425 **C_3H_7N** ***cis*-2-Methylaziridine** **C_1**

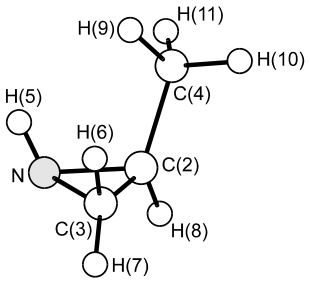
ED, MW, *ab initio* calculations

cis-Propyleneimine

r_z	Å [a])
N–C(2)	1.479(5)
N–C(3)	1.482(5)
N–H	1.014(18)
C(2)–C(3)	1.490(14)
C(2)–C(4)	1.505(9)
C–H	1.089(4)

θ_z	deg [a])
N–C(2)–C(4)	120.2(11)
C–C–C	119.6(10)
C–N–C	60.5 [b])
N–C–C	59.7 [b])
C(2)–N–H	107.6(22)
C(3)–N–H	107.7(22)
N–C–H(6)	119.9(13)
N–C–H(7)	116.1(13)
C–C–H(6)	118.6(13)
C–C–H(7)	121.7(13)
N–C–H(8)	113.7(13)
C(3)–C(2)–H(8)	118.7(13)
C–C–H(9)	110.4(15)
C–C–H(10,11)	111.1(15)
H(8)–C–C–H(9)	–178.4 [c])

The molecule was assumed to exist as a mixture of *trans* and *cis* isomers in the ratio 69:31 estimated by *ab initio* (MP2/6-31G**) method. The barrier height to the N–H inversion was calculated to be 20.0 kcal mol^{-1}. The intra- and inter-conformational differences of some structural parameters were assumed at the values from MP2/6-31G** calculations. The nozzle was at 24 °C.



[a]) Three times the estimated standard errors.
[b]) Dependent parameter.
[c]) Assumed at the MP2/6-31G** value.

Fujiwara, H., Egawa, T., Takeuchi, H., Konaka, S.: J. Mol. Struct. **380** (1996) 63.