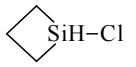
416 **C_3H_7ClSi** **1-Chlorosilacyclobutane** **C_s** (equatorial)
C_s (axial)

ED, *ab initio* and DFT calculations



r_a	Å [a])
Si–C	1.864(2)
Si–Cl	2.059(3)
Si–H	1.470(12)
C–C	1.591(5)
C–H	1.112(4)

θ_a	deg [a])	
H–Si–Cl	106.0(6)	
C–Si–C	80.7(14)	
C–C–Si	85.0 [b])	
C–C–C	98.7(22)	
H–C–H	110.0 [b])	
	equatorial	axial
φ [c])	34.2(25)	21.5(50)
γ_1 [d]) [e])	0.0 [b])	9.6 [b])
γ_2 [e]) [f])	10.0 [b])	10.0 [b])
γ_3 [e]) [g])	7.9 [b])	7.9 [b])

The equatorial conformer was found to be lower in energy than the axial conformer by 3.92(23) kJ mol^{-1}, corresponding to the ratio of the conformers eq : ax = 83(6) : 17(6). The nozzle was at room temperature.
According to MP2/6-31G** calculations, the energy difference is equal to 3.43 kJ mol^{-1}.

[a]) Three times the estimated standard errors.
[b]) Assumed.
[c]) Ring puckering angle.
[d]) Rocking angle of the H–Si–Cl group.
[e]) Rocking angles are positive when the two axial bonds attached to the diagonal atoms are brought closer to each other by rocking.
[f]) Rocking angle of the H–C(2)–H group.
[g]) Rocking angle of the H–C(3)–H group.

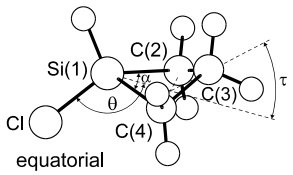
Dakkouri, M., Grosser, M.: J. Mol. Struct. **559** (2001) 7.

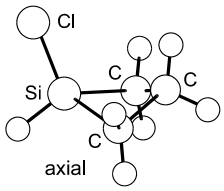
MW **C_s** (equatorial)
C_s (axial)

r_e	Å
Si–C	1.876(2)
Si–Cl	2.068(2)

θ_e	deg
τ_0 [a])	38.0(10)
α_0 [a])	82.3(4)
$\Delta\alpha$ [a])	–2.3(4)
θ_0 [a])	125.4(3)
$\Delta\theta$ [a])	–3.1(2)

Atom	$\lvert a_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
Cl (equatorial)	1.927	0.196
Cl (axial)	1.757	0.360





The potential function of the ring puckering motion was determined: Four vibrational states are localized in the equatorial well, two vibrational states in the axial well, and all remaining higher energy states lie above the interconversion barrier. The equatorial conformer is more stable than the axial one by 185(40) cm^{-1}.

[a]) Parameters of the flexible model, which is based on the potential function: $V(\tau) = (1/2)\Delta E(\tau/\tau_0) + B_0[1 - (\tau/\tau_0)^2]^2$ with $\alpha(\tau) = \alpha_0 + \Delta\alpha(\tau/\tau_0)^2$ and $\theta(\tau) = \theta_0 + \Delta\theta(\tau/\tau_0)$ and $B_0 = 330(15)$ and $\Delta E = 228(8)$ cm^{-1}. See Figure for the definitions of the angles.

Favero, L.B., Maccaferri, G., Caminati, W., Grosser, M., Dakkouri, M.: J. Mol. Spectrosc. **176** (1996) 321.