

r_a	\AA^a	θ_α	deg^a
C–H	1.103(5)	C–C=C	126.1(3)
C=C	1.337(2)	C–C–Cl	115.2(3)
C–C	1.472(4)	C=C–H	118.7(15)
C–Cl	1.745(2)	τ (<i>gauche</i>) ^b	52.3(97)

Mole fractions of the *gauche* conformer are 0.028(67), 0.073(63), and 0.161(58) at the 293, 395 and 593 K, respectively.

These quantities correspond to

$$\Delta E^\circ = E^\circ(\textit{gauche}) - E^\circ(\textit{anti}) = 2.2 \text{ (} 2\sigma = 1.1 \text{) kcal mol}^{-1} \text{ and}$$

$$\Delta S^\circ + R \ln 2 = S^\circ(\textit{gauche}) - S^\circ(\textit{anti}) + R \ln 2$$

$$= 0.35 \text{ (} 2\sigma = 2.2 \text{) cal mol}^{-1} \text{ K}^{-1}.$$

The nozzle temperatures were 293, 395 and 593 K.

The parameters for a model comprising averages of the results from the three temperatures are listed.

^a) Twice the estimated standard errors.

^b) Torsional angle C=C–C=C for the *gauche* conformer; $\tau = 180^\circ$ for the *anti* conformer.

Hagen, K., Hedberg, K., Neisess, J., Gundersen, G.: J. Am. Chem. Soc. **107** (1985) 341.

