

895 $\text{C}_{10}\text{H}_{30}\text{Si}_4$

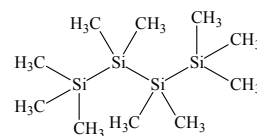
Decamethyltetrasilane

ED, *ab initio* and

DFT calculations

C_2 assumed (*anti*)
 C_2 assumed (*gauche*)
 C_2 assumed (*orthogonal*)

r_a	\AA^a		
	<i>anti</i>	<i>gauche</i>	<i>orthogonal</i>
Si(1)–Si(2)	2.350(6)	2.351(6)	2.345(6)
Si(2)–Si(3)	2.354(6)	2.354(6)	2.359(6)
Si(1)–C	1.893(2)	1.893(2)	1.893(2)
Si(2)–C	1.901(2)	1.903(2)	1.903(2)
C–H (mean)	1.094(2)	1.094(2)	1.095(2)



θ_a	deg^a		
	<i>anti</i>	<i>gauche</i>	<i>orthogonal</i>
Si(1)–Si(2)–Si(3)	112.4(5)	117.0(5)	115.1(5)
Si(2)–Si(1)–C(11)	112.5(15)	112.9(15)	109.4(15)
Si(2)–Si(1)–C(12)	110.2(15)	109.3(15)	109.4(15)
Si(2)–Si(1)–C(13)	111.5(15)	112.0(15)	113.3(15)
Si(1)–Si(2)–C(21)	108.4(14)	110.3(14)	108.2(14)
Si(1)–Si(2)–C(22)	107.9(14)	108.1(14)	109.9(14)
Si(3)–Si(2)–C(21)	107.8(14)	106.0(14)	107.1(14)
Si(3)–Si(2)–C(22)	110.7(14)	109.0(14)	110.3(14)
τ_1^b	163(8)	55 $^\circ$	92 $^\circ$
τ_2^d	44(7)	44 $^\circ$	64 $^\circ$

The molecule was found to exist as a mixture of *anti* (51(6)%) and *gauche* (32(8)%) conformers. The presence of the *orthogonal* conformer (17(14)%) is probable but not certain. Differences between similar parameters in each conformer and differences between parameters of *anti* and *gauche* or *orthogonal* conformers were constrained to the values from B3PW91/6-311G* calculations.

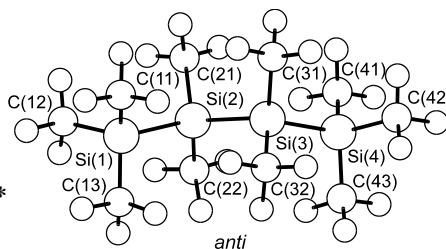
The nozzle temperature was 67(3) °C.

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

^b) Torsional angle Si(1)–Si(2)–Si(3)–Si(4), $\tau_1 = 0^\circ$ for the *syn* position.

^c) Assumed at the value from B3PW91/6-311G* calculations.

^d) Torsional angle Si(3)–Si(2)–Si(1)–C(11), $\tau_2 = 0^\circ$ for the *syn* position.



Belyakov, A.V., Haaland, A., Shorokhov, D.J., West, R.: J. Organomet. Chem. **597** (2000) 87.