

235  
MW

 $\text{C}_2\text{H}_3\text{ClFN}$ 
**Acetonitrile – chlorine fluoride (1/1)**

(weakly bound complex)

 $\text{C}_{3v}$ 

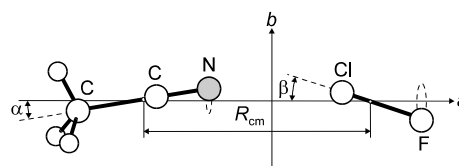
 (effective symmetry class)  
(large-amplitude motion)

 $\text{H}_3\text{C}-\text{C}\equiv\text{N} \cdot \text{ClF}$ 

Isotopic species	$r_0(\text{N}\dots\text{Cl})$ [Å]	$r_0(R_{\text{cm}})$ [Å]	$\theta_0(\alpha_{\text{av}})^{\text{a}}$ [deg]	$\theta_0(\beta_{\text{av}})^{\text{a}}$ [deg]
$\text{CH}_3\text{C}^{14}\text{N} \cdot {}^{35}\text{ClF}$	2.561(2)	4.459(2)	10(2)	7(1)
$\text{CH}_3\text{C}^{14}\text{N} \cdot {}^{37}\text{ClF}$	2.561(2)	4.438(2)	10(2)	7(1)
$\text{CD}_3\text{C}^{14}\text{N} \cdot {}^{35}\text{ClF}$	2.561(2)	4.572(2)	10(2)	7(1)
$\text{CH}_3\text{C}^{15}\text{N} \cdot {}^{35}\text{ClF}$	2.561(2)	4.428(2)	10(2)	7(1)

The intermolecular stretching and bending force constants are  $13.96 \text{ N m}^{-1}$  and  $3.00 \times 10^{-20} \text{ J rad}^{-2}$ , respectively.

<sup>a</sup>) See figure for the definition. Average value.



Page, M.D., Wacławik, E.R., Holloway, J.H., Legon, A.C.: J. Mol. Struct. **509** (1999) 55.