

1192  
ED

**C<sub>3</sub>H<sub>5</sub>Cl**

**3-Chloro-1-propene**  
Allyl chloride

**C<sub>s</sub> (*syn*)**  
**C<sub>1</sub> (*gauche*)**  
**H<sub>2</sub>C=CH-CH<sub>2</sub>Cl**

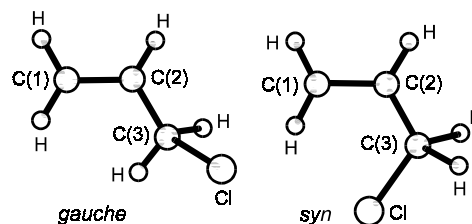
$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C(1)=C(2)	1.341(5)	C=C=C	122.6(13)
C(2)-C(3)	1.506(6)	C-C-Cl	110.0(10)
C-Cl	1.803(5)	Cl-C-H	106.6(24)
C-H	1.081(17) <sup>b)</sup>	$\tau$ <sup>c)</sup>	120.8(54)

The most abundant conformer is *gauche*. At 20 and 90 °C the amount of the *gauche* conformer is 82(9)% and 78(15)%, respectively. The less abundant conformer, *syn* form, has a large root-mean-square torsional amplitude. Parameters of the *gauche* conformer at 90 °C are listed. The nozzle temperatures were 20 and 90 °C.

<sup>a)</sup> Twice the estimated standard errors including a possible scale error.

<sup>b)</sup> Average value.

<sup>c)</sup> Torsion angle C=C-C-Cl,  $\tau = 0^\circ$  for *syn* form when C-Cl is eclipsed with respect to the C=C bond.



Schei, S.H., Shen, Q.: J. Mol. Struct. **128** (1985) 161.

MW

$r_0$	Å		$\theta_0$	deg	
	<i>gauche</i>	<i>syn</i>		<i>gauche</i>	<i>syn</i>
C(1)=C(2)	1.354 <sup>a)</sup>	1.333 <sup>a)</sup>	C=C-C	121.6 <sup>a)</sup>	124.6 <sup>a)</sup>
C(2)-C(3)	1.486 <sup>a)</sup>	1.488 <sup>a)</sup>	C-C-Cl	109.6(20)	115.2 (20)
C-Cl	1.809(20)	1.811(10)	C=C-H	120.0 <sup>a)</sup>	120.0 <sup>a)</sup>
C(1,2)-H	1.080 <sup>a)</sup>	1.080 <sup>a)</sup>	C(2)-C(3)-H <sup>b)</sup>	107.0 <sup>a)</sup>	111.1 <sup>a)</sup>
C(3)-H	1.095 <sup>a)</sup>	1.095 <sup>a)</sup>	H-C(3)-H	111.0 <sup>a)</sup>	108.1 <sup>a)</sup>
			$\tau$ <sup>c)</sup>	122.4 (50)	0.0

<sup>a)</sup> Assumed.

<sup>b)</sup> Both C(2)-C(3)-H angles assumed to be equal.

<sup>c)</sup> C=C-C-Cl dihedral angle.

Hirota, E.: J. Mol. Spectrosc. **35** (1970) 9.