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1,5-Bis(ethylsulfonyl)pentane

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The title compound, $C_9H_{20}O_4S_2$, has been obtained as an unexpected product when attempting to prepare a zinc(II) complex with the disulfoxide ligand 1,5-bis(ethylsulfinyl)-pentane. The average S—C and S=O bond lengths are 1.781 (3) and 1.436 (2) Å, respectively. The two O—S—O angles [118.0 (1) and 117.2 (1)°] are nearly equivalent, with an average value of 117.6 (1)°. The molecular skeleton is almost fully extended in the crystalline state.

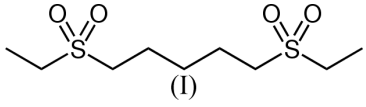
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.112
Data-to-parameter ratio = 13.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Over ten years ago, many bis-sulfone compounds, such as (*Z*)-1,2-bis(benzenesulfonyl)ethylene (Podlaha *et al.*, 1986), *dl*-2,3-bis(ethylsulfonyl)butane (Julia *et al.*, 1986), 1,2-bis(methylsulfonyl)ethane (Mo & Berg, 1982) and bis(phenylsulfonyl)-ethane (Hauback & Mo, 1990) *etc*., were synthesized by the oxidation of their corresponding thioether precursors. In the preparation of the sulfoxide, a sulfone was often obtained because of over-oxidation. During our recent research on complexes containing disulfoxide ligands, a bis-sulfone, namely 1,5-bis(ethylsulfonyl)pentane, (I), was isolated unexpectedly.



(I)

The molecular structure of (I) is shown in Fig. 1. The skeleton is extended, with no crystallographic symmety. The four O atoms (O1–O4) are located on the same side of the molecular chain formed by the C and S atoms. The dihedral angle between the two sulfonyl planes, defined by atoms O1/S1/O2 and O3/S2/O4, is 5.7 (3)°. The S—O bond lengths within each SO_2 group are almost equal, with an average value of 1.438 (7) Å at S1 and 1.433 (2) Å at S2. The average bond length for the four S—C bonds is 1.781 (3) Å. The two O—S—O angles [118.0 (1) and 117.2 (1)°] are nearly equivalent, with an average value of 117.6 (1)°. These bond lengths and angles are all in the normal ranges, and compare well those observed in other analogues (Podlaha *et al.*, 1986; Julia *et al.*, 1986; Mo & Berg, 1982; Hauback & Mo, 1990).

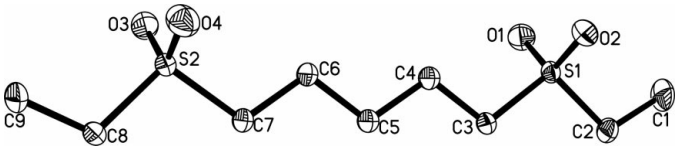


Figure 1
View of the title compound, shown with ellipsoids at the 50% probability level. H atoms have been omitted.

Experimental

1,5-Bis(ethylsulfinyl)pentane was synthesized according to a method described previously (Zhang *et al.*, 1995), and was identified by IR and ^{1}H NMR spectra, and elemental analysis. Further details will be described elsewhere. The crystals of (I) were obtained when attempting to prepare a zinc(II) complex of 1,5-bis(ethylsulfinyl)-pentane, using $Zn(ClO_4)_2{\cdot}6H_2O$ as salt and acetone/chloroform as solvent in an open container. IR spectra were recorded on an FT–IR 170SX (Nicolet) spectrometer (KBr pellet, cm^{-1}): 2944 (*m*), 1309 (*m*), 1289 (*s*), 1139 (*m*), 723 (*m*), 583 (*m*). The reason for the formation of the sulfone is unclear.

Crystal data

$C_9H_{20}O_4S_2$
M_r = 256.37
Triclinic, $P\overline{1}$
a = 5.545 (2) Å
b = 8.187 (3) Å
c = 13.867 (5) Å
α = 96.463 (6)°
β = 96.731 (6)°
γ = 91.288 (6)°
V = 620.8 (4) Å^3
Z = 2
D_x = 1.371 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 925 reflections
θ = 2.8–26.3°
μ = 0.42 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.35 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)
T_{min} = 0.849, T_{max} = 0.920
2545 measured reflections
2181 independent reflections
1766 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 25.0°
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 4$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.01
2181 reflections
157 parameters
Only H-atom U's refined
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.4839P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.433 (2)	S2—O4	1.420 (2)
S1—O2	1.444 (2)	S2—O3	1.445 (2)
S1—C2	1.777 (3)	S2—C7	1.782 (3)
S1—C3	1.780 (3)	S2—C8	1.783 (3)
O1—S1—O2	118.02 (13)	O4—S2—O3	117.19 (14)
O1—S1—C2	109.15 (14)	O4—S2—C7	108.70 (13)
O2—S1—C2	108.85 (13)	O3—S2—C7	108.66 (13)
O1—S1—C3	107.97 (13)	O4—S2—C8	109.90 (13)
O2—S1—C3	108.09 (13)	O3—S2—C8	109.19 (13)
C2—S1—C3	103.85 (13)	C7—S2—C8	102.12 (12)

The H atoms were included in calculated positions, and only their isotropic displacement parameters were allowed to refine.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (1998). *SMART* (Version 5.051) and *SAINT* (Versions 5.01). Bruker AXS Inc., Madison, Wisconsin, USA.
Hauback, B. C. & Mo, F. (1990). *Z. Kristallogr.* **191**, 195–207.
Julia, M., Lauron, H., Stacino, J.-P., Verpeaux, J.-N., Jeannin, Y. & Dromzee, Y. (1986). *Tetrahedron*, **42**, 2475–2484.
Mo, F. & Berg, O. (1982). *Acta Chem. Scand. Ser. A*, **36**, 657–664.
Podlaha, J., Podlahova, J., Kratochvil, B., Tulsani, N. B., Khawaja, A. M. & Maly, K. (1986). *Acta Cryst.* C**42**, 491–493.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Zhang, R. H., Zhan, Y. L. & Chen, J. T. (1995). *Synth. React. Inorg. Met. Org. Chem.* **25**, 283–292.