

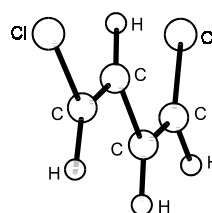
1540
ED

C₄H₄Cl₂

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

C_s (*anti*)
ClHC=CH-CH=CHCl

r_a	\AA^a	θ_α	deg^a
C-H	1.095(6)	C=C-C(<i>cis</i>)	125.6(6)
C=C	1.341(2)	C=C-C(<i>trans</i>)	122.0(6)
C-C	1.456(4)	C=C-Cl(<i>cis</i>)	123.9(3)
C-Cl	1.723(2)	C-C-Cl(<i>trans</i>)	122.9(4)
		τ^b	180.0 ^c



The measurements were made at different temperatures, but the structure of the prevalent *anti* conformer was determined using the 310 K data. The presence of about 5% of *syn* conformer with torsional angle of about 50° at 310 K could not be ruled out. The nozzle temperatures were 283, 310 and 473 K.

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

^b) Torsional angle C=C-C=C.

^c) Assumed.

Gundersen, G., Smith, Z., Thomassen, H.: Acta Chem. Scand., Ser. A **42** (1988) 477.