

1539
ED

C₄H₄Cl₂

(Z,Z)-1,4-Dichloro-1,3-butadiene

C_{2h} (*anti*)
C₁ (*gauche*)
ClHC=CH-CH=CHCl

r_a	Å ^{a)}	θ_α	deg ^{a)}
C-H	1.105(7)	C=C-C	125.1(3)
C=C	1.342(2)	C=C-Cl	123.7(2)
C-C	1.456(4)	C=C-H	124.5(13)
C-Cl	1.731(3)	C-C-H	116(2)
		$\tau(\textit{gauche})$ ^{b)}	59(12) ^{c)}

The *anti* conformer ($\tau(\textit{anti}) = 180^\circ$ (assumed)) was found to be predominate, but a *gauche* form was also identified in small amounts: 4(3), 5(3) and 10(4)% at 283, 314 and 473 K, respectively. This corresponds to *anti-gauche* energy and entropy differences of

$$\Delta E^\circ = E^\circ(\textit{gauche}) - E^\circ(\textit{anti}) = 6(5) \text{ kJ mol}^{-1} \text{ and}$$

$$\Delta S^\circ = S^\circ(\textit{gauche}) - S^\circ(\textit{anti}) = -10(15) \text{ J mol}^{-1} \text{ K}^{-1}.$$

The nozzle temperatures were 283, 314 and 473 K. The parameters are listed for 314 K except for the torsional angle.

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

^{b)} Torsional angle C=C-C=C from the *syn* position.

^{c)} This value was refined only from data for 473 K.

Gundersen, G., Karlsson, F., Smith, Z.,
Thomassen, H.G.: Acta Chem. Scand., Ser. A
40 (1986) 522.

