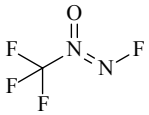
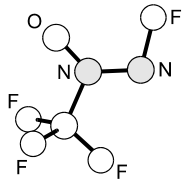
48 **CF_4N_2O** **(*Z*)-1-Fluoro-2-(trifluoromethyl)diazene 2-oxide** **C_s**

ED, *ab initio* and DFT calculations



r_a	Å [a])	θ_a	deg [a])
N=N	1.287(15)	N=N=O	131.2(13)
N=O	1.231(6)	N=N–F	103.5(13)
N–F	1.380(6)	N=N–C	114.0(12)
N–C	1.498(6)	F–C–F	110.4(6)
C–F	1.312(3)	tilt(CF_3) [b])	2.8 [c])

Local C_{3v} symmetry was assumed for the CF_3 group.
One C–F bond is eclipsed with respect to the N=N bond.
The nozzle was at room temperature.



[a]) Three times the estimated standard errors.
[b]) Angle between the C_3 axis of the CF_3 group and the N–C bond direction, away from the N=N bond.
[c]) Assumed at the value from B3LYP/6-31G* calculations.

Leibold, C., Foropoulos, J., Marsden, H.M., Shreeve, J.M., Oberhammer, H.: Inorg. Chem. **41** (2002) 6125.