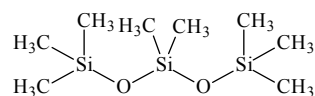


862 **C₈H₂₄O₂Si₃**ED, DFT
calculations**Octamethyltrisiloxane****C₁**

r_a	\AA^a	θ_a	deg^a
Si(1,5)–O	1.650(6) ^b	O–Si–O	107.2(12)
Si(3)–O(2)	1.641(6) ^b	Si(1)–O(2)–Si(3)	165.6(35) ^b
Si(3)–O(4)	1.635(6) ^b	Si(5)–O(4)–Si(3)	163.1(35) ^b
Si(1,5)–C	1.873(2) ^b	C(9)–Si–C(10)	114.3(45)
Si(3)–C	1.865(2) ^b	Si–C–H	111.2(10)
C–H	1.093(3)	O(2)–Si–C(8)	107.8(5) ^b
		O(4)–Si–C(9)	107.8(5) ^b
		O(4)–Si–C(12)	107.8(5) ^b
		O(2)–Si–C(6,7)	109.8(5) ^b
		O(4)–Si–C(11,13)	109.8(5) ^b
		O(2)–Si–C(9,10)	109.8(5) ^b
		Si(1)–O(2)–Si(3)–C(4) ^c	157.0 ^d
		Si(5)–O(4)–Si(3)–O(2) ^c	12.1 ^d
		C(8)–Si(1)–O(2)–Si(3) ^c	166.1 ^d
		C(12)–Si(5)–O(4)–Si(3) ^c	177.4 ^d

Local C_{3v} symmetry was assumed for the methyl groups. According to BPW91/6-311G* calculations, the Si–O–Si fragment is quasilinear with a small potential energy barrier (< 0.5 kJ mol^{−1}) in the linear configuration.

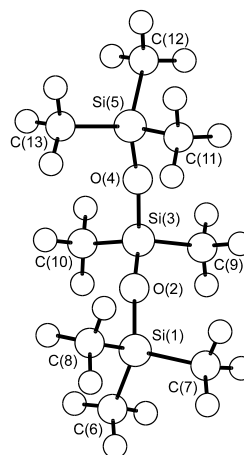
The nozzle temperature was 22 °C.

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

^b) Differences between similar parameters were assumed at the values from BPW91/6-311G* calculations.

^c) Torsional angle, zero degree for the *syn* position, positive value for clockwise rotation looking from the side of rotating atom.

^d) Assumed at the value from BPW91/6-311G* calculations.



Belyakov, A.V., Haaland, A., Shorokhov, D.E., Volden, H.V., West, R.: Zh. Obshch. Khim. **69** No.2 (1999) 244; Russ. J. Gen. Chem. **69** (1999) 235.