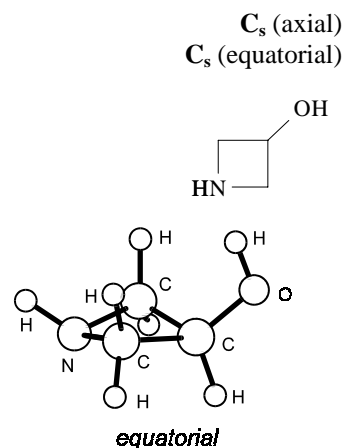


1327 **C₃H₇NO**
ED, *ab initio* calculations
(HF/6-31G**)

3-Azetidinol

r_g	Å ^{a)}	θ_α	deg ^{a)}
O-H	0.971(26)	C-C-C	84.9(9)
N-H	1.033(70)	H-C-H	108.8 ^{b)}
C-H	1.112(19)	C-O-H	110.0 ^{b)}
C-O	1.406(4)	C-C(O)-H	111.5 ^{b)}
C-N	1.486(2)	C-N-H	116.6 ^{b)}
C-C	1.562(7)	C-C-O ^{c)}	117.2(5)
		θ ^{d)}	153.2(23)
		ϕ_1 ^{e)}	180.0 ^{b)}
		ϕ_2 ^{f)}	180.0 ^{b)}



The molecule exists as a mixture of two conformers with the OH group either pseudoequatorial (77(8)%) or pseudoaxial to the four-membered ring.

The temperature of the measurement was 100 °C.

^{a)} Twice the estimated standard errors.

^{b)} Assumed.

^{c)} For the pseudoequatorial conformer.

^{d)} Angle between the CCC and the CNC planes.

^{e)} H-O-C-H torsion angle in the equatorial conformer.

^{f)} H-O-C-H torsion angle in the axial conformer.

Hagen, K., Volden, H.V., Anthoni, U., Christophersen, C., Gajhede, M., Nielsen, P.H.: J. Phys. Chem. **95** (1991) 1597.