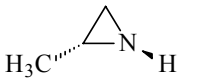
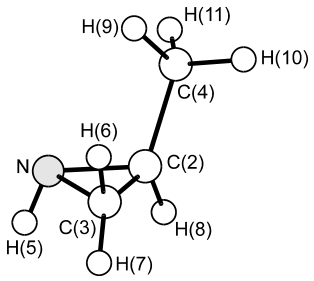
426 **C_3H_7N** ***trans*-2-Methylaziridine** **C_1**
ED, MW, *ab initio* calculations
trans-Propyleneimine



r_z	Å [a])
N–C(2)	1.479(5)
N–C(3)	1.481(5)
N–H	1.012(18)
C(2)–C(3)	1.491(14)
C(2)–C(4)	1.503(9)
C–H (ring)	1.090(4)
C(4)–H	1.088(4)

θ_z	deg [a])
N–C(2)–C(4)	116.2(11)
C–C–C	120.7(11)
C–N–C	60.5 [b])
N–C–C	59.7 [b])
C(2)–N–H	108.5(22)
C(3)–N–H	108.0(22)
N–C–H(6)	115.7(13)
N–C–H(7)	120.2(13)
C–C–H(6)	120.7(13)
C–C–H(7)	119.6(13)
N–C–H(8)	118.0(13)
C(3)–C(2)–H(8)	116.9(13)
C–C–H(9)	109.6(15)
C–C–H(10)	111.0(15)
C–C–H(11)	110.9(15)
H(8)–C–C–H(9)	179.6 [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.
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