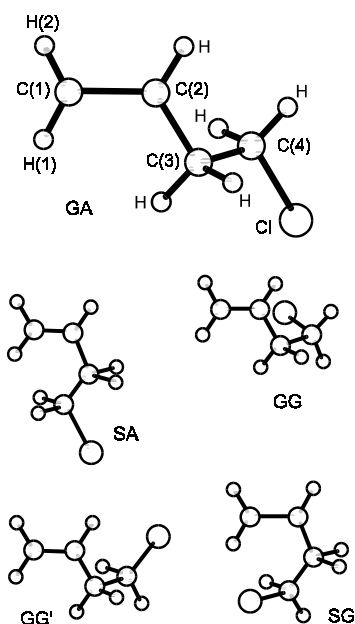


r_a	\AA^a	θ_α	deg^a
C(1)=C(2)	1.339(10)	C(1)=C(2)-C(3)	123.9(21) $^\circ$
C(2)-C(3)	1.508(5)	C(2)-C(3)-C(4)	112.0(21) $^\circ$
C(3)-C(4)	1.528 b	C(3)-C(4)-Cl	111.2(5) $^\circ$
C(4)-Cl	1.794(5)	C(2)=C(1)-H(1)	121.5 d
C-H	1.102(7)	C(2)=C(1)-H(2)	121.0 d
		C(1)=C(2)-H	119.0 d
		C(2)-C(3)-H	109.3 d
		C(4)-C(3)-H	110.2 d
		C(3)-C(4)-H	111.5 d
		Cl-C(4)-H	106.5 d
		C(1)=C(2)-C(3)-C(4)	123.1(26)
		C(2)-C(3)-C(4)-Cl	180.0 e

Molecular mechanics (MM) calculations showed that all the five distinct conformers (see figure) had energy differences of less than 7 kJ mol $^{-1}$. The most abundant form GA is found by the ED experiment to contribute 41(9)% to the conformational mixture, while the two forms with a planar arrangement of all the C atoms, SA and SG, comprise less than 15% together. The experimental data also show the presence of two forms having both the carbon skeleton and the Cl atom in the *gauche* position, GG and GG'. Their total amount is \approx 47%, but the separate amounts remain uncertain. The structure of the most abundant conformer, GA with a *gauche* carbon skeleton and an *anti* Cl atom, is listed. The nozzle temperature was 23 $^\circ\text{C}$.

- a) Twice the estimated standard errors including a systematic error.
 b) Assumed 0.02 \AA larger than C(2)-C(3).
 c) Conformational differences were assumed to be those derived from molecular mechanics calculations for the other forms.
 d) Value from MM calculations.
 e) Assumed.



Schei, S.H.: J. Mol. Struct. **128** (1985) 151.