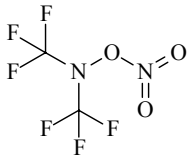
182 $C_2F_6N_2O_3$ **1,1,1-Trifluoro-*N*-(nitrooxy)-*N*-(trifluoromethyl)-methanamine** C_s assumed

ED, *ab initio* and DFT calculations

O-Nitro-*N*,*N*-bis(trifluoromethyl)hydroxylamine

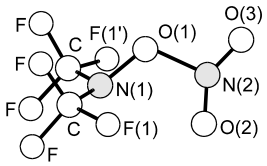


r_a	Å [a])
C–F [b])	1.327(1)
C–N(1)	1.408(8)
N(1)–O(1)	1.392(18)
N=O(2,3) [b])	1.192(4)
O(1)–N(2)	1.597(16)

θ_a	deg [a])
C–N–C	118.9(8)
C–N–O(1)	110.6(19)
N–O(1)–N	106.9(25)
$\sum\alpha$(N(1)) [c])	340.1(21)
O(1)–N=O(2,3) [b])	110.8(17)
O(1)–N=O(2)	114.2(21) [d])
O(1)–N=O(3)	107.5(21) [d])
O(2)=N=O(3)	138.4(24)
F–C–F [b])	108.1(18)
tilt(CF_3) [e])	2.8 [f])
C–N–C–F(1)	172.4(24)

Local C_{3v} symmetry was assumed for the CF_3 groups. The $NONO_2$ skeleton was found to be planar.
The nozzle was at room temperature.

[a]) Three times the estimated standard errors.
[b]) Mean value.
[c]) Sum of the bond angles around the N(1) atom.
[d]) Difference between the O(1)–N=O bond angles was assumed at the value from B3LYP/6-31G* calculations.
[e]) Angle between the C_3 axis of CF_3 group and the N–C bond direction, in the CNC plane and away from the opposite N–C bond.
[f]) Assumed at the value from B3LYP/6-31G* calculations.



Trautner, F., Kirsch, R., Minkwitz, R., Oberhammer, H.: Inorg. Chem. **41** (2002) 7049.