Supporting Information

Aryl-NHC-group 13 Trimethyl Complexes: Structural, Stability and Bonding Insights.

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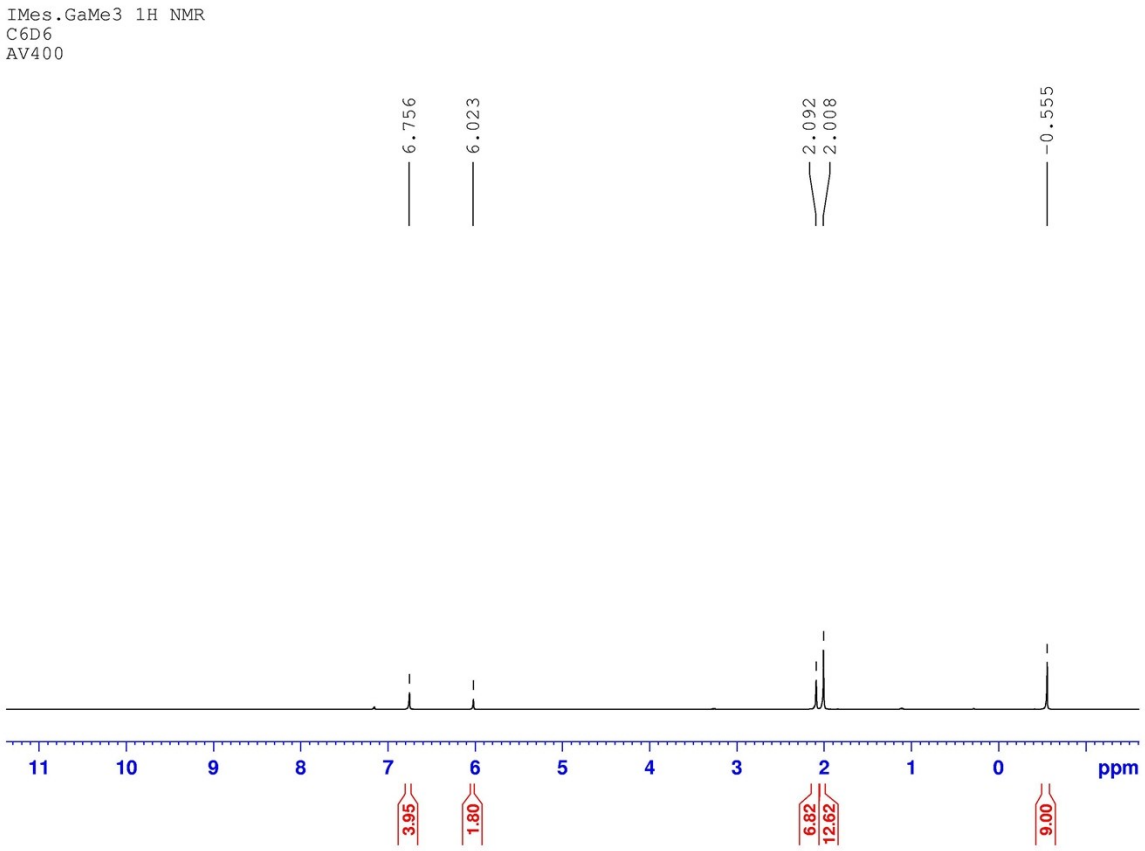
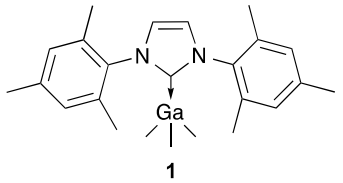
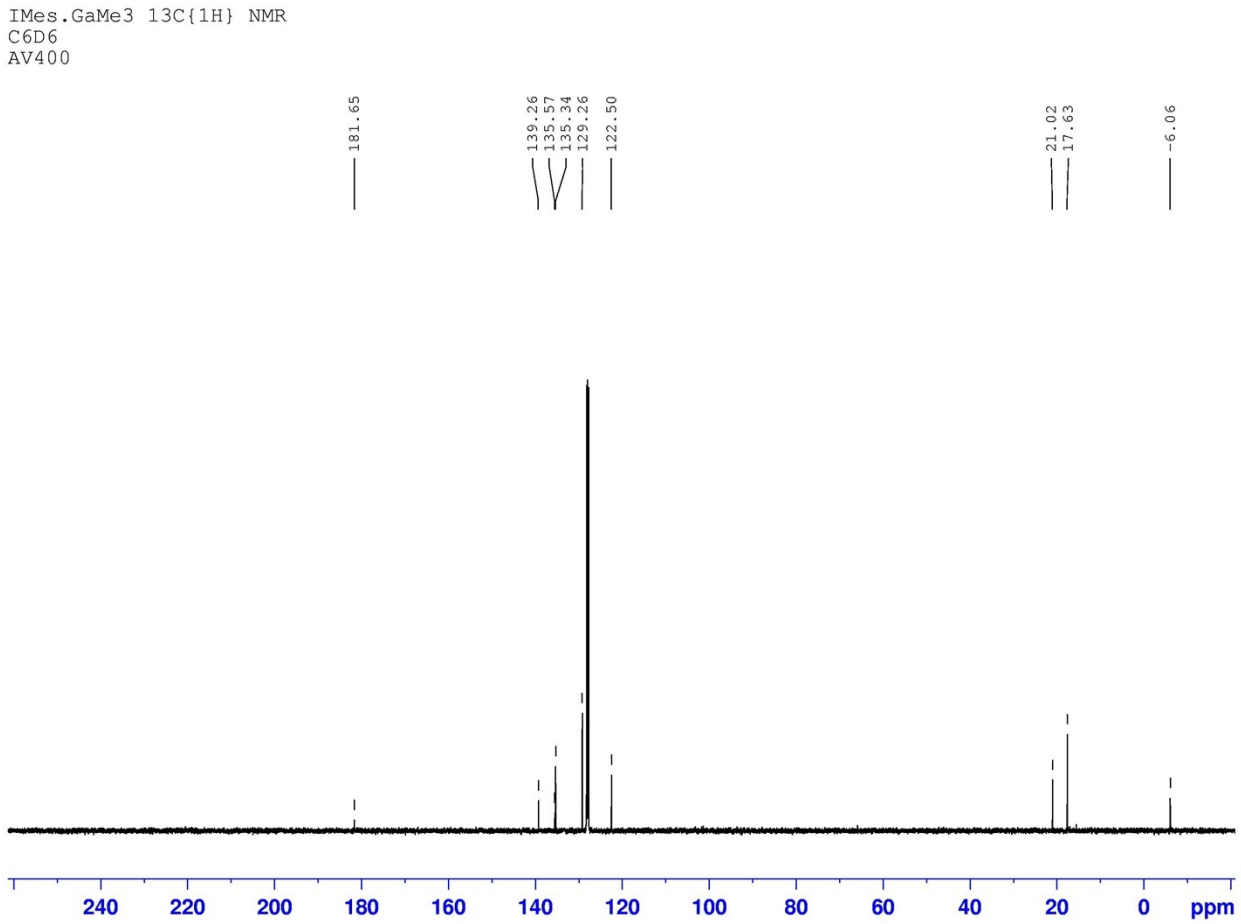
^{1}H and ^{13}C NMR Spectroscopic studies for complexes **1-8**

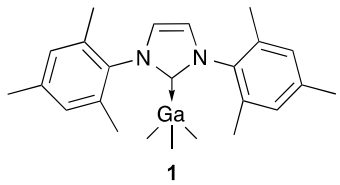




1

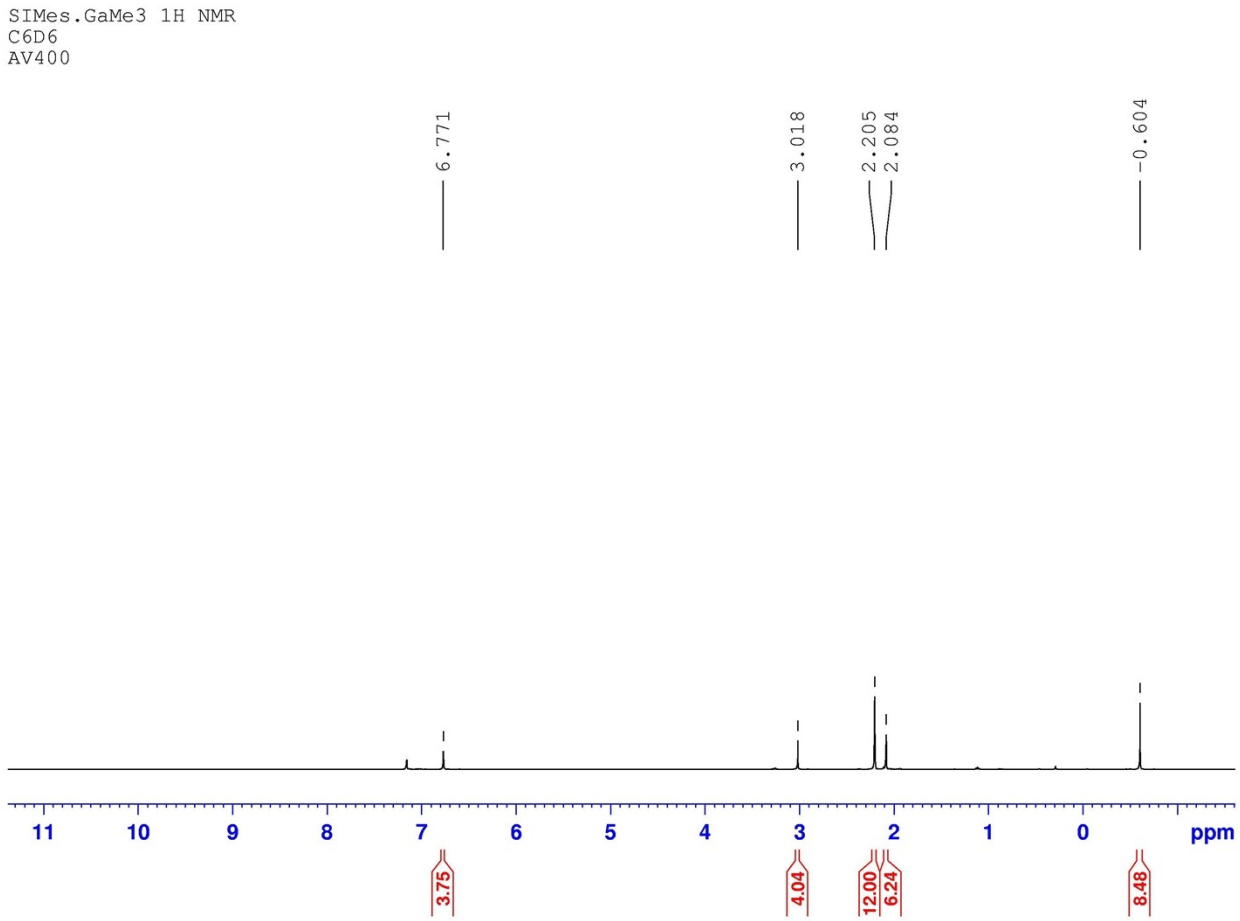
Figure S1. IMes•$GaMe_3$ (**1**) ^{1}H NMR spectrum.





1

Figure S2. IMes•$GaMe_3$ (**1**) $^{13}C\{^1H\}$ NMR spectrum.



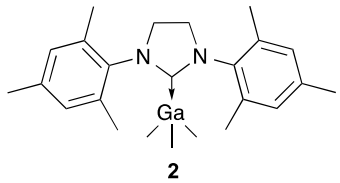


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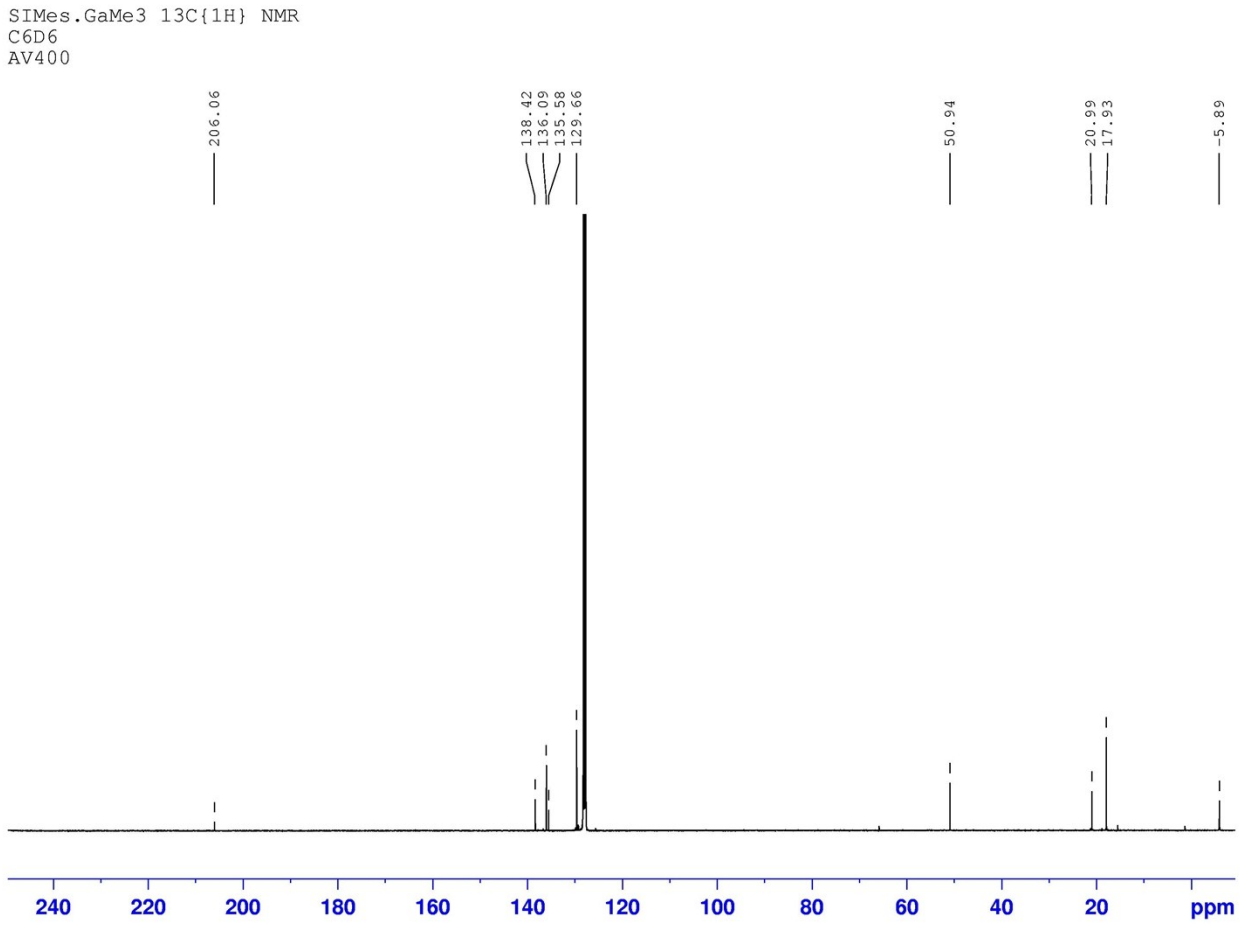
Figure S3. SIMes•$GaMe_3$ (**2**) ^{1}H NMR spectrum.



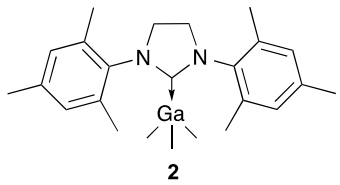


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Figure S4. SIMes•$GaMe_3$ (**2**) $^{13}C\{^1H\}$ NMR spectrum.

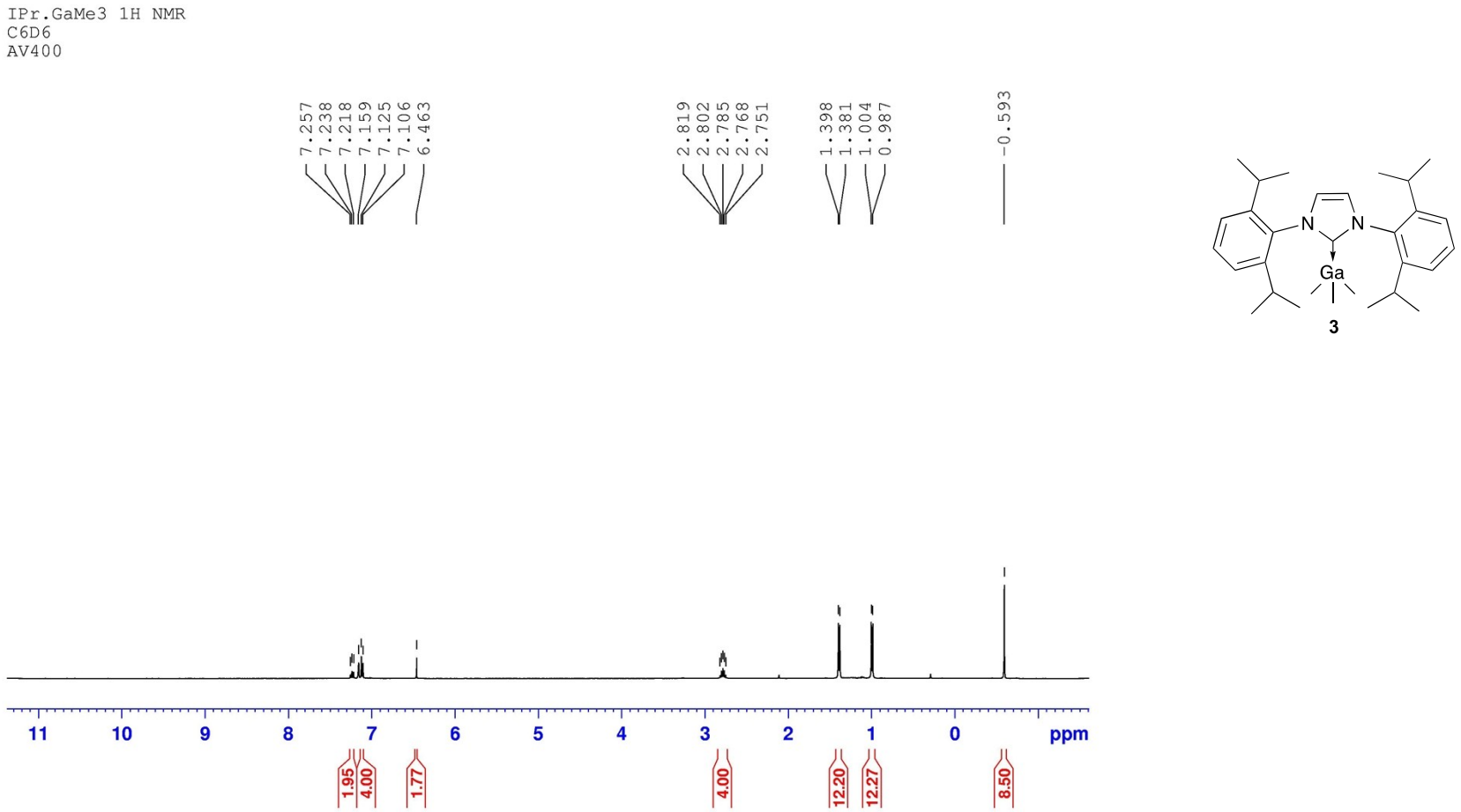
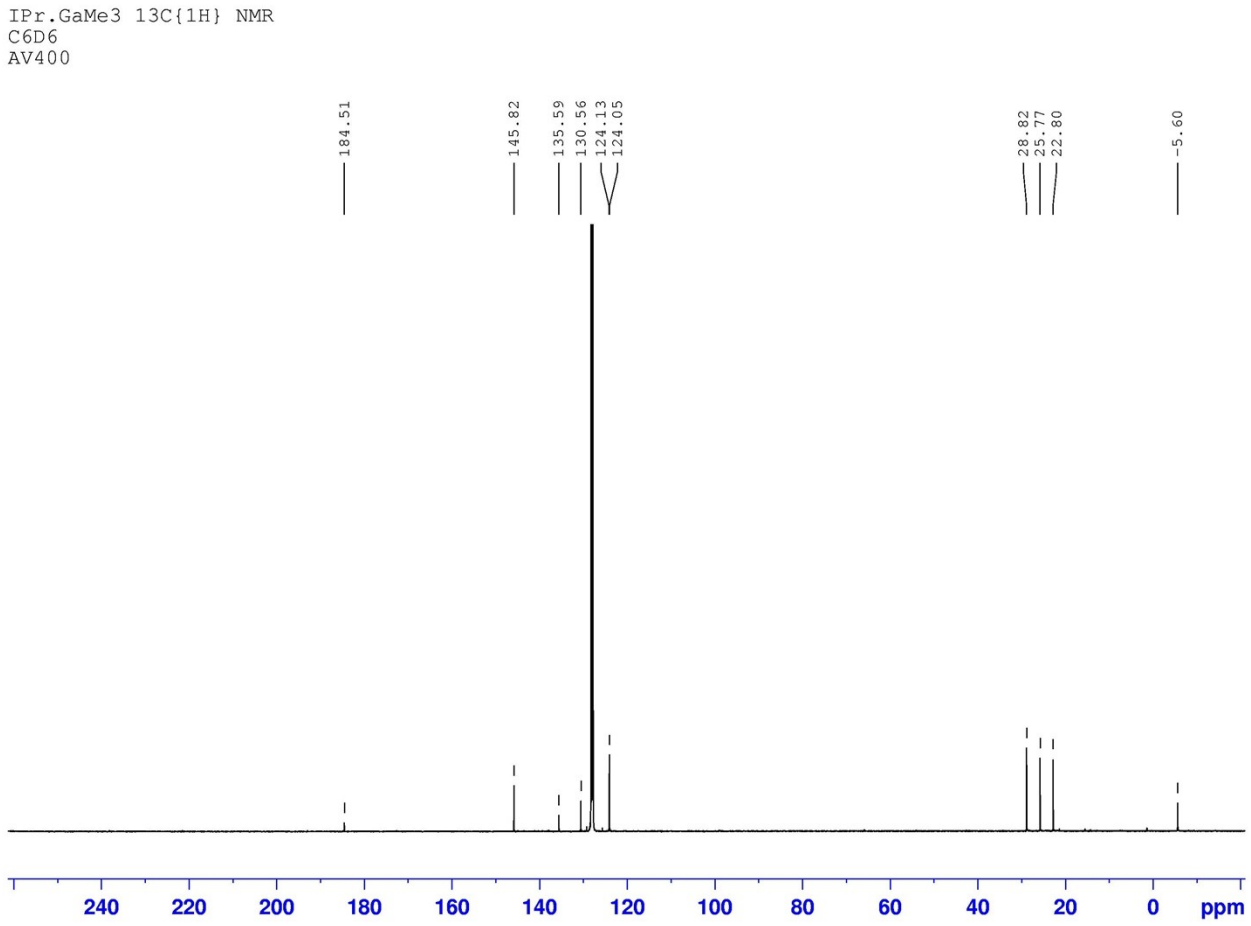


Figure S5. IPr•$GaMe_3$ (**3**) ^1H NMR spectrum.



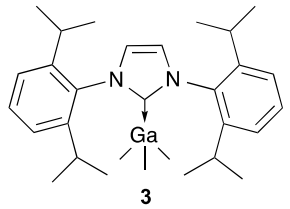


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Figure S6. IPr•$GaMe_3$ (**3**) $^{13}C\{^1H\}$ NMR spectrum.

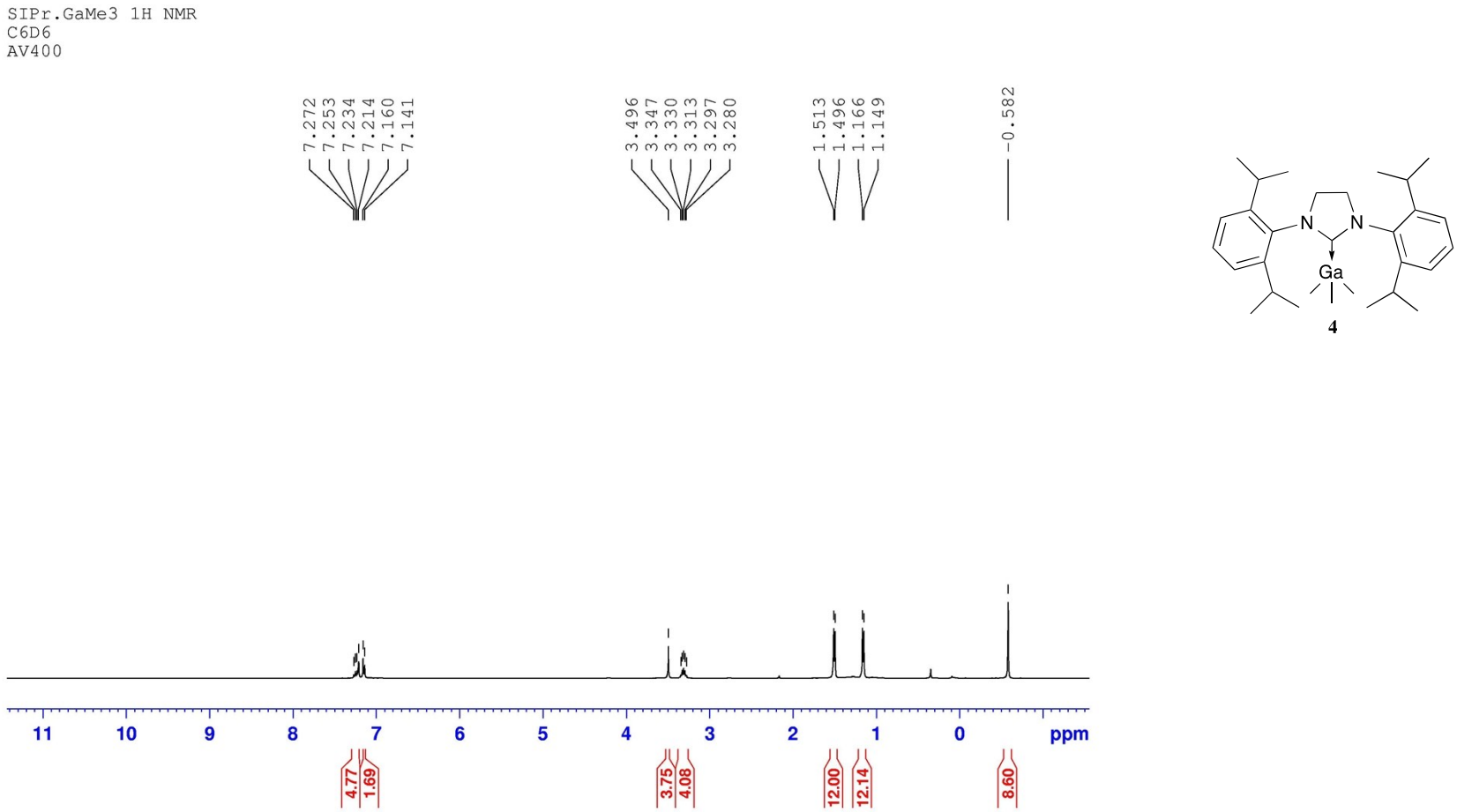
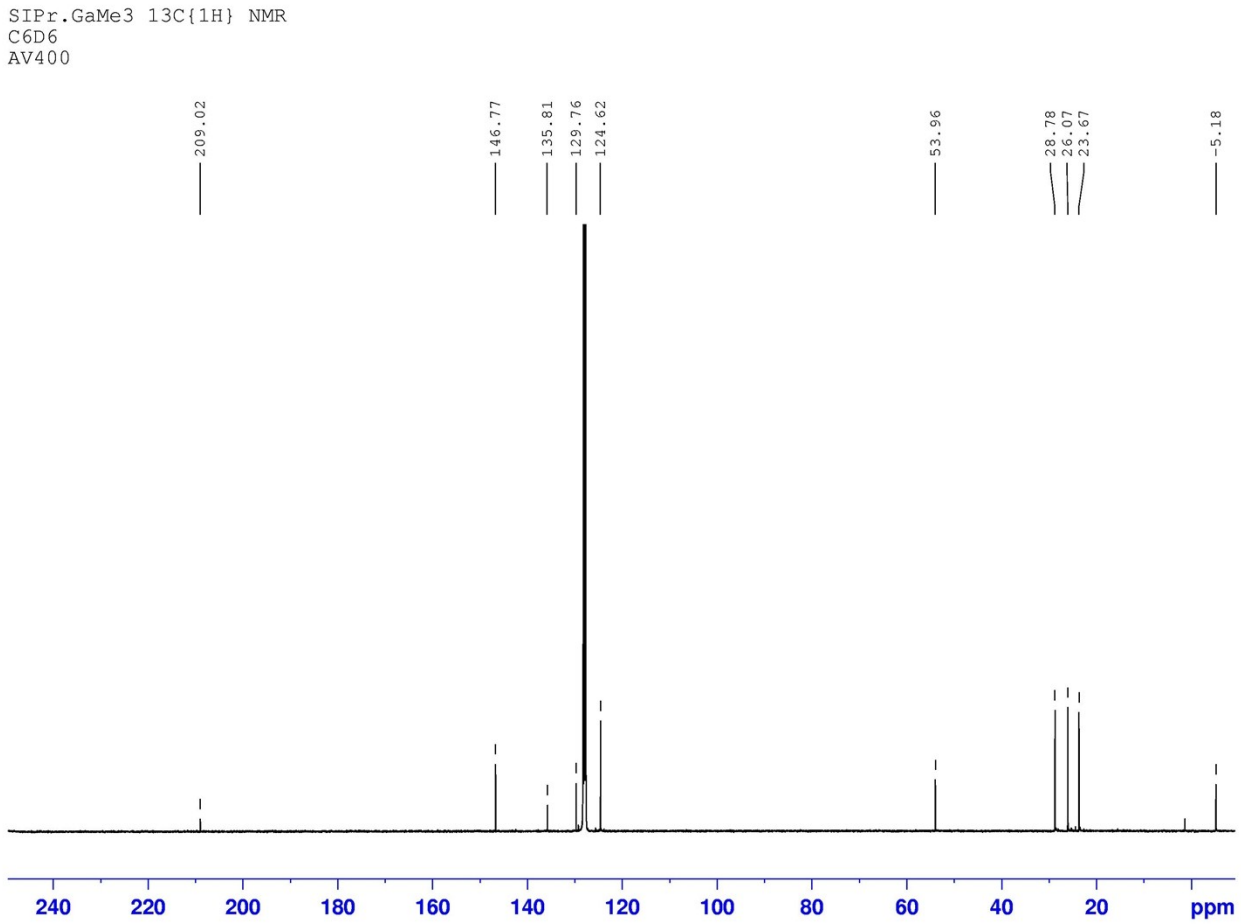


Figure S7. SIPr•$GaMe_3$ (**4**) ^{1}H NMR spectrum.



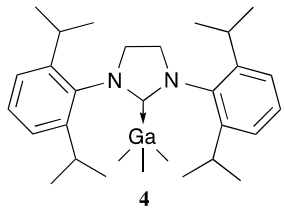


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Figure S8. SIPr•$GaMe_3$ (**4**) $^{13}C\{^1H\}$ NMR spectrum.

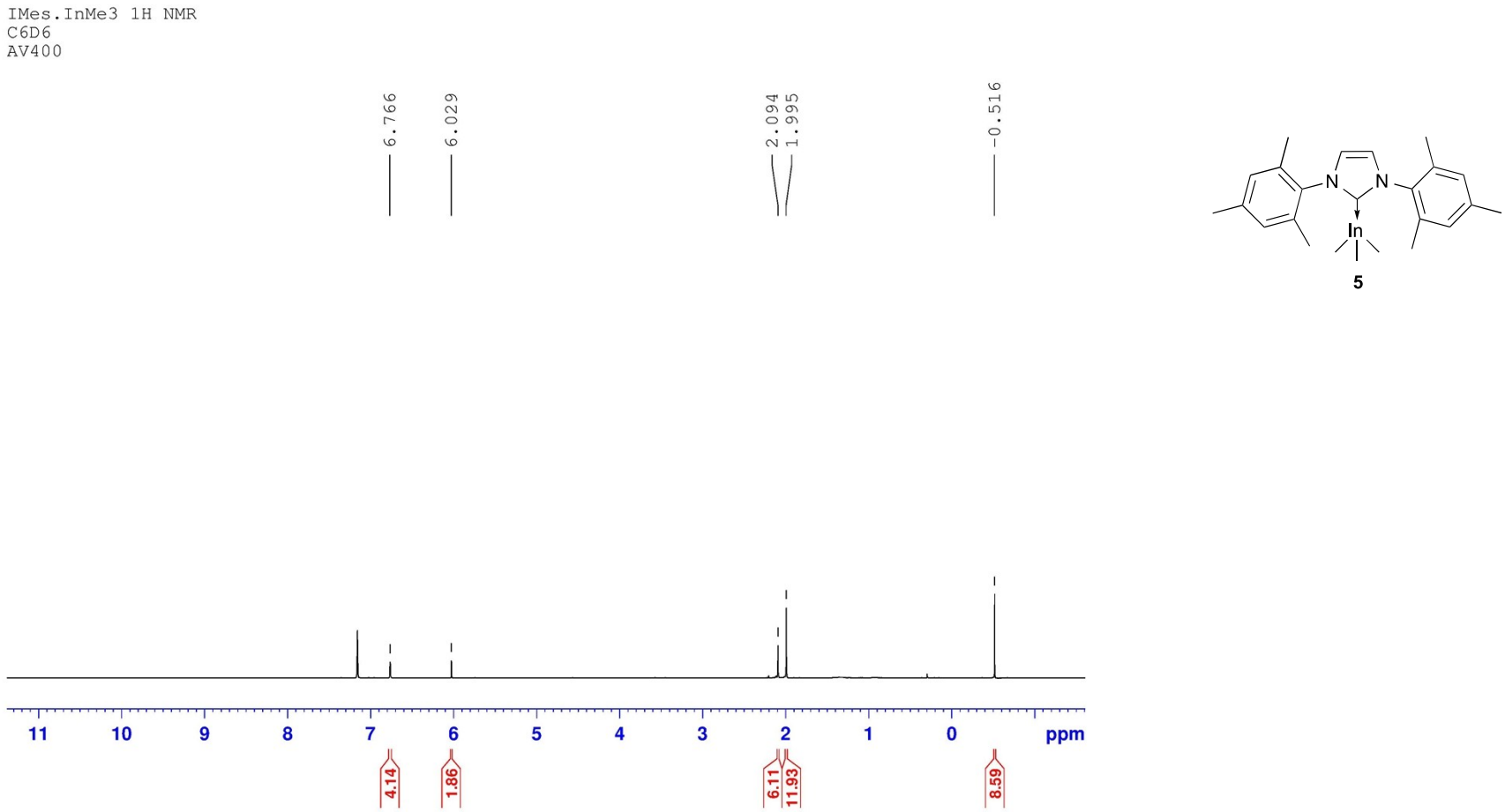
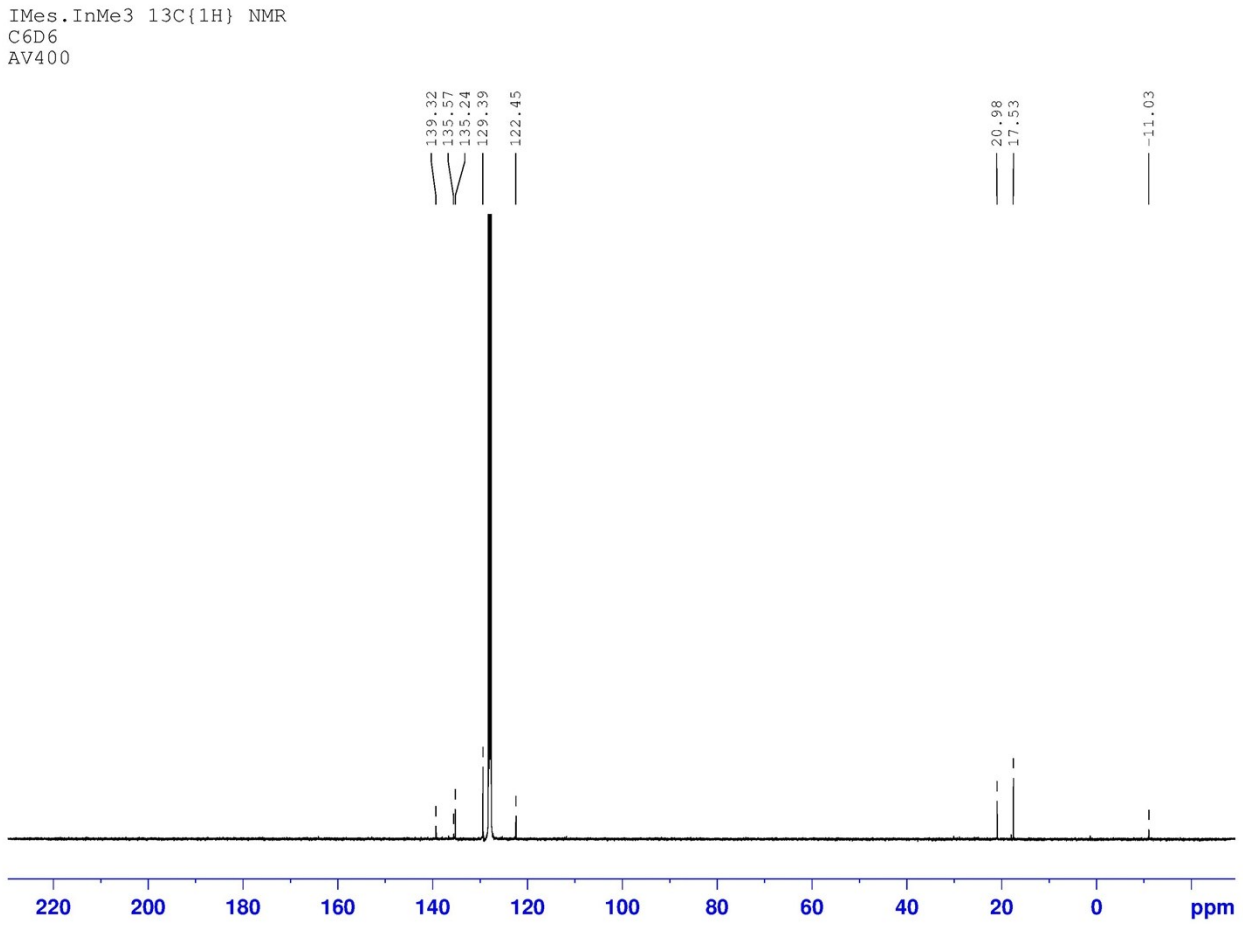


Figure S9. IMes•$InMe_3$ (**5**) ^1H NMR spectrum.



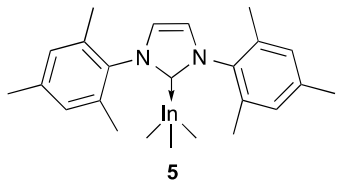


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Figure S10. IMes•$InMe_3$ (**5**) $^{13}C\{^1H\}$ NMR spectrum.

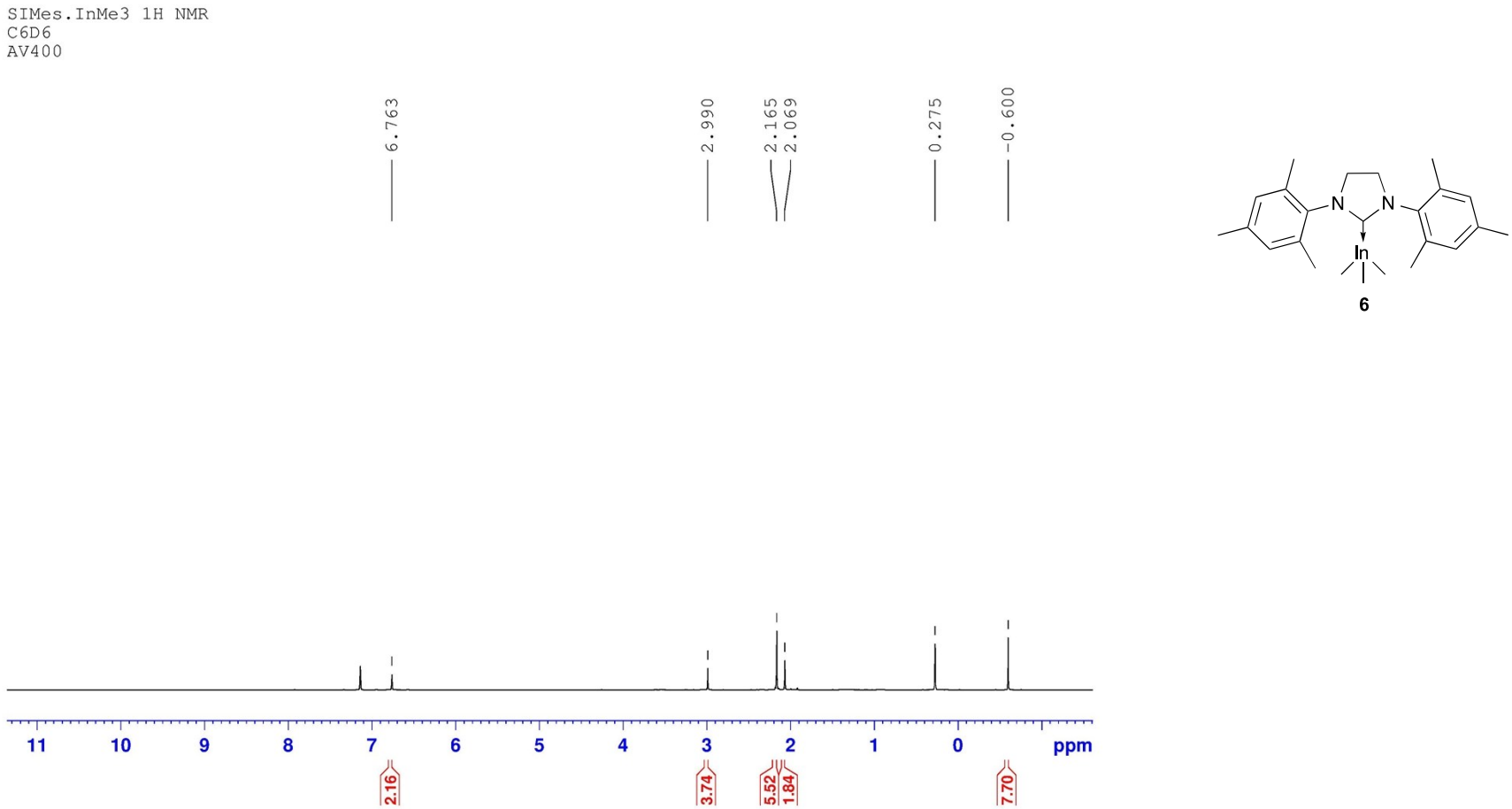
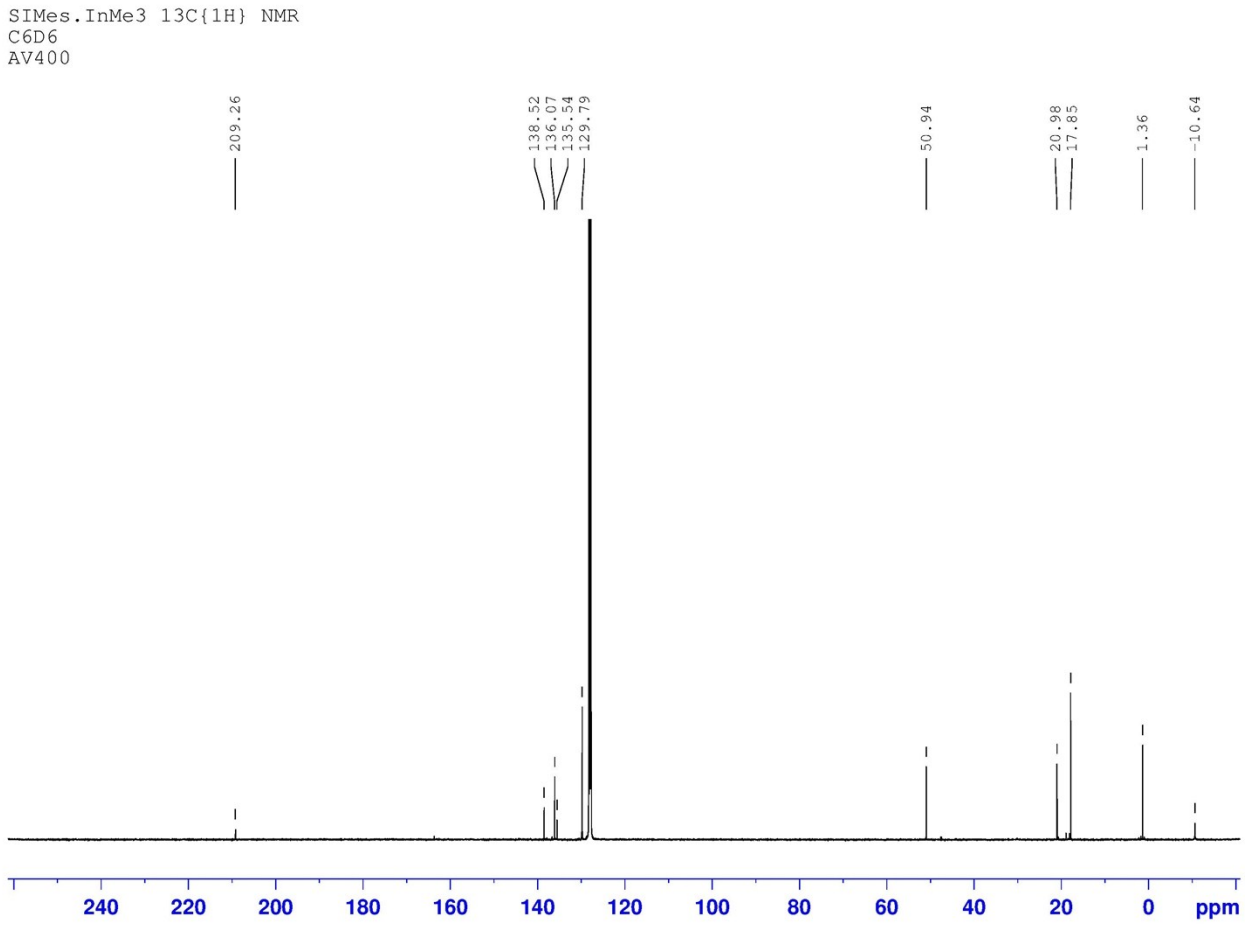


Figure S11. SIMes•$InMe_3$ (**6**) **^{1}H NMR spectrum.**



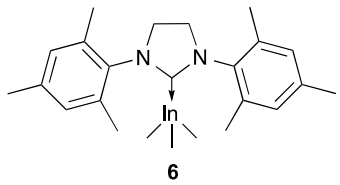


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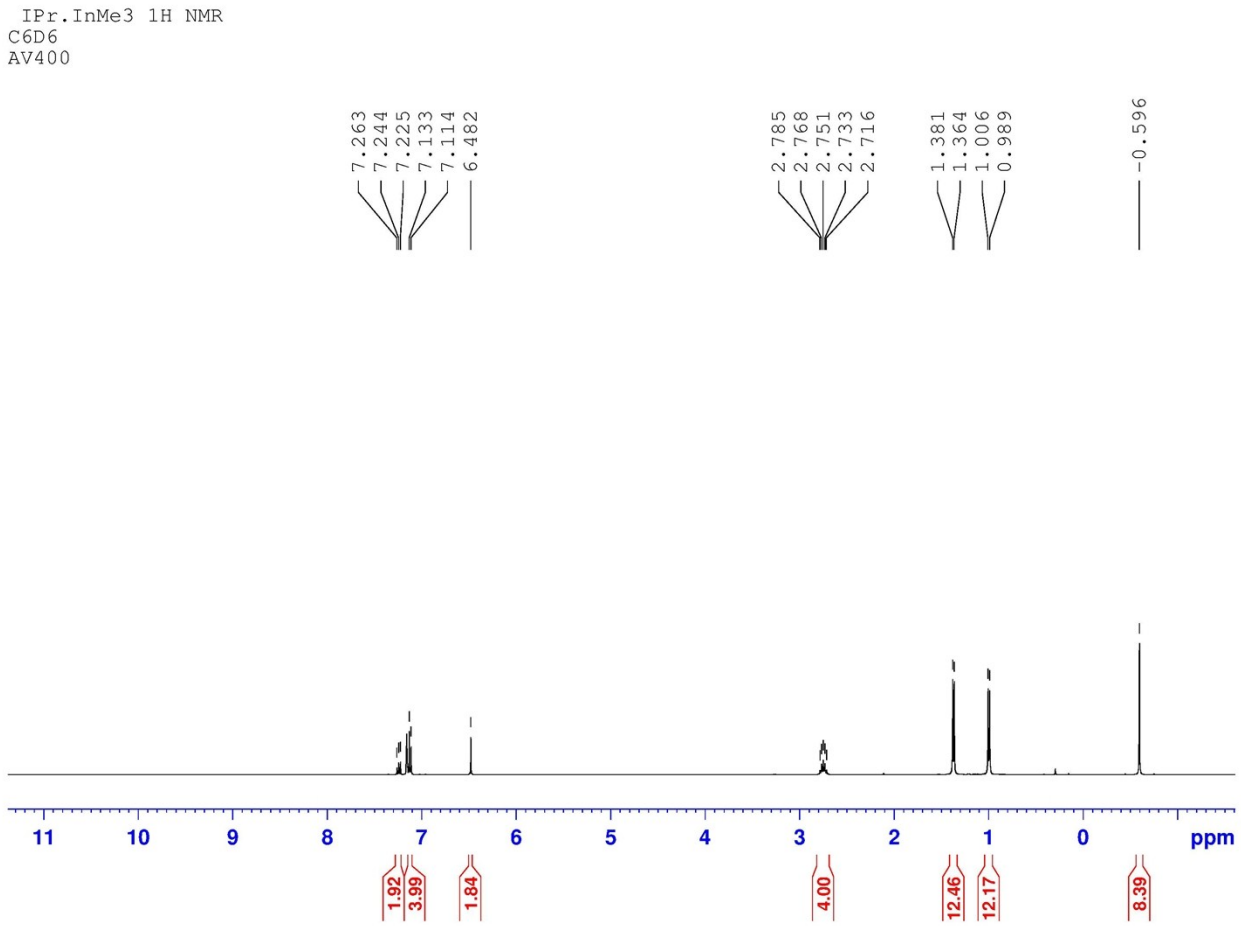
Figure S12. SIMes•$InMe_3$ (**6**) $^{13}C\{^1H\}$ NMR spectrum.



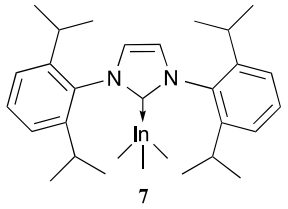


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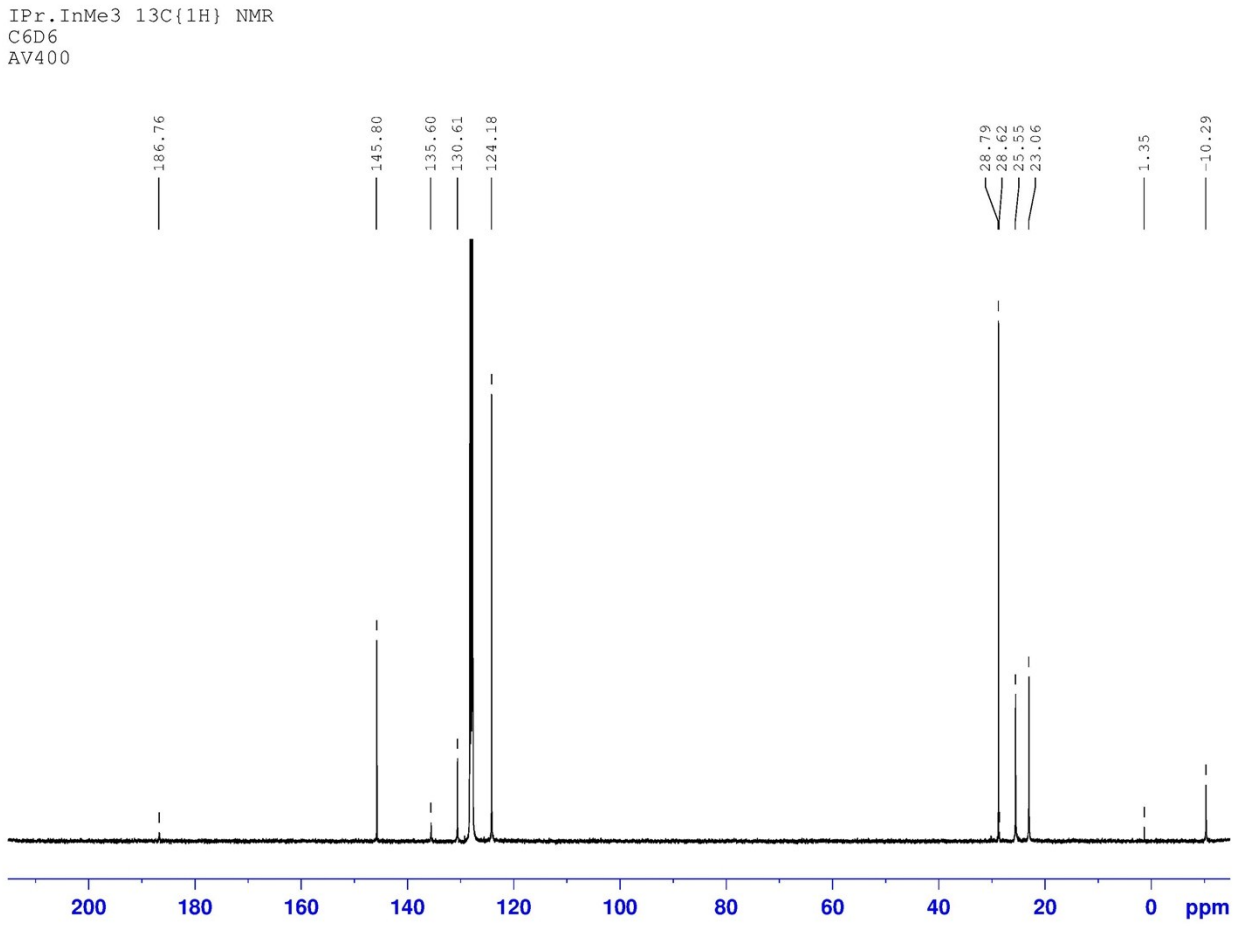
Figure S13. IPr•$InMe_3$ (**7**) ^1H NMR spectrum.



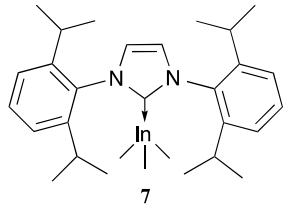


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Figure S14. IPr•$InMe_3$ (**7**) $^{13}C\{^1H\}$ NMR spectrum.

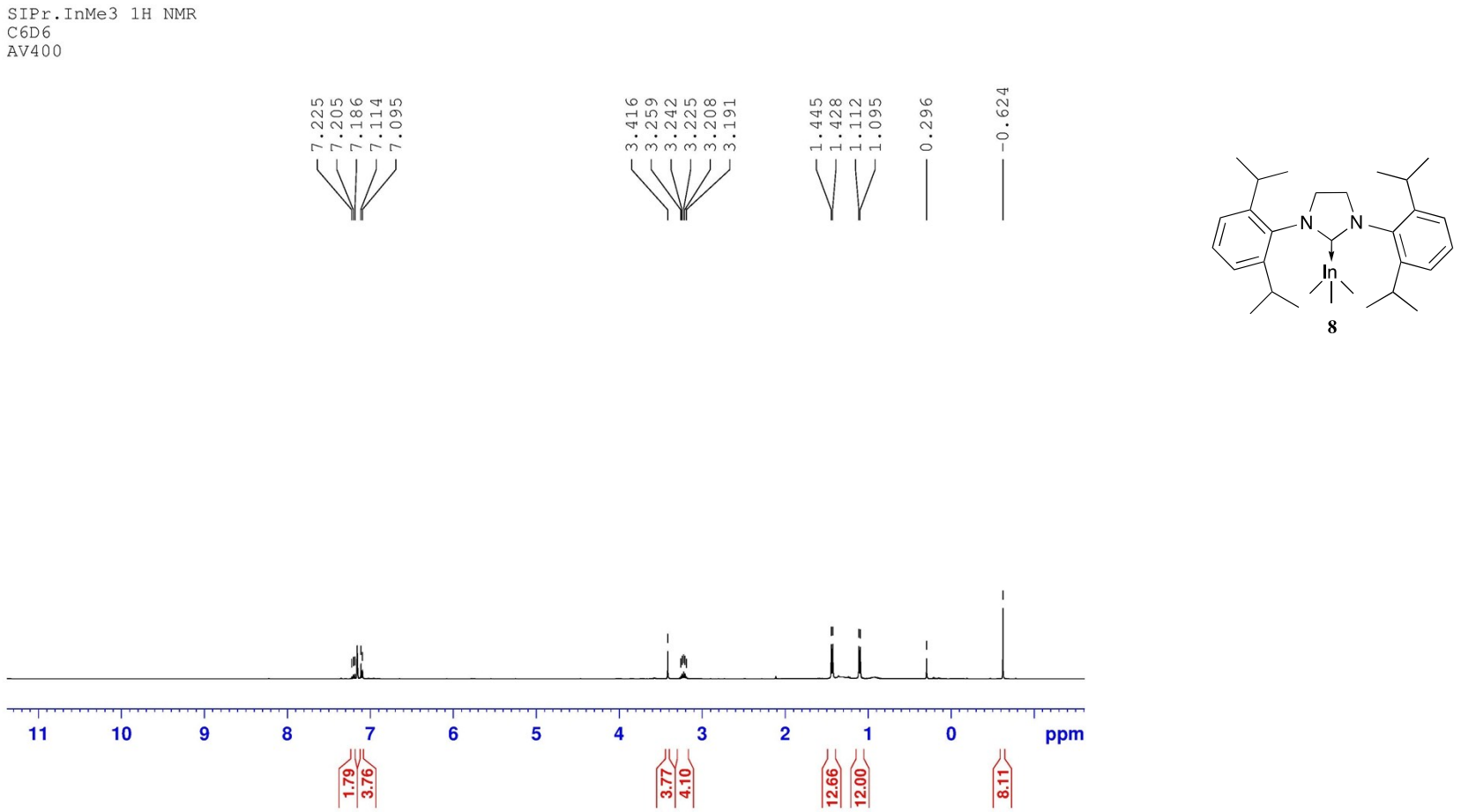
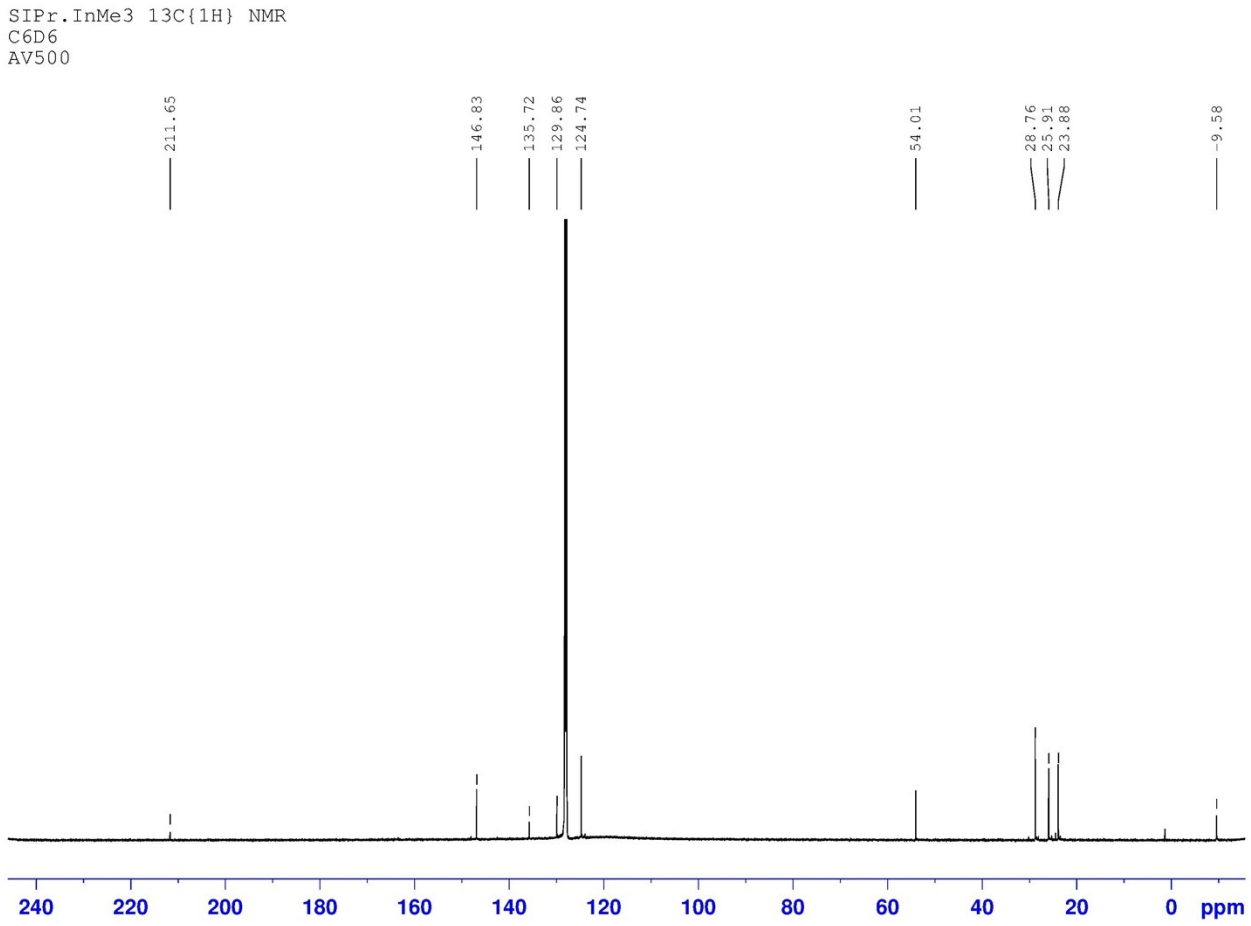


Figure S15. SIPr•$InMe_3$ (**8**) ^1H NMR spectrum.



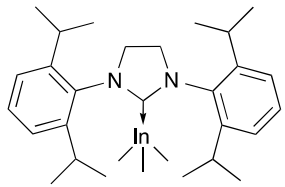


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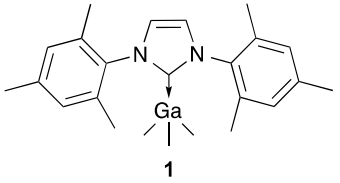
Figure S16. SIPr•$InMe_3$ (**8**) $^{13}C\{^1H\}$ NMR spectrum.

FTIP and HRMS spectroscopic studies for complexes **1-8**



1

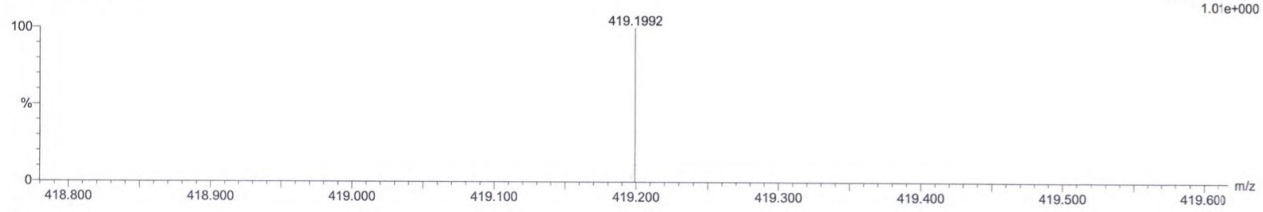
Elemental Composition Report Page 1

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
26 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-30 H: 0-34 N: 0-2 35Cl: 0-1 Ga: 0-1

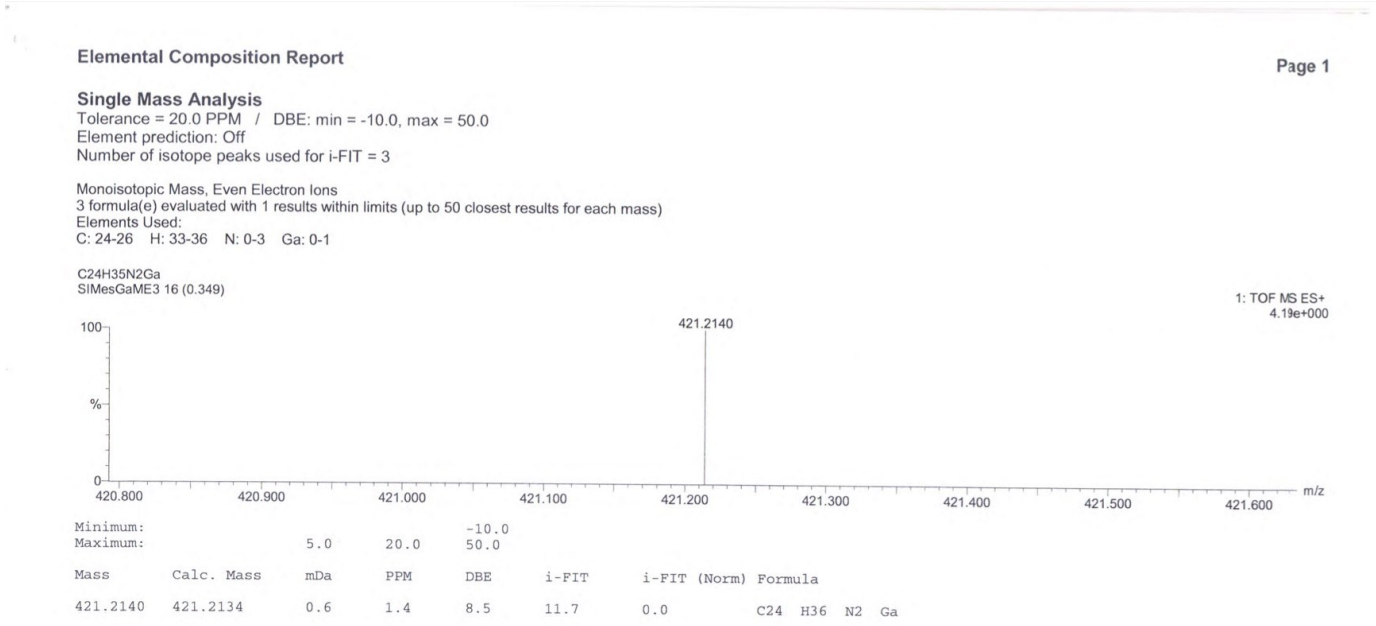
C24H33N2Ga
IMESGAME3 41 (0.920)

1: TOF MS ES+
1.0'e+000



Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
419.1992	419.1978	1.4	3.3	9.5	12.4	0.0	C24 H34 N2 Ga

Figure S17. High resolution mass spectrum of IMes•$GaMe_3$ (**1**).



Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 24-26 H: 33-36 N: 0-3 Ga: 0-1

C24H35N2Ga
SIMesGaME3 16 (0.349)

1: TOF MS ES+
4.19e+000

Minimum:				-10.0			
Maximum:		5.0	20.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
421.2140	421.2134	0.6	1.4	8.5	11.7	0.0	C24 H36 N2 Ga

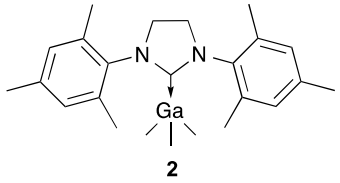


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Figure S18. High resolution mass spectrum of SIMes•$GaMe_3$ (**2**).

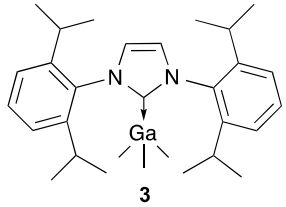

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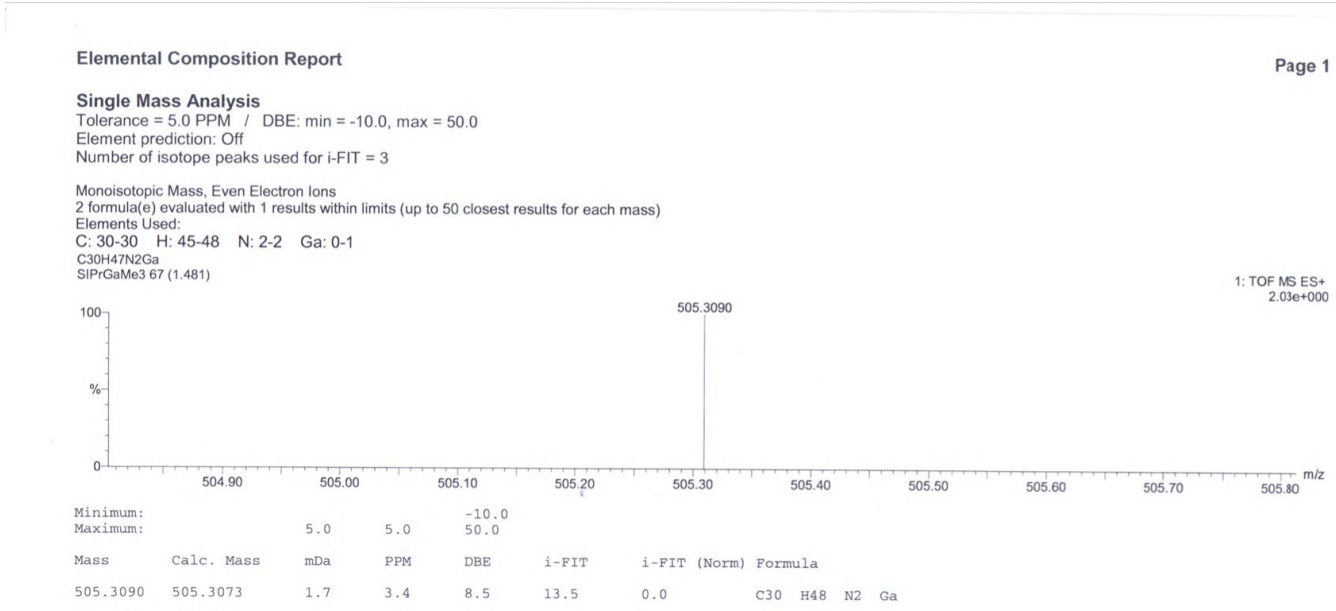
Figure S19. High resolution mass spectrum of IPr•$GaMe_3$ (**3**).



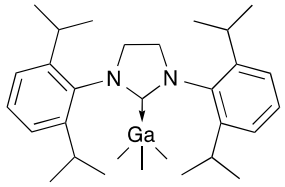


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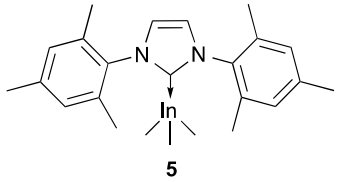
Figure S20. High resolution mass spectrum of SIPr•$GaMe_3$ (**4**).



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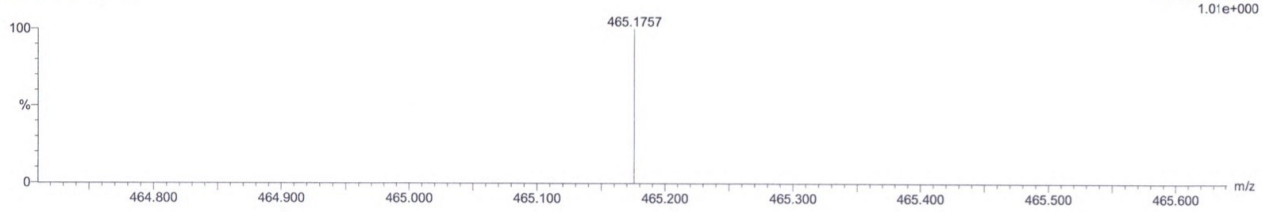
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

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

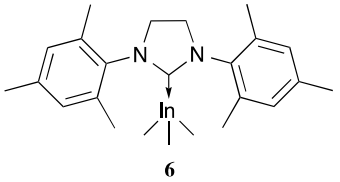
C24H35InN2
IMes-InMe3 45 (0.993)

1: TOF MS ES+
1.01e+000



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
465.1757	465.1761	-0.4	-0.9	9.5	19.6	0.0	C24 H34 N2 In

Figure S21. High resolution mass spectrum of IMes•$InMe_3$ (**5**).



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Elemental Composition Report

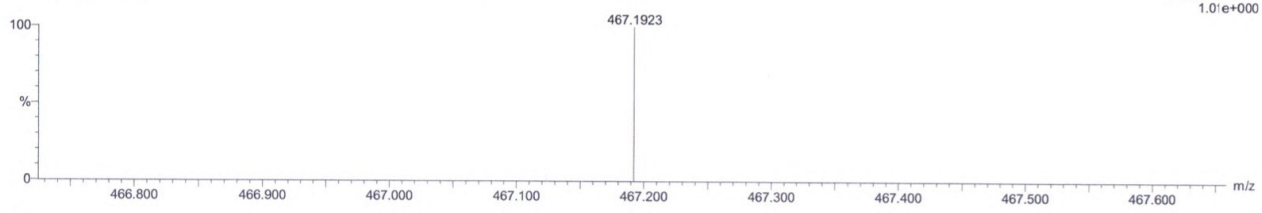
Page 1

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 = 9

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-25 H: 11-36 N: 1-5 In: 0-1

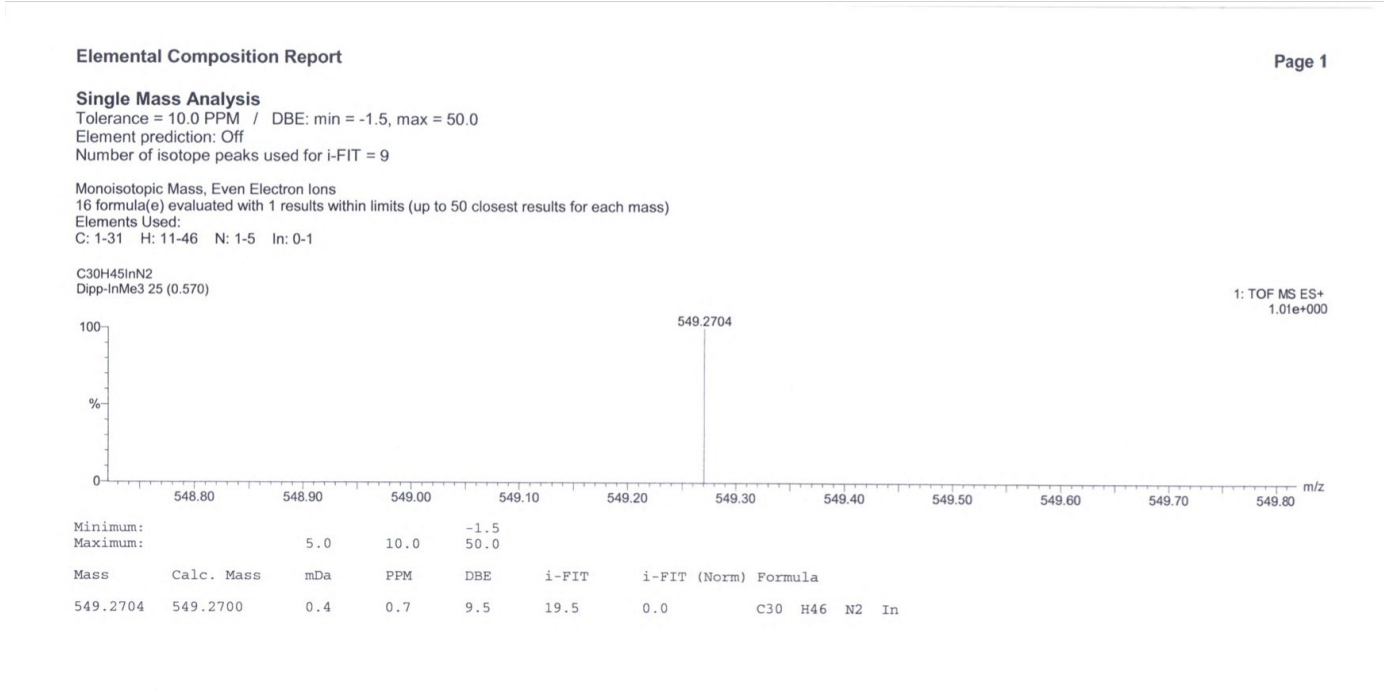
C24H35InN2
SIMes-InMe3 16 (0.350)

1: TOF MS ES+
1.01e+000



Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
467.1923	467.1917	0.6	1.3	8.5	18.9	0.0	C24 H36 N2 In

Figure S22. High resolution mass spectrum of SIMes•$InMe_3$ (**6**).



Elemental Composition Report Page 1

Single Mass Analysis
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Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-31 H: 11-46 N: 1-5 In: 0-1

C30H45InN2
Dipp-InMe3 25 (0.570)

1: TOF MS ES+
1.01e+000

549.2704

100
%
0

548.80 548.90 549.00 549.10 549.20 549.30 549.40 549.50 549.60 549.70 549.80 m/z

Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
549.2704	549.2700	0.4	0.7	9.5	19.5	0.0	C30 H46 N2 In

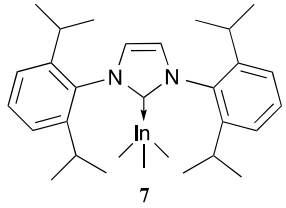

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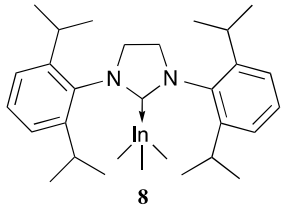
Figure S23. High resolution mass spectrum of IPr•$InMe_3$ (**7**).



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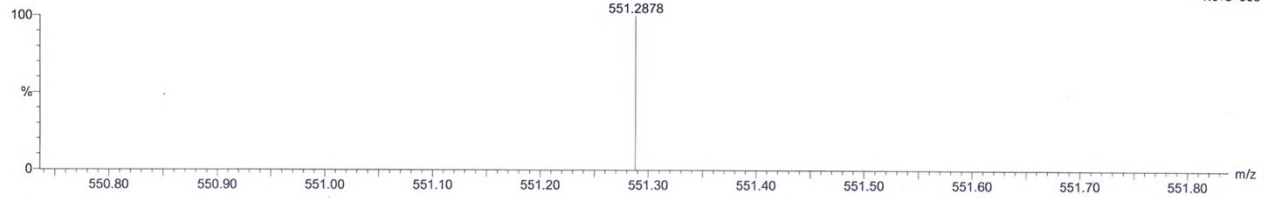
Elemental Composition Report Page 1

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 = 9

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

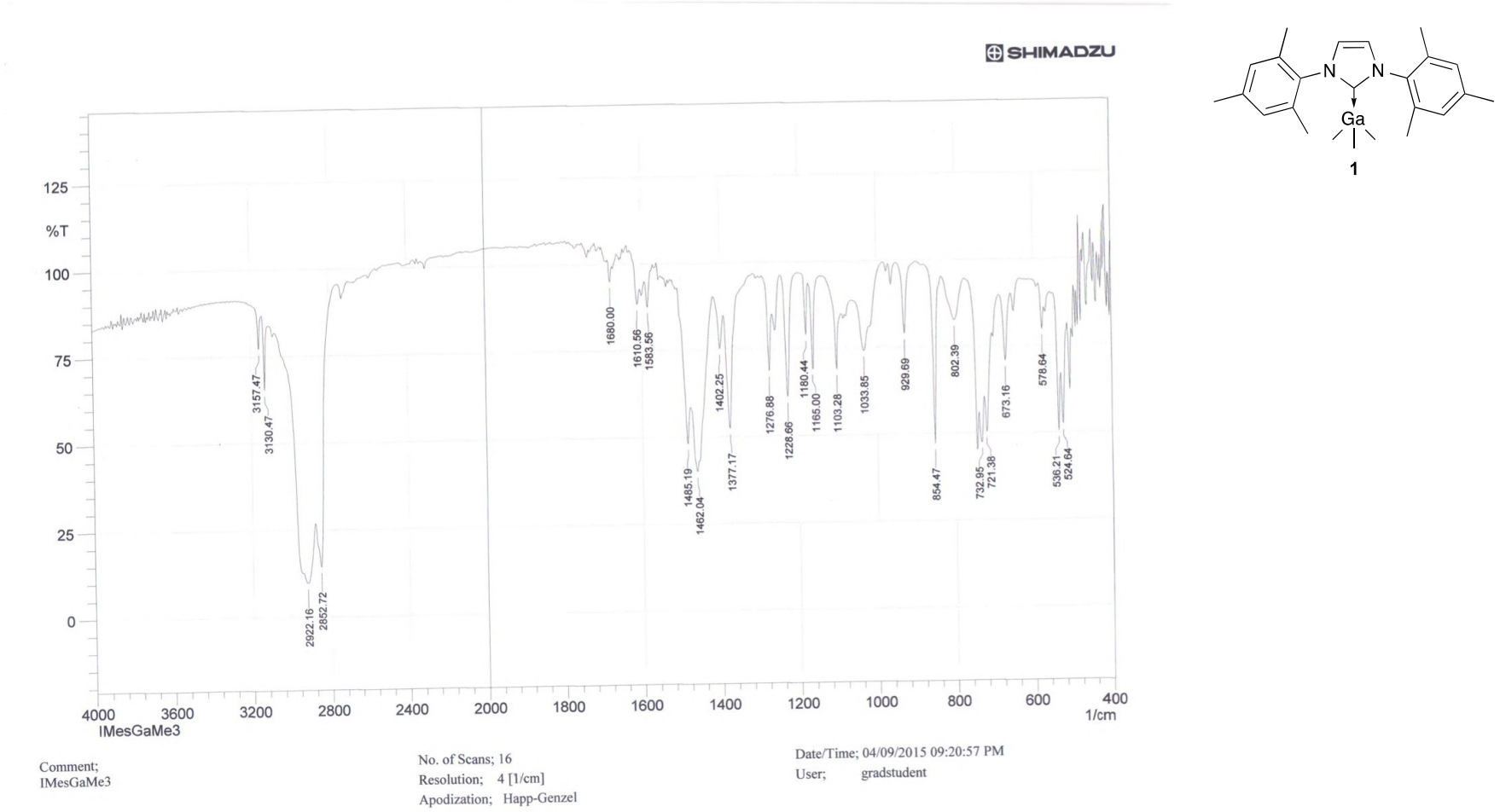
C30H47InN2
SIPrInME3 87 (1.904)

1: TOF MS ES+
1.01e+000



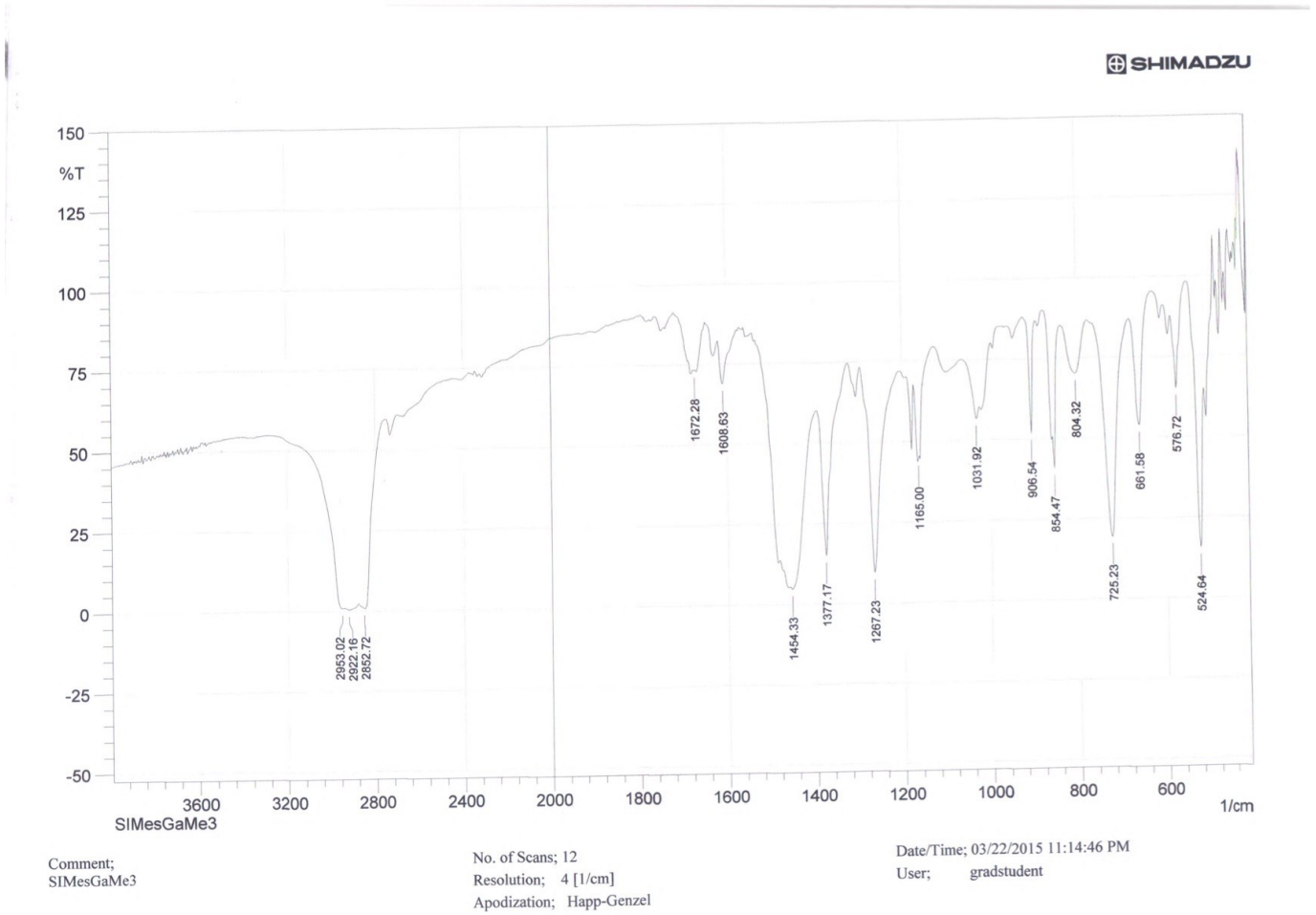
Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
551.2878	551.2856	2.2	4.0	8.5	19.5	0.0	C30 H48 N2 In

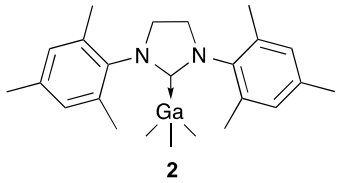
Figure S24. High resolution mass spectrum of SIPr•$InMe_3$ (**8**).



1

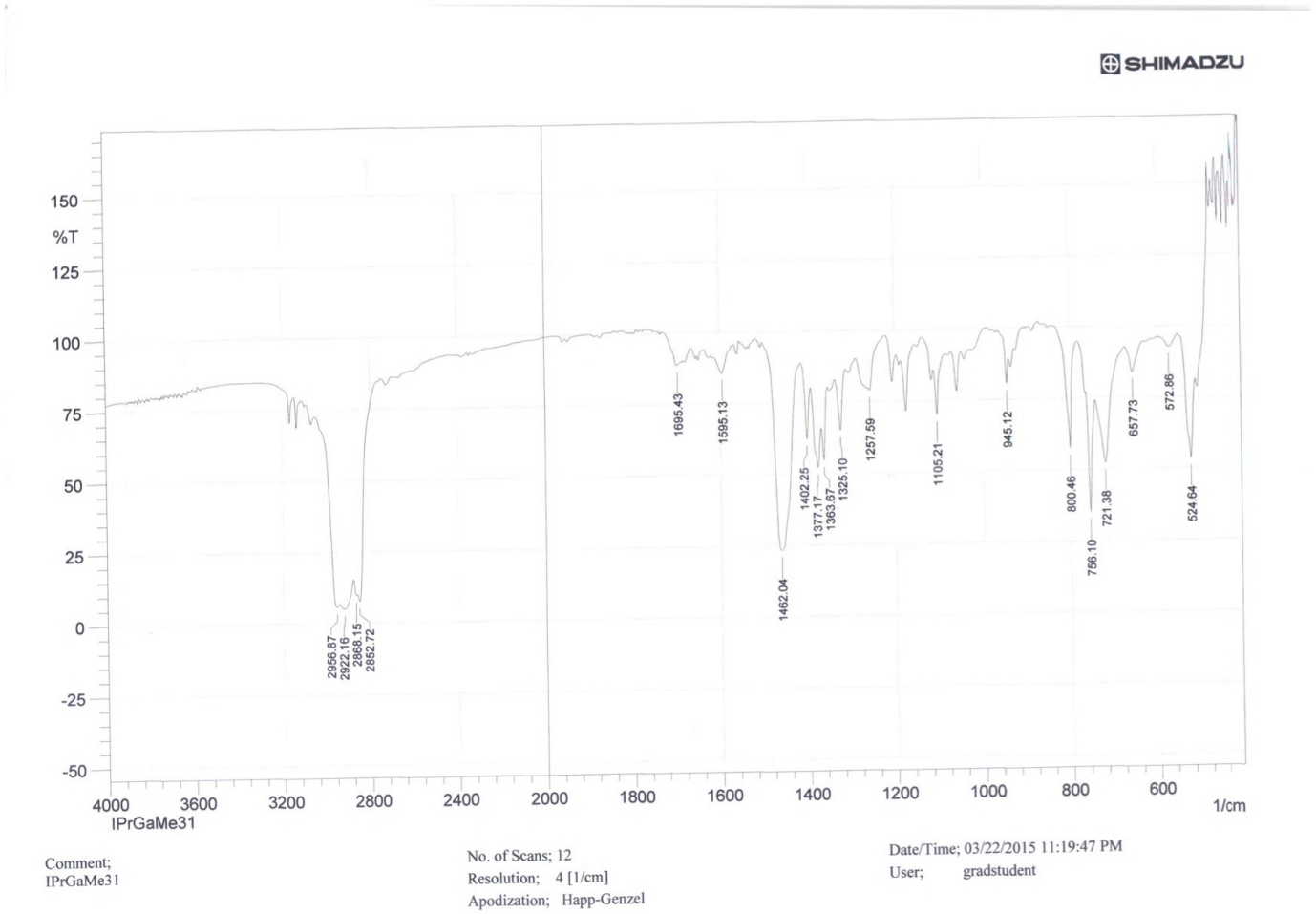
Figure S25. Infrared spectrum of IMes•$GaMe_3$ (**1**).

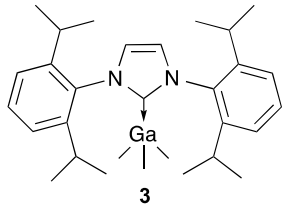




2

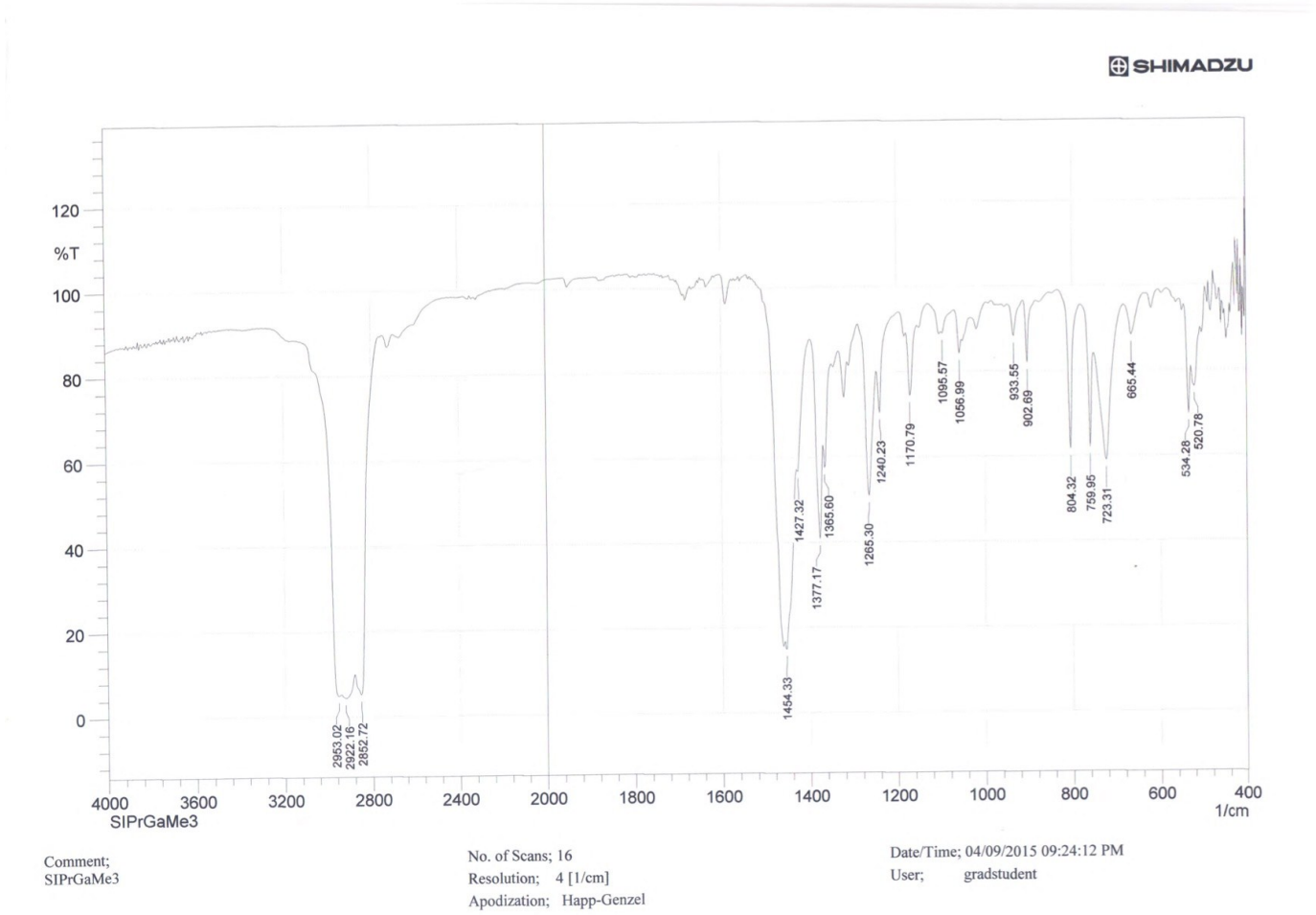
Figure S26. Infrared spectrum of SIMes•$GaMe_3$ (**2**).

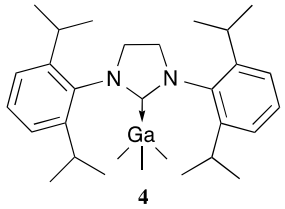




3

Figure S27. Infrared spectrum of IPr•$GaMe_3$ (**3**).





4

Figure S28. Infrared spectrum of SIPr•$GaMe_3$ (**4**).

X-ray single crystal crystallographic studies for complexes **1-8**

Complex 1

A colorless block-like specimen of $C_{24}H_{33}GaN_2$, approximate dimensions 0.180 mm x 0.200 mm x 0.280 mm, was used for the X-ray crystallographic analysis. Instrument description The X-ray intensity data were measured.
Data collection: The total exposure time was 1.34 hours. Integration The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 43057 reflections to a maximum θ angle of 29.13° (0.73 Å resolution), of which 3305 were independent (average redundancy 13.028, completeness = 99.9%, R_{int} = 5.78%, R_{sig} = 2.95%) and 2316 (70.08%) were greater than $2\sigma(F^2)$. Unit cell The final cell constants of a = 23.0884(8) Å, b = 12.3990(4) Å, c = 8.2064(3) Å, volume = 2349.27(14) $Å^3$, are based upon the refinement of the XYZ-centroids of 8838 reflections above 20 σ(I) with 4.821° < 2θ < 45.08°. Scaling Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.922. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7330 and 0.8160.
Structure solution Structure refinement: The final anisotropic full-matrix least-squares refinement on F^2 with 148 variables converged at R1 = 3.39%, for the observed data and wR2 = 9.06% for all data. The goodness-of-fit was 1.009. The largest peak in the final difference electron density synthesis was 0.228 $e^-/Å^3$ and the largest hole was -0.283 $e^-/Å^3$ with an RMS deviation of 0.056 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.185 g/cm^3 and F(000), 888 e^-.

Complex 2

A colorless block-like specimen of $C_{24}H_{35}GaN_2$, approximate dimensions 0.180 mm x 0.200 mm x 0.380 mm, was used for the X-ray crystallographic analysis. Instrument description The X-ray intensity data were measured.
Data collection: The total exposure time was 0.60 hours. Integration The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 63402 reflections to a maximum θ angle of 29.66° (0.72 Å resolution), of which 13086 were independent (average redundancy 4.845, completeness = 99.6%, R_{int} = 8.60%, R_{sig} = 7.51%) and 9875 (75.46%) were greater than $2\sigma(F^2)$. Unit cell The final cell constants of a = 17.6361(8) Å, b = 16.5723(7) Å, c = 15.9218(8) Å, volume = 4653.5(4) $Å^3$, are based upon the refinement of the XYZ-centroids of 9341 reflections above 20 σ(I) with 5.117° < 2θ < 49.63°. Scaling Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.753. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6600 and 0.8140.
Structure solution Structure refinement: The final anisotropic full-matrix least-squares refinement on F^2 with 506 variables converged at R1 = 4.40%, for the observed data and wR2 = 14.40% for all data. The goodness-of-fit was 1.107. The largest peak in the final difference electron density synthesis was 0.750 $e^-/Å^3$ and the largest hole was -0.637 $e^-/Å^3$ with an RMS deviation of 0.185 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.203 g/cm^3 and F(000), 1792 e^-.

Complex 3

A colorless block-like specimen of $C_{30}H_{45}GaN_2$, approximate dimensions 0.180 mm x 0.200 mm x 0.240 mm, was used for the X-ray crystallographic analysis. Instrument description The X-ray intensity data were measured.
Data collection: A total of 605 frames were collected. The total exposure time was 0.67 hours. Integration The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 84170 reflections to a maximum θ angle of 27.75° (0.76 Å resolution), of which 13658 were independent (average redundancy 6.163, completeness = 99.9%, R_{int} = 11.22%, R_{sig} = 9.15%) and 8786 (64.33%) were greater than $2\sigma(F^2)$. Unit cell The final cell constants of a = 16.6315(8) Å, b = 19.4897(10) Å, c = 19.2354(10) Å, β = 111.4316(16)°, volume = 5803.9(5) $Å^3$, are based upon the refinement of the XYZ-centroids of 5374 reflections above 20 σ(I) with 5.559° < 2θ < 42.32°. Scaling Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.821. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8010 and 0.8450.
Structure solution Structure refinement: The final anisotropic full-matrix least-squares refinement on F^2 with 617 variables converged at R1 = 5.30%, for the observed data and wR2 = 18.74% for all data. The goodness-of-fit was 1.046. The largest peak in the final difference electron density synthesis was 1.103 $e^-/Å^3$ and the largest hole was -

1.091 $e^-/Å^3$ with an RMS deviation of 0.355 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.152 g/cm^3 and F(000), 2160 e^-.

Complex 4

A colorless block-like specimen of $C_{30}H_{47}GaN_2$, approximate dimensions 0.220 mm x 0.360 mm x 0.420 mm, was used for the X-ray crystallographic analysis. Instrument description The X-ray intensity data were measured.
Data collection: The total exposure time was 0.95 hours. Integration The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 85651 reflections to a maximum θ angle of 29.60° (0.72 Å resolution), of which 15861 were independent (average redundancy 5.400, completeness = 99.8%, R_{int} = 6.89%, R_{sig} = 5.35%) and 11906 (75.06%) were greater than $2\sigma(F^2)$. Unit cell The final cell constants of a = 9.9188(4) Å, b = 16.6053(7) Å, c = 17.9050(8) Å, α = 83.4019(14)°, β = 75.2437(14)°, γ = 89.8823(14)°, volume = 2831.7(2) $Å^3$, are based upon the refinement of the XYZ-centroids of 9907 reflections above 20 σ(I) with 4.974° < 2θ < 52.96°. Scaling Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.852. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6810 and 0.8120.
Structure solution Structure refinement: The final anisotropic full-matrix least-squares refinement on F^2 with 617 variables converged at R1 = 3.78%, for the observed data and wR2 = 13.84% for all data. The goodness-of-fit was 1.058. The largest peak in the final difference electron density synthesis was 0.663 $e^-/Å^3$ and the largest hole was -0.775 $e^-/Å^3$ with an RMS deviation of 0.218 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.186 g/cm^3 and F(000), 1088 e^-.

Complex 5

A colorless block-like specimen of $C_{24}H_{33}InN_2$, approximate dimensions 0.140 mm x 0.180 mm x 0.240 mm, was used for the X-ray crystallographic analysis. Instrument description The X-ray intensity data were measured.
Data collection: The total exposure time was 0.30 hours. Integration The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 32360 reflections to a maximum θ angle of 31.04° (0.69 Å resolution), of which 13758 were independent (average redundancy 2.352, completeness = 99.8%, R_{int} = 3.95%, R_{sig} = 6.70%) and 9980 (72.54%) were greater than $2\sigma(F^2)$. Unit cell The final cell constants of a = 17.7812(5) Å, b = 16.4794(5) Å, c = 16.1136(4) Å, volume = 4721.7(2) $Å^3$, are based upon the refinement of the XYZ-centroids of 5648 reflections above 20 σ(I) with 4.943° < 2θ < 57.31°. Scaling Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.855. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7930 and 0.8710.
Structure solution Structure refinement: The final anisotropic full-matrix least-squares refinement on F^2 with 506 variables converged at R1 = 4.66%, for the observed data and wR2 = 16.81% for all data. The goodness-of-fit was 1.117. The largest peak in the final difference electron density synthesis was 1.479 $e^-/Å^3$ and the largest hole was -1.971 $e^-/Å^3$ with an RMS deviation of 0.340 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.306 g/cm^3 and F(000), 1920 e^-.

Complex 6

A specimen of $C_{24}H_{35}InN_2$, approximate dimensions 0.120 mm x 0.240 mm x 0.280 mm, was used for the X-ray crystallographic analysis. Instrument description The X-ray intensity data were measured.
Data collection Integration: The integration of the data using an orthorhombic unit cell yielded a total of 23919 reflections to a maximum θ angle of 26.00° (0.81 Å resolution), of which 9282 were independent (average redundancy 2.577, completeness = 100.0%, R_{int} = 5.28%, R_{sig} = 5.90%) and 8056 (86.79%) were greater than $2\sigma(F^2)$. Unit cell The final cell constants of a = 17.7466(7) Å, b = 16.5100(6) Å, c = 16.1725(5) Å, volume = 4738.5(3) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). Scaling The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7660 and 0.8890.
Structure solution Structure refinement: The final anisotropic full-matrix least-squares refinement on F^2 with 505 variables converged at R1 = 3.76%, for the observed data and wR2 = 11.29% for all data. The goodness-of-fit was 1.096. The largest peak in the final difference electron density synthesis was 1.405 $e^-/Å^3$ and the largest hole was -0.467 $e^-/Å^3$ with an RMS deviation of 0.124 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.307 g/cm^3 and F(000), 1936 e^-.

Complex 7

A specimen of $C_{30}H_{45}InN_2$, approximate dimensions 0.390 mm x 0.400 mm x 0.420 mm, was used for the X-ray crystallographic analysis. Instrument description The X-ray intensity data were measured.
Data collection Integration: The integration of the data using a monoclinic unit cell yielded a total of 40592 reflections to a maximum θ angle of 31.07° (0.69 Å resolution), of which 9429 were independent (average redundancy 4.305, completeness = 99.6%, R_{int} = 4.36%, R_{sig} = 4.01%) and 7763 (82.33%) were greater than $2\sigma(F^2)$. Unit cell The final cell constants of a = 10.3930(6) Å, b = 19.4217(9) Å, c = 14.7592(7) Å, β = 98.1212(17)°, volume = 2949.3(3) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). Scaling The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7250 and 0.7410.
Structure solution Structure refinement: The final anisotropic full-matrix least-squares refinement on F^2 with 339 variables converged at R1 = 2.90%, for the observed data and wR2 = 6.81% for all data. The goodness-of-fit was 1.025. The largest peak in the final difference electron density synthesis was 0.586 $e^-/Å^3$ and the largest hole was -0.719 $e^-/Å^3$ with an RMS deviation of 0.079 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.235 g/cm^3 and F(000), 1152 e^-.

Complex 8

A specimen of $C_{30}H_{47}InN_2$, approximate dimensions 0.100 mm x 0.380 mm x 0.420 mm, was used for the X-ray crystallographic analysis. Instrument description The X-ray intensity data were measured.
Data collection Integration: The integration of the data using a monoclinic unit cell yielded a total of 37529 reflections to a maximum θ angle of 31.11° (0.69 Å resolution), of which 9263 were independent (average redundancy 4.051, completeness = 99.7%, R_{int} = 4.84%, R_{sig} = 4.48%) and 7543 (81.43%) were greater than $2\sigma(F^2)$. Unit cell The final cell constants of a = 34.7678(11) Å, b = 9.9342(2) Å, c = 16.8380(5) Å, β = 97.1092(12)°, volume = 5771.0(3) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). Scaling The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7200 and 0.9210.
Structure solution Structure refinement: The final anisotropic full-matrix least-squares refinement on F^2 with 309 variables converged at R1 = 3.18%, for the observed data and wR2 = 8.44% for all data. The goodness-of-fit was 1.091. The largest peak in the final difference electron density synthesis was 0.658 $e^-/Å^3$ and the largest hole was -0.705 $e^-/Å^3$ with an RMS deviation of 0.177 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.267 g/cm^3 and F(000), 2320 e^-.

Table S1. Crystal data for complex **1** (IMes•$GaMe_3$), **2** (SIMes•$GaMe_3$), **3** (IPr•$GaMe_3$), **4** (SIPr•$GaMe_3$) **5** (IMes•$InMe_3$) and **6** (SIMes•$InMe_3$), **7** (IPr•$InMe_3$) and **8** (SIPr•$InMe_3$).

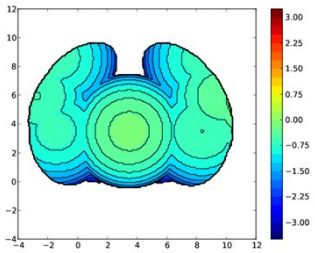
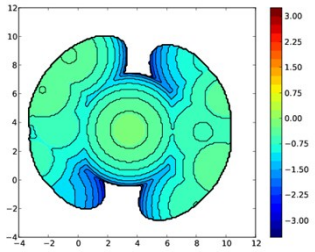
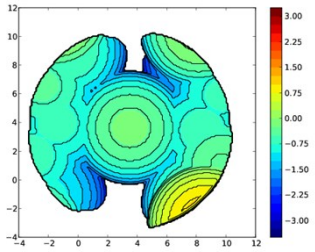
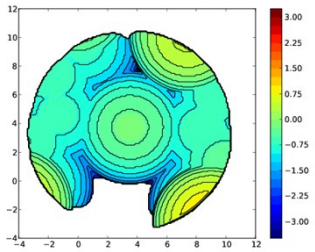
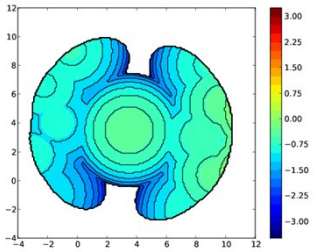
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Formula	$C_{24}H_{33}GaN_2$	$C_{24}H_{35}GaN_2$	$C_{30}H_{45}GaN_2$	$C_{30}H_{47}GaN_2$	$C_{24}H_{33}InN_2$	$C_{24}H_{35}InN_2$	$C_{30}H_{45}InN_2$	$C_{30}H_{47}InN_2$
FW	419.24	421.26	503.40	505.41	464.34	466.36	548.50	550.51
T [K]	292(2)	103(2)	103(2)	103(2)	103(2)	103(2)	103(2)	133(2)
λ [Å]	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal Structure	Orthorhombic	Orthorhombic	Monoclinic	Triclinic	Orthorhombic	Orthorhombic	Monoclinic	Monoclinic
Space Group	Pnma	Pca21	P121/c1	P-`	Pca21	Pca21	P121/n1	C12/c1
a [Å]	22.0884(8)	17.6361(8)	16.6315(8)	9.9188(4)	17.7812(5)	17.7466(7)	10.3930(6)	34.7678(11)
b [Å]	12.3990(4)	16.5723(7)	19.4897(10)	16.6053(7)	16.4794(5)	16.5100(6)	19.4217(9)	9.9342(2)
c [Å]	8.2064(3)	15.9218(8)	19.2354(10)	17.9050(8)	16.1136(4)	16.1725(5)	14.7592(7)	16.8380(5)
α (°)	90	90	90	83.4019(14)	90	90	90	90
β (°)	90	90	111.4316(16)	75.2437(14)	90	90	98.1212(17)	97.1092(12)
γ (°)	90	90	90	89.8823(14)	90	90	90	90
V [Å^3]	2349.27(14)	4653.5(4)	5803.9(5)	2831.7(2)	4721.7(2)	4738.5(3)	2949.3(3)	5771.0(3)
Z	4	8	8	4	8	8	4	8
D_{calcd} [Mg/m^3]	1.185	1.203	1.152	1.186	1.306	1.307	1.235	1.267
μ [mm^{-1}]	1.181	1.193	0.967	0.991	1.011	1.007	0.819	0.838
F(000)	888	1792	2160	1088	1920	1936	1152	2320
Crystal size [mm^3]	0.18x0.20x0.28	0.18x0.20x0.38	0.18x0.20x0.24	0.22x0.36x0.420	0.140x0.180x0.240	1.120x0.240x0.28	0.390x0.400x0.420	0.100x0.380x0.420
θ range [°]	2.63-29.13	1.23-29.66	1.31-27.75	1.18-29.60	1.24-31.04	1.69-26.00	2.78-31.07	1.18-31.11
N	43057	63402	84170	85651	32360	23919	40592	37529
N_{ind} (R_{int})	3305(0.0578)	13086(0.0860)	13658(0.1122)	15861(0.0689)	13758(0.0395)	9282(0.0528)	9429(0.0436)	9263(0.0484)
Max. and min. transmssion	0.8160 & 0.7330	0.8140 & 0.6600	0.8450 & 0.8010	0.8120 & 0.6810	0.8710 & 0.7930	0.8890 & 0.7660	0.7410 & 0.7250	0.9210 & 0.7200
Data, restraints, parameters	3305 / 0 /148	13086 / 1 / 506	13658 / 0 / 617	15861 / 0 / 617	13758 / 1 /506	9282 / 7 / 505	9429 / 123 / 339	9263 / 0 / 309
GOF on F^2	1.009	1.107	1.046	1.058	1.117	1.094	1.027	1.074
Final R indices [I>2σ(I)]	0.0339, 0.0773	0.0440, 0.1034	0.0530, 0.1318	0.0378, 0.1045	0.0466, 0.1175	0.0376, 0.0884	0.0290, 0.0635	0.0318, 0.0733
R indices (all data)	0.0645, 0.0906	0.0744, 0.1440	0.1061, 0.1874	0.0624, 0.1384	0.0842, 0.1681	0.0474, 0.1125	0.0403, 0.0680	0.0459, 0.0848
Largest diff. Peak & hole [eÅ^{-3}]	0.228 & -0.283	0.750 & -0.637	1.103 & -1.091	0.663 & -0.775	1.479 & -1.971	1.403 & -0.467	0.585 & -0.719	0.661 & -0.699
R.M.S deviation from mean [eÅ^{-3}]	0.056	0.185	0.355	0.218	0.340	0.124	0.079	0.177

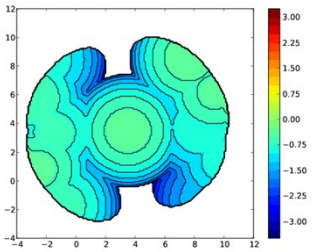
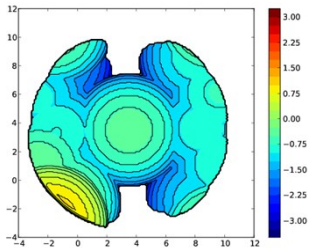
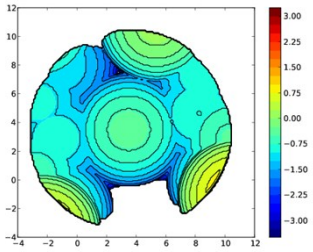
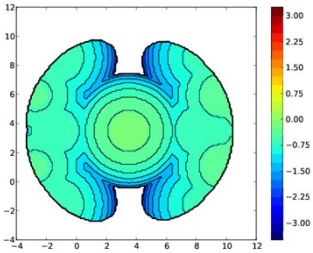
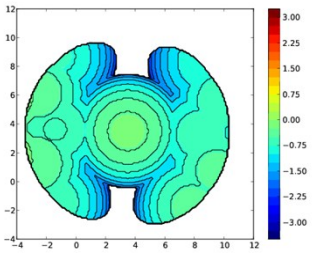
Table S2. Selected M-$C_{carbene}$ bond length

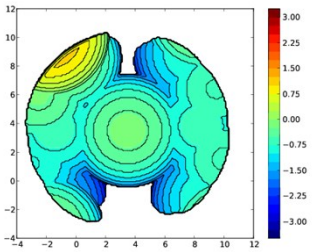
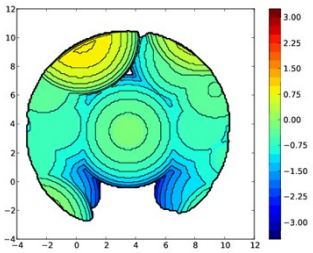
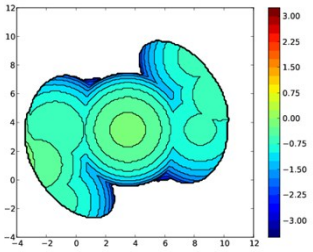
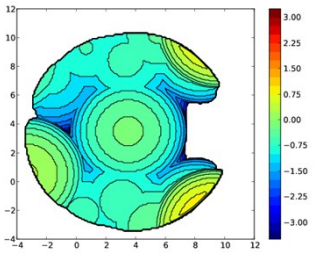
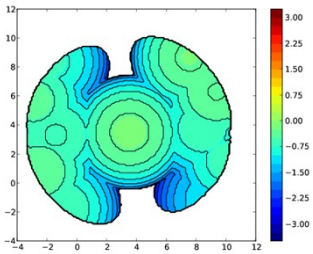
Entries	Complexes	M-$C_{carbene}$ [Å]
1	IMes•$GaMe_3$ (**1**)	2.111(2)
2	SIMes•$GaMe_3$ (**2**)	2.124(5)
3	IPr•$GaMe_3$ (**3**)	2.105(4)
4	SIPr•$GaMe_3$ (**4**)	2.137(2)
5	IMes•$InMe_3$ (**5**)	2.301(8)
6	SIMes•$InMe_3$ (**6**)	2.316(8)
7	IPr•$InMe_3$ (**7**)	2.309(2)
8	SIPr•$InMe_3$ (**8**)	2.342(2)
9	IMes•$GaMe_3$ (**G**)[4a]	2.105(2)
10	IMes•$GaClH_2$[7i]	2.030(3)
11	IMes•$GaCl_2H$[7i]	2.005(6)
12	IMes•$GaCl_3$[7i]	1.954(4)
13	IPr•GaH_3[7i]	2.055(1)
14	IP•$GaCl_3$[7i]	2.016(2)
15	IMes•InH_3[7q]	2.253(5)
16	IMes•InH_2Cl[7q]	2.244(6)
17	IMes•$InBr_3$[7p]	2.195(5)
18	IMes•$InMe_2Cl$ (**R**)[4d]	2.267(2)
19	IPr•$InBr_3$[7p]	2.212(8)

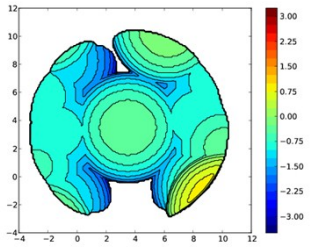
%V_{Bur} and topographic steric map for selected NHC Ga/In alkyl complexes

Table S3. % V_{Bur} and topographic steric map for selected Ga/In complexes. The M-$C_{carbene}$ bond lengths are the experimental values obtained by X-ray single crystal diffraction studies.

Entries	Complexes	M-$C_{carbene}$ [Å]	% V_{bur} [a]	Topographic steric map
1	IMes•$GaMe_3$ (**1**)	2.111(2)	27.9	
2	SIMes•$GaMe_3$ (**2**)	2.125(5)	31.8	
3	IPr•$GaMe_3$ (**3**)	2.105(4)	34.0	
4	SIPr•$GaMe_3$ (**4**)	2.137(2)	35.1	
5	IMes•$InMe_3$ (**5**)	2.301(8)	28.5	

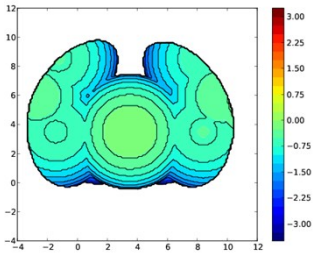
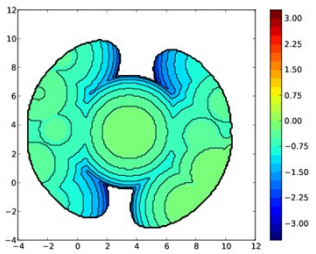
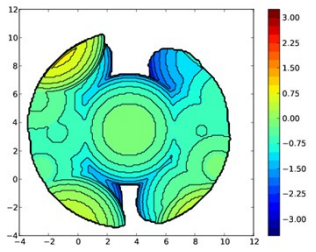
6	SIMes•$InMe_3$ (**6**)	2.316(8)	29.2	
7	IPr•$InMe_3$ (**7**)	2.309(2)	30.2	
8	SIPr•$InMe_3$ (**8**)	2.342(2)	31.4	
9	IMes•$AlMe_3$ (**A**)	2.098(2)	31.7	
10	SIMes•$AlMe_3$ (**B**)	2.112(6)	32.0	

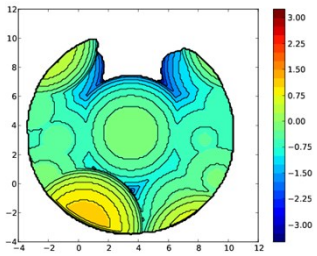
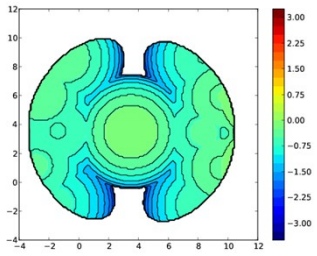
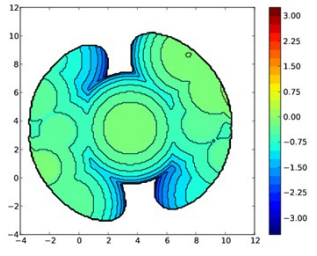
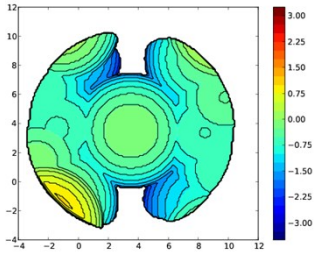
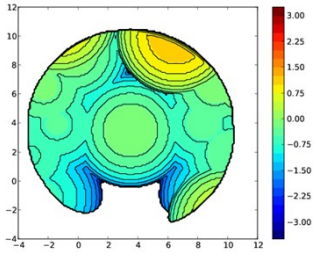
11	IPr•$AlMe_3$ (**C**)	2.103(3)	33.1	
12	SIPr•$AlMe_3$ (**D**)	2.127(2)	36.1	
13	IMes•$GaMe_3$ (**G**)	2.105(2)	28.2	
14	SIPr•$GaMe_3$ (**I**)	2.132(3)	34.7	
15	SIMes•$GaMe_3$ (**J**)	2.121(3)	32.1	

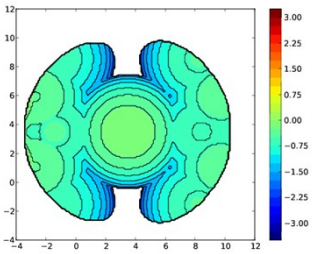
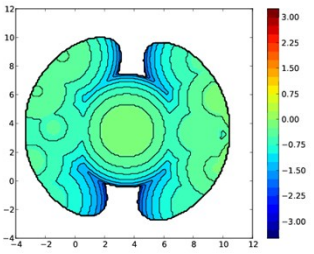
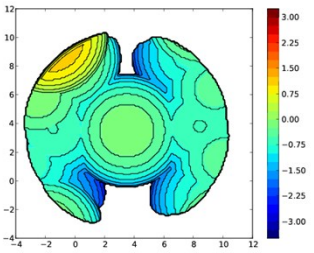
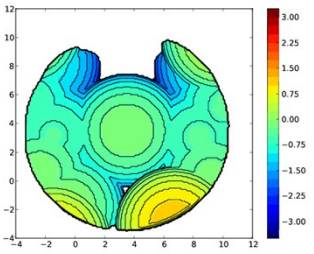
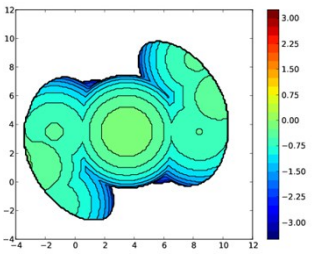
16	IPr•Ga(CH_2SiMe_3)$_3$	2.196(2)	31.9	

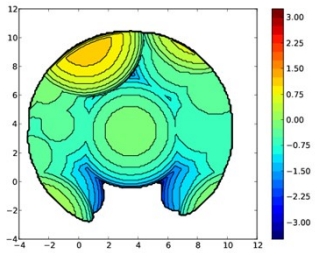
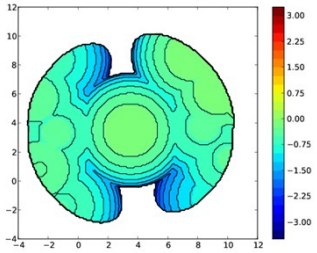
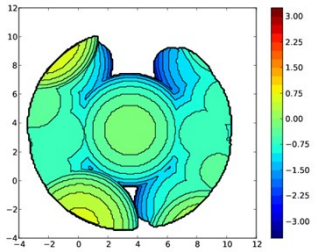
$\%V_{Bur}$ calculations and topographic steric map parameters: All calculations were performed using crystallographic data (CIF). 3.50 Å was selected as the value for the sphere radius; M-$C_{carbene}$ bond distances (**X-ray crystal structure**) were chosen for the metal-ligand bond; mesh spacing for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

Table S4. % V_{Bur} and topographic steric map for selected Ga/In complexes. The M-$C_{carbene}$ bond lengths is set at 2.0 Å. Calculations were performed using the X-ray single crystal structures.

Entries	Complexes	% V_{bur}[a]	Topographic steric map
1	IMes•$GaMe_3$ (**1**)	29.6	
2	SIMes•$GaMe_3$ (**2**)	34.1	
3	IPr•$GaMe_3$ (**3**)	36.2	

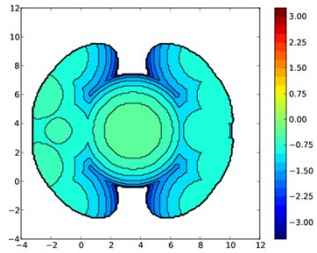
4	SIPr•$GaMe_3$ (**4**)	39.3	
5	IMes•$InMe_3$ (**5**)	34.0	
6	SIMes•$InMe_3$ (**6**)	34.9	
7	IPr•$InMe_3$ (**7**)	35.7	
8	SIPr•$InMe_3$ (**8**)	39.5	

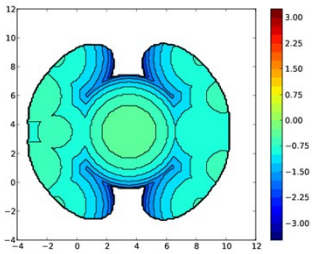
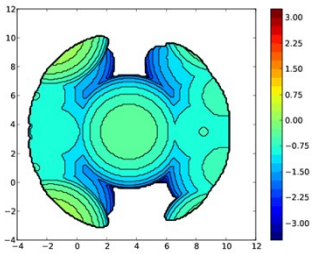
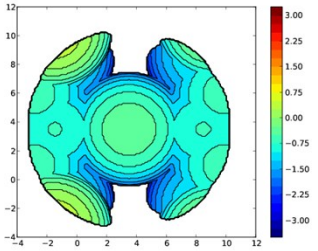
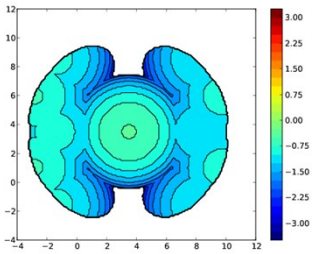
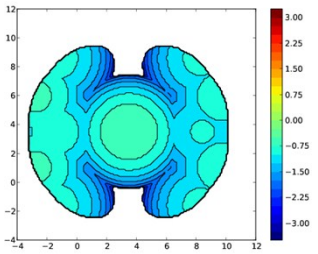
9	IMes•$AlMe_3$ (**A**)	33.7	
10	SIMes•$AlMe_3$ (**B**)	34.1	
11	IPr•$AlMe_3$ (**C**)	35.0	
12	SIPr•$AlMe_3$ (**D**)	38.5	
13	IMes•$GaMe_3$ (**G**)	29.8	

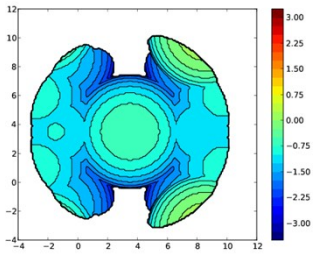
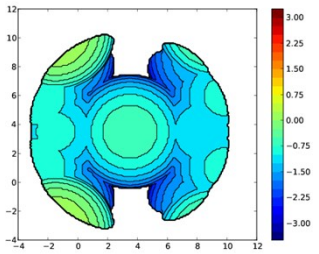
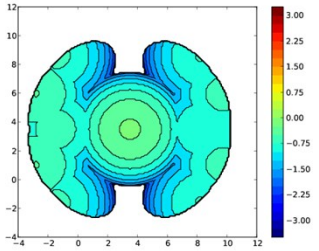
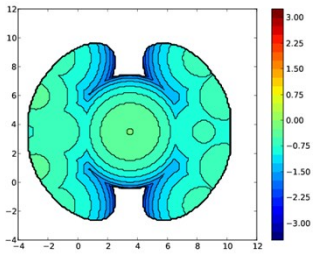
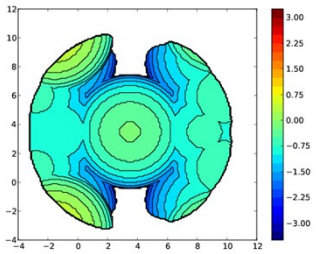
14	SIPr•$GaMe_3$ (**I**)	39.1	
15	SIMes•$GaMe_3$ (**J**)	34.2	
16	IPr•$Ga(CH_2SiMe_3)_3$	36.1	

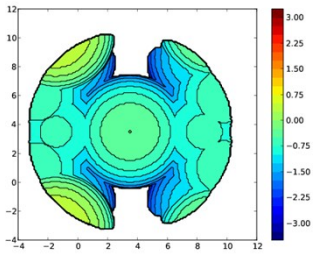
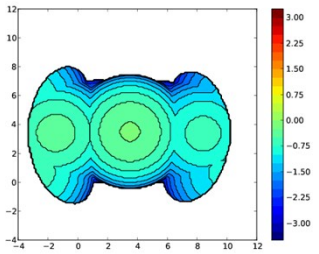
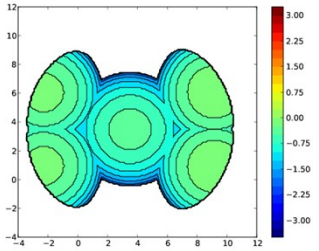
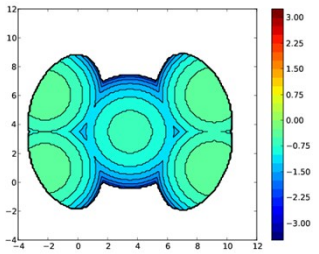
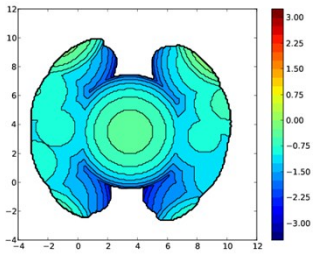
$\%V_{Bur}$ calculations and topographic steric map parameters: All calculations were performed using crystallographic data (CIF). 3.50 Å was selected as the value for the sphere radius; distance of **2.00 Å** was chosen for the metal-ligand bond; mesh spacing for numerical integration was scaled to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

Table S5. % V_{Bur} and topographic steric map for selected Ga/In complexes. Calculations were performed using DFT optimised structure.

Entries	Complexes	M-$C_{carbene}$ [Å]	% V_{bur}[a]	Topographic steric map
1	IMes•$GaMe_3$ (**1**)	2.201	27.4	

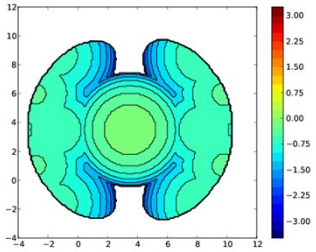
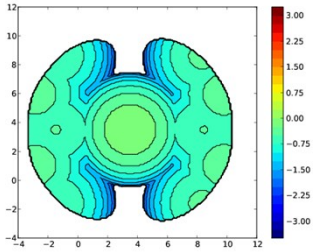
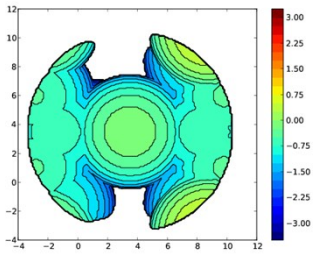
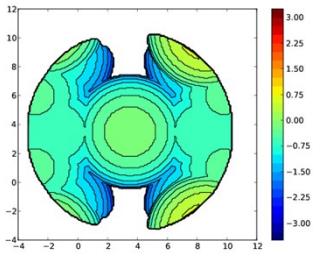
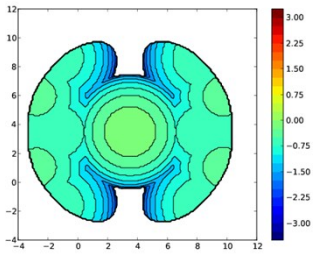
2	SIMes•$GaMe_3$ (**2**)	2.231	28.1	
3	IPr•$GaMe_3$ (**3**)	2.213	28.9	
4	SIPr•$GaMe_3$ (**4**)	2.233	29.5	
5	IMes•$InMe_3$ (**5**)	2.428	25.7	
6	SIMes•$InMe_3$ (**6**)	2.453	26.3	

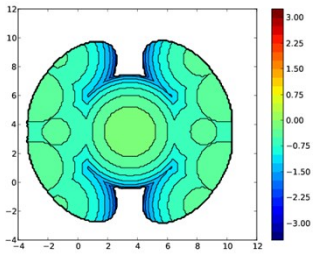
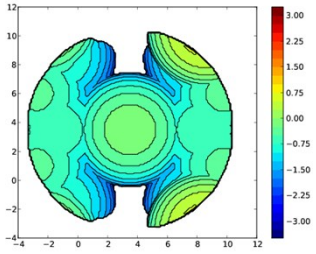
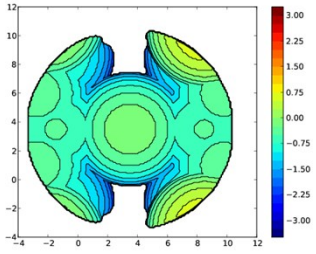
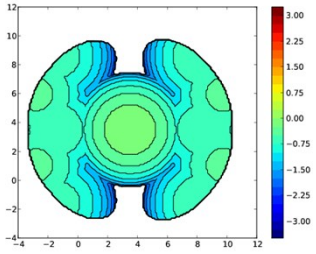
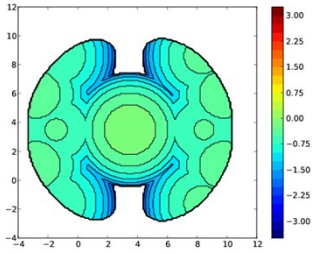
7	IPr•$InMe_3$ (**7**)	2.446	27.1	
8	SIPr•$InMe_3$ (**8**)	2.478	27.7	
9	IMes•$AlMe_3$ (**A**)	2.162	28.9	
10	SIMes•$AlMe_3$ (**B**)	2.188	30.4	
11	IPr•$AlMe_3$ (**C**)	2.165	31.2	

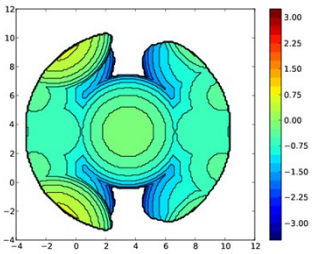
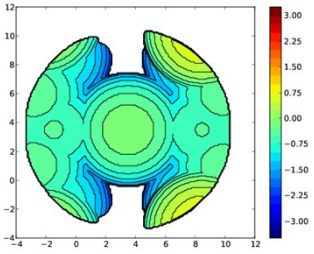
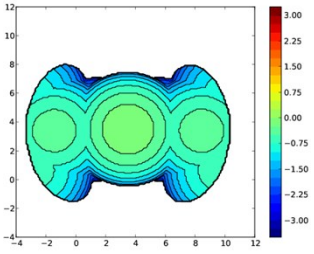
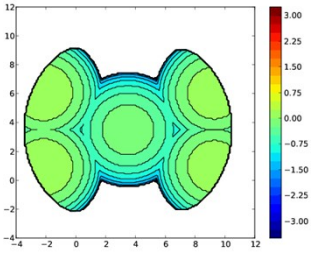
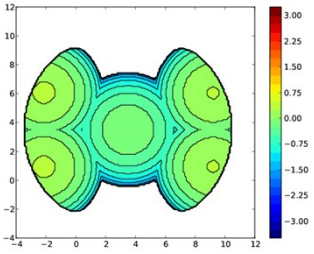
12	SIPr•$AlMe_3$ (**D**)	2.190	32.0	
13	IiPrMe•$GaMe_3$ (**E**)	2.166	25.5	
14	ItBu•$GaMe_3$ (**F**)	2.316	31.6	
15	ItBu•$InMe_3$ (**Q**)	2.558	28.4	
16	IPr•$Ga(CH_2SiMe_3)_3$	2.301	26.2	

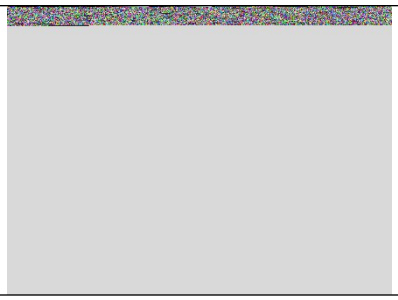
$\%V_{Bur}$ calculations and topographic steric map parameters: All calculations were performed using DFT optimised structure. 3.50 Å was selected as the value for the sphere radius; M-$C_{carbene}$ bond distances (**DFT optimised structure**) were chosen for the metal-ligand bond; mesh spacing for numerical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

Table S6. % V_{Bur} and topographic steric map for selected Ga/In complexes. The M-$C_{carbene}$ bond lengths is set at 2.0 Å. Calculations were performed using DFT optimised structures.

Entries	Complexes	% V_{bur}[a]	Topographic steric map
1	IMes•$GaMe_3$ (**1**)	33.1	
2	SIMes•$GaMe_3$ (**2**)	34.2	
3	IPr•$GaMe_3$ (**3**)	34.7	
4	SIPr•$GaMe_3$ (**4**)	36.0	
5	IMes•$InMe_3$ (**5**)	33.3	

6	SIMes•$InMe_3$ (**6**)	34.4	
7	IPr•$InMe_3$ (**7**)	35.1	
8	SIPr•$InMe_3$ (**8**)	36.2	
9	IMes•$AlMe_3$ (**A**)	32.8	
10	SIMes•$AlMe_3$ (**B**)	33.8	

11	IPr•$AlMe_3$ (**C**)	34.3	
12	SIPr•$AlMe_3$ (**D**)	35.5	
13	IiPrMe•$GaMe_3$ (**E**)	27.8	
14	ItBu•$GaMe_3$ (**F**)	36.7	
15	ItBu•$InMe_3$ (**Q**)	37.5	

16	IPr•Ga(CH_2SiMe_3)$_3$	31.6	

Geometries and Energies.

IMes-GaMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
==========

ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gallium (TZP, 3p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	2.857290	-1.834560	-1.230473
C	2.178841	-1.859944	0.000000
C	2.857290	-1.834560	1.230473
C	4.254108	-1.739210	1.201362
C	4.970528	-1.688771	0.000000
C	4.254108	-1.739210	-1.201362
N	0.741285	-2.047336	0.000000
C	-0.234232	-1.077294	0.000000
N	-1.396693	-1.809665	0.000000
C	-1.149028	-3.181656	0.000000
C	0.199056	-3.330340	0.000000
C	-2.759607	-1.318489	0.000000
C	-3.412011	-1.135246	-1.229695
C	-4.761481	-0.763971	-1.201549
C	-5.456348	-0.582926	0.000000
C	-4.761481	-0.763971	1.201549
C	-3.412011	-1.135246	1.229695
C	-2.685745	-1.305797	-2.540464
C	-2.685745	-1.305797	2.540464
C	-6.925087	-0.231140	0.000000
C	2.120938	-1.921725	2.543596
C	6.479858	-1.627451	0.000000
C	2.120938	-1.921725	-2.543596
Ga	0.066993	1.103053	0.000000
C	1.095022	1.463989	1.704514
C	-1.722193	2.044117	0.000000

C 1.095022 1.463989 -1.704514
H 4.794610 -1.709313 -2.150674
H 4.794610 -1.709313 2.150674
H -5.281531 -0.612559 -2.150621
H -5.281531 -0.612559 2.150621
H -3.374907 -1.174232 3.383100
H -2.225716 -2.301220 2.626437
H -1.877536 -0.566699 2.637701
H -3.374907 -1.174232 -3.383100
H -1.877536 -0.566699 -2.637701
H -2.225716 -2.301220 -2.626437
H -7.197851 0.351046 0.889635
H -7.197851 0.351046 -0.889635
H -7.544548 -1.142047 0.000000
H 6.859803 -1.108761 0.889650
H 2.828838 -1.920508 3.381008
H 1.439303 -1.069265 2.667197
H 1.518158 -2.840042 2.608052
H 2.828838 -1.920508 -3.381008
H 1.518158 -2.840042 -2.608052
H 1.439303 -1.069265 -2.667197
H 1.208533 2.557657 1.797935
H 0.557377 1.124422 2.606250
H 2.106441 1.028447 1.716631
H 1.208533 2.557657 -1.797935
H 2.106441 1.028447 -1.716631
H 0.557377 1.124422 -2.606250
H -1.792024 2.693833 -0.888565
H -2.610242 1.394856 0.000000
H -1.792024 2.693833 0.888565
H 0.821742 -4.216900 0.000000
H -1.951058 -3.909891 0.000000

Net Charge: 0.00

Total Bonding Energy:
-12.864607108939168 hartree
-8072.66 kcal/mol
-33776.02 kJ/mol
Summary Geometry Optimization:

Energy Change : -0.000155
Gradient (Max): 0.000614
Gradient (RMS): 0.000125

SIMes-GaMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
==========
ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gallium (TZP, 3p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	2.868526	-1.822010	-1.227708
C	2.180123	-1.854844	0.000000
C	2.868526	-1.822010	1.227708
C	4.264100	-1.711778	1.200639
C	4.981125	-1.655221	0.000000
C	4.264100	-1.711778	-1.200639
N	0.754980	-2.066951	0.000000
C	-0.238767	-1.149104	0.000000
N	-1.408886	-1.824920	0.000000
C	-1.248744	-3.307149	0.000000
C	0.271088	-3.476612	0.000000
C	-2.753503	-1.310751	0.000000
C	-3.412690	-1.116214	-1.227016
C	-4.758227	-0.731660	-1.201077
C	-5.452582	-0.545182	0.000000
C	-4.758227	-0.731660	1.201077
C	-3.412690	-1.116214	1.227016
C	-2.685468	-1.275383	-2.539027
C	-2.685468	-1.275383	2.539027
C	-6.917378	-0.176896	0.000000
C	2.136948	-1.909523	2.544071
C	6.489765	-1.576500	0.000000
C	2.136948	-1.909523	-2.544071
Ga	0.054714	1.062296	0.000000
C	1.080727	1.427283	1.707030
C	-1.727782	2.019138	0.000000
C	1.080727	1.427283	-1.707030
H	4.804044	-1.671785	-2.150196
H	4.804044	-1.671785	2.150196
H	-5.275533	-0.569842	-2.150222
H	-5.275533	-0.569842	2.150222
H	-3.370503	-1.123152	3.381849
H	-2.237298	-2.274495	2.645676
H	-1.868272	-0.544856	2.623126
H	-3.370503	-1.123152	-3.381849
H	-1.868272	-0.544856	-2.623126
H	-2.237298	-2.274495	-2.645676
H	-7.183475	0.408677	0.889544
H	-7.183475	0.408677	-0.889544
H	-7.547870	-1.080277	0.000000
H	6.863814	-1.053283	0.889597
H	6.934367	-2.584431	0.000000
H	6.863814	-1.053283	-0.889597
H	2.842037	-1.837168	3.380990
H	1.403025	-1.099171	2.641498
H	1.596461	-2.863276	2.646192
H	2.842037	-1.837168	-3.380990
H	1.596461	-2.863276	-2.646192
H	1.403025	-1.099171	-2.641498
H	1.178985	2.522807	1.793666
H	0.546902	1.085678	2.609722
H	2.096400	1.003392	1.716740
H	1.178985	2.522807	-1.793666
H	2.096400	1.003392	-1.716740
H	0.546902	1.085678	-2.609722
H	-1.785244	2.669209	-0.888906
H	-2.623645	1.381798	0.000000
H	-1.785244	2.669209	0.888906
H	0.647387	-4.003085	-0.888626

H 0.647387 -4.003085 0.888626
H -1.733455 -3.736703 -0.888496
H -1.733455 -3.736703 0.888496

Net Charge: 0.00

Total Bonding Energy:
-13.131995442192204 hartree
-8240.45 kcal/mol
-34478.05 kJ/mol
Summary Geometry Optimization:

Energy Change : 0.000024
Gradient (Max): 0.000774
Gradient (RMS): 0.000150

IPr-GaMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
==========

ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gallium (TZP, 3p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C 0.017171 0.063191 -1.239783
C -0.658333 0.048863 0.000000
C 0.017171 0.063191 1.239783
C 1.419125 0.044143 1.207337
C 2.113625 0.029337 0.000000
C 1.419125 0.044143 -1.207337
N -2.109454 0.146216 0.000000
C -3.026020 -0.884085 0.000000
N -4.230272 -0.220669 0.000000
C -4.067187 1.161618 0.000000
C -2.731166 1.391089 0.000000
Ga -2.610936 -3.057812 0.000000
C -4.343373 -4.100095 0.000000
C -5.563607 -0.792652 0.000000
C -6.201268 -1.008426 1.237415
C -7.523418 -1.474477 1.207416
C -8.179734 -1.705094 0.000000
C -7.523418 -1.474477 -1.207416
C -6.201268 -1.008426 -1.237415
C -5.515780 -0.741719 2.573334
H -9.208582 -2.067135 0.000000
C -5.515780 -0.741719 -2.573334
C -0.719838 0.168613 2.573841
C -1.545216 -3.351808 -1.689497
C -1.545216 -3.351808 1.689497
H -1.420656 -4.439450 -1.825664

H -0.538836 -2.909464 -1.631155
H -2.044981 -2.967062 -2.593005
H -2.044981 -2.967062 2.593005
H -1.420656 -4.439450 1.825664
H -0.538836 -2.909464 1.631155
H -4.372117 -4.754258 -0.887391
H -4.372117 -4.754258 0.887391
H -5.269243 -3.506860 0.000000
H -4.471240 -0.473562 2.365681
C -6.165395 0.447618 3.307522
H -8.046060 -1.657731 2.147639
C -5.494734 -1.995581 3.465591
H -8.046060 -1.657731 -2.147639
H -4.471240 -0.473562 -2.365681
C -6.165395 0.447618 -3.307522
C -5.494734 -1.995581 -3.465591
H -4.910847 1.840097 0.000000
H -2.167554 2.314620 0.000000
C -0.054469 -0.631114 -3.705364
H -1.726597 -0.247308 -2.426941
C -0.865284 1.644972 -3.003617
C -0.054469 -0.631114 3.705364
C -0.865284 1.644972 3.003617
H -1.726597 -0.247308 2.426941
H 1.974694 0.042297 -2.145235
H 1.974694 0.042297 2.145235
H -5.637256 0.648585 -4.251746
H -7.218069 0.236671 -3.549628
H -6.138860 1.363983 -2.700082
H -4.932733 -1.792106 -4.389241
H -5.020289 -2.840214 -2.948872
H -6.512134 -2.298345 -3.755340
H -1.419789 1.712081 -3.951960
H -1.401996 2.245115 -2.256808
H 0.125105 2.101158 -3.156418
H -0.692160 -0.601443 -4.600827
H 0.918206 -0.202396 -3.988830
H 0.090389 -1.681520 -3.424577
H -5.637256 0.648585 4.251746
H -6.138860 1.363983 2.700082
H -7.218069 0.236671 3.549628
H -4.932733 -1.792106 4.389241
H -6.512134 -2.298345 3.755340
H -5.020289 -2.840214 2.948872
H -0.692160 -0.601443 4.600827
H 0.090389 -1.681520 3.424577
H 0.918206 -0.202396 3.988830
H -1.419789 1.712081 3.951960
H 0.125105 2.101158 3.156418
H -1.401996 2.245115 2.256808

Net Charge: 0.00

Total Bonding Energy:
-16.420074454451210 hartree
-10303.75 kcal/mol
-43110.90 kJ/mol
Summary Geometry Optimization:

Energy Change : -0.000028
Gradient (Max): 0.000334
Gradient (RMS): 0.000086

SIPr-GaMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
==========

ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gallium (TZP, 3p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	0.021527	0.081494	-1.236386
C	-0.669040	0.061098	0.000000
C	0.021527	0.081494	1.236386
C	1.422086	0.018459	1.205447
C	2.117762	-0.029399	0.000000
C	1.422086	0.018459	-1.205447
N	-2.111146	0.168593	0.000000
C	-3.038685	-0.821168	0.000000
N	-4.254156	-0.227617	0.000000
C	-4.203123	1.259152	0.000000
C	-2.702294	1.538226	0.000000
Ga	-2.639532	-3.018653	0.000000
C	-4.360895	-4.083873	0.000000
C	-5.565334	-0.827087	0.000000
C	-6.212827	-1.047824	1.234639
C	-7.525176	-1.539792	1.206687
C	-8.176950	-1.786896	0.000000
C	-7.525176	-1.539792	-1.206687
C	-6.212827	-1.047824	-1.234639
C	-5.536461	-0.768547	2.572277
H	-9.197810	-2.170945	0.000000
C	-5.536461	-0.768547	-2.572277
C	-0.689679	0.267743	2.575836
H	3.207184	-0.084771	0.000000
C	-0.689679	0.267743	-2.575836
C	-1.581872	-3.350632	-1.685938
C	-1.581872	-3.350632	1.685938
H	-1.491548	-4.444647	-1.797022
H	-0.563373	-2.937369	-1.638079
H	-2.076785	-2.972159	-2.594237
H	-2.076785	-2.972159	2.594237
H	-1.491548	-4.444647	1.797022
H	-0.563373	-2.937369	1.638079
H	-4.369829	-4.739714	-0.886932
H	-4.369829	-4.739714	0.886932
H	-5.303698	-3.518829	0.000000
H	-4.517838	-0.415751	2.360541
C	-6.266321	0.339195	3.357411
H	-8.044527	-1.732509	2.147297
C	-5.405509	-2.046305	3.420734
H	-8.044527	-1.732509	-2.147297

H -4.517838 -0.415751 -2.360541
C -6.266321 0.339195 -3.357411
C -5.405509 -2.046305 -3.420734
H -4.717288 1.649250 0.889667
H -4.717288 1.649250 -0.889667
H -2.369825 2.088655 0.888886
H -2.369825 2.088655 -0.888886
C -0.168744 -0.657616 -3.688348
H -1.752412 0.034419 -2.421686
C -0.572913 1.735563 -3.047730
C -0.168744 -0.657616 3.688348
C -0.572913 1.735563 3.047730
H -1.752412 0.034419 2.421686
H 1.976871 0.014650 -2.144669
H 1.976871 0.014650 2.144669
H -5.727596 0.566858 -4.289572
H -7.286090 0.027368 -3.628871
H -6.350069 1.268154 -2.773913
H -4.863051 -1.829885 -4.353320
H -4.862346 -2.828909 -2.874966
H -6.394940 -2.443610 -3.693155
H -1.157268 1.890490 -3.967399
H -0.923502 2.453863 -2.293143
H 0.476681 1.983253 -3.268502
H -0.770380 -0.516713 -4.598639
H 0.873450 -0.422744 -3.950624
H -0.227729 -1.712696 -3.396776
H -5.727596 0.566858 4.289572
H -6.350069 1.268154 2.773913
H -7.286090 0.027368 3.628871
H -4.863051 -1.829885 4.353320
H -6.394940 -2.443610 3.693155
H -4.862346 -2.828909 2.874966
H -0.770380 -0.516713 4.598639
H -0.227729 -1.712696 3.396776
H 0.873450 -0.422744 3.950624
H -1.157268 1.890490 3.967399
H 0.476681 1.983253 3.268502
H -0.923502 2.453863 2.293143

Net Charge: 0.00

Total Bonding Energy:
-16.685625562411584 hartree
-10470.39 kcal/mol
-43808.10 kJ/mol
Summary Geometry Optimization:

Energy Change : 0.000025
Gradient (Max): 0.000878
Gradient (RMS): 0.000104

IMes-InMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Indium (TZP, 4p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	2.831281	-1.895145	-1.230590
C	2.156356	-1.961856	0.000000
C	2.831281	-1.895145	1.230590
C	4.221409	-1.729795	1.201585
C	4.934266	-1.644483	0.000000
C	4.221409	-1.729795	-1.201585
N	0.724714	-2.186327	0.000000
C	-0.251248	-1.221811	0.000000
N	-1.412296	-1.951717	0.000000
C	-1.164527	-3.323445	0.000000
C	0.185341	-3.470993	0.000000
C	-2.761134	-1.424848	0.000000
C	-3.402737	-1.205777	-1.229734
C	-4.730562	-0.763342	-1.201442
C	-5.414006	-0.543428	0.000000
C	-4.730562	-0.763342	1.201442
C	-3.402737	-1.205777	1.229734
C	-2.685749	-1.408111	-2.541247
C	-2.685749	-1.408111	2.541247
C	-6.858132	-0.101726	0.000000
C	2.095329	-1.989164	2.543314
C	6.437843	-1.499546	0.000000
C	2.095329	-1.989164	-2.543314
In	0.079763	1.183642	0.000000
C	1.201209	1.526338	1.896361
C	-1.913211	2.169814	0.000000
C	1.201209	1.526338	-1.896361
H	4.759130	-1.665717	-2.150785
H	4.759130	-1.665717	2.150785
H	-5.240777	-0.580856	-2.150374
H	-5.240777	-0.580856	2.150374
H	-3.370601	-1.251311	3.383036
H	-2.264265	-2.420315	2.625895
H	-1.849963	-0.700540	2.642192
H	-3.370601	-1.251311	-3.383036
H	-1.849963	-0.700540	-2.642192
H	-2.264265	-2.420315	-2.625895
H	-7.093521	0.496798	0.889481
H	-7.093521	0.496798	-0.889481
H	-7.533341	-0.972004	0.000000
H	6.787904	-0.960061	0.889586
H	6.926472	-2.486742	0.000000
H	6.787904	-0.960061	-0.889586
H	2.803427	-2.001633	3.380427
H	1.425346	-1.127897	2.674531
H	1.480315	-2.899078	2.600778
H	2.803427	-2.001633	-3.380427
H	1.480315	-2.899078	-2.600778
H	1.425346	-1.127897	-2.674531
H	1.329580	2.612577	2.018853
H	0.645797	1.159998	2.773312
H	2.199097	1.065721	1.887177

H 1.329580 2.612577 -2.018853
H 2.199097 1.065721 -1.887177
H 0.645797 1.159998 -2.773312
H -2.001110 2.809406 -0.890919
H -2.758250 1.467217 0.000000
H -2.001110 2.809406 0.890919
H 0.807231 -4.358004 0.000000
H -1.964961 -4.053406 0.000000

Net Charge: 0.00

Total Bonding Energy:
-12.818114208620822 hartree
-8043.49 kcal/mol
-33653.95 kJ/mol
Summary Geometry Optimization:

Energy Change : -0.000001
Gradient (Max): 0.000576
Gradient (RMS): 0.000105

SIMes-InMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Indium (TZP, 4p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C 2.840498 -1.881072 -1.227968
C 2.156833 -1.956865 0.000000
C 2.840498 -1.881072 1.227968
C 4.228044 -1.696299 1.201043
C 4.940537 -1.600883 0.000000
C 4.228044 -1.696299 -1.201043
N 0.738282 -2.206628 0.000000
C -0.255151 -1.294989 0.000000
N -1.424954 -1.964472 0.000000
C -1.267041 -3.448635 0.000000
C 0.255999 -3.618776 0.000000
C -2.754645 -1.413442 0.000000
C -3.402283 -1.182836 -1.227021
C -4.724588 -0.724806 -1.200936
C -5.406711 -0.497944 0.000000
C -4.724588 -0.724806 1.200936
C -3.402283 -1.182836 1.227021
C -2.684389 -1.376239 -2.539688
C -2.684389 -1.376239 2.539688
C -6.845110 -0.037708 0.000000
C 2.107835 -1.978703 2.542810

C 6.441460 -1.430074 0.000000
C 2.107835 -1.978703 -2.542810
In 0.073069 1.136252 0.000000
C 1.187423 1.484057 1.899053
C -1.907581 2.148061 0.000000
C 1.187423 1.484057 -1.899053
H 4.764389 -1.620272 -2.150424
H 4.764389 -1.620272 2.150424
H -5.231135 -0.531641 -2.149961
H -5.231135 -0.531641 2.149961
H -3.363416 -1.196678 3.381926
H -2.278586 -2.393274 2.644423
H -1.837508 -0.680433 2.627360
H -3.363416 -1.196678 -3.381926
H -1.837508 -0.680433 -2.627360
H -2.278586 -2.393274 -2.644423
H -7.072820 0.564014 0.889429
H -7.072820 0.564014 -0.889429
H -7.532047 -0.898842 0.000000
H 6.782114 -0.884296 0.889500
H 6.947817 -2.408330 0.000000
H 6.782114 -0.884296 -0.889500
H 2.811681 -1.914388 3.381376
H 1.378910 -1.163463 2.644703
H 1.560157 -2.928570 2.637207
H 2.811681 -1.914388 -3.381376
H 1.560157 -2.928570 -2.637207
H 1.378910 -1.163463 -2.644703
H 1.298166 2.572802 2.017770
H 0.635783 1.112879 2.776107
H 2.191800 1.038543 1.890791
H 1.298166 2.572802 -2.017770
H 2.191800 1.038543 -1.890791
H 0.635783 1.112879 -2.776107
H -1.982066 2.789002 -0.891182
H -2.763959 1.459990 0.000000
H -1.982066 2.789002 0.891182
H 0.630571 -4.144907 -0.889152
H 0.630571 -4.144907 0.889152
H -1.749483 -3.878657 -0.889036
H -1.749483 -3.878657 0.889036

Net Charge: 0.00

Total Bonding Energy:
-13.085752101978871 hartree
-8211.43 kcal/mol
-34356.64 kJ/mol
Summary Geometry Optimization:

Energy Change : -0.000009
Gradient (Max): 0.000848
Gradient (RMS): 0.000103

IPr-InMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86

Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Indium (TZP, 4p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	0.005287	0.121996	-1.240015
C	-0.669523	0.135514	0.000000
C	0.005287	0.121996	1.240015
C	1.405798	0.057109	1.207593
C	2.099215	0.020315	0.000000
C	1.405798	0.057109	-1.207593
N	-2.118314	0.257936	0.000000
C	-3.031990	-0.770618	0.000000
N	-4.236924	-0.113278	0.000000
C	-4.078411	1.269612	0.000000
C	-2.741885	1.502651	0.000000
In	-2.601908	-3.178382	0.000000
C	-4.547961	-4.257015	0.000000
C	-5.556658	-0.714877	0.000000
C	-6.185418	-0.956167	1.237352
C	-7.490444	-1.468262	1.207197
C	-8.137952	-1.722311	0.000000
C	-7.490444	-1.468262	-1.207197
C	-6.185418	-0.956167	-1.237352
C	-5.506030	-0.679875	2.574455
H	-9.152652	-2.122196	0.000000
C	-5.506030	-0.679875	-2.574455
C	-0.731089	0.236652	2.573530
H	3.188576	-0.036047	0.000000
C	-0.731089	0.236652	-2.573530
C	-1.441686	-3.488901	-1.871402
C	-1.441686	-3.488901	1.871402
H	-1.378747	-4.572188	-2.055221
H	-0.418830	-3.099206	-1.774448
H	-1.919934	-3.026799	-2.746734
H	-1.919934	-3.026799	2.746734
H	-1.378747	-4.572188	2.055221
H	-0.418830	-3.099206	1.774448
H	-4.599282	-4.901988	-0.889899
H	-4.599282	-4.901988	0.889899
H	-5.430267	-3.602900	0.000000
H	-4.480935	-0.345084	2.366152
C	-6.216996	0.449296	3.345065
H	-8.004752	-1.673765	2.147373
C	-5.404087	-1.954321	3.432068
H	-8.004752	-1.673765	-2.147373
H	-4.480935	-0.345084	-2.366152
C	-6.216996	0.449296	-3.345065
C	-5.404087	-1.954321	-3.432068
H	-4.922759	1.947304	0.000000
H	-2.181898	2.428494	0.000000
C	-0.075520	-0.570187	-3.705677
H	-1.742420	-0.168157	-2.425395
C	-0.861770	1.714205	-3.003424
C	-0.075520	-0.570187	3.705677

C -0.861770 1.714205 3.003424
H -1.742420 -0.168157 2.425395
H 1.961058 0.031952 -2.145220
H 1.961058 0.031952 2.145220
H -5.690983 0.656912 -4.288969
H -7.252202 0.170179 -3.592960
H -6.252003 1.380650 -2.761394
H -4.853433 -1.741998 -4.360605
H -4.880203 -2.754562 -2.892437
H -6.400444 -2.327460 -3.712806
H -1.416320 1.786759 -3.951242
H -1.391118 2.320310 -2.256237
H 0.133519 2.159179 -3.157330
H -0.713637 -0.532959 -4.600532
H 0.901335 -0.151579 -3.989955
H 0.058580 -1.622584 -3.426923
H -5.690983 0.656912 4.288969
H -6.252003 1.380650 2.761394
H -7.252202 0.170179 3.592960
H -4.853433 -1.741998 4.360605
H -6.400444 -2.327460 3.712806
H -4.880203 -2.754562 2.892437
H -0.713637 -0.532959 4.600532
H 0.058580 -1.622584 3.426923
H 0.901335 -0.151579 3.989955
H -1.416320 1.786759 3.951242
H 0.133519 2.159179 3.157330
H -1.391118 2.320310 2.256237

Net Charge: 0.00

Total Bonding Energy:
-16.373140876602889 hartree
-10274.30 kcal/mol
-42987.68 kJ/mol
Summary Geometry Optimization:

Energy Change : 0.000040
Gradient (Max): 0.000397
Gradient (RMS): 0.000113

SIPr-InMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Indium (TZP, 4p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C 0.017903 0.144976 -1.236378

C	-0.671884	0.150548	0.000000
C	0.017903	0.144976	1.236378
C	1.416305	0.044932	1.205701
C	2.110469	-0.018880	0.000000
C	1.416305	0.044932	-1.205701
N	-2.111716	0.280687	0.000000
C	-3.035306	-0.707709	0.000000
N	-4.251842	-0.123013	0.000000
C	-4.207990	1.364954	0.000000
C	-2.705940	1.650275	0.000000
In	-2.638279	-3.154105	0.000000
C	-4.582089	-4.240235	0.000000
C	-5.549108	-0.751540	0.000000
C	-6.187134	-0.998455	1.234691
C	-7.484695	-1.528317	1.206485
C	-8.129810	-1.791819	0.000000
C	-7.484695	-1.528317	-1.206485
C	-6.187134	-0.998455	-1.234691
C	-5.515537	-0.711950	2.573236
H	-9.138298	-2.207182	0.000000
C	-5.515537	-0.711950	-2.573236
C	-0.691992	0.331340	2.575721
H	3.198009	-0.103716	0.000000
C	-0.691992	0.331340	-2.575721
C	-1.496456	-3.529055	-1.869749
C	-1.496456	-3.529055	1.869749
H	-1.472107	-4.619081	-2.020815
H	-0.460918	-3.171050	-1.790852
H	-1.969433	-3.078793	-2.753661
H	-1.969433	-3.078793	2.753661
H	-1.472107	-4.619081	2.020815
H	-0.460918	-3.171050	1.790852
H	-4.620804	-4.885951	-0.890112
H	-4.620804	-4.885951	0.890112
H	-5.474959	-3.601486	0.000000
H	-4.504818	-0.336393	2.362615
C	-6.268127	0.374929	3.365554
H	-7.996274	-1.740803	2.146989
C	-5.356765	-1.992196	3.413636
H	-7.996274	-1.740803	-2.146989
H	-4.504818	-0.336393	-2.362615
C	-6.268127	0.374929	-3.365554
C	-5.356765	-1.992196	-3.413636
H	-4.722500	1.753711	0.889974
H	-4.722500	1.753711	-0.889974
H	-2.375650	2.201642	0.889216
H	-2.375650	2.201642	-0.889216
C	-0.188411	-0.615442	-3.677767
H	-1.758391	0.117437	-2.417966
C	-0.554033	1.792241	-3.060956
C	-0.188411	-0.615442	3.677767
C	-0.554033	1.792241	3.060956
H	-1.758391	0.117437	2.417966
H	1.970568	0.021192	-2.144878
H	1.970568	0.021192	2.144878
H	-5.733942	0.607700	-4.299037
H	-7.280856	0.039297	-3.635045
H	-6.371748	1.305424	-2.787791
H	-4.819760	-1.770191	-4.348002
H	-4.796074	-2.759712	-2.863646
H	-6.336847	-2.413938	-3.682747
H	-1.138747	1.948752	-3.980094

H -0.890999 2.521315 -2.310406
H 0.498610 2.021685 -3.287183
H -0.793333 -0.481965 -4.586997
H 0.854875 -0.396397 -3.949494
H -0.256122 -1.665644 -3.370806
H -5.733942 0.607700 4.299037
H -6.371748 1.305424 2.787791
H -7.280856 0.039297 3.635045
H -4.819760 -1.770191 4.348002
H -6.336847 -2.413938 3.682747
H -4.796074 -2.759712 2.863646
H -0.793333 -0.481965 4.586997
H -0.256122 -1.665644 3.370806
H 0.854875 -0.396397 3.949494
H -1.138747 1.948752 3.980094
H 0.498610 2.021685 3.287183
H -0.890999 2.521315 2.310406

Net Charge: 0.00

Total Bonding Energy:
-16.639012104826662 hartree
-10441.14 kcal/mol
-43685.72 kJ/mol
Summary Geometry Optimization:

Energy Change : 0.000016
Gradient (Max): 0.000406
Gradient (RMS): 0.000072

IMes-AlMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Aluminium (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C 2.848943 -1.830516 -1.230675
C 2.172545 -1.880345 0.000000
C 2.848943 -1.830516 1.230675
C 4.240633 -1.679851 1.201341
C 4.954128 -1.598685 0.000000
C 4.240633 -1.679851 -1.201341
N 0.737451 -2.088538 0.000000
C -0.237965 -1.119740 0.000000
N -1.402235 -1.847034 0.000000
C -1.156437 -3.217965 0.000000
C 0.193191 -3.369177 0.000000
C -2.758129 -1.335009 0.000000

C -3.402539 -1.127371 -1.229880
C -4.739204 -0.713024 -1.201538
C -5.427583 -0.509048 0.000000
C -4.739204 -0.713024 1.201538
C -3.402539 -1.127371 1.229880
C -2.677602 -1.304014 -2.540690
C -2.677602 -1.304014 2.540690
C -6.881419 -0.100612 0.000000
C 2.116662 -1.938289 2.544344
C 6.458889 -1.467298 0.000000
C 2.116662 -1.938289 -2.544344
Al 0.061713 1.021272 0.000000
C 1.080753 1.408052 1.691669
C -1.697834 1.994097 0.000000
C 1.080753 1.408052 -1.691669
H 4.779173 -1.626084 -2.150639
H 4.779173 -1.626084 2.150639
H -5.252412 -0.538984 -2.150476
H -5.252412 -0.538984 2.150476
H -3.363354 -1.155237 3.383170
H -2.233806 -2.306072 2.632743
H -1.858096 -0.577012 2.633618
H -3.363354 -1.155237 -3.383170
H -1.858096 -0.577012 -2.633618
H -2.233806 -2.306072 -2.632743
H -7.130652 0.492211 0.889513
H -7.130652 0.492211 -0.889513
H -7.536346 -0.986283 0.000000
H 6.813751 -0.931029 0.889562
H 6.938440 -2.458913 0.000000
H 6.813751 -0.931029 -0.889562
H 2.826973 -1.940117 3.379609
H 1.431467 -1.090210 2.678891
H 1.520057 -2.860776 2.601100
H 2.826973 -1.940117 -3.379609
H 1.520057 -2.860776 -2.601100
H 1.431467 -1.090210 -2.678891
H 1.185166 2.506513 1.760009
H 0.551247 1.098711 2.610673
H 2.101150 0.993335 1.734071
H 1.185166 2.506513 -1.760009
H 2.101150 0.993335 -1.734071
H 0.551247 1.098711 -2.610673
H -1.750758 2.653164 -0.884824
H -2.622029 1.395379 0.000000
H -1.750758 2.653164 0.884824
H 0.814465 -4.256688 0.000000
H -1.959326 -3.945172 0.000000

Net Charge: 0.00

Total Bonding Energy:
-12.914180495086272 hartree
-8103.77 kcal/mol
-33906.18 kJ/mol
Summary Geometry Optimization:

Energy Change : 0.000013
Gradient (Max): 0.000420
Gradient (RMS): 0.000098

SIMes-AlMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Aluminium (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	2.858416	-1.816945	-1.227966
C	2.172618	-1.874511	0.000000
C	2.858416	-1.816945	1.227966
C	4.248009	-1.649381	1.200704
C	4.961410	-1.559640	0.000000
C	4.248009	-1.649381	-1.200704
N	0.750317	-2.108021	0.000000
C	-0.243326	-1.191300	0.000000
N	-1.415742	-1.860880	0.000000
C	-1.258118	-3.343196	0.000000
C	0.263724	-3.516173	0.000000
C	-2.752975	-1.326229	0.000000
C	-3.404303	-1.108779	-1.227170
C	-4.736645	-0.681269	-1.201021
C	-5.424227	-0.471488	0.000000
C	-4.736645	-0.681269	1.201021
C	-3.404303	-1.108779	1.227170
C	-2.678236	-1.273793	-2.539101
C	-2.678236	-1.273793	2.539101
C	-6.873462	-0.046672	0.000000
C	2.130415	-1.926972	2.544347
C	6.464218	-1.406786	0.000000
C	2.130415	-1.926972	-2.544347
Al	0.049130	0.976822	0.000000
C	1.062848	1.366701	1.693238
C	-1.699010	1.971303	0.000000
C	1.062848	1.366701	-1.693238
H	4.785530	-1.585144	-2.150191
H	4.785530	-1.585144	2.150191
H	-5.247080	-0.498331	-2.149972
H	-5.247080	-0.498331	2.149972
H	-3.363371	-1.121969	3.381852
H	-1.861751	-0.542675	-2.626083
H	-2.229937	-2.272710	-2.644071
H	-7.115947	0.549221	0.889405
H	-7.115947	0.549221	-0.889405
H	-7.539063	-0.924386	0.000000
H	6.811369	-0.865219	0.889507
H	6.958644	-2.391132	0.000000
H	6.811369	-0.865219	-0.889507
H	2.837042	-1.861052	3.380385
H	1.394226	-1.119961	2.653705
H	1.594428	-2.884041	2.635255

H 2.837042 -1.861052 -3.380385
H 1.594428 -2.884041 -2.635255
H 1.394226 -1.119961 -2.653705
H 1.152281 2.467183 1.754337
H 0.538443 1.058612 2.615434
H 2.088402 0.965887 1.736984
H 1.152281 2.467183 -1.754337
H 2.088402 0.965887 -1.736984
H 0.538443 1.058612 -2.615434
H -1.737465 2.632482 -0.884347
H -2.636312 1.394035 0.000000
H -1.737465 2.632482 0.884347
H 0.638318 -4.042792 -0.889192
H 0.638318 -4.042792 0.889192
H -1.743154 -3.771106 -0.888986
H -1.743154 -3.771106 0.888986

Net Charge: 0.00

Total Bonding Energy:
-13.180768480651473 hartree
-8271.06 kcal/mol
-34606.10 kJ/mol
Summary Geometry Optimization:

Energy Change : -0.000005
Gradient (Max): 0.000593
Gradient (RMS): 0.000093

IPr-AlMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Aluminium (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C 0.009777 0.041951 -1.240125
C -0.665049 0.051166 0.000000
C 0.009777 0.041951 1.240125
C 1.410216 -0.022350 1.207343
C 2.103640 -0.059721 0.000000
C 1.410216 -0.022350 -1.207343
N -2.115147 0.174309 0.000000
C -3.038857 -0.848118 0.000000
N -4.240128 -0.182301 0.000000
C -4.069567 1.197864 0.000000
C -2.730756 1.420880 0.000000
Al -2.639127 -2.975413 0.000000
C -4.346565 -4.040922 0.000000

C	-5.571553	-0.761128	0.000000
C	-6.204660	-0.988538	1.237494
C	-7.519608	-1.474267	1.207293
C	-8.172329	-1.714956	0.000000
C	-7.519608	-1.474267	-1.207293
C	-6.204660	-0.988538	-1.237494
C	-5.516701	-0.735301	2.574640
H	-9.195071	-2.093835	0.000000
C	-5.516701	-0.735301	-2.574640
C	-0.724175	0.162436	2.574586
H	3.192992	-0.116125	0.000000
C	-0.724175	0.162436	-2.574586
C	-1.579891	-3.309526	-1.672431
C	-1.579891	-3.309526	1.672431
H	-1.466800	-4.403752	-1.780820
H	-0.560865	-2.890681	-1.637048
H	-2.057596	-2.954562	-2.601590
H	-2.057596	-2.954562	2.601590
H	-1.466800	-4.403752	1.780820
H	-0.560865	-2.890681	1.637048
H	-4.360219	-4.705263	-0.882696
H	-4.360219	-4.705263	0.882696
H	-5.306369	-3.501485	0.000000
H	-4.498485	-0.380255	2.366746
C	-6.234780	0.363553	3.380873
H	-8.037791	-1.669521	2.147598
C	-5.389172	-2.031309	3.396160
H	-8.037791	-1.669521	-2.147598
H	-4.498485	-0.380255	-2.366746
C	-6.234780	0.363553	-3.380873
C	-5.389172	-2.031309	-3.396160
H	-4.909785	1.880789	0.000000
H	-2.163073	2.342013	0.000000
C	-0.068569	-0.639866	-3.709855
H	-1.736032	-0.241890	-2.430817
C	-0.850353	1.642293	-2.997989
C	-0.068569	-0.639866	3.709855
C	-0.850353	1.642293	2.997989
H	-1.736032	-0.241890	2.430817
H	1.965101	-0.046572	-2.145125
H	1.965101	-0.046572	2.145125
H	-5.700037	0.555970	-4.323093
H	-7.262419	0.063668	-3.635518
H	-6.290746	1.308060	-2.820281
H	-4.832612	-1.837325	-4.325122
H	-4.860839	-2.808957	-2.829621
H	-6.378615	-2.424445	-3.674382
H	-1.402600	1.720494	-3.946785
H	-1.379933	2.246475	-2.249388
H	0.146194	2.085839	-3.147668
H	-0.707861	-0.600508	-4.603750
H	0.907460	-0.219190	-3.994094
H	0.065854	-1.692826	-3.433504
H	-5.700037	0.555970	4.323093
H	-6.290746	1.308060	2.820281
H	-7.262419	0.063668	3.635518
H	-4.832612	-1.837325	4.325122
H	-6.378615	-2.424445	3.674382
H	-4.860839	-2.808957	2.829621
H	-0.707861	-0.600508	4.603750
H	0.065854	-1.692826	3.433504
H	0.907460	-0.219190	3.994094

H -1.402600 1.720494 3.946785
H 0.146194 2.085839 3.147668
H -1.379933 2.246475 2.249388

Net Charge: 0.00

Total Bonding Energy:
-16.469532412514035 hartree
-10334.79 kcal/mol
-43240.75 kJ/mol
Summary Geometry Optimization:

Energy Change : 0.000003
Gradient (Max): 0.000439
Gradient (RMS): 0.000089

SIPr-AlMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2012.01

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Aluminium (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C 0.018164 0.025920 -1.236665
C -0.671902 0.039210 0.000000
C 0.018164 0.025920 1.236665
C 1.414245 -0.100427 1.205451
C 2.106845 -0.179742 0.000000
C 1.414245 -0.100427 -1.205451
N -2.111201 0.189160 0.000000
C -3.054630 -0.784248 0.000000
N -4.262383 -0.177627 0.000000
C -4.190456 1.306816 0.000000
C -2.682787 1.565701 0.000000
Al -2.689815 -2.943281 0.000000
C -4.396370 -4.011777 0.000000
C -5.577296 -0.771084 0.000000
C -6.221829 -0.997249 1.234920
C -7.533946 -1.489558 1.206722
C -8.186227 -1.734738 0.000000
C -7.533946 -1.489558 -1.206722
C -6.221829 -0.997249 -1.234920
C -5.537109 -0.741714 2.573077
H -9.206419 -2.120450 0.000000
C -5.537109 -0.741714 -2.573077
C -0.684802 0.236061 2.576836
H 3.192329 -0.287199 0.000000
C -0.684802 0.236061 -2.576836
C -1.640428 -3.310363 -1.669456

C -1.640428 -3.310363 1.669456
H -1.564439 -4.409280 -1.762019
H -0.609182 -2.924191 -1.635360
H -2.108452 -2.953414 -2.602114
H -2.108452 -2.953414 2.602114
H -1.564439 -4.409280 1.762019
H -0.609182 -2.924191 1.635360
H -4.399729 -4.676993 -0.882352
H -4.399729 -4.676993 0.882352
H -5.363370 -3.486812 0.000000
H -4.529322 -0.358247 2.362202
C -6.281167 0.321888 3.403275
H -8.051093 -1.688309 2.147245
C -5.366334 -2.044543 3.375973
H -8.051093 -1.688309 -2.147245
H -4.529322 -0.358247 -2.362202
C -6.281167 0.321888 -3.403275
C -5.366334 -2.044543 -3.375973
H -4.698754 1.704317 0.889989
H -4.698754 1.704317 -0.889989
H -2.343625 2.111652 0.889163
H -2.343625 2.111652 -0.889163
C -0.178648 -0.688293 -3.696987
H -1.752452 0.021968 -2.428555
C -0.538129 1.705314 -3.035924
C -0.178648 -0.688293 3.696987
C -0.538129 1.705314 3.035924
H -1.752452 0.021968 2.428555
H 1.967909 -0.133444 -2.144502
H 1.967909 -0.133444 2.144502
H -5.736230 0.528751 -4.336599
H -7.290377 -0.021154 -3.676116
H -6.391164 1.267871 -2.852526
H -4.816487 -1.847791 -4.308484
H -4.814203 -2.796483 -2.797652
H -6.343587 -2.472642 -3.645607
H -1.119581 1.880386 -3.953811
H -0.872165 2.424228 -2.274545
H 0.516502 1.932051 -3.255578
H -0.781096 -0.532867 -4.604282
H 0.865445 -0.464425 -3.961515
H -0.250417 -1.744585 -3.412854
H -5.736230 0.528751 4.336599
H -6.391164 1.267871 2.852526
H -7.290377 -0.021154 3.676116
H -4.816487 -1.847791 4.308484
H -6.343587 -2.472642 3.645607
H -4.814203 -2.796483 2.797652
H -0.781096 -0.532867 4.604282
H -0.250417 -1.744585 3.412854
H 0.865445 -0.464425 3.961515
H -1.119581 1.880386 3.953811
H 0.516502 1.932051 3.255578
H -0.872165 2.424228 2.274545

Net Charge: 0.00

Total Bonding Energy:
-16.734367902935148 hartree
-10500.98 kcal/mol
-43936.08 kJ/mol
Summary Geometry Optimization:

Energy Change : -0.000034
Gradient (Max): 0.000855
Gradient (RMS): 0.000116

IiPrMe-GaMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2014

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Peirdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00
Symmetry: NOSYM

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gallium (TZP, 3p frozen)
Silicon (TZP, 2p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C 6.838794 9.154612 7.478207
C 7.841655 8.160294 7.474188
C 9.006956 8.252782 8.267635
C 9.130459 9.367901 9.108495
C 8.146444 10.351211 9.151322
C 7.016949 10.243527 8.343233
N 7.751781 7.067420 6.517586
C 7.154055 5.830667 6.662529
N 7.462240 5.207665 5.470520
C 8.214727 6.024411 4.630935
C 8.397494 7.194168 5.290242
C 7.112147 3.864969 5.038294
C 5.947702 3.689428 4.263110
C 5.666762 2.394038 3.805347
C 6.519799 1.329910 4.083980
C 7.684332 1.541310 4.818664
C 8.013305 2.811732 5.309073
C 5.050377 4.851682 3.854003
C 9.329422 3.029249 6.049636
C 9.664783 1.901745 7.040001
Ga 5.829120 5.065494 8.381581
C 5.935318 3.048698 8.171326
Si 5.817291 1.807050 9.580741
C 4.211554 1.925147 10.583270
C 10.135359 7.227729 8.210273
C 10.570171 6.746923 9.606096
C 5.633296 9.109052 6.545642
C 4.361528 9.702894 7.172628
C 4.074565 5.922441 7.793411
Si 2.342848 5.324221 8.239511
C 1.998087 5.337279 10.103935
C 6.828159 5.812875 9.986965
Si 6.081694 6.549973 11.548001
C 4.962933 8.029797 11.141033
C 1.057313 6.480670 7.436879
C 1.983538 3.568163 7.607020

C	10.487580	3.211807	5.045421
C	11.343453	7.795219	7.436453
C	5.945013	9.829894	5.216638
C	5.096875	5.306466	12.588777
C	7.479172	7.199606	12.670354
C	5.888565	0.039501	8.870591
C	7.278033	1.982033	10.785747
H	8.543025	5.695798	3.653278
H	8.926061	8.096904	5.011735
H	8.349861	0.701743	5.018851
H	6.279791	0.329474	3.720721
H	4.766942	2.219548	3.215149
H	8.839972	1.718842	7.740085
H	10.555497	2.172119	7.623977
H	9.890594	0.957703	6.523825
H	9.235166	3.958266	6.630448
H	10.611271	2.308398	4.430529
H	11.432357	3.392590	5.577971
H	10.312981	4.058395	4.368404
H	10.014294	9.464541	9.739834
H	8.260515	11.208877	9.816126
H	6.256893	11.023310	8.380792
H	11.023528	7.558784	10.192426
H	11.325212	5.953944	9.509454
H	9.720407	6.347938	10.173353
H	9.765399	6.349815	7.662158
H	11.072318	8.094470	6.414925
H	12.143071	7.043552	7.369784
H	11.752565	8.679381	7.946835
H	4.160833	9.280002	8.165161
H	3.496950	9.488537	6.530083
H	4.428060	10.795972	7.273384
H	5.426349	8.052800	6.323099
H	6.183625	10.888159	5.398499
H	5.072793	9.788841	4.548359
H	6.794633	9.375819	4.690120
H	8.155142	6.386424	12.975880
H	7.074973	7.657327	13.586769
H	8.083683	7.960526	12.154334
H	5.524648	8.801766	10.594175
H	4.564381	8.489474	12.058018
H	4.110071	7.727306	10.517011
H	4.187992	4.968877	12.073454
H	4.784542	5.767763	13.538199
H	5.697839	4.418464	12.833907
H	8.243792	1.920472	10.261842
H	7.257446	1.178647	11.537708
H	7.250026	2.941945	11.320274
H	4.132846	2.886698	11.108651
H	4.177299	1.129665	11.343435
H	3.322029	1.812692	9.946680
H	5.042897	-0.146252	8.191162
H	5.846918	-0.715797	9.670849
H	6.813617	-0.129373	8.298921
H	7.466147	6.620350	9.592510
H	4.124380	6.981968	8.097373
H	7.523581	5.011710	10.294089
H	6.913974	2.840736	7.707882
H	4.100453	5.935051	6.687975
H	5.194547	2.759232	7.405303
H	0.938617	5.104690	10.291477
H	2.597763	4.581856	10.629499

H 2.209500 6.315229 10.559535
H 1.023008 3.211483 8.009264
H 1.910068 3.531664 6.510653
H 2.762410 2.857690 7.915954
H 0.029754 6.148975 7.652375
H 1.160250 7.509888 7.812698
H 1.175266 6.512728 6.343110
H 5.279725 5.701288 4.512907
C 5.355409 5.282050 2.403590
C 3.555208 4.537415 4.013767
H 4.729260 6.139738 2.118767
H 6.406914 5.571591 2.274415
H 5.145523 4.460556 1.703116
H 2.958458 5.435982 3.803943
H 3.223704 3.755998 3.315176
H 3.325897 4.204491 5.032713

Net Charge: 0.00

Total Bonding Energy:
-23.187827037130837 hartree
-14550.58 kcal/mol
-60879.63 kJ/mol
Summary Geometry Optimization:

Energy Change : -0.000039
Gradient (Max): 0.000286
Gradient (RMS): 0.000039

ItBu-GaMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2014

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gallium (TZP, 3p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C 0.285322 -3.548876 0.000000
N 0.778092 -2.255513 0.000000
C -0.242319 -1.323113 0.000000
N -1.386654 -2.108386 0.000000
C -1.065645 -3.456415 0.000000
C 2.262509 -1.975018 0.000000
Ga -0.052752 0.985457 0.000000
C 1.843009 1.762096 0.000000
C -2.837636 -1.660991 0.000000
C -3.107999 -0.852663 -1.272523
C -3.766593 -2.887412 0.000000
C -3.107999 -0.852663 1.272523
C -0.887875 1.651539 1.726116

C -0.887875 1.651539 -1.726116
H -0.315283 2.551586 -1.998605
H -0.805570 0.948443 -2.568066
H -1.940129 1.957033 -1.634309
H -0.315283 2.551586 1.998605
H -1.940129 1.957033 1.634309
H -0.805570 0.948443 2.568066
H 1.912592 2.413015 0.885890
H 2.733038 1.125172 0.000000
H 1.912592 2.413015 -0.885890
H -1.800921 -4.246347 0.000000
H 0.911054 -4.428515 0.000000
H -4.155753 -0.521866 1.279884
H -2.935102 -1.469536 2.165587
H -2.465100 0.028481 1.330177
H -4.155753 -0.521866 -1.279884
H -2.465100 0.028481 -1.330177
H -2.935102 -1.469536 -2.165587
H -4.798891 -2.515546 0.000000
H -3.642576 -3.509599 -0.896901
H -3.642576 -3.509599 0.896901
C 3.050182 -3.297161 0.000000
C 2.607718 -1.223092 -1.295718
C 2.607718 -1.223092 1.295718
H 4.118240 -3.045512 0.000000
H 2.855067 -3.901006 0.896716
H 2.855067 -3.901006 -0.896716
H 3.672710 -0.954648 1.297974
H 2.022657 -0.306347 1.403049
H 2.413748 -1.870880 2.162410
H 3.672710 -0.954648 -1.297974
H 2.413748 -1.870880 -2.162410
H 2.022657 -0.306347 -1.403049

Net Charge: 0.00

Total Bonding Energy:
-9.076753152826154 hartree
-5695.75 kcal/mol
-23831.01 kJ/mol
Summary Geometry Optimization:

Energy Change : 0.000009
Gradient (Max): 0.000748
Gradient (RMS): 0.000147

ItBu-InMe3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2014

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Indium (TZP, 4p frozen)

Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	0.275600	-3.688680	0.000000
N	0.767485	-2.393066	0.000000
C	-0.252710	-1.465137	0.000000
N	-1.392950	-2.245536	0.000000
C	-1.077053	-3.595953	0.000000
C	2.246432	-2.091577	0.000000
In	-0.062601	1.086090	0.000000
C	2.037882	1.871658	0.000000
C	-2.828603	-1.765577	0.000000
C	-3.077794	-0.947822	-1.272363
C	-3.781314	-2.972743	0.000000
C	-3.077794	-0.947822	1.272363
C	-0.982833	1.730521	1.925077
C	-0.982833	1.730521	-1.925077
H	-0.421238	2.622466	-2.239343
H	-0.887607	0.976751	-2.718520
H	-2.039982	2.013613	-1.830724
H	-0.421238	2.622466	2.239343
H	-2.039982	2.013613	1.830724
H	-0.887607	0.976751	2.718520
H	2.139509	2.510201	0.889907
H	2.868825	1.158295	0.000000
H	2.139509	2.510201	-0.889907
H	-1.814474	-4.384586	0.000000
H	0.900296	-4.569625	0.000000
H	-4.118482	-0.596278	1.283684
H	-2.912818	-1.565803	2.166000
H	-2.418564	-0.076647	1.328402
H	-4.118482	-0.596278	-1.283684
H	-2.418564	-0.076647	-1.328402
H	-2.912818	-1.565803	-2.166000
H	-4.808058	-2.585733	0.000000
H	-3.665476	-3.597227	-0.896357
H	-3.665476	-3.597227	0.896357
C	3.048699	-3.403739	0.000000
C	2.583846	-1.322653	-1.286661
C	2.583846	-1.322653	1.286661
H	4.114561	-3.143713	0.000000
H	2.857295	-4.009603	0.896310
H	2.857295	-4.009603	-0.896310
H	3.654865	-1.080488	1.303358
H	2.023794	-0.385694	1.359585
H	2.355072	-1.941788	2.165124
H	3.654865	-1.080488	-1.303358
H	2.355072	-1.941788	-2.165124
H	2.023794	-0.385694	-1.359585

Net Charge: 0.00

Total Bonding Energy:
-9.036385629319275 hartree
-5670.42 kcal/mol
-23725.03 kJ/mol
Summary Geometry Optimization:

Energy Change : -0.000014
Gradient (Max): 0.000896
Gradient (RMS): 0.000179

IPr-Ga(CH2SiMe3)3.out
Energy, Geometry and Frequencies -- Spin Densities still to come
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ADF - Version 2014

GEOMETRY OPTIMIZATION (Threshhold met)
Density Functional: VWN Becke88 Perdew86
Relativistic Corrections: scalar(ZORA,SAPA)
General Accuracy: 5.00
Symmetry: NOSYM

Basis:
Carbon (TZP, 1s frozen)
Nitrogen (TZP, 1s frozen)
Gallium (TZP, 3p frozen)
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

C	-1.057257	-3.418335	-0.194366
C	0.297610	-3.468574	-0.408877
N	0.755137	-2.146063	-0.353287
C	-0.270353	-1.275990	-0.112505
N	-1.378405	-2.067037	-0.012865
C	2.143682	-1.667256	-0.579526
C	2.572162	-1.843848	-2.039745
Ga	-0.044367	0.870424	0.064343
C	0.607650	1.458788	-1.759644
C	-2.728467	-1.485662	0.198170
C	-3.415270	-2.031927	1.452534
C	3.135278	-2.256212	0.427483
C	1.281698	1.107840	1.578269
C	-1.806228	1.762904	0.520940
C	-3.589532	-1.584184	-1.065657
H	-2.513194	-0.425526	0.370213
H	0.591174	2.559101	-1.797796
H	1.636597	1.145016	-1.992706
H	-0.045274	1.095759	-2.568184
H	-1.582093	2.837463	0.619268
H	-2.576532	1.675151	-0.261020
H	-2.244778	1.446804	1.480349
H	1.295246	2.172569	1.859085
H	0.988356	0.539254	2.473940
H	2.317956	0.830800	1.330564
C	-2.021510	-4.557448	-0.124845
C	1.150149	-4.677259	-0.619435
H	-4.515286	-1.011651	-0.918209
H	-3.060021	-1.158134	-1.927325
H	-3.873317	-2.617523	-1.306569
H	-4.307933	-1.426593	1.660293
H	-3.742860	-3.073187	1.340001
H	-2.751080	-1.962753	2.323999
H	2.070380	-0.591455	-0.381669
H	4.091975	-1.724177	0.337749
H	2.771899	-2.124053	1.454543
H	3.333026	-3.321510	0.253293
H	3.538167	-1.344420	-2.194743
H	2.696909	-2.898257	-2.319753
H	1.840065	-1.382998	-2.714295
H	-2.342631	-4.768009	0.906098

H -2.922744 -4.378173 -0.724625
H -1.547040 -5.467345 -0.511647
H 0.514204 -5.547008 -0.824430
H 1.833564 -4.564083 -1.470206
H 1.755898 -4.916134 0.267101

Net Charge: 0.00

Total Bonding Energy:
-9.111243611655306 hartree
-5717.39 kcal/mol
-23921.57 kJ/mol
Summary Geometry Optimization:

Energy Change : -0.000079
Gradient (Max): 0.000495
Gradient (RMS): 0.000097
