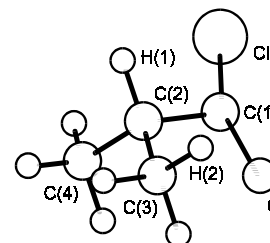


1688 **C₄H₇ClO**
ED, *ab initio* calculations
(HF/6-31G*)

Isobutyryl chloride
2-Methylpropionyl chloride

C₁ (*gauche*)
C_s (*syn*)
Cl(O)C–CH(CH₃)₂

r_g	Å ^{a)}	θ_α	deg ^{a)}
C–H (methyl)	1.108(6)	C(1)–C(2)–C(3)	109.7(8)
C(2)–H ^{b)}	1.088(6)	C(1)–C(2)–C(4)	109.9(8)
C(1)–Cl	1.804(4)	C(3)–C(2)–C(4)	113.8(27)
C(1)–C(2)	1.511(2)	C(2)–C(3,4)–H	111.7(18)
C(2)–C(3) ^{c)}	1.534(2)	C(2)–C(1)=O	127.3(7)
C(2)–C(4) ^{c)}	1.540(2)	C(2)–C(1)–Cl	113.6(5)
C=O	1.186(3)	C(1)–C(2)–H	106.8 ^{d)}
		ϕ_1 ^{e)}	130.1(37)
		ϕ_2 ^{f)}	60 ^{d)}



gauche

The molecule exists as a mixture of the *gauche* (82(12)%) and *syn* conformers. Local C_{3v} symmetry was assumed for the methyl groups. The parameters were given for the *gauche* conformer.

The nozzle temperature was 298 K.

^{a)} Twice the estimated standard errors.

^{b)} Dependent parameter. Difference between C(2)–H and C–H (methyl) was fixed at the *ab initio* value.

^{c)} Dependent parameter. Difference between this parameter and C(1)–C(2) was fixed at the *ab initio* value.

^{d)} Fixed at the *ab initio* value.

^{e)} Dihedral angle O=C–C–H; $\phi_1 = 0^\circ$ for the *syn* position.

^{f)} Dihedral angle H(1)–C(2)–C(3)–H(2).

Aarset, K., Faksnes, L.G., Nygård, I., Hagen, K.: J. Phys. Chem. **98** (1994) 2848.