

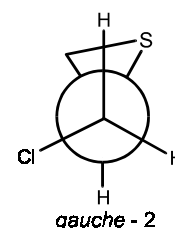
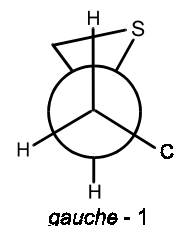
1200  
ED

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

**2-(Chloromethyl)thiirane**  
1-Chloro-2,3-epithiopropene

**C<sub>1</sub> (*gauche*-1)**  
**C<sub>1</sub> (*gauche*-2)**

$r_a$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–H	1.103(12)	C(1)–C(2)–C(3)	114.1(13)
C(2)–C(3)	1.516(24)	C(2)–C(3)–S	114.3(13)
C(1)–C(2)	1.492(23)	C(2)–C(3)–Cl	109.8(12)
C–S	1.822(13)	H–C–H	109.0 <sup>b)</sup>
C–Cl	1.798(23)	C(3)–C(2)–H	110.0 <sup>b)</sup>
		C(2)–C(3)–H	110.8(28)
		C(2)–C(1)–S	65.8(4) <sup>c)</sup>
		C(1)–S–C(2)	48.3(7) <sup>c)</sup>
		$\phi_1$ <sup>d)</sup>	108.5(134)
		$\phi_2$ <sup>d)</sup>	–129.6(48)
		$\tau_1$ <sup>e)</sup>	75.7(134) <sup>c)</sup>
		$\tau_2$ <sup>e)</sup>	–162.4(48) <sup>c)</sup>



The molecule exists as a mixture of *gauche*-2 (82.2(79)%) and *gauche*-1 (17.8(79)%) conformers. The nozzle temperature was 35 °C.

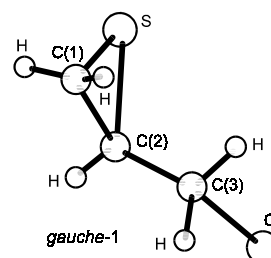
<sup>a)</sup> Twice the estimated standard errors including a systematic error.

<sup>b)</sup> Assumed.

<sup>c)</sup> Dependent parameter.

<sup>d)</sup>  $\phi_1$  and  $\phi_2$  are the C–C torsion angles between the C–Cl bond and the three-membered ring for the *gauche*-1 and the *gauche*-2 conformers, respectively. A positive value of  $\phi$  corresponds to a clockwise rotation of the C–Cl bond in the Newman projections shown in figure;  $\phi = 0^\circ$  for *syn* conformer.

<sup>e)</sup>  $\tau_1$  and  $\tau_2$  are the S–C–C–Cl torsion angles in the *gauche*-1 and *gauche*-2 conformers, respectively;  $\tau = 0^\circ$  for *syn* position.



Shen, Q., Hagen, K.: J. Mol. Struct. **131** (1985) 309.