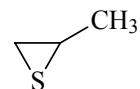


408  
MW $C_3H_6S$ 

Methylthiirane

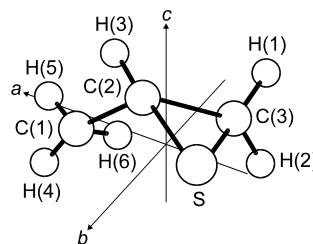
 $C_1$ 

$r_s$	Å	$\theta_s$	deg
C(1)–C(2)	1.5128(62)	C(1)–C(2)–C(3) <sup>a)</sup>	119.96(55)
C(2)–C(3)	1.479(11)	C(1)–C(2)–S	118.22(28)
C(2)–S	1.8124(61)	C(2)–C(3)–S <sup>a)</sup>	65.78(97)
C(3)–S <sup>a)</sup>	1.8176(52)	S–C(2)–C(3)	66.14(97)
		C(2)–S–C(3) <sup>a)</sup>	48.08(95)

$r_0$	Å	$\theta_0$	deg
C(1)–C(2)	1.5169(16)	C(1)–C(2)–C(3) <sup>a)</sup>	119.84(70)
C(2)–C(3)	1.4846(28)	C(1)–C(2)–S	117.52(16)
C(2)–S	1.8268(16)	C(2)–C(3)–S <sup>a)</sup>	66.21(39)
C(3)–S <sup>a)</sup>	1.8202(25)	S–C(2)–C(3)	65.75(8)
		C(2)–S–C(3) <sup>a)</sup>	48.04(47)
		C(1)–C(2)–C(3)–S <sup>b)</sup>	112.38(16)

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
C(1)	1.8246	0.3773	–0.1979
C(2)	0.5955	–0.1611	0.5008
C(3)	–0.2345	–1.1939	–0.1559
S	–1.0280	0.4372	–0.0387

Atom	$a_0$ [Å]	$b_0$ [Å]	$c_0$ [Å]
H(1)	–0.6776	–1.9623	0.4408
H(2)	0.0342	–1.4839	–1.1742
H(3)	0.7586	–0.3327	1.5565
H(4)	1.5142	1.0999	–0.9633
H(5)	2.4701	0.8828	0.5234
H(6)	2.3763	–0.4313	–0.6748



The barrier  $V_3$  hindering the internal rotation of the methyl group was determined to be 13.49(11) kJ mol<sup>–1</sup>.

<sup>a)</sup> Dependent parameters.

<sup>b)</sup> Dihedral angle.

Lorenzo, F.J., López, J.C., Alonso, J.L., Dreizler, H.: J. Chem. Soc., Faraday Trans. **93** (1997) 1863.