

1681 $\text{C}_4\text{H}_7\text{Cl}$
ED, MM calculations

3-Chloro-2-methyl-1-propene

C_1 (*gauche*)
 C_s (*syn*)
 $\text{H}_2\text{C}=\text{C}(\text{CH}_3)-\text{CClH}_2$

r_a	\AA^a	θ_a	deg^a	
$\text{C}(1)=\text{C}(2)$	1.340(6)	$\text{C}(2)=\text{C}(1)-\text{H}$	119.2(39)	
$\text{C}(2)-\text{C}(3)$	1.492(4)	$\text{C}(2)-\text{C}(3)-\text{H}$	112.5 ^c	
$\Delta(\text{C}-\text{C})^b$	0.009 ^c	$\text{C}(2)-\text{C}(4)-\text{H}$	111.0 ^c	
$\text{C}-\text{Cl}$	1.791(5)	φ^d	120.5 ^e	
$\text{C}(1)-\text{H}$	1.098(9)		<i>gauche</i>	<i>syn</i>
$\Delta(\text{C}-\text{H})^b$	0.009 ^c	$\text{C}(1)=\text{C}(2)-\text{C}(3)$	121.5(12)	123 ^e
		$\Delta(\text{C}=\text{C}-\text{C})^b$	-0.5 ^e	-2.9 ^e
		$\text{C}-\text{C}-\text{Cl}$	112.8(4)	114.7 ^e
		τ^f	115.6(28)	

The molecule exists as a mixture of *gauche* (87(7)%) and *syn* (13(7)%) conformers.
The nozzle temperature was 20 °C.

^a) Twice the estimated standard errors.

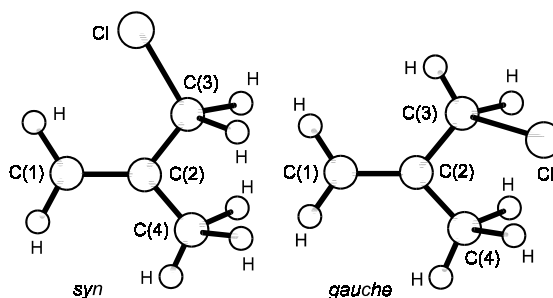
^b) $\Delta(\text{C}-\text{C}) = [\text{C}(2)-\text{C}(4)] - [\text{C}(2)-\text{C}(3)]$,
 $\Delta(\text{C}-\text{H}) = [\text{C}(3,4)-\text{H}] - [\text{C}(1)-\text{H}]$,
 $\Delta(\text{C}=\text{C}-\text{C}) = [\text{C}(1)=\text{C}(2)-\text{C}(3)] - [\text{C}(1)=\text{C}(2)-\text{C}(4)]$.

^c) Assumed.

^d) Angle between projections of
 $\text{C}-\text{Cl}$ and $\text{C}(3)-\text{H}$ on a plane
perpendicular to $\text{C}(2)-\text{C}(3)$ bond.

^e) Fixed at the values from molecular mechanics calculations.

^f) Torsional angle $\text{C}(1)=\text{C}(2)-\text{C}(3)-\text{Cl}$, $\tau = 0^\circ$ for *syn* conformer.



Schei, S.H.: Acta Chem. Scand. Ser. A **37** (1983) 671.