

896 $C_{10}H_{30}Si_5$

Decamethylcyclopentasilane

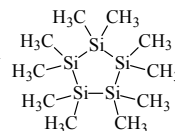
ED,

MM calculations

 C_2 (twist form) C_s (envelope form)

(without H atoms)

r_g	\AA^a	θ_a	deg^a
C–H	1.123(8)	C–Si–C	109.8(13)
Si–C	1.898(2)	H–C–Si	110.9(13)
Si–Si	2.358(3)	H–C–Si–Si	28(8)
q^b	0.68(4)		
		$\varphi=0^\circ$ ^c (envelope form)	$\varphi=90^\circ$ ^c (twist form)
		Si(5)–Si(1)–Si(2) ^d	101.4(8)
		Si(1)–Si(2)–Si(3) ^d	103.1(5)
		Si(2)–Si(3)–Si(4) ^d	105.9(2)
		Si(3)–Si(4)–Si(5) ^d	105.9(2)
		Si(4)–Si(5)–Si(1) ^d	103.1(5)
		τ_1 ^d ^e	26.7(11)
		τ_2 ^d ^f	0.0(8)
		τ_3 ^d ^g	–26.7(11)
		τ_4 ^d ^h	43.1(20)
		τ_5 ^d ⁱ	–43.1(20)



The methyl groups were assumed to have local C_{3v} symmetry. The experimental data were consistent with a pseudorotational model. The precise height of the potential barrier could not be determined. Molecular mechanics (MM3) calculations suggested that the twist form was slightly more stable than the envelope form. The molecular parameters are listed for the two-conformer model with 50% each of the twist and envelope forms.

The nozzle temperature was 85 °C.

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

^b) Puckering amplitude.

^c) Pseudorotational phase angle.

^d) Dependent parameter.

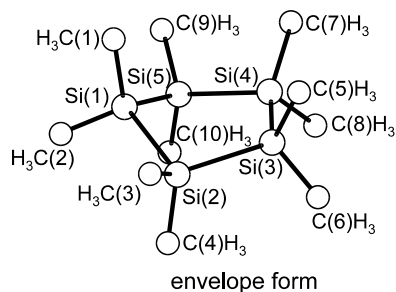
^e) Si(1)–Si(2)–Si(3)–Si(4) torsional angle.

^f) Si(2)–Si(3)–Si(4)–Si(5) torsional angle.

^g) Si(3)–Si(4)–Si(5)–Si(1) torsional angle.

^h) Si(4)–Si(5)–Si(1)–Si(2) torsional angle.

ⁱ) Si(5)–Si(1)–Si(2)–Si(3) torsional angle.



Shen, Q., Bickford, C.: J. Mol. Struct. **446** (1998) 223.