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Electronic Supplementary Information for:

N-Heterocyclic carbene and Cyclic Alkyl(Amino)Carbene Adducts of Gallium Hydrides, Gallium Chlorides and Gallium Hydrochlorides

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1 Experimental Section

General Procedure: All reactions and subsequent manipulations were performed under an argon atmosphere in an IT glovebox or using standard Schlenk techniques. Elemental analyses were performed in the microanalytical laboratory of the Institute of Inorganic Chemistry of the University Würzburg with an Elementar vario micro cube. As most of the compounds presented here are air and moisture sensitive and thermally labile, many of the combustion analyses presented in the following are outside the range generally accepted for analytical purity. However, they are provided here to illustrate the best values obtained to date. NMR spectra were recorded on a Bruker Avance 400 (^{1}H: 400.4 MHz; ^{13}C{^{1}H}: 100.7 MHz) using C_6D_6, thf-d_8 and toluene-d_8 as the solvent. Assignment of the ^{1}H NMR and ^{13}C NMR data was supported by ^{1}H,^{1}H and ^{13}C{^{1}H},^{1}H correlation experiments. ^{13}C NMR spectra were recorded broad band decoupled (^{13}C{^{1}H}). ^{1}H NMR chemical shifts are listed in parts per million (ppm), are reported relative to TMS and were referenced via residual proton resonances of the deuterated solvent (C_6D_5H: 7.16 ppm, d_8-thf: 1.73, 3.58 ppm, toluene-d_8: 2.08 ppm, 7.09). ^{13}C{^{1}H} NMR resonances are reported relative to TMS using the natural-abundance carbon resonances of C_6D_6 (128.06 ppm), d_8-thf (25.37, 67.57 ppm) and toluene-d_8 (20.4 ppm).[1] Infrared spectra were recorded on a Bruker Alpha FT-IR spectrometer (by using an ATR unit) as solids and are reported in cm^{-1}. The NHCs Me_2Im^{Me} (1,3,4,5-tetramethylimidazolin-2-ylidene), *i*Pr_2Im (1,3-di*iso*propylimidazolin-2-ylidene), *i*Pr_2Im^{Me} (1,3-di*iso*propyl-4,5-dimethylimidazolin-2-ylidene), [2] $Dipp_2$Im (1,3-bis-(2,6-di-*iso*-propylphenyl)imidazolin-2-ylidene)[54] and cAAC^{Me}[4] have been prepared according to published procedures. Gallium(III) chloride and lithium hydride were purchased from Sigma Aldrich and used as received. The presented results of the elemental analysis of the compounds 2, 3, 6, 7 and 11 are outside the range viewed as establishing analytical purity, they are provided here to illustrate the best values obtained to date. ^{1}H and ^{13}C{^{1}H} NMR spectra are also provided to this paper as corroborative evidence of purity.

(Me_2Im^{Me})·GaH_3 **1**: $LiGaH_4$ (5.68 mmol) was generated at -78 °C *in situ* from the reaction of $GaCl_3$ (1.00 g, 5,68 mmol) and LiH (904 mg, 114 mmol) in 40 mL EtO_2. Me_2Im^{Me} (705 mg, 5.68 mmol), dissolved in 15 mL EtO_2 was added to this solution. After stirring over night at room temperature, the colorless, cloudy reaction mixture was filtered to remove LiH and all volatiles of the filtrate were removed *in vacuo*. The residue was suspended in 10 ml *n*-hexane, the product was filtered off and dried *in vacuo* to afford **1** (660 mg, 3,35 mmol, 60 %) as a colorless powder. Crystals suitable for X-ray diffraction of compounds **1** were grown by slow evaporation of a saturated solution in benzene. $C_7H_{15}N_2Ga$ (196.93 g/mol): found (calcd.) C 42.52 (42.96), H 7.64 (7.68), N 14.07 (14.23). IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 408 (s), 416 (m), 501 (s), 560 (s), 590 (s), 615 (m), 646 (s), 674 (s), 748 (s, $\nu_{Ga\text{-}H,\ b.}$), 782 (m), 848 (s), 877 (s), 985 (s), 1092 (m), 1127 (m), 1190 (m), 1284 (m), 1311 (m), 1343 (s), 1390 (s), 1403 (s), 1485 (s), 1767 (m, $\nu_{Ga\text{-}H,\ str.}$),1836 (w), 1897 (s), 1906 (s), 1929 (s), 1948 (m), 1986 (w), 2003 (w), 2165 (m), 2825 (s), 2880 (m), 2947 (w, $\nu_{C\text{-}H,str.}$), 2994 (w, $\nu_{C\text{-}H,str.}$), 3097 (w). ^{1}H-NMR (400.4 MHz, C_6D_6, 298 K): δ = 1.16 (s, 6 H, C*H*$_3$), 3.14 (s, 6 H, NCC*H*$_3$CC*H*$_3$N), 4.51 (s, 3 H, Ga*H*$_3$). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 7.9 (*C*H$_3$), 33.8 (NC*C*H$_3$C*C*H$_3$N), 124.9 (N*CC*N), 172.1 (N*C*N).

(*i*Pr_2Im)·GaH_3 **2**: $LiGaH_4$ (5.68 mmol) was generated at -78 °C *in situ* from the reaction of $GaCl_3$ (1.00 g, 5,68 mmol) and LiH (904 mg, 114 mmol) in 40 mL EtO_2. *i*Pr_2Im (778 mg, 778 µL, 5.11 mmol), dissolved in 15 mL EtO_2 was added to this solution. After stirring over night at room temperature, the colorless, cloudy reaction mixture was filtered to remove LiH and all volatiles of the filtrate were removed *in vacuo*. The residue was suspended in 10 ml *n*-hexane, the product was filtered off and dried *in vacuo* to afford **2** (662 mg, 2.94 mmol, 52 %) as a colorless powder. $C_9H_{19}N_2Ga$ (224.99 g/mol): found (calcd.) C 42.73 (48.05), H 8.06 (8.51), N 10.79 (12.45). IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 459 (m), 506 (s), 523 (s), 589 (s), 641 (m), 664 (s), 725 (s, $\nu_{Ga\text{-}H,\ b.}$), 751 (s), 801 (w), 1104 (w), 1115 (m), 1134 (w), 1206 (s), 1369 (m), 1460 (m), 1774

(s, $\nu_{Ga\text{-}H,\ str.}$), 1796 (m), 1846 (m), 2168 (w), 2960 (m, $\nu_{C\text{-}H,str.}$), 3156 (w). ^{1}H-NMR (400.4 MHz, C_6D_6, 298 K): δ = 0.93 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, *i*Pr-CH_3), 4.56 (s, 3 H, Ga-H_3), 5.20 (sept, 2 H, $^3J_{HH}$ = 6.8 Hz, *i*Pr-C*H*), 6.22 (s, 2 H, NC*H*C*H*N). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 22.8 (*i*Pr-*C*H_3), 51.5 (*i*Pr-*C*H), 116.7 (NC*H*C*H*N), 173.3 (N*C*N).

(*i*Pr$_2$Im^{Me})·GaH$_3$ **3**: LiGaH$_4$ (5.68 mmol) was generated at -78 °C *in situ* from the reaction of GaCl$_3$ (1.00 g, 5,68 mmol) and LiH (904 mg, 114 mmol) in 40 mL EtO_2. *i*Pr$_2$Im^{Me} (921 mg,5.11 mmol), dissolved in 15 mL EtO_2 was added to this solution. After stirring over night at room temperature, the colorless, cloudy reaction mixture was filtered to remove LiH and all volatiles of the filtrate were removed *in vacuo*. The residue was suspended in 10 ml *n*-hexane, the product was filtered off and dried *in vacuo* to afford **3** (612 mg, 2.96 mmol, 58 %) as a colorless powder. $C_{11}H_{23}N_2Ga$ (253.04 g/mol): found (calcd.) C 49.48 (52.21), H 8.81 (9.16), N 10.39 (11.07). (ATR): $\tilde{\nu}$ [cm^{-1}] = 518 (s), 558 (m), 733 (s, $\nu_{Ga\text{-}H,\ b.}$), 903 (w), 1105 (w), 1217 (w), 1217 (m), 1370 (w), 1773 (s, $\nu_{Ga\text{-}H,\ str.}$), 2962 (w, $\nu_{C\text{-}H,str.}$). ^{1}H-NMR (400.4 MHz, C_6D_6, 298 K): δ = 1.12 (d, 12 H, $^3J_{HH}$ = 7.1 Hz, *i*Pr-CH_3), 1.52 (s, 6 H, NCCH_3CCH_3N), 4.66 (s, 3 H, Ga-H_3), 5.46 (sept, 2 H, $^3J_{HH}$ = 7.1 Hz, *i*Pr-C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 9.8 (NC*C*H$_3$C*C*H$_3$N), 21.5 (*i*Pr-*C*H$_3$), 52.4 (*i*Pr-*C*H), 125.6 (NC*C*N), 172.7 (N*C*N).

(Dipp$_2$Im^H)·GaH$_3$ **4**: LiGaH$_4$ (1.13 mmol) was generated at -78 °C *in situ* from the reaction of GaCl$_3$ (220 mg, 1.13 mmol) and LiH (90.4 mg, 11.3 mmol) in 40 mL EtO_2. Dipp$_2$Im^H (400 mg, 1.02 mmol), dissolved in 15 mL EtO_2 was added to this solution. After stirring over night at room temperature, the colorless, cloudy reaction mixture was filtered to remove LiH and all volatiles of the filtrate were removed *in vacuo*. The residue was suspended in 10 ml *n*-hexane, the product was filtered off and dried *in vacuo* to afford **4** (273 mg, 2.94 mmol, 59 %) as a colorless powder. Crystals suitable for X-ray diffraction of compounds **4** were grown by slow evaporation of a saturated solution in benzene. $C_{27}H_{42}N_2Ga$ (463.26 g/mol): found (calcd.); C 69.69 (69.84), H 9.00 (9.12), N 6.02 (6.03). IR (ATR): $\tilde{\nu}$ [cm^{-1}] : 458 (m), 522 (m), 619 (w), 716 (s, $\nu_{Ga\text{-}H,\ b.}$), 757 (m), 804 (m),1261 (w), 1322 (m), 1454 (m), 1484 (m), 1790 (s, $\nu_{Ga\text{-}H,\ str.}$), 2932(m). ^{1}H-NMR (400.4 MHz, C_6D_6, 298 K): δ = 1.17 (d, 12 H, $^3J_{HH}$ = 6.9 Hz, *i*Pr-CH_3), 1.53 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, *i*Pr-CH_3), 3.12 (sept, 4 H, $^3J_{HH}$ = 6.9 Hz, *i*Pr-C*H*), 3.36 (s, 4 H, NC*H*C*H*N), 3.58 (s, 3 H, Ga-*H*), 7.08 - 7.24 (m, 6 H, $_{aryl}$C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 24.2 (*i*Pr-*C*H$_3$), 25.4 (*i*Pr-*C*H$_3$), 29.1 (*i*Pr-*C*H), 53.4 (NCH_2CH_2N), 124.6 ($_{aryl}C_{meta}$H), 129.9 ($_{aryl}C_{para}$H), 135.3 ($_{aryl}C_{ipso}$), 146.7 ($_{aryl}C_{ortho}$), 205.9 (N*C*N).

(Me$_2$Im^{Me})·GaH$_2$(cAAC^{Me}H) **5**: A solution of cAAC^{Me} (110 mg, 385 µmol) in 5 mL of thf was added at room temperature to a solution of (Me$_2$Im^{Me})·GaH$_3$ 1 (75 mg, 385 µmol) in 5 mL of thf. After stirring overnight at room temperature, all volatiles were removed *in vacuo* and the residue was suspended in 10 mL of *n*-hexane and stored for crystallization over night at -30 °C. The precipitate was filtered off and dried *in vacuo* to afford **5** (58.0 mg, 121 µmol, 31 %) of a colorless powder. Crystals suitable for X-ray diffraction of compounds **5** were grown by slow evaporation of a saturated solution in benzene. $C_{27}H_{46}N_3Ga$ (482.41 g/mol): found (calcd.) C 65.79 (67.22), H 9.61 (9.61), N 8.66 (8.71). IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 465 (s), 495 (m), 569 (m), 591 (m), 601 (m), 631 (s), 704 (s), 737 (w), 770 (s, $\nu_{Ga\text{-}H,\ b.}$), 796 (s), 849 (m), 1044 (m), 1098 (w), 1110 (m), 1150 (m), 1209 (m), 1248 (m), 1357 (m), 1371 (m), 1381 (m), 1433 (s), 1461 (m), 1746 (m), 1781 (m, $\nu_{Ga\text{-}H,str.}$), 1825 (m), 2858 (w), 2924 (m, $\nu_{C\text{-}H,str.}$). ^{1}H-NMR (400.4 MHz, C_6D_6, 298K): δ = 1.06 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.15 (s, 6 H, $_{NHC}$CH_3), 1.21 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.33 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.37 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.51 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.53 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.83 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.85 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.98 – 2.09 (m, 2 H, $_{cAAC}$CH_2), 3.02 (s, 6 H, $_{NHC}$NCCH_3CCH_3N), 3.69 – 3.76 (s, 1 H, $_{cAAC}$GaC*H* und sept, 1 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-C*H*), 4.54 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-C*H*), 7.10 (m, 3 H, $_{cAAC}$aryl-C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 7.8 ($_{NHC}$CH_3), 24.7 ($_{cAAC}$*i*Pr-CH_3), 25.8 ($_{cAAC}$*i*Pr-CH_3), 26.4 ($_{cAAC}$*i*Pr-CH_3), 27.0 ($_{cAAC}$*i*Pr-CH_3), 27.4 ($_{cAAC}$*i*Pr-C*H*), 29.1 ($_{cAAC}$C(CH_3)$_2$), 29.4 ($_{cAAC}$*i*Pr-C*H*), 29.5 ($_{cAAC}$C(CH_3)$_2$), 29.5 ($_{cAAC}$C(CH_3)$_2$), 31.9 ($_{cAAC}$C(CH_3)$_2$), 33.7 ($_{NHC}$NC*C*H$_3$C*C*H$_3$N), 41.4 ($_{cAAC}$*C*(CH$_3$)$_2$), 61.1 ($_{cAAC}$CH$_2$), 63.4 ($_{cAAC}$*C*(CH$_3$)$_2$),

68.8 ($_{cAAC}$Ga*C*H), 124.1 ($_{cAAC}$aryl-*C*$_{meta}$H), 124.7 ($_{cAAC}$aryl-*C*$_{meta}$H), 124.9 ($_{NHC}$N*C*CH$_3$*C*CH$_3$N) 126.0 ($_{cAAC}$aryl-*C*$_{para}$H), 143.2 ($_{cAAC}$aryl-*C*$_{ipso}$), 152.8 ($_{cAAC}$aryl-*C*$_{ortho}$), 153.2 ($_{cAAC}$aryl-*C*$_{ortho}$), 174.4 ($_{NHC}$N*C*N).

(*i*Pr$_2$Im^{Me})·GaH$_2$(cAAC^{Me}H) **6**: A solution of cAAC^{Me} (113 mg, 395 µmol) in 5 mL of thf was added at room temperature to a solution of (*i*Pr$_2$Im^{Me})·GaH$_3$ (100 mg, 395 µl) in 5 mL of thf. After 5 min stirring at room temperature, all volatiles were removed *in vacuo* and the residue was suspended in 10 mL of *n*-pentane and stored for crystallization over night at -30 °C. The precipitate was filtered off and dried *in vacuo* to afford **6** (64mg, 119 µmol, 30 %) of a colorless powder. Crystals suitable for X-ray diffraction of compounds **6** were grown by slow evaporation of a saturated solution in benzene. $C_{31}H_{54}N_3Ga$ (538.52 g/mol): found (calcd.) C 65.79 (69.14), H 9.61 (10.11), N 8.66 (7.80). IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 462 (s), 498 (s), 522 (s), 568 (s), 605 (m), 636 (s), 648 (m), 686 (s), 706 (s), 752 (s, $\nu_{Ga\text{-}H,\ b.}$), 769 (s), 791 (s), 906 (w), 1046 (m), 1109 (m), 1149 (w), 1208 (s), 1251 (m), 1303 (m), 1319 (m), 1370 (s), 1396 (m), 1433 (s), 1460 (s), 1760 (s, $\nu_{Ga\text{-}H,str.}$), 1813 (s, $\nu_{Ga\text{-}H,str.}$), 2860 (m), 2926 (m), 2970 (s, $\nu_{C\text{-}H,str.}$). ^{1}H-NMR (400.4 MHz, C_6D_6, 298 K): δ = 1.07 (d, 6 H, $^3J_{HH}$ = 7.1 Hz, $_{NHC}$*i*Pr-C*H*$_3$), 1.10 (s, 3 H, $_{cAAC}$C(C*H*$_3$)$_2$), 1.12 (d, 6 H, $^3J_{HH}$ = 7.1 Hz, $_{NHC}$*i*Pr-C*H*$_3$), 1.32 (s, 3 H, $_{cAAC}$C(C*H*$_3$)$_2$), 1.38 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-C*H*$_3$), 1.44 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-C*H*$_3$), 1.49 (s, 3 H, $_{cAAC}$C(C*H*$_3$)$_2$), 1.51 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-C*H*$_3$), 1.51 (s, 6 H, $_{NHC}$NCC*H*$_3$CC*H*$_3$N), 1.79 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-C*H*$_3$), 1.85 (s, 3 H, $_{cAAC}$C(C*H*$_3$)$_2$), 1.95 - 2.09 (m, 2 H, $_{cAAC}$C*H*$_2$), 3.77 (d, 1 H, $^3J_{HH}$ = 3.5 Hz, $_{cAAC}$Ga*CH*), 3.82 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*PrC*H*), 4.51 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*PrC*H*), 5.41 (sept, 2 H, $^3J_{HH}$ = 7.1 Hz, $_{NHC}$*i*PrC*H*), 7.20-7.34 (m, 3 H, $_{cAAC}$aryl-C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 9.9 ($_{NHC}$NC*C*H$_3$C*C*H$_3$N), 21.4 ($_{NHC}$*i*Pr-*C*H$_3$), 21.5 ($_{NHC}$*i*Pr-*C*H$_3$), 25.4 ($_{cAAC}$*i*Pr-*C*H$_3$), 26.0 ($_{cAAC}$*i*Pr-*C*H$_3$), 26.1 ($_{cAAC}$*i*Pr-*C*H$_3$), 27.4 ($_{cAAC}$*i*Pr-*C*H), 27.7 ($_{cAAC}$*i*Pr-*C*H$_3$), 29.1 ($_{cAAC}$C(*C*H$_3$)$_2$), 29.5 ($_{cAAC}$*i*Pr-*C*H), 29.9 ($_{cAAC}$C(*C*H$_3$)$_2$), 30.1 ($_{cAAC}$C(*C*H$_3$)$_2$), 31.8 ($_{cAAC}$C(*C*H$_3$)$_2$), 41.4 ($_{cAAC}$*C*(CH$_3$)$_2$), 52.3 ($_{NHC}$*i*Pr-*C*H), 60.6 ($_{cAAC}$*C*H$_2$), 63.4 ($_{cAAC}$*C*(CH$_3$)$_2$), 69.3 ($_{cAAC}$Ga*C*H), 124.1 ($_{cAAC}$aryl-*C*$_{meta}$H), 124.8 ($_{cAAC}$aryl-*C*$_{meta}$H), 125.6 ($_{NHC}$N*C*CH$_3$*C*CH$_3$N), 126.2 ($_{cAAC}$aryl-*C*$_{para}$H), 142.3 ($_{cAAC}$aryl-*C*$_{ipso}$), 152.7 ($_{cAAC}$aryl-*C*$_{ortho}$), 153.1 ($_{cAAC}$aryl-*C*$_{ortho}$), 175.3 ($_{NHC}$N*C*N).

(Dipp$_2$Im)·GaH$_2$(cAAC^{Me}H) **7**: A solution of cAAC^{Me} (92.8 mg, 325 µmol) in 5 mL of thf was added at room temperature to a solution of (Dipp$_2$Im)·GaH$_3$ (150 mg, 325 µmol) in 5 mL of thf. After 5 min stirring at room temperature, all volatiles were removed *in vacuo* and the residue was suspended in 10 mL of *n*-pentane and stored for crystallization over night at -80 °C. The precipitate was filtered off and dried *in vacuo* to afford **7** (120 mg ,160 µmol, 49 %) of a colorless powder. Crystals suitable for X-ray diffraction of compounds **7** were grown by slow evaporation of a saturated solution in benzene. $C_{47}H_{70}N_3Ga$ (746.83 g/mol): found (calcd.) C 72.33 (75.59), H 9.10 (9.45), N 5.38 (5.63). IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 571 (w), 635 (s), 713 (s), 746 (s, $\nu_{Ga\text{-}H,\ b.}$), 770 (m), 1148 (m), 1210 (m), 1251 (m), 1274 (w), 1322 (m), 1351 (w), 1360 (m), 1383 (m), 1397 (m), 1458 (s), 1781 (m, $\nu_{Ga\text{-}H,str.}$), 1802 (m), 1823 (s), 1845 (s), 2863 (m), 2922 (m), 2961 (s, $\nu_{C\text{-}H,str.}$). ^{1}H-NMR (400.4 MHz, C_6D_6, 298 K): δ = 0.77 (d, 3 H, $^3J_{HH}$ = 6.8 Hz, $_{cAAC}$*i*Pr-C*H*$_3$), 0.92 (m, 12 H, $^3J_{HH}$ = 6.8 Hz, $_{NHC}$*i*Pr-C*H*$_3$), 1.06 (s, 3 H, $_{cAAC}$C(C*H*$_3$)$_2$), 1.18 (s, 3 H, $_{cAAC}$C(C*H*$_3$)$_2$), 1.29-1.32 (m, 12 H, $_{NHC}$*i*Pr-C*H*$_3$, $_{cAAC}$*i*Pr-C*H*$_3$ und $_{cAAC}$C(C*H*$_3$)$_2$), 1.35 (d, 3 H, $^3J_{HH}$ = 6.8 Hz, $_{cAAC}$*i*Pr-C*H*$_3$), 1.41 (d, 6 H, $^3J_{HH}$ = 6.8 Hz, $_{NHC}$*i*Pr-C*H*$_3$),1.43 – 1.44 (m, 6 H, $_{cAAC}$C(C*H*$_3$)$_2$ und $_{cAAC}$*i*Pr-C*H*$_3$), 1.84 - 1.95 (m, 2 H, $_{cAAC}$C*H*$_2$), 2.65 (sept, 2 H, $^3J_{HH}$ = 6.8 Hz, $_{NHC}$*i*Pr-C*H*), 2.81 (sept, 2 H, $^3J_{HH}$ = 6.8 Hz, $_{NHC}$*i*Pr-C*H*), 3.42 (d, 1 H, $^3J_{HH}$ = 4.6 Hz, $_{cAAC}$Ga*CH)*, 3.48 (sept, 1 H, $^3J_{HH}$ = 6.8 Hz, $_{cAAC}$*i*Pr-C*H*), 4.15 (sept, 1 H, $^3J_{HH}$ = 6.8 Hz, $_{cAAC}$*i*Pr-C*H*), 6.41 (s, 2 H, NC*H*C*H*N), 7.05-7.23 (m, 9 H, $_{cAAC}$aryl-C*H* und $_{NHC}$aryl-C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 22.7 ($_{NHC}$*i*Pr-*C*H$_3$), 22.8 ($_{NHC}$*i*Pr-*C*H$_3$), 25.0 ($_{cAAC}$*i*Pr-*C*H$_3$), 25.6 ($_{cAAC}$*i*Pr-*C*H$_3$), 25.9 ($_{cAAC}$*i*Pr-*C*H$_3$), 26.0 ($_{NHC}$*i*Pr-*C*H$_3$), 26.5 ($_{NHC}$*i*Pr-*C*H$_3$), 27.1 ($_{cAAC}$*i*Pr-*C*H$_3$), 27.1 ($_{cAAC}$*i*Pr-*C*H), 28.9 ($_{cAAC}$C(*C*H$_3$)$_2$), 29.0 ($_{NHC}$*i*Pr-*C*H), 29.0 ($_{cAAC}$*i*Pr-*C*H), 29.3 ($_{NHC}$*i*Pr-*C*H), 29.5 ($_{cAAC}$C(*C*H$_3$)$_2$) ,31.3 ($_{cAAC}$C(*C*H$_3$)$_2$) ,31.6 ($_{cAAC}$C(*C*H$_3$)$_2$), 40.8 ($_{cAAC}$*C*(CH$_3$)$_2$), 60.6 ($_{cAAC}$*C*H$_2$), 63.8 ($_{cAAC}$*C*(CH$_3$)$_2$), 67.2 ($_{cAAC}$Ga*C*H), 123.6 ($_{cAAC}$aryl-*C*$_{meta}$H), 124.3 ($_{cAAC}$aryl-*C*$_{meta}$H), 124.4 ($_{NHC}$aryl-*C*$_{meta}$H), 124.4 ($_{NHC}$aryl-*C*$_{meta}$H), 124.7 ($_{NHC}$N*C*H*C*HN), 125.9 ($_{cAAC}$aryl-*C*$_{para}$H), 130.7 ($_{NHC}$aryl-*C*$_{para}$H), 135.9 ($_{NHC}$aryl-*C*$_{ipso}$), 142.0

($_{cAAC}$aryl-C_{ipso}), 145.5 ($_{NHC}$aryl-C_{ortho}), 145.9 ($_{NHC}$aryl-C_{ortho}), 152.6 ($_{cAAC}$aryl-C_{ortho}), 152.7 ($_{cAAC}$aryl-C_{ortho}), 183.6 ($_{NHC}$N*C*N).

(cAAC^{Me}H)$_2$GaH (*meso*-**8**) and (*rac*-**8**): A solution of cAAC^{Me} (100 mg, 346 µmol) in 5 mL of toluene was added at room temperature to a solution of (Dipp$_2$Im^H)·GaH$_3$ (80.0 mg, 173 µmol) in 5 mL of toluene. After 12 h stirring at room temperature, the colorless crystalline residue was filtered off and dried *in vacuo* to afford **8** (38.0 mg ,60.0 µmol, 35 %) of a colorless crystalline powder. Crystals suitable for X-ray diffraction of the compounds **8** were grown by slow evaporation of a saturated solution in benzene. $C_{42}H_{65}GaN_2$ (643.70 g/mol): found (calcd.) C 74.46 (74.64), H 10.08 (10.18), N 4.29 (4.35); IR: (ATR): $\tilde{\nu}$ [cm^{-1}] = 2969 (s), 2948 (m), 1921 (w, $\nu_{Ga\text{-}H,\ str.}$), 1457 (m), 1430 (m), 1381 (m), 1362 (m), 1320 (m), 1305 (m), 1230 (m), 1102 (w), 769 (s, $\nu_{Ga\text{-}H,\ b.}$), 569 (m), 530 (m). Separation of the signals for the isomers *meso*-**8** and *rac*-**8** was not feasible in the ^{1}H and ^{13}C{^{1}H} spectra. ^{1}H-NMR: (400.4 MHz, THF-d$_8$, 298 K, dr(*meso*-**8**:*rac*-**8**) = 1:1.3): δ = 0,63 (s, 3H, C(C*H*$_3$)$_2$), 0.66 (d, 3H, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr-C*H*$_3$), 0.80 (d, 3H, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr-C*H*$_3$), 0.95 (s, 3H, C(C*H*$_3$)$_2$), 1.02 (s, 6H, C(C*H*$_3$)$_2$), 1.10 (s, 3H, C(C*H*$_3$)$_2$), 1.12 (d, 3H, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr-C*H*$_3$), 1.16 (s, 2H, C*H*$_2$), 1.20 (s, 3H, C(C*H*$_3$)$_2$), 1.29 (s, 6H, C(C*H*$_3$)$_2$), 1.35 (d, 3H, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr-C*H*$_3$), 1.43 (s, 3H, C(C*H*$_3$)$_2$), 1.81 (s, 2H, C*H*$_2$), 3.23 (sept, 1H, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr-C*H*), 3.37 (sept, 1H, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr-C*H*), 3.72 (d, 1H, $^3J_{HH}$ = 4.7 Hz, Ga–C*H*), 3.76 (d, 1H, $^3J_{HH}$ = 4.7 Hz, Ga–C*H*), 3.90 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, ^{i}Pr-C*H*), 4.06 (sept, 1H, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr-C*H*), 6.90-7.07 (m, 6H, $_{aryl}$C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, THF-d$_8$, 298 K): δ = 24.4, 25.9, 26.4, 27.2, 27.3, 27.7, 27.8, 28.3, 28.9, 29.8, 30.1, 30.6, 30.9, 31.3, 31.89, 32.5, 42.1, 42. 9, 60.6, 60.8, 64.9, 65.3, 67.7, 67.9, 68.1, , 76.9 (N*C*HC), 77.0 (N*C*HC), 125.3, 125.5, 125.6, 126.2, 127.4, 127.5, 141.2, 142.3, 152.1, 152.2,152.5, 152.5.

(*i*Pr$_2$Im^{Me})·GaH$_2$Cl **9**: To a solution of (*i*Pr$_2$Im^{Me})·GaH$_3$ (500 mg, 1,97 mmol) in 20 mL toluene was added a solution of (*i*Pr$_2$Im^{Me})·GaCl$_3$ (342 mg, 985 µmol) in 10 mL toluene. After the solution was stirred for 24 h at 55 °C all volatiles were removed *in vacuo*. The residue was suspended in 10 mL *n*-hexane, the precipitate filtered off and dried *in vacuo* to afford **9** (652 mg, 2.26 mmol, 77 %) as a colorless powder. $C_{13}H_{23}ClGaN_2$(287.08 g/mol): found (calcd.) C 46.21 (45.80), H 7.76 (8.04), N 9.60 (9.71). IR (ATR): ν [cm-1] = 2995 (w), 2936 (w), 2874 (w), 1890 (w) 1836 (s, $\nu_{Ga\text{-}H,\ str.}$), 1457 (w), 1438 (w), 1387 (w), 1370 (s), 1108 (m), 764 (m, vGa-H, $_{b.}$), 748 (w), 704 (s), 674 (s), 492 (m). ^{1}H-NMR (400.4 MHz, C$_6$D$_6$, 298 K): δ = 1.11 (d, 12 H, $^3J_{HH}$ = 7.1 Hz, *i*Pr-C*H*$_3$), 1.49 (s, 6 H, NCC*H*$_3$CC*H*$_3$N), 5.36 (sept, 2 H, $^3J_{HH}$ = 7.1 Hz, *i*Pr-C*H*), 5.60 (s, 2 H, Ga-*H*$_2$). ^{13}C{^{1}H}-NMR (100.7 MHz, C$_6$D$_6$, 298 K): δ = 9.70 (NC*C*H$_3$C*C*H$_3$N), 21.6 (*i*Pr-*C*H$_3$), 52.5 (*i*Pr-*C*H), 126.0 (NC*C*N), 166.9 (N*C*N).

(Dipp$_2$Im)·GaH$_2$Cl **10**: To a solution of (Dipp$_2$Im)·GaH$_3$ (300 mg, 650 µmol) in 10 mL toluene was added a solution of (Dipp$_2$Im)·GaCl$_3$ (184 mg, 325 µmol) in 10 mL toluene. After the solution was stirred for 24 h at 55 °C all volatiles were removed *in vacuo*. The residue was suspended in 10 mL *n*-hexane, the precipitate filtered off and dried *in vacuo* to afford **10** (349 mg, 702 µmol, 72 %) as a colorless powder. $C_{27}H_{39}ClGaN_2$ (496.80 g/mol): found (calcd.) C 64.67 (65.28) H 7.66 (7.91) N 5.35 (5.64). IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 3153 (w), 3124 (w), 2963 (m), 2928 (w), 2870 (w), 1878 (m, $\nu_{Ga\text{-}H,\ str.}$), 1467 (m), 1112 (m), 803 (m), 757 (m), 732 (s, $\nu_{Ga\text{-}H,\ b.}$), 673 (s). ^{1}H-NMR (400.4 MHz, C$_6$D$_6$, 298 K): δ = 1.00 (d, 12 H, $^3J_{HH}$ = 6.9 Hz, *i*Pr-C*H*$_3$), 1.40 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, *i*Pr-C*H*$_3$), 2.68 (sept, 4 H, $^3J_{HH}$ = 6.9 Hz, *i*Pr-C*H*), 4.66 (s, 3 H, Ga-*H*), 6.46 (s, 2 H, NC*H*C*H*N), 7.08 - 7.27 (m, 6 H, $_{aryl}$C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C$_6$D$_6$, 298 K): δ = 23.1 (*i*Pr-*C*H$_3$), 25.4 (*i*Pr-*C*H$_3$), 29.1 (*i*Pr-*C*H), 124.3 ($_{aryl}$*C*$_{meta}$H), 124.7 (NC*H*C*H*N), 131.1 ($_{aryl}$*C*$_{para}$H), 134.1 ($_{aryl}$*C*$_{ipso}$), 145.7 ($_{aryl}$*C*$_{ortho}$), 181.6 (N*C*N).

(Dipp$_2$Im^H)·GaH$_2$Cl **11**: To a solution of (Dipp$_2$Im^H)·GaH$_3$ (150 mg, 320 µmol) in 10 mL toluene was added a solution of (Dipp$_2$Im^H)·GaCl$_3$ (110 mg, 160 µmol) in 10 mL toluene. After the solution was stirred for 24 h at room temperature all volatiles were removed *in vacuo*. The residue was suspended in 10 mL *n*-hexane, the precipitate filtered off and dried *in vacuo* to

afford **11** (173 mg, 350 µmol, 69 %) as a colorless powder. $C_{27}H_{39}ClGaN_2$ (496.80 g/mol): found (calcd.) C 62.42 (65.01) H 7.89 (8.23) N 5.30 (5.62). IR (ATR): ν [cm-1] = 2959 (m), 2904 (w), 1877 (m, $\nu_{Ga\text{-}H,\ str.}$), 1490 (m), 1455 (m), 1265 (m), 804 (m), 737 (s, vGa-H, $_{b.}$), 631 (w), 447 (m). ^{1}H-NMR (400.4 MHz, C6D6, 298 K): δ = 1.10 (d, 12 H, *i*Pr-C*H*3), 1.50 (d, 12 H, *i*Pr-C*H*3), 3.16 (sept, 4 H, *i*Pr-C*H*), 3.41 (s, 4 H, NC*H*2C*H*2N), 4.56 (s, 2 H, Ga-*H*), 7.05 - 7.21 (m, 6 H, arylC*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C6D6, 298 K): δ = 23.9 (*i*Pr-*C*H3), 25.8 (*i*Pr-*C*H3), 29.2 (*i*Pr-*C*H), 53.7 (N*C*H*C*HN), 124.8 (aryl*C*$_{meta}$H), 130.4 (aryl*C*$_{para}$H), 134.1 (aryl*C*$_{ipso}$), 146.7 (aryl*C*$_{ortho}$), 198.0 (N*C*N).

(*i*Pr$_2$Im^{Me})·GaHCl$_2$ **12**: SiEt$_3$H (820 µL, 5.11 mmol) was added to GaCl$_3$ (900 mg. 5.11 mmol) at -30 °C and the mixture was stirred for 1 h at 5 °C and all volatiles were removed *in vacuo*. A solution of *i*Pr$_2$Im^{Me} (921 mg, 5.11 mmol) in 25 mL EtO_2 was added at -78 °C and stirred overnight. All volatiles were removed, and the residue was suspended in 15 mL *n*-hexane. The precipitate was filtered off and dried *in vacuo* to afford **12** (1.36 g, 4.22 mmol, 83 %) as a colorless powder. Crystals suitable for X-ray diffraction of compounds **12** were grown by slow evaporation of a saturated solution in benzene. $C_{13}H_{22}Cl_2GaN_2$(321.04 g/mol): found (calcd.) C 39.72 (40.91), H 6.49 (6.87), N 8.26 (8.67). IR (ATR): ν [cm-1] = 2980 (w), 2937 (w), 1948 (s, $\nu_{Ga\text{-}H,\ str.}$), 1631 (w), 1464 (m), 1438 (w), 1392 (m), 1372 (m), 1351 (w), 1335 (w), 1290 (w), 1261 (w), 1223 (w), 1201 (w), 1165 (w), 1139 (w), 1108 (m), 1032 (w), 901 (w), 802 (w), 775 (w), 752 (m), 678 (s), 615 (s), 574 (w), 469 (w). ^{1}H-NMR (400.4 MHz, C_6D_6, 298 K): δ = 1.10 (d, 12 H, $^3J_{HH}$ = 7.1 Hz, *i*Pr-CH_3), 1.49 (s, 6 H, NCCH_3CCH_3N), 5.31 (sept, 2 H, $^3J_{HH}$ = 7.1 Hz, *i*Pr-C*H*), 6.18 (s, 1 H, Ga-*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 9.78 (NC*C*H$_3$C*C*H$_3$N), 21.6 (*i*Pr-*C*H$_3$), 52.5 (*i*Pr-*C*H), 126.8 (NC*C*N), 160.7 (N*C*N).

(Dipp$_2$Im)·GaHCl$_2$ **13**: SiEt$_3$H (500 µL, 3.13 mmol) was added to GaCl$_3$ (551 mg. 3.13 mmol) at -30 °C and the mixture was stirred for 1 h at 5 °C and all volatiles were removed *in vacuo*. A solution of Dipp$_2$Im (1.21 g, 3.13 mmol) in 25 mL EtO_2 was added at -78 °C and stirred overnight. All volatiles were removed, and the residue was suspended in 15 mL *n*-hexane. The precipitate was filtered off and dried *in vacuo* to afford **13** (1.20 g, 2.26 mmol, 73 %) as a colorless powder. Crystals suitable for X-ray diffraction of compounds **13** were grown by slow evaporation of a saturated solution in benzene. $C_{27}H_{37}Cl_2GaN_2$ (528.16 g/mol): found (calcd.) C 61.28 (61.16), H 7.18 (7.03), N 5.24 (5.28). IR (ATR): ν [cm-1] = 2963 (m), 1933 (m, $\nu_{Ga\text{-}H,\ str.}$), 1467 (w), 1454 (w), 1364 (w), 1209 (w), 1115 (m), 1061 (w), 800 (m), 755 (s), 614 (s). ^{1}H-NMR (400.4 MHz, C_6D_6, 298 K): δ = 0.97 (d, 12 H, $^3J_{HH}$ = 6.9 Hz, *i*Pr-CH_3), 1.41 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, *i*Pr-CH_3), 2.68 (sept, 4 H, $^3J_{HH}$ = 6.9 Hz, *i*Pr-C*H*), 5.19 (s, 1 H, Ga-*H*), 6.45 (s, 2 H, NC*H*C*H*N), 7.08 - 7.27 (m, 6 H, $_{aryl}$C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 22.9 (*i*Pr-*C*H$_3$), 25.7 (*i*Pr-*C*H$_3$), 29.2 (*i*Pr-*C*H), 124.3 ($_{aryl}$*C*$_{meta}$H), 124.4 (NC*H*C*H*N), 131.5 ($_{aryl}$*C*$_{para}$H), 133.3 ($_{aryl}$*C*$_{ipso}$), 145.7 ($_{aryl}$*C*$_{ortho}$), 167.9 (N*C*N).

(Dipp$_2$Im^H)·GaHCl$_2$ **14**: To a solution of (Dipp$_2$Im^H)·GaH$_3$ (100 mg, 216 µmol) in 10 mL toluene was added a solution of (Dipp$_2$Im^H)·GaCl$_3$ (244 mg, 432 µmol) in 10 mL toluene. After the solution was stirred for 24 h at room temperature all volatiles were removed *in vacuo*. The residue was suspended in 10 mL *n*-hexane, the precipitate filtered off and dried *in vacuo* to afford 14 (270 mg, 508 µmol, 78 %) as a colorless powder. $C_{27}H_{39}Cl_2GaN_2$ (530.17 g/mol): found (calcd.) C 61.79 (60.93) H 7.56 (7.39) N 5.11 (5.26). IR (ATR): ν [cm-1] = 2962 (m), 1925 (m, $\nu_{Ga\text{-}H,\ str.}$), 1488 (s), 1457 (s), 1270 (s), 802 (m), 755 (m), 687 (m), 639 (m). ^{1}H-NMR (400.4 MHz, C6D6, 298 K): δ = 1.08 (d, 12 H, *i*Pr-C*H*3), 1.48 (d, 12 H, *i*Pr-C*H*3), 3.19 (sept, 4 H, *i*Pr-C*H*), 3.46 (s, 4 H, NC*H*2C*H*2N), 5.06 (s, 1 H, Ga-*H*), 7.04 - 7.19 (m, 6 H, arylC*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C6D6, 298 K): δ = 23.9 (*i*Pr-*C*H3), 26,1 (*i*Pr-*C*H3), 29.2 (*i*Pr-*C*H), 54,1 (N*C*H*C*HN), 124.9 (aryl*C*$_{meta}$H), 130.7 (aryl*C*$_{para}$H), 133.2 (aryl*C*$_{ipso}$), 146.8 (aryl*C*$_{ortho}$), 191,1 (N*C*N).

(cAAC^{Me})·GaHCl$_2$ **15**: SiEt$_3$H (300 µL, 1.87 mmol) was added to GaCl$_3$ (328 mg. 1.87 mmol) at -30 °C and the mixture was stirred for 1 h at 5 °C and all volatiles were removed *in vacuo*.

A solution of cAAC^{Me} (539 mg, 1.87 mmol) in 25 mL EtO_2 was added at -78 °C and stirred overnight. All volatiles were removed, and the residue was suspended in 15 mL *n*-hexane. The precipitate was filtered off and dried *in vacuo* to afford **15** (592 mg, 1.39 mmol, 74 %) as a colorless powder. Crystals suitable for X-ray diffraction of compounds **15** were grown by slow evaporation of a saturated solution in benzene. $C_{20}H_{33}Cl_2GaN$ (426.12 g/mol): found (calcd.) C 56.41 (56.11), 7.68 (7.77), 3.19 (3.27).; ^{1}H-NMR (400.4 MHz, C_6D_6, 298 K): δ = 0.74 (s, 6 H, C(CH_3)$_2$), 1.00 (d, 6 H, $^3J_{HH}$ = 7.0 Hz, *i*Pr-CH_3), 1.32 (s, 2 H, CH_2), 1.35 (d, 6 H, $^3J_{HH}$ = 7.0 Hz, *i*Pr-CH_3), 1.68 (s, 6 H, C(CH_3)$_2$), 2.55 (sept, 2 H, $^3J_{HH}$ = 6.6 Hz, *i*Pr-C*H*), 4.98 (s, 1 H, Ga-*H*), 6.89-7.07 (m, 3 H, aryl-C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 23.9 (*i*Pr-*C*H$_3$), 26.5 (*i*Pr-*C*H$_3$), 28.3 (C(*C*H$_3$)$_2$), 29.0 (*i*Pr-*C*H), 29.2 (C(*C*H$_3$)$_2$), 50.3 (*C*(CH$_3$)$_2$), 56.3 (*C*H$_2$), 81.9 (Ga-*C*), 125.5 (aryl-*C*H), 130.8 (aryl-*C*$_{para}$H), 145.3 (aryl-*C*$_{ipso}$H).

(*i*Pr$_2$Im^{Me})·GaHCl(cAAC^{Me}H) (*meso*-**16**) and (*rac*-**16**): A solution of cAAC^{Me} (50 mg, 156 µmol) in 5 mL of toluene was added at room temperature to a solution of (*i*Pr$_2$Im^{Me})·GaH$_2$Cl (50 mg, 156 µl) in 5 mL of toluene. After 5 min stirring at room temperature, all volatiles were removed *in vacuo* and the residue was suspended in 5 mL of *n*-pentane and the precipitate was filtered off and dried *in vacuo* to afford **16** (38 mg, 17.4 mmol, 29 %) as a colorless powder. Crystals suitable for X-ray diffraction of the compounds **16** were grown by slow evaporation of a saturated solution in benzene. $C_{31}H_{53}N_3GaCl$ (571.32 g/mol): found (calcd.) C 65.91 (64.99), H 9.82 (9.32), N 6.76 (7.33) IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 2962 (m), 2872 (w), 1926 (s, $\nu_{Ga\text{-}H,\ str.}$), 1589 (m), 1490 (m), 1456 (w), 1323 (m), 1273 (m), 1185 (m), 1054 (w), 917 (w), 801 (m), 758 (w), 620 (m), 560 (w). Separation of the signals for the isomers meso-16 and rac-16 was not feasible in the ^{1}H and ^{13}C{^{1}H} spectra. ^{1}H-NMR (400.4 MHz, C_6D_6, 298 K, dr(meso-16:rac-16) = 1:0.8)): δ = 0.57 (d, 6 H, $^3J_{HH}$ = 7.1 Hz, $_{NHC}$*i*Pr-CH_3), 0.94 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.03 (d, 6 H, $^3J_{HH}$ = 7.1 Hz, $_{NHC}$*i*Pr-CH_3), 1.07 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.09 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.10 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.18 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.19 (s, 6 H, $_{cAAC}$C(CH_3)$_2$), 1.21 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.27 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.39 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.40 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.45 (s, 6 H, $_{cAAC}$C(CH_3)$_2$), 1.47 (s, 6 H, $_{cAAC}$C(CH_3)$_2$), 1.48 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.49 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.53 (d, 3 H, $_{NHC}$NCCH_3CCH_3N), 1.58 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.62 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.69 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.70 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.86 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.92 - 2.02 (m, 4 H, $_{cAAC}$CH_2), 2.17 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 3.49 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*PrC*H*), 3.69 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*PrC*H*), 3.77 (d, 1 H, $^3J_{HH}$ = 3.5 Hz, $_{cAAC}$GaC*H*), 3.84 (d, 1 H, $^3J_{HH}$ = 3.5 Hz, $_{cAAC}$GaC*H*), 4.38 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*PrC*H*), 4.52 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*PrC*H*), 4.92 (sept, 2 H, $^3J_{HH}$ = 7.1 Hz, $_{NHC}$*i*PrC*H*), 5.37 (b, 1 H, Ga-*H*), 5.46 (sept, 2 H, $^3J_{HH}$ = 7.1 Hz, $_{NHC}$*i*PrC*H*), 5.59 (b, 1 H, Ga-*H*), 6.91-7.41 (m, 3 H, $_{cAAC}$aryl-C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 7.97, 9.84, 9.89, 10.1, 14.4, 21.4, 21.5, 21.63, 21.65, 21.69, 21.7, 21.9, 22.6, 23.1, 25.05, 25.1, 25.2, 25.4, 25.7, 25.8, 25.9, 26.0, 26.1, 26.3, 26.5, 26.6, 26.8, 26.9, 27.3, 27.4, 28.7, 28.9, 29.1, 29.3, 29.5, 29.6, 29.8, 29.92, 29.98, 30.1, 30.8, 31,2, 31.6, 36.91, 31.97, 32.7, 32.8, 41.3, 42.1, 42.2, 42.6, 51.0, 52.4, 52.5, 60.0, 60.6, 61.2, 61.7, 63.3, 63.4, 63.7, 64.5, 69.7 (Ga-*C*), 70.8 (Ga-*C*), 124.2,.124.4, 124.7, 125.00, 125.03, 125.8, 126.1, 126.1, 126.3, 126.7, 126.8, 127.4, 127.9, 128.2, 128.4, 128.6, 128.7, 141.3 (aryl-*C*H), 142.7(aryl-*C*H), 151.6 (aryl-*C*H), 151.8 (aryl-*C*H), 152.3 (aryl-*C*H), 152.4 (aryl-*C*H), 153.3 (aryl-*C*H), 153.9 (aryl-*C*H), 169.6 (N*C*N), 170.0 (N*C*N).

(*i*Pr$_2$Im^{Me})·GaCl$_2$(cAAC^{Me}H) **17**: A solution of cAAC^{Me} (50 mg, 156 µmol) in 5 mL of toluene was added at room temperature to a solution of (*i*Pr$_2$Im^{Me})·GaHCl$_2$ (45 mg, 156 µl) in 5 mL of toluene. After 5 min stirring at room temperature, all volatiles were removed *in vacuo* and the residue was suspended in 5 mL of *n*-pentane and the precipitate was filtered off and dried *in vacuo* to afford **17** (38 mg, 62 µmol, 40 %) as a colorless powder. Crystals suitable for X-ray diffraction of the compounds 17 were grown by slow evaporation of a saturated solution in benzene. $C_{31}H_{52}N_3GaCl_2$ (605.28 g/mol): found (calcd.) C 59.51 (61.20), H 8.62 (8.63), N 6.65 (6.92); IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 2974 (m), 2932 (m), 2869 (w), 1948 (s) 1551 (w), 1468 (m), 1374 (m), 1200 (w), 1133 (w), 1052 (w), 807 (m), 777 (s), 643 (s), 625 (s), 562 (m).^{1}H-NMR (400.4

MHz, C_6D_6, 298 K): δ = 1.03 (d, 6 H, $^3J_{HH}$ = 7.1 Hz, $_{NHC}$*i*Pr-CH_3), 1.09 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.15 (d, 6 H, $^3J_{HH}$ = 7.1 Hz, $_{NHC}$*i*Pr-CH_3), 1.31 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.37 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.39 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.41 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 1.46 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.66 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*Pr-CH_3), 1.95 (d, 6 H, $_{NHC}$NCCH_3CCH_3N), 1.85 (s, 3 H, $_{cAAC}$C(CH_3)$_2$), 2.18 - 2.11 (m, 2 H, $_{cAAC}$CH_2), 3.44 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*PrC*H*), 3.85 (s, 1 H, $^3J_{HH}$ = 3.5 Hz, $_{cAAC}$GaC*H*),4.71 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, $_{cAAC}$*i*PrC*H*), 5.59 (sept, 2 H, $^3J_{HH}$ = 7.1 Hz, $_{NHC}$*i*PrC*H*), 7.13-7.28 (m, 3 H, $_{cAAC}$aryl-C*H*). ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 10.1 ($_{NHC}$NC*C*H$_3$C*C*H$_3$N), 22.2 ($_{NHC}$*i*Pr-*C*H$_3$), 22.8 ($_{NHC}$*i*Pr-*C*H$_3$), 25.0 ($_{cAAC}$*i*Pr-*C*H$_3$), 25.9 ($_{cAAC}$*i*Pr-*C*H$_3$), 26.3 ($_{cAAC}$*i*Pr-*C*H$_3$), 27.3 ($_{cAAC}$*i*Pr-*C*H), 27.6 ($_{cAAC}$*i*Pr-*C*H$_3$), 28.7 ($_{cAAC}$C(*C*H$_3$)$_2$), 28.9 ($_{cAAC}$*i*Pr-*C*H), 32.1 ($_{cAAC}$C(*C*H$_3$)$_2$), 32.8 ($_{cAAC}$C(*C*H$_3$)$_2$), 33.8 ($_{cAAC}$C(*C*H$_3$)$_2$), 42.2 ($_{cAAC}$*C*(CH$_3$)$_2$), 52.4 ($_{NHC}$*i*Pr-*C*H), 60.0 ($_{cAAC}$*C*H$_2$), 64.5 ($_{cAAC}$*C*(CH$_3$)$_2$), 76.0 ($_{cAAC}$Ga*C*H), 124.9 ($_{cAAC}$aryl-*C*$_{meta}$H), 125.0 ($_{cAAC}$aryl-*C*$_{meta}$H), 126.5 ($_{NHC}$N*C*CH$_3$*C*CH$_3$N), 126.8 ($_{cAAC}$aryl-*C*$_{para}$H), 143.9 ($_{cAAC}$aryl-*C*$_{ipso}$), 159.1 ($_{cAAC}$aryl-*C*$_{ortho}$), 153.3 ($_{cAAC}$aryl-*C*$_{ortho}$), 164.5 ($_{NHC}$N*C*N).

(cAAC^{Me}H)$_2$GaCl (*meso*-18) and (*rac*-18): A solution of cAAC^{Me} (116 mg, 402 µmol) in 5 mL of toluene was added at room temperature to a solution of (Dipp$_2$Im^H)·GaH$_2$Cl (100 mg, 201 µmol) in 5 mL of toluene. After 12 h stirring at room temperature, the solution was evaporated to ca. 2 mL and the dark yellow residue was filtered off and dried *in vacuo* to afford 18 (51.0 mg ,74.4 µmol, 37 %) of a dark yellow solid. $C_{40}H_{64}ClGaN_2$ (678.14 g/mol): found (calcd.) C 70.64 (70.85), H 9.67 (9.51), N 4.01 (4.13). Separation of the signals for the isomers *meso*-18 and *rac*-18 was not feasible in the ^{1}H and ^{13}C{^{1}H} spectra. ^{1}H-NMR: (400.4 MHz, C_6D_6, 298 K, dr(meso-18:rac-18) = 1:0.8): δ = 0,93 (s, 3H, C(CH_3)$_2$), 0.98 (d, 6H, $^3J_{HH}$ = 5.7 Hz, ^{i}Pr-CH_3), 1.12 (s, 3H, C(CH_3)$_2$), 1.18 (d, 6H, $^3J_{HH}$ = 5.7 Hz ^{i}Pr-CH_3), 1.21-1.24 (m, 9H, C(CH_3)$_2$), 1.34-1.38 (m, 9H, C(CH_3)$_2$), 1.47-1.49 (m, 6H, ^{i}Pr-CH_3), 1.61 (s, 6H, C(CH_3)$_2$), 1.73-1.86 (m, 4H, CH_2),), 3.09 (sept, 1H, $^3J_{HH}$ = 6.4 Hz, ^{i}Pr-C*H*), 3.19 (sept, 1H, $^3J_{HH}$ = 6.4 Hz, ^{i}Pr-C*H*), 3.84 (s, 1H, Ga–C*H*), 4.10 (s, 1H, Ga–C*H*), 4.15 (sept, 1H, $^3J_{HH}$ = 6.4 Hz, ^{i}Pr-C*H*), 4.37 (sept, 1H, $^3J_{HH}$ = 6.4 Hz, ^{i}Pr-C*H*), 7.02-7.14 (m, 6H, $_{aryl}$C*H*).. ^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6, 298 K): δ = 24.4, 25.9, 26.4, 27.2, 27.3, 27.7, 27.8, 28.3, 28.9, 29.8, 30.1, 30.6, 30.9, 31.3, 31.89, 32.5, 42.1, 42. 9, 60.6, 60.8, 64.9, 65.3, 67.7, 67.9, 68.1, , 76.9 (Ga-*C*), 77.0 (Ga-*C*), 125.3, 125.5, 125.6, 126.2, 127.4, 127.5, 141.2, 142.3, 152.1, 152.2,152.5, 152.5.

2 NMR Spectra

NMR spectra of (Me_2Im^{Me})•GaH_3 1

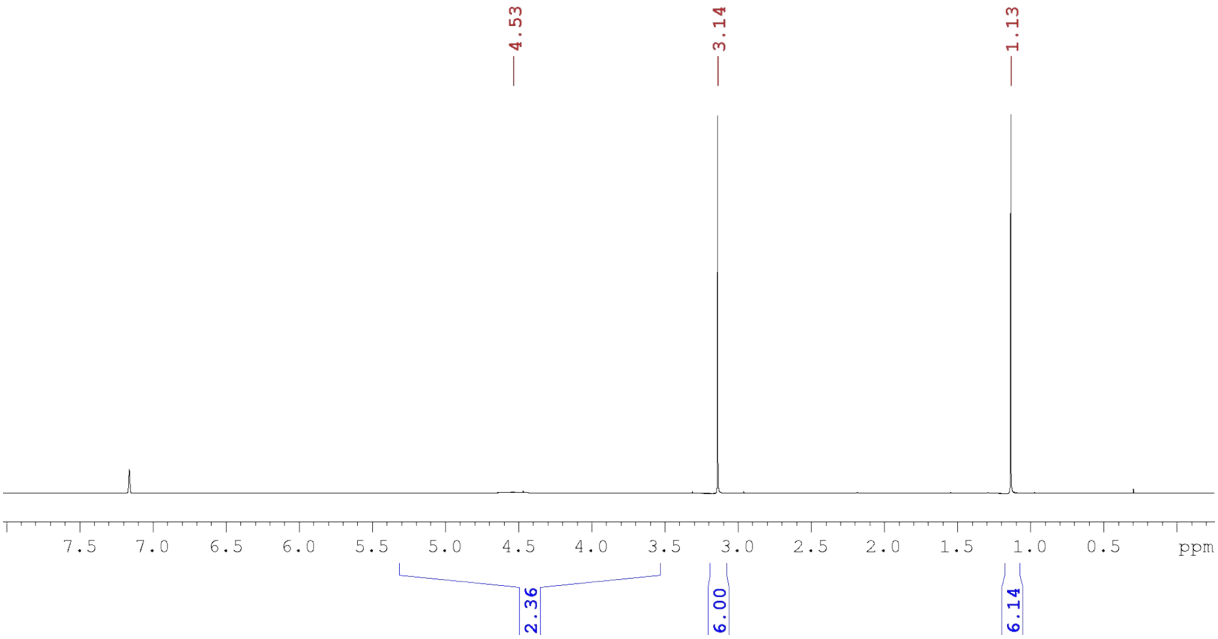

Figure S1: ^{1}H NMR spectrum of $(Me_2Im^{Me})\cdot GaH_3$ **1** in C_6D_6 (400 MHz, 25 °C).

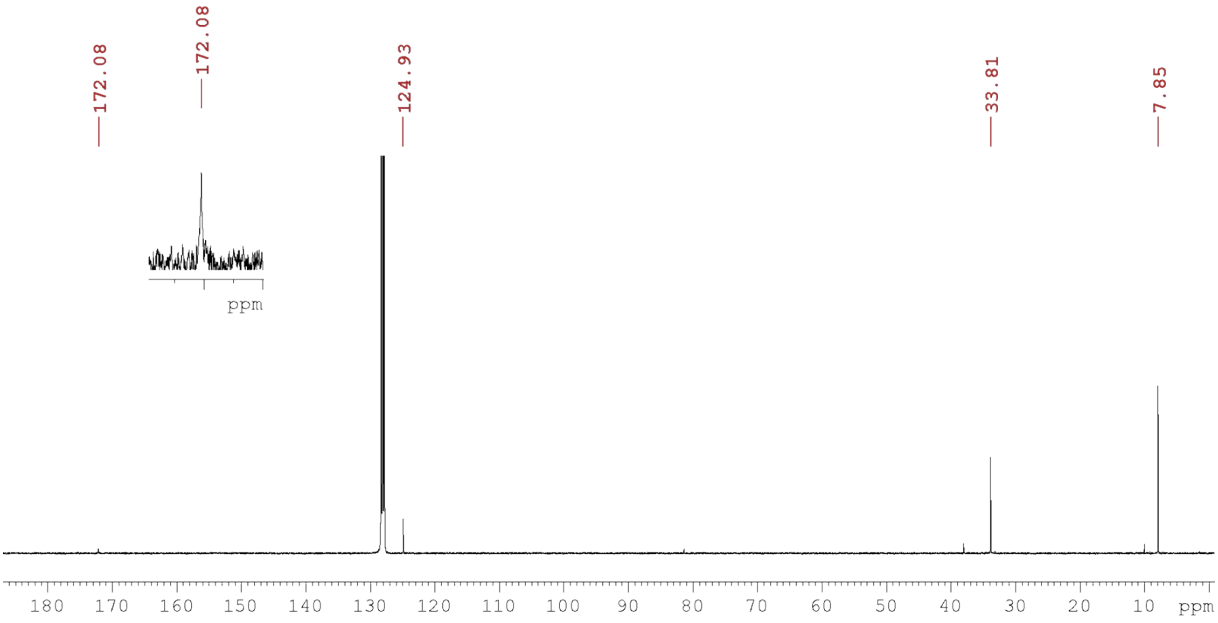

Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of $(Me_2Im^{Me})\cdot GaH_3$ **1** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of (*i*Pr_2Im)•GaH_3 2

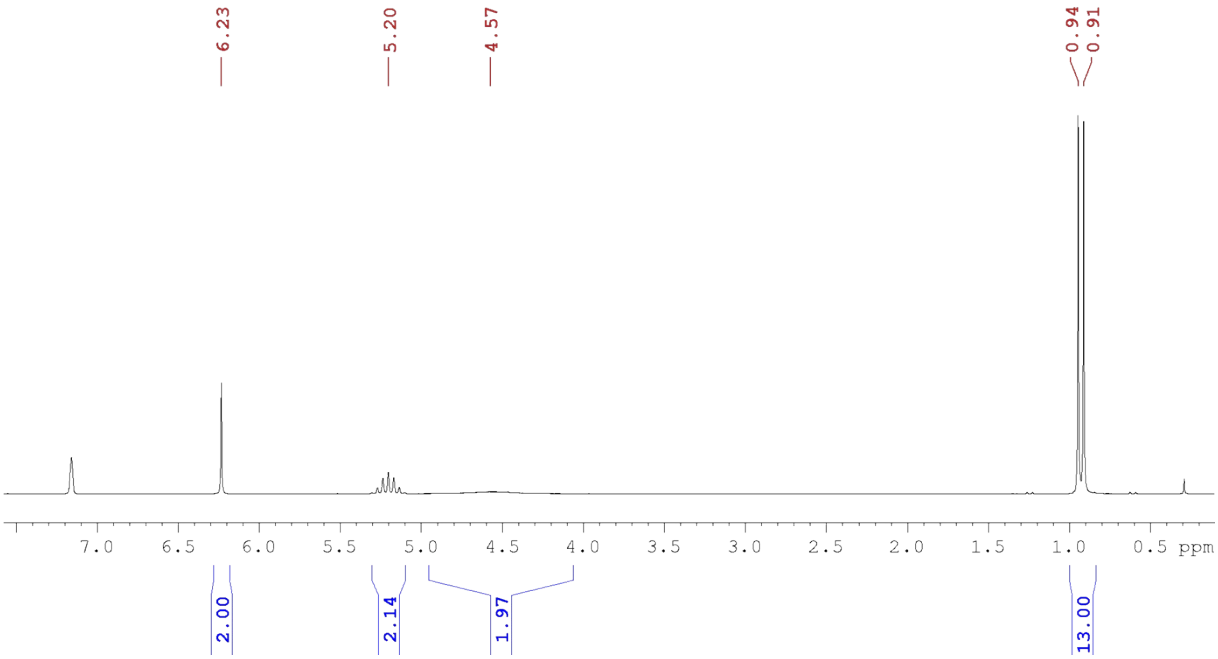

Figure S3: ^{1}H NMR spectrum of (*i*Pr_2Im)·GaH_3 **2** in C_6D_6 (400 MHz, 25 °C).

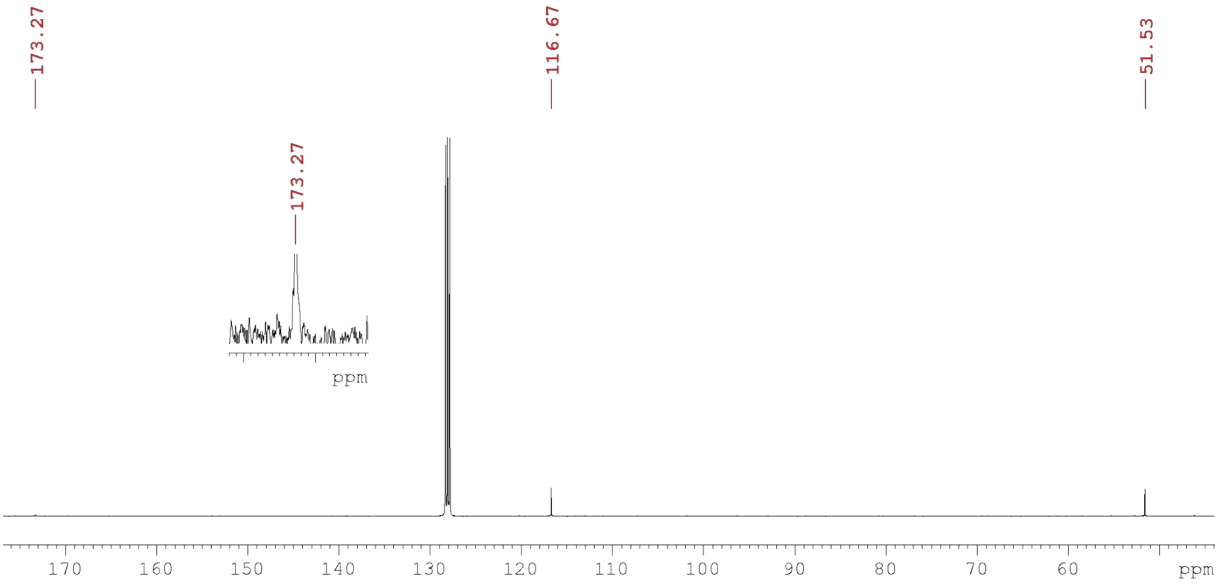

Figure S4: $^{13}C\{^1H\}$ NMR spectrum of (*i*Pr_2Im)·GaH_3 **2** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of (iPr$_2$Im^{Me})•GaH$_3$ 3

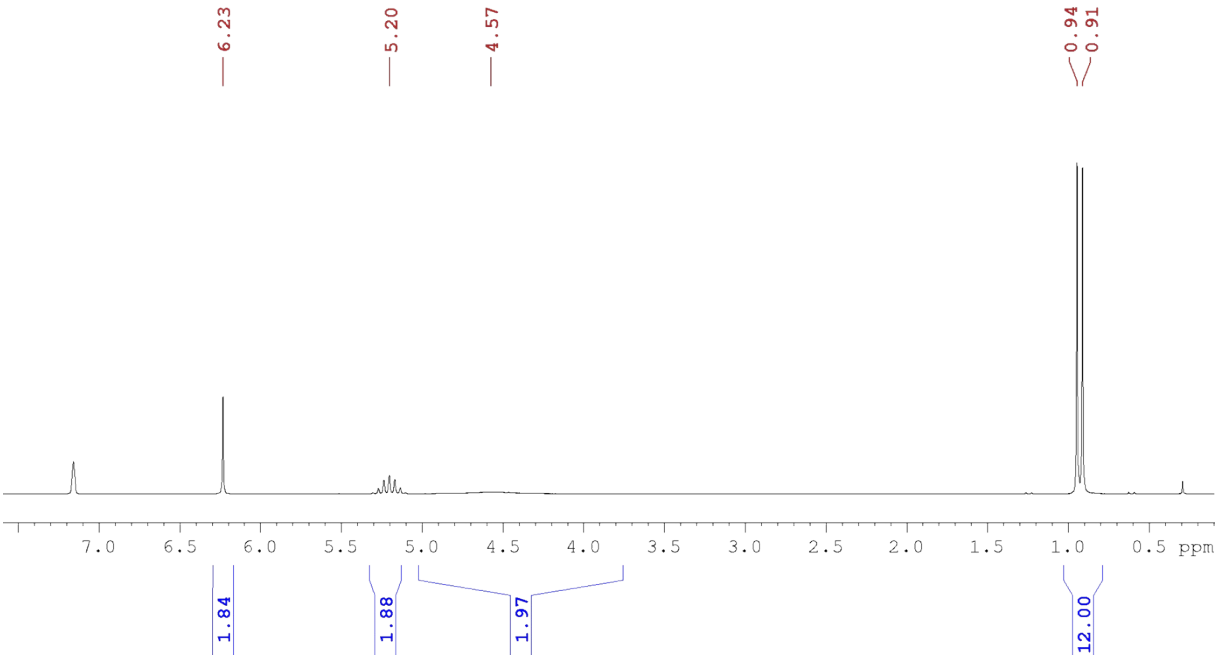

Figure S5: ^{1}H NMR spectrum of (iPr$_2$Im^{Me})·GaH$_3$ **1** in C$_6$D$_6$ (400 MHz, 25 °C).

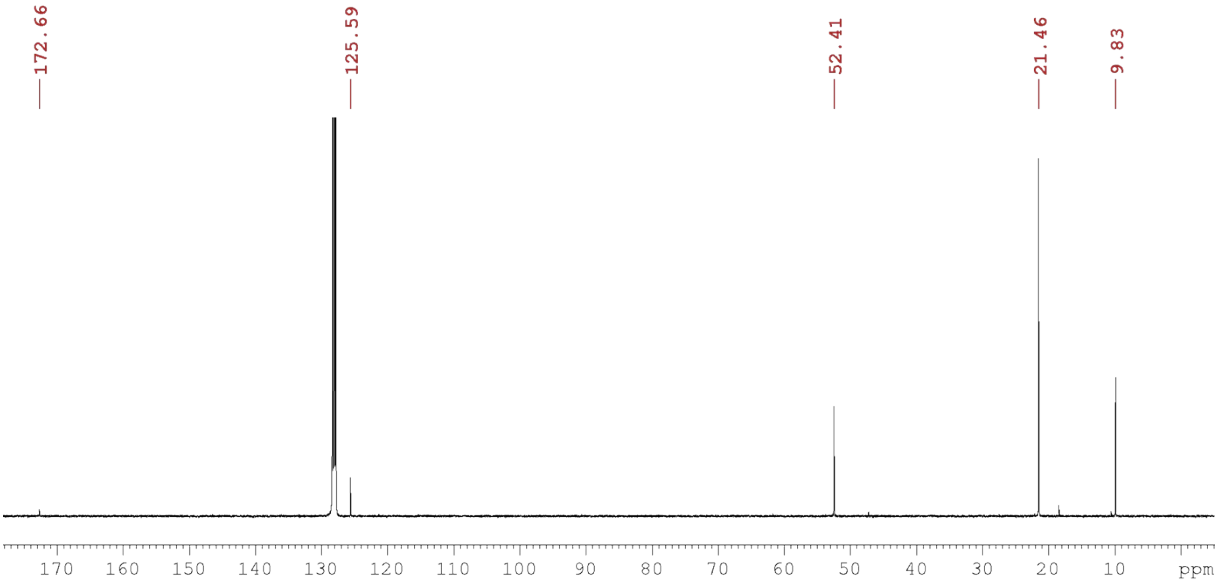

Figure S6: ^{13}C{^{1}H} NMR spectrum of (iPr$_2$Im^{Me})·GaH$_3$ **3** in C$_6$D$_6$ (125.8 MHz, 25 °C).

Solution NMR spectra of $(Dipp_2Im^H)$•GaH_3 4

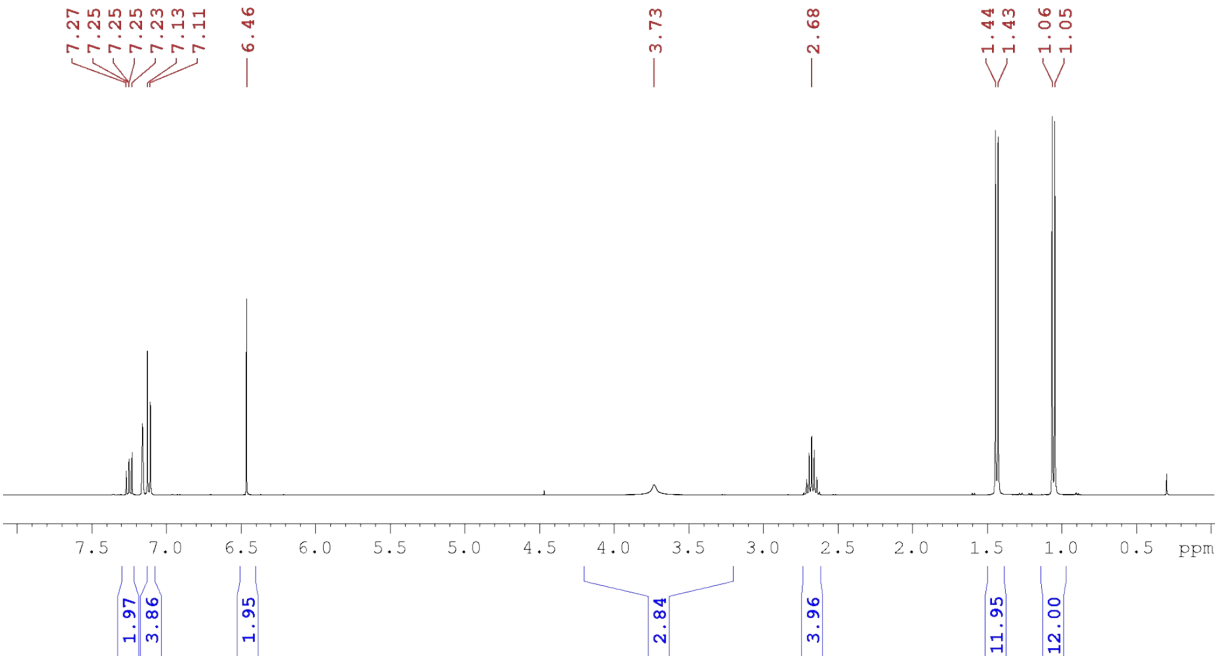

Figure S7: ^1H NMR spectrum of $(Dipp_2Im^H)$·GaH_3 **4** in C_6D_6 (400 MHz, 25 °C).

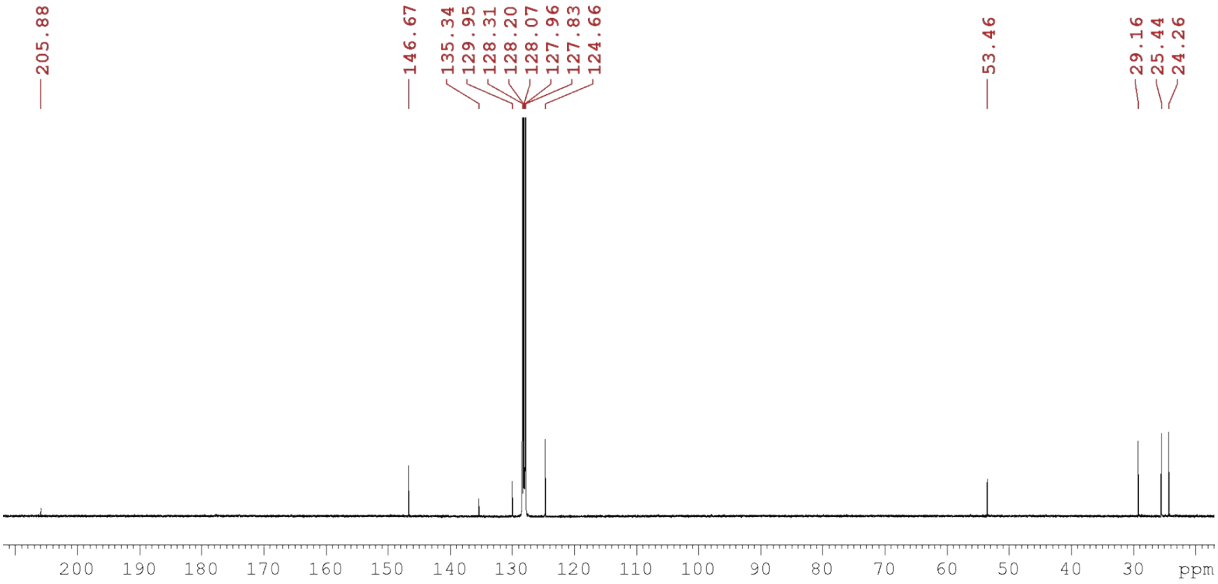

Figure S8: $^{13}C\{^1H\}$ NMR spectrum of $(Dipp_2Im^H)$·GaH_3 **4** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of (Me_2Im^{Me})•GaH_2($cAAC^{Me}H$) 5

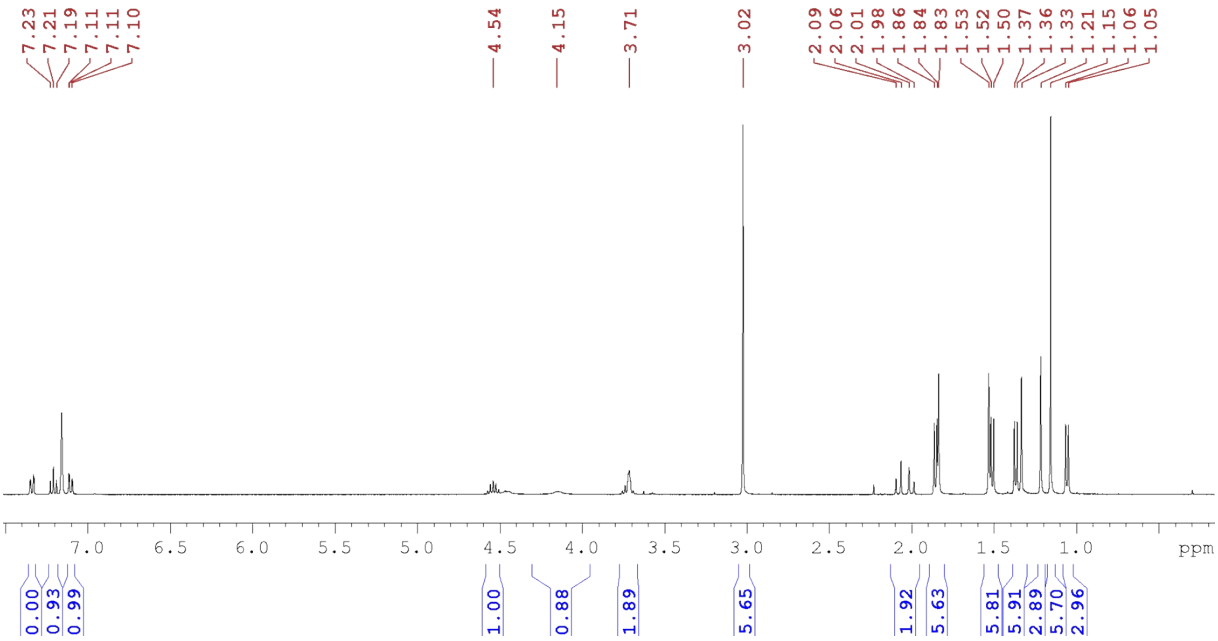

Figure S9: ^{1}H NMR spectrum of (Me_2Im^{Me})•GaH_2($cAAC^{Me}H$) **5** in C_6D_6 (400 MHz, 25 °C).

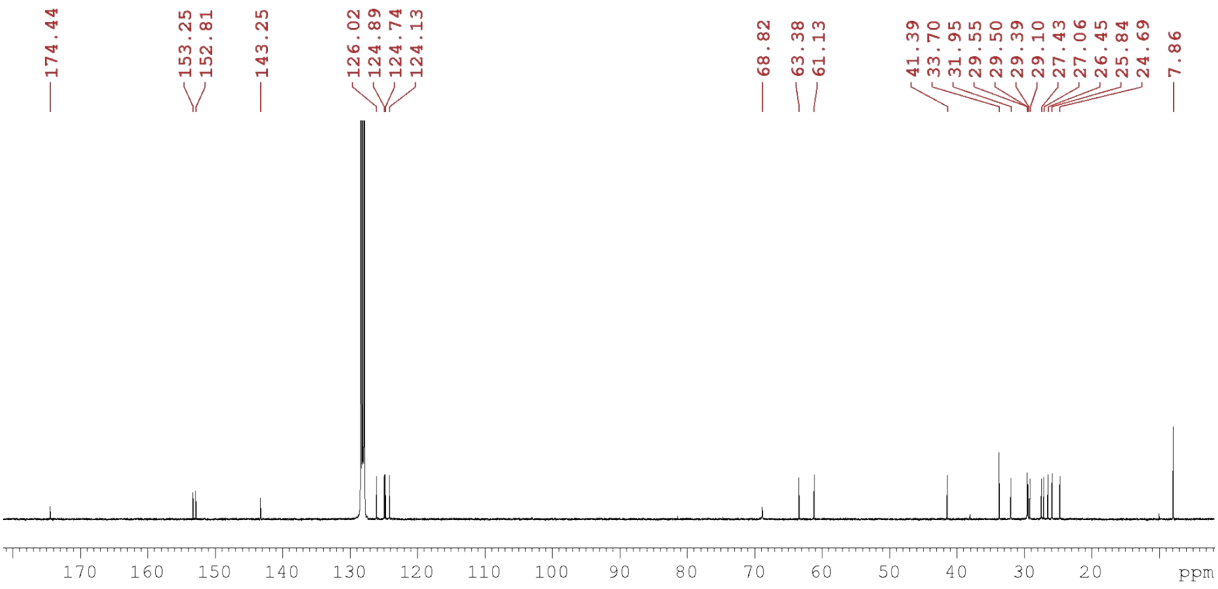

Figure S10: $^{13}C\{^{1}H\}$ NMR spectrum of (Me_2Im^{Me})•GaH_2($cAAC^{Me}H$) **5** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of (*i*Pr$_2$Im^{Me})•GaH$_2$(cAAC^{Me}H) 6

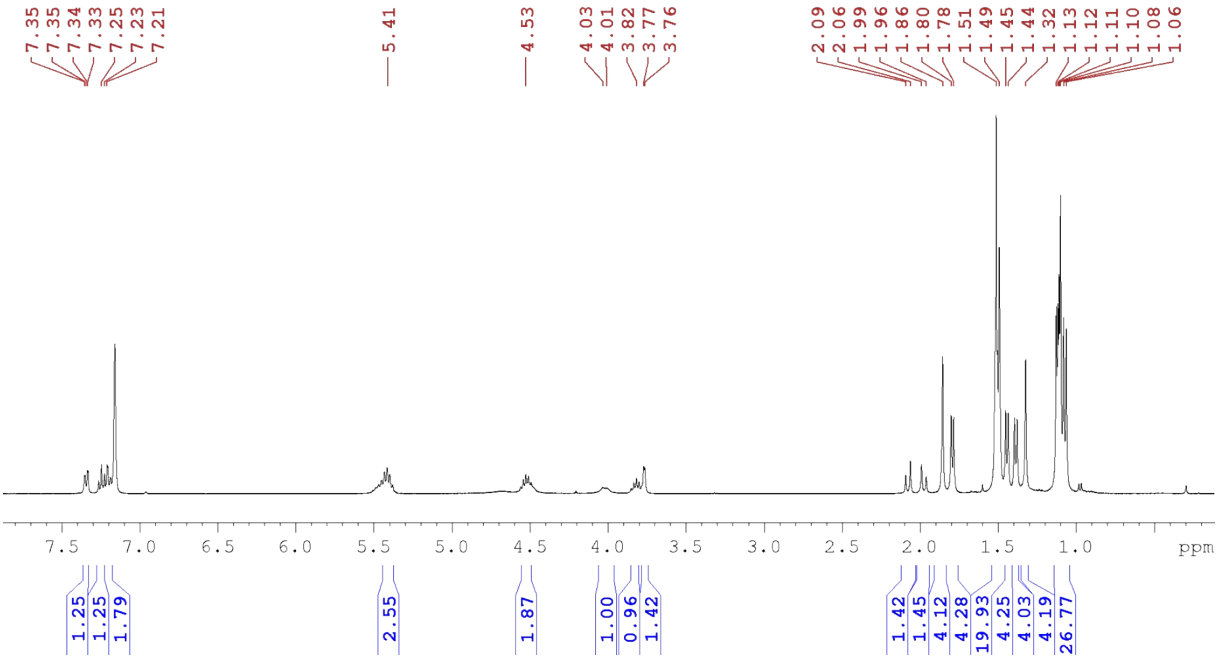

Figure S11: ^{1}H NMR spectrum of (*i*Pr$_2$Im^{Me})•GaH$_2$(cAAC^{Me}H) **6** in C$_6$D$_6$ (400 MHz, 25 °C).

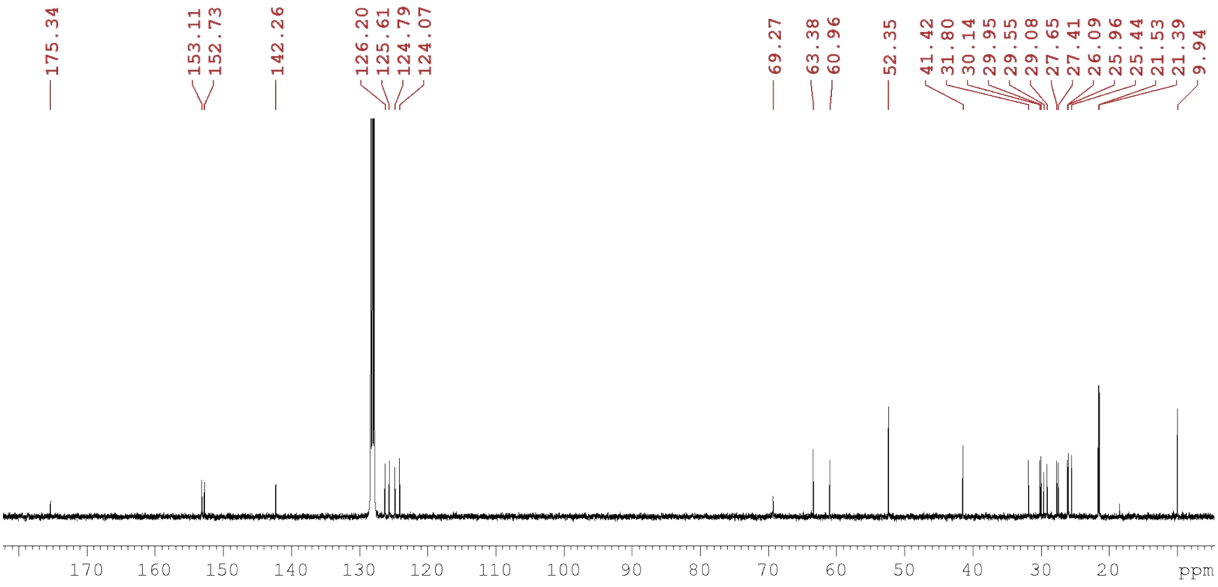

Figure S12: ^{13}C{^{1}H} NMR spectrum of (*i*Pr$_2$Im^{Me})•GaH$_2$(cAAC^{Me}H) **6** in C$_6$D$_6$ (125.8 MHz, 25 °C).

NMR spectra of (Dipp$_2$Im)•GaH$_2$(cAAC^{Me}H) 7

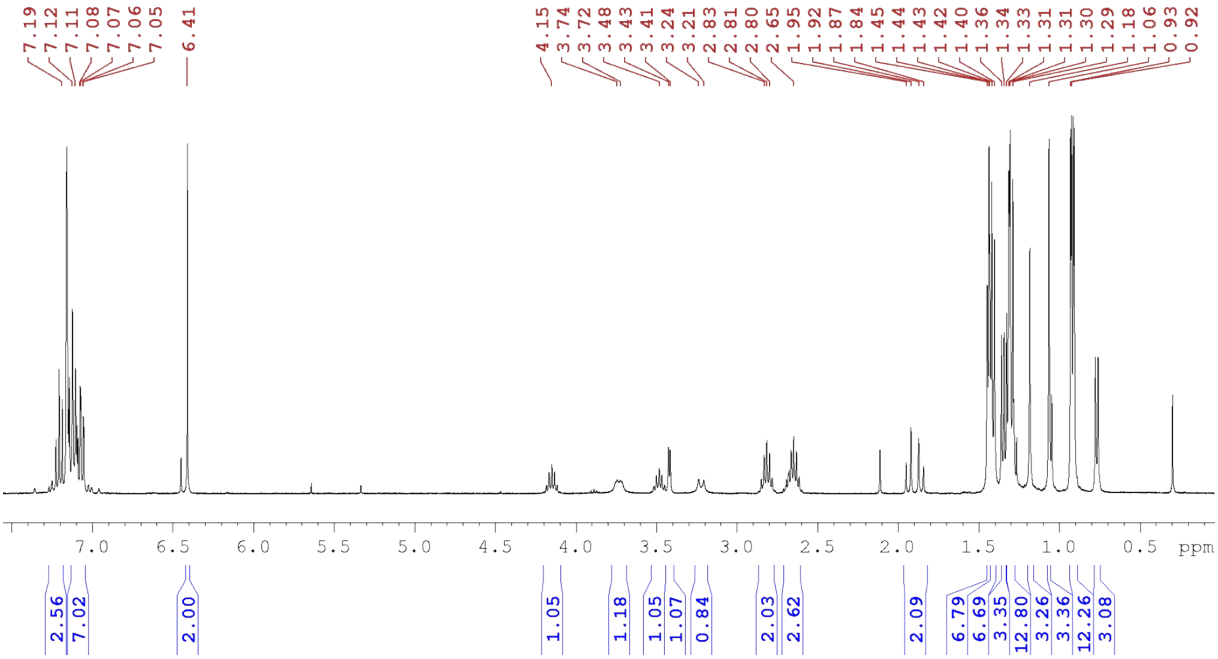

Figure S13: ^{1}H NMR spectrum of (Dipp$_2$Im)•GaH$_2$(cAAC^{Me}H) **7** in C_6D_6 (400 MHz, 25 °C).

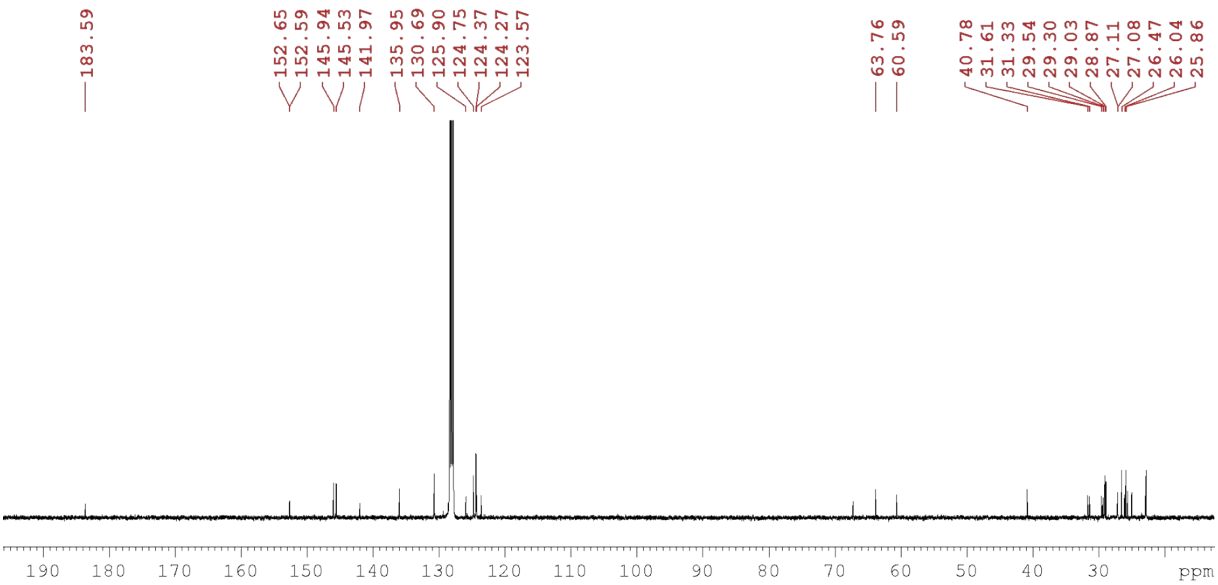

Figure S14: ^{13}C{^{1}H} NMR spectrum of (Dipp$_2$Im)•GaH$_2$(cAAC^{Me}H) **7** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of (cAAC^{Me}H)$_2$GaH 8

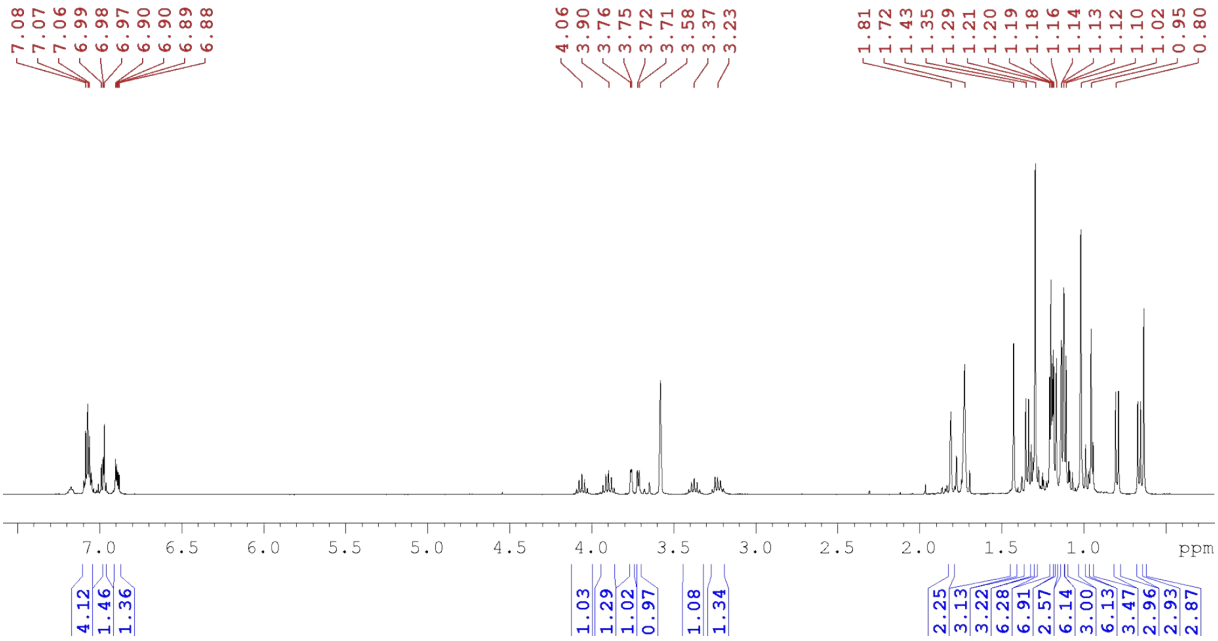

Figure S15: ^{1}H NMR spectrum of (cAAC^{Me}H)$_2$GaH **8** in THF-d8 (400 MHz, 25 °C).

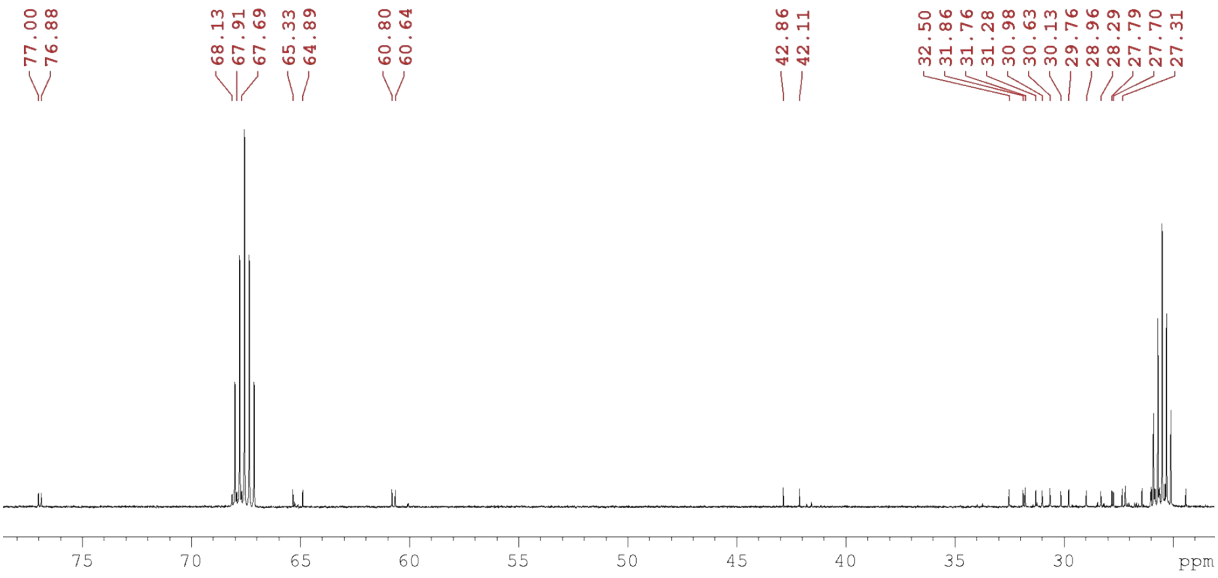

Figure S16: ^{13}C{^{1}H} NMR spectrum of (cAAC^{Me}H)$_2$GaH **8** in THF-d8 (125.8 MHz, 25 °C).

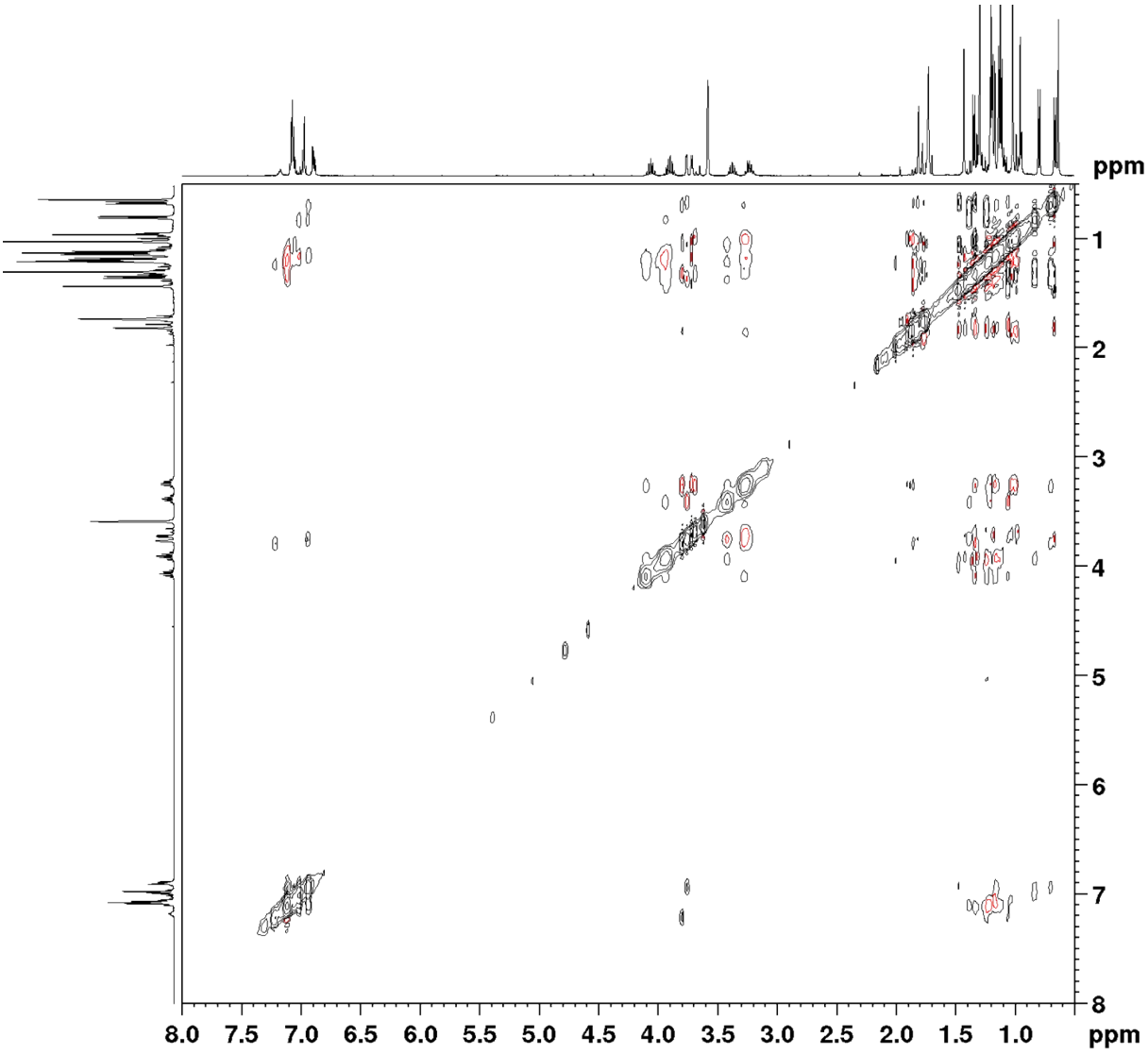

Figure S17: ^{1}H-^{1}H-NOESY/COESY NMR of **8** in thf-d_8 at RT.

NMR spectra of (*i*$Pr_2$$Im^{Me}$)•$GaH_2Cl$ 9

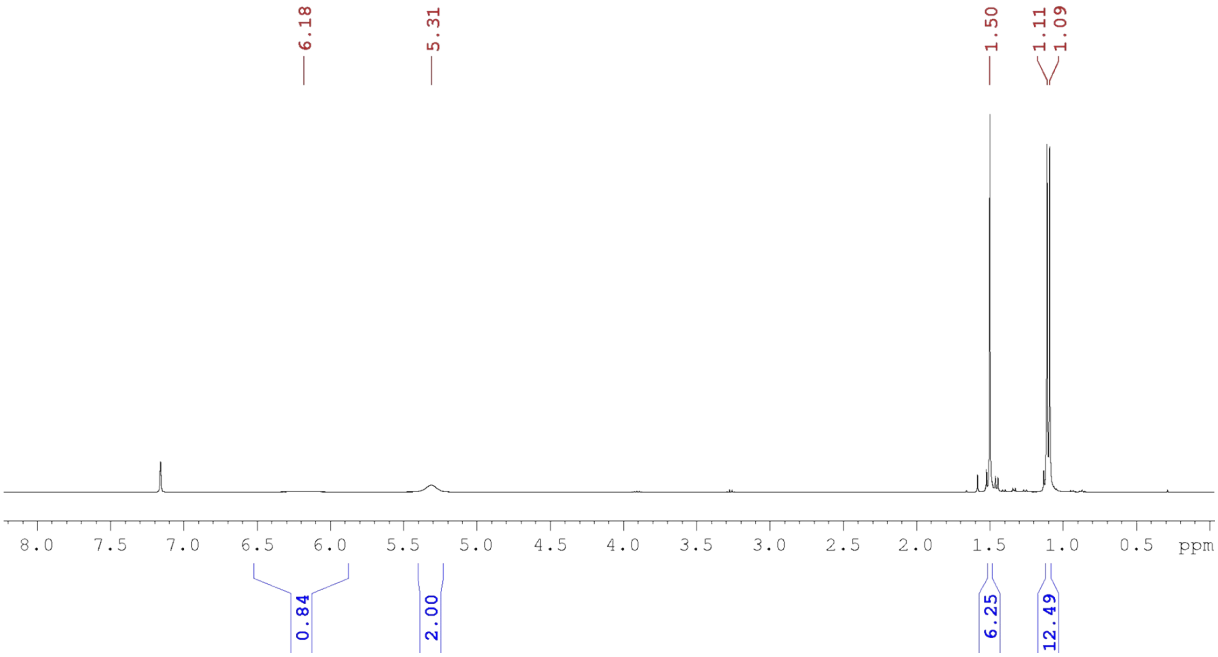

Figure S18: ^{1}H NMR spectrum of (iPr$_2$Im^{Me})•GaH$_2$Cl **9** in C$_6$D$_6$ (400 MHz, 25 °C). 17

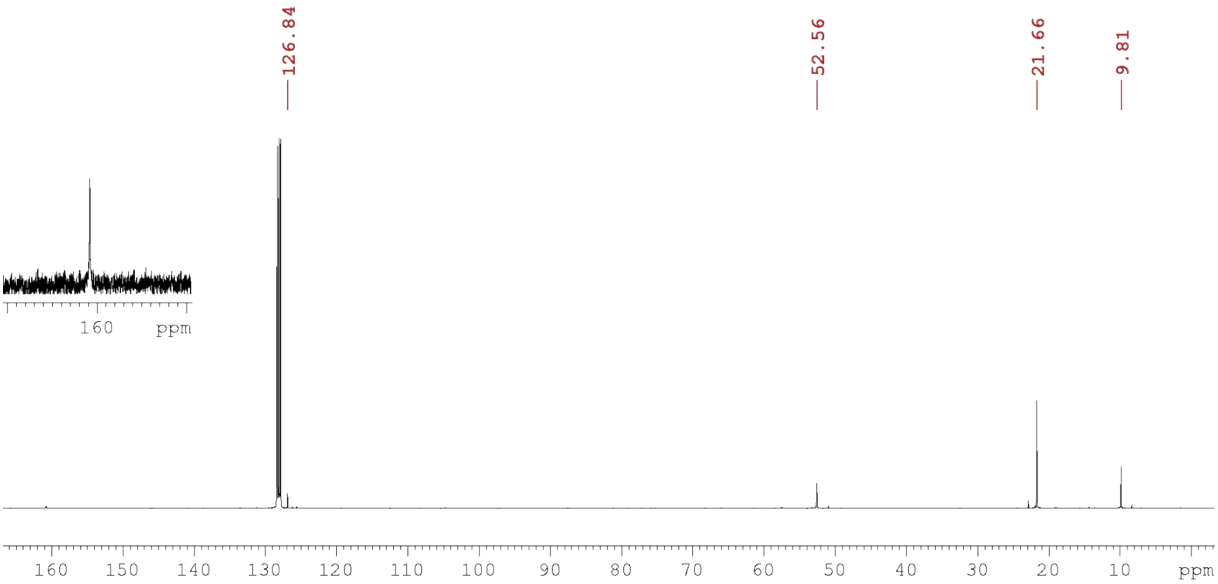

Figure S19: ^{13}C{^{1}H} NMR spectrum of (iPr$_2$Im^{Me})•GaH$_2$Cl **9** in C$_6$D$_6$ (125.8 MHz, 25 °C).

NMR spectra of (Dipp$_2$Im)•GaH$_2$Cl 10

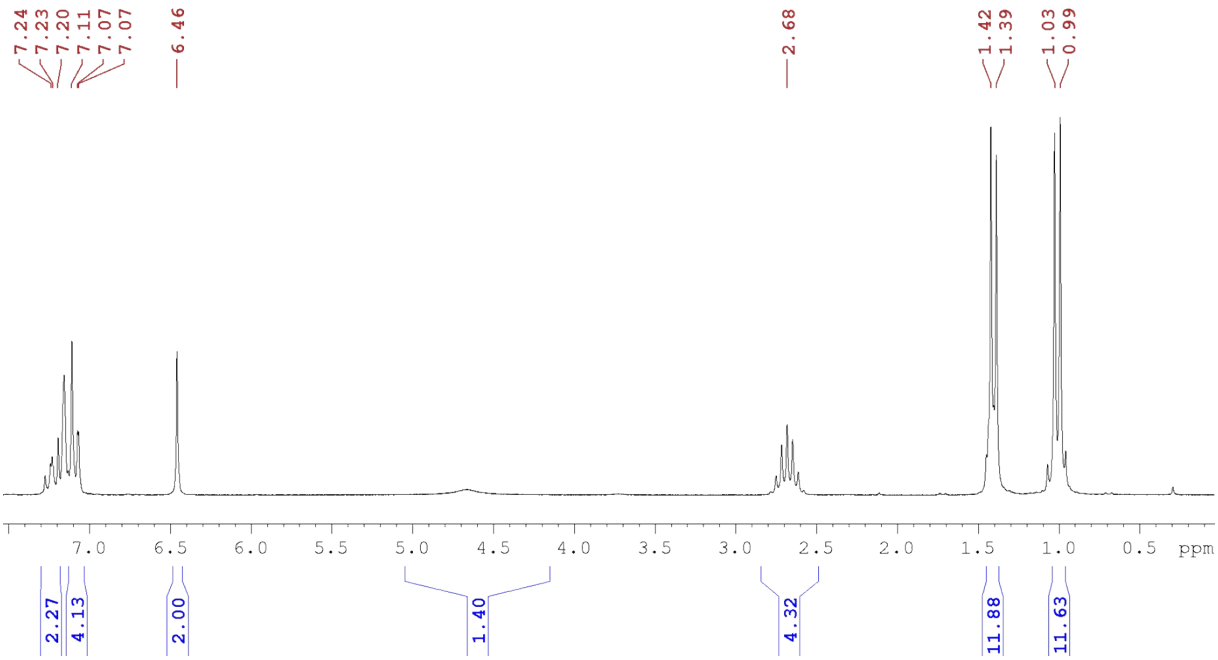

Figure S20: ^{1}H NMR spectrum of (Dipp$_2$Im)•GaH$_2$Cl **10** in C_6D_6 (400 MHz, 25 °C).

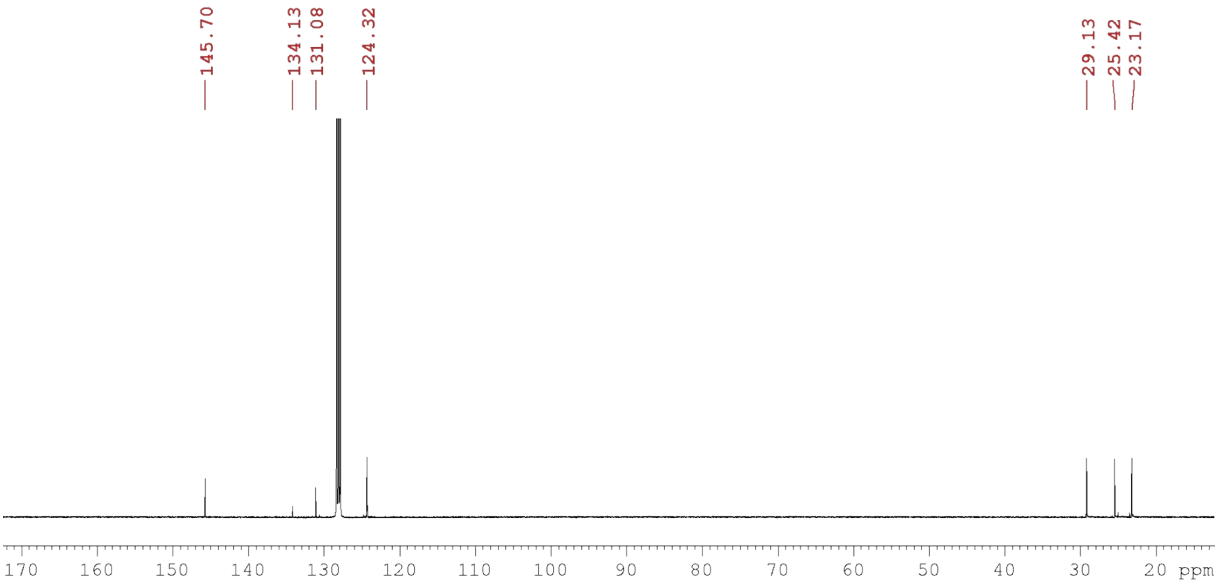

Figure S21: ^{13}C{^{1}H} NMR spectrum of (Dipp$_2$Im)•GaH$_2$Cl **10** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of (Dipp$_2$Im^{H})•GaH$_2$Cl 11

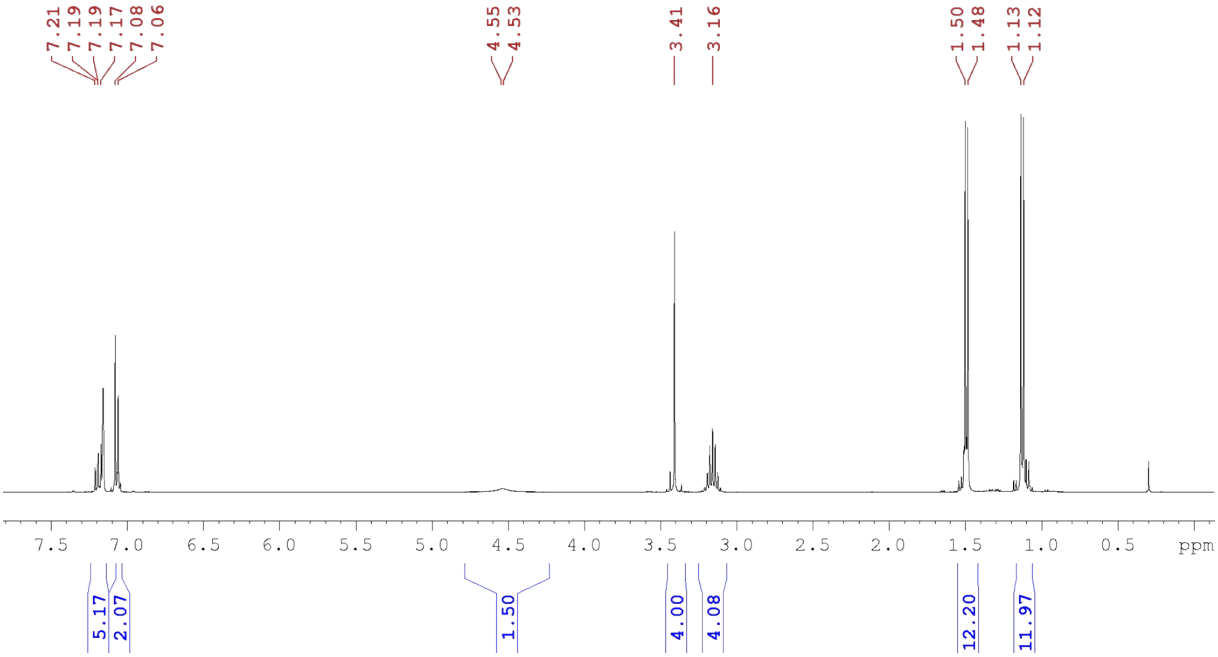

Figure S22: ^{1}H NMR spectrum of (Dipp$_2$Im^{H})•GaH$_2$Cl **11** in C_6D_6 (400 MHz, 25 °C).

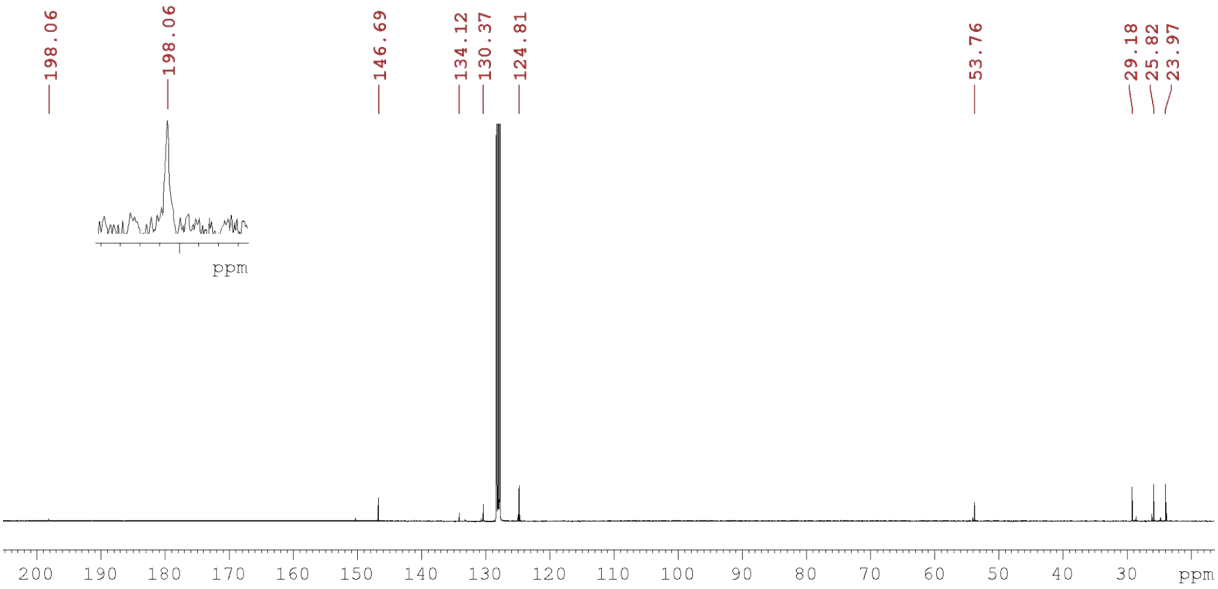

Figure S23: ^{13}C{^{1}H} NMR spectrum of (Dipp$_2$Im^{H})•GaH$_2$Cl **11** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of (iPr$_2$Im^{Me})•GaHCl$_2$ 12

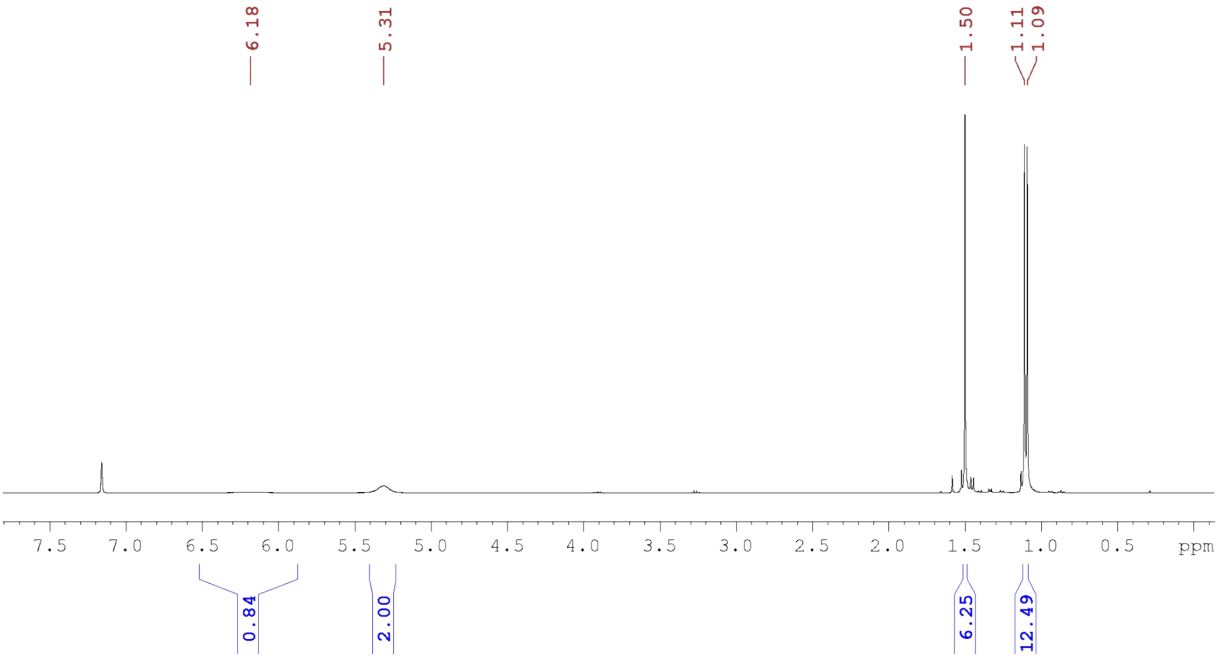

Figure S24: ^{1}H NMR spectrum of (iPr$_2$Im^{Me})•GaHCl$_2$ **12** in C_6D_6 (400 MHz, 25 °C).

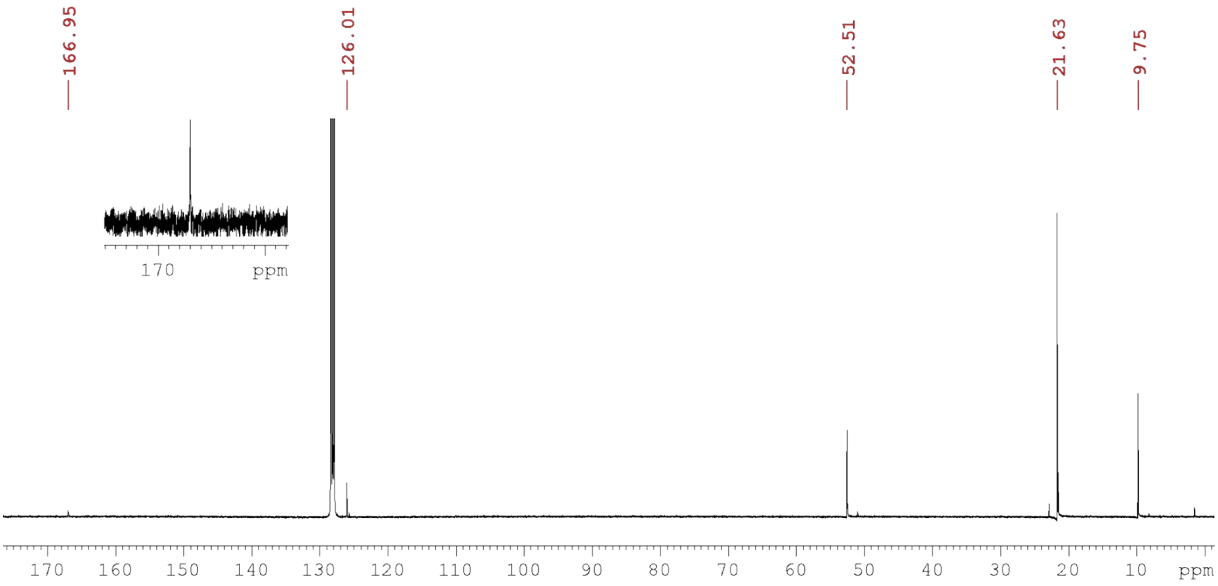

Figure S25: ^{13}C{^{1}H} NMR spectrum of (iPr$_2$Im^{Me})•GaHCl$_2$ **12** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of $(Dipp_2Im)•GaHCl_2$ 13

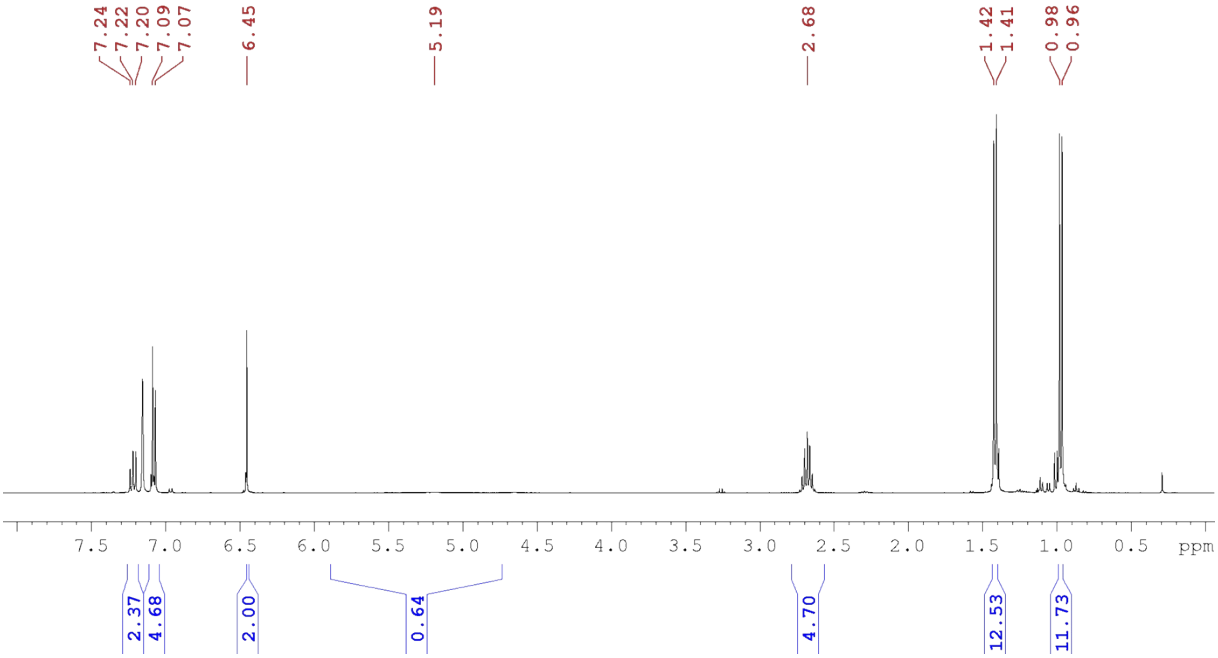

Figure S26: ^{1}H NMR spectrum of $(Dipp_2Im)•GaHCl_2$ **13** in C_6D_6 (400 MHz, 25 °C).

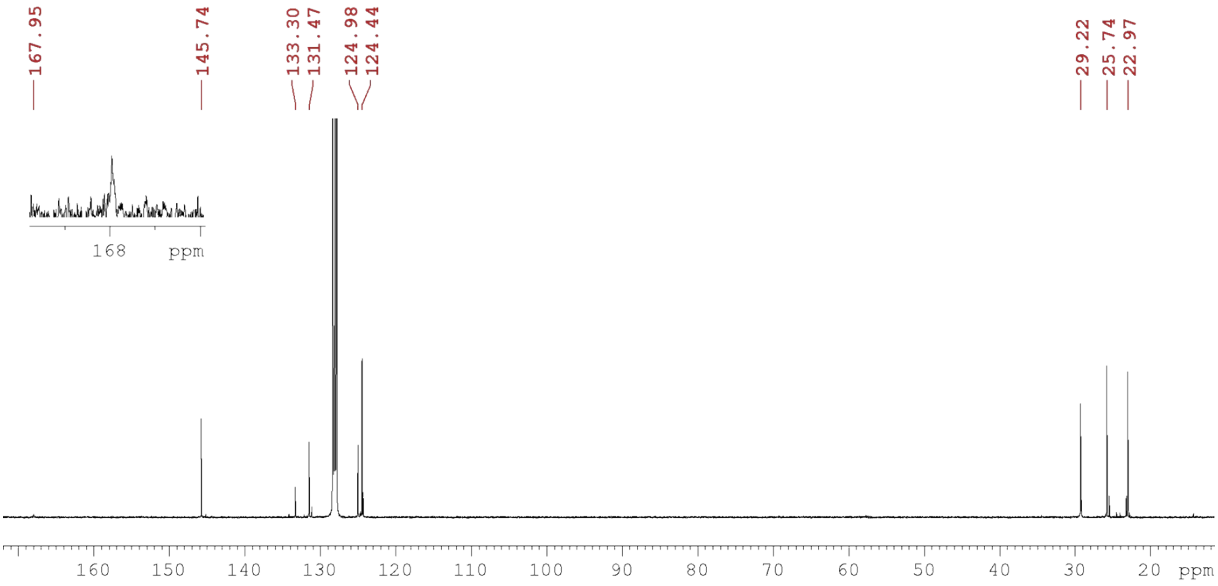

Figure S27: $^{13}C\{^{1}H\}$ NMR spectrum of $(Dipp_2Im)•GaHCl_2$ **14** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of ($Dipp_2Im^H$)•$GaHCl_2$ 14

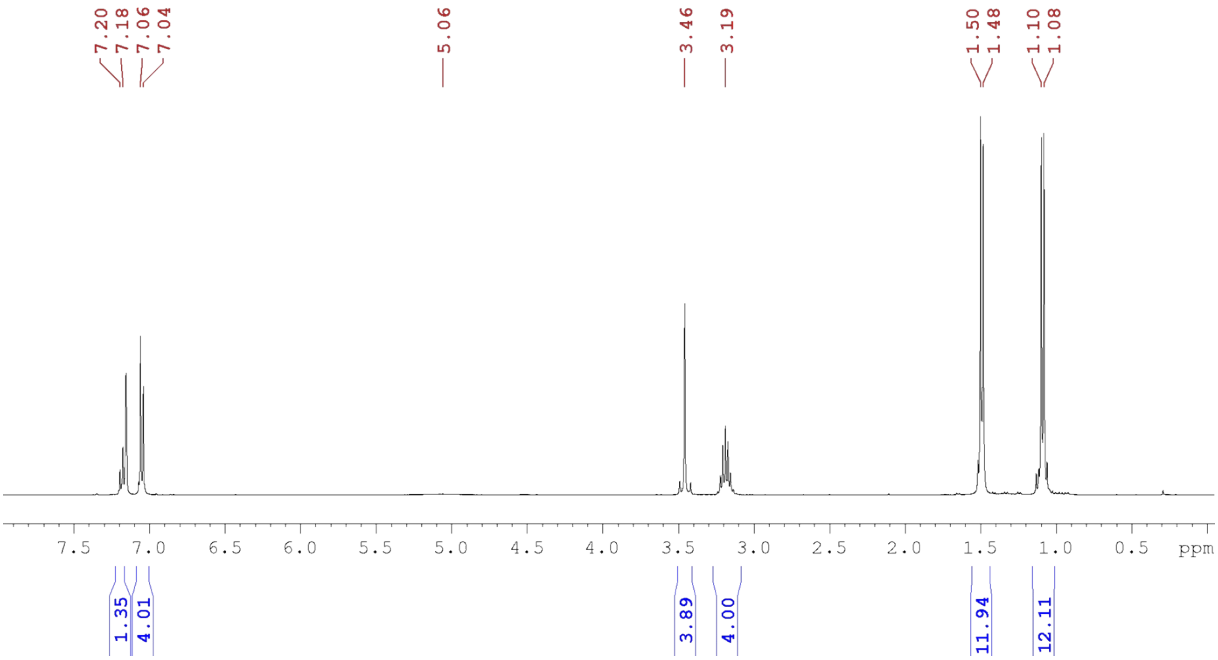

Figure S28: ^1H NMR spectrum of ($Dipp_2Im^H$)•$GaHCl_2$ **14** in C_6D_6 (400 MHz, 25 °C).

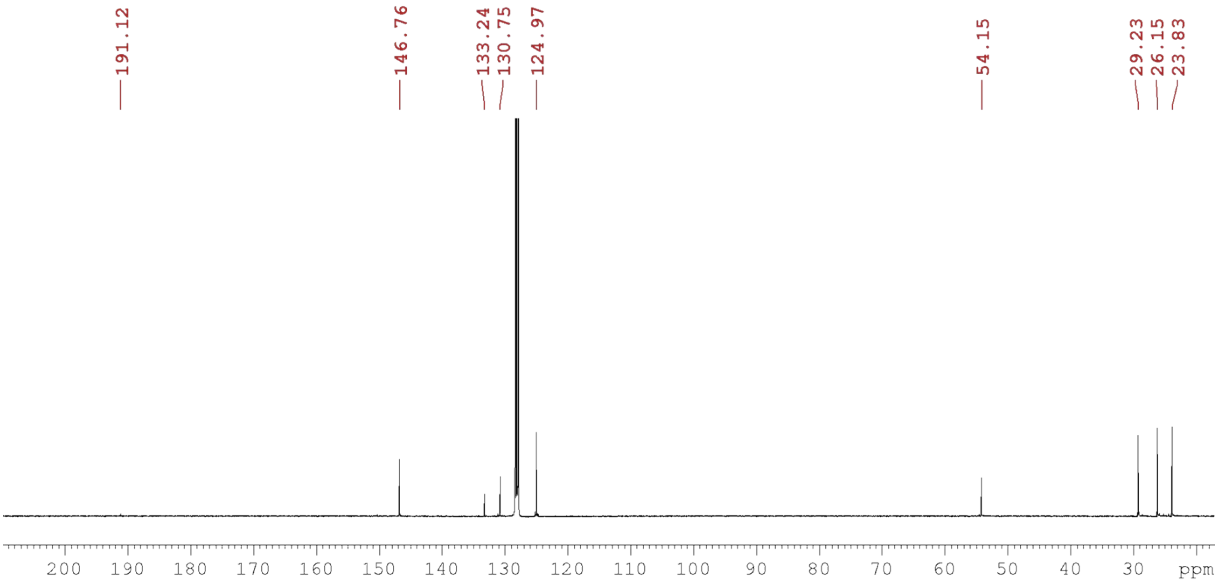

Figure S29: $^{13}C\{^1H\}$ NMR spectrum of ($Dipp_2Im^H$)•$GaHCl_2$ **14** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of (cAAC^{Me})•GaHCl$_2$ 15

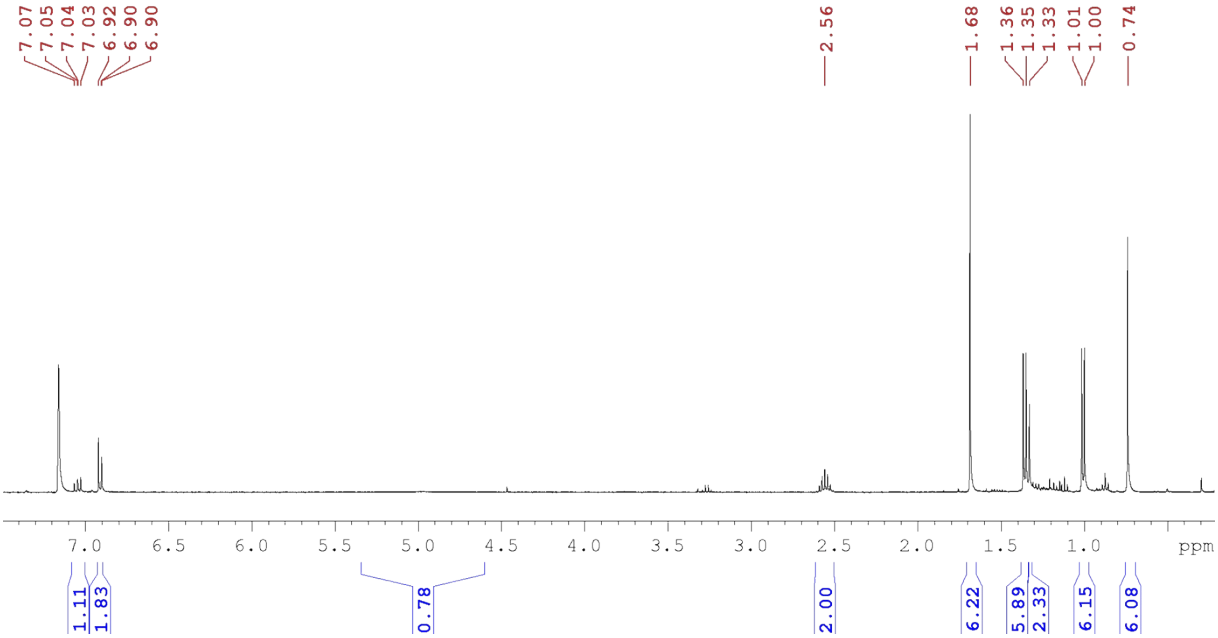

Figure S30: ^{1}H NMR spectrum of (cAAC^{Me})•GaHCl$_2$ **15** in C_6D_6 (400 MHz, 25 °C).

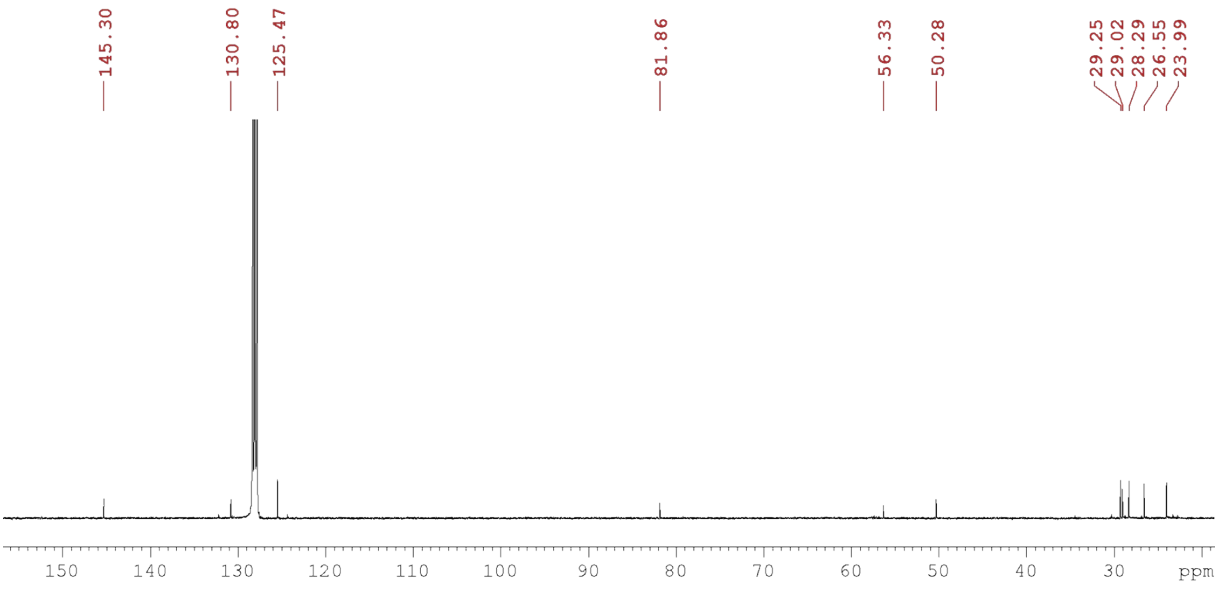

Figure S31: ^{13}C{^{1}H} NMR spectrum of (cAAC^{Me})•GaHCl$_2$ **15** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of (*i*Pr$_2$Im^{Me})•GaHCl(cAAC^{Me}H) 16R/16S

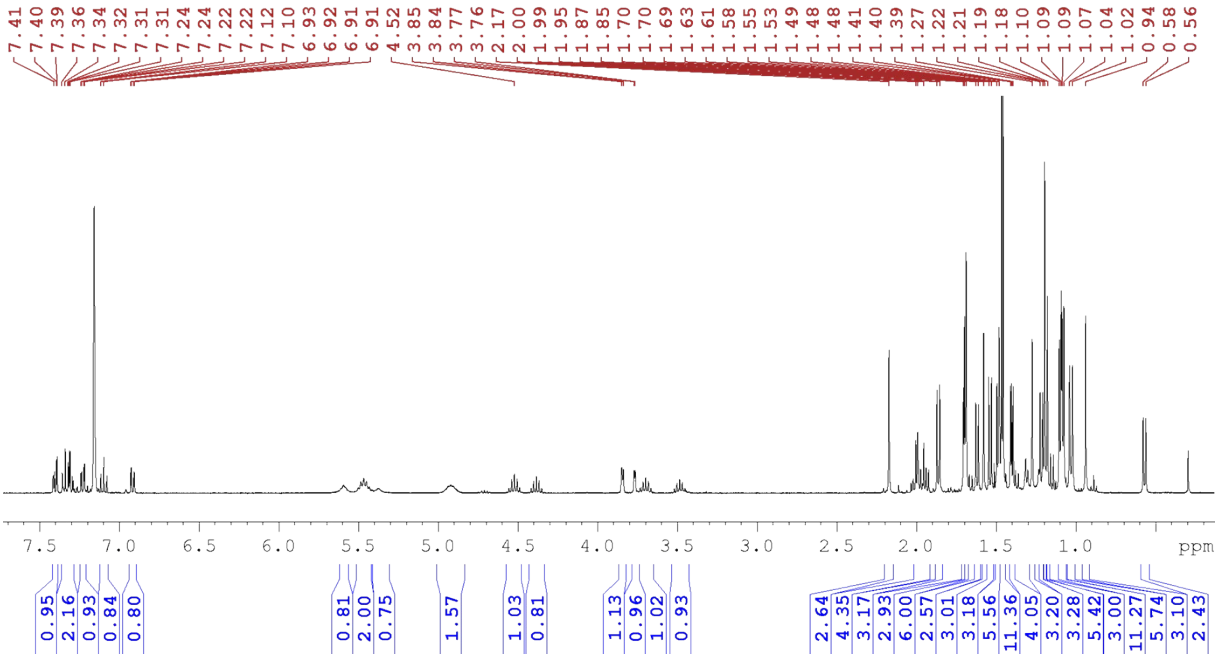

Figure S32: ^{1}H NMR spectrum of (*i*Pr$_2$Im^{Me})•GaHCl(cAAC^{Me}H) **16R/16S** in C_6D_6 (400 MHz, 25 °C).

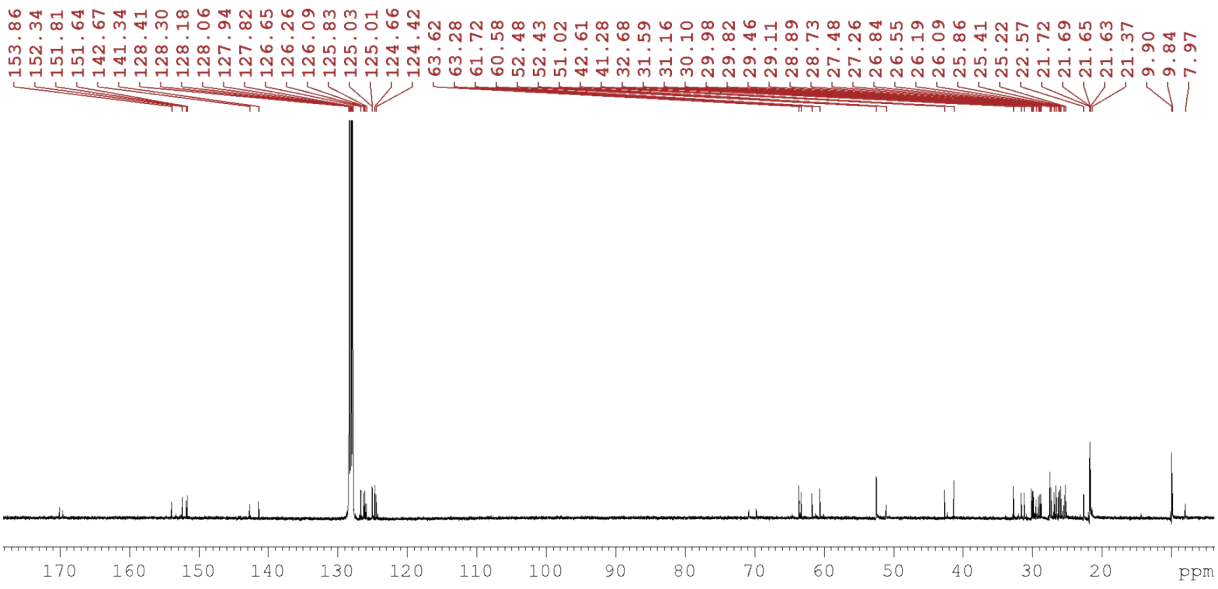

Figure S33: ^{13}C{^{1}H} NMR spectrum of (*i*Pr$_2$Im^{Me})•GaHCl(cAAC^{Me}H) **16R/16S** in C_6D_6 (125.8 MHz, 25 °C).

NMR spectra of (iPr$_2$Im^{Me})•GaCl$_2$(cAAC^{Me}H) 17

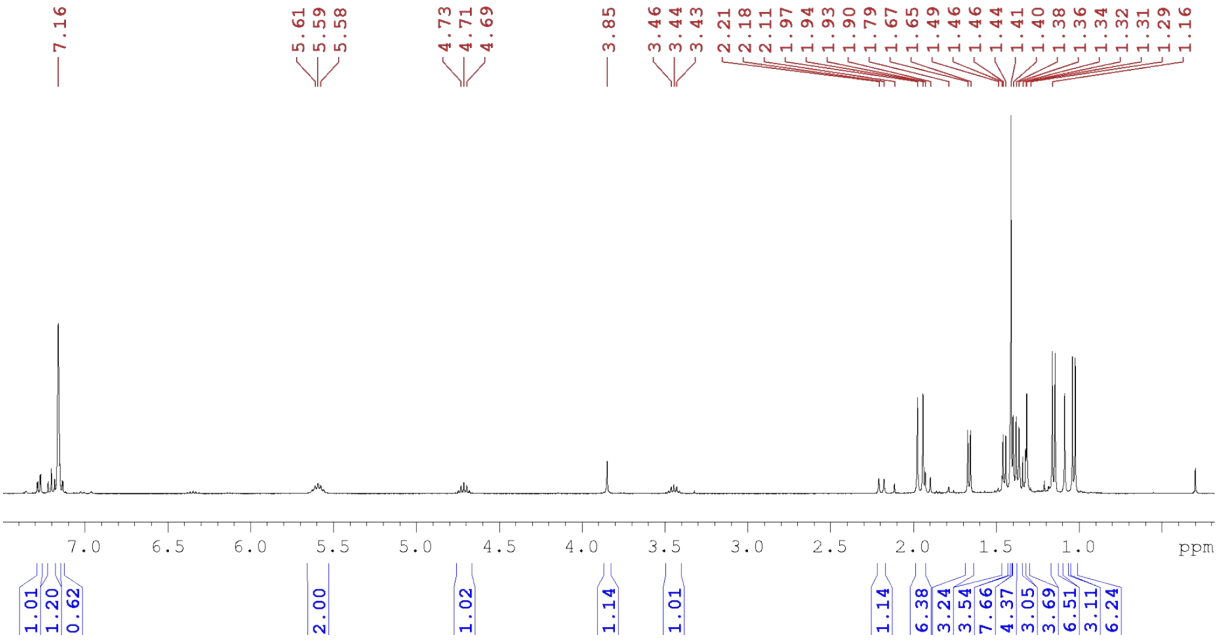

Figure S34: ^{1}H NMR spectrum of (iPr$_2$Im^{Me})•GaCl$_2$(cAAC^{Me}H) **17** in C$_6$D$_6$ (400 MHz, 25 °C).

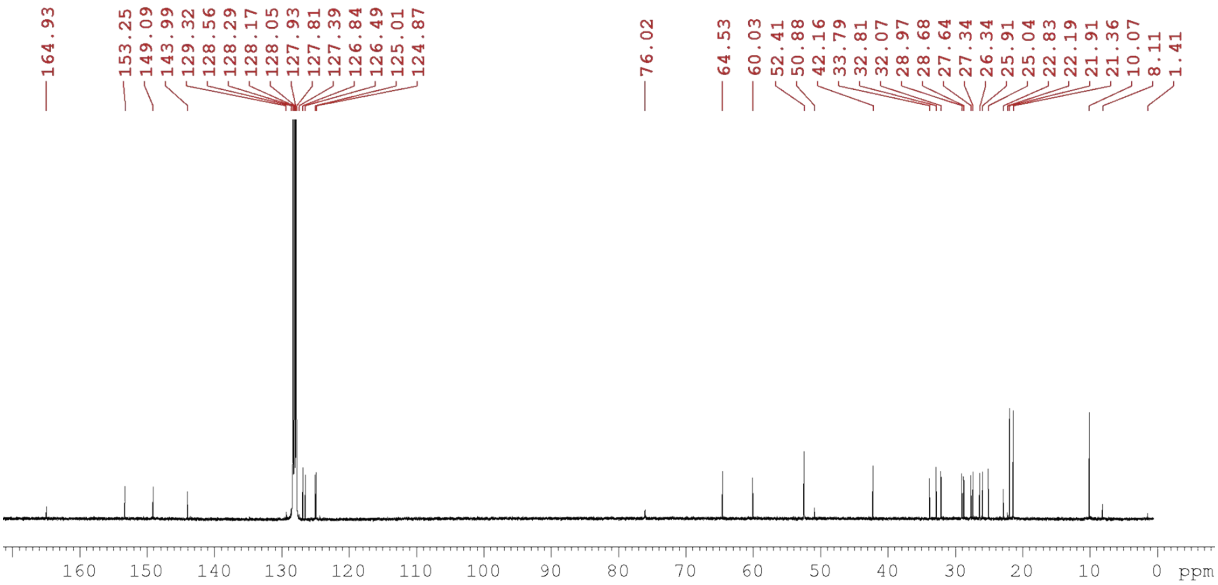

Figure S35: ^{13}C{^{1}H} NMR spectrum of (iPr$_2$Im^{Me})•GaCl$_2$(cAAC^{Me}H) **17** in C$_6$D$_6$ (125.8 MHz, 25 °C).

NMR spectra of (cAAC^{Me}H)$_2$GaCl 18

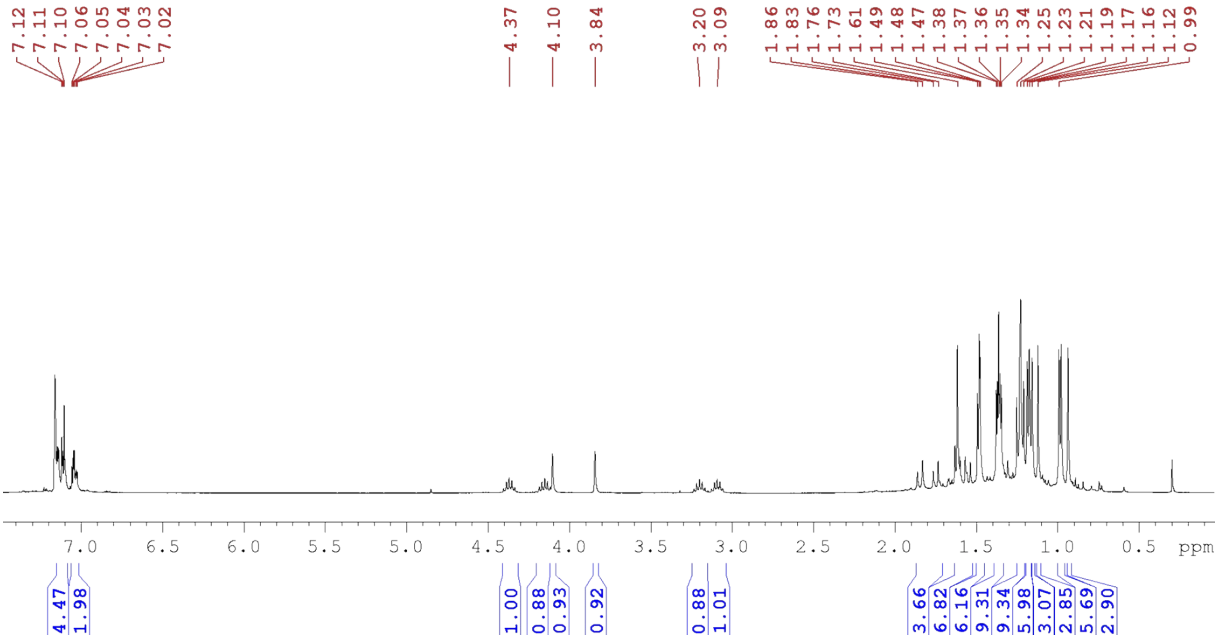

Figure S36: ^{1}H NMR spectrum of (cAAC^{Me}H)$_2$GaCl **18** in C_6D_6 (400 MHz, 25 °C).

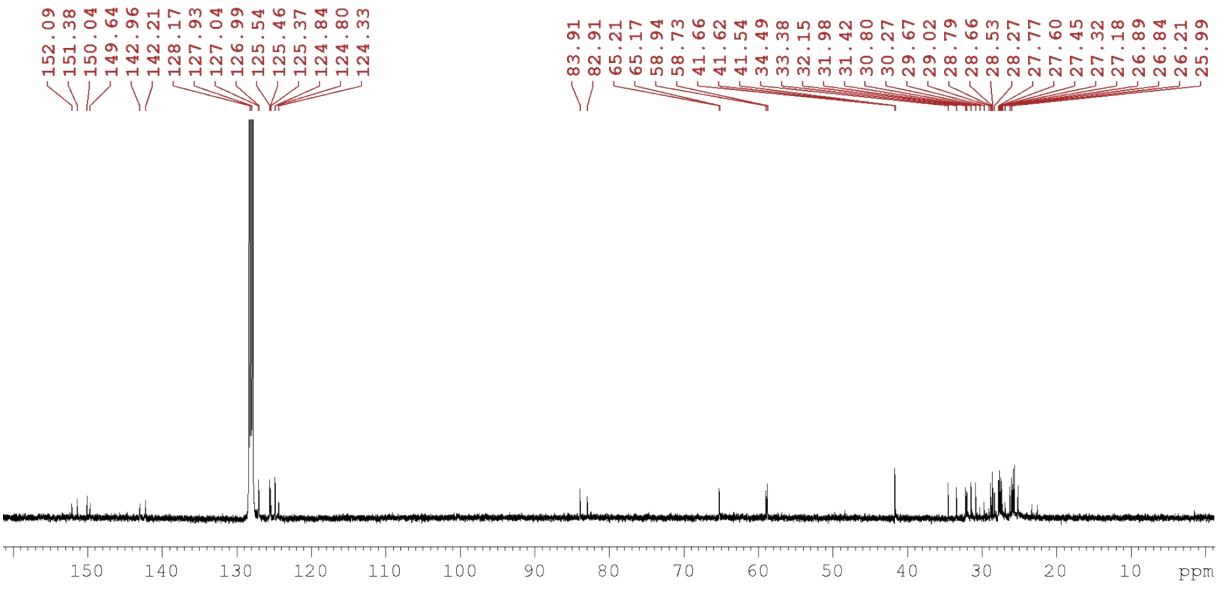

Figure S37: ^{13}C{^{1}H} NMR spectrum of (cAAC^{Me}H)$_2$GaCl **18** in C_6D_6 (125.8 MHz, 25 °C).

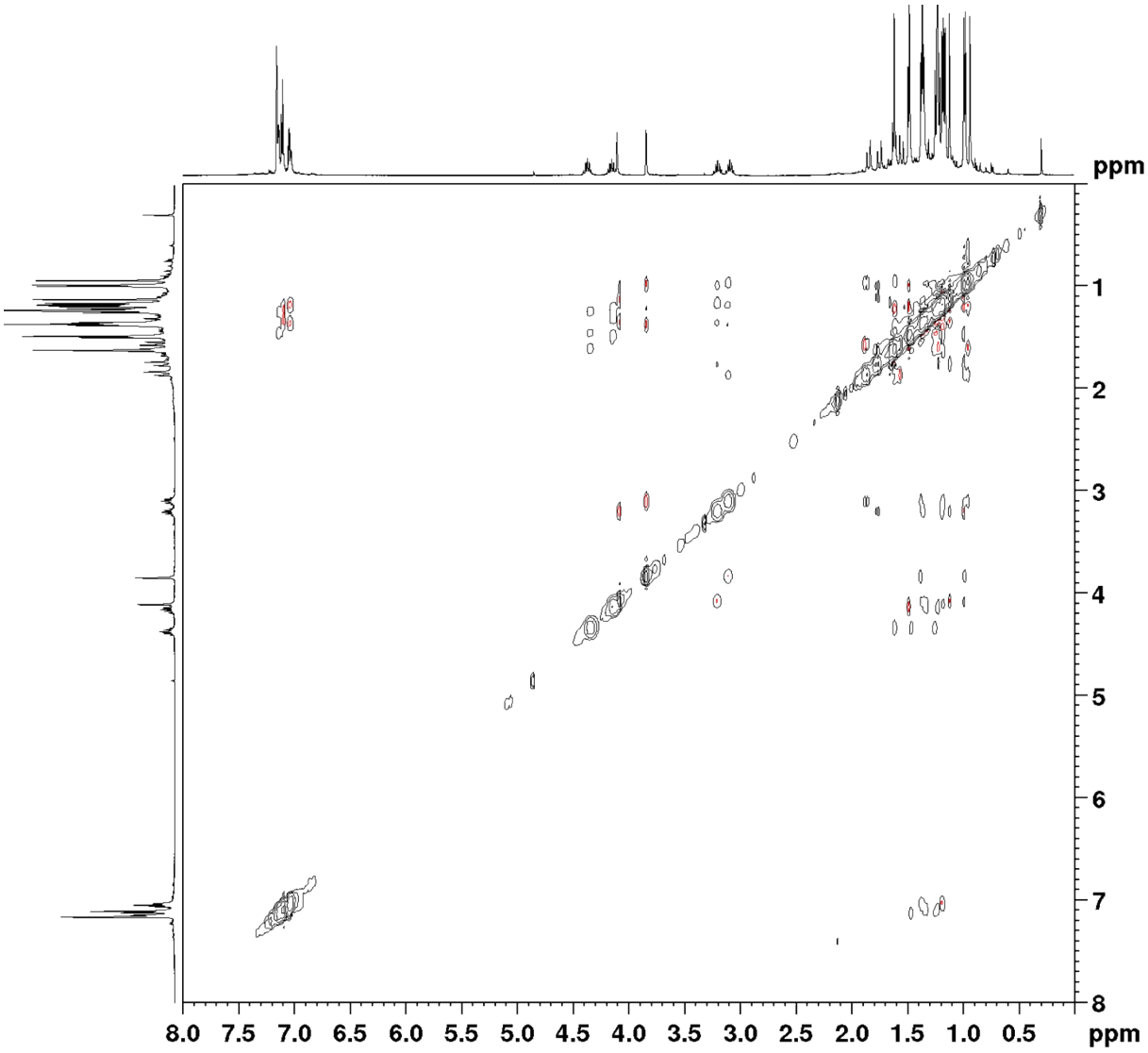

Figure S38: ^{1}H-^{1}H-NOESY/COESY NMR of **18** in C_6D_6 at RT.

3 Crystallographic Data

Crystals were immersed in a film of perfluoropolyether oil on a glass fiber MicroMountTM (MiTeGen) and transferred to a Bruker D8 Apex-1 diffractometer with CCD area detector and graphitemonochromated Mo-Kα radiation or a Bruker D8 Apex-2 diffractometer with CCD area detector and graphite-monochromated Mo-Kα radiation equipped with an Oxford Cryosystems low-temperature device or a Rigaku XtaLAB Synergy-DW diffractometer with HyPix-6000HE detector and monochromated Cu-Kα equipped with an Oxford Cryo 800 cooling unit. Data were collected at 100 K. The images were processed with the Bruker or Crysalis software packages and equivalent reflections were merged. Corrections for Lorentz-polarization effects and absorption were performed if necessary and the structures were solved by direct methods. Subsequent difference Fourier syntheses revealed the positions of all other non-hydrogen atoms. The structures were solved by using the ShelXTL software package.[5] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were usually assigned to idealized positions and were included in structure factors calculations.

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no.s CCDC 2008675 (**1**), 2008679 (**4**), CCDC 2008682 (**5**), CCDC 2008681 (**6**), CCDC 2008676 (**7**), CCDC 1975620 (**8**), CCDC 1975614 (**12**), CCDC 2008677 (**13**), CCDC 2008678 (**15**), CCDC 2008683 (**16**) and CCDC 2008680 (**17**). Copies of the data can be obtained free of charge on application to CCDC.

Crystal Data of $(Me_2Im^{Me})\cdot GaH_3$ **1:** $C_7H_{15}GaN_2$, M_r = 196.93 , colorless block, 0.29 x 0.16 x 0.10 mm, monoclinic group $P2_1/c$, a = 7.49530(10) Å, b = 15.4509(3) Å, c = 8.4772(2) Å, α = 90°, β = 103.862(2)°, γ = 90°, V = 953.14(3) Å^3, T = 100.00 K, Z = 4, $\rho_{calcd.}$ = 1.372 g·cm^{-3}, μ = 3.431, F(000) = 408, 9982 reflections, in h(–8/9), k(-19/16), l(-10/10) measured in the range 5.7460° < θ < 76.5650°, completeness 98.3 %, 6692 independent reflections, 1875 observed reflections (I > 2σ(I)), 107 parameters, 0 restraints; all data: R_1 = 0.0327 and wR_2 = 0.0900, I > 2σ(I): R_1 = 0.0312 and wR_2 = 0.0886, Goof 0.920, largest difference peak/hole 0.45 /-0.60 e·Å^{-3}.

Crystal Data of $(Dipp_2Im^{H})\cdot GaH_3$ **4:** $C_{54}H_{82}Ga_2N_4$, M_r = 926.67 , colorless block, 0.23 x 0.20 x 0.12 mm, triclinic group $P\bar{1}$, a = 12.6504(2) Å, b = 15.3371(3) Å, c = 15.5035(3) Å, α = 63.215(2)°, β = 86.682(2)°, γ = 83.655(2)°, V = 2668.69(10) Å^3, T = 100.01(10) K, Z = 4, $\rho_{calcd.}$ = 1.153 g·cm^{-3}, μ = 1.497, F(000) = 992, 24795 reflections, in h(–16/15), k(-19/19), l(-19/19) measured in the range 3.1970° < θ < 77.2520°, completeness 98.0 %, 11140 independent reflections, 9972 observed reflections (I > 2σ(I)), 581 parameters, 0 restraints; all data: R_1 = 0.0530 and wR_2 = 0.1436, I > 2σ(I): R_1 = 0.0493 and wR_2 = 0.1393, Goof 1.0696, largest difference peak/hole 1.06 /-0.88 e·Å^{-3}.

Crystal Data of $(Me_2Im^{Me})\cdot GaH_2(cAAC^{Me}H)$ **5:** $C_{27}H_{46}GaN_3$, M_r = 964.77 , colorless block, 0.23 x 0.18 x 0.13 mm, triclinic group $P\bar{1}$, a = 9.3195(2) Å, b = 15.9016(3) Å, c = 18.0954(3) Å, α = 100.595(2)°, β = 93.0210(10)°, γ = 91.580(2)°, V = 2630.37(9) Å^3, T = 100.00(10) K, Z = 4, $\rho_{calcd.}$ = 1.218 g·cm^{-3}, μ = 1.546, F(000) = 1040, 30734 reflections, in h(–9/11), k(-19/19), l(-22/22) measured in the range 2.5070° < θ < 77.0490°, completeness 99.9 %, 9987 independent reflections, 9118 observed reflections (I > 2σ(I)), 599 parameters, 0 restraints; all data: R_1 = 0.0366 and wR_2 = 0.094, I > 2σ(I): R_1 = 0.0339 and wR_2 = 0.0918, Goof 0.958, largest difference peak/hole 0.73 /-0.44 e·Å^{-3}.

Crystal Data of $(i Pr_2Im^{Me})\cdot GaH_2(cAAC^{Me}H)$ **6:** $C_{34}H_{57}GaN_3$, M_r = 577.54, colorless block, 0.17 x 0.14 x 0.08 mm, monoclinic group $P2_1/c$, a = 13.71090(10) Å, b = 13.0468(2) Å, c =

18.9477(2) Å, α = 90°, β = 101.9240(10)°, γ = 90°, V = 3316.29(7) Å^3, T = 100.01(10) K, Z = 4, $\rho_{calcd.}$ = 1.157 g·cm^{-3}, μ = 1.303, F(000) = 1252, 20143 reflections, in h(–16/17), k(-16/15), l(-23/23) measured in the range 3.3090° < θ < 76.6690°, completeness 98.3 %, 6940 independent reflections, 6296 observed reflections (I > 2σ(I)), 365 parameters, 0 restraints; all data: R_1 = 0.0378 and wR_2 = 0.0923, I > 2σ(I): R_1 = 0.0344 and wR_2 = 0.0902, Goof 1.097, largest difference peak/hole 0.66 /-0.43 e·Å^{-3}.

Crystal Data of (Dipp$_2$Im)·GaH$_2$(cAAC^{Me}H) **7:** $C_{47}H_{70}GaN_3$, M_r = 746.78, colorless block, 0.24 x 0.15 x 0.13 mm, triclinic group $P\bar{1}$, a = 10.535870(10) Å, b = 12.53250(10) Å, c = 18.49810(10) Å, α = 100.0810(10)°, β = 99.0220(10)°, γ = 112.9620(10)°, V = 2145.48(3) Å^3, T = 100.00(10) K, Z = 2, $\rho_{calcd.}$ = 1.156 g·cm^{-3}, μ = 1.117, F(000) = 808, 29458 reflections, in h(–13/12), k(-15/15), l(-20/23) measured in the range 2.5060° < θ < 76.8670°, completeness 97.9 %, 8955 independent reflections, 8262 observed reflections (I > 2σ(I)), 488 parameters, 0 restraints; all data: R_1 = 0.0362 and wR_2 = 0.0907, I > 2σ(I): R_1 = 0.0337 and wR_2 = 0.0887, Goof 1.00, largest difference peak/hole 0.40 /-0.52 e·Å^{-3}.

Crystal Data of (cAAC^{Me}H)$_2$GaH **8:** $C_{40}H_{65}GaN_2$, M_r = 643.66, colorless block, 0.23 x 0.17 x 0.13 mm, orthorhombic group $P2_1/b2/c2_1/n$, a = 12.56810(10) Å, b = 12.39160(10) Å, c = 23.3708(2) Å, α = 90°, β = 90°, γ = 90°, V = 3639.74(5) Å^3, T = 100(2) K, Z = 4, $\rho_{calcd.}$ = 1.175 g·cm^{-3}, μ = 1.228, F(000) = 1400, 39703 reflections, in h(–15/15), k(-11/15), l(-29/29) measured in the range 2.8030° < θ < 76.9490°, completeness 99.8 %, 3861 independent reflections, 3656 observed reflections (I > 2σ(I)), 225 parameters, 13 restraints; all data: R_1 = 0.0370 and wR_2 = 0.0976, I > 2σ(I): R_1 = 0.0357 and wR_2 = 0.0964, Goof 1.055, largest difference peak/hole 0.70 /-0.39 e·Å^{-3}.

Crystal Data of (*i*Pr$_2$Im^{Me})·GaHCl$_2$ **12:** $C_{11}H_{21}Cl_2GaN_2$, M_r = 321.92, colorless block, 0.21 x 0.18 x 0.12 mm, monoclinic group Cc, a = 14.0953(2) Å, b = 9.46110(10) Å, c = 11.53480(10) Å, α = 90°, β = 105.6090(10)°, γ = 90°, V = 1481.52(3) Å^3, T = 100.00(10) K, Z = 4, $\rho_{calcd.}$ = 1.443 g·cm^{-3}, μ = 5.675, F(000) = 664, 13423 reflections, in h(–17/14), k(-11/11), l(-14/13) measured in the range 5.6980° < θ < 76.3640°, completeness 98.0 %, 2526 independent reflections, 2519 observed reflections (I > 2σ(I)), 156 parameters, 2 restraints; all data: R_1 = 0.0328 and wR_2 = 0.0864, I > 2σ(I): R_1 = 0.0328 and wR_2 = 0.0864, Goof 1.091, largest difference peak/hole 0.57 /-0.31 e·Å^{-3}.

Crystal Data of (Dipp$_2$Im)·GaHCl$_2$ **13:** $C_{27}H_{37}Cl_2GaN_2$, M_r = 530.21, colorless block, 0.29 x 0.15 x 0.09 mm, monoclinic group $P2_1/c$, a = 16.4027(2) Å, b = 19.2302(2) Å, c = 18.9987(2) Å, α = 90°, β = 111.7170(10)°, γ = 90°, V = 5567.36(11) Å^3, T = 100.00(10) K, Z = 8, $\rho_{calcd.}$ = 1.265 g·cm^{-3}, μ = 3.228, F(000) = 2224, 30723 reflections, in h(–20/20), k(-24/24), l(-24/19) measured in the range 2.9230° < θ < 77.2570°, completeness 98.0 %, 11586 independent reflections, 10397 observed reflections (I > 2σ(I)), 601 parameters, 0 restraints; all data: R_1 = 0.0404 and wR_2 = 0.0984, I > 2σ(I): R_1 = 0.0363 and wR_2 = 0.0958, Goof 1.048, largest difference peak/hole 0.64 /-0.47 e·Å^{-3}.

Crystal Data of (cAAC^{Me})·GaHCl$_2$ **15:** $C_{20}H_{32}Cl_2GaN_2$, M_r = 427.08, colorless block, 0.23 x 0.15 x 0.14 mm, monoclinic group Pbca, a = 14.8846(2) Å, b = 14.9936(2) Å, c = 19.0070(3) Å, α = 90°, β = 90°, γ = 90°, V = 4241.86(10) Å^3, T = 100.00(10) K, Z = 8, $\rho_{calcd.}$ = 1.338 g·cm^{-3}, μ = 4.085, F(000) = 1792, 12010 reflections, in h(–10/18), k(-17/18), l(-23/23) measured in the range 3.7660° < θ < 76.6890°, completeness 97.8 %, 4414 independent reflections, 4023 observed reflections (I > 2σ(I)), 229 parameters, 0 restraints; all data: R_1 = 0.0531 and wR_2 = 0.1379, I > 2σ(I): R_1 = 0.0501 and wR_2 = 0.1347, Goof 1.072, largest difference peak/hole 1.49 /-1.03 e·Å^{-3}.

Crystal Data of (iPr$_2$Im^{Me})·GaHCl(cAAC^{Me}H) **16:** $C_{31}H_{53}ClGaN_3$, M_r = 572.93, colorless block, 0.57 x 0.47 x 0.32 mm, triclinic group $P\bar{1}$, a = 9.3866(9) Å, b = 17.0136(17) Å, c = 21.570(2) Å, α = 111.875(4)°, β = 98.356(4)°, γ = 91.005(4)°, V = 3153.1(5) Å^3, T = 100 K, Z = 4, $\rho_{calcd.}$ = 1.207 g·cm^{-3}, μ = 0.980, F(000) = 1232, 13280 reflections, in h(–11/11), k(-21/21), l(-27/27) measured in the range 2.20° < θ < 26.73°, completeness 98.6 %, 13280 independent reflections, 10702 observed reflections (I > 2σ(I)), 685 parameters, 0 restraints; all data: R_1 = 0.0568 and wR_2 = 0.1106, I > 2σ(I): R_1 = 0.0432 and wR_2 = 0.1030, Goof 0.843, largest difference peak/hole 1.24 /-0.59 e·Å^{-3}.

Crystal Data of (iPr$_2$Im^{Me})·GaCl$_2$(cAAC^{Me}H) **17:** $C_{31}H_{52}Cl_2GaN_3$, M_r = 607.37, colorless block, 0.210 x 0.13 x 0.12 mm, monoclinic group $P2_1/c$, a = 15.21640(10) Å, b = 10.86010(10) Å, c = 19.7874(2) Å, α = 90°, β = 92.3350(10)°, γ = 90°, V = 3267.19(5) Å^3, T = 100.01(10) K, Z = 4, $\rho_{calcd.}$ = 1.235 g·cm^{-3}, μ = 2.817, F(000) = 1296, 18634 reflections, in h(–16/18), k(-13/8), l(-23/24) measured in the range 2.9320° < θ < 77.0990°, completeness 100.0 %, 6210 independent reflections, 5730 observed reflections (I > 2σ(I)), 348 parameters, 0 restraints; all data: R_1 = 0.0330 and wR_2 = 0.0822, I > 2σ(I): R_1 = 0.0303 and wR_2 = 0.0803, Goof 1.040, largest difference peak/hole 0.72 /-0.35 e·Å^{-3}.

4 Computational Details

Calculations were carried out using the TURBOMOLE V7.2 2017 program suite, a development of the University of Karlsruhe and the Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.[6] Geometry optimizations were performed using (RI-)DFT calculations[7] on a m4 grid employing the M06-2x [8] functional and a def2-TZVP basis set for gallium and def2-SVP basis sets for C, H, N and Cl atoms. [9]

Cartesian Coordinates of the optimized Geometries

8_int
Energy = -3595.725485041 h

Ga	-0.1437875	-0.5455998	-0.2939767
H	-0.2323805	-0.2099264	-1.8856123
H	0.2520488	0.6863745	0.6399957
N	-2.8974109	-0.7898771	0.5696336
N	2.8261383	-0.7316397	-0.8680103
C	-1.7722110	-1.6718038	0.2553099
H	-2.0133218	-2.2873049	-0.6435648
C	-3.9804379	-1.6000394	1.1440432
C	-5.0365747	-0.7617617	1.8543178
H	-5.8446277	-1.4131807	2.2181337
H	-5.4779996	-0.0240779	1.1656113
H	-4.6189106	-0.2275022	2.7155276
C	-4.6954310	-2.4888808	0.1056278
H	-3.9799172	-3.0555555	-0.5073255
H	-5.3207559	-1.8863902	-0.5668336
H	-5.3474809	-3.2138231	0.6155687
C	-3.1631853	-2.4789294	2.1142044
H	-3.6503796	-3.4454196	2.3184817
H	-3.0727327	-1.9479828	3.0752395
C	-1.7555862	-2.6535680	1.4713341
C	-1.5490640	-4.0995558	1.0172690
H	-1.5049839	-4.7828741	1.8798948
H	-0.6126061	-4.2134297	0.4516664
H	-2.3708925	-4.4305357	0.3648743
C	-0.6745636	-2.2683136	2.4829466
H	-0.7503421	-2.8663949	3.4060330
H	-0.7689391	-1.2042056	2.7538201
H	0.3337172	-2.4182806	2.0613528
C	-2.9783620	0.5590646	0.1233054
C	-3.2246219	0.8643497	-1.2390480
C	-3.6506232	-0.2064781	-2.2292695
H	-3.4719022	-1.1804246	-1.7559959
C	-2.8693735	-0.1747723	-3.5448196
H	-3.1742396	-1.0175788	-4.1836608
H	-1.7888515	-0.2440078	-3.3608265
H	-3.0675399	0.7501096	-4.1085569
C	-5.1540875	-0.0725736	-2.5065017
H	-5.5166424	-0.9086792	-3.1244163
H	-5.3609342	0.8657528	-3.0449316
H	-5.7363747	-0.0492633	-1.5740655
C	-3.1485695	2.1906262	-1.6772658
H	-3.3308662	2.4187392	-2.7298642
C	-2.8518486	3.2220314	-0.7940960
H	-2.7870087	4.2515991	-1.1513489
C	-2.6475351	2.9319465	0.5500776
H	-2.4253382	3.7436370	1.2470961
C	-2.7077829	1.6194023	1.0296373
C	-2.4999105	1.3957492	2.5203071
H	-2.5756992	0.3131839	2.6929486
C	-3.5902444	2.1106665	3.3304458
H	-4.5986439	1.8738614	2.9647078
H	-3.4639608	3.2024269	3.2658553
H	-3.5286378	1.8314703	4.3936235
C	-1.1223794	1.8502481	3.0134180
H	-1.0180956	1.6372013	4.0887713

H	-0.9899049	2.9347288	2.8737838
H	-0.3145778	1.3431965	2.4713045
C	1.7370265	-1.4388052	-0.7404078
C	3.9582104	-1.3906155	-1.6353644
C	4.4833535	-0.4730381	-2.7323845
H	5.2664392	-1.0081413	-3.2889048
H	4.9248664	0.4422145	-2.3128798
H	3.6893858	-0.1981820	-3.4380107
C	5.1141071	-1.7388393	-0.6971214
H	4.8246079	-2.4431468	0.0926354
H	5.5140502	-0.8291386	-0.2272054
H	5.9190724	-2.1994187	-1.2867070
C	3.2336644	-2.6153660	-2.2144153
H	3.8752123	-3.5081817	-2.2120532
H	2.9488399	-2.4098134	-3.2571007
C	1.9601572	-2.8007328	-1.3663405
C	2.1909867	-3.7910685	-0.2101512
H	1.3373624	-3.7984685	0.4796963
H	3.0898077	-3.5432829	0.3708863
H	2.3177619	-4.8046471	-0.6188976
C	0.7592289	-3.2503502	-2.1990986
H	0.9650864	-4.2322858	-2.6512008
H	0.5401864	-2.5290521	-2.9983080
H	-0.1413650	-3.3388003	-1.5740273
C	3.0555202	0.5651075	-0.2564013
C	3.5229085	0.5970491	1.0745175
C	3.5473656	-0.6214316	1.9859775
H	3.3416253	-1.5150151	1.3826202
C	4.8887166	-0.8254243	2.6951891
H	4.8624543	-1.7508366	3.2890924
H	5.1004655	0.0008880	3.3896447
H	5.7282098	-0.8940309	1.9896395
C	2.4123940	-0.4982206	3.0115176
H	1.4505729	-0.3196993	2.5116535
H	2.5986149	0.3457794	3.6934476
H	2.3328320	-1.4149624	3.6149409
C	3.8645370	1.8370468	1.6219348
H	4.2259615	1.8825764	2.6508620
C	3.7262905	3.0103379	0.8903385
H	4.0016060	3.9687309	1.3332405
C	3.1953277	2.9607301	-0.3919690
H	3.0309127	3.8892624	-0.9419871
C	2.8334620	1.7485498	-0.9901203
C	2.1213128	1.8071493	-2.3350784
H	1.8860196	0.7792322	-2.6493753
C	2.9575187	2.4935354	-3.4226202
H	3.9436894	2.0326746	-3.5626011
H	3.1184409	3.5535493	-3.1753822
H	2.4223781	2.4607965	-4.3829601
C	0.7859669	2.5539092	-2.1839728
H	0.1944308	2.4596199	-3.1070408
H	0.9634225	3.6250669	-2.0001174
H	0.1846689	2.1584545	-1.3560070

8_meso

Energy = -3595.749113741 h

Ga	-0.1533141	0.4337504	0.6157398
H	-0.6694401	1.0418619	1.9995872
N	2.5041757	0.4469424	0.9706729
N	-2.3819835	0.0680027	-0.6159361
C	1.6458080	1.0806757	-0.0616361
H	1.8857613	0.6354895	-1.0378934
C	2.0188519	2.5915629	-0.0850088
C	3.2794520	2.6694455	0.8081084
H	3.3324720	3.6198090	1.3609998
H	4.1836839	2.6114778	0.1811329
C	3.2510803	1.4524732	1.7561631
C	4.6616531	0.9785854	2.0957958
H	5.1849412	1.7577352	2.6688327
H	5.2404404	0.7677543	1.1873243
H	4.6356114	0.0629677	2.7046629
C	2.5190817	1.7885574	3.0667617
H	2.9782883	2.6613204	3.5555273

H	2.5743854	0.9417919	3.7656944
H	1.4567245	2.0032315	2.8882061
C	2.9278743	-0.8974958	0.7616637
C	3.7706136	-1.2470234	-0.3265956
C	4.0490737	-2.5945907	-0.5713270
H	4.6861671	-2.8628214	-1.4174763
C	3.5365308	-3.5999845	0.2414950
H	3.7641980	-4.6465007	0.0321983
C	2.7432035	-3.2574932	1.3292087
H	2.3537919	-4.0439780	1.9793504
C	2.4272769	-1.9215668	1.6048714
C	4.4040550	-0.2138060	-1.2456906
H	4.1377059	0.7789273	-0.8593406
C	5.9344530	-0.3239843	-1.2461860
H	6.3770771	0.5110918	-1.8097550
H	6.2618809	-1.2581752	-1.7266692
H	6.3489162	-0.3135014	-0.2284518
C	3.8834045	-0.3243365	-2.6835423
H	4.3337746	0.4547896	-3.3175523
H	2.7909366	-0.2209732	-2.7364445
H	4.1460712	-1.3016971	-3.1172982
C	1.5736709	-1.6176258	2.8243109
H	1.2808727	-0.5597070	2.7651097
C	2.3893950	-1.7982297	4.1104573
H	1.8007965	-1.4983549	4.9906893
H	3.3114145	-1.1997792	4.0919298
H	2.6815588	-2.8524212	4.2371482
C	0.2957101	-2.4591680	2.8831874
H	-0.3557610	-2.1024275	3.6947471
H	0.5175905	-3.5196304	3.0770123
H	-0.2684449	-2.3996939	1.9412764
C	2.3297464	3.0315212	-1.5203484
H	3.1365798	2.4244545	-1.9578534
H	2.6380937	4.0881958	-1.5521345
C	0.9075373	3.5014795	0.4484057
H	0.6032548	3.2409329	1.4707909
H	0.0153384	3.4252439	-0.1935978
C	-1.3817287	-0.9516917	-0.1566835
H	-1.8383663	-1.5626308	0.6329668
C	-1.0067345	-1.8348608	-1.3842682
C	-2.0062419	-1.3785517	-2.4707115
H	-2.8867553	-2.0403494	-2.4832779
H	-1.5637533	-1.4175868	-3.4782325
C	-2.4639994	0.0500055	-2.1014443
C	-1.5261077	1.1201776	-2.6853498
H	-1.4209918	1.0054554	-3.7747958
H	-0.5231392	1.0665275	-2.2357156
H	-1.9260510	2.1245687	-2.4832231
C	-3.8788990	0.3070681	-2.6123255
H	-3.8825755	0.2611585	-3.7110460
H	-4.2461857	1.2955085	-2.3043733
H	-4.5798434	-0.4459899	-2.2294434
C	-3.5295020	0.3770543	0.1864024
C	-4.4650258	-0.6155514	0.5817962
C	-5.5624450	-0.2564708	1.3690216
H	-6.2714562	-1.0293920	1.6747986
C	-5.7857473	1.0621693	1.7441990
H	-6.6587921	1.3282504	2.3421215
C	-4.8852020	2.0378443	1.3410357
H	-5.0586883	3.0764200	1.6301447
C	-3.7518814	1.7213755	0.5826783
C	-4.3572224	-2.0721073	0.1628288
H	-3.5352404	-2.1450605	-0.5544997
C	-4.0399033	-2.9802913	1.3566796
H	-3.9099350	-4.0233598	1.0291056
H	-4.8644446	-2.9574920	2.0857559
H	-3.1257978	-2.6667571	1.8814999
C	-5.6203062	-2.5701367	-0.5497769
H	-5.4566014	-3.5849066	-0.9430845
H	-5.9007676	-1.9187084	-1.3897872
H	-6.4790005	-2.6164567	0.1363892
C	-2.8159341	2.8637791	0.2204546
H	-1.9181600	2.4183973	-0.2333440

C	-2.3855310	3.6613932	1.4554613
H	-1.6653566	4.4440692	1.1744102
H	-1.9166972	3.0081092	2.2044819
H	-3.2449730	4.1625952	1.9248417
C	-3.4429055	3.8048554	-0.8151329
H	-2.7282154	4.5911662	-1.1035663
H	-4.3366839	4.2967994	-0.4005430
H	-3.7510464	3.2723353	-1.7255951
C	0.4327699	-1.6330966	-1.8749280
H	1.1575940	-1.8489630	-1.0742916
H	0.6065562	-0.6087055	-2.2279495
C	-1.1446949	-3.3254530	-1.0472354
H	-0.9307779	-3.9451202	-1.9317592
H	-2.1502534	-3.5824820	-0.6851087
H	-0.4194693	-3.6022380	-0.2649420
H	0.6452918	-2.3122037	-2.7155567
H	1.2330169	4.5538020	0.4458278
H	1.4386705	2.9223231	-2.1592336

8_RR

Energy = -3595.748005021 h

Ga	0.2368423	0.2917697	0.4399269
N	2.7521817	-0.7522875	-0.7385356
N	-2.5533314	0.6939231	0.8806573
C	1.4066499	-0.3282610	-1.0998124
H	1.4132604	0.4916226	-1.8552232
C	0.8445275	-1.5907770	-1.8139707
C	2.1162302	-2.2577697	-2.4120205
H	2.0920927	-2.2581841	-3.5119211
H	2.1783695	-3.3084337	-2.0898788
C	3.3433220	-1.4701466	-1.8882463
C	4.4924579	-2.3866536	-1.4784963
H	4.9255733	-2.8563550	-2.3734928
H	4.1559331	-3.1869512	-0.8082339
H	5.2892079	-1.8165557	-0.9755343
C	3.8618529	-0.5331342	-2.9948960
H	4.2224270	-1.1293044	-3.8461861
H	4.6981561	0.0825780	-2.6319212
H	3.0679095	0.1291638	-3.3711685
C	3.5050991	-0.1117017	0.2889799
C	3.8360891	-0.8412218	1.4630648
C	4.5081072	-0.1959689	2.5054182
H	4.7571667	-0.7604671	3.4072522
C	4.8409348	1.1516150	2.4312973
H	5.3512074	1.6405963	3.2629146
C	4.5142001	1.8684190	1.2877863
H	4.7758203	2.9272209	1.2236683
C	3.8669465	1.2566842	0.2073529
C	3.4581188	-2.3008012	1.6614811
H	2.9447930	-2.6223353	0.7470077
C	2.4821531	-2.4782818	2.8296171
H	2.1656031	-3.5300756	2.9079740
H	2.9543676	-2.1993126	3.7846012
C	4.6931039	-3.1827790	1.8767341
H	4.4069561	-4.2452678	1.9027851
H	5.1775203	-2.9480268	2.8370268
H	5.4400511	-3.0449141	1.0836249
C	3.5685226	2.1094076	-1.0155721
H	3.1946912	1.4468349	-1.7989173
C	2.4686786	3.1297052	-0.7245675
H	2.2448220	3.7384258	-1.6140960
H	2.7523035	3.8082853	0.0952713
H	1.5382360	2.6208142	-0.4293522
C	4.8234152	2.7982196	-1.5604791
H	4.5975925	3.3071507	-2.5094395
H	5.6296762	2.0729993	-1.7413757
H	5.2072681	3.5558462	-0.8608594
C	0.2004500	-2.5298441	-0.7914040
H	-0.7321547	-2.0949174	-0.3882633
H	0.8928789	-2.7246178	0.0429385
C	-0.1852342	-1.2278401	-2.8786640
H	-0.5398411	-2.1276090	-3.4050815
H	0.2367623	-0.5361007	-3.6245130

C -1.4540009 1.3974393 0.1853622
H -1.6743338 1.4645369 -0.8932245
C -1.4625340 2.8447907 0.7498720
C -2.9062194 2.9820710 1.2760288
H -3.5556317 3.3033260 0.4450674
H -2.9919085 3.7404418 2.0696680
C -3.3614641 1.5887210 1.7445194
C -3.0702227 1.3774975 3.2428213
H -3.4942487 2.2040649 3.8327475
H -1.9940616 1.3183745 3.4459583
H -3.5280756 0.4457871 3.6007690
C -4.8660210 1.4027099 1.5410926
H -5.4154683 2.0696396 2.2216142
H -5.1683922 0.3678110 1.7621284
H -5.1685690 1.6382439 0.5131612
C -3.0606697 -0.4824087 0.2590999
C -3.6060540 -0.4394038 -1.0544142
C -3.9373337 -1.6370636 -1.6955127
H -4.3340957 -1.6044771 -2.7133650
C -3.8072959 -2.8641813 -1.0532729
H -4.0805169 -3.7867762 -1.5680498
C -3.3515630 -2.8998397 0.2582908
H -3.2743573 -3.8592025 0.7746950
C -2.9620579 -1.7317702 0.9245575
C -3.9445847 0.8616868 -1.7761906
H -3.7093557 1.6923503 -1.0968897
C -3.1520531 1.0674408 -3.0721459
H -3.4800292 1.9899423 -3.5744239
H -3.3155688 0.2305356 -3.7687722
H -2.0711012 1.1457624 -2.8943621
C -5.4478443 0.9229137 -2.0848755
H -5.7238874 1.9236239 -2.4503829
H -6.0551338 0.6946113 -1.1979425
H -5.7183758 0.1975478 -2.8666705
C -2.4708334 -1.8469809 2.3577291
H -2.0581082 -0.8684832 2.6331780
C -1.3584830 -2.8836272 2.5336320
H -1.0013573 -2.8799573 3.5745608
H -0.4982289 -2.6682596 1.8861878
H -1.7095014 -3.9023942 2.3078052
C -3.6431306 -2.1714053 3.2922284
H -3.3234702 -2.1393436 4.3450441
H -4.0327978 -3.1807345 3.0860857
H -4.4761596 -1.4657542 3.1615934
C -0.4346356 3.0710300 1.8681718
H 0.5923290 3.0473777 1.4687832
H -0.4951998 2.3090411 2.6543795
C -1.2091163 3.8661642 -0.3618765
H -1.2669740 4.8925213 0.0329412
H -1.9562320 3.7650424 -1.1640543
H 0.5218379 -0.1664505 1.9401073
H 1.5881941 -1.8540736 2.7010100
H -0.0771685 -3.4960083 -1.2413617
H -1.0669156 -0.7523551 -2.4198884
H -0.5786907 4.0579698 2.3345118
H -0.2132963 3.7360497 -0.8092859

8_SS

Energy = -3595.749066925 h

Ga -0.1691979 -0.3672834 -0.4983282
N -2.8728663 -0.1166512 0.5699527
N 2.7476307 -0.1873870 -0.5933424
C -2.8950177 1.1975701 0.0136828
C 2.8743238 0.9500340 0.2645995
C -3.3584020 1.4444992 -1.3012910
C 3.2074911 0.7971063 1.6394133
C 2.6788678 2.2659563 -0.2445721
C -1.9618341 -1.1503942 0.0682067
H -2.3396469 -1.6075804 -0.8815883
C -3.3260751 2.7486326 -1.8087061
H -3.6783057 2.9345496 -2.8258839
C -3.8305296 0.3376183 -2.2330515
H -3.8703127 -0.5911297 -1.6558015

C	-2.3636471	2.2730315	0.7743502
C	-4.0498805	-0.7048028	1.2631258
C	1.6809888	-1.1843948	-0.4414660
H	1.8197528	-1.8400716	0.4457033
C	2.8614499	3.3647283	0.6059942
H	2.7189645	4.3705324	0.2051587
C	-2.3663215	3.5627640	0.2340902
H	-1.9657301	4.3932909	0.8160462
C	1.8850194	-2.0757155	-1.6960202
C	3.3484866	1.9251601	2.4537169
H	3.5968144	1.7925094	3.5091446
C	-2.8488444	3.8063534	-1.0475804
H	-2.8355304	4.8182841	-1.4563045
C	-2.1051212	-2.2510590	1.1403875
C	3.1925165	3.2079174	1.9443770
H	3.3215440	4.0795590	2.5883904
C	3.4044281	-0.5595674	2.3022622
H	3.3794303	-1.3238341	1.5190208
C	-5.2305392	0.6033407	-2.7943517
H	-5.5749474	-0.2578138	-3.3864783
H	-5.2336980	1.4811104	-3.4578144
H	-5.9600456	0.7848504	-1.9931407
C	2.2084828	2.5812598	-1.6593982
H	2.0329408	1.6218064	-2.1646401
C	3.9386532	-0.7482507	-1.2916083
C	3.4201285	-2.1189910	-1.7727404
H	3.7856435	-2.3696669	-2.7809805
H	3.7772443	-2.9049808	-1.0880370
C	-3.6240090	-2.1847149	1.4053041
H	-3.8993795	-2.6012202	2.3871655
H	-4.1358755	-2.7867757	0.6376046
C	-1.6959517	2.0375612	2.1228592
H	-2.2271485	1.2182542	2.6152119
C	-5.3662822	-0.5885859	0.4806723
H	-5.6031660	0.4667203	0.2746514
H	-6.1892492	-1.0109022	1.0765285
H	-5.3359188	-1.1341547	-0.4711258
C	-1.3054629	-1.9262675	2.4031587
H	-1.4788209	-0.8935974	2.7367653
H	-0.2292199	-2.0522247	2.2086749
C	-1.6942497	-3.6323754	0.6421210
H	-1.9661290	-4.4042292	1.3788094
H	-0.6059149	-3.6879342	0.4922908
C	-4.2885762	-0.0498080	2.6316532
H	-3.4550853	-0.2316456	3.3225110
H	-5.2000534	-0.4612011	3.0896692
H	-4.4277414	1.0369728	2.5214097
C	-2.8323848	0.1223873	-3.3764120
H	-3.1510083	-0.7155750	-4.0147809
H	-1.8237049	-0.0900730	-2.9944291
H	-2.7573736	1.0216495	-4.0069639
C	0.8879364	3.3673074	-1.6363190
H	0.4656107	3.4328372	-2.6509046
H	1.0513999	4.3961393	-1.2785583
H	0.1313929	2.8987043	-0.9955004
C	3.2307930	3.4018377	-2.4578791
H	2.8693682	3.5546864	-3.4858628
H	4.2188121	2.9304889	-2.5105892
H	3.3627292	4.3969934	-2.0055869
C	-0.2441527	1.5802055	1.9390094
H	0.2896375	1.5449309	2.9009280
H	0.3209017	2.2383272	1.2614255
H	-0.2087376	0.5408402	1.5624659
C	1.3061613	-3.4781168	-1.5391453
H	1.6084669	-4.1114895	-2.3873487
H	0.2056277	-3.4590020	-1.5195486
C	1.2843537	-1.4339031	-2.9541757
H	1.5529998	-0.3724676	-3.0357708
H	0.1811017	-1.5001242	-2.9425283
C	-1.7442295	3.2499330	3.0543205
H	-2.7638123	3.6538726	3.1361388
H	-1.0813641	4.0582199	2.7102016
H	-1.4062932	2.9613942	4.0600473

C	5.1726052	-0.9269589	-0.3956665
H	6.0185239	-1.2836070	-1.0022593
H	5.0051698	-1.6624376	0.4012184
H	5.4644864	0.0304298	0.0628433
C	2.2606685	-0.8557457	3.2765778
H	2.3535017	-1.8695527	3.6953484
H	1.2855706	-0.7750557	2.7790545
H	2.2655556	-0.1412595	4.1151136
C	4.3694772	0.1455552	-2.4580474
H	5.2024304	-0.3205861	-3.0050628
H	4.7230647	1.1098484	-2.0703423
H	3.5501605	0.3317921	-3.1645816
C	4.7521837	-0.6712750	3.0231216
H	4.9057051	-1.6997860	3.3832262
H	4.7937648	-0.0080430	3.8998511
H	5.5898804	-0.4079592	2.3634354
H	-0.2747695	0.9108600	-1.4235017
H	1.6591447	-3.9574369	-0.6129057
H	1.6227727	-1.9545034	-3.8627067
H	-1.5753887	-2.6046704	3.2274819
H	-2.1892142	-3.8820737	-0.3096641

18_int

Energy = -4055.264148296 h

Ga	-0.0859350	0.0400452	-0.0633630
H	-0.3086514	1.1550850	-1.1938498
N	-2.8013167	-0.6014494	0.5967248
N	2.9706366	-0.4462546	-0.6401259
C	-1.5827836	-1.3252460	0.1492036
H	-1.7563763	-1.7790034	-0.8461048
C	-3.4015941	-1.1631987	1.8232874
C	-3.7836715	-0.0810776	2.8357957
H	-4.1316024	-0.5525524	3.7674200
H	-4.6050730	0.5353424	2.4450416
H	-2.9270292	0.5638283	3.0716565
C	-4.6778993	-1.9898145	1.5765419
H	-4.5107230	-2.8892813	0.9730482
H	-5.4264458	-1.3671324	1.0629925
H	-5.1079148	-2.3083814	2.5378921
C	-2.2385967	-1.9988490	2.3735630
H	-2.5869664	-2.8310954	3.0059426
H	-1.6083947	-1.3408259	2.9933732
C	-1.3981025	-2.4823568	1.1796950
C	-1.9001603	-3.8280536	0.6309359
H	-1.8396316	-4.6068351	1.4077516
H	-1.2779753	-4.1563542	-0.2170159
H	-2.9372516	-3.7907959	0.2780591
C	0.0466354	-2.6931581	1.6386401
H	0.0844078	-3.4362962	2.4516264
H	0.4732742	-1.7561048	2.0167854
H	0.6830840	-3.0660885	0.8226220
C	-3.5551161	0.2038799	-0.3092333
C	-4.2522627	-0.3810064	-1.4033968
C	-4.2256632	-1.8736750	-1.6942467
H	-3.6992970	-2.3571587	-0.8668756
C	-3.4525305	-2.1732623	-2.9837308
H	-3.3573336	-3.2592704	-3.1385023
H	-2.4442344	-1.7368668	-2.9571896
H	-3.9719480	-1.7510835	-3.8581225
C	-5.6285466	-2.4845733	-1.7701258
H	-5.5625167	-3.5788866	-1.8714933
H	-6.1844868	-2.1061522	-2.6410630
H	-6.2163588	-2.2572569	-0.8706381
C	-4.9916739	0.4259783	-2.2728197
H	-5.5176168	-0.0368364	-3.1115718
C	-5.0816147	1.7990759	-2.0822493
H	-5.6752824	2.4145636	-2.7605897
C	-4.3973012	2.3777540	-1.0225565
H	-4.4477790	3.4594891	-0.8784997
C	-3.6191183	1.6158976	-0.1421241
C	-2.8375890	2.3786198	0.9183846
H	-2.2521884	1.6470983	1.4878546
C	-3.7448454	3.1585500	1.8793257

H -4.5132335 2.5318752 2.3472470
H -4.2595254 3.9752905 1.3490425
H -3.1416482 3.6144037 2.6791505
C -1.8496807 3.3665737 0.2833457
H -1.1893813 3.7825037 1.0595455
H -2.3815202 4.2029860 -0.1977325
H -1.2237405 2.8795301 -0.4738696
C 1.7234855 -0.7212565 -0.8850002
C 3.9774554 -1.0438060 -1.6143653
C 4.9787538 -0.0046108 -2.1019506
H 5.6572708 -0.4925258 -2.8163359
H 5.5805578 0.4034481 -1.2776483
H 4.4759053 0.8187609 -2.6226970
C 4.7310135 -2.1831506 -0.9379349
H 4.0547635 -2.9476952 -0.5314313
H 5.3556671 -1.7908494 -0.1267767
H 5.3921445 -2.6586299 -1.6758384
C 3.0534039 -1.5176917 -2.7407881
H 3.3705605 -2.4915172 -3.1395697
H 3.0841987 -0.7942025 -3.5689885
C 1.6302427 -1.5642660 -2.1496904
C 1.1985473 -2.9917911 -1.7838842
H 0.1954200 -2.9912435 -1.3350373
H 1.8944148 -3.4669322 -1.0767992
H 1.1660568 -3.6021988 -2.6981360
C 0.6065456 -0.9729479 -3.1268100
H 0.6193412 -1.5569594 -4.0592120
H 0.8353862 0.0756705 -3.3622431
H -0.4104376 -1.0054990 -2.7119731
C 3.4687030 0.4185887 0.4182820
C 3.8923632 -0.1242086 1.6495001
C 3.5987356 -1.5416612 2.1275295
H 3.0498056 -2.0714532 1.3332917
C 4.8524932 -2.3440235 2.4987239
H 4.5606490 -3.3429123 2.8550283
H 5.3925962 -1.8500324 3.3202276
H 5.5579907 -2.4737263 1.6699547
C 2.6919659 -1.4762075 3.3686891
H 1.8535664 -0.7845387 3.2208043
H 3.2682269 -1.1285379 4.2396485
H 2.2990845 -2.4756140 3.6057243
C 4.5158824 0.7388399 2.5579785
H 4.8526197 0.3406765 3.5168102
C 4.6812286 2.0893568 2.2848454
H 5.1669434 2.7410381 3.0123165
C 4.1865192 2.6134038 1.0976588
H 4.2679696 3.6845332 0.9060498
C 3.5703994 1.8001904 0.1430071
C 2.9756829 2.4807753 -1.0829240
H 2.5901053 1.7084563 -1.7660938
C 3.9971035 3.3394654 -1.8404641
H 4.9141853 2.7908419 -2.0938821
H 4.2911232 4.2136288 -1.2411237
H 3.5506150 3.7207534 -2.7705328
C 1.7877205 3.3572925 -0.6601285
H 1.2494271 3.7260788 -1.5459219
H 2.1440098 4.2290196 -0.0894568
H 1.0831548 2.8069717 -0.0250695
Cl 0.4070232 1.0088617 1.9194323

18_meso

Energy = -4055.286628221 h

Ga -0.1109423 0.3903980 0.6305536
N 2.6287051 0.4294818 1.0640552
N -2.4791549 0.0626250 -0.7104112
C 1.7179752 1.1075985 0.1316571
H 1.9225225 0.7458197 -0.8892692
C 2.0472440 2.6256826 0.2053285
C 3.3651756 2.6604312 1.0145053
H 3.4462645 3.5731313 1.6242752
H 4.2234414 2.6551312 0.3231755
C 3.4129675 1.3812272 1.8768747
C 4.8455536 0.8984899 2.0867014

H	5.3974520	1.6334099	2.6903974
H	5.3708861	0.7698506	1.1318005
H	4.8608172	-0.0636706	2.6201546
C	2.7726088	1.6093373	3.2566010
H	3.2559281	2.4538184	3.7710637
H	2.8962150	0.7166249	3.8871214
H	1.6958975	1.8089151	3.1784990
C	2.9989582	-0.9113810	0.7632236
C	3.7815426	-1.2148633	-0.3823743
C	3.9973702	-2.5522022	-0.7255879
H	4.5888147	-2.7873382	-1.6138086
C	3.4747741	-3.5898276	0.0404022
H	3.6505913	-4.6275136	-0.2480523
C	2.7366888	-3.2934635	1.1796518
H	2.3388628	-4.1067591	1.7908655
C	2.4870284	-1.9676667	1.5561769
C	4.4057501	-0.1416605	-1.2616246
H	4.1808266	0.8320694	-0.8050540
C	5.9310569	-0.2904315	-1.3301819
H	6.3748950	0.5611232	-1.8674545
H	6.2123432	-1.2068474	-1.8703441
H	6.3840651	-0.3447255	-0.3306210
C	3.8261867	-0.1491569	-2.6810712
H	4.2605009	0.6668156	-3.2786237
H	2.7338063	-0.0305142	-2.6823623
H	4.0577820	-1.0973497	-3.1905286
C	1.6876200	-1.7039448	2.8201385
H	1.4712214	-0.6278849	2.8549471
C	2.5155388	-2.0500074	4.0628451
H	1.9696171	-1.7803030	4.9793092
H	3.4779327	-1.5178020	4.0648579
H	2.7330632	-3.1290733	4.0991998
C	0.3491357	-2.4463324	2.8420645
H	-0.2551735	-2.1097716	3.6964572
H	0.4879635	-3.5353654	2.9262964
H	-0.2348014	-2.2556447	1.9285210
C	2.2492518	3.1764471	-1.2103106
H	3.0385348	2.6253476	-1.7446172
H	2.5307063	4.2401968	-1.1817763
C	0.9557394	3.4589126	0.8821525
H	0.7398447	3.1273662	1.9051383
H	0.0182085	3.3879182	0.3091934
C	-1.4524156	-0.8644722	-0.1734342
H	-1.8893034	-1.4401925	0.6548447
C	-1.0211233	-1.8157479	-1.3329895
C	-2.0264061	-1.4775823	-2.4544112
H	-2.8791530	-2.1739682	-2.4195848
H	-1.5753792	-1.5717131	-3.4542719
C	-2.5441368	-0.0477393	-2.1854879
C	-1.6373830	1.0132788	-2.8345471
H	-1.4892225	0.8130068	-3.9065317
H	-0.6487455	1.0423891	-2.3509764
H	-2.0822381	2.0122731	-2.7297185
C	-3.9644765	0.1134196	-2.7201617
H	-3.9595304	-0.0043755	-3.8136095
H	-4.3794951	1.1013192	-2.4788147
H	-4.6326285	-0.6444228	-2.2900757
C	-3.6078741	0.4320487	0.0855003
C	-4.5248319	-0.5378863	0.5682786
C	-5.6068640	-0.1341169	1.3545292
H	-6.3032425	-0.8877843	1.7297415
C	-5.8264707	1.2058969	1.6474283
H	-6.6851202	1.5071640	2.2495049
C	-4.9403170	2.1580271	1.1628422
H	-5.1136218	3.2110618	1.3917710
C	-3.8224425	1.7978185	0.4014634
C	-4.3991264	-2.0193703	0.2545752
H	-3.5909814	-2.1321365	-0.4755557
C	-4.0378071	-2.8272070	1.5073165
H	-3.8730487	-3.8864564	1.2558438
H	-4.8563968	-2.7797808	2.2417362
H	-3.1329788	-2.4413215	1.9996468
C	-5.6684682	-2.5896462	-0.3888008

H	-5.5005690	-3.6315808	-0.7012000
H	-5.9733573	-2.0112120	-1.2727057
H	-6.5126066	-2.5885366	0.3167070
C	-2.9011382	2.9132597	-0.0691791
H	-1.9841859	2.4374899	-0.4576385
C	-2.5131852	3.8694296	1.0637806
H	-1.8108731	4.6310292	0.6931186
H	-2.0425983	3.3319324	1.8981668
H	-3.3927187	4.4065615	1.4477670
C	-3.5403069	3.7137531	-1.2122667
H	-2.8353822	4.4617561	-1.6067798
H	-4.4313124	4.2481366	-0.8473057
H	-3.8609601	3.0718256	-2.0435198
C	0.4176304	-1.5846119	-1.8141231
H	1.1407400	-1.7737712	-1.0044987
H	0.5716567	-0.5613525	-2.1827390
C	-1.1089823	-3.2840459	-0.8982043
H	-0.8718398	-3.9515553	-1.7410719
H	-2.1095250	-3.5457836	-0.5248947
H	-0.3799489	-3.4893041	-0.0979313
H	0.6597291	-2.2719600	-2.6394990
H	1.2472370	4.5202104	0.9155809
H	1.3184929	3.0909488	-1.7947365
Cl	-0.8890711	0.9644296	2.6289903

18_RR

Energy = -4055.283381146 h

Ga	0.2475272	0.4191452	0.4299478
N	2.7790306	-0.7562875	-0.7124804
N	-2.5873227	0.7275179	0.8539064
C	1.4344013	-0.3155650	-1.0276620
H	1.4297951	0.5158678	-1.7744676
C	0.8343272	-1.5580938	-1.7458972
C	2.0846520	-2.2085450	-2.4058296
H	2.0165130	-2.1921736	-3.5037314
H	2.1645976	-3.2628546	-2.1007677
C	3.3266005	-1.4222891	-1.9151822
C	4.5139143	-2.3290685	-1.6057729
H	4.9218072	-2.7299909	-2.5448294
H	4.2323834	-3.1792272	-0.9737582
H	5.3144322	-1.7645612	-1.1028115
C	3.7753874	-0.4337920	-3.0088940
H	4.0872331	-0.9913634	-3.9041504
H	4.6306576	0.1683825	-2.6688935
H	2.9624838	0.2426716	-3.3119210
C	3.5418445	-0.1810708	0.3459167
C	3.8899432	-0.9806796	1.4664697
C	4.5176264	-0.3807828	2.5616172
H	4.7753413	-0.9944966	3.4280112
C	4.7918195	0.9817536	2.5866538
H	5.2603620	1.4334468	3.4626693
C	4.4668468	1.7606635	1.4839962
H	4.6948549	2.8293336	1.4931811
C	3.8657487	1.1973853	0.3526289
C	3.5987101	-2.4717313	1.5437363
H	3.0908874	-2.7466896	0.6112314
C	2.6596046	-2.8317802	2.6993512
H	2.4641893	-3.9152325	2.7018713
H	3.1070189	-2.5707565	3.6712042
C	4.8961918	-3.2808332	1.6632832
H	4.6848705	-4.3590717	1.5974292
H	5.3783309	-3.0965960	2.6357291
H	5.6194607	-3.0205979	0.8787023
C	3.6039311	2.1022339	-0.8416756
H	3.2220168	1.4791831	-1.6536852
C	2.5419000	3.1590708	-0.5420910
H	2.3900969	3.8251244	-1.4051116
H	2.8168715	3.7773720	0.3261605
H	1.5707961	2.6896527	-0.3185839
C	4.8959413	2.7566233	-1.3424005
H	4.7093558	3.3133872	-2.2731540
H	5.6710006	2.0022594	-1.5397057
H	5.3013984	3.4645215	-0.6038143

C	0.2309248	-2.5144615	-0.7154041
H	-0.6950498	-2.0935747	-0.2848871
H	0.9483896	-2.7054506	0.0984413
C	-0.2341558	-1.1669006	-2.7604818
H	-0.6144432	-2.0531651	-3.2914670
H	0.1605188	-0.4606922	-3.5081595
C	-1.4948114	1.4219277	0.1574042
H	-1.6791353	1.4025067	-0.9312141
C	-1.5634494	2.9105159	0.6097545
C	-3.0117204	3.0217597	1.1289195
H	-3.6814340	3.2610382	0.2865635
H	-3.1250325	3.8243111	1.8735791
C	-3.4001746	1.6410384	1.6915296
C	-3.0480852	1.5112177	3.1862398
H	-3.4237422	2.3790719	3.7492462
H	-1.9653151	1.4239606	3.3409824
H	-3.5118252	0.6114086	3.6131638
C	-4.9004570	1.3923995	1.5382096
H	-5.4546546	2.0796018	2.1942353
H	-5.1619454	0.3630647	1.8249063
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Cl	0.6888045	0.1070990	2.5584381

18_SS

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H	4.5300656	3.0295572	-1.6592615
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H	-2.8318179	-3.6022385	-1.0722885
Cl	-0.2314019	0.9597229	-2.5074296

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