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Crystal structure of 2-benzenesulfonamido-3-hydroxypropanoic acid

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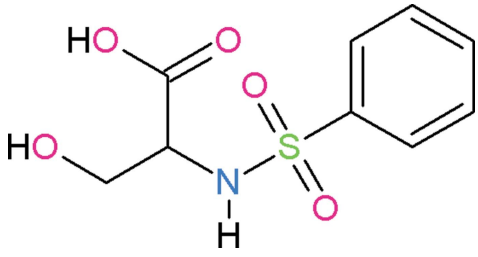
In the title compound, $C_9H_{11}NO_5S$, the O═S═O plane of the sulfonyl group is twisted at a dihedral angle of 52.54 (16)° with respect to the benzene ring. The dihedral angle between the carboxylic acid group and the benzene ring is 49.91 (16)°. In the crystal, C—H···O, N—H···O and O—H···O hydrogen bonds link the molecules into (001) sheets.

Keywords: crystal structure; benzenesulfonamido; propanoic acid; sulfonyl group; O—H···O hydrogen bonds.

CCDC reference: 1433189

1. Related literature

For related structures, see: Aguilar-Castro *et al.* (2004); Arshad *et al.* (2009, 2012); Zolotarev *et al.* (2014).



2. Experimental

2.1. Crystal data

$C_9H_{11}NO_5S$
M_r = 245.25
Orthorhombic, $P2_12_12_1$
a = 5.0464 (4) Å
b = 9.9752 (8) Å
c = 21.4701 (17) Å
V = 1080.78 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 296 K
0.40 × 0.20 × 0.18 mm

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.890, T_{max} = 0.950
5013 measured reflections
2354 independent reflections
1978 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.093
S = 1.03
2354 reflections
149 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack x determined using 919 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.05 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^{i}	0.84 (5)	1.81 (5)	2.621 (4)	164 (5)
O3—H3···O5^{i}	0.82	1.96	2.754 (3)	164
N1—H1A···O4^{ii}	0.86	2.39	3.066 (4)	136
C2—H2···O2^{iii}	0.98	2.48	3.425 (5)	162
C6—H6···O5^{iv}	0.93	2.52	3.342 (5)	148
C7—H7···O2^{v}	0.93	2.58	3.347 (5)	141

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x+1, y, z$; (iii) $x-1, y, z$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, -z$; (v) $x-\frac{1}{2}, -y+\frac{3}{2}, -z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7530).

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supporting information

Acta Cryst. (2015). E**71**, o902–o903 [doi:10.1107/S2056989015020149]

Crystal structure of 2-benzenesulfonamido-3-hydroxypropanoic acid

Nabila Jabeen, Misbah Mushtaq, Muhammad Danish, Muhammad Nawaz Tahir and Muhammad Asam Raza

S1. Comment

The title compound (I), (Fig. 1) has been synthesized for complexation and other studius.

The crystal structures of *N*-((4-methylphenyl)sulfonyl)serine (Zolotarev *et al.*, 2014), *N(S)*-(*p*-toluenesulfonyl)-*L*-alanine (Aguilar-Castro *et al.*, 2004), 2-benzenesulfonamido-3-methylbutyric acid (Arshad *et al.*, 2012) and (2*R*)-2-benzenesulfonamido-2- phenylethanoic acid (Arshad *et al.*, 2009) have been reported which are related to the title compound.

The aminoacetic acid moiety B (C1/C2/N1/O1/O2) is roughly planar with r.m.s. deviation of 0.0588 Å. The dihedral angle between the benzene ring and B is 52.96 (14)°. The sulfonyl group *C* (S1/O4/O5) is oriented at a dihedral angle of 52.54 (16)° with the parent benzene ring. In the crystal, the molecules are linked into a two-dimensional polymeric network (Table 2, Fig. 2) due to H-bondings of C–H···O, N–H···O and O–H···O types with base vectors [100], [010] and in the plane (001).

S2. Experimental

The title compound was prepared by using equimolar ratio of *L*-serine and benzenesulfonyl chloride in 40 ml water. The benzenesulfonyl chloride disolved in distilled water was added pinch by pinch in the *L*-serine already disolved in distilled water and stirred at 296–298 K, while keeping the pH of the reaction mixture was maintained at 8–9 by adding 1.0 *M* sodium bicarbonate solution. The 1.0 *M* HCl solution was added after an hour which resulted in the form of white precipitates. The precipitates obtained were filtered and dried from which colourless needles of (I) were obtained after recrystallization from ethanol solution after 48 h. Yield: 68% Melting point: 493 K.

S3. Refinement

The coordinates of H-atom of carboxyl group were refined. The other H-atoms were positioned geometrically (O—H = 0.82, N—H = 0.86, C–H = 0.93—0.98 Å) and refined as riding with U_{iso}(H) = xU_{eq}(C, N, O), where x = 1.5 for hydroxy and x = 1.2 for all other H-atoms.

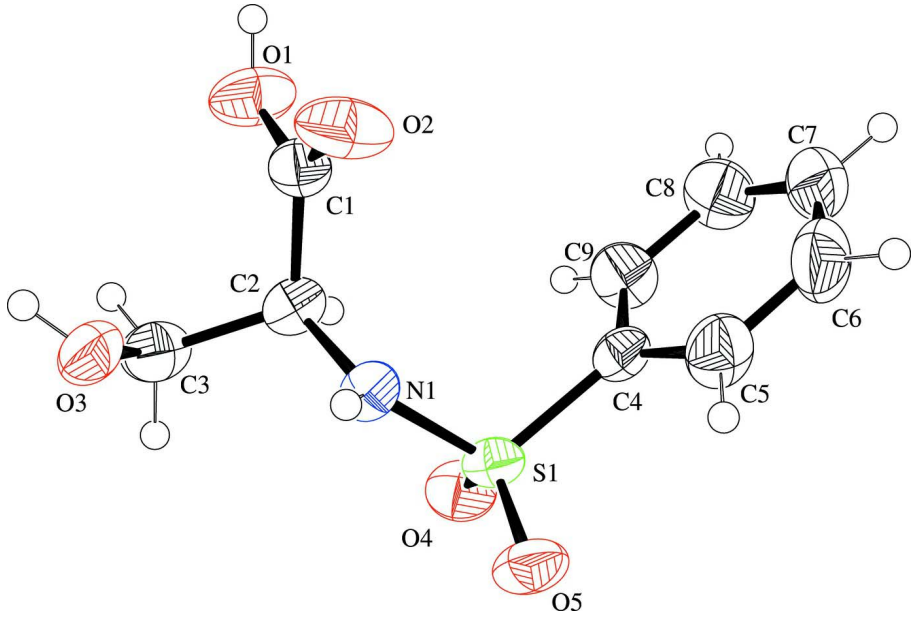

Figure 1

View of the asymmetric unit of title compound with displacement ellipsoids drawn at the 50% probability level.

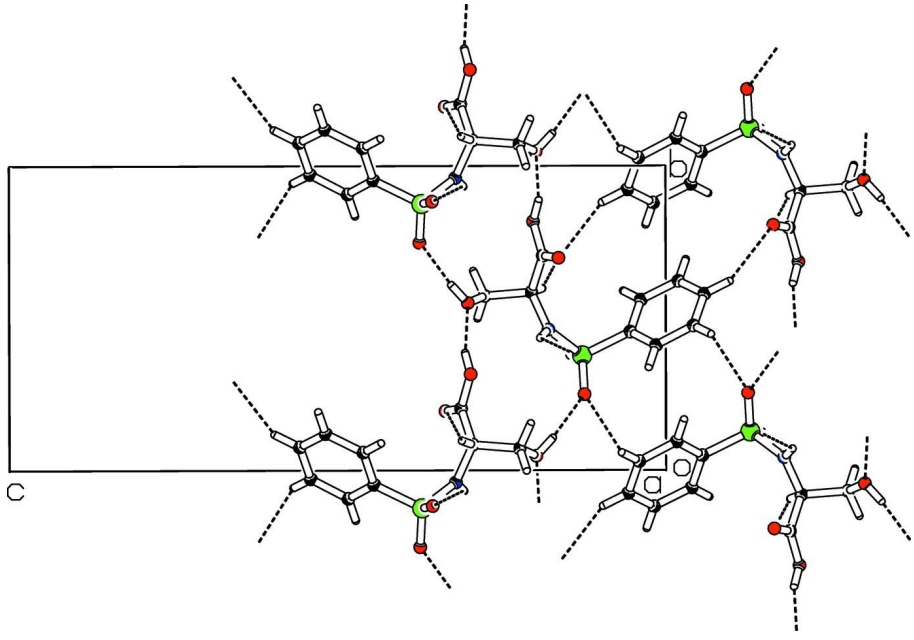

Figure 2

The partial packing (*PLATON*; Spek, 2009), which shows that molecules form two dimensional polymeric network.

2-Benzenesulfonamido-3-hydroxypropanoic acid

Crystal data

$C_9H_{11}NO_5S$
$M_r = 245.25$
Orthorhombic, $P2_12_12_1$
$a = 5.0464$ (4) Å
$b = 9.9752$ (8) Å
$c = 21.4701$ (17) Å
$V = 1080.78$ (15) Å^3
$Z = 4$

$F(000) = 512$
$D_x = 1.507$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1978 reflections
$\theta = 2.8–27.1°$
$\mu = 0.31$ mm^{-1}
$T = 296$ K
Needle, colorless
0.40 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.80 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.890$, $T_{max} = 0.950$
5013 measured reflections
2354 independent reflections
1978 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 27.1°$, $\theta_{min} = 2.8°$
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 12$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.093$
$S = 1.03$
2354 reflections
149 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.1053P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Absolute structure: Flack *x* determined using 919 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.05 (5)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.68841 (17)	0.37500 (8)	0.12794 (3)	0.0362 (2)
O1	0.7864 (6)	0.8154 (3)	0.20233 (14)	0.0624 (8)
H1	0.871 (11)	0.885 (5)	0.194 (2)	0.094*
O2	1.1199 (6)	0.6949 (3)	0.16402 (14)	0.0651 (8)
O3	0.9705 (7)	0.5474 (2)	0.30216 (11)	0.0583 (8)
H3	1.0059	0.6065	0.3274	0.087*
O4	0.4135 (5)	0.3816 (3)	0.14371 (11)	0.0504 (6)
O5	0.8178 (6)	0.2474 (2)	0.12476 (11)	0.0502 (6)

N1	0.8462 (6)	0.4600 (2)	0.17945 (11)	0.0368 (6)
H1A	0.9985	0.4323	0.1920	0.044*
C1	0.9047 (8)	0.7029 (3)	0.18768 (14)	0.0406 (8)
C2	0.7369 (7)	0.5833 (3)	0.20543 (14)	0.0384 (8)
H2	0.5583	0.5962	0.1886	0.046*
C3	0.7171 (9)	0.5712 (4)	0.27649 (16)	0.0530 (10)
H3A	0.6444	0.6533	0.2936	0.064*
H3B	0.5990	0.4981	0.2873	0.064*
C4	0.7318 (7)	0.4526 (3)	0.05482 (14)	0.0365 (8)
C5	0.9275 (9)	0.4077 (4)	0.01556 (16)	0.0542 (10)
H5	1.0338	0.3355	0.0269	0.065*
C6	0.9645 (11)	0.4717 (4)	−0.04132 (17)	0.0653 (12)
H6	1.0988	0.4436	−0.0679	0.078*
C7	0.8028 (10)	0.5765 (4)	−0.05829 (16)	0.0609 (11)
H7	0.8250	0.6180	−0.0967	0.073*
C8	0.6103 (9)	0.6193 (4)	−0.01864 (17)	0.0618 (12)
H8	0.5028	0.6909	−0.0301	0.074*
C9	0.5718 (9)	0.5581 (4)	0.03840 (17)	0.0512 (9)
H9	0.4395	0.5879	0.0652	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0337 (4)	0.0291 (3)	0.0459 (4)	−0.0024 (4)	−0.0051 (4)	0.0017 (3)
O1	0.061 (2)	0.0327 (13)	0.0933 (19)	0.0046 (14)	0.0105 (17)	−0.0028 (13)
O2	0.054 (2)	0.0441 (14)	0.097 (2)	0.0024 (14)	0.0283 (17)	0.0134 (14)
O3	0.089 (2)	0.0342 (13)	0.0514 (14)	0.0014 (15)	−0.0182 (15)	−0.0063 (10)
O4	0.0350 (13)	0.0529 (14)	0.0634 (14)	−0.0087 (13)	−0.0019 (13)	0.0046 (12)
O5	0.0590 (17)	0.0282 (11)	0.0635 (14)	0.0039 (11)	−0.0118 (16)	0.0015 (10)
N1	0.0325 (16)	0.0352 (14)	0.0428 (12)	0.0059 (13)	−0.0089 (14)	−0.0030 (11)
C1	0.042 (2)	0.0349 (17)	0.0444 (17)	0.0068 (17)	−0.0013 (18)	0.0026 (14)
C2	0.0300 (19)	0.0357 (16)	0.0496 (16)	0.0040 (14)	−0.0014 (16)	−0.0043 (13)
C3	0.059 (3)	0.0427 (19)	0.0569 (19)	−0.005 (2)	0.025 (2)	−0.0085 (15)
C4	0.036 (2)	0.0331 (15)	0.0405 (14)	−0.0015 (16)	−0.0064 (16)	−0.0051 (12)
C5	0.059 (3)	0.051 (2)	0.0528 (19)	0.018 (2)	0.001 (2)	−0.0045 (16)
C6	0.081 (3)	0.069 (3)	0.0457 (19)	0.011 (3)	0.014 (2)	−0.011 (2)
C7	0.080 (3)	0.062 (2)	0.0400 (16)	0.000 (3)	−0.006 (2)	0.0020 (16)
C8	0.071 (3)	0.057 (2)	0.058 (2)	0.014 (2)	−0.011 (2)	0.0106 (19)
C9	0.048 (2)	0.050 (2)	0.0560 (19)	0.0159 (19)	0.003 (2)	0.0046 (17)

Geometric parameters (Å, º)

S1—O4	1.429 (3)	C3—H3A	0.9700
S1—O5	1.432 (2)	C3—H3B	0.9700
S1—N1	1.605 (3)	C4—C9	1.373 (5)
S1—C4	1.764 (3)	C4—C5	1.374 (5)
O1—C1	1.310 (4)	C5—C6	1.391 (5)
O1—H1	0.84 (5)	C5—H5	0.9300

O2—C1	1.201 (4)	C6—C7	1.375 (6)
O3—C3	1.413 (5)	C6—H6	0.9300
O3—H3	0.8200	C7—C8	1.360 (6)
N1—C2	1.458 (4)	C7—H7	0.9300
N1—H1A	0.8600	C8—C9	1.382 (5)
C1—C2	1.512 (5)	C8—H8	0.9300
C2—C3	1.534 (5)	C9—H9	0.9300
C2—H2	0.9800		

O4—S1—O5	119.67 (16)	C2—C3—H3A	109.7
O4—S1—N1	107.09 (15)	O3—C3—H3B	109.7
O5—S1—N1	106.03 (14)	C2—C3—H3B	109.7
O4—S1—C4	108.12 (15)	H3A—C3—H3B	108.2
O5—S1—C4	106.92 (15)	C9—C4—C5	121.0 (3)
N1—S1—C4	108.64 (14)	C9—C4—S1	119.5 (3)
C1—O1—H1	115 (4)	C5—C4—S1	119.5 (3)
C3—O3—H3	109.5	C4—C5—C6	119.1 (4)
C2—N1—S1	121.4 (2)	C4—C5—H5	120.5
C2—N1—H1A	119.3	C6—C5—H5	120.5
S1—N1—H1A	119.3	C7—C6—C5	120.1 (4)
O2—C1—O1	124.8 (4)	C7—C6—H6	119.9
O2—C1—C2	124.1 (3)	C5—C6—H6	119.9
O1—C1—C2	111.1 (3)	C8—C7—C6	119.7 (4)
N1—C2—C1	110.9 (3)	C8—C7—H7	120.1
N1—C2—C3	109.8 (3)	C6—C7—H7	120.1
C1—C2—C3	110.4 (3)	C7—C8—C9	121.1 (4)
N1—C2—H2	108.5	C7—C8—H8	119.4
C1—C2—H2	108.5	C9—C8—H8	119.4
C3—C2—H2	108.5	C4—C9—C8	118.9 (4)
O3—C3—C2	110.0 (3)	C4—C9—H9	120.6
O3—C3—H3A	109.7	C8—C9—H9	120.6

O4—S1—N1—C2	−37.2 (3)	N1—S1—C4—C9	−83.5 (3)
O5—S1—N1—C2	−166.0 (2)	O4—S1—C4—C5	−148.5 (3)
C4—S1—N1—C2	79.4 (3)	O5—S1—C4—C5	−18.4 (3)
S1—N1—C2—C1	−114.8 (3)	N1—S1—C4—C5	95.6 (3)
S1—N1—C2—C3	122.8 (3)	C9—C4—C5—C6	0.7 (6)
O2—C1—C2—N1	−11.0 (5)	S1—C4—C5—C6	−178.4 (3)
O1—C1—C2—N1	170.0 (3)	C4—C5—C6—C7	−1.4 (6)
O2—C1—C2—C3	111.1 (4)	C5—C6—C7—C8	1.4 (7)
O1—C1—C2—C3	−68.0 (4)	C6—C7—C8—C9	−0.8 (7)
N1—C2—C3—O3	59.3 (4)	C5—C4—C9—C8	−0.1 (6)
C1—C2—C3—O3	−63.3 (4)	S1—C4—C9—C8	179.1 (3)
O4—S1—C4—C9	32.4 (3)	C7—C8—C9—C4	0.1 (7)
O5—S1—C4—C9	162.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3^{i}	0.84 (5)	1.81 (5)	2.621 (4)	164 (5)
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Symmetry codes: (i) −*x*+2, *y*+1/2, −*z*+1/2; (ii) *x*+1, *y*, *z*; (iii) *x*−1, *y*, *z*; (iv) *x*+1/2, −*y*+1/2, −*z*; (v) *x*−1/2, −*y*+3/2, −*z*.