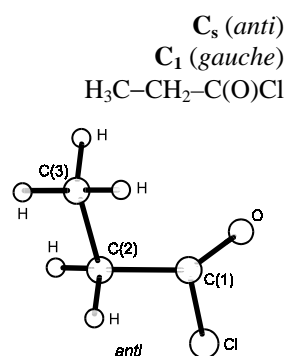


1194
ED, MW

C₃H₅ClO

Propionyl chloride

r_a	Å ^{a)}	θ_α	deg ^{a)}
C–H	1.123(11)	C–C=O	127.1(6)
C=O	1.181(5)	C–C–Cl	112.0(3)
C(2)–C(1)	1.522(13)	C–C–C	112.3(8)
C(2)–C(3)	1.526(15)	τ (<i>gauche</i>) ^{b)}	120.0(77)
C–Cl	1.800(6)		



The molecule exists as a mixture of *anti* and *gauche* conformers. The geometrical parameters listed in the table are consistent with the rotational constants observed only for the *anti* conformer. Energy difference $\Delta E = E(\textit{gauche}) - E(\textit{anti}) = 6(2) \text{ kJ mol}^{-1}$ and entropy difference $\Delta S = 7(6) \text{ J mol}^{-1} \text{ K}^{-1}$.

Different nozzle temperatures: 293, 367 and 488 K. The mole fraction of the *anti* conformer at 488 K was 0.53(11). The parameters at 488 K are listed.

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

^{b)} Torsional angle C–C–C–Cl; $\tau = 0^\circ$ for *anti* conformer.

Dyngeseth, S., Schei, S.H., Hagen, K.: J. Mol. Struct. **116** (1984) 257.