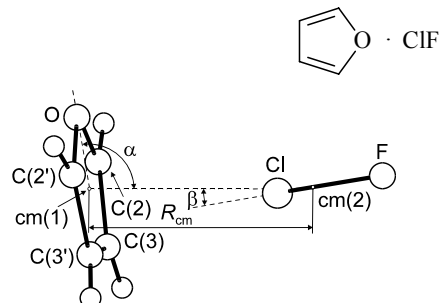


506
MW**C₄H₄ClFO****Furan – chlorine fluoride (1/1)**
(weakly bound complex)**C₁**
(effective symmetry class)
(large-amplitude motion)

r_0	Å	θ_0	deg
O...Cl	2.762(5) ^{a)}	α ^{b)}	99.5(8)
R_{cm}	3.6127(4)	β ^{b)}	-17.7(21)
		γ ^{c)}	57.3(41)
		δ ^{d)}	68.4(10)



Transitions allowed by all three components μ_a , μ_b and μ_c of the electric dipole moment were observed, those associated with μ_c exhibiting a small doubling (*ca.* 20 kHz). The geometry obtained by fitting the principal moments of inertia of the three observed isotopomers is consistent with the direction cosines θ_{az} ($\alpha = a, b, c$) relating the ClF axis (z) to the principal inertial axis system, which are derived by diagonalizing the Cl nuclear quadrupole coupling tensor (of which all five components were derived from the observed spectra), and has the ClF subunit approximately perpendicular to one of the C(2)–C(3) bonds of furan. The doubling of the c -type transitions is interpreted in terms of a motion in which the interaction switches from C(2)–C(3) to C(2')–C(3').

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

^{b)} See figure for the definition.

^{c)} Dihedral angle Cl–cm(2)...cm(1)...O, where cm(1) and cm(2) are the centers of mass of the furan and the ClF subunits, respectively.

^{d)} Dihedral angle cm(2)...cm(1)...O–C(2), where cm(1) and cm(2) are the centers of mass of the furan and the ClF subunits, respectively.

Cooke, S.A., Corlett, G.K., Holloway, J.H., Legon, A.C.: J. Chem. Soc., Faraday Trans. **94** (1998) 2675.