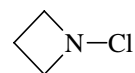


1239 **C₃H₆ClN**
ED, MW, vibrational
spectroscopy

1-Chloroazetidine
N-Chloroazetidine

C_s assumed



	r_g [Å] ^{a)}	r_z [Å] ^{a)}	θ_z	deg ^{a)}
N–C	1.487(3)	1.485(3)	C–N–C	90.4(4)
C–C	1.554(3)	1.551(3)	C–N–Cl	115.0(2)
N–Cl	1.745(2)	1.741(2)	N–C–H(1)	115.8(23)
C–H	1.114(4)	1.098(4)	N–C–H(2)	111.0(21)
			C–C–H(1)	119.4(21)
			C–C–H(2)	109.6(32)
			C–C–C	85.6 ^{b)}
			H–C–H ^{c)}	111.4 ^{b)}
			ϕ ^{d)}	32.4(17)
			τ ^{e)}	5.5 ^{b)}

Only the equatorial conformer was found at room temperature.

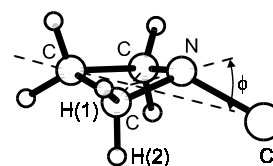
^{a)} Three times the estimated standard errors.

^{b)} Dependent parameter.

^{c)} All H–C–H angles were assumed to be equal.

^{d)} Ring dihedral angle (see figure).

^{e)} Angle between the bisectors of the adjacent H–C–H and C–C–C angles.



Fujiwara, H., Egawa, T., Takeuchi, H., Konaka, S.: J. Mol. Struct. **301** (1993) 113.