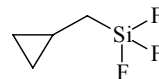


551 **C₄H₇F₃Si**ED, *ab initio*
calculations**(Cyclopropylmethyl)trifluorosilane****C₁ (*ac*)**
C_s assumed (*sp*)

r_a	Å ^{a)} ^{b)}	θ_a	deg ^{a)}	
			<i>ac</i>	<i>sp</i>
C(1)–C(2)	1.520 ^{c)}	Si–C(4)–C(1)	115.0(12)	123.4(37)
C(2)–C(3)	1.500 ^{c)}	F(6)–Si–C	111.3(24)	109.0 ^{c)}
C(1)–C(4)	1.548(12)	F(7,8)–Si–C	110.0 ^{c)}	115.9(64)
Si–C(4)	1.837(5)	H–C(1)–C(4)	110.5 ^{c)}	113.0 ^{c)}
Si–F	1.593(1)	H–C(4)–H	106.3(18)	106.3(18)
C–H	1.095(8)	H–C–H (ring)	113.0 ^{c)}	113.0 ^{c)}
		φ ^{d)}	129.5(17)	124.6(53)
		τ_1 ^{e)}	170.0(54)	180.0 ^{c)}
		τ_2 ^{f)}	115.7(29)	0.0 ^{c)}



The molecule was found to exist as a mixture of *ac* and *sp* conformers with respect to the C(1)–C(4) bond in the ratio of 75(12):25(12).

The nozzle temperature was 40 °C.

^{a)} Three times the estimated standard errors.

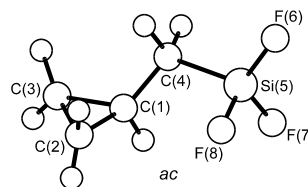
^{b)} Bond lengths of the *ac* and *sp* conformers were assumed to be equal.

^{c)} Assumed.

^{d)} Angle between the C(1)–C(4) bond and the ring plane.

^{e)} Torsional angle F(6)–Si–C(4)–C(1), $\tau_1 = 0^\circ$ for the *syn* position.

^{f)} Torsional angle Si–C(4)–C(1)–X (X is the center of the ring), $\tau_2 = 0^\circ$ for the *syn* position.



Dakkouri, M.: J. Mol. Struct. **413-414** (1997) 133.