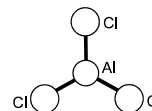


## Structure Data of Free Polyatomic Molecules

<b>8</b>	<b>AlCl<sub>3</sub></b>	<b>Aluminum trichloride</b>	<b>D<sub>3h</sub> assumed</b>
	ED, <i>ab initio</i>	Aluminum(III) chloride	AlCl <sub>3</sub>
	calculations		

$$\frac{r_g}{\text{Al-Cl}} \quad \text{\AA}^a) \quad 2.063(3)$$

$$\frac{r_\alpha}{\text{Al-Cl}} \quad \text{\AA}^a) \quad 2.052(3)$$



The monomeric (71(3) mol%) and dimeric (29(3) mol%) forms were found to be present in the vapor. The structural parameters of Al<sub>2</sub>Cl<sub>6</sub> molecule were constrained to the values obtained in the study at 150 °C, the difference between  $r_\alpha(\text{Al-Cl})$  in the monomer and  $r_\alpha(\text{Al-Cl(t)})$  in the dimer was assumed at the values from HF/6-31G(d) calculations. The nozzle temperature was 400 °C.

<sup>a</sup>) Twice the estimated standard error.

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

Replaces [II/25A\(2, 4\)](#)