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4-Benzenesulfonamidobenzoic acid

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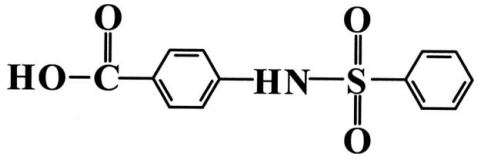
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.065; wR factor = 0.199; data-to-parameter ratio = 18.5.

In the molecule of the title sulfonamide compound, $C_{13}H_{11}NO_4S$, the dihedral angle between the planes of the benzene ring and the carboxyl substituent group is 6.7 (4)°. The two aromatic rings are inclined at 45.36 (15)° to one another. In the crystal, adjacent molecules are linked *via* classical intermolecular N—H···O and O—H···O, and non-classical C—H···O hydrogen bonds, which stabilize the crystal structure.

Related literature

For the biological activity and pharmaceutical applications of sulfonamide derivatives, see: Innocenti *et al.* (2004); Parai *et al.* (2008); Rathish *et al.* (2009); Selvam *et al.* (2001). For related structures of sulfonamide derivatives with 4–aminobenzoic acid, see: Arshad *et al.* (2009); Khan *et al.* (2009); Nan & Xing (2006).



Experimental

Crystal data

$C_{13}H_{11}NO_4S$
M_r = 277.30
Monoclinic, $P2_1/c$
a = 5.2050 (3) Å
b = 37.726 (2) Å
c = 7.3781 (4) Å
β = 117.510 (3)°
V = 1284.98 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 295 K
0.26 × 0.21 × 0.19 mm

Data collection

Bruker CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.935, T_{max} = 0.958
13550 measured reflections
3185 independent reflections
2633 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.199
S = 1.10
3185 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O8^{i}	0.81	2.28	3.054 (4)	162
O5—H5···O6^{ii}	0.82	1.82	2.625 (3)	168
C18—H18···O5^{iii}	0.93	2.58	3.413 (4)	150
C19—H19···O6^{iv}	0.93	2.48	3.348 (4)	155

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2179).

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supplementary materials

Acta Cryst. (2009). E**65**, o3086 [**doi:10.1107/S1600536809047291**]

4-Benzenesulfonamidobenzoic acid

H. M. A. Sharif, G.-Y. Dong, M. N. Arshad and I. U. Khan

Comment

Benzene sulfonamide derivative have shown antimalarial (Parai *et al.*, 2008), carbonic anhydrase inhibitors (Innocenti *et al.*, 2004), anti*HIV* (Selvam *et al.*, 2001) and antiinflamatory (Rathish *et al.*, 2009) activities. In continuation of synthesis and structural studies of different benzene sulfonamide derivative (Khan *et al.*, 2009; Arshad *et al.*, 2009), we report here the molecular and crystal structures of title compound. The molecular structure of the title compound, **I**, is illustrated in Fig. 1. In **I**, phenyl and *p*–aminobenzoic acid moieties are connected through the SO_2 group. The structure of **I** is comparable with 4–(tosylamino)benzoic acid, (Nan & Xing, 2006). The dihedral angle between the planes of the benzene ring and the carboxyl substituent group is 6.7 (4)°. The two aromatic rings (C20–C25 and C14–C19) are inclined at 45.36 (15)° to one another. The torsion angle C14—N2—S1—C20 in the central part of the molecule is 70 (1)°.

In the crystal, adjacent molecules are linked *via* intermolecular classical N—H···O and O—H···O and non–classical C—H···O hydrogen bonds (Tab. 1, Fig. 2), which stabilize the crystal structure.

Experimental

The 4–amino benzoic acid (1 g, 7.3 mmol) was dissolved in distilled water (10 ml). The pH of the solution was adjusted at 8–9 using 1*M* Na_2CO_3. Benzene sulfonylchloride (1.29 g, 7.3 mmol) was added to the above solution and stirred at room temperature until all the suspended benzene sulfonyl chloride was consumed. On completion of the reaction the pH was adjusted 1–2, using 1*N* HCl acid. The precipitate obtained was filtered, washed with distilled water, dried and recrystalized in methanol to yield colourless crystals.

Refinement

All H atoms were positioned geometrically an refined using a riding model with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic, O—H = 0.82Å and U_{iso}(H) = 1.5U_{eq}(O) for the OH group and N—H = 0.81Å and U_{iso}(H) = 1.2U_{eq}(N) for the NH group.

Figures

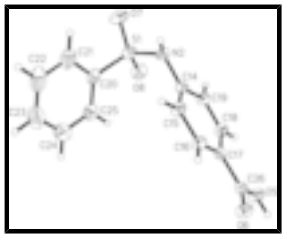

Fig. 1. The molecular structure of **I** with the atom numbering scheme. Displacement ellipsoids are drawn at 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

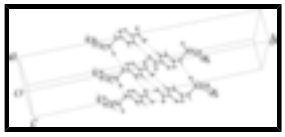

Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines and H atoms not involved in hydrogen bonding omitted for clarity.

4-Benzenesulfonamidobenzoic acid

Crystal data

$C_{13}H_{11}NO_4S$	$F_{000} = 576$
$M_r = 277.30$	$D_x = 1.433$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 5008 reflections
$a = 5.2050$ (3) Å	$\theta = 3.0$–25º
$b = 37.726$ (2) Å	$\mu = 0.26$ mm^{-1}
$c = 7.3781$ (4) Å	$T = 295$ K
$\beta = 117.510$ (3)º	Block, colourless
$V = 1284.98$ (13) Å^3	0.26 × 0.21 × 0.19 mm
$Z = 4$	

Data collection

Bruker CCD diffractometer	3185 independent reflections
Radiation source: fine–focus sealed tube	2633 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 295$ K	$\theta_{max} = 28.4$º
φ and ω scans	$\theta_{min} = 1.1$º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -4\rightarrow6$
$T_{min} = 0.935$, $T_{max} = 0.958$	$k = -50\rightarrow45$
13550 measured reflections	$l = -9\rightarrow9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.065$	H-atom parameters constrained
$wR(F^2) = 0.199$	$w = 1/[\sigma^2(F_o^2) + (0.0878P)^2 + 1.4857P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} < 0.001$
3185 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
172 parameters	$\Delta\rho_{min} = -0.36$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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	0.27263 (17)	0.36345 (2)	0.53929 (12)	0.0443 (3)
O5	−0.4876 (5)	0.48980 (7)	−0.2675 (3)	0.0496 (6)
H5	−0.5699	0.5003	−0.3768	0.074*
O6	−0.2171 (5)	0.47077 (6)	−0.4087 (3)	0.0464 (5)
O7	0.4834 (6)	0.35320 (8)	0.7386 (4)	0.0693 (8)
O8	−0.0109 (5)	0.37334 (7)	0.5034 (4)	0.0557 (6)
N2	0.4098 (5)	0.39697 (7)	0.4738 (4)	0.0408 (6)
H2	0.5771	0.3942	0.5010	0.049*
C14	0.2360 (6)	0.41529 (7)	0.2848 (4)	0.0344 (6)
C15	0.2845 (6)	0.41056 (8)	0.1173 (5)	0.0411 (7)
H15	0.4269	0.3949	0.1242	0.049*
C16	0.1192 (6)	0.42930 (8)	−0.0615 (5)	0.0406 (6)
H16	0.1543	0.4267	−0.1735	0.049*
C17	−0.0980 (5)	0.45182 (7)	−0.0728 (4)	0.0319 (5)
C18	−0.1453 (6)	0.45608 (8)	0.0961 (4)	0.0375 (6)
H18	−0.2921	0.4710	0.0884	0.045*
C19	0.0239 (6)	0.43826 (8)	0.2754 (4)	0.0386 (6)
H19	−0.0049	0.4417	0.3895	0.046*
C20	0.2370 (7)	0.32889 (8)	0.3691 (5)	0.0456 (7)
C21	0.4682 (10)	0.30652 (11)	0.4110 (8)	0.0731 (12)
H21	0.6402	0.3090	0.5314	0.088*
C22	0.4401 (13)	0.28042 (13)	0.2715 (11)	0.0938 (18)
H22	0.5934	0.2650	0.2995	0.113*
C23	0.1881 (15)	0.27699 (14)	0.0918 (10)	0.0938 (17)
H23	0.1703	0.2594	−0.0015	0.113*
C24	−0.0327 (15)	0.29943 (14)	0.0524 (9)	0.1009 (19)
H24	−0.2033	0.2972	−0.0692	0.121*
C25	−0.0115 (10)	0.32565 (11)	0.1883 (7)	0.0724 (12)
H25	−0.1653	0.3411	0.1574	0.087*
C26	−0.2763 (6)	0.47182 (7)	−0.2629 (4)	0.0340 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0400 (4)	0.0527 (5)	0.0429 (4)	0.0102 (3)	0.0214 (3)	0.0115 (3)
O5	0.0442 (12)	0.0658 (15)	0.0422 (11)	0.0254 (11)	0.0228 (10)	0.0118 (10)
O6	0.0505 (12)	0.0567 (13)	0.0380 (11)	0.0155 (10)	0.0255 (10)	0.0054 (9)
O7	0.0665 (17)	0.087 (2)	0.0466 (14)	0.0161 (15)	0.0193 (13)	0.0233 (13)
O8	0.0467 (13)	0.0653 (15)	0.0681 (16)	0.0086 (11)	0.0376 (12)	0.0058 (12)
N2	0.0281 (11)	0.0490 (14)	0.0410 (13)	0.0053 (10)	0.0121 (10)	0.0076 (10)
C14	0.0279 (12)	0.0365 (14)	0.0357 (13)	0.0003 (10)	0.0122 (10)	0.0004 (10)
C15	0.0350 (14)	0.0452 (16)	0.0460 (15)	0.0146 (12)	0.0210 (12)	0.0041 (12)
C16	0.0410 (15)	0.0483 (16)	0.0395 (14)	0.0095 (12)	0.0247 (12)	0.0008 (12)
C17	0.0277 (12)	0.0343 (13)	0.0342 (13)	0.0010 (10)	0.0146 (10)	−0.0026 (10)
C18	0.0361 (14)	0.0393 (14)	0.0421 (14)	0.0095 (11)	0.0223 (12)	0.0009 (11)
C19	0.0416 (15)	0.0437 (15)	0.0360 (14)	0.0073 (12)	0.0226 (12)	−0.0003 (11)
C20	0.0475 (17)	0.0407 (15)	0.0560 (18)	0.0068 (13)	0.0303 (15)	0.0121 (13)
C21	0.054 (2)	0.058 (2)	0.108 (4)	0.0152 (18)	0.038 (2)	0.003 (2)
C22	0.089 (4)	0.059 (3)	0.156 (6)	0.019 (2)	0.076 (4)	−0.001 (3)
C23	0.130 (5)	0.066 (3)	0.101 (4)	0.008 (3)	0.067 (4)	−0.011 (3)
C24	0.122 (5)	0.076 (3)	0.074 (3)	0.019 (3)	0.019 (3)	−0.015 (3)
C25	0.074 (3)	0.060 (2)	0.066 (2)	0.022 (2)	0.017 (2)	0.0007 (19)
C26	0.0307 (13)	0.0361 (13)	0.0346 (13)	0.0023 (10)	0.0146 (10)	−0.0031 (10)

Geometric parameters (Å, °)

S1—O7	1.423 (3)	C17—C26	1.482 (4)
S1—O8	1.423 (2)	C18—C19	1.379 (4)
S1—N2	1.632 (3)	C18—H18	0.9300
S1—C20	1.760 (4)	C19—H19	0.9300
O5—C26	1.279 (3)	C20—C25	1.368 (5)
O5—H5	0.8186	C20—C21	1.383 (5)
O6—C26	1.249 (3)	C21—C22	1.383 (7)
N2—C14	1.440 (3)	C21—H21	0.9300
N2—H2	0.8048	C22—C23	1.374 (8)
C14—C19	1.380 (4)	C22—H22	0.9300
C14—C15	1.382 (4)	C23—C24	1.347 (8)
C15—C16	1.390 (4)	C23—H23	0.9300
C15—H15	0.9300	C24—C25	1.376 (7)
C16—C17	1.386 (4)	C24—H24	0.9300
C16—H16	0.9300	C25—H25	0.9300
C17—C18	1.386 (4)		
O7—S1—O8	120.12 (17)	C14—C19—C18	119.7 (3)
O7—S1—N2	106.43 (16)	C14—C19—H19	120.1
O8—S1—N2	107.42 (14)	C18—C19—H19	120.1
O7—S1—C20	108.24 (17)	C25—C20—C21	119.8 (4)
O8—S1—C20	107.64 (16)	C25—C20—S1	120.2 (3)
N2—S1—C20	106.21 (14)	C21—C20—S1	119.9 (3)

C26—O5—H5	109.5	C20—C21—C22	119.1 (5)
C14—N2—S1	119.58 (19)	C20—C21—H21	120.4
C14—N2—H2	115.3	C22—C21—H21	120.5
S1—N2—H2	113.4	C23—C22—C21	120.7 (5)
C19—C14—C15	120.5 (3)	C23—C22—H22	119.6
C19—C14—N2	118.7 (3)	C21—C22—H22	119.6
C15—C14—N2	120.7 (2)	C24—C23—C22	119.2 (5)
C14—C15—C16	119.6 (3)	C24—C23—H23	120.4
C14—C15—H15	120.2	C22—C23—H23	120.4
C16—C15—H15	120.2	C23—C24—C25	121.4 (5)
C17—C16—C15	119.9 (3)	C23—C24—H24	119.3
C17—C16—H16	120.0	C25—C24—H24	119.3
C15—C16—H16	120.0	C20—C25—C24	119.7 (4)
C18—C17—C16	119.7 (3)	C20—C25—H25	120.1
C18—C17—C26	119.9 (2)	C24—C25—H25	120.1
C16—C17—C26	120.4 (2)	O6—C26—O5	123.0 (3)
C19—C18—C17	120.4 (3)	O6—C26—C17	120.2 (2)
C19—C18—H18	119.8	O5—C26—C17	116.8 (2)
C17—C18—H18	119.8		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O8^{i}	0.81	2.28	3.054 (4)	162
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Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*−1, −*y*+1, −*z*−1; (iii) −*x*−1, −*y*+1, −*z*; (iv) *x*, *y*, *z*+1.

Fig. 1

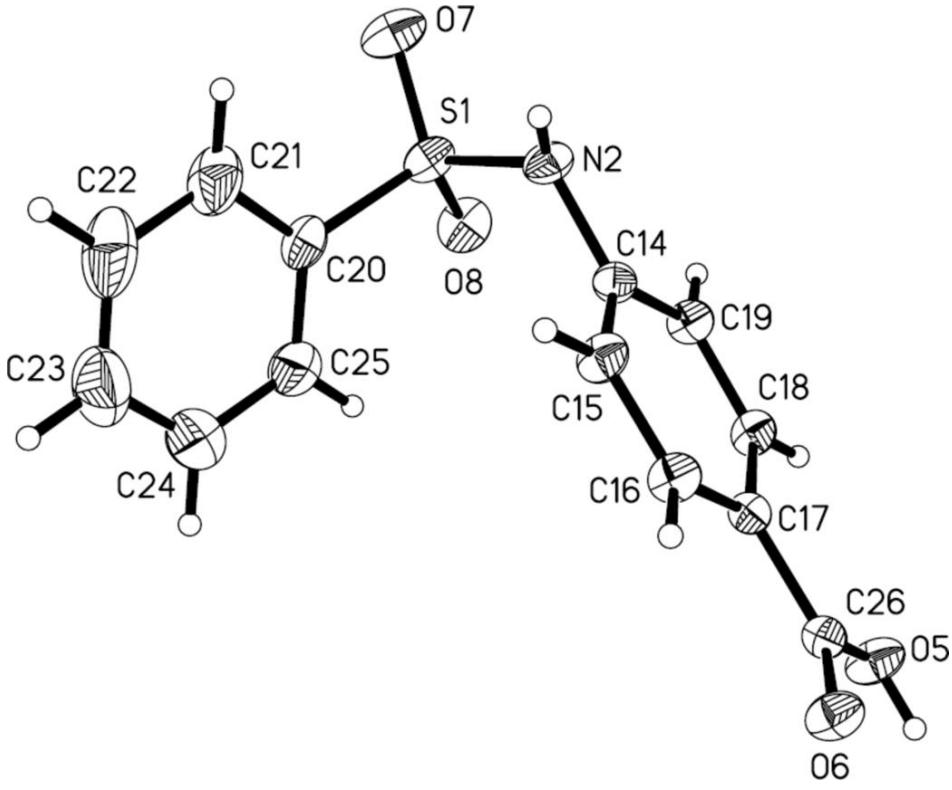
O7
S1
C21
N2
C22
C20
O8
C14
C19
C23
C25
C15
C18
C24
C16
C17
C26
O5
O6

Fig. 2