

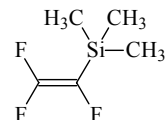
**653**      **C<sub>5</sub>H<sub>9</sub>F<sub>3</sub>Si**ED, *ab initio*  
calculations**Trifluoro(trimethylsilyl)ethene**

Trimethyl(trifluorovinyl)silane

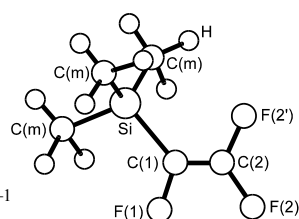
Trimethyl(trifluoroethenyl)silane

**C<sub>s</sub>** (staggered)

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C–H	1.100(5)	C(1)=C(2)–F(2)	127.7(6)
C=C	1.310[20] <sup>b)</sup>	C(1)=C(2)–F(2')	122.0(6)
C(2)–F	1.324(5) <sup>c)</sup>	C(2)=C(1)–F(1)	118.0(8)
C(1)–F	1.365(5) <sup>c)</sup>	C(2)=C(1)–Si	127.7(13)
C(1)–Si	1.877(10)	C(m)–Si–C(m)	113.0(10)
Si–C(m)	1.865(4)	H–C–H	109.2(9)
		tilt(Si(CH <sub>3</sub> ) <sub>3</sub> ) <sup>d)</sup>	0 <sup>e)</sup>



Local C<sub>3v</sub> symmetry was assumed for the Si(CH<sub>3</sub>)<sub>3</sub> unit. Staggered conformation with respect to the opposite Si–C bonds was assumed for the methyl groups. The Si(CH<sub>3</sub>)<sub>3</sub> group undergoes a large-amplitude torsional motion about the staggered conformation with respect to the C(2)=C(1) bond. According to HF/3-21G\* calculations, the eclipsed conformation ( $\alpha$ (C(2)=C(1)–Si–C(m)) = 0°) is 0.42 kcal mol<sup>–1</sup> less stable than the staggered conformation ( $\alpha$ (C=C–Si–C) = 60°). The nozzle was at room temperature.



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

<sup>b)</sup> Not refined, but varied within the given range estimated by the *ab initio* method.

<sup>c)</sup> Difference between C(1)–F and C(2)–F was assumed at the *ab initio* value.

<sup>d)</sup> Tilt angle between the C<sub>3</sub> axis of the Si(CH<sub>3</sub>)<sub>3</sub> group and the C(1)–Si bond direction.

<sup>e)</sup> Found to be close to zero within a large error limit and set to zero in the final refinements.

Ritter, S.K., Kirchmeier, R.L., Shreeve, J.M., Oberhammer, H.: Inorg. Chem. **35** (1996) 4067.