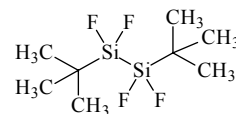


856 **C₈H₁₈F₄Si₂**ED, IR, Ra, *ab initio*
calculations**1,2-Bis(1,1-dimethylethyl)-1,1,2,2-tetrafluorodisilane** **C_{2h} (*anti*)**1,2-Di-*t*-butyltetrafluorodisilane

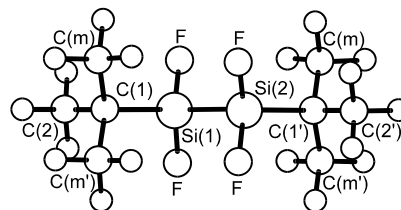
r_a	Å ^{a)}	θ_a	deg ^{a)}
Si–Si	2.346(6)	Si–Si–F	108.7(3)
Si–C	1.872(3)	F–Si–F	107(2)
Si–F	1.600(2)	Si–Si–C	114.6(7)
C–C	1.537(3)	C–C–C	110.2(5)
C–H	1.135(2)	C–C–H	109.5(10)
		Si–C–C–H	180 ^{b)}
		Si–Si–C–C	192.5(17)
		C–Si–Si–C	184(7)
		tilt(<i>t</i> -butyl) ^{c)}	3.7(6)

The *ab initio* (MP2/6-31G*) studies and spectroscopic measurements consistently supported the presence of a single (*anti*) conformer only. The ED data were fully consistent with a single *anti* conformer with a large-amplitude torsional motion over a range of 140...220°. Local C_{3v} symmetry for the methyl groups and local C₃ symmetry for the *t*-butyl groups were assumed. The SiSiF₂C fragments were assumed to have local C_s symmetry. The nozzle temperature was 293 K.

^{a)} Estimated standard errors.

^{b)} Assumed at the value from HF/6-31G* calculations.

^{c)} Tilt angle between the C₃ axis of the *t*-butyl group and the Si–C bond; positive tilt leads to a single Si(1)–C(1)–C(2) angle and two equivalent (Si(1)–C(1)–C(m) and Si(1)–C(1)–C(m')) larger angles.



Smart, B.A., Robertson, H.E., Mitzel, N.W., Rankin, D.W.H., Zink, R., Hassler, K.: J. Chem. Soc., Dalton Trans. (1997) 2475.

See also: Zink, R., Hassler, K., Mitzel, N., Smart, B.A., Rankin, D.W.H., in: "Organosilicon Chemistry. From Molecules to Materials", Vol. III, p. 248, N. Auner and J. Weis, Eds., Weinheim: Wiley-VCH, 1997.