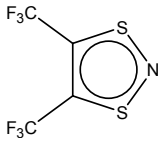
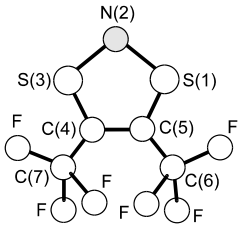
477 **$C_4F_6NS_2$** **4,5-Bis(trifluoromethyl)-1,3,2-dithiazolyl** **C_{2v}** assumed

ED, DFT calculations



r [a])	Å [b])	θ [a])	deg [b])
C(4)=C(5)	1.324(7)	C=C–S [c])	114.8(3)
C–S	1.749(3)	C–S–N [c])	96.5(6)
S–N	1.634(2)	S–N–S	117.3(5)
C–C(6,7)	1.481(3)	C=C–C	127.3(3)
C–F	1.330(2)	F–C–F	107.4(2)
		tilt(CF_3) [d])	1.5(6)



Local C_{3v} symmetry and staggered position were assumed for the CF_3 groups. The ring was assumed to be planar.
The nozzle was at room temperature.

[a]) Unidentified, possibly r_a and θ_a.
[b]) Three times the estimated standard errors including a systematic error.
[c]) Dependent parameter.
[d]) Tilt angle between the C_3 axis of the CF_3 group and the C–C bond direction, away from the C(4)=C(5) bond.

Brownridge, S., Du, H., Fairhurst, S.A., Haddon, R.C., Oberhammer, H., Parsons, S., Passmore, J., Schriver, M.J., Sutcliffe, L.H., Westwood, N.P.C.: J. Chem. Soc., Dalton Trans. (2000) 3365.

Replaces II/25C (**3**, 1472)