

1177
MW

C₃H₄S

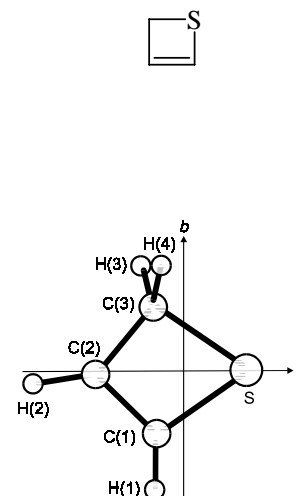
2H-Thiete

C_s

r_s	Å ^{a)}	θ_s	deg ^{a)}
C(1)–S	1.770(3)	C(2)=C(1)–S	97.6
C(3)–S	1.850(3)	C(3)–C(2)=C(1)	99.2
C(1)=C(2)	1.355	S–C(1)=C(2)	89.3(6)
C(2)–C(3)	1.500(3)	C(3)–S–C(1)	73.9(6)
C(1)–H	1.079(3)	C(2)–C(3)–H	115.7(6)
C(3)–H	1.092(1)	H–C(3)–H	111.0(6)

r_0	Å	θ_0	deg
C(1)–S	1.770(3)	C(2)=C(1)–S	97.87 ^{b)}
C(3)–S	1.853(3)	C(3)–C(2)=C(1)	99.27 ^{b)}
C(1)=C(2)	1.350 ^{b)}	S–C(1)=C(2)	89.14(6)
C(2)–C(3)	1.501(3)	C(3)–S–C(1)	73.72(6)
C(1)–H	1.079(3)	C(3)–C(2)–H	132.32(9)
C(2)–H	1.080 ^{c)}	C(2)–C(3)–H	115.87(6)
C(3)–H	1.092(1)	H–C(3)–H	110.93(6)

Atom	a_s [Å]	b_s [Å]	c_s [Å]	a_0 [Å] ^{d)}	b_0 [Å] ^{d)}	c_0 [Å] ^{d)}
C(1)	–0.4318	1.0659	0.0	–0.4353	1.0652	0.0
C(2)	–1.3776	0.0949	0.0	–1.3779	0.0997	0.0
C(3)	–0.4843	–1.1096	0.0	–0.4871	–1.1088	0.0
S	0.9885	0.0094	0.0	0.9882	0.0136	0.0
H(1)	–0.4610	2.1441	0.0	–0.4610	2.1439	0.0
H(2)	–	–	0.0	–2.452	0.211	0.0
H(3)	–0.5225	–1.7267	–0.8996	–0.5227	–1.7267	–0.8996
H(4)	–0.5225	–1.7267	0.8996	–0.5227	–1.7267	0.8996



^{a)} Uncertainties for r_s parameters were not estimated in the original paper and were taken to be identical to those for r_0 parameters.

^{b)} Redundant parameters.

^{c)} Assumed.

^{d)} C_s symmetry was assumed as was $r(\text{C}(2)\text{--H}(2)) = 1.080$ Å.

Rodler, M., Bauder, A.: J. Mol. Struct. **117** (1984) 141.