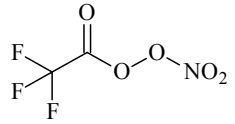
174 **$C_2F_3NO_5$** **Nitro trifluoroacetyl peroxide** **C_1**

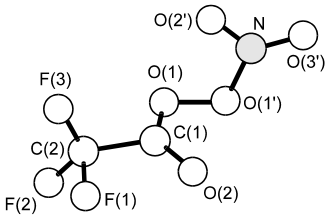
ED, MW, *ab initio* and DFT calculations



r_a	Å [a])	θ_a	deg [a])
C(1)=O(2)	1.180 [b])	O(1)–C=O(2)	126.7(18)
N=O(2',3') [c])	1.199(3)	O(1)–C–C	106.5(18)
C–C	1.535 [b])	O(2')=N=O(3')	136.0 [d])
O(1)–C(1)	1.360 [d])	Δ(ONO) [e])	7.2 [f])
O(1')–N	1.526(10)	O(1')–O(1)–C	107.6(20)
O(1)–O(1')	1.408(8)	O(1)–O(1')–N	109.9(15)
C–F [c])	1.328(3)	F–C–F	108.0(3)
		τ_1 [g])	–5.2 [f])
		τ_2 [h])	2.3 [f])
		τ_3 [i])	85.8(29)
		τ_4 [j])	–1.0 [f])

The molecule was found to exist as the *syn* conformer with C(1)=O(2) bond in the *syn* position with respect to the O(1)–O(1') bond. Local C_{3v} symmetry was assumed for the CF_3 group.
The nozzle was at room temperature.

[a]) Three times the estimated standard errors including a systematic error.
[b]) Constrained to the value for similar molecules.
[c]) Mean value.
[d]) Assumed.
[e]) [O–N=O(2')] – [O–N=O(3')].
[f]) Assumed at the value from B3PW91/6-311+G* or MP2/6-31G* calculations.
[g]) Torsional angle O(1')–O(1)–C(1)=O(2).
[h]) Torsional angle O(1)–O(1')–N=O(2').
[i]) Torsional angle C(1)–O(1)–O(1')–N.
[j]) Torsional angle O(2)=C–C–F(1).



Hermann, A., Niemeyer, J., Mack, H.-G., Kopitzky, R., Beuleke, M., Willner, H., Christen, D., Schäfer, M., Bauder, A., Oberhammer, H.: Inorg. Chem. **40** (2001) 1672.