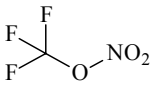
42 **CF_3NO_3** **Trifluoromethanol nitrate** **C_s**

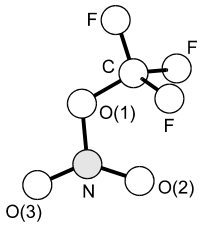
ED, *ab initio* and DFT calculations

Trifluoromethyl nitrate



r_a	Å [a])	θ_a	deg [a])
N–O(1)	1.493(6)	O(1)–N=O(2)	115.0(11)
N=O(2)	1.187(2) [b])	O(1)–N=O(3)	107.8(12)
N=O(3)	1.183(2) [b])	N–O(1)–C	117.0(6)
O(1)–C	1.397(8)	F–C–F	108.8(4)
C–F	1.321(2)	tilt(CF_3) [c])	5.4 (8)

Local C_{3v} symmetry was assumed for the CF_3 group.
The nozzle was at room temperature.



[a]) Three times the estimated standard errors.
[b]) Difference between the N=O(2) and N=O(3) bond lengths was assumed at the value from B3LYP/6-31G* calculations.
[c]) Tilt angle between the C_3 axis of the CF_3 group and the O–C bond direction, defined positive when the CF_3 group is tilted away from O(2).

Sander, S., Willner, H., Oberhammer, H., Argüello, G.A.: Z. Anorg. Allg. Chem. **627** (2001) 655.