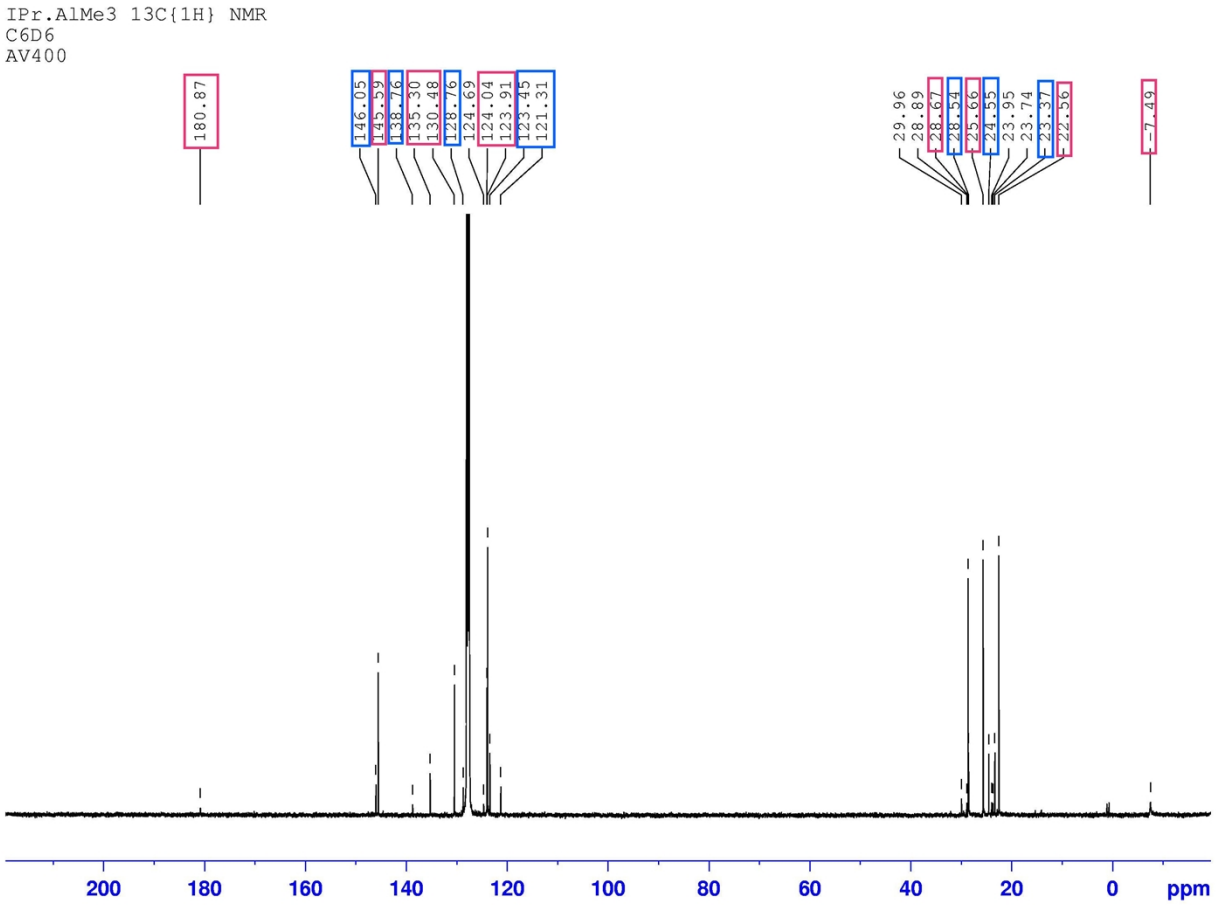
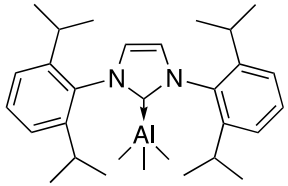


Figure S8. IPr•AlMe$_3$ (3) $^{13}C\{^1H\}$ NMR spectrum.



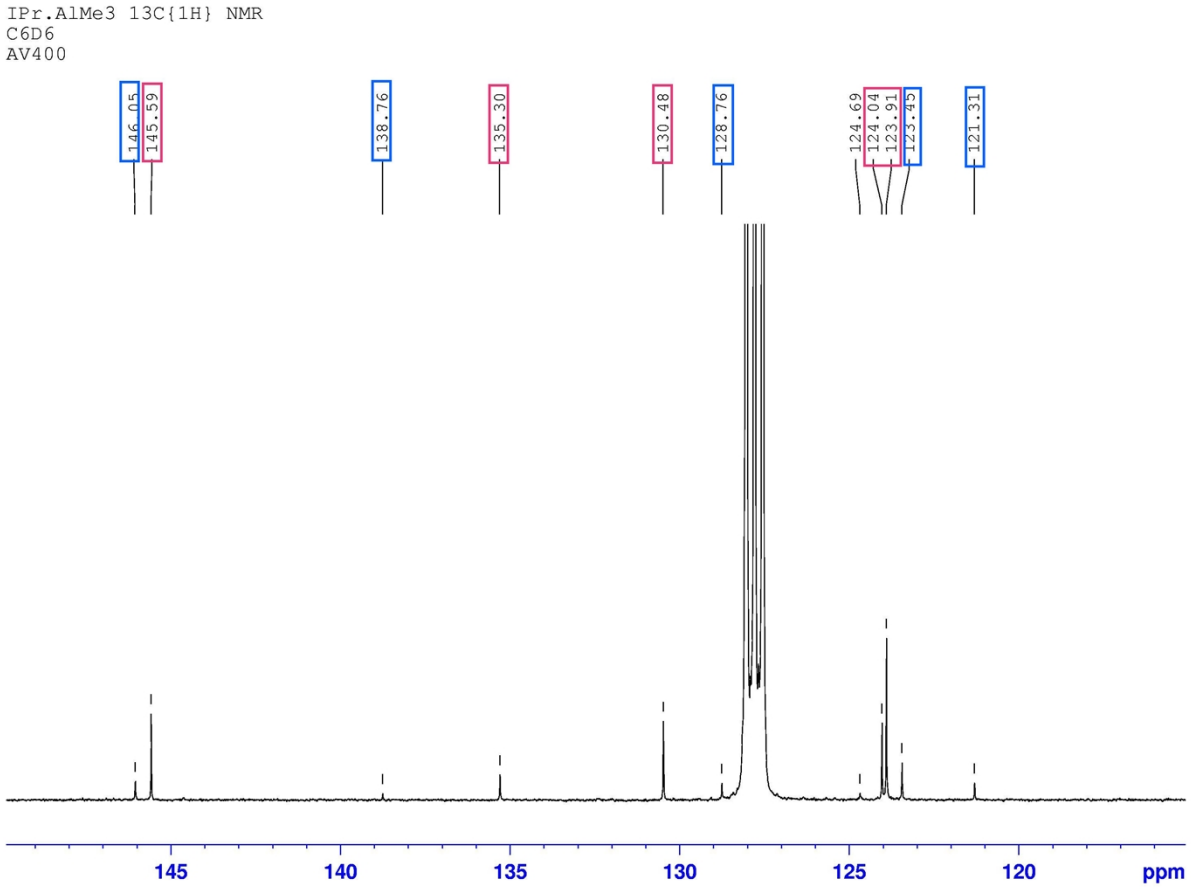
3

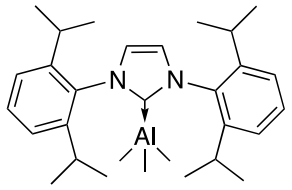
Red – Compound

- 181.1 ($C_{carbene}$, weak)
- 145.8 (*Ar*)
- 135.3 (*Ar*)
- 130.5 (*Ar*)
- 124.0 (N*C*H)
- 123.9 (*Ar*)
- 28.7 (*C*H(CH$_3$)$_2$)
- 25.7 (CH(*C*H$_3$)$_2$)
- 22.6 (CH(*C*H$_3$)$_2$)
- -7.5 (Al*Me*$_3$, broad)

IPr – 146, 138.8, 128.8, 123.5, 121.3, 28.5, 24.6, 23.4

Unknown – 124.7, 30.0, 28.9, 24.0, 23.8





3

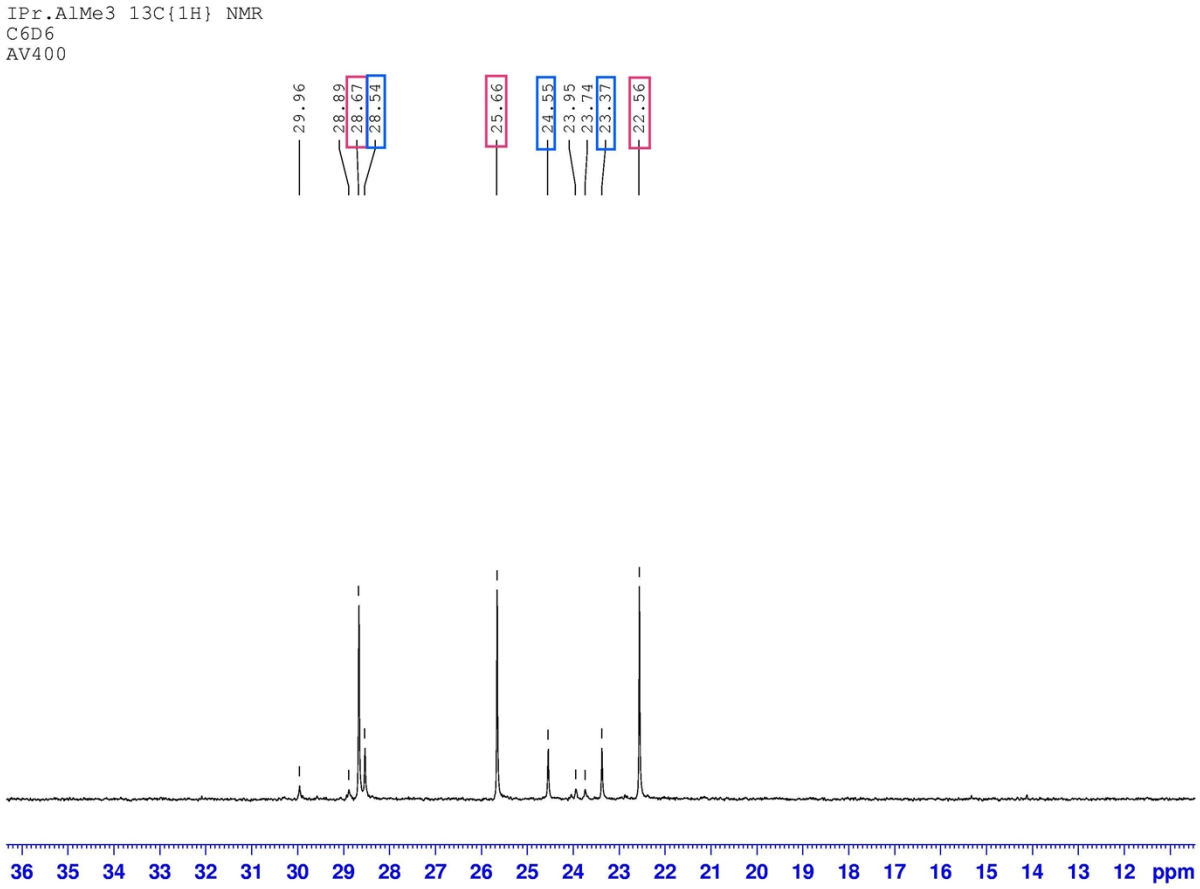
Red – Compound

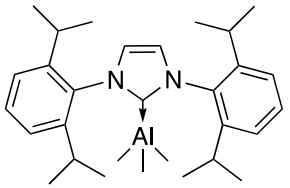
- 145.6 (*Ar*)
- 135.3 (*Ar*)
- 130.5 (*Ar*)
- 124.0 (N*C*H)
- 123.9 (*Ar*)

IPr – 146, 138.8, 128.8, 123.5, 121.3

Unknown – 124.7

Figure S9. IPr•AlMe$_3$ (3) $^{13}C\{^1H\}$ NMR spectrum (expanded spectrum).





3

Red – Compound

- 28.7 ($\mathit{C}H(CH_3)_2$)
- 25.7 ($CH(\mathit{C}H_3)_2$)
- 22.6 ($CH(\mathit{C}H_3)_2$)

IPr – 28.5, 24.6, 23.4

Unknown – 30.0, 28.9, 24.0, 23.8

Figure S10. IPr•$AlMe_3$ (3) $^{13}C\{^1H\}$ NMR spectrum (expanded spectrum)

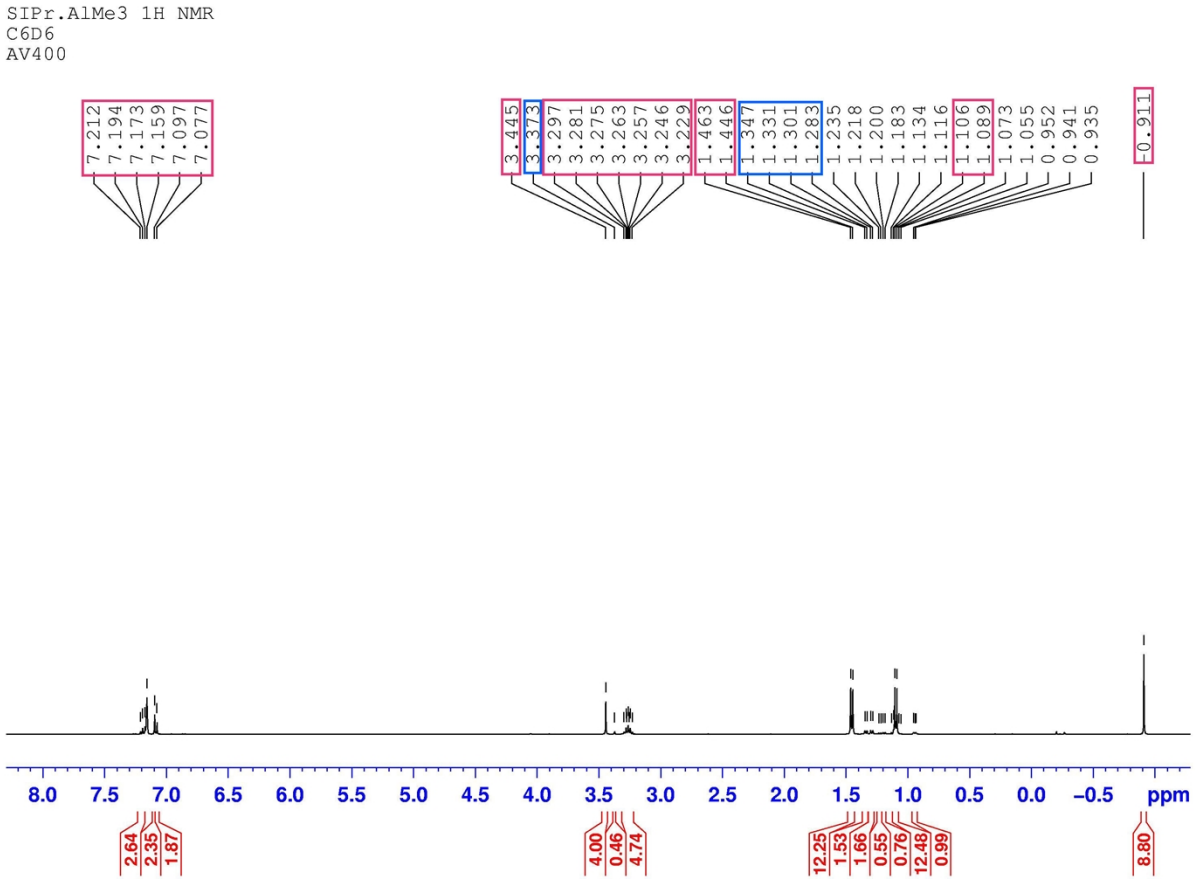
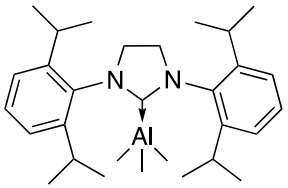


Figure S11. SIPr•AlMe$_3$ (4) ^{1}H NMR spectrum.



4

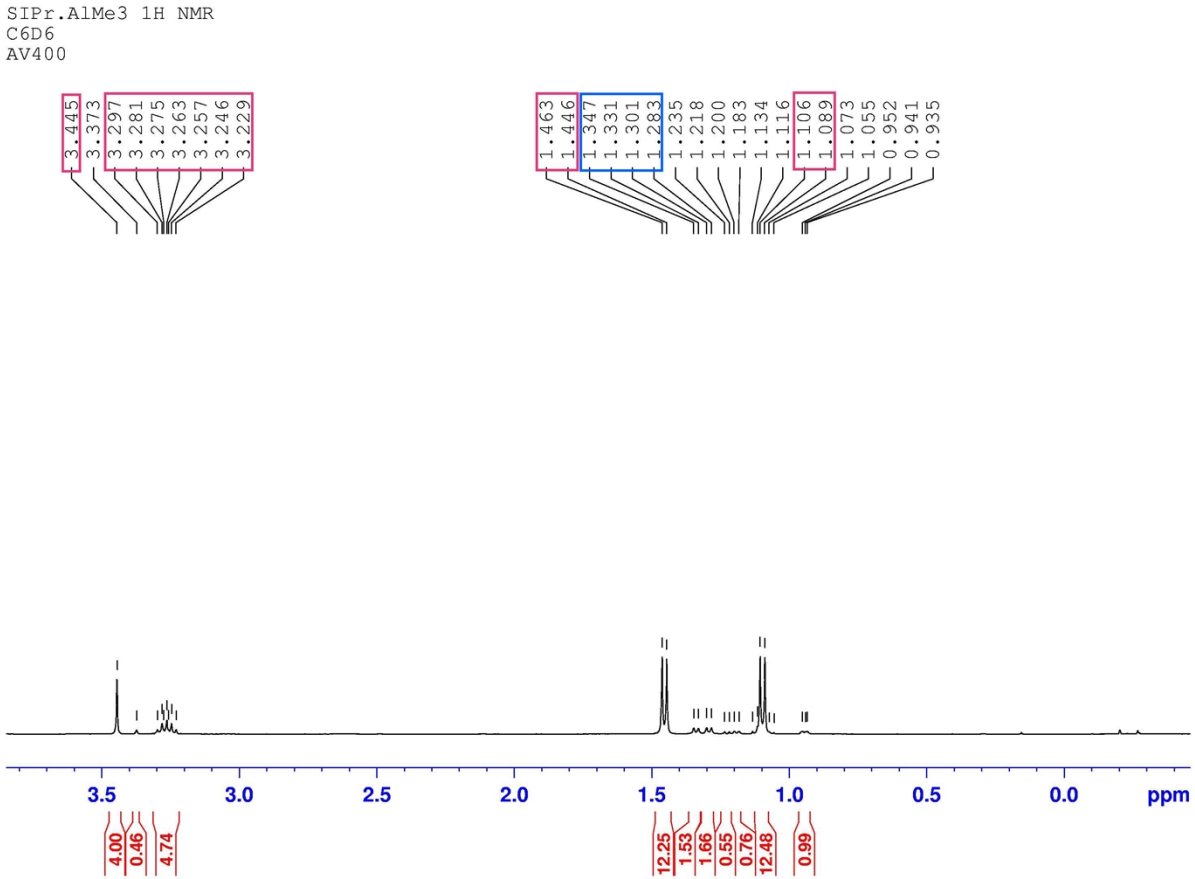
Red – Compound

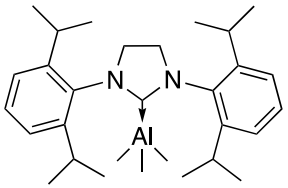
- 7.19-7.21 (m, 2H, *p*-C_6H_3)
- 7.16-7.17 (m, 2H, *m*-C_6H_3)
- 7.08-7.10 (m, 2H, *m*-C_6H_3)
- 3.45 (s, 4H, NCH_2)
- 3.23-3.30 (p, 4H, $J_{H\text{-}H}$ = 6.8 Hz, $CH(CH_3)_2$)
- 1.45-1.46 (d, 12H, $J_{H\text{-}H}$ = 6.8 Hz, $CH(CH_3)_2$)
- 1.09-1.11 (d, 12H, $J_{H\text{-}H}$ = 6.8 Hz, $CH(CH_3)_2$)
- -0.91 (s, 9H, $AlCH_3$)

Other

- SIPr 3.37, 1.28 – 1.34

Rest unknown species





4

Red – Compound

- 3.45 (s, 4H, NCH_2)
- 3.23-3.30 (p, 4H, $J_{H\text{-}H}$ = 6.8 Hz, $CH(CH_3)_2$)
- 1.45-1.46 (d, 12H, $J_{H\text{-}H}$ = 6.8 Hz, $CH(CH_3)_2$)
- 1.09-1.11 (d, 12H, $J_{H\text{-}H}$ = 6.8 Hz, $CH(CH_3)_2$)

Other

- SIPr 3.37, 1.28 – 1.34

Rest unknown species

Figure S12. SIPr•$AlMe_3$ (4) ^{1}H NMR spectrum (expanded spectrum)

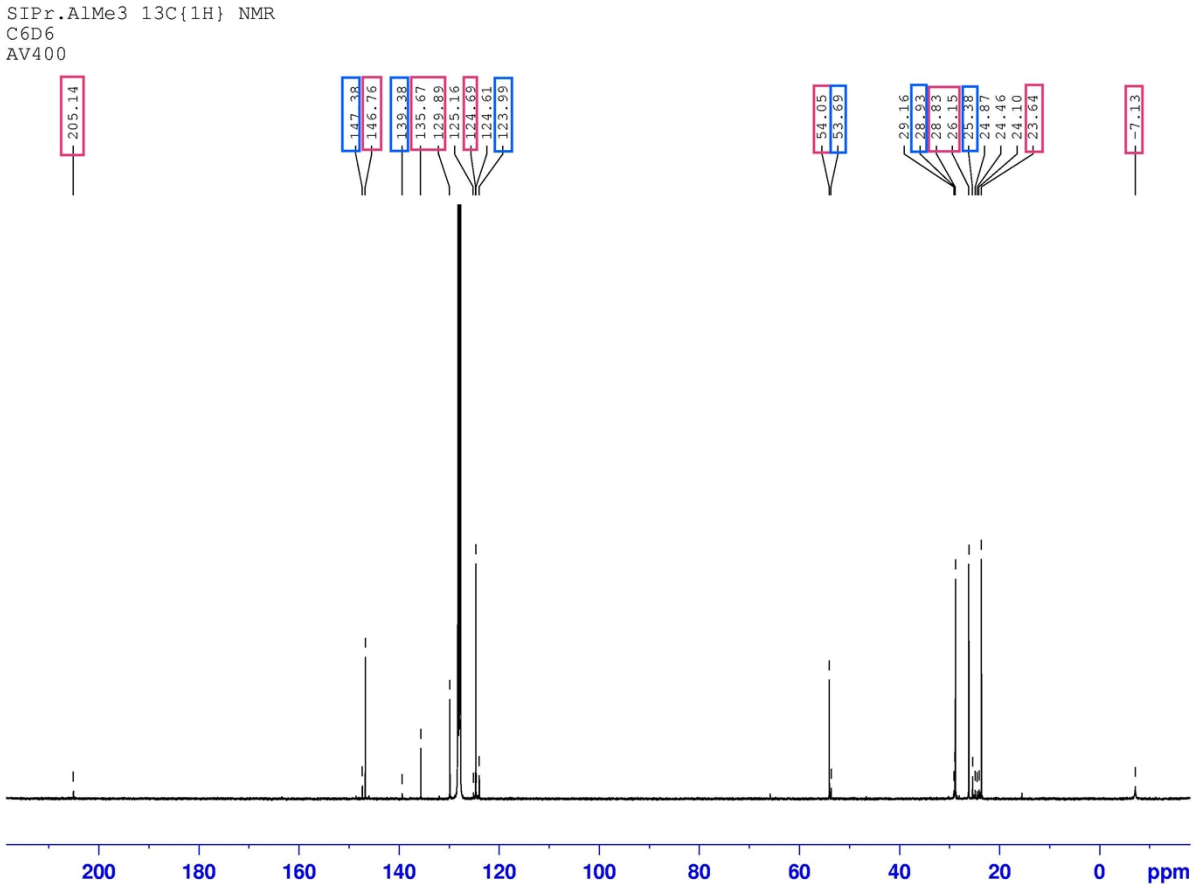
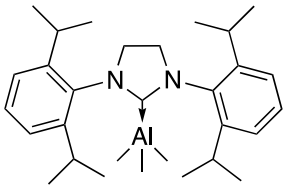


Figure S13. SIPr•AlMe$_3$ (4) $^{13}C\{^1H\}$ NMR spectrum



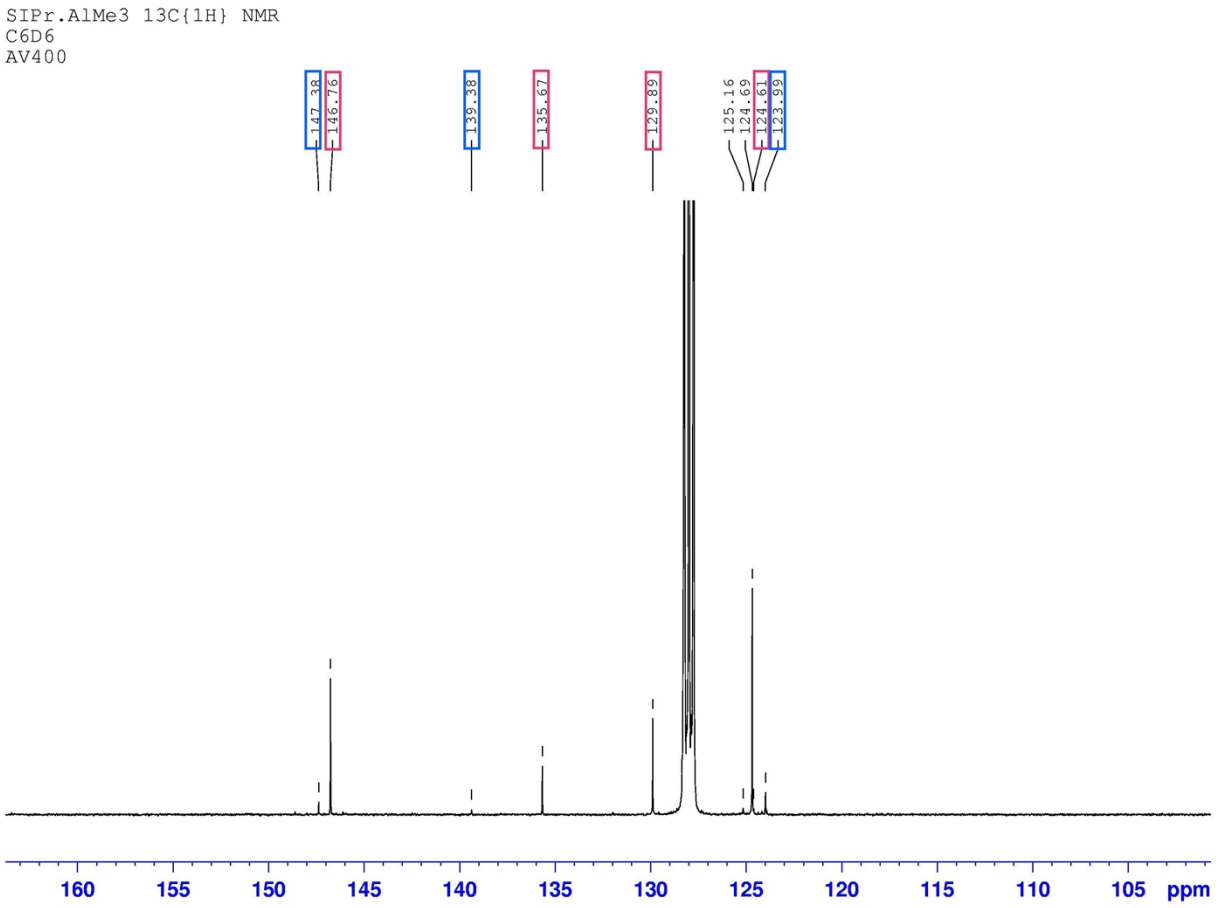
4

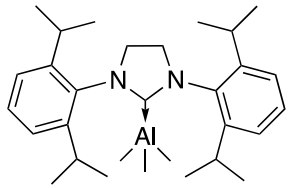
Red – Compound

- 205.1 ($C_{carbene}$, weak)
- 146.8 (*Ar*)
- 135.7 (*Ar*)
- 129.9 (*Ar*)
- 124.7 (Ar)
- 54.1 (N*C*H)
- 28.8 (*C*H(CH$_3$)$_2$)
- 26.2 (CH(*C*H$_3$)$_2$)
- 23.6 (CH(*C*H$_3$)$_2$)
- -7.1 (Al*Me*$_3$, broad)

SIPr – 147.4, 139.4, 124.0, 53.7, 28.9, 25.4

Unknown – 125.2, 124.6, 29.2, 24.9, 24.5, 24.1



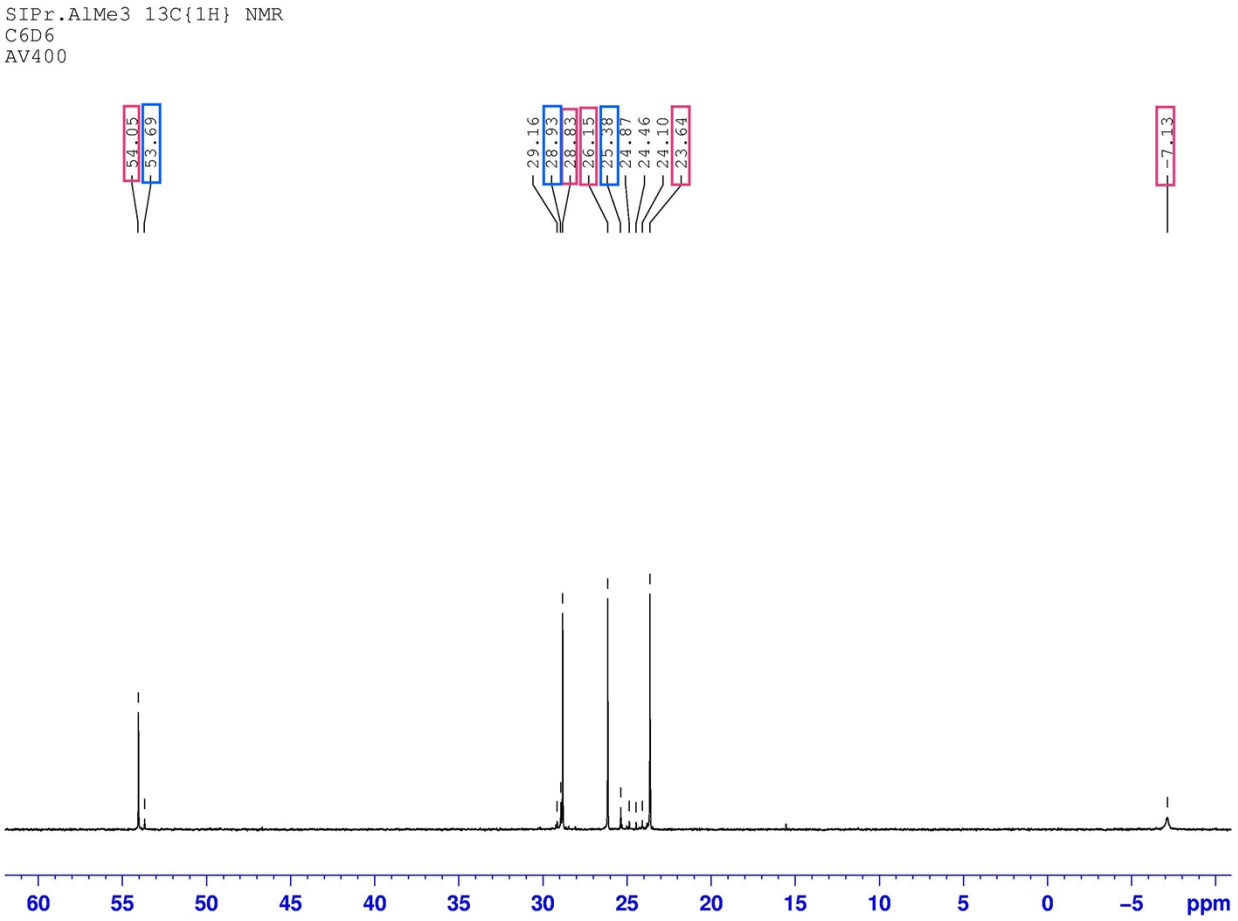


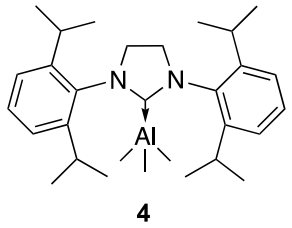
4

Red – Compound
- 146.8 (*Ar*)
- 135.7 (*Ar*)
- 129.9 (*Ar*)
- 124.7 (Ar)

SIPr – 147.4, 139.4, 124.0
Unknown – 125.2, 124.6

Figure S14. SIPr•$AlMe_3$ (4) $^{13}C\{^1H\}$ NMR spectrum (expanded)





4

Red – Compound

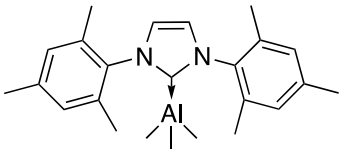
- 54.1 (N*C*H)
- 28.8 (*C*H(CH$_3$)$_2$)
- 26.2 (CH(*C*H$_3$)$_2$)
- 23.6 (CH(*C*H$_3$)$_2$)
- -7.1 (Al*Me*$_3$, broad)

SIPr –53.7, 28.9, 25.4

Unknown –29.2, 24.9, 24.5, 24.1

Figure S15. SIPr•AlMe$_3$ (4) ^{13}C{^{1}H} NMR spectrum (expanded)

High-resolution mass spectra for 1-4



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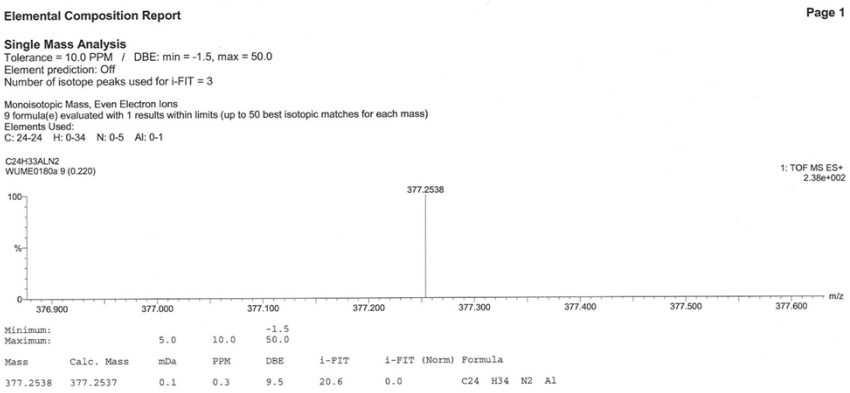


Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 24-24 H: 0-34 N: 0-5 Al: 0-1

C24H33ALN2
WUME0180a 9 (0.220)

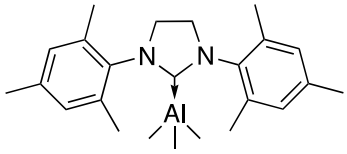
1: TOF MS ES+
2.38e+002

377.2538

100
%
0
376.900 377.000 377.100 377.200 377.300 377.400 377.500 377.600 m/z

Minimum:		5.0	10.0	-1.5			
Maximum:				50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
377.2538	377.2537	0.1	0.3	9.5	20.6	0.0	C24 H34 N2 Al

Figure S18. High resolution mass spectrum of IMes•$AlMe_3$ (1)



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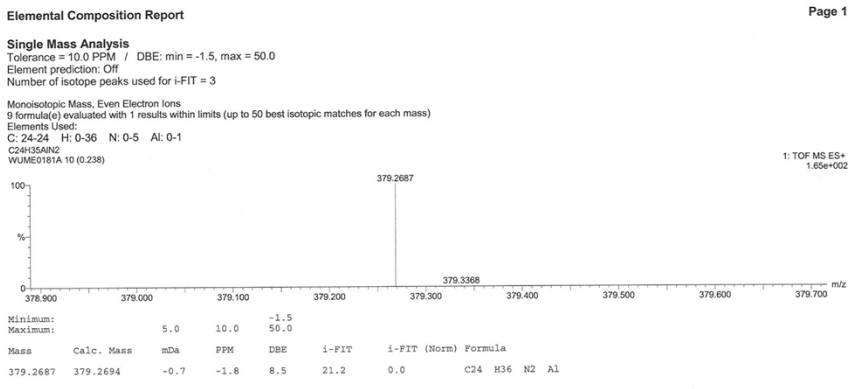


Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 24-24 H: 0-36 N: 0-5 Al: 0-1

C24H35AlN2
WUME0181A 10 (0.238)

1: TOF MS ES+
1.65e+002

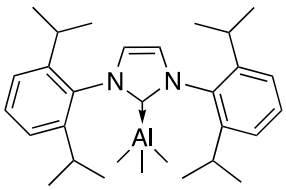
379.2687

379.3368

100
%
0
378.900 379.000 379.100 379.200 379.300 379.400 379.500 379.600 379.700 m/z

Minimum:		5.0	10.0	-1.5			
Maximum:				50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
379.2687	379.2694	-0.7	-1.8	8.5	21.2	0.0	C24 H36 N2 Al

Figure S19. High resolution mass spectrum of SIMes•$AlMe_3$ (2)



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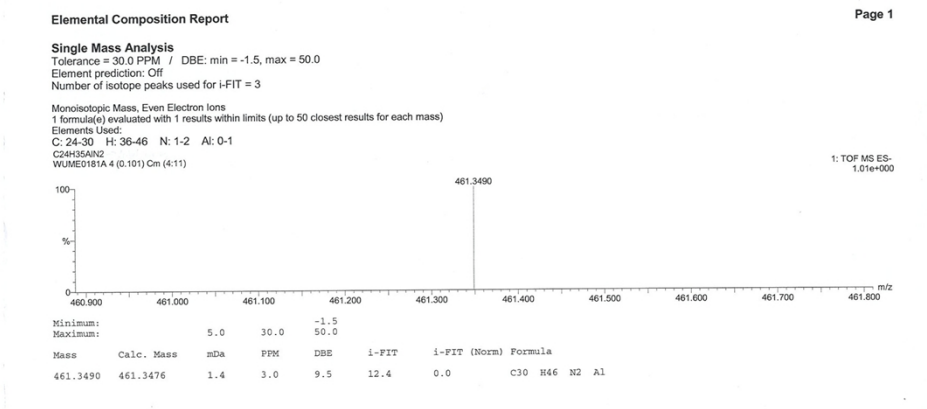

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 24-30 H: 36-46 N: 1-2 Al: 0-1

C24H35AlN2
WUME0181A 4 (0.101) Cm (4:11)

1: TOF MS ES-
1.01e+000

461.3490

100
%
0
460.900 461.000 461.100 461.200 461.300 461.400 461.500 461.600 461.700 461.800
m/z

Minimum:				-1.5			
Maximum:		5.0	30.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
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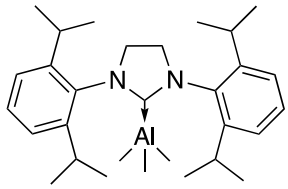
Figure S20. High resolution mass spectrum of Dipp•$AlMe_3$ (3)



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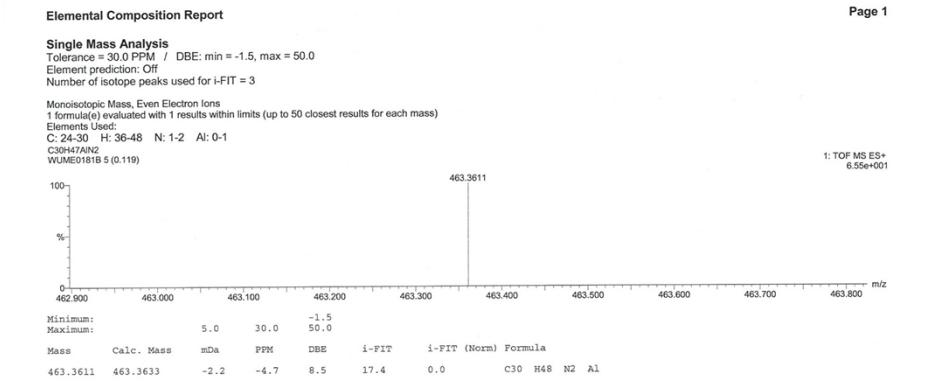


Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 24-30 H: 36-48 N: 1-2 Al: 0-1

C30H47AlN2
WUME0181B 5 (0.119)

1: TOF MS ES+
6.55e+001

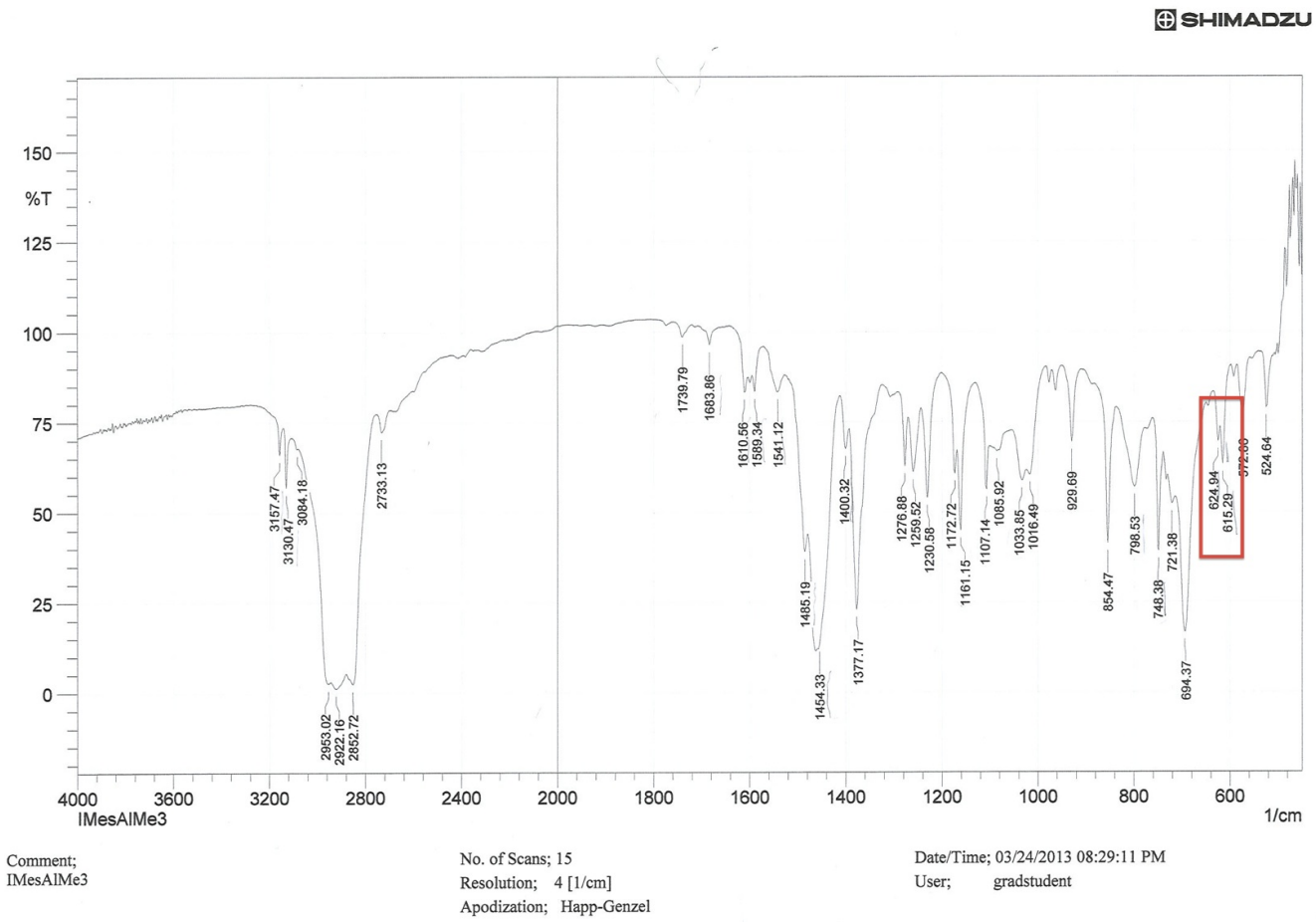
463.3611

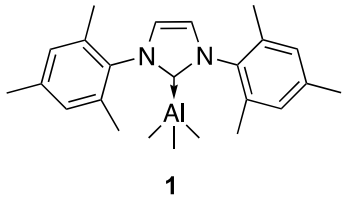
100
%
0
462.900 463.000 463.100 463.200 463.300 463.400 463.500 463.600 463.700 463.800
m/z

Minimum:				-1.5			
Maximum:		5.0	30.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
463.3611	463.3633	-2.2	-4.7	8.5	17.4	0.0	C30 H48 N2 Al

Figure S21. High resolution mass spectrum of SIPr•$AlMe_3$ (4)

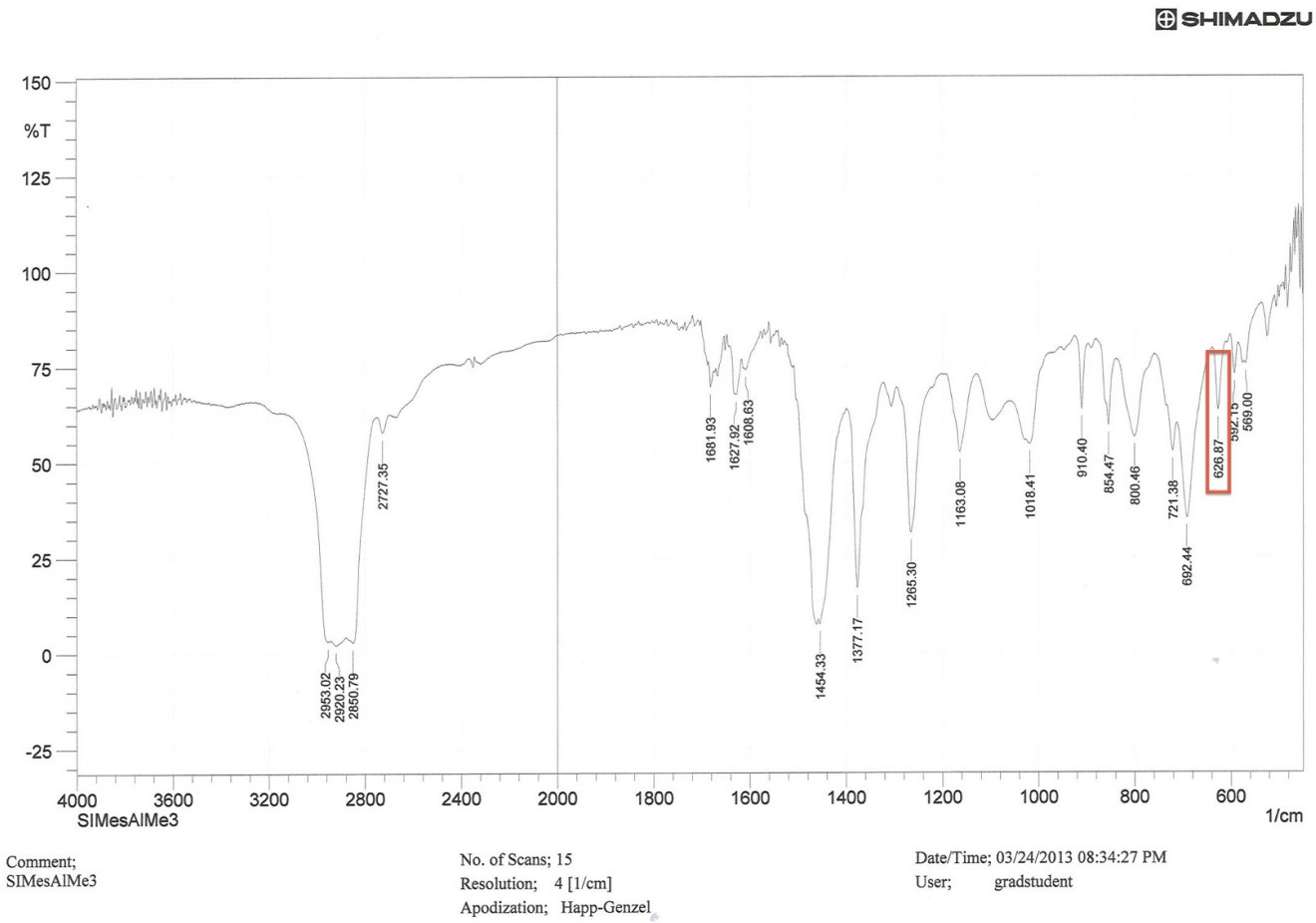
IR Spectra for 1-4

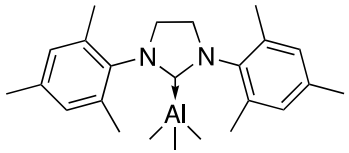




1

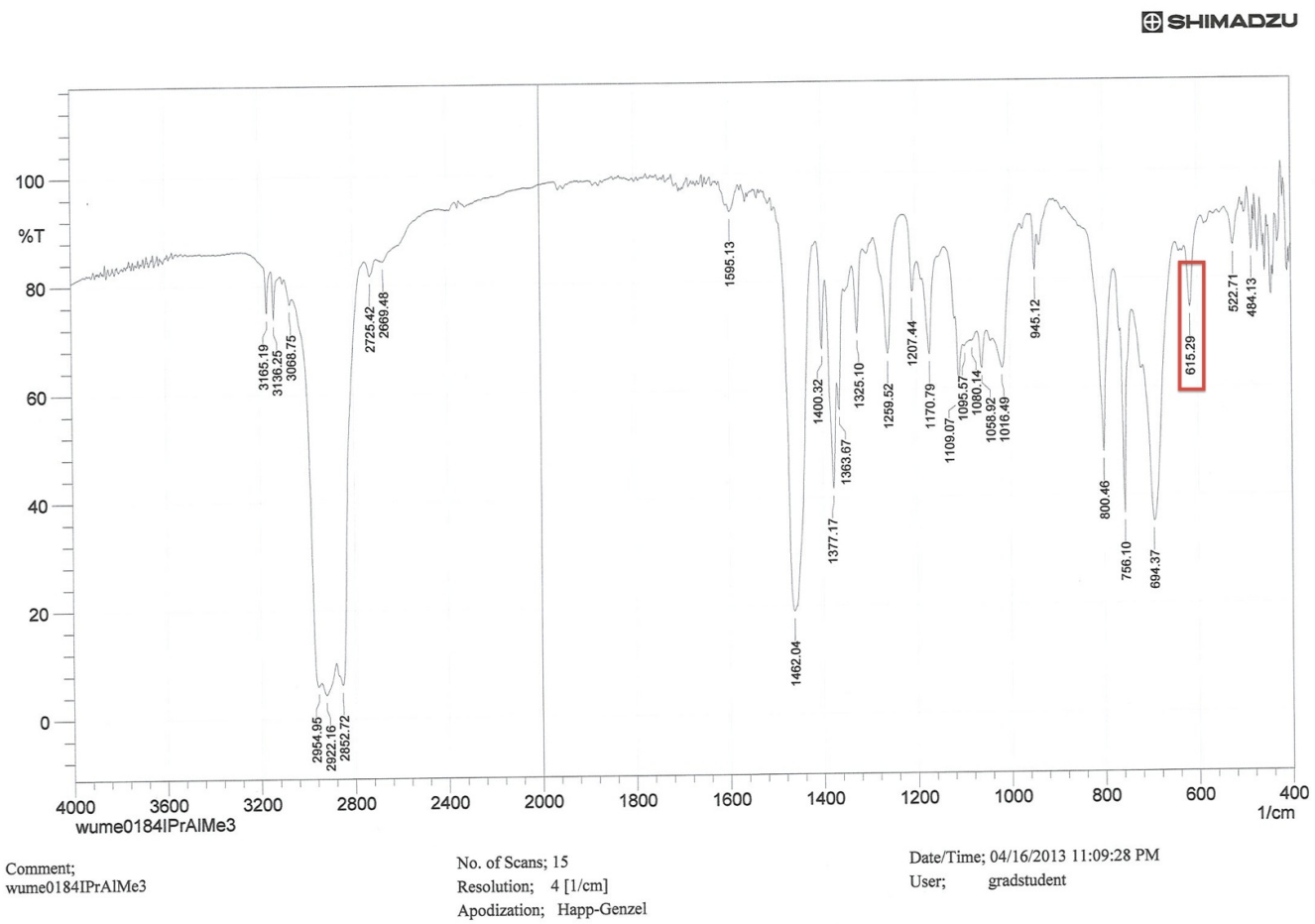
Figure S22. Infrared spectrum of IMes•$AlMe_3$ (1)

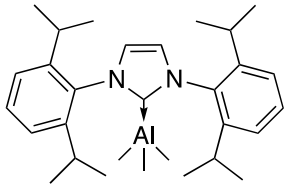




2

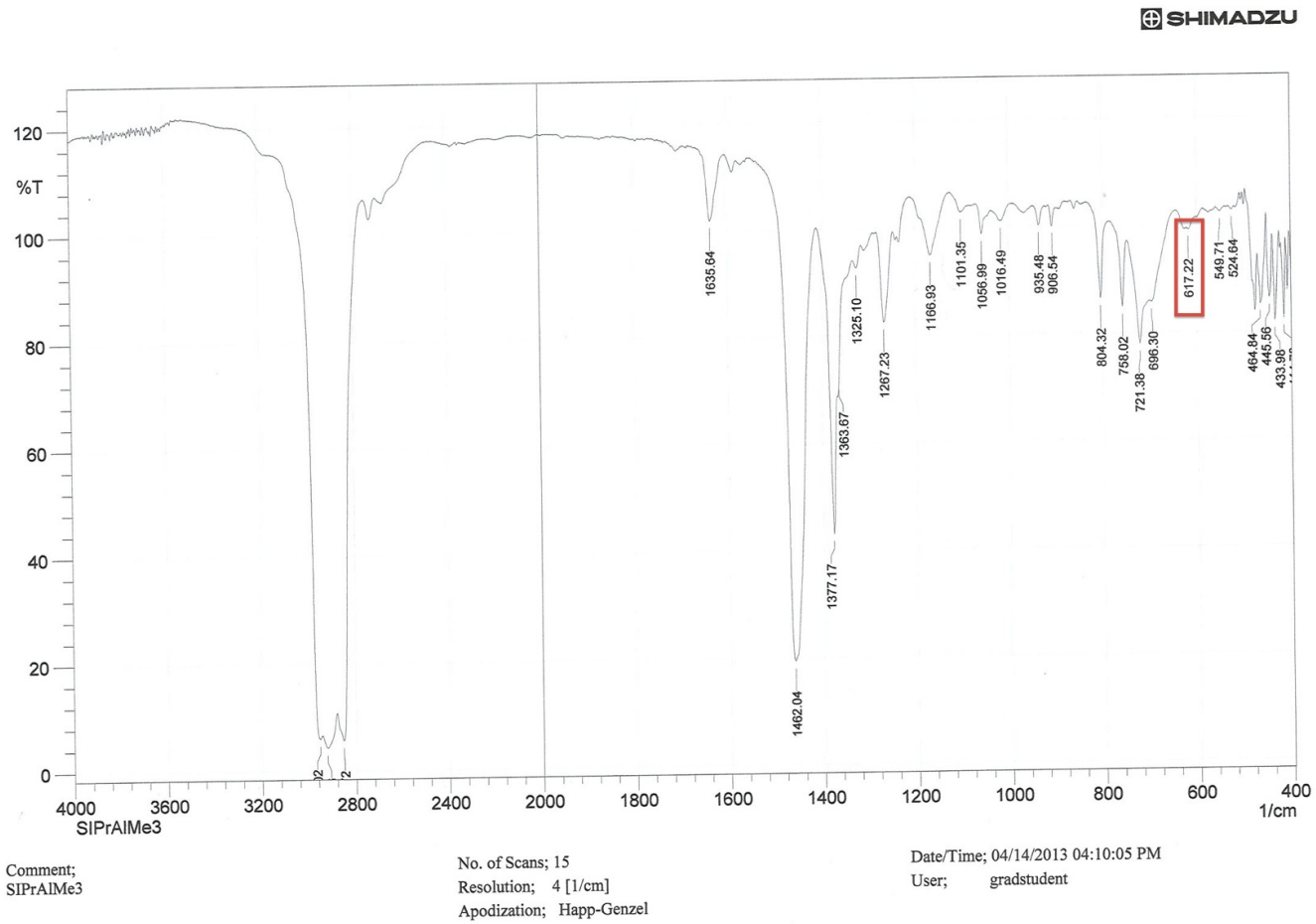
Figure S23. Infrared spectrum of SIMes•AlMe$_3$ (2)

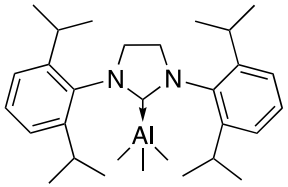




3

Figure S24. Infrared spectrum of Dipp•$AlMe_3$ (3)





4

Figure S25. Infrared spectrum of SIPr•AlMe$_3$ (4)

Decomposition profile for 4

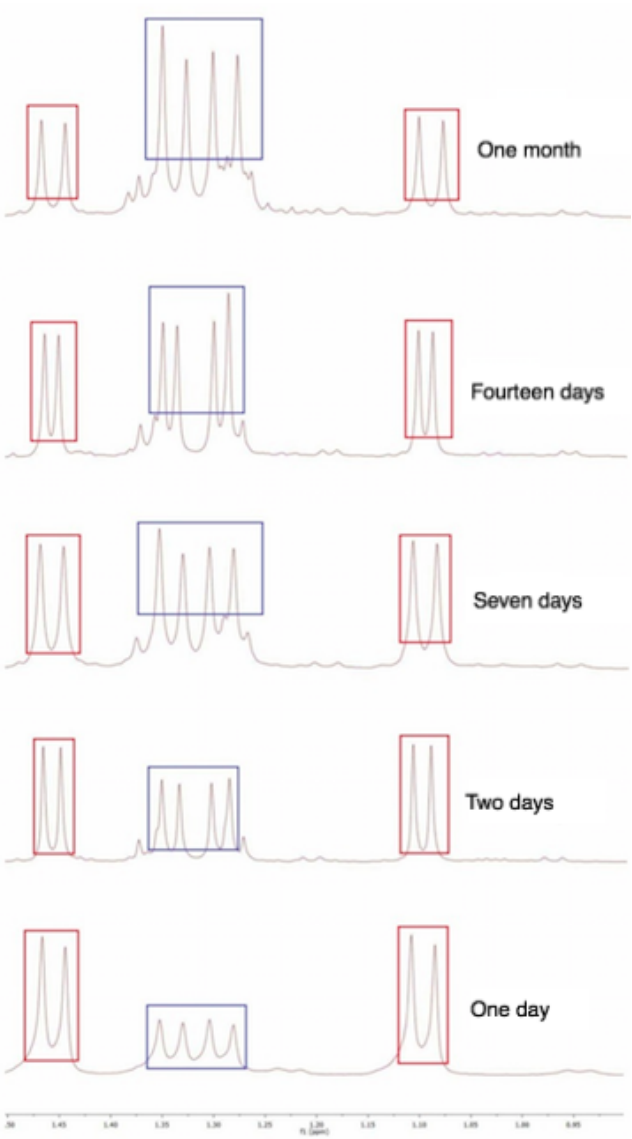


Figure S26. ^{1}H NMR spectrum showing the decomposition of SIPr.AlMe3 conducted at 60°C for 1 month. Red represents our complex; blue represents the carbene.

Summarised tables for selected Al Complexes

Table S1. Al-$C_{carbene}$ bond length and % V_{bur} for selected Al complexes.

Entries	Complex	Al-$C_{carbene}$ [Å]	% V_{bur}[a]
1	**1**	2.098(2)	33.7
2	**2**	2.112(6)	34.1
3	**3**	2.103(3)	35.0
4	**4**	2.127(2)	38.5
5	**A**	2.124(6)	27.2
6	**B**	2.162(2)	36.9
7	**C**	2.097(2)	33.6
8	**D**	2.074(2)	N.A.
9	**E**	2.078(3)	N.A.
10	IMes•AlH_3[1]	2.034(3)	35.2
11	IMes•$AlCl_3$[2]	2.017(2)	33.1
12	Dipp•AlH_3[3]	2.056(2)	40.1
13	Dipp•AlI_3[4]	2.031(2)	33.5

[a] Bidentate ligands were not considered in the %V_{bur} comparison.

Table S2. Selected ^{1}H and ^{13}C NMR chemical shifts for selected complexes

Entries	Complex[a]	^{1}H [AlCH_3] (ppm)
1	1	-0.78
2	2	-0.86
3	3	-0.86
4	4	-0.91
5	A	-0.09
6	B	-0.73
7	$Me_3Al•PMe_3$	-0.41
8	$Me_3Al•PMe_2Ph$	-0.35
9	$Me_3Al•PEt_3$	-0.15
10	$Me_3Al•P(CH_2CH_2CN)_3$	-0.16
11	$Me_3Al•PMePh_2$	-0.22
12	$Me_3Al•P(C_6H_4Me\text{-}p)_3$	-0.02
13	$Me_3Al•PPh_3$	-0.09
14	$Me_3Al•P(C_6H_4F\text{-}p)_3$	-0.14
15	$Me_3Al•PPh_2(C_6H_{11})$	-0.07
16	$Me_3Al•PPh(C_6H_{11})_2$	-0.12
17	$Me_3Al•P(CH_2Ph)_3$	-0.28
18	$Me_3Al•P(C_6H_{11})_3$	-0.19
19	$Me_3Al•PtBu_3$	-0.17
20	$Me_3Al•P(C_6H_4Me\text{-}o)_3$	-0.31

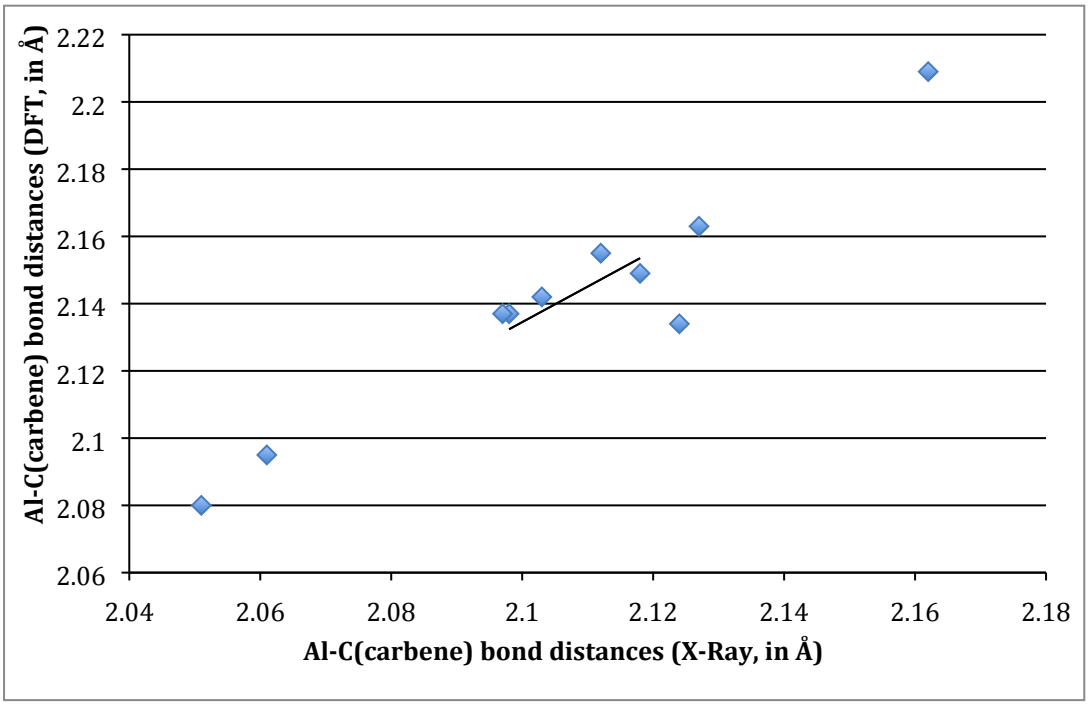
[a] ^{1}H and ^{13}C chemical shift for trimethylaluminium phosphines were obtained from ref 7.

Table S3. Al-$C_{carbene}$ bond lengths, $\%V_{Bur}$ and dissociation energies for optimized structures.[a]

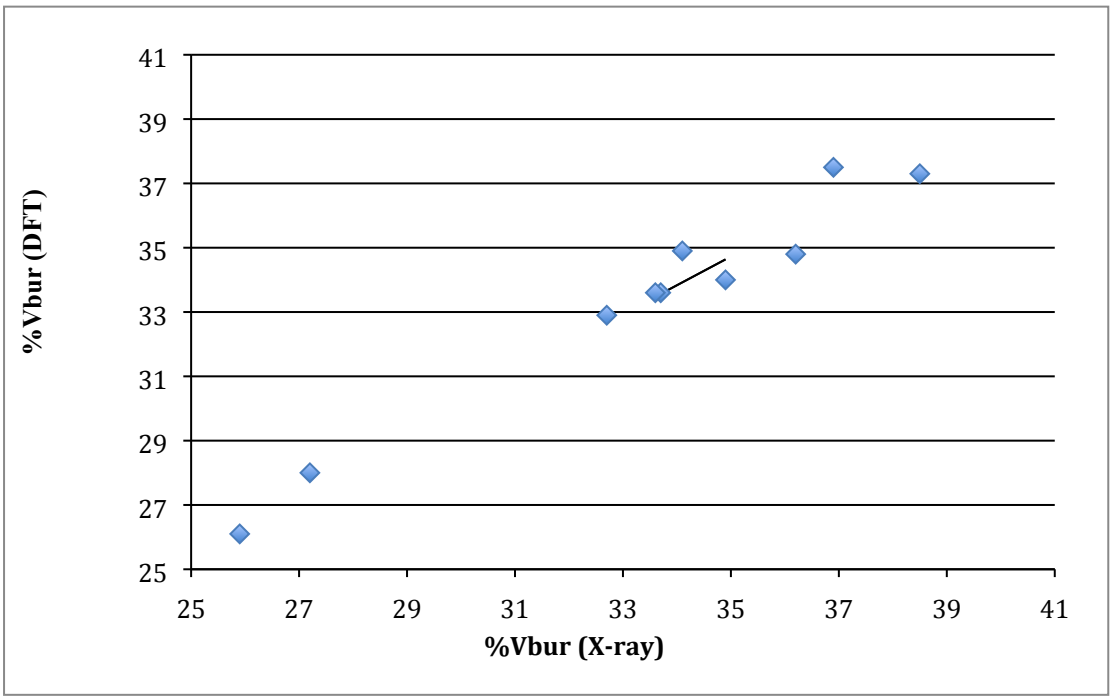
Entries[a]	Complex[a]	Al-$C_{carbene}$ [Å]	$\%V_{Bur}$ R=optimized	$\%V_{Bur}$ R=2.0 Å
1	IMes•$AlMe_3$ (**1**)	2.137	31.1	33.6
2	SIMes•$AlMe_3$ (**2**)	2.155	31.8	34.9
3	Dipp•$AlMe_3$ (**3**)	2.142	32.1	34.8
4	SIPr•$AlMe_3$ (**4**)	2.163	33.3	37.3
5	IPr•$AlMe_3$ (**A**)	2.134	26.2	28.0
6	ItBu•$AlMe_3$ (**B**)	2.209	34.2	37.5
7	IMes•$AlMe_3$ (**C**)	2.137	31.1	33.6
8	IMes•$Al(C_6F_5)_3$	2.095	31.1	32.9
9	IMe•$Al(C{\equiv}CtBu)_3$	2.080	25.2	26.1
10	Dipp•$Al((CH_2)_3CH_3)_3$	2.149	31.3	34.0
11	SItBu•$AlMe_3$	2.229	33.3	37.6

[a]Structures were optimized using PBE0/6-311G(d,p) model chemistry

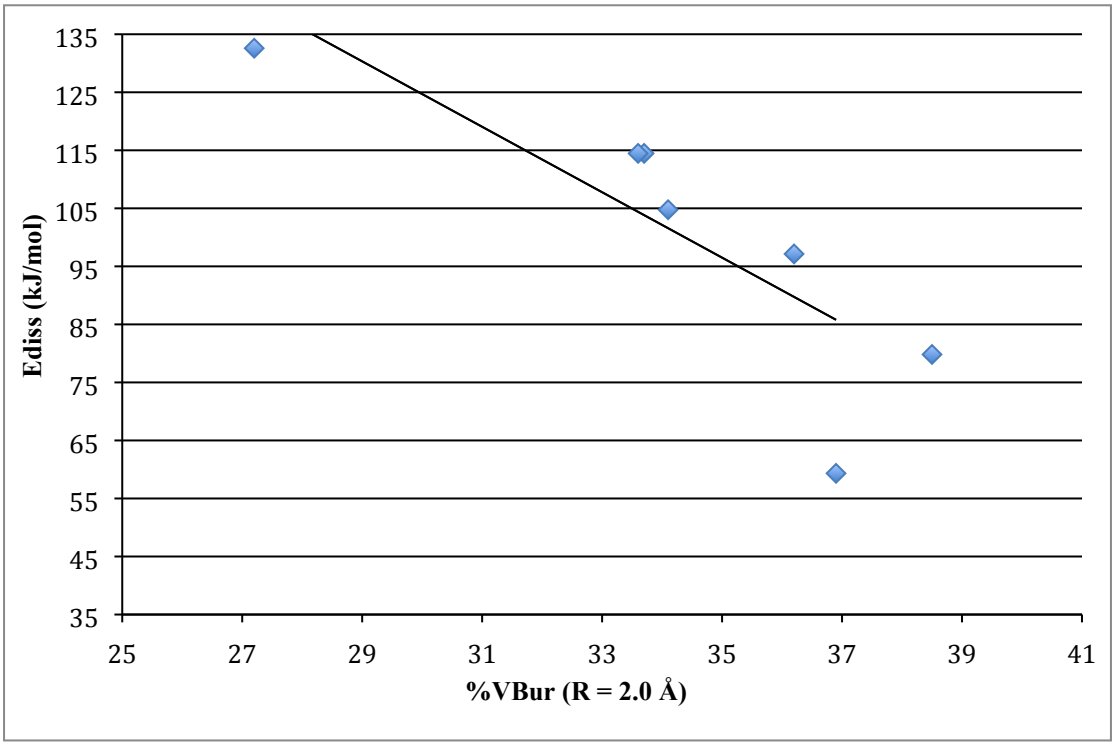
Graph of Al-$C_{carbene}$ bond distances of DFT optimized structures *vs.* Al-$C_{carbene}$ bond distances of X-ray structures.



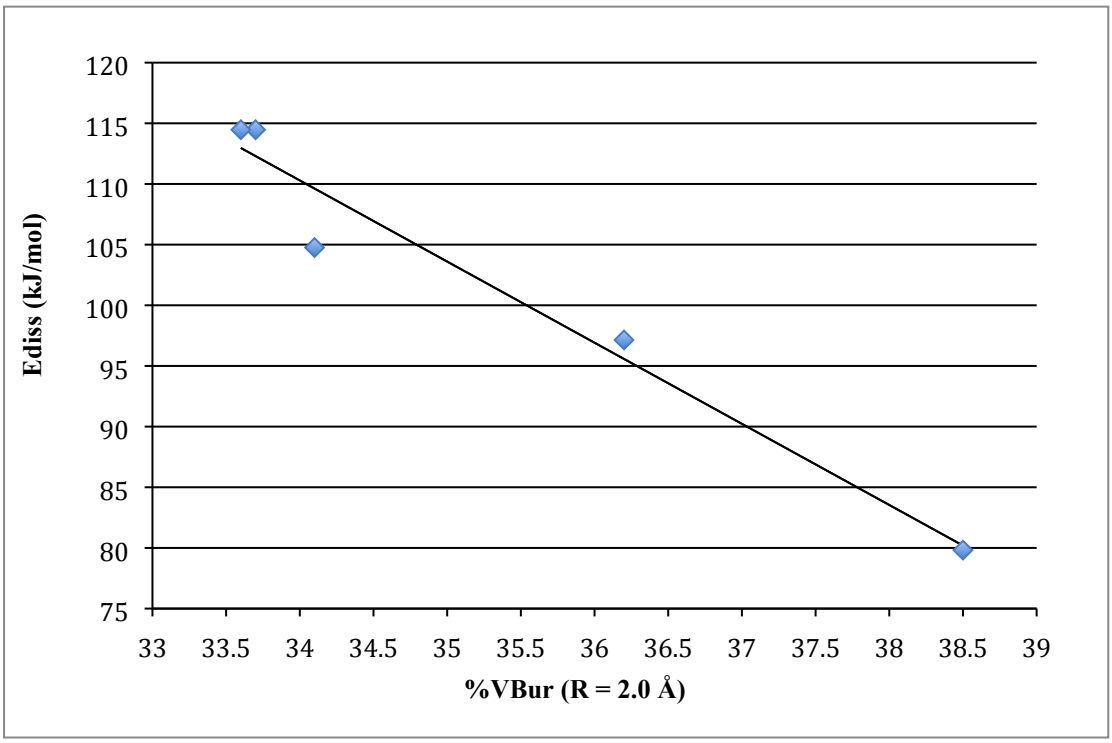
Graph of %V_{Bur} of all NHC•AlR_3 DFT optimized structures *vs.* %V_{Bur} of all the X-ray structures.



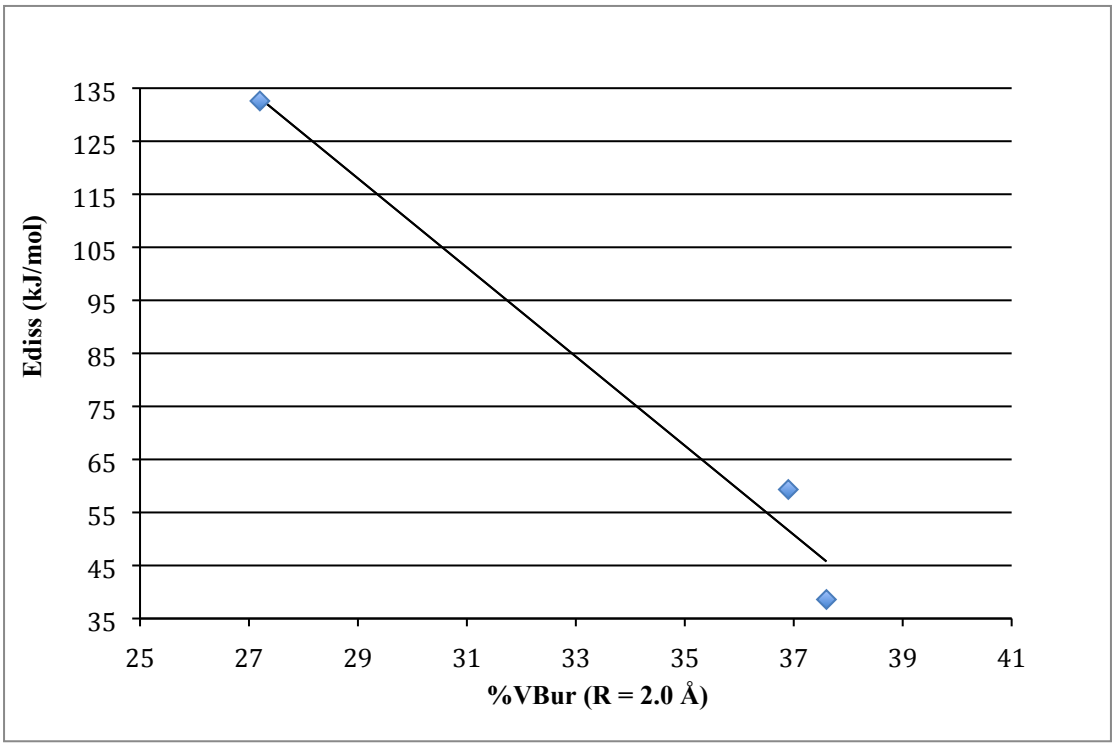
Graph of %V_{Bur} of all NHC•$AlMe_3$ complexes *vs.* their dissociation energy (excluding SitBu).



Graph of $\%V_{Bur}$ of all aryl-NHC•$AlMe_3$ complexes *vs.* their dissociation energy.

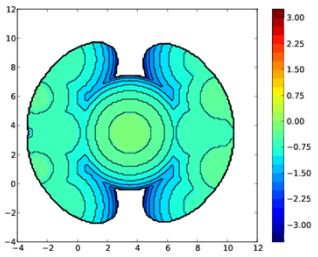
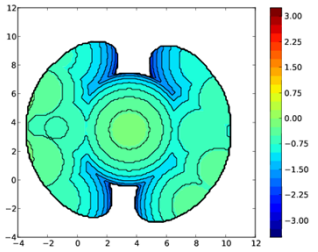
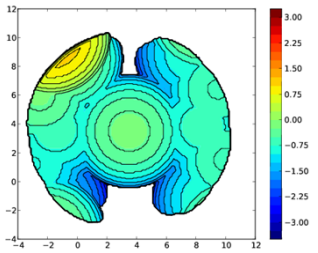
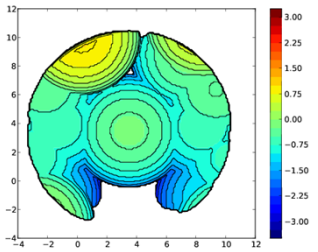
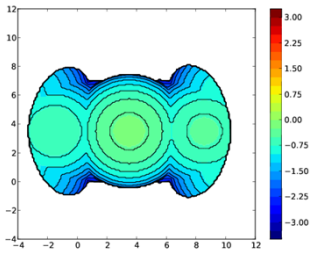


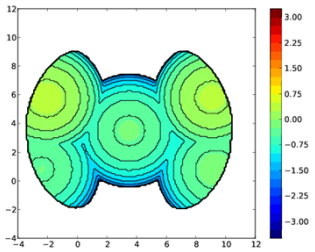
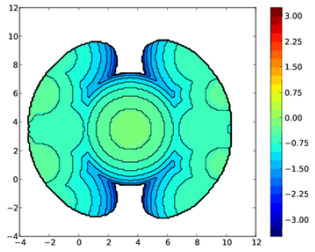
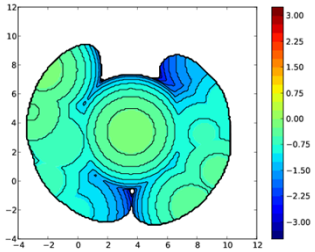
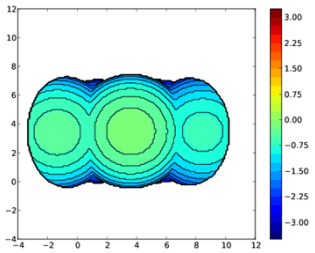
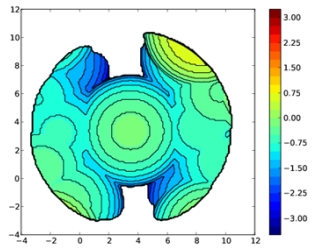
Graph of $\%V_{Bur}$ of all alkyl-NHC•$AlMe_3$ complexes *vs.* their dissociation energy (including SitBu).



$\%V_{Bur}$ and topographic steric map for selected NHC Al alkyl complexes

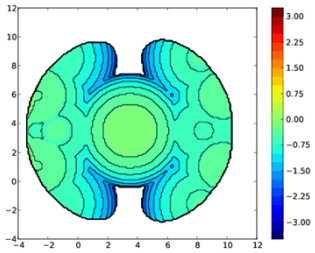
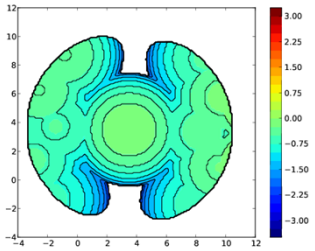
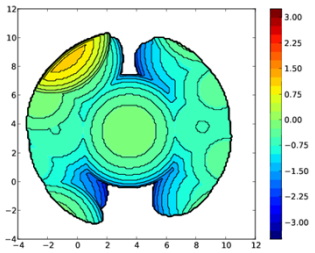
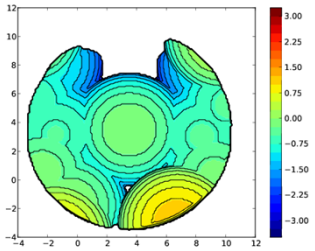
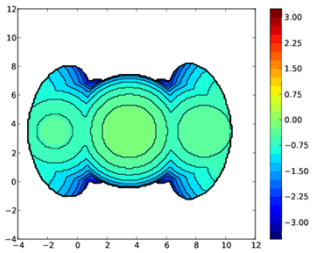
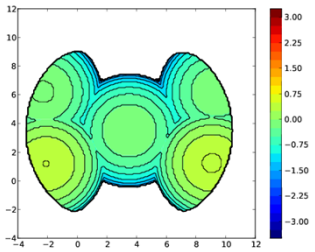
Table S4. % V_{Bur} and topographic steric map for selected Al complexes. The Al-$C_{carbene}$ bond lengths are the experimental values obtained by X-ray single crystal diffraction studies.

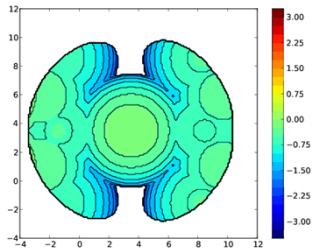
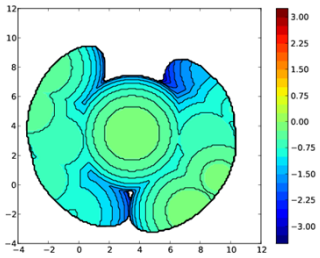
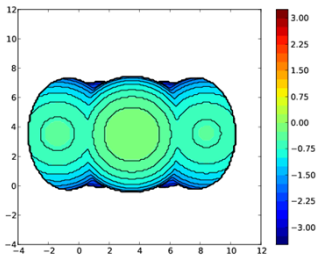
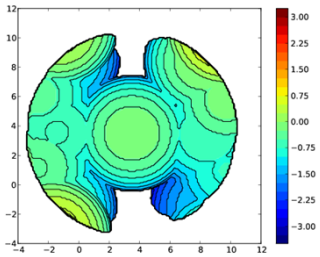
Entries	Complexes	Al-$C_{carbene}$ [Å]	% V_{bur}[a]	Topographic steric map
1	IMes•$AlMe_3$ (1)	2.098(2)	31.7	
2	SIMes•$AlMe_3$ (2)	2.112(6)	32.0	
3	Dipp•$AlMe_3$ (3)	2.103(3)	33.1	
4	SIPr•$AlMe_3$ (4)	2.127(2)	36.1	
5	IPr•$AlMe_3$ (A)	2.124(6)	25.5	

6	ItBu•$AlMe_3$ (B)	2.162(2)	34.3	
7	IMes•$AlMe_3$ (C)	2.097(2)	31.8	
8	IMes•$Al(C_6F_5)_3$	2.061(3)	31.2	
9	IMes•$Al(C{\equiv}CtBu)_3$	2.051(2)	25.3	
10	Dipp•$Al((CH_2)_3CH_3)_3$	2.118(2)	32.6	

$\%V_{Bur}$ calculations and topographic steric map parameters: All calculations were performed using crystallographic data (CIF). 3.50 Å was selected as the value for the sphere radius; Al-$C_{carbene}$ bond distances (**X-ray crystal structure**) were chosen for the metal-ligand bond; mesh spacing for numerical integration was scaled to 0.05; hydrogen atoms were omitted for the calculations; and bondi radii was scaled by 1.17.

Table S5. % V_{Bur} and topographic steric map for selected Al complexes. The Al-$C_{carbene}$ bond length is set at 2.0Å.

Entries	Complexes	% V_{bur}[a]	Topographic steric map
1	IMes•$AlMe_3$ (1)	33.7	
2	SIMes•$AlMe_3$ (2)	34.1	
3	Dipp•$AlMe_3$ (3)	35.0	
4	SIPr•$AlMe_3$ (4)	38.5	
5	IPr•$AlMe_3$ (A)	27.2	
6	ItBu•$AlMe_3$ (B)	36.9	

7	IMes•$AlMe_3$ (C)	33.6	
8	IMes•$Al(C_6F_5)_3$	32.7	
9	IMes•$Al(C{\equiv}CtBu)_3$	25.9	
10	Dipp•$Al((CH_2)_3CH_3)_3$	34.9	

$\%V_{Bur}$ calculations and topographic steric map parameters: All calculations were performed using crystallographic data (CIF). 3.50 Å was selected as the value for the sphere radius; distance of **2.00 Å** was chosen for the metal-ligand bond; mesh spacing for numerical integration was scaled to 0.05; hydrogen atoms were omitted for the calculations; and bondi radii was scaled by 1.17.

Crystal Structure Report for 1 & 2

Complex 1

A specimen of $C_{24}H_{33}AlN_2$, approximate dimensions 0.380 mm x 0.400 mm x 0.400 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using an orthorhombic unit cell yielded a total of 27611 reflections to a maximum θ angle of 37.04° (0.59 Å resolution), of which 5968 were independent (average redundancy 4.627, completeness = 99.5%, R_{int} = 9.65%) and 3425 (57.39%) were greater than $2\sigma(F^2)$. The final cell constants of a = 22.9414(9) Å, b = 12.2109(5) Å, c = 8.0965(3) Å, volume = 2268.11(15) Å^3, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9610 and 0.9630.

The final anisotropic full-matrix least-squares refinement on F^2 with 148 variables converged at R1 = 5.52%, for the observed data and wR2 = 16.08% for all data. The goodness-of-fit was 0.971. The largest peak in the final difference electron density synthesis was 0.499 e$^-$/Å^3 and the largest hole was -0.341 e$^-$/Å^3 with an RMS deviation of 0.069 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.103 g/cm^3 and F(000), 816 e$^-$.

Complex 2

A specimen of $C_{24}H_{35}AlN_2$, approximate dimensions 0.120 mm x 0.220 mm x 0.280 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using an orthorhombic unit cell yielded a total of 38760 reflections to a maximum θ angle of 28.26° (0.75 Å resolution), of which 11323 were independent (average redundancy 3.423, completeness = 99.8%, R_{int} = 12.67%, R_{sig} = 10.17%) and 6399 (56.51%) were greater than $2\sigma(F^2)$. The final cell constants of a = 17.7329(18) Å, b = 16.5921(14) Å, c = 15.9863(16) Å, volume = 4703.6(8) Å^3, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9740 and 0.9890.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P c a 21, with Z = 8 for the formula unit, $C_{24}H_{35}AlN_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 505 variables converged at R1 = 7.04%, for the observed data and wR2 = 19.32% for all data. The goodness-of-fit was 0.979. The largest peak in the final difference electron density synthesis was 0.333 e$^-$/Å^3 and the largest hole was -0.346 e$^-$/Å^3 with an RMS deviation of 0.078 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.069 g/cm^3 and F(000), 1648 e$^-$.

Table 5. Crystal data for complex **1** (IMes•$AlMe_3$) and **2** (SIMes•$AlMe_3$).

	1	**2**
Formula	$C_{24}H_{33}AlN_2$	$C_{24}H_{35}AlN_2$
FW	376.50	378.52
T [K]	103(2)	103(2)
λ [Å]	0.71073	0.71073
Crystal Structure	Orthorhombic	Orthorhombic
Space Group	Pnma	Pca21
a [Å]	22.9414(9)	17.7329(18)
b [Å]	12.2109(5)	16.5921(14)
c [Å]	8.0965(3)	15.986316)
α (°)	90	90
β (°)	90	90
γ (°)	90	90
V [Å^3]	2268.11(15)	4703.6(8)
Z	4	8
D_{calcd} [Mg/m^3]	1.103	1.069
μ [mm^{-1}]	0.1	0.096
F(000)	816	1648
Crystal size [mm^3]	0.38x0.40x0.40	1.120x0.220x0.280
θ range [°]	1.77-37.04	1.68-28.26
N	27611	38760
N_{ind} (R_{int})	5968(0.0965)	11323(0.1267)
Max. and min.	0.9630 & 0.9610	0.9890 & 0.9740

transmssion		
Data, restraints, parameters	5968 / 0 /148	11323 / 1 / 505
GOF on F^2	0.971	0.979
Final R indices [I>2σ(I)]	0.0552, 0.1339	0.0704, 0.1503
R indices (all data)	0.1098, 0.1608	0.1465, 0.1932
Largest diff. Peak & hole [eÅ^{-3}]	0.333 & -0.346	0.333 & -0.346
R.M.S deviation from mean [eÅ^{-3}]	0.079	0.078

Crystal Structure Report for 3 & 4

Complex 3

A specimen of $C_{30}H_{45}AlN_2$, approximate dimensions 0.180 mm x 0.220 mm x 0.260 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a monoclinic unit cell yielded a total of 56158 reflections to a maximum θ angle of 28.78° (0.74 Å resolution), of which 15123 were independent (average redundancy 3.713, completeness = 99.5%, R_{int} = 13.60%) and 6812 (45.04%) were greater than 2σ(F^2). The final cell constants of a = 16.6982(12) Å, b = 19.5345(14) Å, c = 19.2491(14) Å, β = 111.602(3)°, volume = 5837.9(7) Å^3, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9780 and 0.9840.

The final anisotropic full-matrix least-squares refinement on F^2 with 782 variables converged at R1 = 7.71%, for the observed data and wR2 = 22.92% for all data. The goodness-of-fit was 0.970. The largest peak in the final difference electron density synthesis was 0.677 e$^-$/Å^3 and the largest hole was -0.677 e$^-$/Å^3 with an RMS deviation of 0.266 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.048 g/cm^3 and F(000), 2016 e$^-$.

Complex 4

A specimen of $C_{30}H_{47}AlN_2$, approximate dimensions 0.300 mm x 0.310 mm x 0.320 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a monoclinic unit cell yielded a total of 19383 reflections to a maximum θ angle of 30.51° (0.70 Å resolution), of which 8679 were independent (average redundancy 2.233, completeness = 99.0%, R_{int} = 6.44%) and 5152 (59.36%) were greater than 2σ(F^2). The final cell constants of a = 17.8289(13) Å, b = 10.1831(7) Å, c = 16.5889(10) Å, β = 107.807(2)°, volume = 2867.5(3) Å^3, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9720 and 0.9740.

The final anisotropic full-matrix least-squares refinement on F^2 with 309 variables converged at R1 = 6.35%, for the observed data and wR2 = 19.37% for all data. The goodness-of-fit was 1.007. The largest peak in the final difference electron density synthesis was 0.481 e$^-$/Å^3 and the largest hole was -0.560 e$^-$/Å^3 with an RMS deviation of 0.150 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.072 g/cm^3 and F(000), 1016 e$^-$.

Table 14. Crystal data for complex 3 (Dipp•$AlMe_3$) and 4 (SIPr•$AlMe_3$).

	3	**4**
Formula	$C_{30}H_{45}AlN_2$	$C_{30}H_{47}AlN_2$
FW	460.66	462.67
T [K]	103(2)	103(2)
λ [Å]	0.71073	0.71073
Crystal Structure	Monoclinic	Monoclinic
Space Group	P121/c1	P121/c1
a [Å]	16.6982(12)	17.8289(13)
b [Å]	19.5345(14)	10.1831(7)
c [Å]	19.2491(14)	16.5889(10)
α (°)	90	90
β (°)	111.602(3)	107.807(2)
γ (°)	90	90
V [Å^3]	5837.9(7)	2867.5(3)
Z	8	4

D_{calcd} [Mg/m^3]	1.048	1.072
μ [mm^{-1}]	0.088	0.090
F(000)	2016	1016
Crystal size [mm^3]	0.180x0.220x0.260	0.300x0.310x0.320
θ range [°]	1.54-28.78	2.33-30.51
N	56158	19383
N_{ind} (R_{int})	5968(0.0965)	8679(0.0644)
Max. and min. transmssion	0.9840 & 0.9780	0.9740 & 0.9720
Data, restraints, parameters	15123 / 1030 /782	8679 / 0 / 309
GOF on F^2	0.970	1.007
Final R indices [I>2σ(I)]	0.0771, 0.1611	0.0635, 0.1510
R indices (all data)	0.1898, 0.2292	0.1204, 0.1937
Largest diff. Peak & hole [eÅ^{-3}]	0.677 & -0.677	0.481 & -0.560
R.M.S deviation from mean [eÅ^{-3}]	0.266	0.150

Crystal Structure Report for 5

A specimen of $C_{15}H_{22.25}NO_2$, approximate dimensions 0.100 mm x 0.120 mm x 0.360 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a monoclinic unit cell yielded a total of 22109 reflections to a maximum θ angle of 28.32° (0.75 Å resolution), of which 7192 were independent (average redundancy 3.074, completeness = 99.6%, R_{int} = 10.91%, R_{sig} = 15.05%) and 3550 (49.36%) were greater than 2σ(F^2). The final cell constants of a = 10.653(2) Å, b = 17.656(3) Å, c = 15.577(3) Å, β = 98.900(6)°, volume = 2894.6(10) Å^3, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9740 and 0.9930.

The final anisotropic full-matrix least-squares refinement on F^2 with 345 variables converged at R1 = 7.75%, for the observed data and wR2 = 21.37% for all data. The goodness-of-fit was 1.021. The largest peak in the final difference electron density synthesis was 0.352 e$^-$/Å^3 and the largest hole was -0.378 e$^-$/Å^3 with an RMS deviation of 0.070 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.141 g/cm^3 and F(000), 1082 e$^-$.

Table 16. Selected bond lengths and angles in complex **5.**

	5
Formula	$C_{15}H_{22.25}NO_2$
FW	248.59
T [K]	103(2)
λ [Å]	0.71073
Crystal Structure	Monoclinic
Space Group	P121/c1
a [Å]	10.653(2)
b [Å]	17.656(3)
c [Å]	15.577(3)
α (°)	90
β (°)	98.900(6)
γ (°)	90
V [Å^3]	2894.6(10)
Z	8
D_{calcd} [Mg/m^3]	1.141
μ [mm^{-1}]	0.075
F(000)	1082
Crystal size [mm^3]	0.100x0.120x0.360
θ range [°]	2.66-28.32
N	22109
N_{ind} (R_{int})	7192(0.1091)
Max. and min. transmssion	0.9930 & 0.9740
Data, restraints, parameters	7192 / 1 /345
GOF on F^2	1.021
Final R indices [I>2σ(I)]	0.0775, 0.1758
R indices (all data)	0.1706, 0.2137
Largest diff. Peak & hole [eÅ^{-3}]	0.352 & -0.378
R.M.S deviation from mean [eÅ^{-3}]	0.070

Cartesian Coordinates for optimised complexes at the PBE0/6-311G(d,p) model chemistry

$AlMe_3$

Al	0.000100	0.000000	-0.000100
C	-0.829200	1.780400	0.000100
H	-1.482300	1.912100	0.871900
H	-0.104100	2.600000	0.005500
H	-1.472900	1.915700	-0.878100
C	1.956600	-0.172100	-0.000300
H	2.303600	-1.209900	-0.017400
H	2.398800	0.338300	-0.864900
H	2.394000	0.306500	0.884900
C	-1.127500	-1.608300	0.000200
H	-0.927200	-2.230100	-0.881400
H	-0.910700	-2.242900	0.868500
H	-2.199600	-1.389900	0.011500

IMes

C	-0.674600	-0.008400	1.917200
C	0.674600	0.010900	1.917200
C	0.000000	-0.000100	-0.279100
H	-1.383700	-0.023100	2.729100
H	1.383700	0.026600	2.729100
N	-1.057600	-0.013500	0.582600
N	1.057600	0.014300	0.582600
C	-2.420500	-0.028500	0.153700
C	-3.173100	1.144900	0.237600
C	-2.966300	-1.217300	-0.339300
C	-4.505300	1.102000	-0.167700
C	-4.299900	-1.210000	-0.736500
C	-5.088200	-0.064700	-0.651900
H	-5.097700	2.011700	-0.114100
H	-4.733400	-2.127300	-1.126500
C	2.420500	0.028800	0.153700
C	3.172800	-1.144800	0.238100
C	2.966600	1.217200	-0.339800
C	4.505000	-1.102600	-0.167200
C	4.300200	1.209300	-0.737100
C	5.088200	0.063800	-0.651900
H	5.097100	-2.012400	-0.113200
H	4.734000	2.126300	-1.127500
C	-2.132100	-2.457700	-0.457800
H	-1.298400	-2.291600	-1.145700
H	-1.698100	-2.739100	0.506900
H	-2.731800	-3.294000	-0.821900
C	-2.558100	2.427000	0.717700
H	-2.321900	2.391900	1.786000
H	-1.621300	2.628900	0.190900
H	-3.237400	3.265200	0.552100
C	-6.533500	-0.095900	-1.058800
H	-7.159400	-0.488600	-0.249700
H	-6.900500	0.903700	-1.302800
H	-6.687800	-0.737000	-1.930500
C	2.557300	-2.426500	0.718700
H	2.319400	-2.390400	1.786600
H	1.621300	-2.629100	0.190700
H	3.237000	-3.264800	0.555000
C	2.132800	2.457700	-0.459000
H	1.299100	2.291500	-1.147000
H	1.698700	2.739700	0.505500
H	2.732700	3.293700	-0.823500
C	6.533600	0.094300	-1.058500

H	6.689400	0.740200	-1.926400
H	7.160200	0.480800	-0.247000
H	6.898500	-0.904600	-1.308400

SIMes

C	-0.757000	-0.085600	2.021600
C	0.757000	0.085200	2.021600
C	-0.000000	0.000000	-0.226000
H	-1.069100	-1.075600	2.375800
H	1.270900	-0.668200	2.622300
N	-1.070700	0.058500	0.586400
N	1.070700	-0.058600	0.586400
C	-2.415900	-0.000500	0.127800
C	-3.252500	1.106400	0.308000
C	-2.892700	-1.169300	-0.483200
C	-4.575900	1.021100	-0.121000
C	-4.218500	-1.206000	-0.901500
C	-5.080200	-0.125700	-0.723000
H	-5.224000	1.884600	0.007000
H	-4.589100	-2.107900	-1.382200
C	2.415900	0.000400	0.127800
C	3.252500	-1.106400	0.308000
C	2.892700	1.169300	-0.483100
C	4.576000	-1.021100	-0.121000
C	4.218500	1.206100	-0.901300
C	5.080200	0.125800	-0.722800
H	5.224100	-1.884500	0.007000
H	4.589100	2.108100	-1.381900
C	-1.992800	-2.349400	-0.701900
H	-1.165300	-2.084300	-1.365600
H	-1.547400	-2.692400	0.237800
H	-2.547900	-3.182500	-1.138000
C	-2.741900	2.377100	0.922800
H	-2.768200	2.337300	2.018200
H	-1.708800	2.569800	0.624400
H	-3.355900	3.226600	0.616600
C	-6.515700	-0.208100	-1.156900
H	-7.119900	-0.740400	-0.413800
H	-6.951300	0.785700	-1.284100
H	-6.615300	-0.746400	-2.103100
C	2.742000	-2.377200	0.922700
H	2.768300	-2.337500	2.018000
H	1.708900	-2.569900	0.624300
H	3.356000	-3.226600	0.616400
C	1.992800	2.349500	-0.701600
H	1.165400	2.084500	-1.365500
H	1.547200	2.692200	0.238100
H	2.547900	3.182700	-1.137500
C	6.515600	0.208300	-1.157100
H	6.614100	0.739500	-2.107500
H	7.118400	0.748000	-0.418100
H	6.953600	-0.785300	-1.276600
H	-1.270900	0.667700	2.622400
H	1.069100	1.075200	2.376000

Dipp

C	-0.664900	-0.009800	1.867900
C	0.683200	-0.079800	1.874800
C	0.025000	0.049100	-0.322800
H	-1.380000	-0.005600	2.674500
H	1.386900	-0.151400	2.688300
N	-1.038100	0.065600	0.533900
N	1.075600	-0.041500	0.544300
C	-2.404600	0.118700	0.110500

C	-2.972800	1.361600	-0.202600
C	-3.135200	-1.075100	0.039700
C	-4.311000	1.384300	-0.591500
C	-4.472500	-0.998500	-0.347300
C	-5.057500	0.217900	-0.659200
H	-4.775400	2.330900	-0.846700
H	-5.060400	-1.908700	-0.412400
C	2.445500	-0.111800	0.132800
C	2.985700	-1.361600	-0.200700
C	3.201600	1.067200	0.092800
C	4.323200	-1.406200	-0.590800
C	4.535300	0.970000	-0.301300
C	5.091800	-0.253400	-0.639700
H	4.769700	-2.357100	-0.860100
H	5.145200	1.865700	-0.348500
C	-2.514900	-2.425600	0.338400
H	-1.469700	-2.261200	0.612200
C	-2.161200	2.640300	-0.182200
H	-1.244900	2.441700	0.380800
C	2.137000	-2.616800	-0.199100
H	1.284400	-2.436500	0.463000
C	2.581900	2.417600	0.391600
H	1.672000	2.244400	0.973700
H	-6.099100	0.257600	-0.961600
H	6.131800	-0.309000	-0.945100
C	-2.523500	-3.317800	-0.904800
H	-3.544900	-3.543700	-1.227500
H	-2.005300	-2.833800	-1.736100
H	-2.023100	-4.268500	-0.695200
C	-3.202300	-3.113200	1.519300
H	-3.172300	-2.489400	2.417200
H	-4.252600	-3.329900	1.300000
H	-2.708900	-4.062700	1.749100
C	2.876200	-3.842300	0.334900
H	3.681800	-4.160000	-0.334300
H	3.311200	-3.653500	1.320500
H	2.184100	-4.684700	0.424800
C	1.580900	-2.870300	-1.603900
H	0.994700	-2.012700	-1.943500
H	2.395700	-3.038500	-2.316100
H	0.937700	-3.756500	-1.608700
C	-2.887500	3.792800	0.510200
H	-2.225800	4.660900	0.585300
H	-3.774700	4.110500	-0.046200
H	-3.204600	3.519000	1.520400
C	-1.750000	3.015700	-1.608700
H	-1.133600	3.920300	-1.607500
H	-1.176700	2.205800	-2.066200
H	-2.632100	3.207400	-2.228900
C	3.488300	3.324900	1.221400
H	3.819000	2.832100	2.140100
H	4.378900	3.633700	0.665500
H	2.950900	4.236300	1.499500
C	2.166600	3.093900	-0.918400
H	3.041700	3.282400	-1.549100
H	1.473000	2.461000	-1.477100
H	1.678700	4.053800	-0.719600

SIPr

C	0.750500	0.135900	1.963600
C	-0.750600	-0.135300	1.963600
C	-0.000000	0.000100	-0.287700
H	1.001800	1.131400	2.349300
H	-1.321000	0.601400	2.535700
N	1.069900	0.055400	0.525500

N	-1.070000	-0.055100	0.525400
C	2.415200	0.212600	0.082400
C	3.268700	-0.901100	0.094400
C	2.867300	1.479000	-0.324600
C	4.590500	-0.726400	-0.313000
C	4.194000	1.603200	-0.732900
C	5.051600	0.513600	-0.723900
H	5.264600	-1.577600	-0.318900
H	4.563500	2.568500	-1.062700
C	-2.415100	-0.212500	0.082400
C	-3.268900	0.901000	0.094400
C	-2.867000	-1.479100	-0.324700
C	-4.590700	0.726000	-0.313000
C	-4.193800	-1.603500	-0.732900
C	-5.051500	-0.514100	-0.723900
H	-5.265000	1.577000	-0.318800
H	-4.563000	-2.568900	-1.062700
C	1.936400	2.673200	-0.379400
H	1.074300	2.447500	0.255900
C	2.779700	-2.280300	0.486400
H	1.740400	-2.180200	0.811000
C	-2.780200	2.280300	0.486300
H	-1.740900	2.180400	0.811000
C	-1.935900	-2.673100	-0.379500
H	-1.073800	-2.447200	0.255800
H	6.082300	0.631800	-1.042800
H	-6.082200	-0.632600	-1.042700
C	1.407800	2.862700	-1.804300
H	2.231100	3.064600	-2.497800
H	0.884500	1.963300	-2.137500
H	0.712200	3.707400	-1.848200
C	2.576100	3.955500	0.151000
H	2.986300	3.816100	1.155400
H	3.385600	4.307000	-0.496000
H	1.830500	4.755200	0.194800
C	-3.585000	2.868700	1.646200
H	-4.630900	3.029800	1.367000
H	-3.574800	2.207800	2.517800
H	-3.172000	3.836700	1.946800
C	-2.782900	3.219300	-0.722400
H	-2.172900	2.812600	-1.532800
H	-3.797500	3.368000	-1.105700
H	-2.381600	4.200400	-0.448300
C	3.584200	-2.868700	1.646500
H	3.171000	-3.836600	1.947200
H	4.630200	-3.030000	1.367400
H	3.574100	-2.207600	2.518000
C	2.782400	-3.219500	-0.722100
H	2.380800	-4.200500	-0.447900
H	2.172600	-2.812800	-1.532600
H	3.797000	-3.368500	-1.105300
C	-2.575300	-3.955500	0.151000
H	-2.985500	-3.816200	1.155400
H	-3.384800	-4.307200	-0.496000
H	-1.829600	-4.755100	0.194700
C	-1.407400	-2.862400	-1.804400
H	-2.230700	-3.064500	-2.497800
H	-0.884300	-1.962900	-2.137600
H	-0.711600	-3.707000	-1.848400
H	1.320900	-0.600800	2.535800
H	-1.001900	-1.130800	2.349500

IPr•$AlMe_3$

Al	0.688600	2.195100	-0.072600
C	-0.839800	3.493100	-0.070800

C	1.707800	2.301500	-1.796600
C	0.000400	0.175900	-0.025500
C	-1.225700	-1.723000	-0.010600
C	0.088900	-2.083200	-0.008000
C	-2.438000	0.534000	0.013100
C	-3.402100	0.267700	-1.135300
N	-1.251600	-0.335300	-0.024700
N	0.817400	-0.902400	-0.017200
C	-2.420700	-2.608400	-0.038600
C	0.663100	-3.454900	-0.041900
C	2.282000	-0.758900	0.028200
C	2.972200	-1.441900	-1.144200
H	-1.492200	3.465500	-0.953500
H	-1.480400	3.468100	0.820400
H	1.090900	2.008400	-2.656400
H	2.632100	1.712800	-1.855500
H	2.002100	3.344900	-1.972700
H	-2.021700	1.530400	-0.131400
H	-2.869500	0.219300	-2.088300
H	-4.116400	1.093000	-1.192800
H	-3.975900	-0.652600	-1.005800
H	-3.180400	-2.302700	0.683200
H	-2.128400	-3.629500	0.211000
H	-2.889400	-2.634800	-1.027000
H	1.464800	-3.589400	0.686400
H	1.061900	-3.707100	-1.029200
H	-0.113700	-4.184700	0.191200
H	2.438300	0.314400	-0.085600
H	2.503500	-1.157000	-2.088900
H	2.970500	-2.530900	-1.060600
H	4.015500	-1.117700	-1.177100
C	1.777000	2.401000	1.599400
H	1.238400	2.069700	2.497400
H	2.750100	1.894300	1.605800
H	1.990700	3.467800	1.749800
C	2.844400	-1.159300	1.385400
H	2.332500	-0.619200	2.184200
H	2.762700	-2.232500	1.575600
H	3.904900	-0.896900	1.427300
C	-3.106300	0.512600	1.381700
H	-2.381700	0.744900	2.165500
H	-3.892000	1.272200	1.411800
H	-3.568500	-0.451200	1.611000
H	-0.379800	4.491400	-0.076000

ItBu•$AlMe_3$

C	0.000000	-0.288200	-0.075900
C	-0.672800	-2.439100	0.093700
H	-1.352800	-3.267100	0.162100
C	0.673300	-2.439000	0.093800
H	1.353500	-3.266800	0.162200
C	-2.521100	-0.748300	-0.070400
C	-2.837800	0.205600	1.078000
H	-2.654200	-0.286700	2.037100
H	-3.892800	0.489300	1.032600
H	-2.245800	1.117700	1.042900
C	-3.395000	-1.990900	0.105100
H	-3.257800	-2.716500	-0.701400
H	-4.437600	-1.667400	0.076200
H	-3.230500	-2.482000	1.068400
C	-2.802500	-0.159400	-1.450600
H	-2.167800	0.700000	-1.654400
H	-3.845000	0.164500	-1.510200
H	-2.633100	-0.917500	-2.221200
C	2.521300	-0.747900	-0.070300

C	3.395400	-1.990200	0.105700
H	3.230800	-2.481100	1.069100
H	4.437900	-1.666600	0.077000
H	3.258500	-2.716100	-0.700600
C	2.802700	-0.159400	-1.450700
H	2.633200	-0.917700	-2.221100
H	3.845200	0.164400	-1.510500
H	2.168000	0.700000	-1.654700
C	2.837900	0.206600	1.077700
H	2.245800	1.118600	1.042000
H	3.892800	0.490300	1.032200
H	2.654200	-0.285200	2.037000
N	-1.076000	-1.129200	-0.009100
N	1.076200	-1.129000	-0.009000
C	-1.550800	2.834900	-0.820600
H	-2.577000	2.631000	-0.500000
H	-1.530500	2.772600	-1.916600
H	-1.364600	3.893900	-0.587000
C	0.000200	2.123900	2.068600
H	-0.000000	1.184600	2.634900
H	-0.877100	2.693400	2.402300
H	0.877900	2.692900	2.402100
C	1.549500	2.834900	-0.822000
H	1.362500	3.894100	-0.590200
H	1.529600	2.770900	-1.917900
H	2.575800	2.632200	-0.500800
Al	-0.000200	1.915900	0.066300

$Al(C_6F_5)_3$

Al	-0.000100	-0.000500	-0.000400
C	0.802000	1.782000	-0.001000
C	0.202100	2.852700	-0.648100
C	0.751900	4.123000	-0.661600
C	1.954000	4.337700	-0.001000
C	2.589200	3.294900	0.659700
C	2.001400	2.041700	0.646400
C	-1.945000	-0.196300	0.000800
C	-2.769100	0.713100	0.648100
C	-4.148400	0.596100	0.661700
C	-4.734500	-0.475200	0.001200
C	-3.948100	-1.409300	-0.659500
C	-2.572900	-1.250900	-0.646300
C	1.142800	-1.586300	-0.000700
C	0.765200	-2.757000	0.641400
C	1.556600	-3.892700	0.654900
C	2.780400	-3.861900	-0.000000
C	3.198500	-2.711400	-0.655100
C	2.373100	-1.600100	-0.642100
F	-0.948200	2.666600	-1.305900
F	0.158900	5.126200	-1.294400
F	2.497300	5.542800	-0.001100
F	3.733700	3.514900	1.292300
F	2.623500	1.056500	1.304200
F	-2.226600	1.744200	1.305900
F	-4.910600	1.477600	1.294400
F	-6.049800	-0.606800	0.001500
F	-4.520800	-2.424400	-1.292000
F	-1.837100	-2.154500	-1.303800
F	-0.401800	-2.805500	1.294000
F	1.171900	-4.995800	1.282300
F	3.552600	-4.934800	0.000300
F	4.366900	-2.697300	-1.282000
F	2.790700	-0.509000	-1.294200

IMes•Al(C_6F_5)$_3$

Al	0.031700	0.118300	-0.232500
C	0.010800	-0.542600	1.754900
C	-0.598200	-1.207800	3.821300
H	-1.281700	-1.537100	4.585900
C	0.736500	-1.003700	3.840600
H	1.464700	-1.108900	4.627300
C	2.481800	-0.476500	2.193800
C	3.111900	0.766500	2.198800
C	4.456200	0.810000	1.823100
H	4.953400	1.775500	1.800200
C	5.165700	-0.329400	1.472700
C	4.509800	-1.559800	1.537800
H	5.053600	-2.467100	1.289300
C	3.174800	-1.662400	1.900300
C	2.422700	2.041100	2.579000
H	1.466700	1.876300	3.072600
H	2.235400	2.646300	1.687200
H	3.061000	2.627200	3.245000
C	6.588300	-0.247700	1.004800
H	7.064500	0.678900	1.331500
H	6.625700	-0.271100	-0.089400
H	7.179900	-1.089300	1.373600
C	2.516000	-3.008600	1.981600
H	3.142800	-3.766600	1.509100
H	1.545600	-3.021700	1.482300
H	2.355800	-3.311200	3.022200
C	-2.394900	-1.155900	2.148700
C	-2.705800	-2.343600	1.478300
C	-4.034800	-2.558600	1.126100
H	-4.289600	-3.470700	0.593800
C	-5.036700	-1.642800	1.433100
C	-4.689600	-0.504800	2.155600
H	-5.460000	0.212800	2.421100
C	-3.377700	-0.240300	2.536800
C	-1.666000	-3.367300	1.136400
H	-2.137000	-4.331800	0.939200
H	-0.943900	-3.503600	1.946200
H	-1.106500	-3.085300	0.241700
C	-6.446000	-1.859800	0.968200
H	-6.685700	-2.923000	0.896300
H	-6.585600	-1.420200	-0.025400
H	-7.166600	-1.386800	1.639100
C	-3.053700	1.001500	3.311800
H	-3.964900	1.565700	3.514900
H	-2.370700	1.647600	2.758700
H	-2.581500	0.773500	4.272500
C	0.029900	2.131900	-0.320100
C	-0.277300	3.026300	0.685700
C	-0.353500	4.397600	0.502000
C	-0.126600	4.915400	-0.763400
C	0.163500	4.060000	-1.815600
C	0.227500	2.698300	-1.568900
C	1.729300	-0.668000	-0.992800
C	2.842100	0.091500	-1.324600
C	4.006000	-0.448600	-1.850000
C	4.092500	-1.816000	-2.046100
C	3.017000	-2.622400	-1.711800
C	1.877800	-2.029800	-1.194600
C	-1.694700	-0.375500	-1.157300
C	-1.854500	-1.293200	-2.184600
C	-3.073200	-1.551800	-2.796500
C	-4.195800	-0.850100	-2.388700
C	-4.081900	0.107400	-1.394900
C	-2.844100	0.322000	-0.813900

F	-0.534600	2.578500	1.933600
F	-0.643500	5.216200	1.511900
F	-0.193600	6.225300	-0.968100
F	0.367900	4.556400	-3.032000
F	0.485600	1.899800	-2.617600
F	2.854600	1.415000	-1.115900
F	5.057500	0.322100	-2.128500
F	5.212500	-2.353100	-2.517100
F	3.107400	-3.943700	-1.852700
F	0.891400	-2.871100	-0.827400
F	-0.807300	-1.987000	-2.647000
F	-3.178400	-2.457200	-3.765900
F	-5.378000	-1.094000	-2.944200
F	-5.161800	0.783000	-1.002100
F	-2.791100	1.270900	0.137400
N	-1.026400	-0.926600	2.542000
N	1.095400	-0.603800	2.572600

$Al(C{\equiv}CtBu)_3$

Al	-0.001100	-0.004400	-0.007900
C	1.581300	-1.044800	-0.008000
C	2.600100	-1.711600	-0.005700
C	0.109300	1.886100	-0.006700
C	0.178900	3.101700	-0.003900
C	-1.694000	-0.853100	-0.006000
C	-2.783600	-1.396700	-0.001100
C	3.826400	-2.510700	0.000200
C	0.264300	4.563000	0.000900
C	-4.093100	-2.050500	0.002900
C	4.432000	-2.483900	1.412200
H	3.735900	-2.903400	2.142800
H	5.352800	-3.075800	1.430800
H	4.670700	-1.461300	1.714600
C	3.494300	-3.957000	-0.395800
H	3.056000	-3.996100	-1.396100
H	4.406700	-4.562200	-0.393100
H	2.782800	-4.399200	0.305900
C	4.823900	-1.911500	-1.003000
H	4.409900	-1.916100	-2.014400
H	5.069800	-0.880100	-0.739100
H	5.746800	-2.500200	-1.003700
C	0.893400	5.022700	1.325200
H	1.897400	4.607800	1.443800
H	0.964200	6.115000	1.341700
H	0.287900	4.702100	2.176500
C	-1.145600	5.156200	-0.139200
H	-1.090800	6.249700	-0.137100
H	-1.612300	4.834900	-1.073600
H	-1.785700	4.839500	0.687900
C	1.140700	5.019200	-1.175600
H	2.148200	4.604100	-1.094500
H	0.713300	4.696300	-2.128100
H	1.213800	6.111500	-1.181200
C	-5.133700	-1.098300	0.611100
H	-5.201800	-0.174600	0.031300
H	-6.117800	-1.577800	0.618200
H	-4.868900	-0.837200	1.638700
C	-4.013300	-3.338200	0.836700
H	-4.987500	-3.837600	0.842700
H	-3.273200	-4.026100	0.420600
H	-3.731200	-3.117400	1.869200
C	-4.483900	-2.392400	-1.443400
H	-4.541700	-1.488900	-2.055300
H	-3.752300	-3.066400	-1.895800
H	-5.462400	-2.883000	-1.455600

IMe

N	-1.054900	-0.704500	0.000000
N	1.055000	-0.704400	-0.000100
C	0.000000	-1.561900	-0.000000
C	-0.679400	0.635000	0.000000
C	0.679400	0.635000	-0.000100
C	-2.421400	-1.167100	-0.000000
H	-2.388700	-2.255300	0.000000
H	-2.958000	-0.822700	-0.889600
H	-2.958200	-0.822600	0.889400
C	2.421400	-1.167100	0.000100
H	2.388800	-2.255200	0.000100
H	2.958100	-0.822600	0.889600
H	2.958300	-0.822700	-0.889300
C	-1.654000	1.755200	0.000100
H	-1.133100	2.714500	-0.000100
H	-2.302500	1.732100	0.883000
H	-2.302800	1.731900	-0.882700
C	1.653800	1.755300	-0.000000
H	1.132700	2.714600	-0.000800
H	2.303000	1.731900	-0.882500
H	2.302000	1.732800	0.883200

IMe•Al(C≡CtBu)$_3$

Al	0.250900	0.113200	-0.289400
N	-0.088300	-0.803700	2.704100
C	2.182800	-0.059800	-0.153600
N	-1.942700	-0.334000	1.758800
C	3.398300	-0.144000	-0.151300
C	-0.582000	-1.199100	-1.459700
C	-1.085500	-2.043500	-2.179400
C	-0.346800	1.936100	-0.627000
C	-0.718000	3.077500	-0.838300
C	-0.610900	-0.356500	1.544600
C	-1.077300	-1.066800	3.637900
C	-2.260200	-0.770900	3.032900
C	1.326300	-0.987300	2.966100
H	1.887900	-0.730100	2.067800
H	1.525000	-2.028800	3.228500
H	1.642800	-0.341900	3.789300
C	-2.921800	0.041500	0.754200
H	-2.458700	0.731200	0.048700
H	-3.762300	0.541500	1.237100
H	-3.271800	-0.841900	0.215600
C	-0.775400	-1.569600	5.000700
H	-1.697800	-1.713400	5.564900
H	-0.148600	-0.868700	5.561500
H	-0.251300	-2.530400	4.970300
C	-3.653900	-0.856200	3.535600
H	-3.664400	-1.269800	4.544800
H	-4.272200	-1.502200	2.904400
H	-4.132100	0.128000	3.575300
C	-1.152400	4.451600	-1.110600
C	-1.150200	4.693500	-2.628400
H	-0.150000	4.548300	-3.043600
H	-1.473800	5.717900	-2.845500
H	-1.829000	4.000300	-3.132600
C	-2.569400	4.658300	-0.559800
H	-3.271700	3.962900	-1.027400
H	-2.906900	5.680100	-0.762100
H	-2.591600	4.492500	0.520700
C	-0.188000	5.435300	-0.430400
H	0.829100	5.299400	-0.805300
H	-0.173500	5.278900	0.651700

H	-0.497200	6.467400	-0.628900
C	4.862200	-0.235000	-0.170100
C	5.366100	-0.701300	1.203900
H	5.071600	0.004000	1.985900
H	6.458600	-0.774100	1.199200
H	4.956800	-1.684100	1.454400
C	5.294100	-1.241400	-1.246500
H	4.944400	-0.925200	-2.232500
H	4.878000	-2.231300	-1.042600
H	6.386400	-1.320500	-1.272700
C	5.447900	1.149200	-0.490000
H	5.151600	1.879300	0.267500
H	5.091300	1.504900	-1.459800
H	6.542100	1.100600	-0.517400
C	-1.660700	-3.060300	-3.066900
C	-3.121000	-3.328800	-2.673600
H	-3.185800	-3.677800	-1.639400
H	-3.554300	-4.094900	-3.325500
H	-3.717800	-2.417900	-2.769400
C	-0.848000	-4.358300	-2.940700
H	0.199000	-4.187200	-3.204400
H	-1.255600	-5.126300	-3.607000
H	-0.881500	-4.736600	-1.915300
C	-1.604500	-2.556100	-4.516400
H	-0.571200	-2.366900	-4.817900
H	-2.165700	-1.624100	-4.621400
H	-2.034600	-3.301200	-5.194400

$Al((CH_2)_3CH_3)_3$

Al	0.072900	-0.729000	0.137000
C	0.006100	1.094600	0.897700
H	-0.821700	1.165800	1.617500
H	0.921800	1.300100	1.468700
C	-0.172800	2.186300	-0.170000
H	-1.085700	2.000200	-0.754000
H	0.654400	2.148500	-0.893700
C	-0.246500	3.600900	0.399800
H	-1.076500	3.650100	1.115800
H	0.664900	3.796600	0.978500
C	-0.421000	4.671900	-0.668100
H	-0.469500	5.673300	-0.231000
H	-1.342200	4.514600	-1.238800
H	0.412100	4.660800	-1.378700
C	1.797700	-1.619100	-0.232000
H	1.802300	-1.917000	-1.292500
H	1.806500	-2.577300	0.311500
C	3.074000	-0.836800	0.087700
H	3.079000	0.114700	-0.462000
H	3.086100	-0.556400	1.150100
C	4.361800	-1.591000	-0.231200
H	4.359700	-1.864900	-1.294100
H	4.365300	-2.538100	0.323400
C	5.621200	-0.799500	0.093700
H	6.526800	-1.364300	-0.145700
H	5.662700	-0.542200	1.157300
H	5.655800	0.137400	-0.472000
C	-1.591000	-1.677800	-0.347000
H	-1.610200	-1.766600	-1.445500
H	-1.509000	-2.719000	0.001100
C	-2.911600	-1.073200	0.136600
H	-2.914900	-1.007100	1.233500
H	-3.001500	-0.036200	-0.215400
C	-4.149300	-1.848300	-0.306800
H	-4.066100	-2.883600	0.048200
H	-4.158300	-1.906200	-1.402800

C	-5.453600	-1.237900	0.187100
H	-6.321400	-1.814900	-0.145300
H	-5.575600	-0.214100	-0.181900
H	-5.481900	-1.197600	1.281100

Dipp•Al($(CH_2)_3CH_3)_3$

Al	-0.258200	-0.294500	1.168600
C	-2.257800	-0.520900	1.181300
H	-2.736800	0.341100	0.694000
H	-2.585600	-1.387900	0.590900
C	-2.833100	-0.646800	2.596800
H	-2.516700	0.208600	3.211500
H	-2.415900	-1.530800	3.098200
C	-4.357000	-0.739300	2.647700
H	-4.782500	0.148900	2.161900
H	-4.680600	-1.595600	2.041500
C	-4.913000	-0.869000	4.059800
H	-6.005700	-0.932400	4.064500
H	-4.627900	-0.009500	4.676000
H	-4.526600	-1.766800	4.554100
C	0.804100	-1.947100	1.601100
H	1.858000	-1.645400	1.703600
H	0.783600	-2.663600	0.765000
C	0.382500	-2.678800	2.878400
H	0.368600	-1.979300	3.726600
H	-0.652000	-3.036900	2.780500
C	1.268900	-3.866600	3.249000
H	2.302600	-3.515000	3.366300
H	1.283600	-4.573500	2.408500
C	0.826100	-4.585600	4.516600
H	1.479700	-5.429800	4.757300
H	-0.193000	-4.973600	4.413700
H	0.831200	-3.906600	5.376000
C	0.234200	1.251200	2.354100
H	0.135800	0.821300	3.365900
H	1.295900	1.524500	2.280100
C	-0.644500	2.500300	2.279000
H	-0.445900	3.047600	1.344600
H	-1.702300	2.207300	2.217200
C	-0.492200	3.469500	3.450200
H	0.559400	3.771100	3.539200
H	-0.727200	2.933500	4.378700
C	-1.373400	4.706400	3.335600
H	-1.255200	5.374000	4.194600
H	-2.431600	4.430600	3.273600
H	-1.132800	5.281900	2.434400
C	0.357200	0.127100	-0.846400
N	-0.402400	0.105800	-1.972500
N	1.605600	0.413100	-1.309700
C	0.346700	0.367700	-3.101100
H	-0.091700	0.386200	-4.084500
C	1.613800	0.562900	-2.681800
H	2.514200	0.793100	-3.225000
C	-1.806800	-0.192200	-2.069200
C	-2.720500	0.870000	-2.052500
C	-4.066800	0.558800	-2.228500
H	-4.803000	1.355100	-2.214400
C	-4.480700	-0.751400	-2.411300
H	-5.535100	-0.972100	-2.541100
C	-3.553200	-1.780200	-2.422800
H	-3.888300	-2.802600	-2.562400
C	-2.193200	-1.525300	-2.255000
C	-2.284100	2.312100	-1.881200
H	-1.261800	2.307500	-1.491500
C	-3.146600	3.071900	-0.873400

H	-3.191200	2.552000	0.085900
H	-4.169500	3.209700	-1.237000
H	-2.726700	4.066700	-0.698900
C	-2.271200	3.035000	-3.232100
H	-1.610800	2.542500	-3.951000
H	-1.929300	4.067600	-3.111600
H	-3.275900	3.060800	-3.666000
C	-1.199700	-2.669900	-2.301600
H	-0.215600	-2.279200	-2.027600
C	-1.093600	-3.237500	-3.720100
H	-0.804200	-2.467800	-4.441400
H	-2.049600	-3.657800	-4.047900
H	-0.346500	-4.036200	-3.757400
C	-1.542500	-3.769500	-1.295200
H	-1.600700	-3.373000	-0.279300
H	-0.773000	-4.547000	-1.313600
H	-2.498500	-4.247300	-1.530600
C	2.819400	0.514300	-0.537700
C	3.171300	1.759800	0.005600
C	4.375400	1.835500	0.703000
H	4.673200	2.776500	1.150000
C	5.196400	0.727200	0.838200
H	6.126500	0.808500	1.391300
C	4.836300	-0.481900	0.267600
H	5.490600	-1.339400	0.375100
C	3.642800	-0.617900	-0.440200
C	2.318800	2.998600	-0.198700
H	1.275300	2.673700	-0.260800
C	2.417600	3.997700	0.951500
H	2.243400	3.520800	1.917700
H	1.666600	4.782100	0.823700
H	3.395000	4.490200	0.977400
C	2.685700	3.696200	-1.514800
H	2.544200	3.047900	-2.382000
H	3.732600	4.015700	-1.499000
H	2.064000	4.585400	-1.657900
C	3.311200	-1.932800	-1.122200
H	2.228500	-1.963400	-1.280000
C	3.686000	-3.159400	-0.290800
H	3.259400	-3.112600	0.712200
H	4.771200	-3.274600	-0.206600
H	3.306200	-4.062400	-0.777600
C	4.000500	-2.012300	-2.490500
H	3.714800	-1.189300	-3.149200
H	3.742200	-2.949500	-2.993200
H	5.088400	-1.982300	-2.372200

SitBu

C	0.755200	1.652000	0.089100
C	-0.755200	1.652000	-0.089100
H	1.040900	1.962600	1.104000
H	1.262500	2.303900	-0.624000
H	-1.262600	2.303800	0.624000
H	-1.040800	1.962700	-1.104000
N	-1.071000	0.232600	0.130000
N	1.071000	0.232600	-0.130200
C	0.000000	-0.567500	-0.000100
C	2.449100	-0.272100	-0.005900
C	-2.449100	-0.272100	0.006000
C	-2.801900	-0.438200	-1.475800
H	-3.830300	-0.792500	-1.594600
H	-2.711900	0.510200	-2.015400
H	-2.126100	-1.162900	-1.936800
C	-2.547600	-1.618800	0.716700
H	-1.836800	-2.327100	0.291300

H	-2.315500	-1.507700	1.779500
H	-3.563500	-2.013200	0.618100
C	-3.410900	0.715200	0.667000
H	-4.421900	0.299900	0.661200
H	-3.124700	0.899000	1.706900
H	-3.446900	1.673400	0.140300
C	3.410900	0.715400	-0.666500
H	3.446500	1.673600	-0.139900
H	4.422000	0.300400	-0.660300
H	3.125100	0.899200	-1.706500
C	2.547800	-1.618600	-0.717000
H	1.837300	-2.327300	-0.291900
H	2.315700	-1.507200	-1.779800
H	3.563900	-2.012800	-0.618600
C	2.801600	-0.438500	1.475800
H	3.829900	-0.793200	1.594700
H	2.711800	0.509700	2.015700
H	2.125500	-1.163200	1.936500

SItBu•$AlMe_3$

C	0.718500	-2.354500	-0.667500
C	-0.769400	-2.417000	-0.408600
H	0.958000	-2.365600	-1.738200
H	1.248600	-3.175800	-0.189600
H	-1.333700	-2.781200	-1.269800
H	-1.002600	-3.054400	0.449700
N	-1.100800	-1.018500	-0.115100
N	1.077200	-1.054900	-0.093500
C	-0.003000	-0.253600	0.030600
C	2.508500	-0.740500	0.139800
C	-2.529200	-0.680600	0.125700
C	-3.235400	-1.903300	0.729600
H	-4.269100	-1.624000	0.944500
H	-3.266900	-2.759400	0.051400
H	-2.772500	-2.210900	1.671700
C	-2.664400	0.445200	1.143800
H	-2.174200	0.177200	2.083000
H	-2.251600	1.387200	0.792800
H	-3.726600	0.609600	1.345400
C	-3.195800	-0.337500	-1.207400
H	-4.254700	-0.110800	-1.052800
H	-2.721100	0.526700	-1.669200
H	-3.134600	-1.184000	-1.899300
C	3.209400	-2.005100	0.656800
H	3.302600	-2.781300	-0.107000
H	4.221900	-1.735400	0.965000
H	2.693100	-2.419400	1.528100
C	2.643600	0.311600	1.235700
H	2.205800	1.269400	0.965000
H	2.175200	-0.038100	2.159500
H	3.705500	0.483500	1.431200
C	3.174900	-0.313900	-1.169100
H	4.235100	-0.103700	-1.000400
H	3.112100	-1.114600	-1.913300
H	2.707300	0.581200	-1.574900
Al	0.024700	1.974500	-0.031900
C	-1.451900	2.630900	-1.229200
H	-2.496900	2.600200	-0.905500
H	-1.208700	3.694800	-1.364500
H	-1.403700	2.194900	-2.236100
C	1.613200	2.694200	-1.031300
H	1.402200	3.774200	-1.048000
H	2.627600	2.594800	-0.633300
H	1.638000	2.391500	-2.086400
C	-0.049700	2.571200	1.878900

H	0.797900	3.227600	2.114000
H	-0.956800	3.153800	2.084600
H	-0.027900	1.754800	2.610700

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