

Structure Data of Free Polyatomic Molecules

77	BaBr₂	Barium dibromide	C_{2v}
	ED, vibrational spectroscopy, <i>ab initio</i> calculations	Barium(II) bromide	BaBr ₂

r_g	Å ^{a)}	θ_a	deg ^{a)}
Ba–Br	2.911(6)	Br–Ba–Br	137.0(25)
r_e ^{b)}	Å ^{a)}	θ_e ^{b)}	deg ^{a)}
Ba–Br	2.899(7)	Br–Ba–Br	137.1(49)

The nozzle temperature was 1399...1412 K.

^{a)} Estimated total error.

^{b)} Estimated from a joint analysis of ED data and vibrational frequencies from MP2 calculations. Anharmonic (via diagonal cubic force constants) and nonlinear kinematic effects were taken into account.

Hargittai, M., Kolonits, M., Schultz, G.: J. Mol. Struct. **567-568** (2001) 241.