

1748  
MW

**C<sub>4</sub>H<sub>8</sub>OS**

**1,4-Oxathiane**

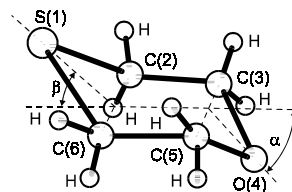
**C<sub>s</sub>**

$r_0$	$\text{\AA}^a$	$\theta_0$	deg <sup>a)</sup>
C–S	1.829(10)	C–S–C	95.7(20)
C–O	1.420(10)	C–O–C	115.6(20)
C–C	1.526(10)	H–C–H <sup>b)</sup>	120.9(30)
C–H	1.095(10)	$\alpha$ <sup>c)</sup>	56.4(30)
		$\beta$ <sup>c)</sup>	48.6(20)

<sup>a)</sup> Uncertainties were not estimated in the original paper.

<sup>b)</sup> Assumed to share a common bisector with the interior ring angle.

<sup>c)</sup> See figure.



Kitchin, R.W., Avirah, T.K., Malloy, T.B., Cook, R.L.: J. Mol. Struct. **24** (1975) 337.

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$r_a$	$\text{\AA}^a$	$\theta_a$	deg <sup>a)</sup>
C–S	1.826(4)	C–S–C	97.1(20)
C–O	1.418(4)	C–O–C	115.1(22)
C–C	1.521(6)	H–C–H	124.2(35)
C–H	1.093(4)	C–C–S	111.4(10)
		H–C–O	110.4(18)
		H–C–C	109.0(18)
		C–C–O	113.2(17)
		$\tau_1$ <sup>b)</sup>	63.5(20)
		$\tau_2$ <sup>c)</sup>	51.2(28)
		$\tau_3$ <sup>d)</sup>	60.1(12)

The molecule has a chair form; no appreciable amount of the twist-boat form is shown to be present.

The nozzle temperature was 60...80 °C.

<sup>a)</sup> Estimated total errors.

<sup>b)</sup> Dihedral angle C(2)–C(3)–O(4)–C(5).

<sup>c)</sup> Dihedral angle C(6)–S(1)–C(2)–C(3).

<sup>d)</sup> Dihedral angle S(1)–C(2)–C(3)–O(4).

Schultz, G., Hargittai, I., Hermann, L.: J. Mol. Struct. **14** (1972) 353.