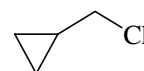


1685  
MW

**C<sub>4</sub>H<sub>7</sub>Cl**

**(Chloromethyl)cyclopropane**

**C<sub>s</sub> (*cis*)**  
**C<sub>1</sub> (*gauche*)**



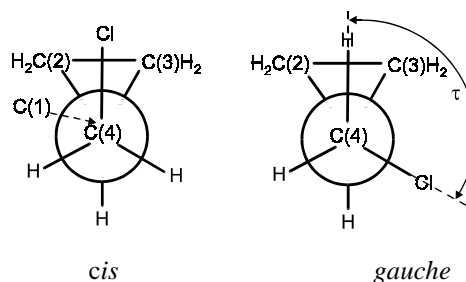
$r_0$	Å <sup>a)</sup>	$\theta_0$	deg <sup>a)</sup>
C(1)–C(2,3),		C(1)–C(2)–C(3),	
C(2)–C(3)	1.514 <sup>b)</sup>	C(2)–C(3)–C(1)	60 <sup>b)</sup>
C(1)–C(4)	1.522 <sup>b)</sup>	H–C(2,3)–H	116 <sup>b)</sup>
C(1,2,3)–H	1.082 <sup>b)</sup>	H–C(1)–C(4)	116 <sup>b)</sup>
C(4)–H	1.091 <sup>b)</sup>	C(1)–C(4)–Cl	109.45 <sup>b)</sup>
C(4)–Cl	1.791(10)	C(1)–C(4)–H	109.45 <sup>b)</sup>
		$\tau$ <sup>c)</sup>	120.2(50)

Structural parameters are given for the *gauche* conformer.

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

<sup>b)</sup> Assumed.

<sup>c)</sup> Torsional angle around the C(1)–C(4) bond, see figure;  $\tau = 0^\circ$  for the *cis* conformer.



Mohammadi, M.A., Brooks, W.V.F.: J. Mol. Spectrosc. **73** (1978) 347 (*gauche*).

Fujiwara, F.G., Chang, J.C., Kim, H.: J. Mol. Struct. **41** (1977) 177 (*cis* and *gauche* conformers).

ED

$r_a$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–C (ring, average)	1.519(3)	$\phi(\text{Cl–C–H})$ <sup>b)</sup>	120 <sup>c)</sup>
$\Delta(\text{C–C})$ <sup>d)</sup>	0.00 <sup>e)</sup>	C(2,3)–C(1)–C(4)	117.2(9)
C–Cl	1.798(5)	C–C–H (ring)	116.0(15)
C–H (average)	1.087(9)	C(1)–C(4)–Cl	112.6(7)
		C(1)–C(4)–H	110.3(32)
		$\tau$ <sup>f)</sup>	116.0(38)

The predominant conformer is *gauche* (96(9)%). The amount of the *cis* conformer is very small, if any.

The nozzle temperature was 45 °C.

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

<sup>b)</sup> Angle between projections of C(4)–Cl and C(4)–H on the plane perpendicular to the C(1)–C(4) bond.

<sup>c)</sup> Assumed.

<sup>d)</sup>  $\Delta(\text{C–C}) = [\text{C(1)–C(4)}] - [\text{C–C(ring)}]$ .

<sup>e)</sup> Assumed by taking the MW results into consideration.

<sup>f)</sup> Torsional angle around the C(1)–C(4) bond, see figure;  $\tau = 0^\circ$  for the *cis* conformer.

Schei, S.H.: Acta Chem. Scand. Ser. A **37** (1983) 15.