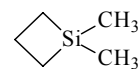


678 **C₅H₁₂Si**ED, *ab initio*
calculations**1,1-Dimethyl-1-silacyclobutane****C_s**

r_a	$\text{\AA}^a)$	θ_a	$\text{deg}^a)$
Si–C(m)	1.872(2)	C(2)–Si–C(4)	79.2(11)
Si–C(2,4)	1.885(2)	C(m)–Si–C(m)	109.9(47)
C–C	1.563(4)	Si–C(m)–H	113.9(17)
C–H (average)	1.115(3)	Si–C–H(ax)	108.6(32)
		Si–C–H(eq)	118.2(32)
		C–C(2)–H(ax)	107.2(32)
		C–C(2)–H(eq)	112.1(32)
		C–C–C	99.9(14)
		Si–C–C	86.8(6)
		H–C(3)–H	107.6 ^{b)}
		$\delta(\text{Si})$ ^{c)}	3.9 ^{b)}
		$\delta(\text{C}(3))$ ^{d)}	4.2 ^{b)}
		$\delta(\text{C}(2))$ ^{e)}	4.2 ^{b)}
		ρ_{ax} ^{f)}	0.9 ^{g)}
		ρ_{eq} ^{f)}	14.2 ^{g)}
		φ_e ^{h)}	29.7(45)

Large-amplitude ring puckering motion was described using a dynamic model. The relaxation of the molecular geometry was estimated by the HF/6-311G** method. The potential function was found to be well described as $V(\varphi) = V_0[(\varphi/\varphi_e)^2 - 1]^2$, where $V_0 = 1.3(12) \text{ kcal mol}^{-1}$ is the energy difference between the planar and equilibrium configurations. The nozzle temperature was 20 °C.

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

^{b)} Assumed using the results of HF/6-311G** calculations.

^{c)} Angle between the bisector of the C(m)–Si–C(m) angle and the C(2)SiC(4) plane. See figure.

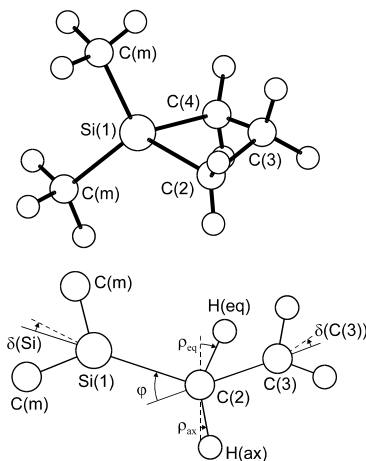
^{d)} Angle between the bisector of the H–C(3)–H angle and the CCC plane. See figure.

^{e)} Angle between the bisector of the H–C(2)–H angle and the SiCC plane.

^{f)} Deviations of the C–H(eq) and C–H(ax) bonds from the position where the bisector of the Si–C–C angle lies in the H(eq)CH(ax) plane. See figure.

^{g)} Dependent parameter.

^{h)} Ring puckering angle (acute dihedral angle between the C(2)SiC(4) and CCC planes) in the equilibrium position.



Novikov, V.P., Tarasenko, S.A., Samdal, S., Shen, Q., Vilkov, L.V.: J. Mol. Struct. **477** (1999) 71.

See also: Novikov, V.P., Tarasenko, S.A., Samdal, S., Vilkov, L.V.: Zh. Strukt. Khim. **41** No.2 (2000) 269; J. Struct. Chem. (Engl. Transl.) **41** (2000) 217.

Replaces [II/25D \(3, 2074\)](#)