

Structure Data of Free Polyatomic Molecules

78	BeBr₂	Beryllium dibromide	D_{∞h}
ED		Beryllium(II) bromide	BeBr ₂

r_g	$\text{\AA}^a)$	θ_g	$\text{deg}^a)$
Be–Br	1.944(6)	Br–Be–Br	163.5(22)

The dynamic model taking into account quartic anharmonicity of the bending vibration and the coupling of stretching and bending vibrations was also used in the analysis. The vapor contained *ca.* 30 mol% of Br₂.

The temperature of the measurements was 800(10) K.

^{a)} 2.5 times the estimated standard error including a systematic error.

Giricheva, N.I., Girichev, G.V., Girichev, A.G., Shlykov, S.A.: Struct. Chem. **11** (2000) 313.

ED, *ab initio*
calculations

$r_e^a)$	$\text{\AA}^b)$
Be–Br	1.928(6)

ED intensity curves were taken from [1].

^{a)} Anharmonic correction (via diagonal cubic force constants) was determined by fitting to the experimental intensity curves. Nonlinear kinematic effect was also taken into account.

^{b)} 2.5 times the estimated standard error including a systematic error.

Vogt, N.: Spectroscopy in the 21st Century, Hayama, Japan (2001) P116.

[1] Giricheva, N.I., Girichev, G.V., Girichev, A.G., Shlykov, S.A.: Struct. Chem. **11** (2000) 313.