Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

(Benzylsulfonyl)methanol

Peter C. Healy,[a]* Wendy A. Loughlin,[a] Bláthín M. Sweeney[a] and Ian D. Jenkins[b]

[a]School of Science, Griffith University, Nathan, Brisbane 4111, Australia, and [b]AstraZeneca R&D, Griffith University, Don Young Rd, Mt Gravatt Research Park, Nathan, Brisbane 4111, Australia

Correspondence e-mail: p.healy@sct.gu.edu.au

The structure of the title compound, $C_8H_{10}O_3S$, (I), has been determined as part of an investigation into the synthesis and characterization of α-hydroxy sulfones. Compound (I) is novel and its X-ray structure is the first recorded for a simple α-hydroxy sulfone. In the crystals of (I), pairs of molecules are linked by intermolecular $O-H\cdots O_{\rm sulfonyl}$ hydrogen bonds around a centre of symmetry to form a dimer.

Received 3 January 2002
Accepted 8 January 2002
Online 11 January 2002

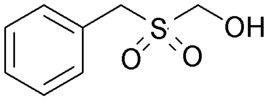
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.101
Data-to-parameter ratio = 14.4

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

Comment

The title compound, (I), is an α-hydroxy sulfone. It was obtained as a crystalline compound which decomposed very slowly upon standing. This result was considered unusual in that simple α-hydroxy sulfones such as this have been reported as being unstable and easily subject to cleavage (Field & Settlage, 1951; Bredereck *et al.*, 1954). In the crystals, pairs of centrosymmetrically related molecules are associated through intermolecular hydrogen-bonding interactions between the α-hydroxyl groups and one of the sulfone O atoms so as to form a dimer [$H\cdots O3^{i}$ = 1.99 Å, $O1\cdots O3^{i}$ = 2.783 (4) Å and $O1-H\cdots O3^{i}$ = 161°; symmetry code: (i) $-x$, $1-y$, $1-z$]. This hydrogen-bonding motif can be described using graph-set notation (Bernstein *et al.*, 1995) as $R_2^2(10)$. The S1—C1 bond distance of 1.799 (3) Å is 0.02 Å longer than the S1—C2 bond distance of 1.779 (3) Å. This is consistent with the influence of the electron-withdrawing O atom attached to atom C1.



(I)

Experimental

The title compound was prepared by the reaction of benzylmagnesium chloride with sulfur dioxide followed by quenching with sulfuric acid to yield benzylsulfinic acid (van Allen *et al.*, 1966). Immediate treatment with formaldehyde (Bredereck & Bäder, 1954) yielded (I) upon work-up as a solid powder. Crystals were isolated as colourless needles by slow evaporation of an ether solution of (I).

DOI: 10.1107/S1600536802000429

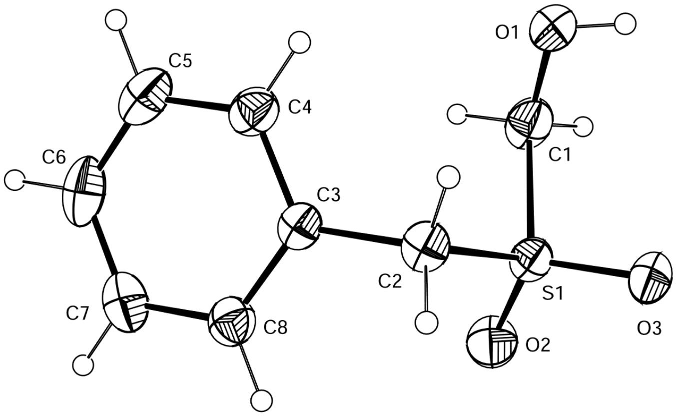


Figure 1
ORTEP-3 (Farrugia, 1997) plot showing the atomic numbering scheme for (I). Displacement ellipsoids are drawn at the 30% probability level for non-H atoms.

Crystal data

$C_8H_{10}O_3S$
$M_r = 186.23$
Monoclinic, $P2_1/n$
$a = 22.758$ (11) Å
$b = 7.160$ (7) Å
$c = 5.422$ (2) Å
$\beta = 91.88$ (3)°
$V = 883.0$ (10) Å^3
$Z = 4$
$D_x = 1.401$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 12.6$–17.4°
$\mu = 0.33$ mm^{-1}
$T = 295$ K
Prismatic, colourless
0.30 × 0.20 × 0.15 mm

Data collection

Rigaku AFC-7*R* diffractometer
$\omega/2\theta$ scans
1795 measured reflections
1565 independent reflections
1155 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\rm max} = 25.0°$
$h = -13 \rightarrow 27$
$k = 0 \rightarrow 8$
$l = -6 \rightarrow 6$
3 standard reflections every 150 reflections intensity decay: 3.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.101$
$S = 1.05$
1565 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 0.1986P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.25$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.23$ e Å^{-3}

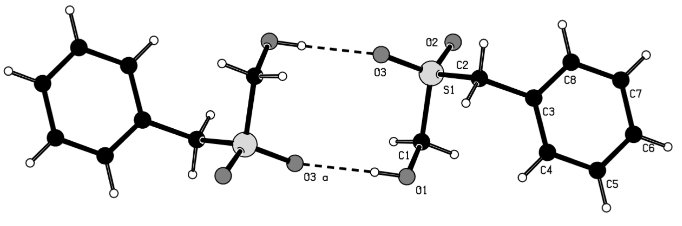


Figure 2
The hydrogen-bonding scheme for the dimer.

H atoms were placed at calculated positions with C—H distances set to 0.95 Å, except for the hydroxyl H atom, which was located from a difference synthesis, and O—H was set to 0.82 Å. All H atoms were constrained in the refinement.

Data collection: *MSC/AFC*-7 *Diffractometer Control Software* (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC*-7 *Diffractometer Control Software*; data reduction: *teXsan for Windows* (Molecular Structure Corporation, 1997–2001); program(s) used to solve structure: *teXsan for Windows*; program(s) used to refine structure: *teXsan for Windows* and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2001) and *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *teXsan for Windows* and *PLATON*.

The authors thank the Australian Research Council for financial assistance.

References

Allen, R. T. van, Scott, R. B. & Brockelbank, E. L. (1966). *J. Org. Chem.* **31**, 2357–2365.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bredereck, H. & Bäder, E. (1954). *Chem. Ber.* **87**, 129–139.
Bredereck. H., Bäder, E. & Wohnhas, A. (1954). *Makromol. Chem.* **12**, 100–109.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Field, L. & Settlage, P. H. (1951). *J. Am. Chem. Soc.* **73**, 5870–5872.
Molecular Structure Corporation (1999). *MSC/AFC*-7 *Diffractometer Control Software for Windows*. Version 1.02. MSC, 9009 New Trails Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1997–2001). *teXsan for Windows*. Version 1.06. MSC, 9009 New Trails Drive, The Woodlands, TX 77381, USA.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2001). *PLATON* for Windows. Version 121201. University of Utrecht, The Netherlands.