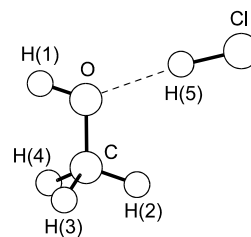


135
MW**CH₅ClO****Methanol – hydrogen chloride (1/1)**
(weakly bound complex)**C_s**
(effective symmetry class)
(large-amplitude motion)
CH₃OH · HCl

r_0	Å	θ_0	deg
O...Cl	3.13(10)	C–O...H(5)	116(5)
R_{cm} ^{a)}	3.44(2)	O...H(5)–Cl	172(5)

Atom	a_0	b_0	c_0
H(1)	1.962	–1.377	0.0
O	1.400	–0.618	0.0
C	2.217	0.550	0.0
H(2)	1.543	1.412	0.0
H(3)	2.853	0.604	0.888
H(4)	2.853	0.604	–0.888
Cl	–1.654	0.067	0.0
H(5)	–0.430	–0.322	0.0



An apparently low barrier (74 cm^{–1}) of the CH₃ internal rotation is ascribed to a large-amplitude wagging motion of the hydroxyl hydrogen. Assuming that the methyl group torsional barrier does not change upon complexation (*i.e.*, 373 cm^{–1}), an estimate for the hydroxyl torsional barrier of 155(5) cm^{–1} was obtained.

^{a)} Uncertainty was not estimated in the original paper.

Tan, X.-Q., Ioannou, I.I., Kuczkowski, R.L.: J. Mol. Struct. **356** (1995) 105.

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