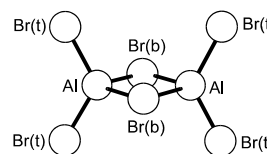


11 **Al₂Br₆**ED, *ab initio*
calculations**Di- μ -bromo-bis(dibromoaluminum)**Di- μ -bromo-tetrabromodialuminum
Dialuminum hexabromide**D_{2h}** assumed

r_g	\AA^a
Al–Br(b)	2.433(7)
Al–Br(t)	2.234(4)

r_a	\AA^a	θ_a	deg ^a
Al–Br(b)	2.426(7)	Br(b)–Al–Br(b)	91.6(6)
Al–Br(t)	2.221(4)	Br(t)–Al–Br(t)	122.1(31)
Al–Br (average)	2.323(4)		

No monomeric species of AlBr₃ molecule were detected in the vapor. The effect of the ring puckering large-amplitude mode on the interatomic distances was handled by a dynamic model composed of a set of pseudoconformers. The differences between corresponding structural parameters in the pseudoconformers were constrained to the values from HF/6-31G(d) calculations. The nozzle temperature was 167 °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.

ED

r_g	\AA^a	θ_a	deg ^a
Al–Br(b)	2.421(5)	Br(b)–Al–Br(b)	93.3(2)
Al–Br(t)	2.227(5)	Br(t)–Al–Br(t)	119.6(7)
		φ^b	19.3(13)

The ED investigation was coupled with a quadrupole mass spectrometric experiment. The nozzle temperature was 360 K.

^a) Estimated total errors.

^b) Effective dihedral angle of the four-membered ring between the Br(b)AlBr(b) planes due to the large-amplitude puckering vibration.

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

Replaces I/25A(2, 17)