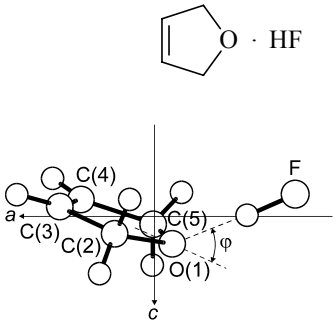
550 **C_4H_7FO** **2,5-Dihydrofuran – hydrogen fluoride (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)

r_0	Å [a])
O(1)...H	1.674(2)
H–F	0.925595 [a])
C(2)–O(1)	1.43 [b])
C(2)–C(3)	1.50 [b])
C(3)=C(4)	1.35 [b])
C(2)–H(8)	1.095 [b])
C(3)–H(6)	1.085 [b])

θ_0	deg [a])
C(5)–O(1)–C(2)	111.9(1)
O(1)–C(2)–C(3)	104.1(1)
C(2)–C(3=C(4)	109.34 [b])
H(8)–C(2)–O(1)	110.42 [b])
H(8)–C(2)–C(3)	110.42 [b])
H(6)–C(3)=C(4)	125.33 [b])
φ [c])	46.34(4)
ϕ [d])	0.0 [b])



All the observed lines are split into two components due to the tunneling of HF between the two equivalent hydrogen-bonding sites at the oxygen atom. A value for the barrier to HF inversion of 100 cm^{-1} was calculated from an analysis of the rotational constants of both tunneling states on the basis of a simple one-dimensional model. An analysis using a flexible model gives the potential barrier V = 100(3) cm^{-1}, r(O...H) = 1.661(1) Å, and φ_{min} = 47.89(3) deg.

[a]) Estimated standard errors.
[b]) Assumed.
[c]) See figure for the definition.
[d]) Dihedral angle between the OC(2)C(5) and C(2)C(3)C(4)C(5) planes.

López, J.C., Blanco, S., Lesarri, A., Sanz, M.E., Lorenzo, F.J., Alonso, J.L.: J. Chem. Phys. **114** (2001) 9421.

Replaces II/25C (**3**, 1696)