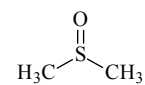


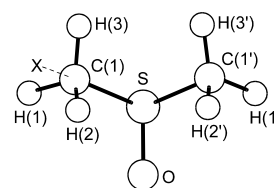
**302 C<sub>2</sub>H<sub>6</sub>OS**ED, MW, *ab initio* and  
DFT calculations**Sulfinylbismethane**

Dimethyl sulfoxide

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

$r_{av}$	Å <sup>a)</sup>	$\theta_{av}$	deg <sup>a)</sup>
C–S	1.807(1)	C–S–C	96.6(6)
S=O	1.484(2)	C–S=O	106.6(1)
C–H	1.093(1)	tilt(CH <sub>3</sub> ) <sup>b)</sup>	1.9(45)
C(1)...X <sup>c)</sup>	0.338(1)	$\phi$ <sup>d)</sup>	115.4(5)
		C(1')–S–C(1)...X <sup>c)</sup>	159(11)
		H(1)–C(1)...X...C(1') <sup>c)</sup>	176.3(14)

Local C<sub>3v</sub> symmetry was assumed for the methyl groups.  
The nozzle temperature was 70 °C.



<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> Angle between the C<sub>3</sub> axis of the methyl group and the C–S bond direction, positive values when the methyl groups are tilted away from each other.

<sup>c)</sup> X is the midpoint of the plane spanned by the methyl hydrogen atoms.

<sup>d)</sup> Angle between the CSC plane and the S=O bond.

Typke, V., Dakkouri, M.: J. Mol. Struct. **599** (2001) 177.

MW

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

$r_s$	Å	$\theta_s$	deg
S–C	1.799(2)	C–S–C	96.56(20)
S=O	1.485(2)	$\phi$ <sup>a)</sup>	64.49(8)
C–H(1)	1.096(4)	S–C–H(1)	106.03(33)
C–H(2)	1.097(4)	S–C–H(2)	108.16(11)
C–H(3)	1.093(3)	S–C–H(3)	109.49(22)
		H(1)–C–H(2)	112.11(64)
		H(1)–C–H(3)	110.06(35)
		H(2)–C–H(3)	110.84(29)
		C–S–C–H(1) <sup>b)</sup>	178.01(56)
		C–S–C–H(2) <sup>b)</sup>	57.59(28)
		C–S–C–H(3) <sup>b)</sup>	–63.29(33)

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
S	0.00	0.1433	0.4202
O	0.00	1.4025	–0.3667
C	±1.3425	–0.8664	–0.2227
H(1)	±2.2695	–0.3536	0.0604
H(2)	±1.2259	–0.9375	–1.3116
H(3)	±1.3065	–1.8571	0.2377

<sup>a)</sup> The angle between the C–S–C plane and the S=O bond.

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

Typke, V.: J. Mol. Struct. **384** (1996) 35.

See also: Feder, W., Dreizler, H., Rudolph, H.D., Typke, V.: Z. Naturforsch. **24a** (1969) 266.

Replaces [II/25B\(3, 892\)](#)