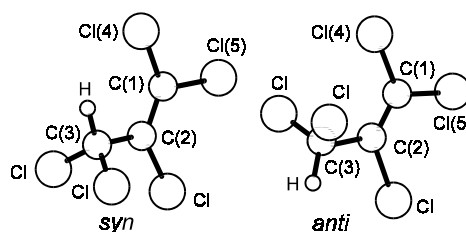


$r_g$	$\text{\AA}^a$	$\theta_\alpha$	$\text{deg}^a$
C–H	1.095 <sup>b)</sup>	C–C=C	124.6(13)
C=C	1.341(10)	C(2)=C(1)–Cl(4)	121.5(17)
C–C	1.497(13)	C(2)=C(1)–Cl(5)	123.2(12)
C–Cl (mean)	1.745(3)	C(3)–C(2)–Cl	114.4(18)
$\Delta(\text{C–Cl})^c$	0.041(11)	C(2)–C(3)–Cl	112.7(17)
C(1)–Cl <sup>e)</sup>	1.724(5)	Cl–C(3)–Cl	109.4(22)
C(3)–Cl <sup>e)</sup>	1.765(7)	C(2)–C(3)–H	109 <sup>b)</sup>
		$\phi_1^d$	0 <sup>b)</sup>
		$\phi_2^d$	180 <sup>b)</sup>

The majority (89(11)%) of the molecules have a *syn* conformation, while the rest (11(11)%) have an *anti* conformation. The nozzle was at 331 K.



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

<sup>b)</sup> Assumed.

<sup>c)</sup>  $\Delta(\text{C–Cl}) = (\text{C(3)–Cl}) - (\text{C(1,2)–Cl})$ .

<sup>d)</sup>  $\phi_1$  and  $\phi_2$  are the H–C(3)–C(2)=C(1) torsional angles in the *syn* and *anti* conformers, respectively.

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

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