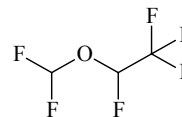


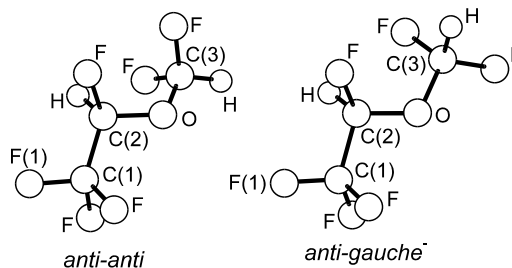
346 **C₃H₂F₆O**ED, *ab initio* and DFT
calculations**2-(Difluoromethoxy)-1,1,1,2-tetrafluoroethane****C₁ (*anti-anti*)****C₁ (*anti-gauche*[−])**

r_a	Å ^{a)}	θ_a	deg ^{a)}
O–C(2)	1.375(9)	C(1)–C(2)–O	105.8(19)
O–C(3)	1.354 ^{b)}	C(2)–O–C(3)	119.7(24)
C(1)–C(2)	1.528(10)	F–C(1)–F	107.4(5)
C(1)–F	1.336(3)	C(1)–C(2)–F	108.3(7)
C(2)–F	1.363 ^{b)}	O–C(2)–F	110.9 ^{c)}
C(3)–F	1.354 ^{b)}	O–C(3)–F	111.4 ^{c)}
C–H (mean)	1.100 ^{d)}	F–C(3)–F	106.3 ^{e)}
		tilt (CF ₃) ^{f)}	1.1 ^{e)}
		τ_1 ^{g)}	−146(4)
		τ_2 ^{h)}	176(11)
		τ_3 ⁱ⁾	−177.6 ^{e)}



The molecule was found to exist as a mixture of *anti-anti* and *anti-gauche*[−] conformers in the ratio of 80(8):20. These conformers possess near *anti* configuration of the C–C–O–C skeleton and *anti* or *gauche* configuration of C–O–C(3)–H unit. Local C_{3v} symmetry was assumed for the CF₃ group and C_{2v} for CHF₂. The structural parameters of the *anti-gauche*[−] conformer were coupled to those of the *anti-anti* conformer using the respective theoretical differences. All angles involving hydrogen atoms were assumed at the calculated values. The structural parameters are listed for the *anti-anti* conformer.

The nozzle was at room temperature.



^{a)} Three times the estimated standard errors.

^{b)} Differences in the O–C and C–F bond lengths were assumed at the values from MP2/6-311G(2d) calculations.

^{c)} Difference between the O–C–F and C(1)–C(2)–F bond angles was assumed at the value from MP2/6-311G(2d) calculations.

^{d)} Assumed.

^{e)} Assumed at the value from *ab initio* calculations.

^{f)} Angle between the C₃ axis of CF₃ group and C(1)–C(2) bond, away from the F atom at C(2).

^{g)} Torsional angle C(1)–C(2)–O–C(3), $\tau_1 = 0^\circ$ for the *syn* position.

^{h)} Torsional angle C(2)–O–C(3)–H, $\tau_2 = 0^\circ$ for the *syn* position.

ⁱ⁾ Torsional angle F(1)–C(1)–C(2)–O, $\tau_3 = 0^\circ$ for the *syn* position.

Hermann, A., Mack, H.-G., Oberhammer, H.: J. Fluor. Chem. **101** (2000) 223.