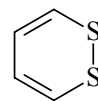


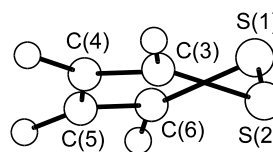
516
MW $C_4H_4S_2$

1,2-Dithiin

 C_2 

r_s	\AA	θ_s	deg
S-S	2.051(3)	S-S-C	98.7(2)
S-C	1.759(4)	S-C=C	121.4(2)
C=C	1.353(3)	C=C-C	124.2(2)
C-C	1.451(4)	S-S-C=C ^{a)}	41.2
		S-C=C-C ^{a)}	-0.3
		C=C-C=C ^{a)}	29.0
		C-S-S-C ^{a)}	53.9

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$	$c_s [\text{\AA}]$
S(1)	0.956	-0.969	-0.337
S(2)	0.956	0.969	0.337
C(3)	-0.594	1.478	-0.320
C(6)	-0.594	-1.478	0.320
C(4)	-1.6768	0.668	-0.282
C(5)	-1.6768	-0.668	0.282



The molecule has a twisted conformation about the S-S bond.

^{a)} Dihedral angle. Dependent parameters.

Gillies, J.Z., Gillies, C.W., Cotter, E.A., Block, E., DeOrazio, R.: J. Mol. Spectrosc. **180** (1996) 139.

Replaces [II/25C \(3, 1571\)](#)