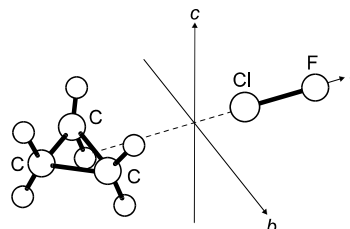
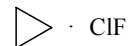


392  
MW $\text{C}_3\text{H}_6\text{ClF}$ **Cyclopropane – chlorine fluoride (1/1)**  
(weakly bound complex) $\text{C}_{2v}$   
(effective symmetry class)  
(large-amplitude motion)

$r_0$	$\text{\AA}^{\text{a}}$	
	$(\text{CH}_2)_3 \cdot ^{35}\text{ClF}$	$(\text{CH}_2)_3 \cdot ^{37}\text{ClF}$
$R_{\text{cm}}$	3.9697(10)	3.9488(10)
$\text{M} \dots \text{Cl}^{\text{b}}$	2.9578(10)	2.9575(10)
$k_{\sigma} [\text{N m}^{-1}]^{\text{c}}$	9.91	9.74



The distance from the cyclopropane centre of mass to the Cl nucleus was also reported to be 3.395(1) Å. A detailed interpretation of the observed molecular constants leads to the conclusion that the three C nuclei, the Cl nucleus and the F nucleus are coplanar and that in the equilibrium conformation the axis of ClF coincides or nearly coincides with the *a*-axis of the complex, with Cl closer than F to the cyclopropane ring. It is most likely that the *a*-axis coincides with a median of the  $\text{C}_3$  equilateral triangle.

<sup>a</sup>) Uncertainties were not all estimated in the original paper.

<sup>b</sup>) M indicates the midpoint of the C–C internuclear line.

<sup>c</sup>) Intermolecular stretching force constant.

Hinds, K., Holloway, J.H., Legon, A.C.: J. Chem. Soc., Faraday Trans. **93** (1997) 373.