

1695 C₄H₇FOMW, *ab initio* calculations
(RHF/3-21G, 6-31G*)**Isobutyryl fluoride**

2-Methylpropionyl fluoride

C₁ (*gauche*)F(O)C–CH(CH₃)₂

r_0	Å ^{a)}	θ_0	deg ^{a)}
C(2)–H	1.098(50)	C(1)–C(2)–H	105.5(50)
C(1)–C(2)	1.503(20)	O=C(1)–C(2)	128.7(30)
C(1)=O	1.180(20)	F–C(1)–C(2)	111.3(30)
C(1)–F	1.338(20)	F–C(1)=O	120.0(30)
C(2)–C(3)	1.527(20)	C(1)–C(2)–C(3)	110.7(30)
C(2)–C(3')	1.537(20)	C(1)–C(2)–C(3')	110.4(30)
C(3)–H ^{b)}	1.094(50)	C(3)–C(2)–C(3')	110.0(30)
		H–C(3)–C(2) ^{b)}	110.6(50)
		τ (F–C(1)–C(2)=O) ^{c)}	180.0 ^{d)}
		τ (O=C(1)–C(2)–H) ^{c)}	118.5(50)
		τ (C(3)–C(2)–C(1)–H) ^{c)}	118.5(50)
		τ (C(3')–C(2)–C(1)–H) ^{c)}	117.1(50)
		τ (C(3')–C(2)–C(1)–C(3) ^{c)}	124.4(50)
		τ (H(s)–C(3,3')–C(2)–C(1)) ^{b)} ^{c)} ^{e)}	180.0 ^{d)}
		τ (H(s)–C(3,3')–C(2)–H(a)) ^{c)}	120.0 ^{d)}

The observed rotational constants
were assigned to the *gauche* conformer,
 τ (F–C(1)–C(2)–H) = 61.5(50)°.

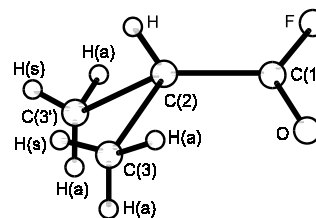
^{a)} Uncertainties were not estimated in the original paper.

^{b)} Average values for the methyl C–H bond distances and
angles are given.

^{c)} τ (A–B–C–D) denotes the dihedral angle between the
ABC and BCD planes.

^{d)} Assumed.

^{e)} H(s) represents H atoms *anti* to the C(1) atom with respect to the C(2)–C(3,3') bond.



Durig, J.R., Guirgis, G.A., Brewer, W.E., Baranovic, G.: J. Phys. Chem. **96** (1992) 7547.