Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Benzenesulfonamide

B. Thimme Gowda,[a]* Roopa Nayak,[a] Jozef Kožíšek,[b] Miroslav Tokarčík[c] and Hartmut Fuess[d]

[a]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, [b]Department of Physical Chemistry, Slovak University of Technology, Radlinského 9, SK-812 37 Bratislava, Slovak Republic, [c]Department of Chemical Physics, Slovak University of Technology, Radlinského 9, 812 37 Bratislava, Slovak Republic, and [d]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287, Darmstadt, Germany
Correspondence e-mail: gowdabt@yahoo.com

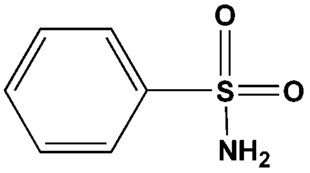
Received 29 April 2007; accepted 16 May 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.016 Å; R factor = 0.074; wR factor = 0.260; data-to-parameter ratio = 11.3.

The structure of the title compound (BSA), $C_6H_7NO_2S$, closely resembles those of other aryl sulfonamides. The geometric parameters in BSA are similar except for some difference in the S=O bond lengths. Molecules are connected by N—H···O hydrogen bonds into layers parallel to the bc plane, with an interlayer distance of 7.734 (2) Å.

Related literature

For related literature, see: Gowda & Shetty (2004); Gowda *et al.* (2002, 2003, 2005, 2007); Jones & Weinkauf (1993); Kumar *et al.* (1992); O'Connor & Maslen (1965).



Experimental

Crystal data

$C_6H_7NO_2S$
M_r = 157.19
Monoclinic, Pc
a = 8.304 (2) Å
b = 5.534 (1) Å
c = 8.237 (2) Å
β = 111.36 (3)°
V = 352.52 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 295 (2) K
0.52 × 0.46 × 0.09 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006; Clark & Reid, 1995)
$T_{\min}$ = 0.812, $T_{\max}$ = 0.956
2613 measured reflections
1003 independent reflections
621 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.260
S = 1.01
1003 reflections
93 parameters
5 restraints
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.19 e Å^{-3}
$\Delta\rho_{\min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983), with 356 Friedel pairs
Flack parameter: −0.1 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1$^{\rm i}$	0.89	2.20	2.932 (14)	139
N1—H1B···O2$^{\rm ii}$	0.89	2.17	3.016 (17)	158

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

BTG gratefully thanks the Alexander von Humboldt Foundation, Bonn, Germany, for the extensions of his research fellowship. JK and MT thank the Grant Agency of the Slovak Republic (grant No. 1/2449/05).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2171).

References

Clark, R. C. & Reid, J. S. (1995). *Acta Cryst.* A**51**, 887–897.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Gowda, B. T., Damodara, N. & Jyothi, K. (2005). *Int. J. Chem. Kinet.* **37**, 572–582.
Gowda, B. T., Jyothi, K. & D'Souza, J. D. (2002). *Z. Naturforsch. Teil A*, **57**, 967–973.
Gowda, B. T., Jyothi, K., Kozisek, J. & Fuess, H. (2003). *Z. Naturforsch. Teil A*, **58**, 656–660.
Gowda, B. T. & Shetty, M. (2004). *J. Phys. Org. Chem.* **17**, 848–864.
Gowda, B. T., Srilatha, Foro, S., Kozisek, J. & Fuess, H. (2007). *Z. Naturforsch. Teil A*, **62**. In the press.
Jones, P. G. & Weinkauf, A. (1993). *Z. Kristallogr.* **208**, 128–129.
Kumar, S. V., Senadhi, S. E. & Rao, L. M. (1992). *Z. Kristallogr.* **202**, 1–6.
O'Connor, B. H. & Maslen, E. N. (1965). *Acta Cryst.* **18**, 363–366.
Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

doi:10.1107/S1600536807024221

supplementary materials

Acta Cryst. (2007). E**63**, o2967 [**doi:10.1107/S1600536807024221**]

Benzenesulfonamide

B. T. Gowda, **R. Nayak**, **J. Kozísek**, **M. Tokarcík** and **H. Fuess**

Comment

The chemistry of sulfonamides is of interest as they show distinct physical, chemical and biological properties. Many arylsulfonamides and their N-halo compounds exhibit pharmacological, fungicidal and herbicidal activities due to their oxidizing action in aqueous, partial aqueous and non-aqueous media. Thus N-halo arylsulfonamides are of interest in synthetic, mechanistic, analytical and biological chemistry (Gowda *et al.*, 2002; 2003; 2005; 2007; Gowda & Shetty, 2004). In the present work, the structure of benzenesulfonamde (BSA) has been determined to explore the substituent effects on the solid state structures of sulfonamides and N-halo arylsulfonamides (Gowda *et al.*, 2003, 2007). The structure of BSA (Fig. 1) closely resembles those of other aryl sulfonamides (Gowda *et al.*, 2003; Jones & Weinkauf, 1993; Kumar *et al.*, 1992; O'Connor & Maslen, 1965). The parent sulphonamide, BSA crystallizes in monoclinic *Pc* space group in contrast to orthorhombic Pbca space group observed with 4-fluorobenzenesulfonamide (Jones & Weinkauf, 1993) and 4-aminobenzenesulfonamide (O'Connor & Maslen, 1965) and monoclinic P21/n space group observed with 4-chlorobenzenesulfonamide and 4-bromobenzenesulfonamide (Gowda *et al.*, 2003), and 4-methylbenzenesulfonamide (Kumar *et al.*, 1992). The bond parameters in BSA are similar except for some slight differences in the S—O bond lengths.

Molecules are connected by N—H···O hydrogen bonds into layers parallel to the *bc*-plane (Fig.2), with interlayer distance 7.734 (2) Å.

Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2002, 2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Gowda *et al.*, 2002). Single crystals of the title compound were obtained from a slow evaporation of its ethanolic solution and used for X-ray diffraction studies at room temperature.

Refinement

Monoclinic crystal (1) was refined as twinned, with two twin domains (fractional contributions 84 and 16 percent). The non-merohedral twinning was analysed using TwinRotMat routine within *WinGX* package. It was found that 22 percent of total reflections were overlapped with rotation matrix (1.000 0.000 0.734) (0.000 − 1.000 0.000) (0.000 0.000 − 1.000) Using the above twin matrix a HKLF5 file was generated which was subsequenly used in the *SHELXL97* refinement of the structure. The BASF parameter was refined to final value 0.154.

Hydrogen atoms attached to carbons were positioned geometrically and treated as riding with C–H = 0.93 Å. H atoms attached to N1 atom were placed in positions with N–H bond distance restrained to 0.89 (2)Å and H–H restrained to 1.50 (3) Å. In the last stage of refinement, these H were treated as riding on their parent N atom with U_{iso}(H)=1.2 U_{eq}(N).

Although the N atom has an elongated ellipsoids, no reasonable disordered model could be defined.

Owing to the poor quality of the data, the absolute structure couldn't be reliably defined and any references to the Flack parameter have been omitted. The Friedel pairs were merged.

Figures

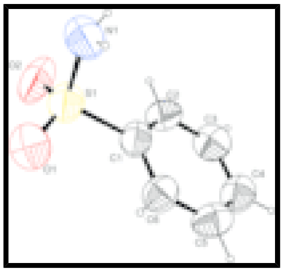


Fig. 1. *ORTEP* view of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

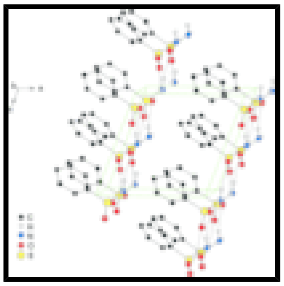


Fig. 2. Packing of the title compound viewed down the *b* axis, showing molecular layers parallel to the *bc*-plane. Within a layer the molecules are connected by N—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bondings have been omitted for clarity.

Benzenesulfonamide

Crystal data

$C_6H_7NO_2S$

$M_r = 157.19$

Monoclinic, *Pc*

Hall symbol: P -2yc

$a = 8.304\ (2)$ Å

$b = 5.534\ (1)$ Å

$c = 8.237\ (2)$ Å

$\beta = 111.36\ (3)$°

$V = 352.52\ (15)$ Å^3

$Z = 2$

$F_{000} = 164$

$D_x = 1.481$ Mg m^{-3}

Mo *K*α radiation
$\lambda = 0.71073$ Å

Cell parameters from 706 reflections

$\theta = 2.0$–30.0°

$\mu = 0.39$ mm^{-1}

$T = 295\ (2)$ K

Plate, colourless

0.52 × 0.46 × 0.09 mm

Data collection

Oxford Diffraction Xcalibur diffractometer

Monochromator: graphite

$T = 295(2)$ K

Rotation method data acquisition using ω and phi scans

Absorption correction: analytical

621 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.086$

$\theta_{\max} = 25.7$°

$\theta_{\min} = 4.5$°

$h = -10 \rightarrow 10$

(CrysAlis RED; Oxford Diffraction, 2006; Clark & Reid, 1995)	
$T_{\min} = 0.812$, $T_{\max} = 0.956$	$k = -6\rightarrow 6$
2613 measured reflections	$l = -10\rightarrow 8$
1003 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.074$	$w = 1/[\sigma^2(F_o^2) + (0.1777P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.260$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.01$	$\Delta\rho_{\max} = 0.19$ e Å^{-3}
1003 reflections	$\Delta\rho_{\min} = -0.31$ e Å^{-3}
93 parameters	Extinction correction: none
5 restraints	Absolute structure: Flack (1983), with 356 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.1 (3)
Secondary atom site location: difference Fourier map	

Special details

Experimental. Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by Clark & Reid, 1995).

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	$U_{\text{iso}}*/U_{\text{eq}}$
O1	1.1057 (12)	0.6751 (12)	0.7719 (12)	0.124 (2)
O2	1.0908 (12)	1.0728 (16)	0.6495 (18)	0.153 (4)
S1	1.0618 (2)	0.8225 (4)	0.6248 (2)	0.1057 (11)
C1	0.8412 (11)	0.7887 (19)	0.4996 (12)	0.095 (3)
C2	0.7597 (12)	0.9503 (16)	0.3760 (14)	0.096 (2)
H2	0.8191	1.0812	0.3544	0.115*
C3	0.5887 (15)	0.919 (2)	0.2829 (17)	0.111 (3)
H3	0.5293	1.0355	0.2016	0.134*

C4	0.5006 (14)	0.717 (2)	0.3070 (17)	0.111 (3)
H4	0.3844	0.6934	0.2395	0.133*
C5	0.5888 (16)	0.5511 (17)	0.4325 (17)	0.109 (3)
H5	0.5307	0.4170	0.4519	0.130*
C6	0.7579 (12)	0.5802 (16)	0.5278 (13)	0.096 (2)
H6	0.8182	0.4656	0.6100	0.115*
N1	1.1731 (11)	0.734 (3)	0.5134 (11)	0.149 (4)
H1A	1.1665	0.5763	0.4933	0.179*
H1B	1.1408	0.8270	0.4185	0.179*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.131 (6)	0.116 (5)	0.115 (5)	0.014 (4)	0.035 (5)	−0.001 (4)
O2	0.092 (5)	0.168 (7)	0.185 (9)	−0.035 (5)	0.036 (6)	−0.078 (7)
S1	0.0844 (13)	0.126 (2)	0.1070 (17)	0.0067 (16)	0.0350 (11)	−0.0243 (18)
C1	0.071 (4)	0.122 (7)	0.094 (6)	0.000 (5)	0.032 (4)	−0.032 (5)
C2	0.083 (5)	0.098 (6)	0.114 (7)	0.003 (4)	0.045 (5)	0.011 (5)
C3	0.099 (6)	0.116 (7)	0.121 (7)	0.026 (6)	0.043 (6)	0.007 (7)
C4	0.082 (5)	0.126 (7)	0.129 (9)	0.000 (5)	0.044 (5)	−0.029 (7)
C5	0.114 (8)	0.088 (6)	0.137 (10)	−0.008 (5)	0.062 (7)	0.005 (6)
C6	0.092 (6)	0.087 (5)	0.109 (7)	−0.003 (4)	0.036 (5)	−0.006 (5)
N1	0.067 (4)	0.283 (13)	0.097 (6)	0.045 (7)	0.029 (4)	−0.020 (7)

Geometric parameters (Å, °)

O1—S1	1.394 (8)	C3—H3	0.9300
O2—S1	1.408 (9)	C4—C5	1.376 (16)
S1—N1	1.597 (8)	C4—H4	0.9300
S1—C1	1.755 (9)	C5—C6	1.346 (15)
C1—C2	1.339 (13)	C5—H5	0.9300
C1—C6	1.407 (15)	C6—H6	0.9300
C2—C3	1.356 (16)	N1—H1A	0.8885
C2—H2	0.9300	N1—H1B	0.8901
C3—C4	1.393 (18)		
O1—S1—O2	118.2 (7)	C4—C3—H3	119.4
O1—S1—N1	107.3 (6)	C5—C4—C3	118.7 (10)
O2—S1—N1	106.2 (8)	C5—C4—H4	120.7
O1—S1—C1	109.5 (5)	C3—C4—H4	120.7
O2—S1—C1	106.1 (6)	C6—C5—C4	121.0 (9)
N1—S1—C1	109.2 (4)	C6—C5—H5	119.5
C2—C1—C6	122.0 (9)	C4—C5—H5	119.5
C2—C1—S1	120.4 (8)	C5—C6—C1	118.3 (9)
C6—C1—S1	117.5 (8)	C5—C6—H6	120.9
C1—C2—C3	118.7 (9)	C1—C6—H6	120.9
C1—C2—H2	120.6	S1—N1—H1A	113.4
C3—C2—H2	120.6	S1—N1—H1B	106.0
C2—C3—C4	121.2 (10)	H1A—N1—H1B	115.1

C2—C3—H3	119.4

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.89	2.20	2.932 (14)	139
N1—H1B···O2^{ii}	0.89	2.17	3.016 (17)	158

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

Fig. 1

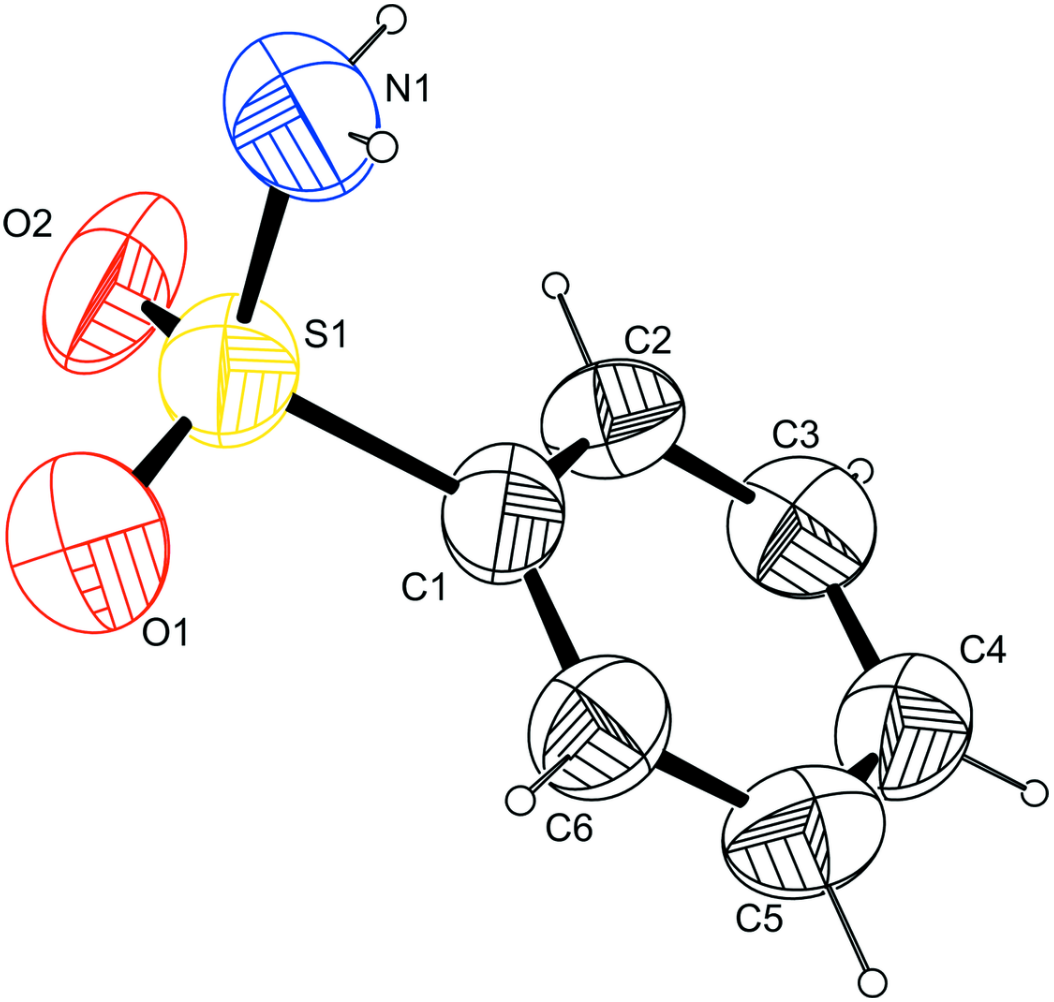


Fig. 2