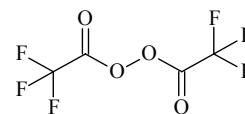


478 C₄F₆O₄ED, vibrational spectroscopy,
ab initio and DFT calculations**Bis(trifluoroacetyl) peroxide****C₂ assumed**

r_a	Å ^{a)}	θ_a	deg ^{a)}
O–O	1.426(10)	O–O–C	107.5(11)
O–C	1.361(12)	O–C=O	130.3(12)
C=O	1.190(4)	O–C–C	104.5(12)
C–C	1.547(6)	F–C–F	108.7(4)
C–F	1.326(3)	tilt(CF ₃) ^{b)}	0.5 ^{c)}
		τ (CF ₃) ^{d)}	–22.8(29)
		O–O–C=O ^{e)}	–11.5(30)
		C–O–O–C ^{e)}	86.5(32)



The molecule was found to exist as a *syn-syn* conformer. Local C_{3v} symmetry for the CF₃ groups and planarity of the carbonyl groups were assumed. According to the results of quantum chemical calculations (B3PW91/6-31G*, HF/6-31G* and MP2/6-31G*), the *syn-anti* conformer is less stable than *syn-syn* by 3.6 kcal mol^{–1} or more.

The nozzle was at room temperature.

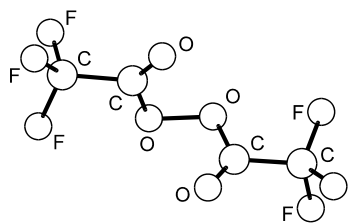
^{a)} Three times the estimated standard errors.

^{b)} Angle between the C₃ axis of the CF₃ group and the C–C bond direction toward the C=O bond.

^{c)} Assumed at the value from MP2/6-31G* calculations.

^{d)} Torsional angle of the CF₃ group around the C–C bond, $\tau = 0^\circ$ when one C–F bond is eclipsed with respect to the C=O bond.

^{e)} Zero degree for the *syn* position. A positive value means a counter-clockwise rotation of the nearer bond with respect to the farther bond.



Kopitzky, R., Willner, H., Hermann, A., Oberhammer, H.: Inorg. Chem. **40** (2001) 2693.