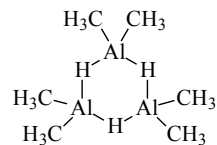


764 **C₆H₂₁Al₃**ED, *ab initio*
calculations**Tri- μ -hydrohexamethyltrialuminum**Cyclo-tri- μ -hydrido-1:2 κ^2 H;1:3 κ^2 H;2:3 κ^2 H-
hexamethyl-1 κ^2 C,2 κ^2 C,3 κ^2 C-trialuminum**D_{3h}** assumed

r_a	Å ^{a)}	θ_a	deg ^{a)}
Al–C	1.958(3)	Al–C–H	110.1(31)
C–H	1.120(2) ^{b)}	H(b)–Al–C	108.3(14)
Al–H(b)	1.711(23)	C–Al–C ^{c)}	143.3(27)
Al...Al	3.153(8)	Al–H(b)–Al ^{c)}	134.3(36)
		H(b)–Al–H(b) ^{c)}	105.7(36)
		H–C–H ^{c)}	108.8(16)
		tilt(CH ₃) ^{d)}	0 ^{e)}



It was found that the vapor consisted of the dimeric (70(4)%), [(CH₃)₂AlH]₂, and trimeric, [(CH₃)₂AlH]₃, molecules. Each of the Al–CH₃ fragments was assumed to have C_{3v} symmetry. The temperature of the vapor was 327 K.

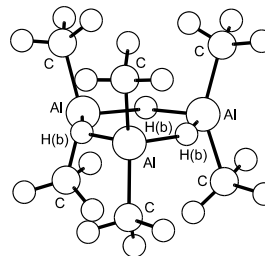
^{a)} Estimated standard errors.

^{b)} Assumed to be equal to that in the dimeric molecule at 327 K.

^{c)} Dependent parameter.

^{d)} Angle between the C₃ axis of the methyl group and the Al–C bond direction.

^{e)} Assumed at the value from MP2/6-31G* calculations.



Downs, A.J., Greene, T.M., Collin, S.E., Whitehurst, L.A., Brain, P.T., Morrison, C.A., Pulham, C.R., Smart, B.A., Rankin, D.W.H., Keys, A., Barron, A.R.: *Organometallics* **19** (2000) 527.