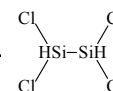


157 **Cl₄H₂Si₂**ED, IR, Ra, *ab initio*
calculations**1,1,2,2-Tetrachlorodisilane****C₂ (*gauche*)****C_{2h} (*anti*)**

| r_g | $\text{\AA}^a)$ | | θ_a | $\text{deg}^a)$ | |
|--------------------------|---------------------|---------------------|-----------------------------------|---------------------|---------------------|
| | <i>gauche</i> | <i>anti</i> | | <i>gauche</i> | <i>anti</i> |
| Si–Si | 2.310(8) | 2.309(8) | Si–Si–Cl ^{b)} | 108.9(4) | 108.2(4) |
| Si–Cl ^{b)} | 2.039(2) | 2.042(2) | Si–Si–H | 111.5 ^{c)} | 112.8 ^{c)} |
| Si–H | 1.511 ^{c)} | 1.510 ^{c)} | <i>P</i> (Cl–Si–Cl) ^{d)} | 119.6(7) | 118.8(7) |
| Si–Cl(3,8) ^{e)} | 2.036(2) | 2.042(2) | Si–Si–Cl(3,8) ^{e)} | 110.0(4) | 108.2(4) |
| Si–Cl(4,7) ^{e)} | 2.043(2) | 2.042(2) | Si–Si–Cl(4,7) ^{e)} | 107.9(4) | 108.2(4) |
| | | | Cl–Si–Cl ^{e)} | 109.7(3) | 109.7(3) |
| | | | H–Si–Cl ^{e)} | 108.9(5) | 108.9(5) |
| | | | $\tau^f)$ | 60 ^{g)} | 180 ^{g)} |



The molecule exists as a mixture of *gauche* (80%) and *anti* conformers. The torsional potential function was described by V_1 and V_3 constants; they were estimated to be: $V_1 = -0.6(2)$ kcal mol⁻¹ from the IR/Ra energy difference of the conformers [1] and $V_3 = 1.5(5)$ kcal mol⁻¹ from the ED analysis based on the dynamic model. Differences between the parameters of conformers were assumed at the values from HF/6-31G(d) calculations.

The nozzle temperature was 296 K.

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

^{b)} Average value.

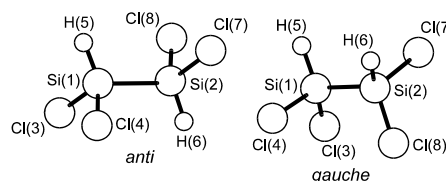
^{c)} Estimated according to results from MP2/6-31G(d) calculations.

^{d)} Projection of Cl–Si–Cl angle on a plane perpendicular to the Si–Si bond.

^{e)} Dependent parameter.

^{f)} H–Si–Si–H torsional angle.

^{g)} Assumed.



Johansen, T.H., Hagen, K., Stølevik, R.: J. Mol. Struct. **485-486** (1999) 121.

[1] Ernst, M., Schenzel, K., Jähn, A., Köll, W., Hassler, K.: J. Raman Spectrosc. **28** (1997) 589.