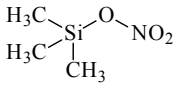
453 **$C_3H_9NO_3Si$** **Trimethylsilanol nitrate** **C_s** assumed

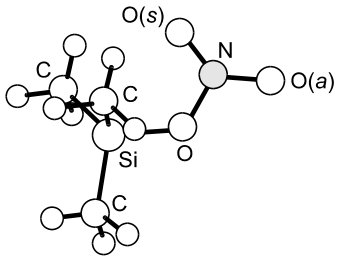
ED, *ab initio* and DFT calculations

Trimethylsilyl nitrate



r_a	Å [a])	θ_a	deg [a])
C–H	1.095(6)	C–Si–C	112.1(6)
N=O (mean)	1.210(2)	Si–O–N	120.1(9)
Δ(N=O) [b])	0.020[20] [c])	O–N=O (mean)	111.5(5)
N=O(*a*)	1.200(11)	Δ(O–N=O) [d])	1.6(30)
N=O(*s*)	1.220(11)	O–N=O(*a*)	112.3(16)
N–O	1.383(5)	O–N=O(*s*)	110.7(16)
Si–O	1.715(4)	H–C–H	108.0 [e])
Si–C	1.820(2)	tilt($SiMe_3$) [f])	5.3(12)

Local C_{3v} symmetry and no tilt were assumed for the methyl groups. Local C_{3v} symmetry and staggered orientation with respect to the NO_3 group were assumed for the $Si(CH_3)_3$ group. The nozzle was at room temperature.



[a]) Three times the estimated standard errors including a systematic error.
[b]) [N=O(*s*)] – [N=O(*a*)].
[c]) Not refined, but varied within the given range.
[d]) [O–N=O(*a*)] – [O–N=O(*s*)].
[e]) Estimated according to the results of HF/3-21G* and B3LYP/6-31G* calculations.
[f]) Angle between the C_3 axis of the $Si(CH_3)_3$ group and the Si–O bond, in the SiON plane and away from the O(*s*) atom.

Hertel, T., Jakob, J., Minkwitz, R., Oberhammer, H.: Inorg. Chem. **37** (1998) 5092.