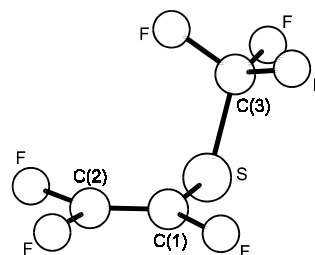


1021 C₃F₆SED, *ab initio* calculations
(HF/3-21G*)**1,1,2-Trifluoro-2-[(trifluoromethyl)thio]ethene****C₁**

r_a	Å ^{a)}	θ_α	deg ^{a)}
C(1)=C(2)	1.302(19)	C(2)=C(1)-S	120.0(9)
S-C(1)	1.719(9)	C(2)=C(1)-F	119.5(4)
S-C(3)	1.820(10)	C(1)=C(2)-F ^{b)}	125.5(11)
C(3)-F	1.331(2)	C(1)-S-C(3)	101.7(7)
C(1)-F ^{b)}	1.354(6)	F-C(3)-F	108.9(4)
C(2)-F ^{b)}	1.314(6)	C(2)=C(1)-S-C(3)	96.9(12)
		tilt (CF ₃) ^{c)}	3.9(8)



Planarity of the F₂C=C(F)S skeleton, local C_{2v} symmetry of the CF₂ group and local C_{3v} symmetry of the CF₃ group were assumed. The CF₃ group was fixed at the staggered position with respect to the C(1)-S bond. Differences in similar parameters were constrained to *ab initio* values. The nozzle was at room temperature.

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

^{b)} Dependent parameter.

^{c)} Tilt angle of the CF₃ group away from the C(1) atom.

Olleta, A., Haas, A., Oberhammer, H.: Chem. Ber. **128** (1995) 803.