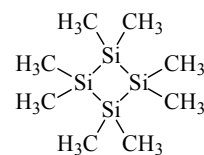


863 **C₈H₂₄Si₄**ED, *ab initio*
calculations**Octamethylcyclotetrasilane****D_{2d}**

r_a	Å ^{a)}	θ_a	deg ^{a)}
Si–C (average)	1.894(3)	C–Si–C	109.5(6)
Si–C(ax)	1.892(3) ^{b)}	Si–Si–Si	88.2(2)
Si–C(eq)	1.896(3) ^{b)}	Si–C–H	111.7(6)
Si–Si	2.363(3)	$\delta^c)$	4.1 ^{d)}
C–H	1.104(3)	$\phi_e^c)$	28.3(19)

Experimental ED intensities from [1] were reanalyzed. The dynamic model was used to describe the large-amplitude ring puckering motion, relaxation of the molecular geometry estimated from HF/6-311G** calculations being taken into account. The potential function of the ring puckering was described as $V(\varphi) = V_0[(\varphi/\varphi_e)^2 - 1]^2$ with a refined constant V_0 of 1.0(5) kcal mol⁻¹, where φ is the ring puckering angle. Staggered conformations were assumed for the methyl groups.

The nozzle was at 74 °C.

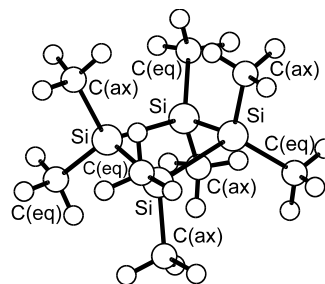
^{a)} Three times the estimated standard errors including a systematic error.

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

^{c)} Angle between the bisector of the C–Si–C angle and the SiSiSi plane, positive for the motion of the C(ax) atom towards the symmetry axis.

^{d)} Assumed at the value from HF/6-311G** calculations.

^{e)} Acute angle between the SiSiSi planes in equilibrium position.



Novikov, V.P., Tarasenko, S.A., Samdal, S., Vilkov, L.V.: Struct. Chem. **11** (2000) 111.

[1] Mastryukov, V.S., Strelkov, S.A., Vilkov, L.V., Kolonits, M., Rozsondai, B., Schuster, H.G., Hengge, E.: J. Mol. Struct. **238** (1990) 433.

See also: Novikov, V.P., Tarasenko, S.A., Samdal, S., Vilkov, L.V.: Mendeleev Commun. (1999) 217.

Replaces [II/25D \(3, 2633\)](#)