

1013 C₃F₄O₂ED, *ab initio* calculations(HF/3-21G, HF/6-31G**) **Difluoromalonyl difluoride**

r_a	Å ^{a)}	θ_α	deg ^{a)}
C–F(mean)	1.328(2)	C–C–C	110.6(5)
ΔCF ^{b)}	–0.02(1) ^{c)}	F(m)–C–F(m) ^{d)}	107.9(7)
C–F(c) ^{d)}	1.323(6) ^{e)}	C–C=O	128.2(7)
C–F(m) ^{d)}	1.333(6)	C–C–F(c)	107.7(5)
C–C	1.531(4)	F(c)–C=O ^{d)}	124.1(9) ^{e)}
C=O	1.168(3)	$\delta(C-C-C=O)$	120.0(16)

The molecule exists as a mixture of two conformers, *W-gauche* 70(15)% and *S-gauche* 30(15)%. The *S-gauche* conformer possesses C₁ symmetry with one C=O bond eclipsing one vicinal C–F bond and the other C=O bond eclipsing the opposite C–C bond. The parameters for the *W-gauche* conformer are listed. The nozzle was at room temperature.

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

^{b)} $\Delta CF = (C-F(c)) - (C-F(m))$; F(c), carbonyl fluorine; F(m), methylene fluorine.

^{c)} Fixed in the analysis but varied within the range of ± 0.01 Å.

^{d)} F(c), carbonyl fluorine; F(m), methylene fluorine.

^{e)} Dependent parameter.

Jin, A., Mack, H.-G., Waterfeld, A., Oberhammer, H.: J. Am. Chem. Soc. **113** (1991) 7847.

C₂ (*W-gauche*)
C₁ (*S-gauche*)
F(O)C–CF₂–C(O)F

