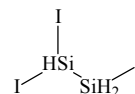


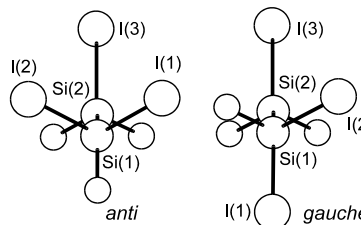
**261**      **H<sub>3</sub>I<sub>3</sub>Si<sub>2</sub>**ED, *ab initio* and DFT  
calculations**1,1,2-Triiododisilane****C<sub>s</sub>** (*anti*)**C<sub>1</sub>** (*gauche*)

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
Si–Si	2.329(12)	Si–Si–I (average)	109.9(4)
Si–I (average) <sup>b)</sup>	2.449(3)	Si–Si–I(1,2) ( <i>anti</i> ) <sup>c)</sup>	109.2(4)
Si–H (average)	1.527 <sup>d)</sup>	Si–Si–I(3) ( <i>anti</i> ) <sup>c)</sup>	111.2(4)
		I–Si–I	110.5(4)
		I–Si–H	109.0(2)
		Si–Si–H (average)	110.1 <sup>d)</sup>
		$\tau$ ( <i>anti</i> ) <sup>c)</sup>	180
		$\tau$ ( <i>gauche</i> ) <sup>c)</sup>	79.8 <sup>f)</sup>



The molecule was found to exist as a mixture of *anti* and *gauche* conformers. The population of the *anti* conformer was estimated to be 51% by ED and 64% by IR and Ra spectroscopy. In contrast, theoretical calculations (B3LYP/3-21G\*, MP2/SBK, *etc.*) predicted that the *gauche* conformer (90%) was more stable;  $\Delta E_0 = 1.1$  kcal mol<sup>−1</sup>. The origin of this discrepancy has not been understood.

The nozzle temperature was 325 K.



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

<sup>b)</sup> Differences in the Si–I bond lengths were assumed at the values from B3LYP/3-21G\* calculations.

<sup>c)</sup> Difference between the Si–Si–I(1,2) and Si–Si–I(3) bond angles was assumed at the value from B3LYP/3-21G\* calculations.

<sup>d)</sup> Estimated value.

<sup>e)</sup> H–Si–Si–I(3) torsional angle.

<sup>f)</sup> Calculated from the refined parameters of three-term cosine potential function ( $V_1 = 0.7(11)$  kcal mol<sup>−1</sup>,  $V_2 = -0.4(10)$  kcal mol<sup>−1</sup>,  $V_3 = 0.4(6)$  kcal mol<sup>−1</sup>).

Johansen, T.H., Hagen, K., Hassler, K., Tekautz, G., Stølevik, R.: J. Mol. Struct. **509** (1999) 237.