

99	Br₂H₂	Hydrogen bromide dimer	C_s
MW		(weakly bound complex)	(effective symmetry class)
			(large-amplitude motion)
			HBr · DBr

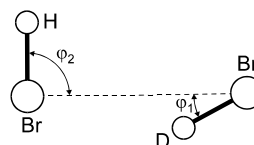
r_0	\AA^a			
	H ⁷⁹ Br · D ⁷⁹ Br	H ⁷⁹ Br · D ⁸¹ Br	H ⁸¹ Br · D ⁷⁹ Br	H ⁸¹ Br · D ⁸¹ Br
Br...Br	4.13632(50)	4.13615(50)	4.13634(50)	4.13618(50)
R_{cm}	4.1018(5)	4.1024(5)	4.1018(5)	4.1025(5)
θ_0	deg			
	H ⁷⁹ Br · D ⁷⁹ Br	H ⁷⁹ Br · D ⁸¹ Br	H ⁸¹ Br · D ⁷⁹ Br	H ⁸¹ Br · D ⁸¹ Br
φ_1^b	0.0	0.0	0.0	0.0
$\varphi_1(\text{eff})^b)^c$	$\pm 28.077(2)$	$\pm 28.072(2)$	$\pm 28.067(2)$	$\pm 28.061(2)$
φ_2^b	90	90	90	90
$\varphi_2(\text{eff})^b)^c$	$90 \pm 24.777(1)$	$90 \pm 24.799(1)$	$90 \pm 24.769(1)$	$90 \pm 24.769(1)$

In the hydrogen halide dimers, allowed transitions are across the inversion doublet caused by the geared interchange of the donor and acceptor of the hydrogen bond. In (HBr)₂, however, because of the low inversion potential barrier, the inversion frequency is in the infrared. In order to investigate the hydrogen bromide dimer with the high precision allowed by an FT microwave experiment, the inversion motion was quenched by substituting deuterium for one of the hydrogen atoms. Using the measurements of the nuclear quadrupole coupling constants of the bromine nuclei, the wide-amplitude bending motions of the hydrogen-bonded deuterium have been determined as has the wide-amplitude bending angle of the nonbonding hydrogen atom. The Br...Br–D angle undergoes excursions of 28° about zero, and the H–Br...Br angle oscillates 25° about its 90° equilibrium angle. The intermolecular stretching, HBr bending and DBr bending force constants are 3.528 N m^{−1}, 0.177×10^{−20} N m and 0.344×10^{−20} N m, respectively.

^{a)} Uncertainties were not estimated in the original paper.

^{b)} See figure for the definition.

^{c)} Amplitude of oscillation.



Chen, W., Walker, A.R.H., Novick, S.E., Tao, F.-M.: J. Chem. Phys. **106** (1997) 6240;
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Replaces [II/25A\(2, 195\)](#)