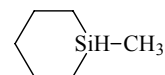


755 C₆H₁₄SiED, ¹³C NMR, *ab initio*
and DFT calculations**1-Methylsilacyclohexane**C_s assumed (equatorial)C_s assumed (axial)

<i>r_a</i>	Å ^{a)}	<i>θ_a</i>	deg ^{a)}
Si–C (mean)	1.865(2)	C(2)–Si–C(6)	102.8(20)
Si–C(2)	1.867(4) ^{b)}	C(3)–C(4)–C(5)	116.7(34)
Si–C(7)	1.862(4) ^{b)}	Si–C(2)–C(3)	110.5(16)
C–C (mean)	1.531(2)	C(2)–C(3)–C(4)	112.4(27)
C(2)–C(3)	1.534(3) ^{b)}	C(2)–Si–C(7)	112.5(24)
C(3)–C(4)	1.528(3) ^{b)}	C(2)–Si–H	108.8 ^{c)}
C–H	1.104(3)	H–C–H (ring)	106.0 ^{c)}
Si–H	1.510 ^{d)}	H–C–H (methyl)	107.7 ^{c)}
		<i>φ</i> ₁ ^{e)}	46.0(31)
		<i>φ</i> ₂ ^{f)}	55.9(20)
		Si–C(2)–C(3)–C(4)	56.6(10)
		C(2)–C(3)–C(4)–C(5)	62.9(9)
		C(2)–Si–C(6)–C(5)	49.8(28)



The molecule was found to exist as a mixture of equatorial (68(7)%) and axial (32(7)%) conformers. Differences in the structural parameters of these conformers were assumed at the values from B3LYP/6-31G* calculations, which predicted $\Delta E(\text{axial} - \text{equatorial}) = 0.42 \text{ kcal mol}^{-1}$. Local C_{3v} symmetry was assumed for the methyl group. The CH₂ groups were assumed to be symmetric with respect to the bisector of the adjacent endocyclic angle. The nozzle temperature was 298 K.

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

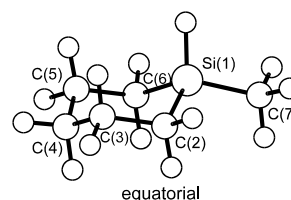
^{b)} Differences in the C–C and Si–C bond lengths were set to the values from B3LYP/6-31G* calculations.

^{c)} Assumed at the value from B3LYP/6-31G* calculations.

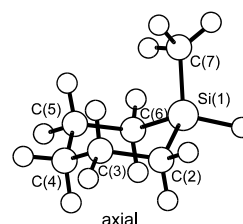
^{d)} Assumed at the value for 1,3,5-trisilacyclohexane.

^{e)} Flap angle of the Si atom from the C(2)C(3)C(5)C(6) plane, *i.e.*, the dihedral angle between the C(2)C(3)C(5)C(6) and C(2)SiC(6) planes.

^{f)} Flap angle of the C(4) atom from the C(2)C(3)C(5)C(6) plane, *i.e.*, the dihedral angle between the C(2)C(3)C(5)C(6) and C(3)C(4)C(5) planes.



equatorial



axial

Arnason, I., Kvaran, A., Jonsdottir, S., Gudnason, P.I., Oberhammer, H.: J. Org. Chem. **67** (2002) 3827.