Electronic Supplementary Material (ESI) for Dalton Transactions.

Self-reducing Precursors for Aluminium Metal Thin Films: Evaluation of Stable Aluminium Hydrides for Vapor Phase Aluminium Deposition

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Supplementary Information

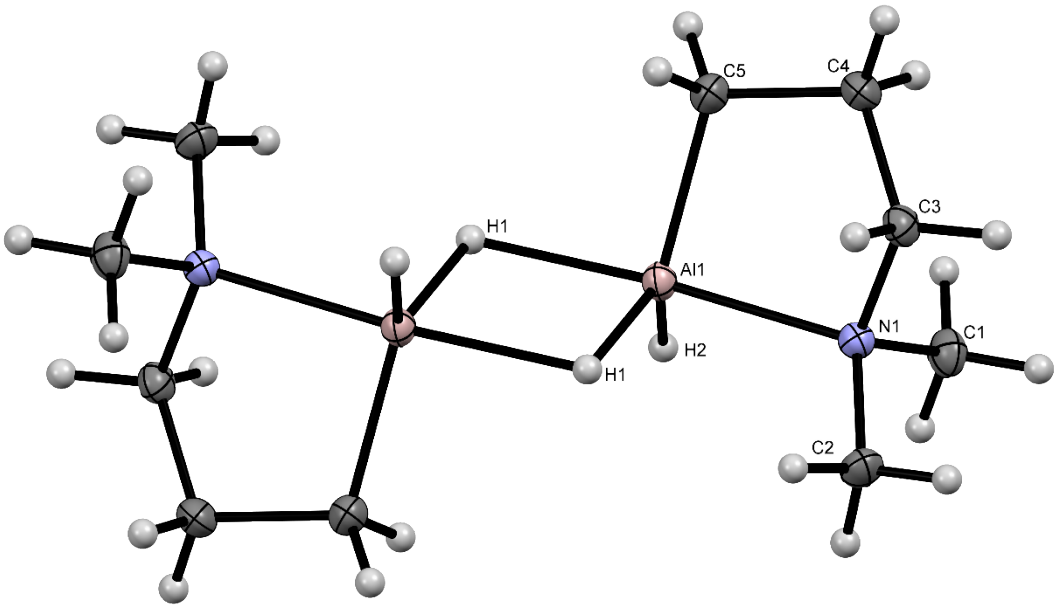

Fig._SI 1 Solid state structure with the displacement ellipsoid plot (50 % probability) of $[Al(DMP)H_2]_2$ (**1**).

Table_SI 1 Crystallographic data and structure refinement for $[Al(DMP)H_2]_2$ (**1**).

Empirical formula	$C_{10}\ H_{28}\ Al_2\ N_2$	
Formula weight	230.30	
Temperature	293(2) K	
Wavelength l	1.54184 Å (Cu Kα)	
Crystal system	triclinic	
Space group	P -1 (no. 2)	
Unit cell dimensions	a = 7.0931(5) Å	α = 65.927(7)°
	b = 7.1791(6) Å	β = 79.774(6)°
	c = 7.9448(6) Å	γ = 85.949(6)°
Volume	363.51(5) $Å^3$	
Z	1	
Density r(calculated)	1.052 g/cm^3	
Absorption coefficient μ	1.569 mm^{-1}	
F(000)	128	
Crystal size	0.297 x 0.189 x 0.185 mm^3	
Theta range for data collection	6.184 to 73.010°	
Index ranges	-8 <= h <= 8, -8 <= k< = 8, -9 <= l< = 7	
Reflections collected	4027	
Independent reflections	1414 [R_{int} = 0.0146, R_{sigma} = 0.0149]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	multi-scan	
Max. and min. transmission	1.00000 and 0.86950	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	1414 / 0 / 101	
Goodness-of-fit on F^2	1.067	
Final R indices [I > 2 σ(I)]	R_1 = 0.0237, wR_2 = 0.0633	
R indices (all data)	R_1 = 0.0249, wR_2 = 0.0643	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.247 and -0.157 $e^-Å^{-3}$	

Table_SI 2 Selected bond distances and bond angles for $[Al(DMP)H_2]_2$ (**1**). Hydrogen H1* is corresponding to dimer molecule.

Bond length (Å)	
Al1 – N1	2.125(1)
Al1 – C5	1.986(1)
Al1 – H2	1.54(1)
Al1 – H1	1.59(1)
Al1 – H1*	1.92(2)
N1 – C1	1.481(1)
N1 – C2	1.479(2)
N1 – C3	1.493(1)
C3 - C4	1.524(2)
C4 – C5	1.538(2)
Bond angle (°)	
N1 – Al1 – H2	96.9(6)
N1 – Al1 – H1	93.4(5)
H1 – Al1 – H2	115.1(8)
H1 – Al1 – H1*	75.2(7)
C1 – N1 – C2	108.73(9)
C1 – N1 – C3	109.59(9)
C2 – N1 – C3	109.83(9)
C1 – N1 – Al1	110.66(7)
C2 – N1 – Al1	114.53(7)
C3 – N1 – Al1	103.35(7)
N1 – C3 – C4	110.26(9)
C3 – C4 – C5	109.5(1)
C4 – C5 – Al1	108.40(8)
C5 – Al1 – H1	128.1(6)
C5 – Al1 – H2	116.2(5)
C5 – Al1 – N1	87.37(4)

Table_SI 3 Summarized onsets of volatilization ($T_{vol.}$) determined by 1 % mass loss taken from TGA for compound 1 – 9.

No.	Name	$T_{vol.}$ (°C)
1	$[Al(DMP)H_2]_2$	74.1
2	Al(DMP)HCl	87.5
3	Al(DMP)HMe	56.8
4	$AlH_3{:}NMe_3$	51.5
5	$[AlH_2NMe_2]_3$	58.4
6	AlH_2NEt_2	47.9
7	$Al(Me_2NCH_2CH_2N^tBu)H_2$	67.2
8	$[Al(Me_2NCH_2CH_2NMe)H_2]_2$	116.9
9	$Al(Me_2NCH_2CH_2NH)H_2$	78.9

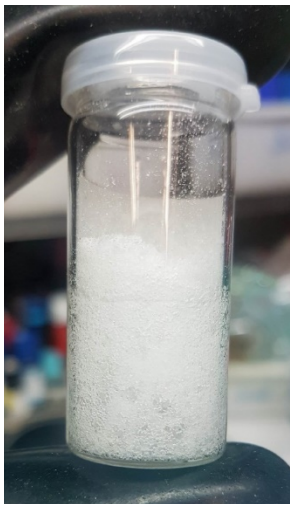

Fig._SI 2 Compound 9 after one week of storage at room temperature under inert conditions. The formation of a foam like, brittle solid was observed.