

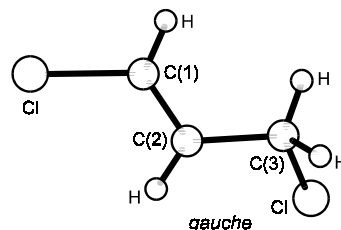
1141
ED

C₃H₄Cl₂

***trans*-1,3-Dichloro-1-propene**
(*E*)-1,3-Dichloro-1-propene

C_s (*syn*)
C₁ (*gauche*)
ClHC=CH-CClH₂

r_g	Å ^{a)}	θ_α	deg ^{a)}
C-H	1.072(12)	C(2)=C(1)-Cl	124(2)
C(1)=C(2)	1.338(6)	C(2)-C(3)-Cl	110(2)
C(2)-C(3)	1.508(8)	C(1)=C(2)-C(3)	121(1)
C(1)-Cl	1.716(5)	τ^b	119(7)
C(3)-Cl	1.801(6)		



The molecule exists as a mixture of *syn* (or near-*syn*) and *gauche* (83(10)% at 25 °C) conformers with the latter being lower in energy. The energy and entropy differences between the *syn* and *gauche* conformers were found to be 0.6(8) kcal mol⁻¹ and 2.5(20) cal mol⁻¹ K⁻¹, respectively. Measurements were made at nozzle temperatures of 25, 80 and 180 °C; the structure for 25 °C is listed.

^{a)} Twice the estimated standard errors.

^{b)} C(1)=C(2)-C(3)-Cl torsion angle of the *gauche* conformer; $\tau = 0^\circ$ for the *syn* form.

Shen, Q., Nunn, C.: J. Mol. Struct. **212** (1989) 143.