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Reactivity of halfsandwich rare-earth metal methylaluminates toward potassium (2,4,6-tri-*tert*-butylphenyl)amide and 1-adamantylamine

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Table S1. Crystallographic Parameters for complexes **2a**, **3**, **4**, **5**, **7** and **8**.

	2a	**3**	**4**	**5**	**7**	**8**
formula	$C_{76}H_{140}Al_2N_2Y_2$	$C_{35}H_{61}AlNOY$	$C_{26}H_{42}Al_2LuN$	$C_{39}H_{56}AlLuN_2$	$C_{32}H_{46}AlN_2Y$	$C_{13}H_{26}AlN$
M_r [g mol^{-1}]	1313.69	627.74	597.53	754.80	574.60	223.33
T [K]	100(2)	123(2)	173.(2)	153.(2)	100(2)	100(2)
λ [Å]	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
cryst system	monoclinic	monoclinic	triclinic	triclinic	triclinic	monoclinic
space group	C2/c	$P2_1/n$	P−1	P−1	P−1	$P2_1/c$
a [Å]	49.639(1)	19.151(1)	9.1367(3)	12.1090(3)	9.4592(4)	6.8749(3)
b [Å]	12.3116(3)	8.9975(5)	12.1049(4)	13.6700(3)	12.2445(5)	19.6763(8)
c [Å]	35.971(2)	24.183(1)	13.2803(4)	13.7168(3)	14.0256(6)	12.1047(5)
α [°]	90	90	77.756(1)	105.191(1)	68.379(2)	90
β [°]	131.598(1)	108.305(1)	81.137(1)	113.695(1)	80.349(1)	124.608(2)
γ [°]	90	90	88.071(1)	106.489(1)	82.208(2)	90
V [Å^3]	16439.4	3956.0(4)	1418.24(8)	1801.47(7)	1484.0(1)	1347.7(1)
Z	8	4	2	2	2	4
F(000)	5728	1352	604	776	608	496
ρ_{calcd} [g cm^{-3}]	1.063	1.054	1.399	1.392	1.286	1.101
μ [mm^{-1}]	1.463	1.519	3.554	2.792	2.017	0.123
R_1 (obsd)[a]	0.0687	0.0413	0.0143	0.0179	0.0346	0.0383
wR_2 (all)[b]	0.1579	0.0950	0.0372	0.0420	0.0933	0.1049
S[c]	1.165	1.031	1.106	1.034	1.035	1.113

[a] $R1 = \Sigma(||F_0|-|F_c||)/\Sigma|F_0|$, $F_0 > 4\sigma(F_0)$. [b] $wR2 = \{\Sigma[w(F_0^2-F_c^2)^2/\Sigma[w(F_0^2)^2]\}^{1/2}$. [c] $S = [\Sigma w(F_0^2-F_c^2)^2/(n_0-n_p)]^{1/2}$.

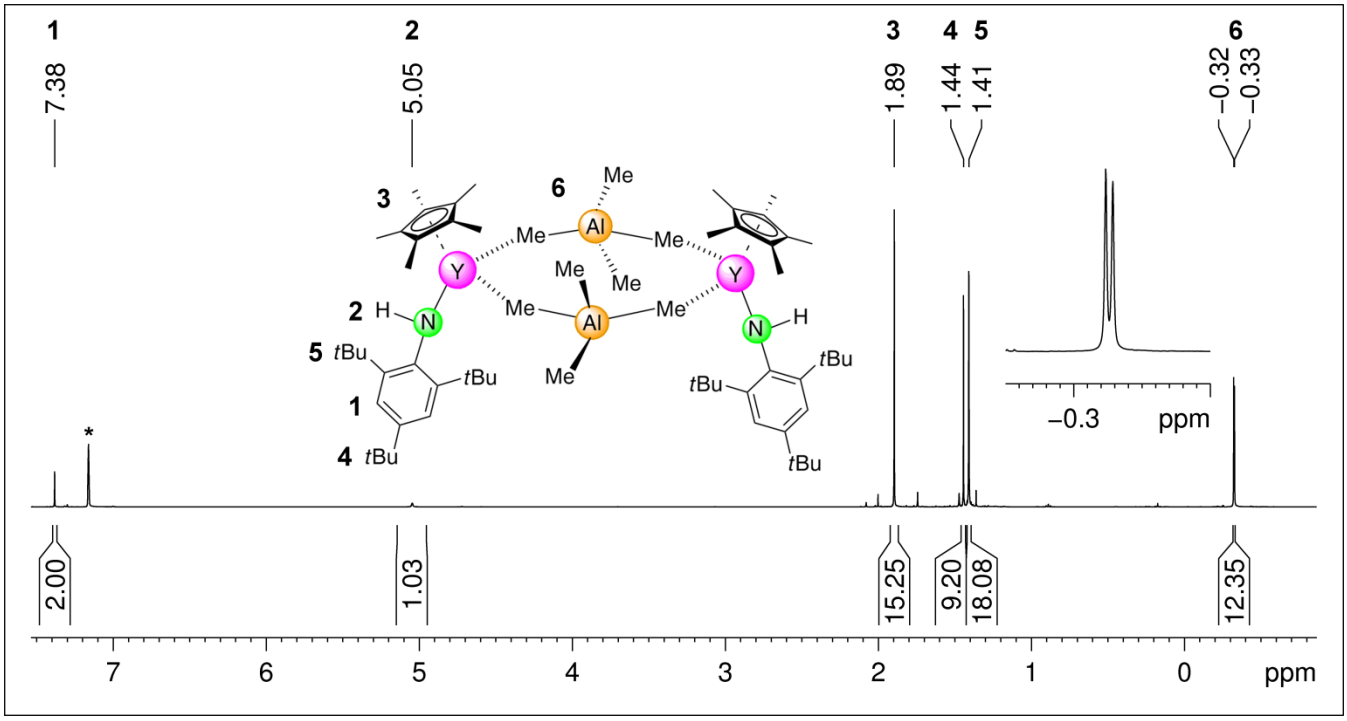

Figure S1. ^{1}H NMR spectrum (500 MHz) of {Cp*Y[NH(mes*)](AlMe$_4$)}$_2$ (**2a**) in C_6D_6 at 26 °C.

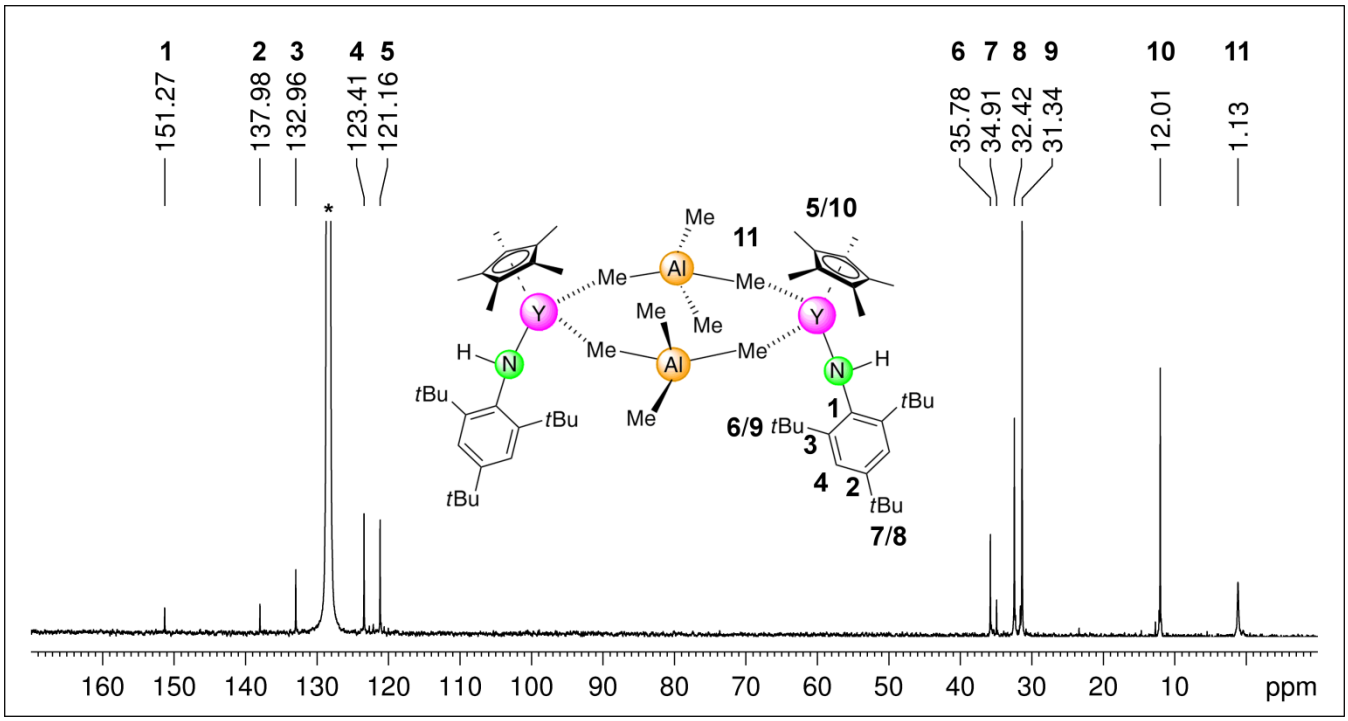

Figure S2. ^{13}C{^{1}H} NMR spectrum (126 MHz) of {Cp*Y[NH(mes*)](AlMe$_4$)}$_2$ (**2a**) in C_6D_6 at 26 °C.

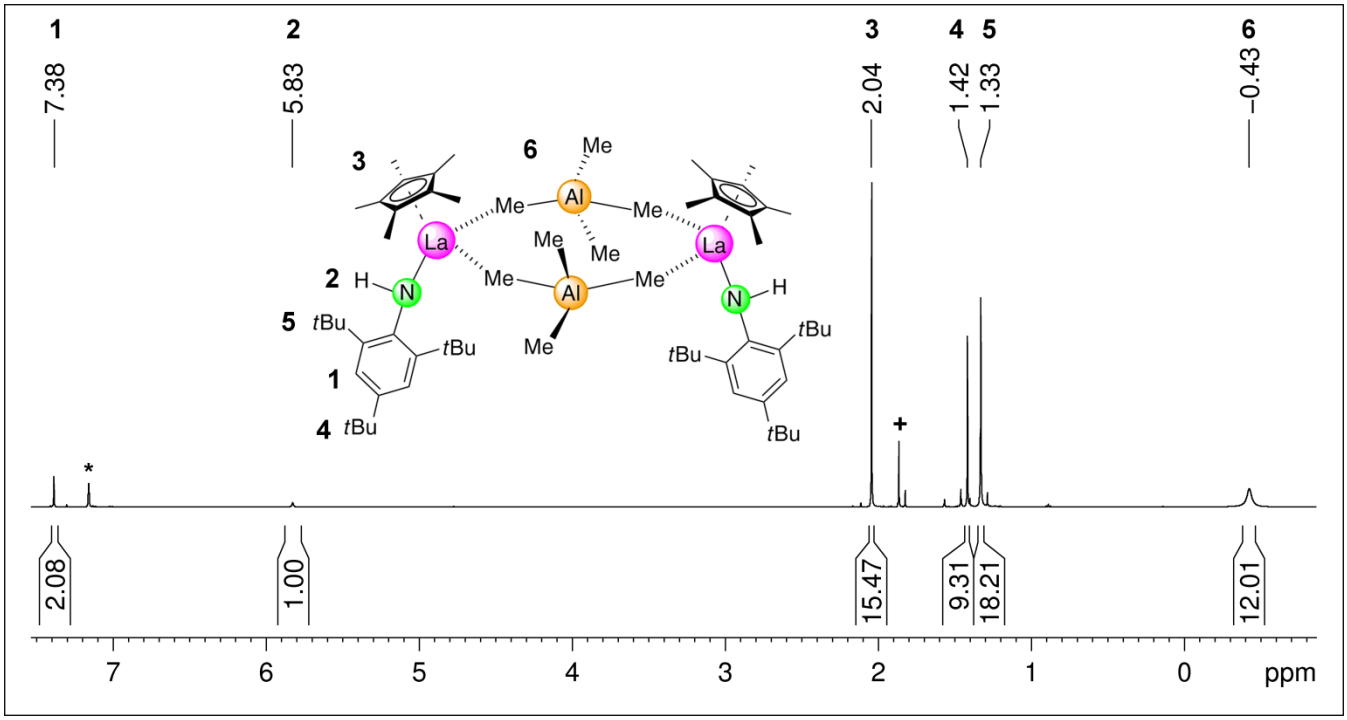

Figure S3. ^{1}H NMR spectrum (500 MHz) of $\{Cp^*La[NH(mes^*)](AlMe_4)\}_x$ (**2b**) in C_6D_6 at 26 °C (+ impurity).

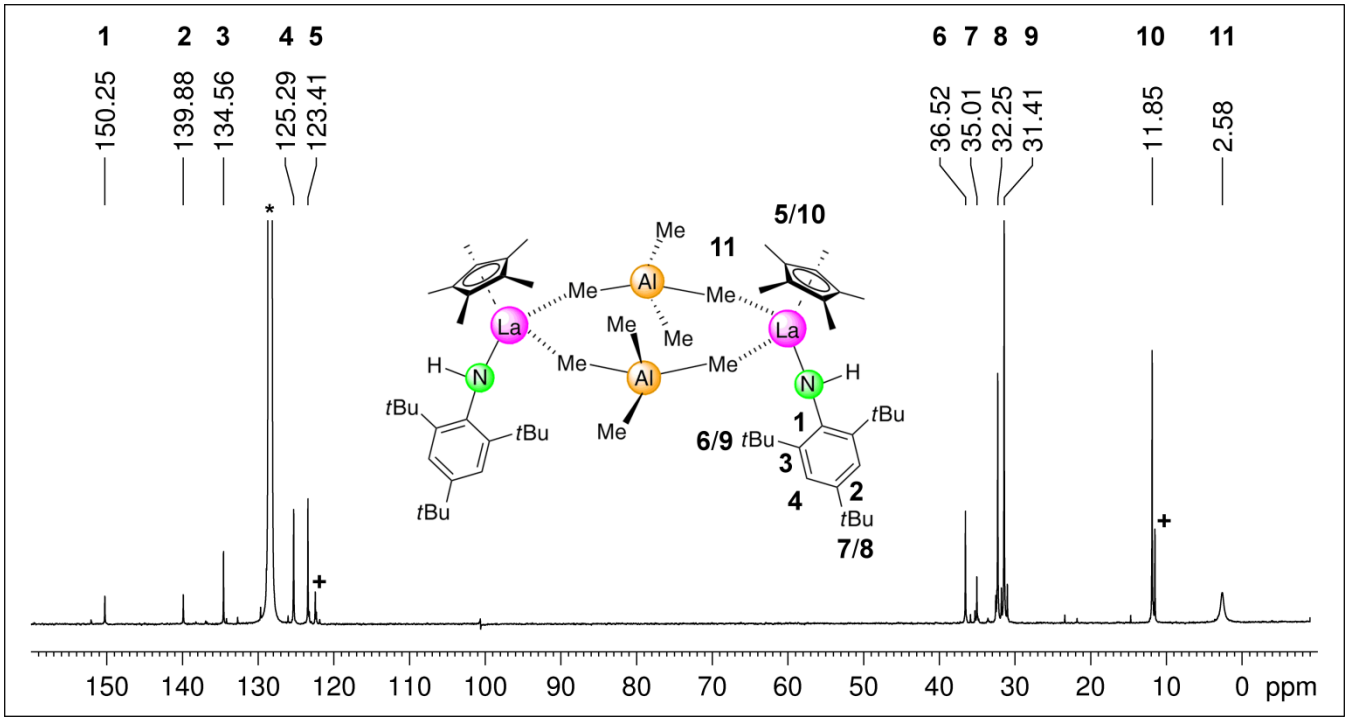

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz) of $\{Cp^*La[NH(mes^*)](AlMe_4)\}_x$ (**2b**) in C_6D_6 at 26 °C (+ impurity).

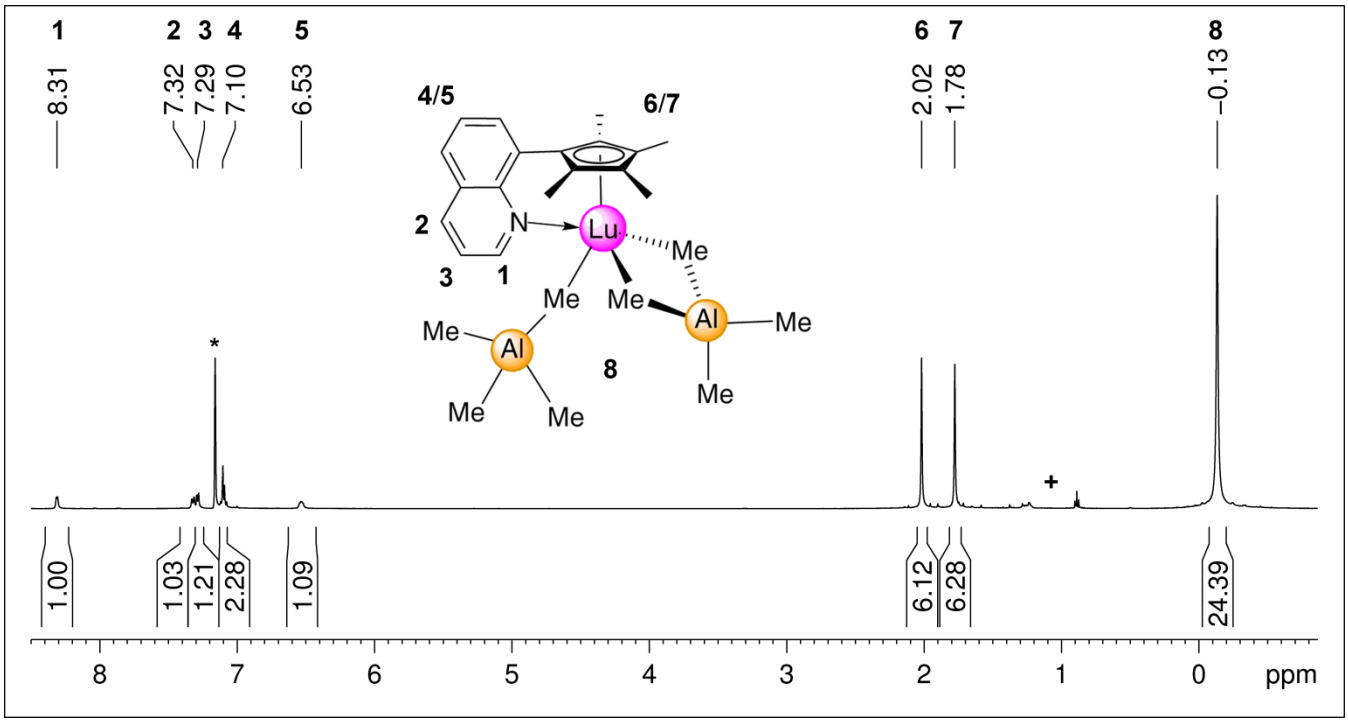

Figure S5. ^{1}H NMR spectrum (500 MHz) of $Cp^{Q}Lu(AlMe_4)_2$ (**4**) in C_6D_6 at 26 °C (+ *n*-hexane).

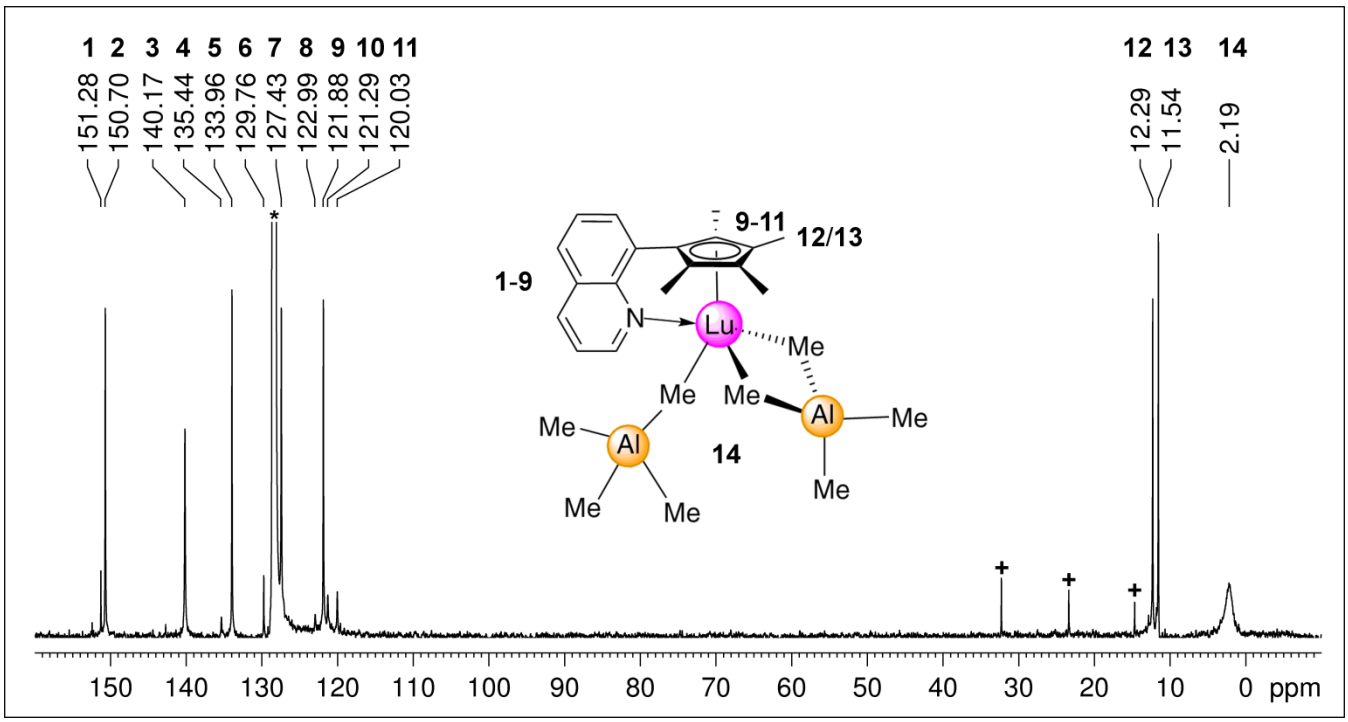

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz) of $Cp^{Q}Lu(AlMe_4)_2$ (**4**) in C_6D_6 at 26 °C (+ *n*-hexane).

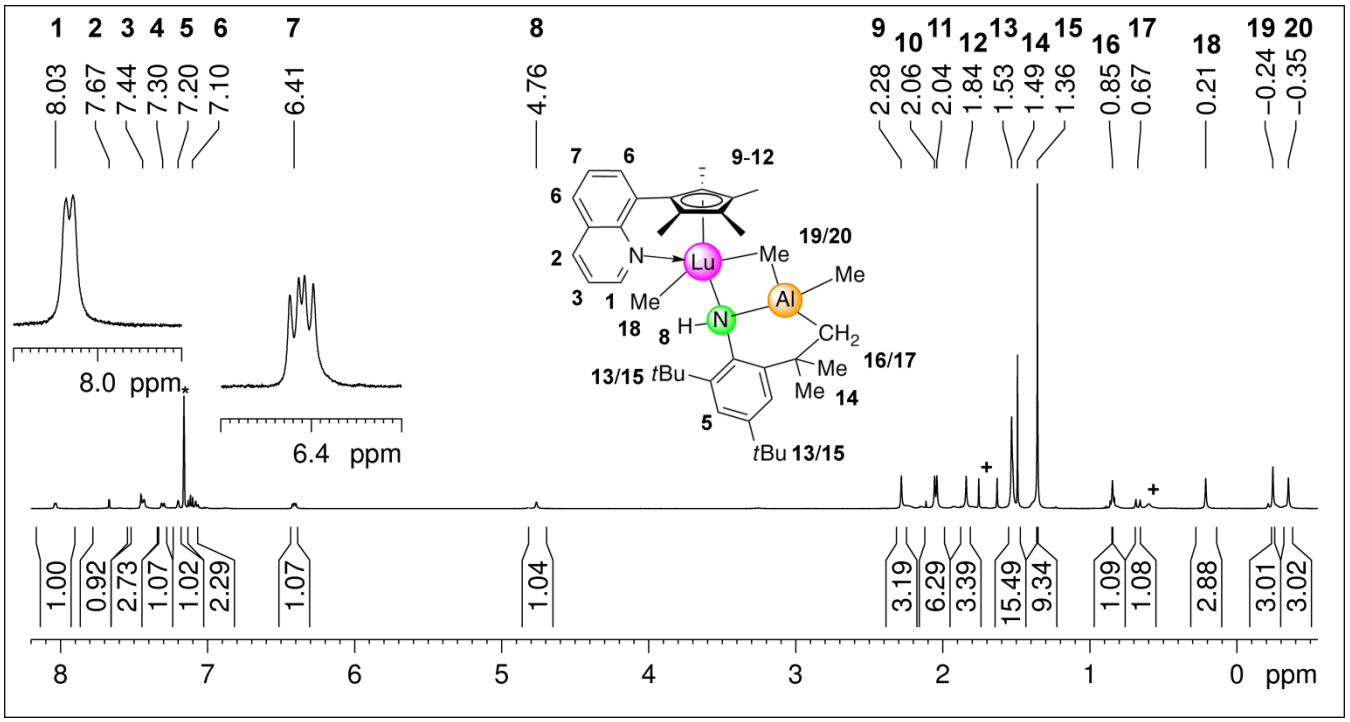

Figure S7. ^{1}H NMR spectrum (500 MHz) of $Cp^{Q}LuMe\{NH[C_6H_2tBu_2\text{-}2,4\text{-}(CMe_2CH_2)\text{-}6]\}(AlMe_2)$ (**5**) in C_6D_6 at 26 °C (+ contaminated by a small amount of decomposition material).

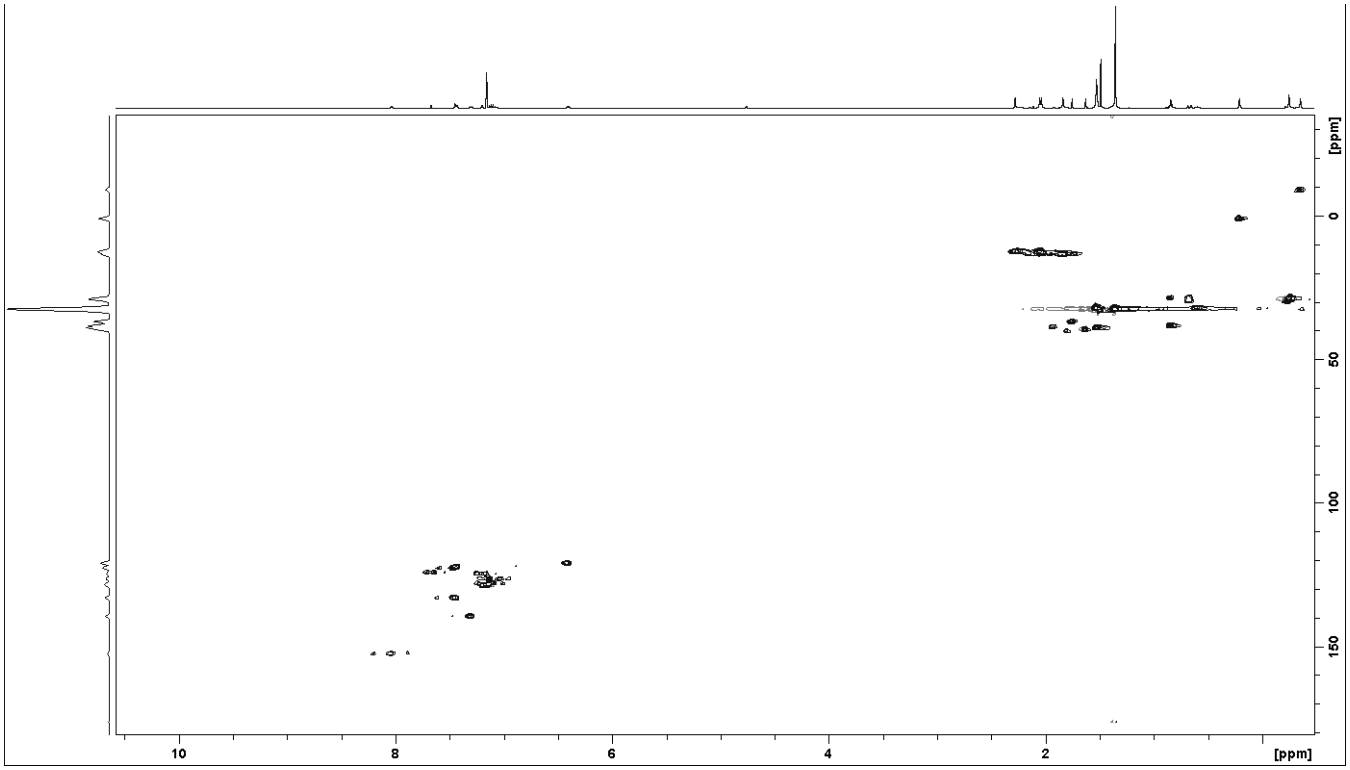

Figure S8. $^{1}H^{13}C$ HSQC NMR spectrum (500 MHz) of $Cp^{Q}LuMe\{NH[C_6H_2tBu_2\text{-}2,4\text{-}(CMe_2CH_2)\text{-}6]\}(AlMe_2)$ (**5**) in C_6D_6 at 26 °C (1D ^{13}C NMR spectrum (126 MHz) on the left edge of the contour plot, 1D ^{1}H NMR spectrum (500 MHz) shown on the top).

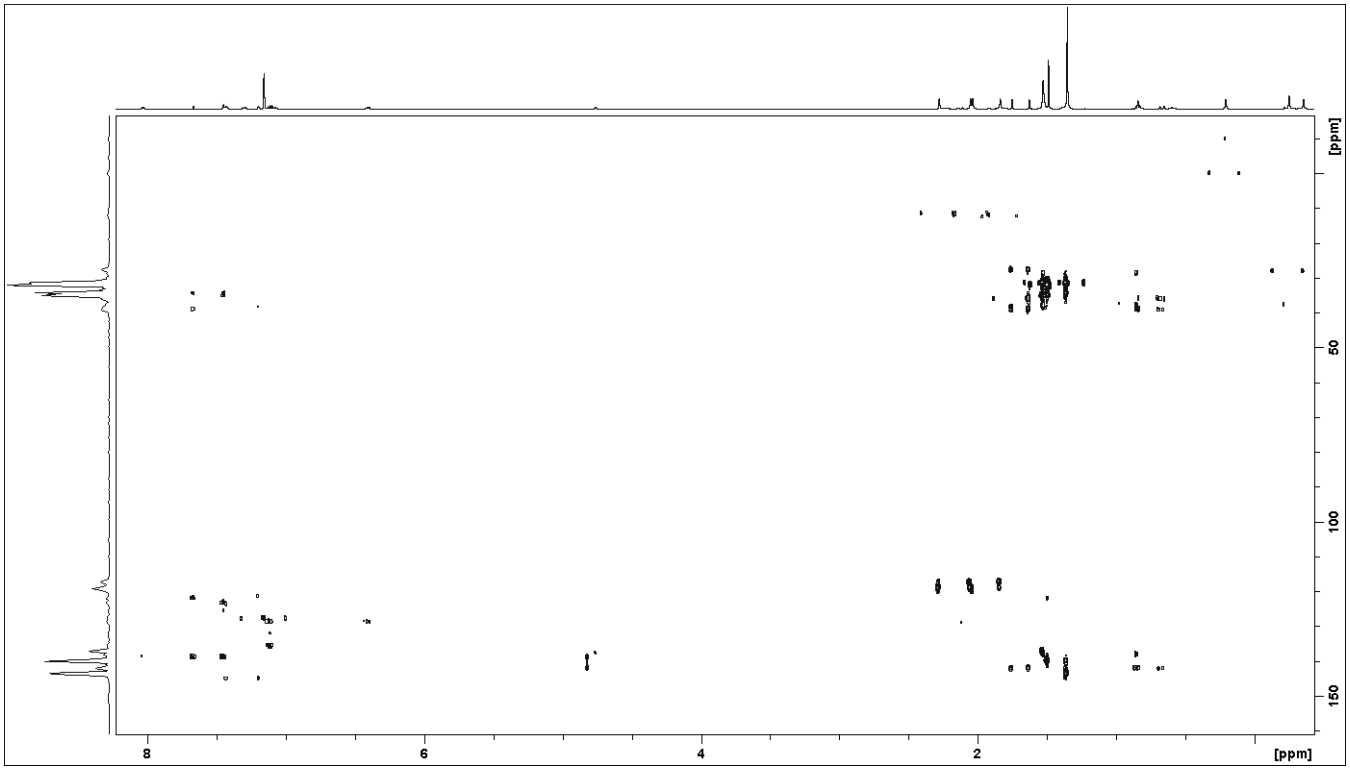

Figure S9. $^{1}H^{13}C$ HMBC NMR spectrum (500 MHz) of $Cp^{Q}LuMe\{NH[C_6H_2tBu_2\text{-}2,4\text{-}(CMe_2CH_2)\text{-}6]\}(AlMe_2)$ (**5**) in C_6D_6 at 26 °C (1D ^{13}C NMR spectrum (126 MHz) on the left edge of the contour plot, 1D ^{1}H NMR spectrum (500 MHz) shown on the top).

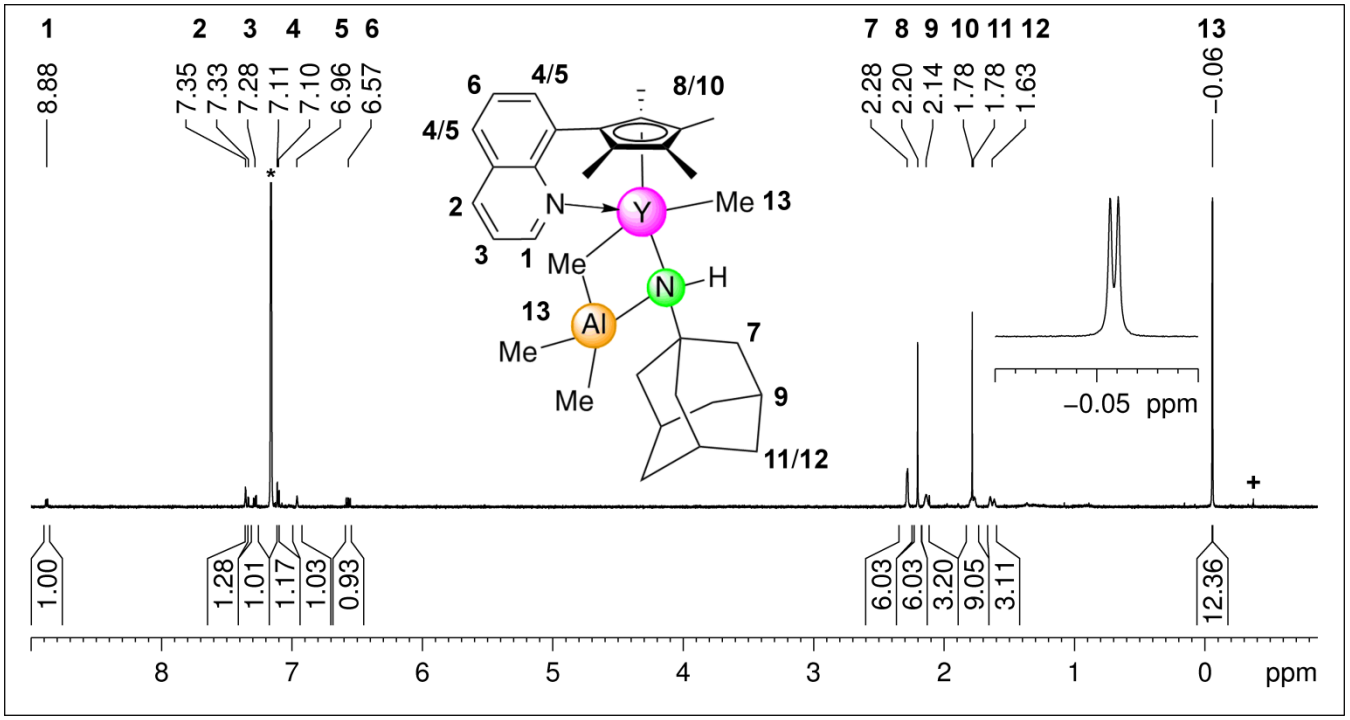

Figure S10. ^{1}H NMR spectrum (400 MHz) of $Cp^{Q}Y[NH(Ad)](AlMe_3)$ (**7**) in C_6D_6 at 26 °C (+ co-product **8**).

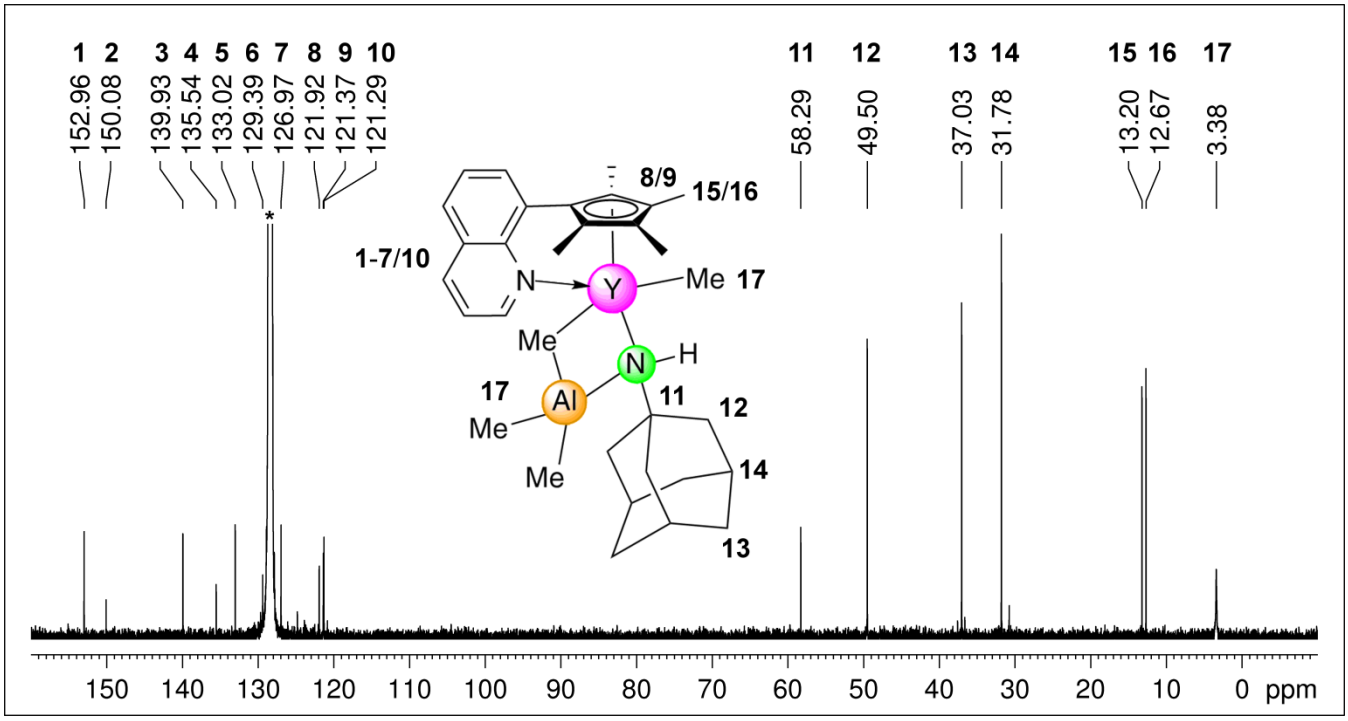

Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz) of $Cp^{Q}Y[NH(Ad)](AlMe_3)$ (**7**) in C_6D_6 at 26 °C.

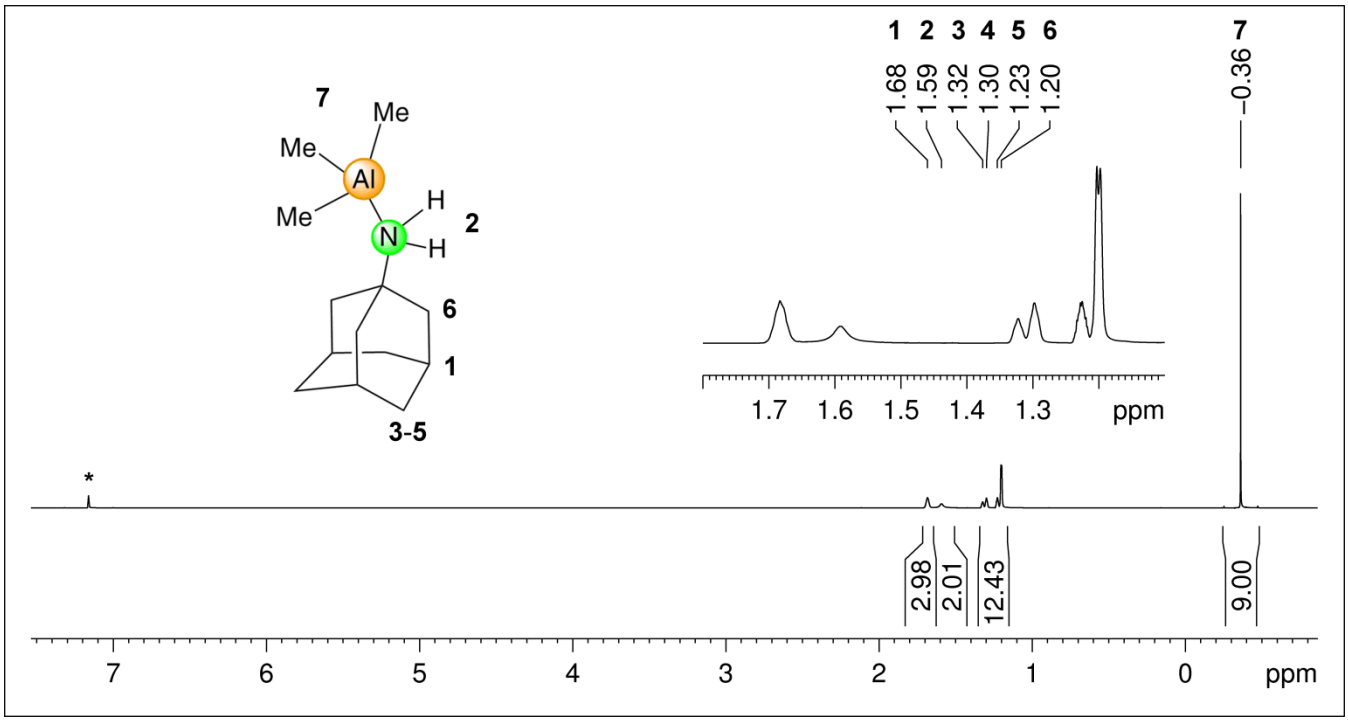

Figure S12. ^{1}H NMR spectrum (500 MHz) of $Me_3Al{\cdot}NH_2(Ad)$ (**8**) in C_6D_6 at 26 °C.

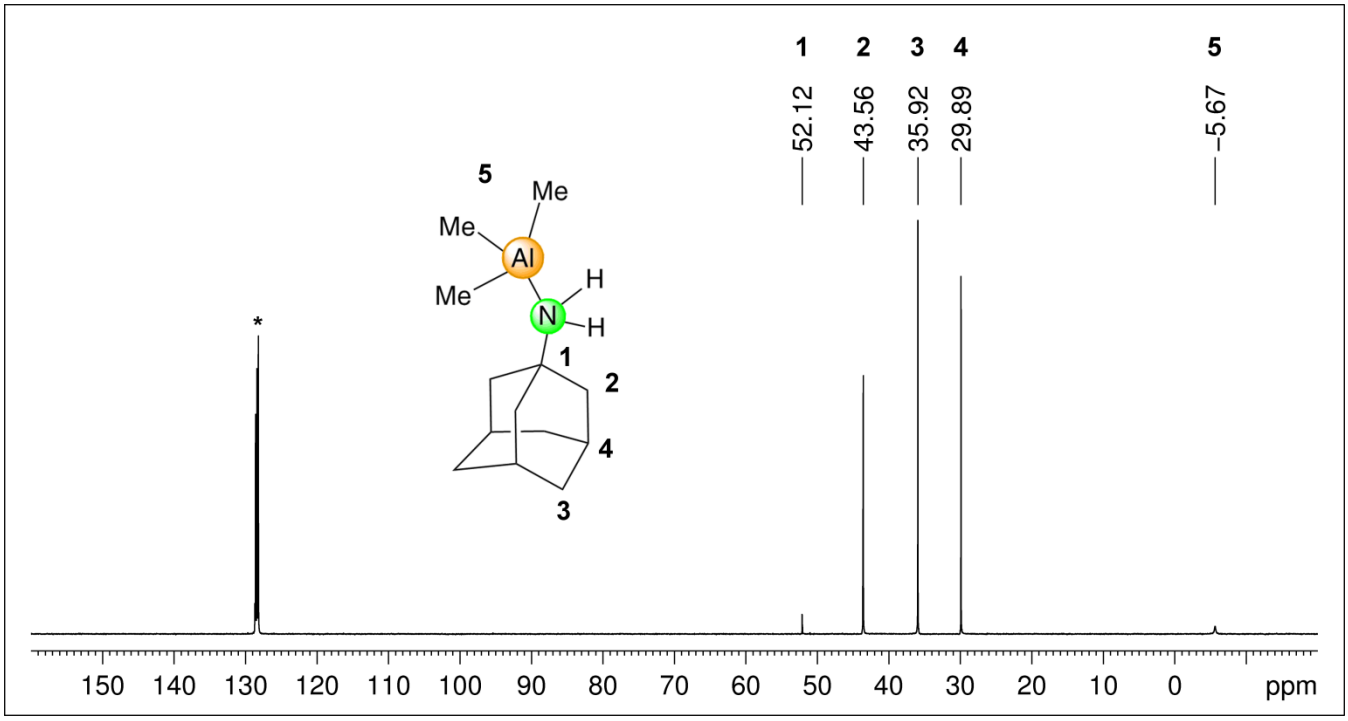

Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz) of $Me_3Al{\cdot}NH_2(Ad)$ (**8**) in C_6D_6 at 26 °C.