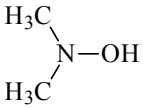
311 **C_2H_7NO** ***N*-Hydroxy-*N*-methylmethanamine** **C_s** assumed

ED, *ab initio* calculations

N,*N*-Dimethylhydroxylamine

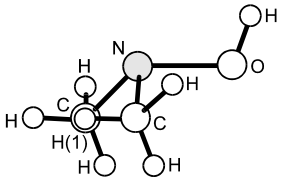


r_α	Å [a])
N–O	1.448(11)
N–C	1.463(7)
C–H	1.116(6)
O–H	1.011(25)

θ_α	deg [a])
C–N–C	110.4(15)
C–N–O	106.7(4)
N–C–H	107.4(7)
N–O–H	101.1(15)
twist(CH_3) [b])	9.3(13)
tilt(CH_3) [c])	–2.3(12)

According to results of MP2/6-311G** calculations ($\Delta E = E(syn) - E(anti) = 11.8$ kJ mol^{-1}) [1], the molecule was assumed to exist as *anti* conformer (O–H group is *anti* with respect to the bisector of the C–N–C angle). Local C_{3v} symmetry was assumed for the CH_3 groups. The ED analysis was carried out by applying flexible restraints based on the results of *ab initio* calculations.
The nozzle was at 293 K.

[a]) Estimated standard errors.
[b]) H(1)–C–N–O torsional angle from the *anti* position, positive value for the clockwise rotation.
[c]) Angle between the C–N bond and the C_3 axis of the methyl group in the CNC plane; positive values represent displacements of the CH_3 groups away from one another.



Mitzel, N.W., Smart, B.A., Parsons, S., Robertson, H.E., Rankin, D.W.H.: J. Chem. Soc., Perkin Trans. **2** (1996) 2727.
[1] Gange, D.M., Kallel, E.A.: J. Chem. Soc., Chem. Commun. (1992) 824.