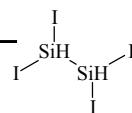


240 **H₂I₄Si₂**
1,1,2,2-Tetraiododisilane
C₂ (*gauche*)

 ED, *ab initio* and DFT
calculations

C_{2h} (*anti*)

r_g	$\text{\AA}^a)$		θ_α	deg ^{a)}	
	<i>anti</i>	<i>gauche</i>		<i>anti</i>	<i>gauche</i>
Si–Si	2.364(30)	2.363(30)	Si(2)–Si(1)–I(3)	107.2(4)	109.4(4)
Si–I(3)	2.450(6)	2.433(6)	Si(2)–Si(1)–I(4)	107.2(4)	106.0(4)
Si–I(4)	2.450(6)	2.449(6)	Si–Si–H	110.9 ^{b)}	109.5 ^{b)}
Si–H	1.531 ^{b)}	1.529 ^{b)}	I–Si–I	111.7(3)	111.2(3)
			I–Si–H	109.9(2)	110.3(2)
			H–Si–Si–H	180.0	59(20) ^{c)}



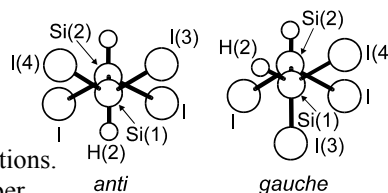
Molecular structure determined in [1] was reinvestigated. The molecule was found to exist as a mixture of *gauche* (77.4%) and *anti* (22.6%) conformers with $\Delta E(\textit{gauche} - \textit{anti}) = -0.74$ kcal mol⁻¹. Dynamic model was used in the ED analysis. Differences in the parameters of the conformers and pseudoconformers were assumed at the values from B3LYP/3-21G* calculations.

The nozzle temperature was 428 K.

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

^{b)} Estimated or taken from B3LYP/3-21G* calculations.

^{c)} Uncertainty was not estimated in the original paper.



Johansen, T.H., Hassler, K., Tekautz, G., Hagen, K.: J. Mol. Struct. **598** (2001) 171.

[1] Röhmen, E., Hagen, K., Stølevik, R., Hassler, K., Pöschl, M.: J. Mol. Struct. **244** (1991)

41.

Replaces [II/25A\(2, 699\)](#)