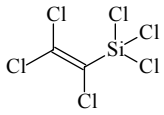
171 **C_2Cl_6Si** **Trichloro(trichloroethenyl)silane** **C_s** (*syn*)
ED, *ab initio* calculations Perchlorovinylsilane **C_s** (*anti*)

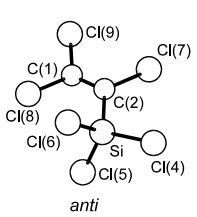


r_g	Å [a])
C=C	1.349(12)
C–Si	1.863(13)
C(2)–Cl	1.725(5)
C(1)–Cl(8)	1.714(5)
C(1)–Cl(9)	1.711(5)
Si–Cl(4)	2.015(3)
Si–Cl(5,6)	2.022(3)

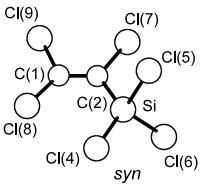
θ_α	deg [a])
C=C–Si	124.0(12)
C=C–Cl (mean)	121.6(4)
Cl(5)–Si–Cl(6) [b])	116.9(71)
C–Si–Cl (mean)	111.1(15)
C(2)–Si–Cl(4)	110.7(15)
C(2)–Si–Cl(5,6)	111.3(15)
C(1)=C(2)–Cl(7)	119.0(4)
C(2)=C(1)–Cl(8)	121.8(4)
C(2)=C(1)–Cl(9)	124.1(4)
Si–C(2)–Cl(7)	117.1(14)
Cl–C(1)–Cl	114.0(7)
τ[Cl(4)–Si–C(2)=C(1)]	180 [c])

The molecule exists as a mixture of *anti* (*ca*. 80%) and *syn* conformers. The estimate of conformational energy difference ($\Delta E^0 = E^0(anti) - E^0(syn) = -1.04(58)$ kcal mol^{-1}) was based on the V_3 potential constant from ED. According to HF/6-31G(d) calculations, $\Delta E^0 = E^0(anti) - E^0(syn) = -1.43$ kcal mol^{-1}. Structural differences of two conformers were assumed at the values from HF/6-31G(d) calculations. The structural parameters are listed for the *anti* conformer.
The nozzle temperature was 373 K.

[a]) Twice the estimated standard errors including a systematic error.
[b]) Cl–Si–Cl angle projected on the plane perpendicular to the C–Si bond.
[c]) τ[Cl(4)–Si–C(2)=C(1)] = 0° for the *syn* conformer.



anti



syn

Johansen, T.H., Hagen, K., Hassler, K., Richardson, A., Pätzold, U., Stølevik, R.:
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