Electronic Supplementary Material (ESI) for Faraday Discussions.

Supporting Information

Alkali metal···methyl short contacts in aluminates: more than agostic interactions

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1. Spectroscopic data for 1

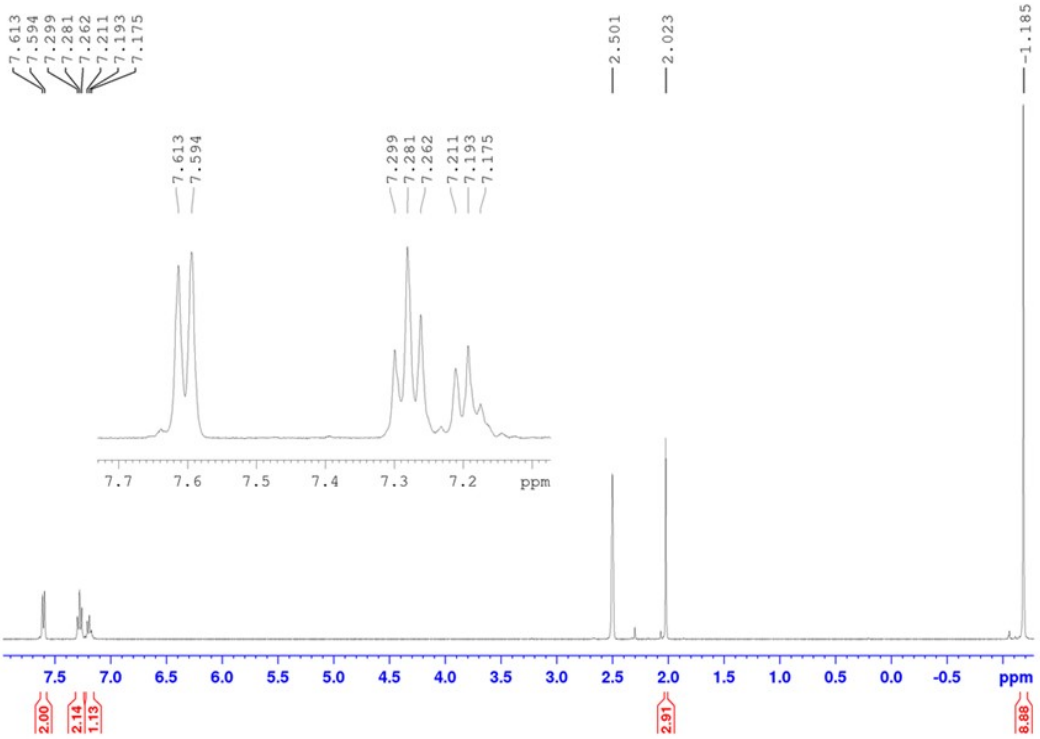

Figure S1 ^{1}H (400 MHz, DMSO-d_6) NMR spectrum of complex [$NaAlMe_3(Ox)$] (**1**). δ -1.19 (s, 9H, $AlCH_3$), 2.02 (s, 3H, C_8H_3), 7.19 (t, 1H, J=7.5Hz, C_4H), 7.28 (t, 2H, J=7.5Hz, $C_{3,5}H$), 7.60 (d, 2H, J=7.5Hz, $C_{2,6}H$)

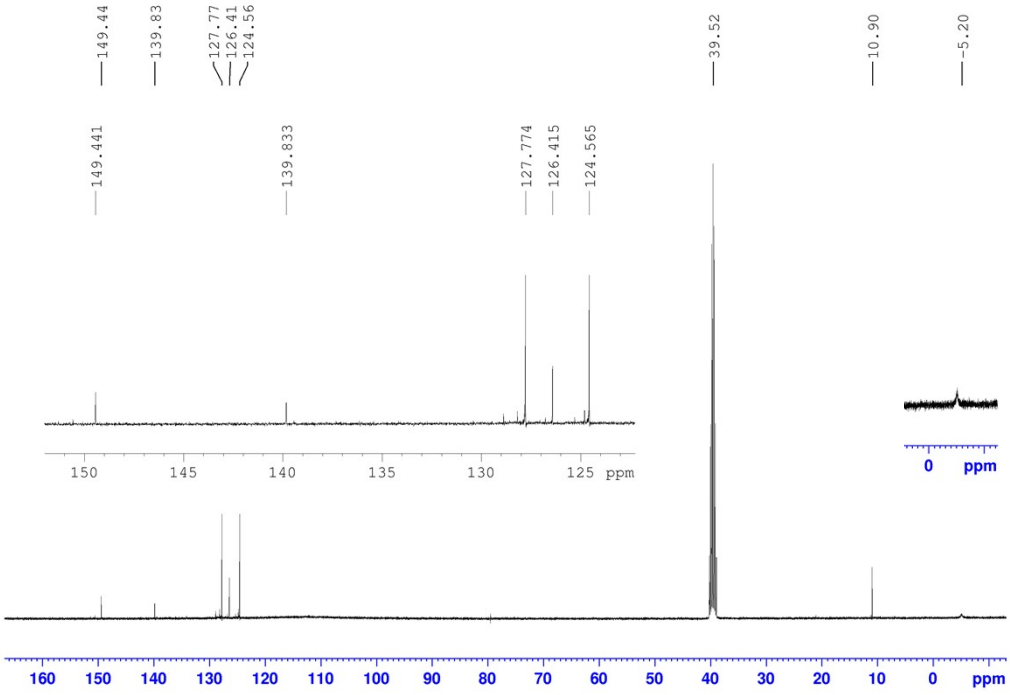

Figure S2 ^{13}C (100.6 MHz, DMSO-d_6) NMR spectrum of complex [$NaAlMe_3(Ox)$] (**1**). δ -5.2 ($AlCH_3$), 10.9 (C_8H_3), 124.6 ($C_{2,6}H$), 126.4 (C_4H), 127.8 ($C_{3,5}H$), 139.8 (C_1), 149.4 (C_7)

2. Single-Crystal X-ray Data for 1.

Table S1 Crystallographic data for [$NaAlMe_3(Ox)$] (**1**)

	[$NaAlMe_3(Ox)$]
Empirical formula	$C_{11}H_{17}AlNaNO$
Formula weight	229.22
Color, shape	Yellow/block
Crystal size (mm)	0.41 x 0.34 x 0.21
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	9.5855(4)
b (Å)	11.0763(5)
c (Å)	13.1896(7)
α (°)	90
β (°)	99.386(4)
γ (°)	90
V (Å^3)	1381.62(11)
Z	4
$\rho_{calcd.}$ (mg m^{-3})	1.102
F_{000}	488
μ (mm^{-1})	0.155
θ Range (°)	3.061 to 27.502
Reflns. Collected	6142
Indep. Reflns./R(int)	3171/0.0331
Data/restraints/param	3171 / 0 / 172
R_1/wR_2 (I > 2σ(I)) [a]	0.0420/0.1043
R_1/wR_2 (all data)[a]	0.0754/0.1140
GOF	1.031
Max/min $\Delta\rho$ (e.Å^{-3})	0.342 and -0.291

[a] $R_1 = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; GOF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$

Table S2 Bond lengths (Å) and angles (°) for **[NaAlMe$_3$(Ox)]** (**1**)

Bond lengths (Å)			
Al(1)-O(1)	1.8299(13)	Na-C(3)	2.757(2)
Al(1)-C(2)	1.978(2)	Na-O(1)	2.7766(15)
Al(1)-C(1)	1.985(2)	Na-C(2)#1	3.094(2)
Al(1)-C(3)	1.989(2)	Na-Na#1	3.7777(14)
Al(1)-Na#1	3.3743(9)	N(1)-C(10)	1.282(2)
Al(1)-Na	3.3753(9)	N(1)-O(1)	1.4104(19)
Na-O(1)#1	2.2573(14)	C(4)-C(10)	1.499(3)
Na-N(1)	2.3489(17)	C(10)-C(11)	1.486(3)
Na-C(1)#2	2.701(2)		
Angles (°)			
O(1)-Al(1)-C(2)	101.30(8)	O(1)#1-Na-Al(1)	95.56(4)
O(1)-Al(1)-C(1)	106.88(9)	N(1)-Na-Al(1)	53.61(4)
C(2)-Al(1)-C(1)	113.73(10)	C(1)#2-Na-Al(1)	132.87(6)
O(1)-Al(1)-C(3)	109.98(8)	C(3)-Na-Al(1)	36.10(5)
C(2)-Al(1)-C(3)	112.44(11)	O(1)-Na-Al(1)	32.81(3)
C(1)-Al(1)-C(3)	111.81(10)	C(2)#1-Na-Al(1)	134.92(6)
O(1)-Al(1)-Na#	138.69(4)	Al(1)#1-Na-Al(1)	111.93(2)
C(2)-Al(1)-Na#	164.59(7)	O(1)#1-Na-Na#1	46.88(4)
C(1)-Al(1)-Na#1	131.91(8)	N(1)-Na-Na#1	60.10(4)
C(3)-Al(1)-Na#1	112.19(7)	C(1)#2-Na-Na#1	171.14(6)
O(1)-Al(1)-Na	55.30(5)	C(3)-Na-Na#1	85.98(5)
C(2)-Al(1)-Na	117.85(7)	O(1)-Na-Na#1	36.40(3)
C(1)-Al(1)-Na	127.67(7)	C(2)#1-Na-Na#1	84.36(5)
C(3)-Al(1)-Na	54.75(7)	Al(1)#1-Na-Na#1	55.98(2)
Na#1-Al(1)-Na	68.07(2)	Al(1)-Na-Na#1	55.95(2)
O(1)#1-Na-N(1)	103.04(6)	C(10)-N(1)-O(1)	114.55(15)
O(1)#1-Na-C(1)#2	125.49(7)	C(10)-N(1)-Na	142.21(12)
N(1)-Na-C(1)#2	124.13(7)	O(1)-N(1)-Na	91.76(9)
O(1)#1-Na-C(3)	109.03(6)	N(1)-O(1)-Al(1)	114.80(10)
N(1)-Na-C(3)	84.19(6)	N(1)-O(1)-Na#1	127.30(9)
C(1)#2-Na-C(3)	101.93(7)	Al(1)-O(1)-Na#1	110.87(6)
O(1)#1-Na-O(1)	83.28(5)	N(1)-O(1)-Na	57.73(8)
N(1)-Na-O(1)	30.51(4)	Al(1)-O(1)-Na	91.89(6)
C(1)#2-Na-O(1)	150.73(7)	Na#1-O(1)-Na	96.72(5)
C(3)-Na-O(1)	68.87(5)	Al(1)-C(1)-Na#3	167.86(12)

O(1)#1-Na-C(2)#1 64.62(5)	Al(1)-C(2)-Na# 180.14(7)
N(1)-Na-C(2)#1 90.06(7)	Al(1)-C(3)-Na 89.16(8)
C(1)#2-Na-C(2)#1 87.79(7)	N(1)-C(10)-C(11) 115.43(16)
C(3)-Na-C(2)#1 170.28(7)	N(1)-C(10)-C(4) 124.03(17)
O(1)-Na-C(2)#1 102.40(6)	C(11)-C(10)-C(4) 120.54(17)
O(1)#1-Na-Al(1)#1 30.45(3)	C(16)-C(11)-C(12) 117.87(18)
N(1)-Na-Al(1)#1 92.03(4)	C(16)-C(11)-C(10) 121.53(17)
C(1)#2-Na-Al(1)#1 115.19(6)	C(12)-C(11)-C(10) 120.60(18)
C(3)-Na-Al(1)#1 136.86(6)	C(13)-C(12)-C(11) 120.4(2)
O(1)-Na-Al(1)#1 86.54(3)	C(14)-C(13)-C(12) 120.6(2)
C(2)#1-Na-Al(1)#1 35.27(4)	C(13)-C(14)-C(15) 119.3(2)
C(14)-C(15)-C(16) 120.7(2)	C(15)-C(16)-C(11) 121.0(2)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+2,-z #2 x,-y+3/2,z-1/2 #3 x,-y+3/2,z+1/2