

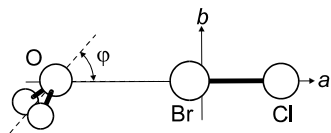
86 MW	<b>BrClH<sub>2</sub>O</b>	<b>Bromine chloride – water (1/1)</b> (weakly bound complex)	<b>C<sub>2v</sub></b> (effective symmetry class) (large-amplitude motion) BrCl · H <sub>2</sub> O
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$r_0$	Å	$\theta_0$	deg
		$\varphi^a$	

O...Br 2.7809(3)

48.0(2)

The zero-point state of the complex is effectively planar (C<sub>2v</sub>) with a low potential energy barrier to the motion that interconverts the two equivalent equilibrium conformers of C<sub>s</sub> symmetry. The intermolecular stretching force constant is 12.08 N m<sup>-1</sup>.



<sup>a</sup>) See figure for the definition.

Davey, J.B., Legon, A.C.: Phys. Chem. Chem. Phys. **3** (2001) 3006.