Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(methylsulfonyl)methane

Riad Awad,[a] Eyad Mallah,[a]* Wael Abu Dayyih,[a] Kamal Sweidan[b] and Manfred Steimann[c]

[a]Faculty of Pharmacy and Medical Science, University of Petra, Amman, Jordan, [b]Department of Chemistry, Faculty of Science, The University of Jordan, Amman, Jordan, and [c]University of Tübingen, Inorganic Chemistry, Auf der Morgenstelle 18, 72076 Tübingen, Germany
Correspondence e-mail: eyad782002@yahoo.com

Received 6 June 2014; accepted 11 July 2014

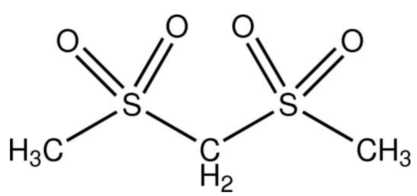
Edited by V. V. Chernyshev, Moscow State University, Russia

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(S–C) = 0.002 Å; R factor = 0.031; wR factor = 0.073; data-to-parameter ratio = 12.5.

In the title compound, $C_3H_8O_4S_2$, the two central S—C(H$_2$) bond lengths are almost identical [1.781 (2) and 1.789 (2) Å]. In the crystal, each molecule utilizes CH_2 and CH_3 bonds to form weak C—H···O hydrogen bonds to six other molecules, thus linking molecules into a three-dimensional network.

Related literature

For the structures of similar compounds, see: Berthou *et al.* (1972); Glidewell *et al.* (1995, 1996); Meehan *et al.* (1997); Zhang *et al.* (2009). For information of the use of the title compound in the food industry, see: Awaleh *et al.* (2007); Gereben & Pusztai (2012).



Experimental

Crystal data

$C_3H_8O_4S_2$
M_r = 172.21
Monoclinic, $P2_1/n$
a = 11.0496 (18) Å
b = 5.793 (3) Å
c = 11.0496 (6) Å
β = 96.77 (3)°
V = 702.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.70 mm^{-1}
T = 173 K
0.25 × 0.05 × 0.05 mm

Data collection

Stoe IPDS diffractometer
9692 measured reflections
1441 independent reflections
1274 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.073
S = 1.10
1441 reflections
115 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O4^{i}	0.94 (2)	2.55 (2)	3.342 (3)	142.3 (18)
C1—H1B···O4^{ii}	0.92 (2)	2.43 (2)	3.254 (3)	149.1 (19)
C2—H2C···O5^{iii}	0.89 (3)	2.51 (3)	3.365 (3)	160.3 (19)
C3—H3A···O6^{iv}	0.96 (2)	2.56 (2)	3.339 (3)	138.1 (18)
C3—H3A···O7^{v}	0.96 (2)	2.45 (2)	3.206 (3)	135.5 (18)
C3—H3B···O6^{vi}	0.96 (2)	2.27 (2)	3.184 (3)	159.2 (19)

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x, y+1, z$; (iii) $-x-\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x, -y+2, -z$; (vi) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *IPDS* (Stoe & Cie, 2008); cell refinement: *X-AREA* (Stoe & Cie, 2008); data reduction: *IPDS*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the University of Petra for financial support and the University of Tübingen for technical assistance.

Supporting information for this paper is available from the IUCr electronic archives (Reference: CV5464).

References

Awaleh, M. O., Badia, A. & Brisse, F. (2007). *Inorg. Chem.* **46**, 3185–3191.
Berthou, J., Jéminet, G. & Laurent, A. (1972). *Acta Cryst.* B**28**, 2480–2485.
Gereben, O. & Pusztai, L. (2012). *J. Phys. Chem. B*, **116**, 9114–9121.
Glidewell, C., Ferguson, G., Nikas, S. & Varvoglis, A. (1996). *Acta Cryst.* C**52**, 1488–1490.
Glidewell, C., Lightfoot, P. & Patterson, I. L. J. (1995). *Acta Cryst.* C**51**, 1648–1651.
Meehan, P. R., Gregson, R. M., Glidewell, C. & Ferguson, G. (1997). *Acta Cryst.* C**53**, 1975–1978.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stoe & Cie (2008). *IPDS*, *X-AREA* and *X-RED32*, Stoe & Cie, Darmstadt, Germany.
Zhang, B., Chen, X., Kang, H., Sun, F., Wang, Y., Liu, J. & Wang, D. (2009). *Acta Cryst.* E**65**, o3198.

supporting information

Acta Cryst. (2014). E**70**, o877 [doi:10.1107/S1600536814016201]

Bis(methylsulfonyl)methane

Riad Awad, Eyad Mallah, Wael Abu Dayyih, Kamal Sweidan and Manfred Steimann

S1. Comment

The title compound, bis (methylthio) methane (I), is an odorous constituent of truffle which considered as an essential food and industrial flavor used as a primary aromatic ingredient in the truffle oil when combined in an olive oil base (Gereben & Pusztai, 2012; Awaleh *et al.*, 2007).

In (I) (Fig. 1), the two central C—S bond distances [1.781 (2) Å and 1.789 (2) Å] are very close to those reported by Glidewell *et al.* (1995) for $(PhSO_2)_2CH_2$ [1.786 Å], but smaller than the corresponding distances in the $(PhSO_2)_2CBr_2$ [1.863 Å] and $(PhSO_2)_2CI)_2$ [1.854 Å], respectively. This fact could be attributed due to the large size of halogen atoms Br and I relative to the hydrogen atom in the prepared molecule. The S2—C3—S1 angle of 117.20 (10)° and the two O—S—O angles of 118.02 (8)° and 108.72 (9)° entirely consistent with those reported previously by Lucchi *et al.* (1985). The overall conformation is close to the corresponding conformations reported for similar compounds (Berthou *et al.*, 1972; Glidewell *et al.*, 1995).

S2. Experimental

The title compound was prepared by addition of Bis (methylthio) methane (2.00 ml, 19.58 mmol) to a solution containing acetic acid (16.00 ml, 279.76 mmol) with stirring at 0°C for 15 min. After that (17.00 ml, 720 mmol) of hydrogen peroxide was added drop wise at room temperature, and then the mixture was heated for 3 h at 55°C, the whit precipitate was formed, washed with methanol and dried *in vacuo*. Yield after recystallization from dichloromethane / diethyl ether 2.72 g (82%), as colorless plate crystals.

S3. Refinement

H atoms were found on electron density map and isotropically refined.

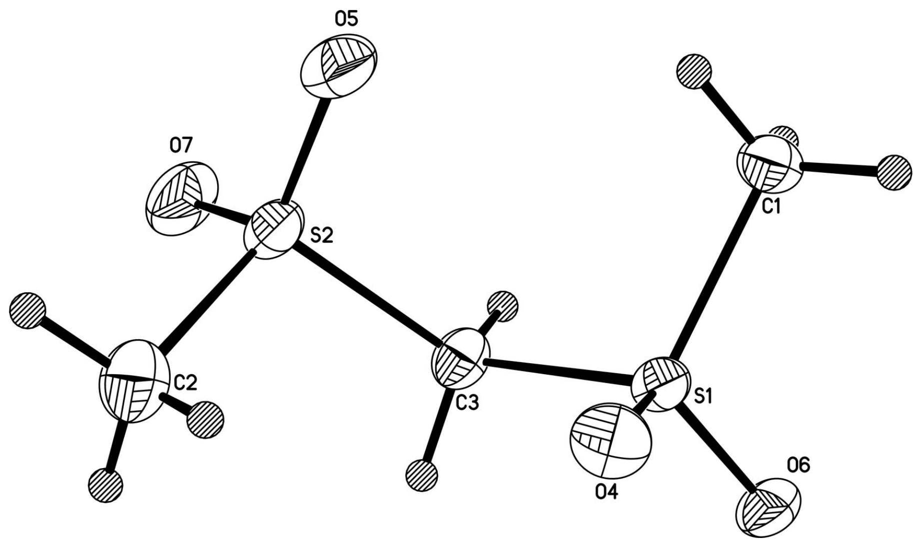


Figure 1

The molecular structure of (I) showing the atomic numbering and 50% probability displacement ellipsoids.

Bis(methylsulfonyl)methane

Crystal data

$C_3H_8O_4S_2$
$M_r = 172.21$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 11.0496$ (18) Å
$b = 5.793$ (3) Å
$c = 11.0496$ (6) Å
$\beta = 96.77$ (3)°
$V = 702.3$ (3) Å^3
$Z = 4$
$F(000) = 360$
$D_x = 1.629$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 5.7$–16.2°
$\mu = 0.70$ mm^{-1}
$T = 173$ K
Needle, colourless
0.25 × 0.05 × 0.05 mm

Data collection

Stoe IPDS diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
πhi scans
9692 measured reflections
1441 independent reflections
1274 reflections with $I > 2\sigma(I)$
$R_{int} = 0.074$
$\theta_{max} = 26.3°$, $\theta_{min} = 3.7°$
$h = -13 \rightarrow 13$
$k = -6 \rightarrow 7$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.073$
$S = 1.10$
1441 reflections
115 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0285P)^2 + 0.429P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0073 (18)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
S1	0.16353 (4)	1.01190 (7)	0.35533 (4)	0.01773 (15)
S2	−0.07227 (4)	1.00358 (8)	0.18190 (4)	0.02323 (16)
C1	0.11691 (19)	1.2396 (3)	0.44401 (18)	0.0233 (4)
H1A	0.033 (2)	1.226 (4)	0.448 (2)	0.034 (6)*
H1B	0.137 (2)	1.376 (4)	0.409 (2)	0.030 (6)*
H1C	0.160 (2)	1.220 (4)	0.524 (2)	0.037 (6)*
C2	−0.0862 (2)	0.7028 (4)	0.1665 (2)	0.0349 (5)
H2A	−0.052 (2)	0.634 (5)	0.239 (2)	0.041 (7)*
H2B	−0.046 (3)	0.657 (5)	0.099 (3)	0.048 (7)*
H2C	−0.166 (3)	0.673 (5)	0.158 (2)	0.049 (8)*
C3	0.08763 (16)	1.0559 (3)	0.20496 (16)	0.0210 (4)
H3A	0.127 (2)	0.955 (4)	0.153 (2)	0.028 (6)*
H3B	0.103 (2)	1.214 (4)	0.1858 (19)	0.027 (6)*
O4	0.12487 (12)	0.7950 (2)	0.40149 (12)	0.0254 (3)
O5	−0.12516 (12)	1.0780 (3)	0.28823 (13)	0.0325 (4)
O6	0.29086 (11)	1.0408 (2)	0.34274 (12)	0.0248 (3)
O7	−0.11405 (14)	1.1120 (3)	0.06711 (13)	0.0360 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0156 (2)	0.0170 (2)	0.0206 (2)	0.00100 (16)	0.00237 (15)	0.00051 (16)
S2	0.0151 (2)	0.0293 (3)	0.0248 (3)	0.00225 (17)	0.00043 (17)	−0.00117 (18)
C1	0.0216 (9)	0.0220 (9)	0.0267 (9)	0.0008 (7)	0.0044 (7)	−0.0055 (8)
C2	0.0240 (11)	0.0325 (12)	0.0479 (14)	−0.0070 (9)	0.0031 (10)	−0.0062 (10)
C3	0.0170 (8)	0.0243 (9)	0.0218 (9)	−0.0013 (7)	0.0024 (7)	0.0023 (7)
O4	0.0295 (7)	0.0196 (6)	0.0273 (7)	−0.0003 (5)	0.0047 (5)	0.0038 (5)
O5	0.0189 (7)	0.0465 (9)	0.0327 (8)	0.0046 (6)	0.0053 (5)	−0.0066 (7)
O6	0.0145 (6)	0.0274 (7)	0.0325 (7)	0.0017 (5)	0.0019 (5)	−0.0021 (6)
O7	0.0273 (7)	0.0492 (10)	0.0292 (7)	0.0091 (7)	−0.0061 (6)	0.0039 (7)

Geometric parameters (Å, º)

S1—O6	1.4398 (13)	S2—O5	1.4386 (14)
S1—O4	1.4397 (14)	S2—O7	1.4416 (15)
S1—C1	1.7563 (19)	S2—C2	1.756 (2)
S1—C3	1.7889 (18)	S2—C3	1.7811 (19)
O6—S1—O4	118.02 (8)	O5—S2—C2	109.70 (11)
O6—S1—C1	108.72 (9)	O7—S2—C2	109.39 (11)
O4—S1—C1	109.82 (10)	O5—S2—C3	108.90 (9)
O6—S1—C3	104.48 (8)	O7—S2—C3	105.13 (9)
O4—S1—C3	109.10 (8)	C2—S2—C3	104.87 (10)
C1—S1—C3	105.96 (10)	S2—C3—S1	117.20 (10)
O5—S2—O7	117.99 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O4^{i}	0.94 (2)	2.55 (2)	3.342 (3)	142.3 (18)
C1—H1*B*···O4^{ii}	0.92 (2)	2.43 (2)	3.254 (3)	149.1 (19)
C2—H2*C*···O5^{iii}	0.89 (3)	2.51 (3)	3.365 (3)	160.3 (19)
C3—H3*A*···O6^{iv}	0.96 (2)	2.56 (2)	3.339 (3)	138.1 (18)
C3—H3*A*···O7^{v}	0.96 (2)	2.45 (2)	3.206 (3)	135.5 (18)
C3—H3*B*···O6^{vi}	0.96 (2)	2.27 (2)	3.184 (3)	159.2 (19)

Symmetry codes: (i) −*x*, −*y*+2, −*z*+1; (ii) *x*, *y*+1, *z*; (iii) −*x*−1/2, *y*−1/2, −*z*+1/2; (iv) −*x*+1/2, *y*−1/2, −*z*+1/2; (v) −*x*, −*y*+2, −*z*; (vi) −*x*+1/2, *y*+1/2, −*z*+1/2.