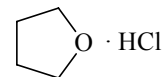
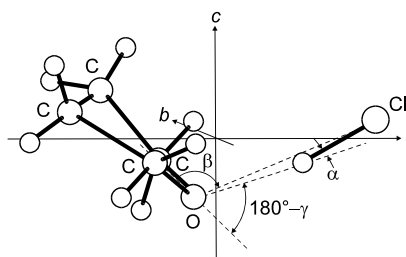


577
MW C_4H_8ClO **Tetrahydrofuran – hydrogen chloride (1/1)**
(weakly bound complex) C_s
(effective symmetry class)
(large-amplitude motion)

Ring form	$r_0(O...Cl)$ [Å] ^{a)}	$r_0(O...H)$ ^{b)} [Å]	$\theta_0(\varphi)$ ^{c)} [deg]	$\theta_0(\beta)$ ^{d)} [deg] ^{a)}	$\theta_0(\gamma)$ ^{b) d)} [deg]	$\theta_0(\alpha)$ ^{b) d)} [deg]
T5–	2.894(5)	1.625	54	136.1(1)	122.7	11.5
B3+	2.963(3)	1.690	72	125.87(6)	119.5	9.9
T1+	3.057(3)	1.781	90	112.65(5)	116.2	8.4
B4–	3.146(5)	1.868	108	99.7(1)	113.2	7.0
T2–	3.232(5)	1.952	126	89.7(1)	110.5	6.1

The vibrational energy difference between the members of the tunneling doublet, $\Delta E = 3.550(25)$ MHz, was determined from the analysis of the α -type Coriolis coupling interaction between them. The tunneling splittings were not observed for the species $C_4D_8O \cdot H^{35}Cl$.

From the analysis of all the available data, these splittings were ascribed to pseudorotation within the tetrahydrofuran subunit. The spectroscopic constants were interpreted in terms of a geometry in which tetrahydrofuran has a conformation close to the twisted ring-form with HCl lying on the plane bisector to the COC ring angle. One minimum and three transition structures were located and characterized at the MP2/6-31G** level. The geometric parameters and rotational constants of the minimum agreed well with those determined from the spectroscopic data. The transition structures correspond to interconversion between equivalent conformations, the first one *via* an inversion motion and the remaining two *via* pseudorotation movements. One of these latter two is responsible for the splittings detected by microwave spectroscopy.



^{a)} Estimated standard errors.

^{b)} Derived parameters.

^{c)} Pseudorotation angle.

^{d)} See figure for the definition.

López, J.C., Alonso, J.L., Lorenzo, F.J., Rayón, V.M., Sordo, J.A.: J. Chem. Phys. **111** (1999) 6363.