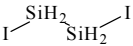


**272**      **H<sub>4</sub>I<sub>2</sub>Si<sub>2</sub>****1,2-Diiododisilane****C<sub>2</sub>** (*gauche*)ED, *ab initio* and DFT  
calculations**C<sub>2h</sub>** (*anti*)

$r_g$	$\text{\AA}^a)$		$\theta_\alpha$	$\text{deg}^a)$		
	<i>anti</i>	<i>gauche</i>		<i>anti</i>	<i>gauche</i>	
Si–Si	2.315(26)	2.325(26)	Si–Si–I	107.5(10)	109.3(10)	
Si–I	2.447(6)	2.434(6)	Si–Si–H	110.8 <sup>b)</sup>	110.2 <sup>b)</sup>	
Si–H	1.528 <sup>b)</sup>	1.533 <sup>b)</sup>	I–Si–H	109.8(5)	109.2(5)	
			I–Si–Si–I	180	61(11) <sup>c)</sup>	

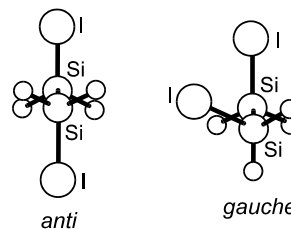
The molecular structure determined in [1] was reinvestigated. The molecule was found to exist as a mixture of *gauche* (60%) and *anti* (40%) conformers with  $\Delta E(\textit{gauche} - \textit{anti}) = 0.14 \text{ kcal mol}^{-1}$ . The dynamic model was used in the ED analysis. Differences in the parameters of the conformers and pseudoconformers were assumed at the values from B3LYP/3-21G\* calculations.

The nozzle temperature was 328 K.

<sup>a)</sup> Twice the estimated standard errors including a systematic error.

<sup>b)</sup> Estimated or taken from B3LYP/3-21G\* calculations.

<sup>c)</sup> Uncertainty was not estimated in the original paper.



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

[1] Røhmen, E., Hagen, K., Stølevik, R., Hassler, K., Pöschl, M.: J. Mol. Struct. **244** (1991) 41.

Replaces [II/25A\(2, 747\)](#)