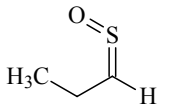
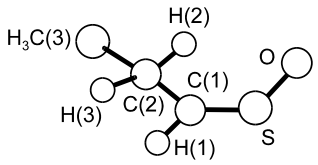
405 **C_3H_6OS** **(*Z*)-Propanethial *S*-oxide** **C_1**
MW



r_s	Å	θ_s	deg
C(1)=S	1.585(6)	C(2)–C(1)=S	126.7(3)
C(1)–C(2)	1.513(7)	C(3)–C(2)–C(1)	112.6(4)
C(2)–C(3)	1.536(3)	H(3)–C(2)–C(1)	99.9(2) [108.2(2)] [a]
C(2)–H(3)	1.216(7) [1.088(7)] [a]	S=C(1)–C(2)–C(3) [b]	118.4(2) [c]
		S=C(1)–C(2)–H(3) [b]	351.2(4) [c]

r_0	Å	θ_0	deg
S=O	1.470(2) [1.473(2)] [a]	C(1)=S=O	113.7(2) [113.8(2)] [a]
C(1)=S	1.593(4) [1.578(4)] [a]	C(2)–C(1)=S	126.2(1) [126.5(1)] [a]
C(1)–C(2)	1.515(5) [1.524(5)] [a]	C(3)–C(2)–C(1)	112.6(2) [112.4(1)] [a]
C(2)–C(3)	1.539(2) [1.544(2)] [a]	H(3)–C(2)–C(1)	100.2(3) [108.1(3)] [a]
C(2)–H(3)	1.207(6) [1.078(5)] [a]	S=C(1)–C(2)–C(3) [b]	118.4(2) [118.5(2)] [a]
		S=C(1)–C(2)–H(3) [b]	351.3(3) [357.2(4)] [a]

Atom	a_s [Å]	b_s [Å]	c_s [Å]
S	1.212	–0.399	0.128
C(1)	–0.296	–0.765	–0.190
C(2)	–1.398	0.195	–0.581
C(3)	–2.5546	0.208	0.430
H(3)	–0.745	1.208	–0.742



The isomer was found to exist as the *skew* conformer shown in the figure.

[a]) From the rotational constants, which were adjusted for bond and torsional shrinkage effects.
[b]) Dihedral angle.
[c]) Uncertainties were not estimated in the original paper.

Gillies, J.Z., Cotter, E., Gillies, C.W., Warner, H.E., Block, E.: J. Phys. Chem. A **103** (1999) 4948.