

1577 C₄H₅Cl

 ED, MW, *ab initio*
 calculations (HF/4-21G)

2-Chloro-1,3-butadiene

 C_s (*anti*)
 C₁ (*synclinal*)
 H₂C=CCl-CH=CH₂

r_a	Å ^{a)}	θ_α	deg ^{a)}
C(1)=C(2)	1.344(2)	C(1)=C(2)-C	123.5(1)
C(3)=C(4)	1.344(2)	C(4)=C(3)-C	125.6(2)
C(2)-C(3)	1.469(3)	C-C-Cl	117.2(1)
C-Cl	1.742(2)	$\tau(\text{anti})$ ^{b)}	180
C(1)-H(1)	1.098(2)	$\tau(\text{synclinal})$ ^{b)}	27(11)

Some *ab initio* constraints were used in defining the positions of hydrogen atoms and for a difference $r(\text{C}(1)=\text{C}(2)) - r(\text{C}(3)=\text{C}(4))$ parameter.

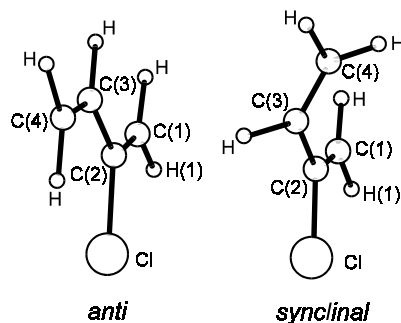
$E(\text{synclinal}) - E(\text{anti}) = 6.4(12) \text{ kJ mol}^{-1}$,

$S(\text{synclinal}) - S(\text{anti}) = -6(3) \text{ J K}^{-1} \text{ mol}^{-1}$.

Mole fractions of the *synclinal* conformer at different nozzle temperatures: 25(5)% at 655 K, 18(5)% at 565 K, 7(4)% at 298 K. Data at 298 K are listed.

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

^{b)} Torsional angle C(1)=C(2)-C(3)=C(4).

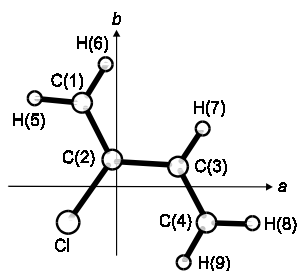


Gundersen, G., Thomassen, H.G., Boggs, J.E., Peng, C.: J. Mol. Struct. **243** (1991) 385.

MW

r_s	Å	θ_s	deg
C(1)=C(2)	1.349(5)	C(1)=C(2)-C(3)	123.9(6)
C(3)=C(4)	1.341(4)	C(4)=C(3)-C(2)	125.8(3)
C(2)-C(3)	1.447(9)	C(1)=C(2)-Cl	118.4(7)
C-Cl	1.741(9)	C(2)=C(1)-H(5)	121.7(5)
C(1)-H(5)	1.085(4)	C(2)=C(1)-H(6)	119.8(5)
C(1)-H(6)	1.069(5)	C(4)=C(3)-H(7)	119.3(7)
C(3)-H(7)	1.08(2)	C(3)=C(4)-H(8)	120.5(4)
C(4)-H(8)	1.079(2)	C(3)=C(4)-H(9)	120.1(2)
C(4)-H(9)	1.097(4)		

Atom	a_s [Å]	b_s [Å]
C(1)	-0.7299	1.7862
C(2)	-0.0465	0.6048
C(3)	1.3616	0.4758
C(4)	2.0467	-0.6745
H(5)	-1.8154	1.8404
H(6)	-0.1690	2.6990
H(7)	1.9003	1.4156
H(8)	3.1266	-0.6690
H(9)	1.5149	-1.6342
Cl	-1.0216	-0.8607



Cederbalk, P., Karlsson, F.: Acta Chem. Scand. Ser. A **35** (1981) 7.