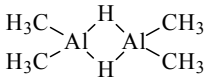
614 **$C_4H_{14}Al_2$** **Di-μ-hydrotetramethyldialuminum** **D_{2h}** assumed

ED, *ab initio* and DFT calculations

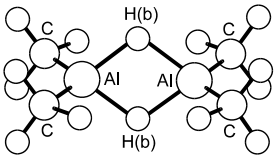
Di-μ-hydrido-bis[dimethylaluminum(III)]



r_a	Å [a])
Al–C	1.952(2)
C–H	1.114(2)
Al–H(b)	1.776(7)
Al...Al	2.625(6)

θ_a	deg [a])
Al–C–H	109.0(7)
Al…Al–C	121.2(2)
C–Al–C [b])	117.7(4)
Al–H(b)–Al [b])	95.3(6)
H(b)–Al–H(b) [b])	84.7(6)
H–C–H [b])	110.0(7)
tilt(CH_3) [c])	0 [d])
twist(CH_3) [e])	0 [d])
wag(CH_3) [f])	0 [d])

Each of the Al–CH_3 fragments was assumed to have C_{3v} symmetry.
The temperature of the vapor was 470 K.



[a]) Estimated standard errors.
[b]) Dependent parameter.
[c]) Angle between the C_3 axis of the methyl group and the Al–C bond direction in the Al_2C_4 plane.
[d]) Assumed at the value from MP2/6-31G* calculations.
[e]) Twist angle of CH_3 group from D_{2h} overall configuration.
[f]) Angle between the C_3 axis of the methyl group and the Al–C bond direction in a plane perpendicular to the Al_2C_4 plane.

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.

Replaces II/25C (**3**, 1865)