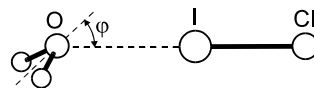


## Structure Data of Free Polyatomic Molecules

<b>131</b> MW	<b>ClH<sub>2</sub>IO</b>	<b>Iodine chloride – water (1/1)</b> (weakly bound complex)	<b>C<sub>s</sub></b> (effective symmetry class) (large-amplitude motion) ICl · H <sub>2</sub> O
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$r_0$	Å	$\theta_0$	deg
O...I	2.838(3)	$\varphi^a$	46(2)

In the zero-point state the complex is effectively planar, with a very low potential energy barrier at the planar geometry (C<sub>2v</sub>) separating two equivalent equilibrium conformers of C<sub>s</sub> symmetry. The intermolecular stretching force constant  $k_\sigma$  is 15.6 N m<sup>-1</sup>.



<sup>a</sup>) The out-of-plane angle, see figure for the definition.

Davey, J.B., Legon, A.C., Wacławik, E.R.: Phys. Chem. Chem. Phys. **2** (2000) 1659.