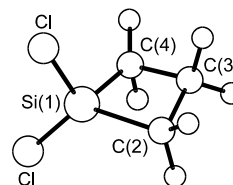


396 **C₃H₆Cl₂Si**ED, *ab initio*
calculations**1,1-Dichloro-1-silacyclobutane**

1,1-Dichloro-1-siletane

C_s

r_a	Å ^{a)}	θ_a	deg ^{a)}
Si–Cl(ax)	2.043(2) ^{b)}	Cl–Si–Cl	105.2(8)
Si–Cl(eq)	2.038(2) ^{b)}	C–Si–C	81.1(10)
Si–C	1.860(3)	Si–C–H(ax)	109.7(54)
C–C	1.557(4)	Si–C–H(eq)	118.9(54)
C–H	1.091(8)	C–C(2)–H(ax)	100.9(63)
		C–C(2)–H(eq)	105.3(63)
		H–C(3)–H	108.0 ^{c)}
		C–C–C	102.0(15)
		Si–C–C	85.7(12)
		H–C(2)–H	125.7(91)
		Cl(ax)–Si–C	114.7(4)
		Cl(eq)–Si–C	120.2(4)
		H(ax)–C(3)–C	110.0 ^{c)}
		H(eq)–C(3)–C	113.4 ^{c)}
		δ [H–C(2)–H] ^{d)}	5.1 ^{c)}
		δ_1 ^{e)}	4.1 ^{c)}
		δ_2 ^{f)}	3.0 ^{c)}
		ρ (ax) ^{g)}	3.0(30)
		ρ (eq) ^{g)}	21.5(40)
		ϕ_e ^{h)}	25.9(26)



The ring puckering was described as a large-amplitude motion using dynamic model with the potential function $V(\varphi) = V_0[(\varphi/\varphi_e)^2 - 1]^2$. The barrier height V_0 was found to be equal to 0.57(32) kcal mol^{−1}.

The nozzle temperature was 20 °C.

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

^{b)} Difference between the Si–Cl(ax) and Si–Cl(eq) bond lengths was assumed at the value from HF/6-311+G** calculations.

^{c)} Assumed from HF/6-311+G** calculations.

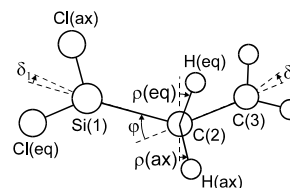
^{d)} Angle between the bisector of the H–C(2)–H angle and the SiC(2)C(3) plane.

^{e)} Angle between the bisector of the Cl–Si–Cl angle and the C(2)SiC(4) plane, see figure.

^{f)} Angle between the bisector of the H–C(3)–H angle and the C(2)C(3)C(4) plane, see figure.

^{g)} See Newman projection for definition.

^{h)} Ring puckering angle for the equilibrium conformation.



Novikov, V.P., Tarasenko, S.A., Samdal, S., Vilkov, L.V.: J. Mol. Struct. **445** (1998) 207.

Replaces [II/25C \(3, 1248\)](#)