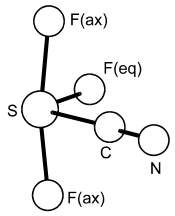
44 **CF_3NS** **Sulfur cyanide trifluoride** **C_s** assumed
ED Cyanotrifluorosulfur $N{\equiv}C{-}SF_3$

r_a	Å [a])
C≡N	1.159(4)
S–F (mean)	1.622(2)
Δ(S–F) [b])	0.105(5)
S–F(eq) [c])	1.552(4)
S–F(ax) [c])	1.657(3)
S–C	1.736(8)

θ_α	deg [a])
F(ax)–S–F(eq)	86.9(3)
F(ax)–S–C	86.0(4)
F(ax)–S–F(ax) [c])	169.0(6)
F(eq)–S–C	98.7(8)
S–C≡N [d])	171(4)



The experimental bond lengths were reproduced well by values from HF/3-21G*, HF/6-31G* or MP2/6-31G* calculations. The bond angles were reproduced by these methods within about ±3°.
The nozzle was probably at room temperature.

[a]) Three times the estimated standard errors.
[b]) [S–F(ax)] – [S–F(eq)].
[c]) Dependent parameter.
[d]) Bent in the equatorial plane F(eq)–S–C, away from the F(eq) atom.

Mack, H.-G., Oberhammer, H., Jacobs, J., Kronberg, M., Willner, H.: Inorg. Chem. **35** (1996) 806.