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## Structure Reports

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## 5-Amino-2-methylbenzenesulfonamide

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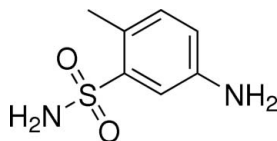
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Key indicators: single-crystal X-ray study;  $T = 294$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.040;  $wR$  factor = 0.120; data-to-parameter ratio = 12.9.

In the crystal structure of the title compound,  $\text{C}_7\text{H}_{10}\text{N}_2\text{O}_2\text{S}$ , a benzoic acid derivative, intermolecular  $\text{N}-\text{H}\cdots\text{O}$  interactions link the molecules into a three-dimensional network.

## Related literature

For bond-length data, see: Allen *et al.* (1987).

## Experimental

## Crystal data

 $\text{C}_7\text{H}_{10}\text{N}_2\text{O}_2\text{S}$  $M_r = 186.23$ Orthorhombic, *Iba*2 $a = 10.679$  (2) Å $b = 22.431$  (5) Å $c = 7.1980$  (14) Å $V = 1724.2$  (6) Å<sup>3</sup> $Z = 8$ Mo  $K\alpha$  radiation $\mu = 0.34$  mm<sup>-1</sup> $T = 294$  K

0.30 × 0.20 × 0.10 mm

## Data collection

Enraf–Nonius CAD-4 diffractometer

Absorption correction:  $\psi$  scan (North *et al.*, 1968) $T_{\min} = 0.906$ ,  $T_{\max} = 0.967$ 

1587 measured reflections  
1432 independent reflections  
1369 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.044$

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.040$  $wR(F^2) = 0.120$  $S = 1.00$ 

1432 reflections

111 parameters

1 restraint

3 standard reflections  
frequency: 120 min  
intensity decay: 1%

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.29$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.35$  e Å<sup>-3</sup>Absolute structure: Flack (1983),  
576 Friedel pairs

Flack parameter: 0.04 (14)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1B}\cdots\text{O2}^{\text{i}}$	0.86	2.27	2.996 (4)	142
$\text{N1}-\text{H1C}\cdots\text{O1}^{\text{ii}}$	0.86	2.16	3.001 (4)	164
$\text{N2}-\text{H2C}\cdots\text{O1}^{\text{iii}}$	0.86	2.60	3.278 (4)	137

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2722).

## References

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**supplementary materials**

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## 5-Amino-2-methylbenzenesulfonamide

X.-J. Ma, Z. Fang, L.-L. Ren and P. Wei

### Comment

Some derivatives of benzoic acid are important chemical materials. We report herein the crystal structure of the title compound.

In the molecule of the title compound, (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Ring A (C2-C7) is, of course, planar. Atoms S, O1, N2 and C1 are 0.013 (3), -0.102 (3), -0.027 (3) and -0.032 (3) Å away from the plane of ring A, respectively.

In the crystal structure, intermolecular N-H...O interactions (Table 1) link the molecules into a three-dimensional network (Fig. 2), in which they may be effective in the stabilization of the structure.

### Experimental

For the preparation of the title compound, ammonium hydroxide (25 ml) was added to *N*-acetylamino-2-toluenesulfonyl chloride (10.7 g). The mixture was cooled down, and sulfuric acid solution (10 ml, 20%) was slowly added. The mixture was kept at 273–278 K for 5 min. The corresponding sulfonamide was collected, washed with ice water and dried to give a crystalline crude colorless solid (yield; 67%). Then, hydrochloric acid (15 ml, 18%) was added to *N*-acetyltoluenesulfonamide (5.6 g) and the mixture was refluxed for 20 min. The resulting solution was diluted with an equal volume of water and sodium carbonate until pH = 8. After cooling, the precipitate was collected and washed with ice water (yield; 3.9 g). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

### Refinement

H atoms were positioned geometrically, with N-H = 0.86 Å (for NH<sub>2</sub>) and C-H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C,N})$ , where  $x = 1.5$  for methyl H and  $x = 1.2$  for all other H atoms.

### Figures

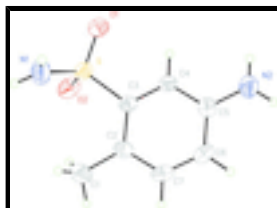


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

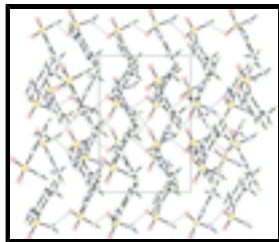


Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

## 5-Amino-2-methylbenzenesulfonamide

### Crystal data

$C_7H_{10}N_2O_2S$

$M_r = 186.23$

Orthorhombic, *Iba2*

Hall symbol: *I 2 -2c*

$a = 10.679$  (2) Å

$b = 22.431$  (5) Å

$c = 7.1980$  (14) Å

$V = 1724.2$  (6) Å<sup>3</sup>

$Z = 8$

$F_{000} = 784$

$D_x = 1.435$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 25 reflections

$\theta = 10\text{--}14^\circ$

$\mu = 0.34$  mm<sup>-1</sup>

$T = 294$  K

Block, colorless

$0.30 \times 0.20 \times 0.10$  mm

### Data collection

Enraf-Nonius CAD-4  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 294$  K

$\omega/2\theta$  scans

Absorption correction:  $\psi$  scan  
(North *et al.*, 1968)

$T_{\min} = 0.906$ ,  $T_{\max} = 0.967$

1587 measured reflections

1432 independent reflections

1369 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 25.3^\circ$

$\theta_{\min} = 1.8^\circ$

$h = -12 \rightarrow 0$

$k = -26 \rightarrow 8$

$l = -8 \rightarrow 8$

3 standard reflections

every 120 min

intensity decay: 1%

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.120$

$S = 1.00$

1432 reflections

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.35P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.29$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.35$  e Å<sup>-3</sup>

111 parameters Extinction correction: SHELXL97 (Sheldrick, 2008),  
 $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$   
 1 restraint Extinction coefficient: 0.019 (2)  
 Primary atom site location: structure-invariant direct methods Absolute structure: Flack (1983), 576 Friedel pairs  
 Secondary atom site location: difference Fourier map Flack parameter: 0.04 (14)

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{iso}^*/U_{eq}$
S	0.16988 (6)	0.09021 (3)	0.64671 (14)	0.0332 (3)
O1	0.06327 (19)	0.12096 (9)	0.5690 (4)	0.0469 (6)
N1	0.1216 (3)	0.05631 (12)	0.8282 (5)	0.0495 (8)
H1B	0.1362	0.0189	0.8419	0.059*
H1C	0.0810	0.0755	0.9123	0.059*
C1	0.4280 (3)	0.06855 (16)	0.8644 (6)	0.0527 (9)
H1D	0.5127	0.0686	0.9089	0.079*
H1E	0.4210	0.0420	0.7604	0.079*
H1F	0.3730	0.0555	0.9618	0.079*
O2	0.2333 (2)	0.04672 (10)	0.5348 (4)	0.0511 (7)
N2	0.3024 (3)	0.30886 (10)	0.6676 (5)	0.0489 (8)
H2B	0.2329	0.3169	0.6125	0.059*
H2C	0.3532	0.3372	0.6962	0.059*
C2	0.3922 (2)	0.13040 (13)	0.8053 (4)	0.0316 (6)
C3	0.2794 (2)	0.14549 (11)	0.7132 (4)	0.0272 (6)
C4	0.2507 (2)	0.20373 (11)	0.6649 (5)	0.0287 (6)
H4A	0.1767	0.2118	0.6017	0.034*
C5	0.3323 (3)	0.25064 (13)	0.7103 (5)	0.0318 (7)
C6	0.4439 (3)	0.23609 (14)	0.8042 (5)	0.0357 (7)
H6A	0.4997	0.2662	0.8367	0.043*
C7	0.4711 (3)	0.17810 (14)	0.8483 (4)	0.0363 (7)
H7A	0.5458	0.1701	0.9098	0.044*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S	0.0294 (4)	0.0314 (4)	0.0390 (5)	-0.0021 (2)	-0.0014 (3)	-0.0050 (3)

## supplementary materials

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O1	0.0350 (11)	0.0441 (12)	0.0615 (15)	-0.0049 (10)	-0.0151 (11)	0.0014 (11)
N1	0.0459 (16)	0.0367 (14)	0.066 (2)	0.0010 (12)	0.0155 (16)	0.0131 (13)
C1	0.0487 (19)	0.0423 (17)	0.067 (2)	0.0114 (15)	-0.016 (2)	0.0051 (18)
O2	0.0447 (14)	0.0482 (13)	0.0603 (17)	-0.0016 (10)	0.0036 (12)	-0.0242 (12)
N2	0.0561 (15)	0.0312 (12)	0.059 (2)	-0.0070 (11)	-0.0146 (18)	0.0069 (14)
C2	0.0283 (14)	0.0348 (15)	0.0317 (15)	0.0046 (11)	0.0002 (12)	-0.0003 (11)
C3	0.0236 (12)	0.0307 (13)	0.0273 (13)	0.0010 (10)	0.0024 (11)	-0.0021 (11)
C4	0.0249 (12)	0.0330 (13)	0.0281 (15)	-0.0009 (10)	-0.0035 (12)	0.0019 (11)
C5	0.0374 (14)	0.0322 (14)	0.0258 (14)	0.0000 (10)	0.0029 (12)	0.0010 (11)
C6	0.0309 (13)	0.0422 (16)	0.0339 (15)	-0.0101 (12)	-0.0014 (13)	-0.0054 (13)
C7	0.0248 (14)	0.0503 (17)	0.0338 (16)	0.0022 (11)	-0.0052 (12)	-0.0034 (11)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

S—O2	1.435 (2)	N2—H2B	0.8600
S—O1	1.444 (2)	N2—H2C	0.8600
S—N1	1.597 (3)	C2—C7	1.397 (4)
S—C3	1.770 (3)	C2—C3	1.416 (4)
N1—H1B	0.8600	C3—C4	1.386 (4)
N1—H1C	0.8600	C4—C5	1.405 (4)
C1—C2	1.501 (4)	C4—H4A	0.9300
C1—H1D	0.9600	C5—C6	1.408 (4)
C1—H1E	0.9600	C6—C7	1.370 (5)
C1—H1F	0.9600	C6—H6A	0.9300
N2—C5	1.379 (4)	C7—H7A	0.9300
O2—S—O1	118.64 (18)	C7—C2—C3	115.7 (3)
O2—S—N1	106.75 (16)	C7—C2—C1	119.5 (3)
O1—S—N1	106.85 (15)	C3—C2—C1	124.8 (3)
O2—S—C3	108.43 (14)	C4—C3—C2	122.1 (2)
O1—S—C3	106.92 (12)	C4—C3—S	116.5 (2)
N1—S—C3	108.98 (17)	C2—C3—S	121.4 (2)
S—N1—H1B	120.0	C3—C4—C5	120.7 (3)
S—N1—H1C	120.0	C3—C4—H4A	119.7
H1B—N1—H1C	120.0	C5—C4—H4A	119.7
C2—C1—H1D	109.5	N2—C5—C4	120.9 (3)
C2—C1—H1E	109.5	N2—C5—C6	121.5 (3)
H1D—C1—H1E	109.5	C4—C5—C6	117.6 (3)
C2—C1—H1F	109.5	C7—C6—C5	120.7 (3)
H1D—C1—H1F	109.5	C7—C6—H6A	119.7
H1E—C1—H1F	109.5	C5—C6—H6A	119.7
C5—N2—H2B	120.0	C6—C7—C2	123.3 (3)
C5—N2—H2C	120.0	C6—C7—H7A	118.4
H2B—N2—H2C	120.0	C2—C7—H7A	118.4
C7—C2—C3—C4	1.5 (5)	C2—C3—C4—C5	-1.6 (5)
C1—C2—C3—C4	178.9 (3)	S—C3—C4—C5	-179.5 (2)
C7—C2—C3—S	179.3 (2)	C3—C4—C5—N2	-177.9 (3)
C1—C2—C3—S	-3.3 (5)	C3—C4—C5—C6	0.7 (5)
O2—S—C3—C4	123.0 (3)	N2—C5—C6—C7	178.9 (3)
O1—S—C3—C4	-6.0 (3)	C4—C5—C6—C7	0.3 (5)

N1—S—C3—C4	-121.1 (3)	C5—C6—C7—C2	-0.3 (5)
O2—S—C3—C2	-54.9 (3)	C3—C2—C7—C6	-0.6 (5)
O1—S—C3—C2	176.1 (3)	C1—C2—C7—C6	-178.1 (3)
N1—S—C3—C2	61.0 (3)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1B $\cdots$ O2 <sup>i</sup>	0.86	2.27	2.996 (4)	142
N1—H1C $\cdots$ O1 <sup>ii</sup>	0.86	2.16	3.001 (4)	164
N2—H2C $\cdots$ O1 <sup>iii</sup>	0.86	2.60	3.278 (4)	137

Symmetry codes: (i)  $x, -y, z+1/2$ ; (ii)  $-x, y, z+1/2$ ; (iii)  $x+1/2, -y+1/2, z$ .

Fig. 1

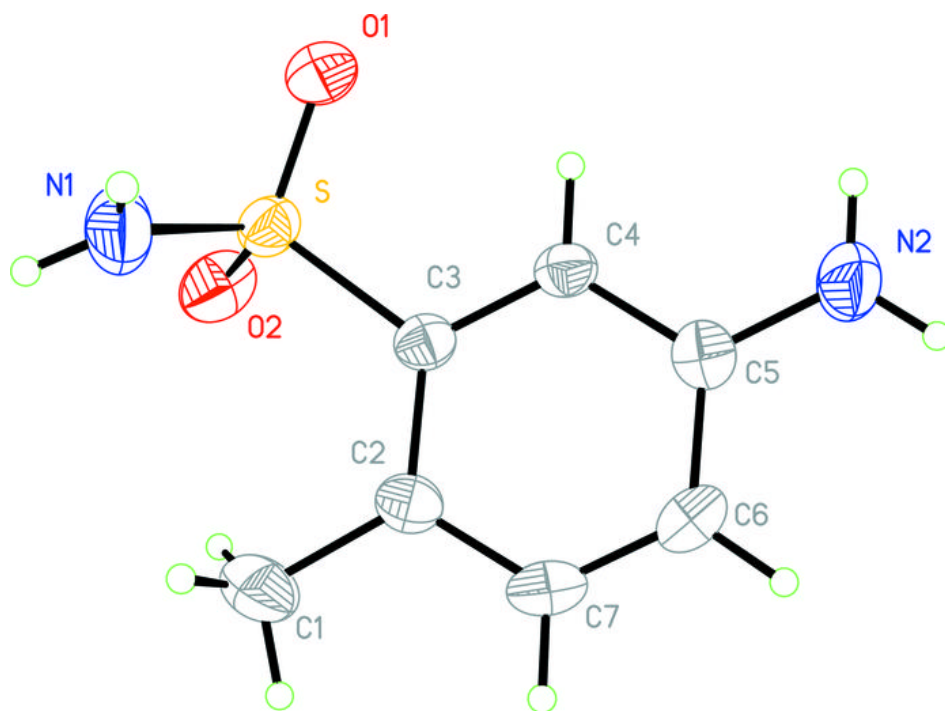




Fig. 2

