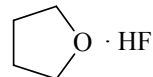
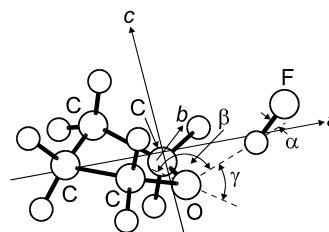


581
MW C_4H_8FO **Tetrahydrofuran – hydrogen fluoride (1/1)**
(weakly bound complex) C_s
(effective symmetry class)
(large-amplitude motion)

Ring form	$r_0(O...F)$ [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–	2.5988(25)	1.556	54	149.719(66)	43.36	14.5
B3+	2.5182(17)	1.606	72	138.658(43)	47.48	12.4
T1+	2.5979(17)	1.682	90	125.140(42)	51.27	10.1
B4–	2.6896(29)	1.770	108	110.495(70)	56.19	7.8
T2–	2.7666(41)	1.845	126	99.795(97)	59.66	6.3

The rotational spectra of $C_4H_8O \cdot HF$ and $C_4H_8O \cdot DF$ exhibit small tunneling splittings, which were not observed for $C_4D_8O \cdot HF$ and the four single ^{13}C isotopomers. From the analysis of these observations in terms of symmetry considerations, these splittings were ascribed to pseudorotation within the tetrahydrofuran subunit of the complex and not to HF inversion. The spectroscopic parameters of the complex were interpreted in terms of a geometry in which tetrahydrofuran has a conformation close to the twisted ring form, with HF lying on the plane bisector to the COC ring angle.



^{a)} Estimated standard errors.

^{b)} Derived parameters.

^{c)} Pseudorotation angle.

^{d)} See figure for the definition.

Alonso, J.L., López, J.C., Blanco, S.B., Lesarri, A., Lorenzo, F.J.: J. Chem. Phys. **113** (2000) 2760.