

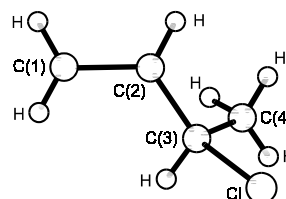
1683 **C₄H₇Cl**
ED, MM and *ab initio*

3-Chloro-1-butene

C₁ (all conformers)
H₂C=CH-CHCl-CH₃

(HF/4-21) calculations

r_a	\AA^a	θ_α	deg^a
C(1)=C(2)	1.337(6)	C(1)=C(2)-C(3)	122.9(21)
C(2)-C(3)	1.503(4)	C(2)-C(3)-C(4)	112.6(22)
C(3)-C(4)	1.522(5)	C(2)-C(3)-Cl	109.9(2)
C-Cl	1.813(4)	τ_1^b	120.3(21)
		τ_2^c	-119.4(29)



The most stable conformer (76(10)% and 62(10)% at 20 and 180 °C, respectively) has the C(3)-H bond eclipsing the C(2)=C(1) bond. The conformer with the C(3)-Cl bond eclipsing the C(2)=C(1) bond was also present. Molecular mechanics and *ab initio* calculations indicated the existence of the third conformer with the C(3)-C(4) bond eclipsing the C(2)=C(1) bond. Planarity of the H₂C=CH-C fragment and local C_{3v} symmetry of the CH₃ groups were assumed, and several angles or angular differences were adopted from results of theoretical calculations. The parameters of the predominant conformer (H eclipsing C=C) at 20 °C are listed.

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

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

^{c)} Dihedral angle C=C-C-Cl from the *syn* position.

Schei, S.H.: J. Mol. Struct. **118** (1984) 319.