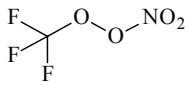
43 **CF_3NO_4** **Trifluoromethyl peroxonitrate** **C_1**

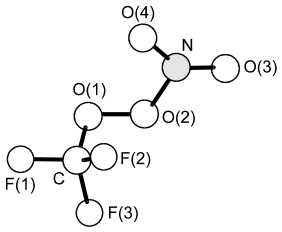
ED, *ab initio* and DFT calculations



r_a	Å [a])	θ_a	deg [a])
O–O	1.414(8)	O(1)–O(2)–N	108.4(13)
O–N	1.523(7)	O(2)–O(1)–C	107.7(14)
O–C	1.378[12] [b])	O(3)=N=O(4)	135.2(21)
N=O(3,4) [c])	1.187(3)	Δ(O–N=O) [d])	7.9 [e])
C–F	1.322(3)	F–C–F	108.8(9)
		tilt(CF_3) [f])	4.6 [e])
		τ(C–O–O–N) [g])	105.1(16)
		τ[O–O–N=O(3)] [g])	178.3 [e])
		τ[O–O–C–F(l)] [g])	181.8 [e])

Local C_{3v} symmetry was assumed for the CF_3 group. The O–NO_2 group was assumed to be planar.

The nozzle was at room temperature.



[a]) Three times the estimated standard errors including a systematic error.

[b]) Not refined but varied within the given range.

[c]) N=O(3) and N=O(4) bond lengths were assumed to be equal.

[d]) [O(2)–N=O(4)] – [O(2)–N=O(3)].

[e]) Assumed at the value from B3PW91/6-311+G* calculations.

[f]) Angle between the C_3 axis and the O–C bond direction away from the O(1)–O(2) bond.

[g]) Zero degree for the *syn* position.

Kopitzky, R., Willner, H., Mack, H.-G., Pfeiffer, A., Oberhammer, H.: Inorg. Chem. **37** (1998) 6208.