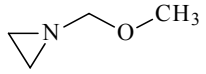
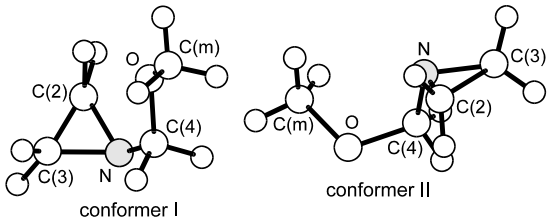
589 **C_4H_9NO** **1-(Methoxymethyl)aziridine** **C_1** (conformer I)
ED, *ab initio* and DFT calculations **C_1** (conformer II)



r [a])	Å [b])	θ [a])	deg [b])
C(4)–O	1.421(7)	C–O–C	114.3(22)
C(m)–O [c])	1.409(7)	O–C–N	113.4(12)
C(2)–N	1.456(9)	C(2)–N–C(4)	116.8(4)
C(4)–N [c])	1.434(9)	C(2)–N–C(3)	61.9(4)
C–H (average)	1.098(4)	τ(C–N) [d])	–11(4)
C–C [c])	1.500(9)	τ(C–O) [e])	167(6)

The molecule was found to exist as a mixture of conformers I (67(12)%) and II (33(12)%). Local C_{3v} symmetry was assumed for the methyl group and C_{2v} for the aziridine unit. Structural parameters are listed for conformer I. Independent parameters of conformer II were assumed to be equal to the corresponding parameters of conformer I. Torsional angles of conformer II were determined to be τ(C–N) = 120(7)° and τ(C–O) = 80(9)°.
The nozzle was at room temperature.



[a]) Unidentified, possibly r_a and θ_{h1}.
[b]) Estimated standard errors.
[c]) Dependent parameter, differences in the C–O and C–N bond lengths were assumed at the values from B3LYP/cc-pVTZ calculations.
[d]) Torsional angle O–C(4)–N–C(2), 0° for the *syn* position.
[e]) Torsional angle N–C(4)–O–C(m), 0° for the *syn* position.

Shishkov, I.F., Khristenko, L.V., Vilkov, L.V., Dakkouri, M., Kadorkina, G.K., Dormov, P.E., Kostyanovsky, R.G.: Mendeleev Commun. (2000) 217.