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2-(Benzenesulfonamido)acetic acid

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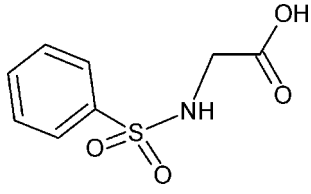
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.116; data-to-parameter ratio = 18.1.

The title compound, $C_8H_9NO_4S$, is of interest as a precursor to biologically active sulfur-containing heterocyclic cmpounds. The crystal structure displays the classical O—H···O intermolecular hydrogen bonding typical for carboxylic acids forming dimers. Symmetry-related dimers are, in turn, linked through head-to-tail pairs of intermolecular N—H···O interactions, giving rise to a zigzag chain along the c axis.

Related literature

For the synthesis and biological evaluation of sulfur-containing heterocyclic compounds, see: Zia-ur-Rehman *et al.* (2005, 2006, 2007, 2008); Wen *et al.* (2005). For related structures, see: Wen *et al.* (2006); Zhang *et al.* (2006). For bond-length data, see: Allen *et al.* (1987). For background information, see: Berredjem *et al.* (2000); Esteve & Bidal (2002); La Roche & Co (1967*a*,*b*); Lee & Lee (2002); Martinez *et al.* (2000); Soledade *et al.* (2006); Xiao & Timberlake (2000). For related literature, see: Gowda *et al.* (2007*a*,*b*,*c*); Kayser *et al.* (2004); La Roche & Co (1967); Vaichulis (1977).



Experimental

Crystal data

$C_8H_9NO_4S$
M_r = 215.23
Monoclinic, $P2_1/n$
a = 8.5181 (3) Å
b = 11.1302 (4) Å
c = 10.6414 (4) Å
β = 112.600 (2)°
V = 931.42 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 296 (2) K
0.36 × 0.16 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.889, T_{max} = 0.952
10301 measured reflections
2338 independent reflections
1644 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.116
S = 1.03
2338 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.20	3.054 (3)	174
O3—H8···O4^{ii}	0.82	1.86	2.678 (2)	178

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors are grateful to the Higher Education Commission of Pakistan for their grant to purchase the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2721).

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Acta Cryst. (2008). E**64**, o2283–o2284 [doi:10.1107/S1600536808035721]

2-(Benzenesulfonamido)acetic acid

Muhammad Nadeem Arshad, Islam Ullah Khan and Muhammad Zia-ur-Rehman

S1. Comment

Sulfonamide is an important functionality found in many naturally occurring as well as synthetic compounds which possess numerous types of biological activities *e.g.*, anticonvulsant, antihypertensive, herbicidal and antimalarial (Soledade *et al.*, 2006; Esteve & Bidal, 2002; Xiao & Timberlake, 2000; Martinez *et al.*, 2000; Berredjem *et al.*, 2000; Lee & Lee, 2002) activities. In addition, these are found useful as anticancer (La Roche & Co, 1967) and antitubercular (Vaichulis, 1977) agents. These are also assumed as safe antibiotics during Pregnancy (Kayser *et al.*, 2004).

In the present paper, the structure of the title compound has been determined as a part of our ongoing research on the synthesis and biological evaluation of sulfur containing heterocyclic compounds (Zia-ur-Rehman *et al.*, 2005, 2006, 2007, 2008). In the molecule of (**I**) (Fig. 1), bond lengths and bond angles are almost similar to those in the related sulfonamide molecules (Gowda *et al.*, 2007*a*,*b*,*c*) and the bond lengths are within normal ranges (Allen *et al.*, 1987). In the crystal structure, each molecule is linked to an inersion related one through head-to-tail pairs of O—H···O intermolecular hydrogen bonds giving rise to dimeric motifs typical for carboxylic acids. Neighbouring dimers are further arranged into zigzag chains along *c* axis through head-to-tail pairs of N—H···O intermolecular interactions.

S2. Experimental

A mixture of *N*-benzenesulfonyl glycine methyl ester (1.0 g; 4.5 mmoles) and aqueous sodium hydroxide solution (10%; 10.0 ml) was refluxed for a peiod of one hour, cooled and acidified with 1 N hydrochloric acid. A white precipitate obtained was washed with water, dried and recrystallized from methanol to obtain colourless crystals suitable for X-ray studies; m.p. 435-436K.

S3. Refinement

All H atoms were placed in idealized positions, (C-H = 0.93-97 Å, O-H = 0.82Å, and N-H = 0.86Å), and included in the refinement in a riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C and N) and U_{iso}(H) = 1.5U_{eq}(O).

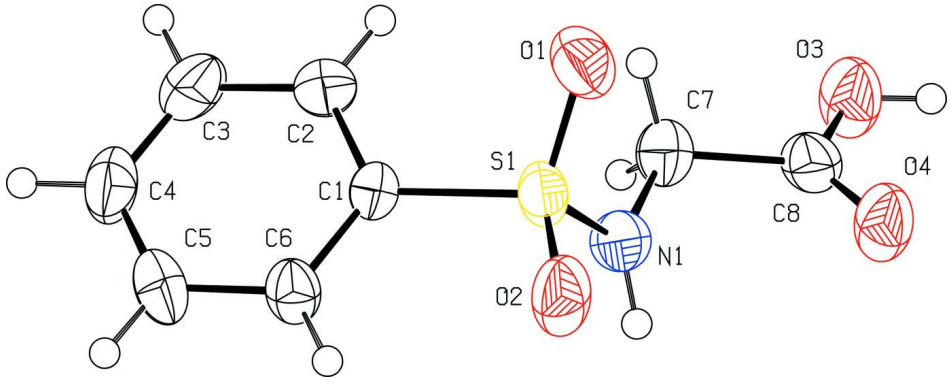

Figure 1

The molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

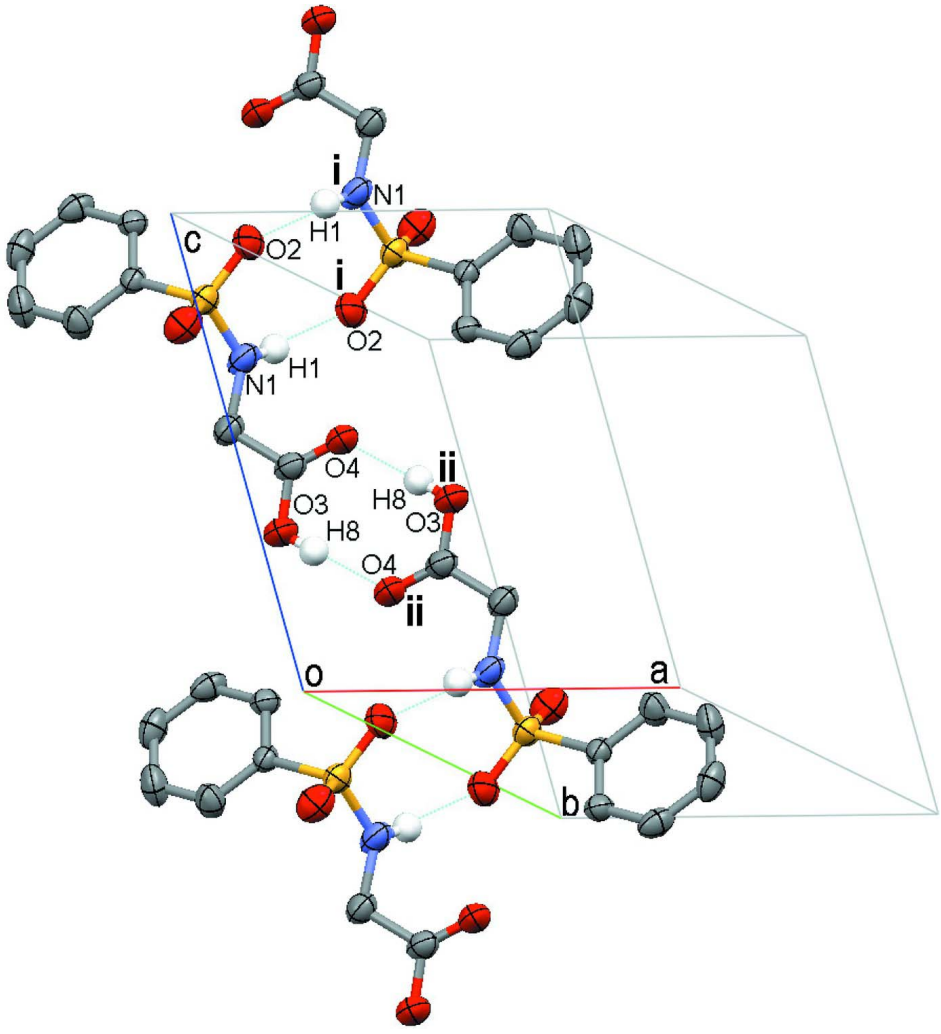

Figure 2

Part of the crystal structure, viewed approximately along the *b* axis, showing hydrogen bond interactions (dashed lines) along the [0 0 1] direction. H atoms not involved in hydrogen bonding have been omitted for clarity. Symmetry codes as given in Table 1.

2-(Benzenesulfonamido)acetic acid

Crystal data

$C_8H_9NO_4S$
$M_r = 215.23$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.5181\ (3)$ Å
$b = 11.1302\ (4)$ Å
$c = 10.6414\ (4)$ Å
$\beta = 112.600\ (2)°$
$V = 931.42\ (6)$ Å^3
$Z = 4$

$F(000) = 448$
$D_x = 1.535$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2708 reflections
$\theta = 2.8–26.2°$
$\mu = 0.34$ mm^{-1}
$T = 296$ K
Cubes, colourless
0.36 × 0.16 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.889, T_{max} = 0.952
10301 measured reflections
2338 independent reflections
1644 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 28.4°, θ_{min} = 2.6°
h = −11→11
k = −14→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.116
S = 1.03
2338 reflections
128 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
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 0.3567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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	0.16488 (6)	0.67470 (5)	0.09397 (5)	0.04003 (18)
O1	0.1794 (2)	0.77973 (15)	0.17404 (17)	0.0549 (4)
O2	0.01764 (18)	0.65761 (17)	−0.02937 (16)	0.0570 (5)
O3	0.2307 (2)	0.51175 (18)	0.53583 (15)	0.0586 (5)
H8	0.1631	0.5017	0.5728	0.088*
O4	−0.0061 (2)	0.52365 (18)	0.34770 (15)	0.0573 (5)
N1	0.1740 (3)	0.56105 (19)	0.18822 (18)	0.0518 (5)
H1	0.1223	0.4965	0.1497	0.062*
C1	0.3436 (2)	0.66945 (18)	0.04972 (19)	0.0319 (4)
C2	0.5008 (3)	0.7030 (2)	0.1452 (2)	0.0474 (6)
H2	0.5119	0.7290	0.2313	0.057*
C3	0.6406 (3)	0.6970 (2)	0.1100 (3)	0.0575 (7)
H3	0.7476	0.7174	0.1736	0.069*
C4	0.6226 (3)	0.6612 (2)	−0.0184 (3)	0.0519 (6)
H4	0.7171	0.6593	−0.0418	0.062*
C5	0.4666 (3)	0.6282 (2)	−0.1123 (2)	0.0463 (5)

H5	0.4558	0.6039	−0.1988	0.056*
C6	0.3255 (2)	0.6309 (2)	−0.07854 (19)	0.0386 (5)
H6	0.2197	0.6070	−0.1413	0.046*
C7	0.2639 (3)	0.5602 (2)	0.3340 (2)	0.0456 (5)
H7A	0.3143	0.6385	0.3640	0.055*
H7B	0.3550	0.5015	0.3585	0.055*
C8	0.1465 (3)	0.5299 (2)	0.4048 (2)	0.0429 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0364 (3)	0.0515 (4)	0.0382 (3)	−0.0005 (2)	0.0210 (2)	−0.0011 (2)
O1	0.0665 (11)	0.0495 (10)	0.0606 (10)	0.0057 (8)	0.0376 (9)	−0.0035 (8)
O2	0.0327 (7)	0.0894 (14)	0.0493 (9)	−0.0016 (8)	0.0161 (7)	0.0003 (9)
O3	0.0539 (10)	0.0876 (14)	0.0368 (8)	−0.0090 (9)	0.0200 (7)	0.0061 (9)
O4	0.0496 (9)	0.0886 (14)	0.0364 (8)	−0.0138 (9)	0.0196 (7)	0.0028 (8)
N1	0.0702 (13)	0.0551 (13)	0.0395 (10)	−0.0230 (10)	0.0314 (9)	−0.0075 (9)
C1	0.0307 (9)	0.0338 (11)	0.0337 (9)	−0.0008 (8)	0.0153 (8)	0.0032 (8)
C2	0.0428 (11)	0.0554 (15)	0.0445 (12)	−0.0114 (10)	0.0171 (9)	−0.0138 (11)
C3	0.0350 (11)	0.0646 (17)	0.0718 (17)	−0.0140 (11)	0.0195 (11)	−0.0136 (14)
C4	0.0448 (12)	0.0513 (15)	0.0737 (16)	0.0012 (10)	0.0384 (12)	0.0036 (12)
C5	0.0544 (13)	0.0525 (14)	0.0430 (12)	0.0104 (11)	0.0308 (10)	0.0079 (10)
C6	0.0359 (10)	0.0494 (13)	0.0309 (10)	0.0026 (9)	0.0135 (8)	0.0044 (9)
C7	0.0501 (12)	0.0490 (14)	0.0441 (12)	−0.0058 (10)	0.0251 (10)	0.0018 (10)
C8	0.0550 (13)	0.0431 (13)	0.0344 (10)	−0.0059 (10)	0.0213 (10)	−0.0010 (9)

Geometric parameters (Å, º)

S1—O1	1.4237 (17)	C2—H2	0.9300
S1—O2	1.4376 (16)	C3—C4	1.374 (4)
S1—N1	1.598 (2)	C3—H3	0.9300
S1—C1	1.7590 (19)	C4—C5	1.370 (3)
O3—C8	1.316 (2)	C4—H4	0.9300
O3—H8	0.8200	C5—C6	1.381 (3)
O4—C8	1.207 (3)	C5—H5	0.9300
N1—C7	1.443 (3)	C6—H6	0.9300
N1—H1	0.8600	C7—C8	1.502 (3)
C1—C6	1.382 (3)	C7—H7A	0.9700
C1—C2	1.385 (3)	C7—H7B	0.9700
C2—C3	1.380 (3)		
O1—S1—O2	119.98 (11)	C5—C4—C3	120.6 (2)
O1—S1—N1	107.60 (10)	C5—C4—H4	119.7
O2—S1—N1	106.46 (10)	C3—C4—H4	119.7
O1—S1—C1	107.60 (10)	C4—C5—C6	120.1 (2)
O2—S1—C1	107.00 (9)	C4—C5—H5	119.9
N1—S1—C1	107.66 (10)	C6—C5—H5	119.9
C8—O3—H8	109.5	C5—C6—C1	119.04 (19)

C7—N1—S1	123.95 (16)	C5—C6—H6	120.5
C7—N1—H1	118.0	C1—C6—H6	120.5
S1—N1—H1	118.0	N1—C7—C8	111.13 (18)
C6—C1—C2	121.18 (19)	N1—C7—H7A	109.4
C6—C1—S1	119.67 (15)	C8—C7—H7A	109.4
C2—C1—S1	119.14 (15)	N1—C7—H7B	109.4
C3—C2—C1	118.7 (2)	C8—C7—H7B	109.4
C3—C2—H2	120.7	H7A—C7—H7B	108.0
C1—C2—H2	120.7	O4—C8—O3	124.5 (2)
C4—C3—C2	120.3 (2)	O4—C8—C7	123.80 (19)
C4—C3—H3	119.8	O3—C8—C7	111.68 (19)
C2—C3—H3	119.8		

O1—S1—N1—C7	−28.4 (2)	S1—C1—C2—C3	179.16 (19)
O2—S1—N1—C7	−158.27 (18)	C1—C2—C3—C4	1.5 (4)
C1—S1—N1—C7	87.27 (19)	C2—C3—C4—C5	−1.6 (4)
O1—S1—C1—C6	−141.46 (18)	C3—C4—C5—C6	0.1 (4)
O2—S1—C1—C6	−11.3 (2)	C4—C5—C6—C1	1.3 (4)
N1—S1—C1—C6	102.82 (18)	C2—C1—C6—C5	−1.3 (3)
O1—S1—C1—C2	39.3 (2)	S1—C1—C6—C5	179.46 (17)
O2—S1—C1—C2	169.46 (18)	S1—N1—C7—C8	121.9 (2)
N1—S1—C1—C2	−76.44 (19)	N1—C7—C8—O4	−9.4 (3)
C6—C1—C2—C3	−0.1 (3)	N1—C7—C8—O3	170.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.20	3.054 (3)	174
O3—H8···O4^{ii}	0.82	1.86	2.678 (2)	178

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