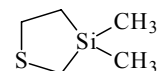


676 **C₅H₁₂SSi**ED, *ab initio*
calculations**3,3-Dimethyl-1-thia-3-silacyclopentane**

3,3-Dimethyl-3-silathiophane

C₁ (probably distorted
₁T⁵ conformer, see
comment)

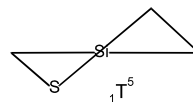
r_g	Å ^{a)}	θ_α	deg ^{a)}
S(1)–C(2)	1.828(5)	C(5)–S(1)–C(2)	98.6(8)
C(2)–Si(3)	1.898(6)	S(1)–C(2)–Si(3)	107.3(4)
Si(3)–C(4)	1.887 ^{b)}	C(2)–Si(3)–C(4)	97.7(6)
C(4)–C(5)	1.541(7)	Si(3)–C(4)–C(5)	112.0(10)
C(5)–S(1)	1.830 ^{b)}	C(4)–C(5)–S(1)	109.0(6)
Si(3)–C(6)	1.875 ^{b)}	C(2)–Si(3)–C(6)	112.7(4)
Si(3)–C(7)	1.872 ^{b)}	C(2)–Si(3)–C(7)	113.6 ^{b)}
C–H ^{c)}	1.112(3)	C(4)–Si(3)–C(6)	113.7 ^{b)}
		C(4)–Si(3)–C(7)	114.5 ^{b)}
		C(6)–Si(3)–C(7)	104.8(12)
		H–C–H ^{c)}	112.3(20)
		Si–C–H ^{c)}	116.4(10)
		S(1)–C(2)–Si(3)–C(4)	15.7(26)
		C(2)–Si(3)–C(4)–C(5)	10.1(28)
		Si(3)–C(4)–C(5)–S(1)	327.4(26)
		C(4)–C(5)–S(1)–C(2)	40.2(20)
		C(5)–S(1)–C(2)–Si(3)	328.1(22)
		q_o ^{d)}	10.7(6)
		ϕ ^{e)}	168.1(44)
		τ ^{f)}	±36(6)



Two local minima with ₁T⁵ and ₄T⁵ conformations of the ring could not be distinguished on the basis of ED data alone. However, the model with the five-membered ring having a distorted ₁T⁵ form agreed with the results of *ab initio* calculations and had a slightly lower *R*-factor than the ₄T⁵ form. Each CH₂ group in the ring was assumed to have local C_{2v} symmetry with one of the symmetry planes formed by the carbon of the CH₂ group and the two adjacent atoms in the ring. It was assumed that the methyl groups have local C_{3v} symmetry and no tilt and rotate in the opposite directions.

The nozzle temperature was 21 °C.

According to HF/6-311++G** calculations, the barrier to pseudorotation is equal to 9.6 kJ mol^{−1}.



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

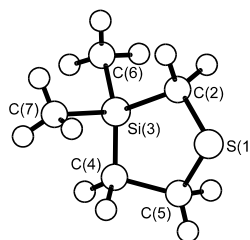
^{b)} Differences in the C–S bond lengths, C–Si bond lengths and exocyclic C–Si–C bond angles were assumed at the values from MP2/6-311++G** calculations.

^{c)} Mean value.

^{d)} Pseudorotation puckering amplitude.

^{e)} Pseudorotation phase angle.

^{f)} Torsional angle of the methyl group, H–C(6,7)–Si–C(7,6); $\tau = 0^\circ$ for the eclipsed position.



Borisenko, K.B., Samdal, S., Suslova, E.N., Sipachev, V.A., Shishkov, I.F., Vilkov, L.V.:
Acta Chem. Scand. **52** (1998) 975.

Replaces [II/25D \(3, 2073\)](#)

Structure Data of Free Polyatomic Molecules
