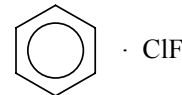


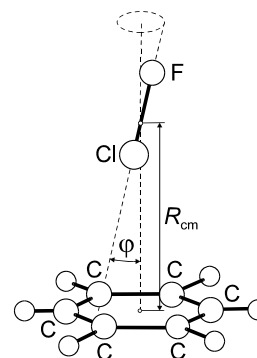
717
MW**C₆H₆ClF****Benzene – chlorine fluoride (1/1)**
(weakly bound complex)**C_{6v}**
(effective symmetry class)
(large-amplitude motion)

Isotopic species	$r_0(R_{\text{cm}})$ [Å] ^{a)}	$r_0(*\dots\text{Cl})$ [Å] ^{a) b)}	$\theta_0(\varphi)$ [deg] ^{c)}
C ₆ H ₆ · ³⁵ ClF	3.765(3)	3.313(3)	14.40(5)
C ₆ H ₆ · ³⁷ ClF	3.745(3)	3.313(3)	14.39(5)
C ₆ D ₆ · ³⁵ ClF	3.760(3)	3.300(3)	13.95(8)



The observed spectra were established to be of the symmetric-top type, but with large centrifugal distortion effects. At equilibrium, the ClF axis is inclined at an angle of $\varphi \approx 14^\circ$ to the C_6 axis of benzene, with the two axes intersecting at the ClF center of mass. The Cl atom lies closer to the benzene ring than does the F atom. The extrapolation of the ClF internuclear axis intersects the plane of the benzene ring at a point (*) that lies at a distance of *ca.* 0.24 Å inside the ring from the center of a C–C bond.

The conformation with $\varphi = 0^\circ$ (ClF axis and benzene C_6 axis coincident) corresponds to a potential energy maximum, concentric with which is an approximately circular valley corresponding to $\varphi \approx 14^\circ$. This type of potential energy surface is consistent with the symmetric-top nature of the observed spectra, with the relatively small energy separation of the $\nu = 0$ and 1 states, and with large, but oppositely signed, centrifugal distortion effects in the two states originating in a Coriolis interaction between them. The intermolecular stretching force constant is 4.48 N m⁻¹.



^{a)} Uncertainties were not estimated in the original paper.

^{b)} * denotes the point where the extrapolation of the ClF internuclear axis intersects the plane of the benzene ring.

^{c)} See figure for the definition.

Cooke, S.A., Evans, C.M., Holloway, J.H., Legon, A.C.: J. Chem. Soc., Faraday Trans. **94** (1998) 2295.