

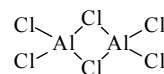
Structure Data of Free Polyatomic Molecules

12 **Al₂Cl₆**

 ED, *ab initio*
calculations

Di- μ -chloro-bis(dichloroaluminum)

 Di- μ -chloro-tetrachlorodialuminum
Dialuminum hexachloride

D_{2h} assumed


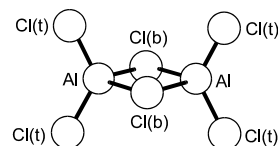
r_g	Å ^{a)}
Al–Cl(b)	2.250(3)
Al–Cl(t)	2.061(2)

r_α	Å ^{a)}	θ_α	deg ^{a)}
Al–Cl(b)	2.242(3)	Cl(b)–Al–Cl(b)	90.0(8)
Al–Cl(t)	2.048(2)	Cl(t)–Al–Cl(t)	122.1(31)
Al–Cl (average)	2.145(2)		

No monomeric species of AlCl₃ molecule were detected in the vapor. The effect of the large-amplitude ring puckering mode on the interatomic distances was handled by a dynamic model composed of a set of pseudoconformers. The differences between corresponding structure parameters in the pseudoconformers were constrained to the values from HF/6-31G(d) calculations.

The nozzle temperature was 150 °C.

^{a)} Twice the estimated standard errors including a systematic error.



Aarset, K., Shen, Q., Thomassen, H., Richardson, A.D., Hedberg, K.: J. Phys. Chem. A **103** (1999) 1644.

Replaces [II/25A\(2, 18\)](#)