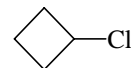


1686 **C₄H₇Cl**
ED, MW, *ab initio*
calculations (HF/4-21G)

Chlorocyclobutane
Cyclobutyl chloride

C_s (equatorial)
C_s (axial)

r_α	\AA^a	θ_α	deg a
C–C (average)	1.553(2)	H–C–Cl	107(2)
$\Delta(\text{C–C})^b$	0.015 c	H–C–H	110(2)
C–Cl	1.788(4)	C(4)–C(1)–C(2) (eq)	89.0 c
C–H	1.082(4)	C(4)–C(1)–C(2) (ax)	89.4 c
		φ (eq) d	30(5)
		φ (ax) d	–21(8)
		α (eq) e	132(1)
		α (ax) e	121(5)



The equatorial and axial conformers are found to be present.

$$\Delta H^\circ = H^\circ(\text{axial}) - H^\circ(\text{equatorial}) \approx 4...5 \text{ kJ mol}^{-1}, \Delta S^\circ = S^\circ(\text{ax}) - S^\circ(\text{eq}) \approx 0 \text{ J mol}^{-1} \text{ K}^{-1}.$$

Different nozzle temperatures, 21, 220 and 430 °C.

The temperature-average values are given

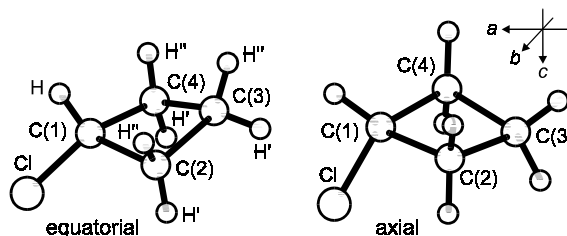
a) Twice the estimated standard errors, some of them slightly larger than those of the original data or roughly estimated.

b) $[\text{C}(2)\text{--C}(3)] - [\text{C}(1)\text{--C}(2)]$.

c) Assumed.

d) Ring puckering angle, dihedral angle between the C(2)C(1)C(4) and C(2)C(3)C(4) planes.

e) Angle between the C(2)C(1)C(4) plane and the C(1)–Cl bond.



Jonvik, T.: J. Mol. Struct. **172** (1988) 213.

MW

C_s (equatorial)

r_0	\AA	θ_0	deg
C(1)–C(2)	1.525(10)	H–C–Cl	114(3)
C(2)–C(3)	1.550(10)	C(4)–C(1)–C(2)	90.8(10)
C–Cl	1.775(10)	H'–C(2)–H''	112(2)
C(1)–H	1.10(2)	H'–C(3)–H''	110(2)
C(2)–H a)	1.085(20)	H'–C(2)–C(1)	114(2)
C(3)–H a)	1.10(2)	H''–C(2)–C(1)	115(2)
		φ^b	135(2)
		α^c	20(2)

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$	$c_s [\text{\AA}]$
Cl	1.661	0.0	0.092
C(1)	0.028	0.0	–0.454
H	–0.16	0.0	–1.548
C(2,4)	–0.980	± 1.086	0.033
H'	–0.667	± 1.527	0.973
H''	–1.172	± 1.839	–0.725
C(3)	–2.077	0.0	0.169
H'	–2.592	0.0	1.141
H''	–2.814	0.0	–0.648

a) There is no difference in the distances of C–H' and C–H''.

b) Angle between the C(2)C(1)C(4) plane and the C(2)C(3)C(4) plane.

c) Angle between the C(2)C(1)C(4) plane and the C(1)–Cl bond.

Kim, H., Gwinn, W.D.: J. Chem. Phys. **44** (1966) 865.