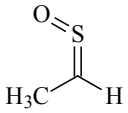
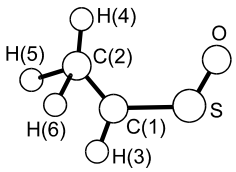
272 **C_2H_4OS** **(*Z*)-Methylsulfine** **C_s**
MW (*Z*)-Ethanethial *S*-oxide



r_s [a])	Å	θ_s [a])	deg
C=S	1.618(3)	C=S=O	113.9(2)
S=O	1.477(4)	H(3)–C=S	113(3)
C(1)–H(3)	1.077(25)	C–C=S	125.4(2)
C–C	1.493(3)	H(5,6)–C(2)–C(1)	110.1(2)
C(2)–H(5,6)	1.096(2)	H(4)–C(2)–C(1)	111.0(1)
C(2)–H(4)	1.076(3)		

r_0	Å	θ_0	deg
C=S	1.619(3)	C=S=O	113.8(1)
S=O	1.478(2)	H(3)–C=S	117(2)
C(1)–H(3)	1.077(17)	C–C=S	125.1(2)
C–C	1.498(3)	H(5,6)–C(2)–C(1)	110.3(2)
C(2)–H(5,6)	1.078(1)	H(4)–C(2)–C(1)	109.6(1)
C(2)–H(4)	1.087(3)		

Atom	a_s [Å]	b_s [Å]	c_s [Å]
O	1.1705	0.9449	0.0
S	0.7048	–0.4569	0.0
C(1)	–0.9056	–0.6121	0.0
H(3)	–1.2335	–1.6380	0.0
C(2)	–1.8821	0.5166	0.0
H(5,6)	–2.5320	0.4530	±0.8804
H(4)	–1.3740	1.4650	0.0



The CH_3 torsional potential barrier was determined to be 285.6(3) cm^{-1}. Spectra of the normal isotopomer of the *E*-isomer were also observed, for which no torsional splitting was resolved.

[a]) Except for O and H(3) coordinates, which were determined by using five moment relations in least-squares fit, fixing C(1)–H(3) to 1.077 Å.

Gillies, J.Z., Gillies, C.W., Grabow, J.-U., Hartwig, H., Block, E.: J. Phys. Chem. **100** (1996) 18708.