

1105
ED, MW

C₃H₃F₃Si

3,3,3-Trifluoro-1-silyl-1-propyne
4,4,4-Trifluoro-1-silabut-2-yne

C_{3v} assumed
F₃C–C≡C–SiH₃

r_z	Å ^{a)}	θ_z	deg ^{a)}
Si–H	1.473(21)	H–Si–C	107 ^{b)}
Si–C	1.827(6)	F–C–C	110.3(4)
C≡C	1.218(8)	ϕ ^{c)}	0.0 ^{b)}
C–C	1.482(8)		
C–F	1.341(3)		

Local C_{3v} symmetry for the CF₃ and SiH₃ groups and a linear C–C≡C–Si skeleton were assumed. It was impossible to distinguish between a free-rotation model and the various fixed-conformation models.

The nozzle temperature was 333 K.

^{a)} Estimated standard errors.

^{b)} Fixed in the least-squares analysis.

^{c)} Twist angle; $\phi = 0^\circ$ when CF₃ group is staggered with respect to the SiH₃ group.

Anderson, D.W.W., Cradock, S., Ebsworth, E.A.V., Green, A.R., Rankin, D.W.H., Robiette, A.G.: J. Organomet. Chem. **271** (1984) 235.