

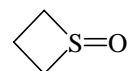
1271  
MW

**C<sub>2</sub>H<sub>6</sub>OS**

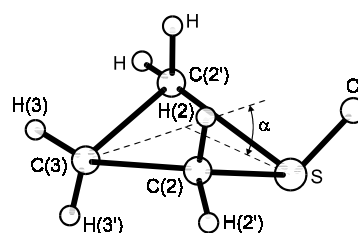
**Thietane 1-oxide**  
Trimethylene sulfoxide

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

$r_s$	Å	$\theta_s$	deg
S=O	1.4749(34)	C(2)–S–C(2')	75.68(25)
C(2)–S	1.8360(32)	C(2)–C(3)–C(2')	93.88(37)
C(2)–C(3)	1.5416(54)	S–C(2)–C(3)	89.62(8)
C(2)–H(2)	1.0994(96)	O=S–C(2)	113.35(45)
C(2)–H(2')	1.0751(86)	H(2)–C(2)–H(2')	110.70(222)
C(3)–H(3)	1.0870(71)	H(2)–C(2)–S	106.00(180)
C(3)–H(3')	1.0982(78)	H(2')–C(2)–S	116.72(145)
		H(3)–C(3)–H(3')	108.75(276)
		$\alpha^a$	34.88(62)



Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
O	–1.7839	0.0	0.4218
S	–0.5714	0.0	–0.4180
C(2)	0.7406	$\pm 1.1263$	$\pm 0.1986^b$
C(3)	1.7777	0.0	$\pm 0.0503^b$
H(2)	0.5177	$\pm 1.2978$	1.2619
H(2')	0.8587	$\pm 2.0604$	–0.3201
H(3)	2.6113	0.0	0.7169
H(3')	2.1744	0.0	–1.0047



The equatorial conformer was observed.

<sup>a</sup>) As defined in figure.

<sup>b</sup>) The sign is difficult to determine. First and second moment conditions were used to estimate the structure listed above.

Bevan, J.W., Legon, A.C., Millen, D.J.: Proc. Roy. Soc. (London) Ser. A **354** (1977) 491.