

1057
ED

$C_3H_2Cl_4$

(*E*)-1,2,3,3-Tetrachloro-1-propene

C_s (*syn*)
 C_s (*anti*)
 $CHCl=CCl-CHCl_2$

r_g	Å ^{a)}	θ_α	deg ^{a)}
C–H	1.047(36)	C–C=C	125.7(15)
C=C	1.340(11)	C(2)=C(1)–Cl	124.4(19)
C–C	1.489(12)	C(2)=C(1)–H	118 ^{b)}
C–Cl (mean)	1.751(2)	C(3)–C(2)–Cl	116.6(23)
$\Delta(C-Cl)$ ^{c)}	0.046(9)	C(2)–C(3)–Cl	111.8(20)
C(1,2)–Cl ^{d)}	1.728(5)	Cl–C(3)–Cl	110.3(7)
C(3)–Cl ^{d)}	1.774(5)	C(2)–C(3)–H	107 ^{b)}
		τ_1 ^{e)}	0 ^{b)}
		τ_2 ^{e)}	180 ^{b)}

The majority (87(13)%) of the molecules have a *syn* conformation, while the rest (13(13)%) have an *anti* conformation.
The nozzle was at 338 K.

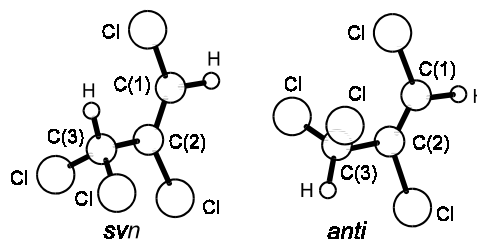
^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Assumed.

^{c)} $(C(3)-Cl) - (C(1,2)-Cl)$.

^{d)} Dependent parameter.

^{e)} τ_1 and τ_2 are the H–C(3)–C(2)=C(1) torsion angles in the *syn* and *anti* conformers, respectively.



Kaleem, H., Lund, A., Schei, S.H., de Meijere, A., Hagen, K., Stølevik, R.: J. Phys. Chem. **96** (1992) 8357.