

1198
ED

C₃H₅ClO₂S

(Z)-2-Chlorovinyl methyl sulfone

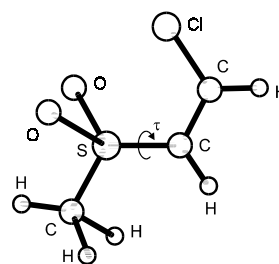
C_s (*anti*)
C₁ (*gauche*)
HCIC=CH-SO₂-CH₃

r_g	Å ^{a)}	θ_a	deg ^{a)}
S=O	1.437(3)	O=S=O	120.3(10)
S-C (average)	1.766(10)	O=S-C(vinyl)	111.1(7)
C-H (average)	1.116(5)	C=C-S	127.6(10)
		C-S-C	101.2(15)
		C=C-Cl	124.3(10)
		C=C-H	120(2)
		S-C-H	108(2)
		$\tau(\textit{anti})$ ^{b)}	180(47)
		$\tau(\textit{gauche})$ ^{b)}	80(19)

The molecule exists as a mixture of *anti* and *gauche* conformers. Mole fraction of the *anti* conformer is 0.305(35). The energy difference is $\Delta E = E(\textit{anti}) - E(\textit{gauche}) \approx 0.4 \text{ kJ mol}^{-1}$. The nozzle temperature was $\approx 101^\circ \text{C}$.

^{a)} Estimated total errors.

^{b)} C-S-C=C torsion angle; $\tau = 0^\circ$ corresponds to a *synperiplanar* chain whose plane bisects the O=C=O angle.



anti

Vajda, E., Hargittai, I., Hnyk, D.: J. Mol. Struct. **162** (1987) 75.