

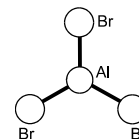
7 AlBr_3 ED, *ab initio*
calculations**Aluminum tribromide**

Aluminum(III) bromide

 D_{3h} assumed **AlBr_3**

$$\frac{r_g}{\text{Al-Br}} \quad \text{\AA}^{\text{a)}} \\ 2.221(3)$$

$$\frac{r_\alpha}{\text{Al-Br}} \quad \text{\AA}^{\text{a)}} \\ 2.210(3)$$



The monomeric (92(4) mol%) and dimeric (8(4) mol%) forms were found to be present in the vapor. The structural parameters of Al_2Br_6 molecule were constrained to the values obtained in the study at 167 °C, and the difference between $r_\alpha(\text{Al-Br})$ in the monomer and $r_\alpha(\text{Al-Br(t)})$ in the dimer was assumed at the values from HF/6-31G(d) calculations. The nozzle temperature was 330 °C.

^{a)} Twice the estimated standard error.

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

ED

$$\frac{r_g}{\text{Al-Br}} \quad \text{\AA}^{\text{a)}} \\ 2.231(5)$$

$$\frac{r_\alpha}{\text{Al-Br}} \quad \text{\AA}^{\text{a)}} \\ 2.216(5)$$

The ED investigation was coupled with quadrupole mass spectrometric experiment. The nozzle temperature was 830 K.

^{a)} Estimated total error including a systematic error.

Hargittai, M., Kolonits, M., Gödörházy, L.: Chem. Phys. Lett. **257** (1996) 321.