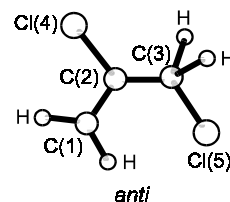


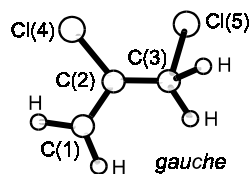
$r_a$	$\text{\AA}^a$	$\theta_\alpha$	$\text{deg}^a$
C–H	1.101(20)	C(3)–C(2)=C(1)	127.6(11)
$\Delta(C-H)^b$	0.005 <sup>c</sup>	C(3)–C(2)–Cl	110.2(10)
C(1)=C(2)	1.334(9)	C(2)–C(3)–Cl	113.1(12)
C(2)–C(3)	1.504(13)	H–C(3)–H	109.5 <sup>d</sup>
C–Cl	1.764(6)	C(2)–C(1)–H	120.0 <sup>d</sup>
$\Delta(C-Cl)^c$	0.024(39)	$\varphi^f$	124.0 <sup>d</sup>
		$\tau(gauche)^g$	108.9(34)
		$\phi^h$	10.4



The molecule exists as a mixture of two conformers with the chlorine atoms *anti* (54.7(82)%) or *gauche* to each other and with the *anti* form the more stable.

$$\Delta E^0 = E^0(gauche) - E^0(anti) = 0.7(3) \text{ kcal mol}^{-1}.$$

The measurements were made at 24, 90 and 273 °C. The results obtained from the data at 24 °C are listed.



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

<sup>b</sup>)  $\Delta(C-H) = [C(3)-H] - [C(1)-H]$ .

<sup>c</sup>) Determined by *R*-factor optimization.

<sup>d</sup>) Fixed at assumed value.

<sup>e</sup>)  $\Delta(C-Cl) = [C(3)-Cl] - [C(2)-Cl]$ .

<sup>f</sup>) Angle between the plane C(3)HH and C(2)–C(3) bond.

<sup>g</sup>) Torsional angle Cl–C–C–Cl;  $\tau = 0^\circ$  for the *anti* conformer.

<sup>h</sup>) The calculated value of the r.m.s. amplitude for the torsional oscillation in the *anti* form.

Trongmo, Ø., Shen, Q., Hagen, K., Seip, R.: J. Mol. Struct. **71** (1981) 185.