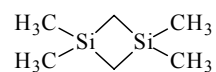


756 **C₆H₁₆Si₂**ED, *ab initio*
calculations**1,1,3,3-Tetramethyl-1,3-disilacyclobutane****D_{2h}**

r_a	Å ^{a)}	θ_a	deg ^{a)}
Si–C(m)	1.853(4)	C(m)–Si–C(m)	109.2(14)
Si–C(2,4)	1.910(5)	C(2)–Si–C(4)	92.2(4)
C–H (average)	1.084(5)	Si–C–H	113.8(13)
		H–C(2,4)–H	107.9 ^{b)}
		φ_e ^{c)}	0
		$\delta(C)$ ^{d)}	0 ^{b)}
		$\delta(H)$ ^{e)}	0 ^{b)}

Large-amplitude motion (ring puckering) was described using a dynamic model. The relaxation of the molecular geometry was estimated by HF/6-311G** method. The potential function was found to be well described as $V(\varphi) = A\varphi^2$ with $A = 4.9(18) \times 10^{-4}$ kcal mol⁻¹ deg⁻². The nozzle temperature was 20 °C.

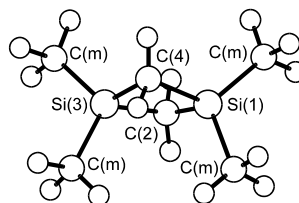
^{a)} Three times the estimated standard errors including a systematic error.

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

^{c)} Ring puckering angle (acute dihedral angle between two C(2)SiC(4) planes) at the minimum of the potential function.

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

^{e)} Angle between the bisector of H–C(2,4)–H angle and the SiCSi plane.



Novikov, V.P., Tarasenko, S.A., Samdal, S., Shen, Q., Vilkov, L.V.: J. Mol. Struct. **485–486** (1999) 135.

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 \(3, 2374\)](#)