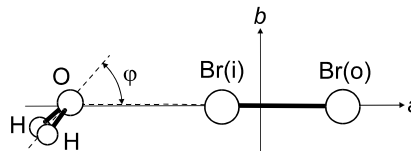


100 MW	Br₂H₂O	Dibromine – water (1/1) (weakly bound complex)	C_s (effective symmetry class) (large-amplitude motion) Br ₂ · H ₂ O
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r_0	Å	θ_0	deg
O...Br(i) ^{a)}	2.8506(1)	φ ^{b)}	46.8(1)

The complex has C_s symmetry with a pyramidal configuration at O. The intermolecular stretching force constant is 9.8 N m⁻¹.



^{a)} Bromine atom that is closer to the water O atom.

^{b)} Angle between the C₂ axis of H₂O and the O...Br-Br.

Legon, A.C., Thumwood, M.A., Wacławik, E.R.: Chem. Eur. J. **8** (2002) 940.