

1300
MW

$\text{C}_3\text{H}_7\text{Cl}$

Cyclopropane – hydrogen chloride (1/1)
(weakly bound complex)

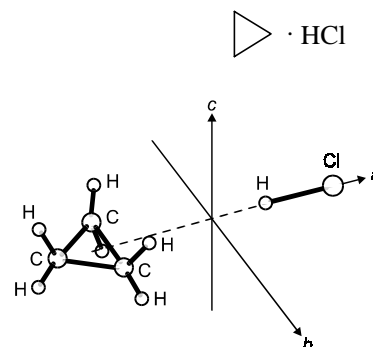
C_{2v}
(effective symmetry class)
(large-amplitude motion of HCl)

Isotopic species	$r_0(\text{centroid} \dots \text{Cl}) [\text{\AA}]^{\text{a)}}$	$\gamma_0 [\text{deg}]^{\text{a) b)}$
$\text{C}_3\text{H}_6 \cdot \text{H}^{35}\text{Cl}$	4.004(3)	21.2(5)
$\text{C}_3\text{H}_6 \cdot \text{H}^{37}\text{Cl}$	4.004(3)	21.1(5)
$\text{C}_3\text{H}_6 \cdot \text{D}^{35}\text{Cl}$	4.001(3)	19.0(5)

HCl lies in the plane of the ring along the C_2 axis.

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

^{b)} Instantaneous angle between the HCl bond direction and the a axis. Average angle.



Legon, A.C., Aldrich, P.D., Flygare, W.H.: J. Am. Chem. Soc. **104** (1982) 1486.

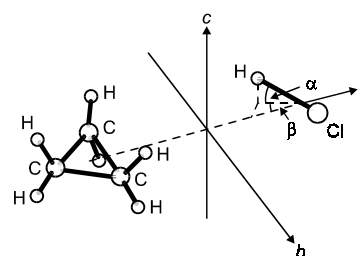
MW

Isotopic species	$\theta_0 [\text{deg}]^{\text{a)}}$	$\alpha_0 [\text{deg}]^{\text{b)}}$	$\beta_0 [\text{deg}]^{\text{b)}}$
$\text{C}_3\text{H}_6 \cdot \text{H}^{35}\text{Cl}$	21.15(1) ^{c)}	15.35(5) ^{c)}	15.25(5) ^{c)}

^{a)} Angle between the HCl subunit and the a -axis of the complex; $\cos \theta = \cos \alpha \cos \beta$. Average angle.

^{b)} See figure for definition. Average angle.

^{c)} Obtained from eQq , the nuclear quadrupole coupling constant. Average angle.



Aldrich, P.D., Kukolich, S.G., Campbell, E.J., Read, W.G.: J. Am Chem. Soc. **105** (1983) 5569.