

137
MW**ClH₅O₂****Hydrogen chloride – water (1/2)**
(weakly bound complex)**C₁**
(large-amplitude motion)
HCl · 2H₂O

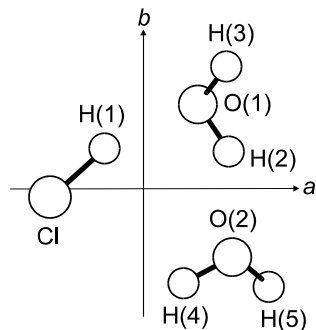
r_s	Å	θ_s	deg
Cl...O(1)	3.083(5)	Cl...O(1)...O(2)	70.34(11)
O(1)...O(2)	2.810(2)	Cl...O(2)...O(1)	58.59(12)
Cl...O(2)	3.402(3)		

r_0	Å	θ_0	deg
Cl...O(1)	3.0801(13)	Cl...O(1)...O(2)	70.68(3)
O(1)...O(2)	2.8085(9)	Cl...O(1)–H(2)	91.2(3)
Cl...O(2)	3.4132(15)	H(4)–O(2)...O(1)	94(2)
O(1)...H(1)	1.828(7)	Cl...O(2)...O(1)	58.38(4)
O(2)...H(2)	1.934(2)	O(1)–H(2)...O(2)	149.5(4)
Cl...H(4)	2.69(2)	Cl...H(4)–O(2)	132(2)
		Cl–H(1)...O(1)	163(2)
		Cl–H(1)...a ^a	43.1 ^b
		H(3)–O(1)–H(2)...O(2) ^c	156.2(3)
		H(5)–O(2)–H(4)...Cl ^c	156.2(3)
		H(1)–Cl...O(2)...O(1) ^c	0.0 ^b
		H(4)–O(2)...O(1)...Cl ^c	0.0 ^b
		H(2)–O(1)...Cl...O(2) ^c	0.0 ^b

r_{av}^d	Å	θ_{av}^d	deg
Cl...O(1)	3.0840(11)	Cl...O(1)...O(2)	70.58(2)
O(1)...O(2)	2.8151(8)	Cl...O(1)–H(2)	91.3(2)
Cl...O(2)	3.4152(13)	H(4)–O(2)...O(1)	103(2)
O(1)...H(1)	1.831(6)	Cl...O(2)...O(1)	58.39(3)
O(2)...H(2)	1.943(2)	O(1)–H(2)...O(2)	149.1 (4)
Cl...H(4)	2.81(2)	Cl...H(4)–O(2)	122(2)
		Cl–H(1)...O(1)	164(2)
		Cl–H(1)...a ^a	43.1 ^b
		H(3)–O(1)–H(2)...O(2) ^c	144.1(2)
		H(5)–O(2)–H(4)...Cl ^c	144.1(2)
		H(1)–Cl...O(2)...O(1) ^c	0.0 ^b
		H(4)–O(2)...O(1)...Cl ^c	0.0 ^b
		H(2)–O(1)...Cl...O(2) ^c	0.0 ^b

Atom	a_s [Å]	b_s [Å]	c_s [Å]
Cl	–1.4743	–0.1707	0.033i ^c
O(1)	1.0936	1.5325	0.058i ^c
H(2)	1.6168	0.5510	0.1625
O(2)	1.7710	–1.1945	0.045i ^c

Atom	a_{av} [Å]	b_{av} [Å]	c_{av} [Å]
Cl	–1.4815	–0.1630	0.0009
H(1)	–0.5446	0.7145	–0.0228
O(1)	1.0921	1.5357	–0.0429
H(2)	1.6425	0.7434	–0.0178
H(3)	1.5711	2.1851	0.4863
O(2)	1.7739	–1.1944	0.0404
H(4)	0.9136	–1.6313	0.0511
H(5)	2.3373	–1.7728	–0.4881



The rotational transitions are split into components belonging to four low-lying vibration-rotation-tunneling substates. The trimer is bound strongly enough to attenuate the dynamics of the water subunits to a level such that the differences in rotational constants between the four states are below 1 MHz. The complex is near planar, as evidenced by inertial defect of -0.5 u \AA^2 . The three monomers are bound in a triangular arrangement through O...HO and O...HCl hydrogen bonds and a primarily dispersive OH...Cl bond. All atoms, with the exception of two nonbonded hydrogen atoms, lie near a common plane.

^{a)} Inertial a axis.

^{b)} Assumed.

^{c)} Dihedral angle.

^{d)} r^* and θ^* in the original paper.

^{e)} Imaginary values.

Kisiel, Z., Białkowska-Jaworska, E., Pszczółkowski, L., Milet, A., Struniewicz, C., Moszynski, R., Sadlej, J.: J. Chem. Phys. **112** (2000) 5767.