

1768
MW

C₄H₈S

Tetrahydrothiophene

C₂

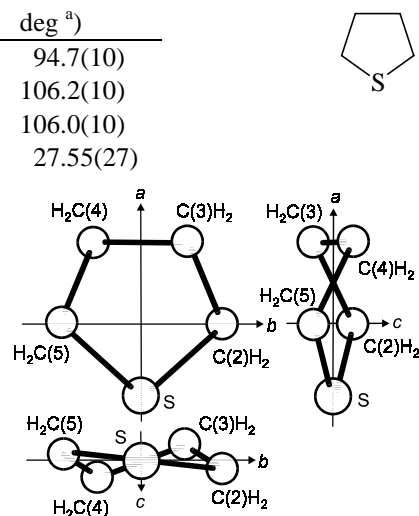
r_s	Å ^{a)}	θ_s	deg ^{a)}
C(3)–C(4)	1.527(2)	C(2)–S–C(5)	94.7(10)
C(2)–C(3)	1.538 ^{b)}	S–C(2)–C(3)	106.2(10)
C(2)–S	1.821(10)	C(2)–C(3)–C(4)	106.0(10)
		$\tau^c)$	27.55(27)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
S	–1.2323	0.0	0.0
C(2)	–	1.3316	0.1373
C(3)	1.3442	0.7097	–0.2818
C(4)	1.3442	–0.7097	0.2818
C(5)	–	–1.3316	–0.1373

^{a)} Uncertainties were not estimated in the original paper.

^{b)} Assumed.

^{c)} Twist angle between the C(2)SC(5) plane and the C(3)–C(4) bond.



Mamleev, A.Kh., Pozdeev, N.M.: Zh. Strukt. Khim. **20** (1979) 1114; Russ. J. Struct. Chem. (Engl. Transl.) **20** (1979) 949.

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r_a	Å ^{a)}	θ_a	deg ^{a)}
C–C	1.532(4)	C–S–C	93.4(10)
C–S	1.835(4)	S–C–C	106.1(8)
C–H	1.117(10)	C–C–C	105.0(10)
		$\tau_1^b)$	14.8(10)
		$\tau_2^c)$	–40.4(24)
		$\tau_3^d)$	52.5(32)

The nozzle temperature was ≈ 52 °C.

^{a)} Estimated standard errors, twice those in the original data. The scale factor has been readjusted.

^{b)} Torsional angle C(5)–S–C(2)–C(3).

^{c)} Torsional angle S–C(2)–C(3)–C(4).

^{d)} Torsional angle C(2)–C(3)–C(4)–C(5).

Náhlavská, Z., Náhlavský, B., Seip, H.M.: Acta Chem. Scand. **23** (1969) 3534.