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2-Amino-4-methylbenzenesulfonamide

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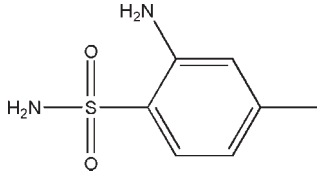
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.132; data-to-parameter ratio = 13.2.

In the crystal of the title compound, $C_7H_{10}N_2O_2S$, the molecules are linked by two strong N—H···O hydrogen bonds. The molecular structure is stabilized by an intramolecular N—H···O hydrogen bond. The C/S/N plane makes a dihedral angle of 69.7 (2)° with the aromatic ring plane.

Related literature

For the anticonvulsant activity of the title compound and its derivatives, see: Monzani *et al.* (1985); Tait *et al.* (1993). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_7H_{10}N_2O_2S$
M_r = 186.23
Monoclinic, $P2_1/c$
a = 9.873 (5) Å
b = 9.151 (4) Å
c = 10.408 (5) Å
β = 114.689 (6)°
V = 854.4 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 273 K
0.16 × 0.13 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.948, T_{max} = 0.967
4115 measured reflections
1449 independent reflections
1338 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.132
S = 1.10
1449 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O2^{i}	0.86	2.15	3.003 (4)	174
N2—H2A···O1^{ii}	0.86	2.27	2.975 (4)	139
N1—H1B···O2	0.86	2.60	3.080 (5)	117

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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: BX2239).

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Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tait, A., Parenti, C., Zanoli, P., Veneri, C., Truzzi, C., Brandoli, C., Baraldi, M. & Di Bella, M. (1993). *Farmaco*, **48**, 1463–1473.

supporting information

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S1. Comment

The title compound (I), Figure1, was prepared and tested for anticonvulsant activity in mice, (Monzani, *et al.*,1985). In addition, its derivatives was studied using indomethacin as a reference drug (Tait, *et al.*,1993). We report here its crystal and molecular structure. The molecules are linked by two strong N—H···O generating a graph-set motif $R^4_4(16)$ ring (Bernstein, *et al.*, 1995) and is stabilized by one N—H···O intramolecular hydrogen bonds (Table1, Figure 2). The C2/S1/N2 plane makes a dihedral angle of 69.7 (2)° with the aromatic ring plane.

S2. Experimental

The title compound was synthesized according to method described by Monzani, *et al.,1985.T*he single crystals suitable for X-ray diffraction were obtained by spontaneous evaporation of the solvent.

S3. Refinement

All the H atoms attached to C atoms were placed in geometrical positions and constrained to ride on their parent atoms with C—H distance in the range 0.93–0.98 Å, They were treated as riding atoms, with U_{iso}(H) = 1.2U_{eq}(C).

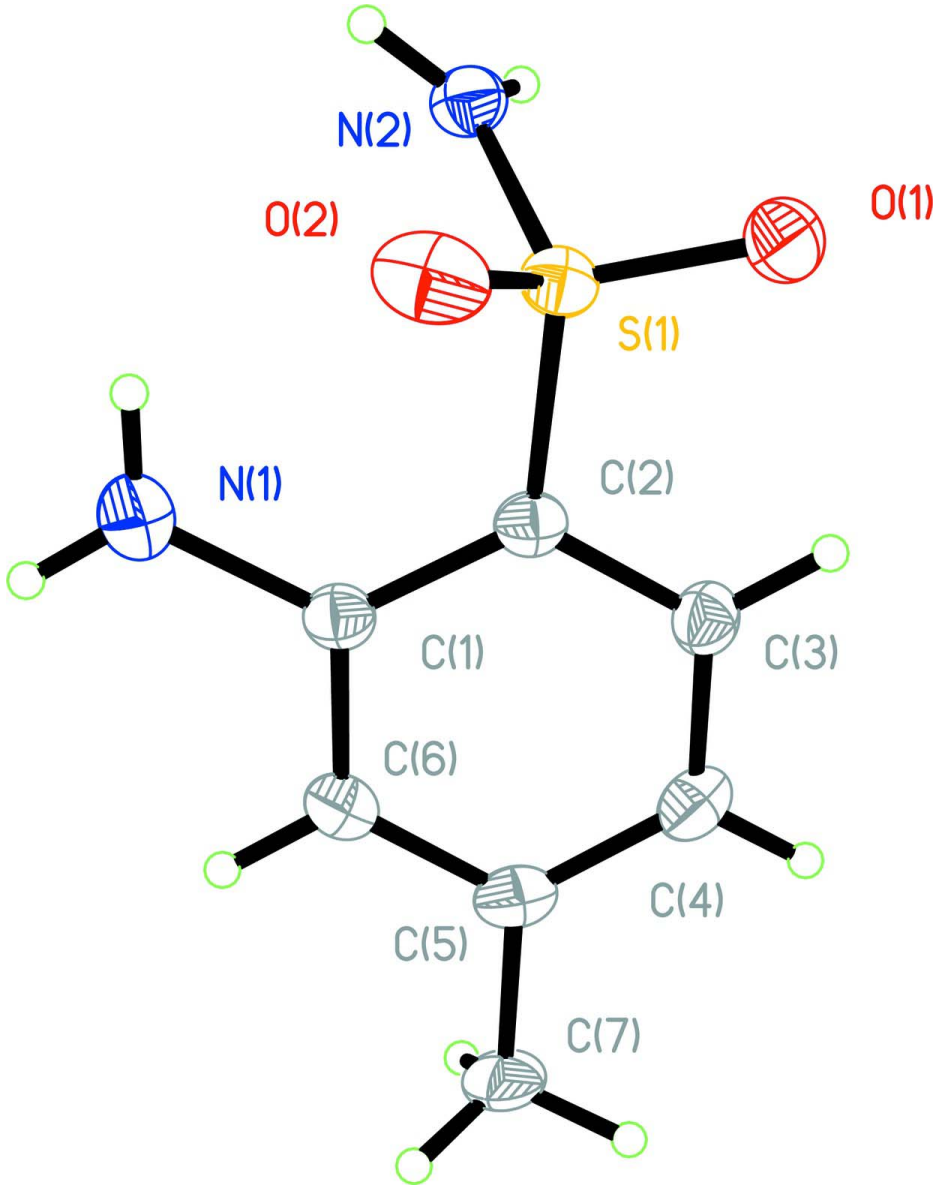

Figure 1

The structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

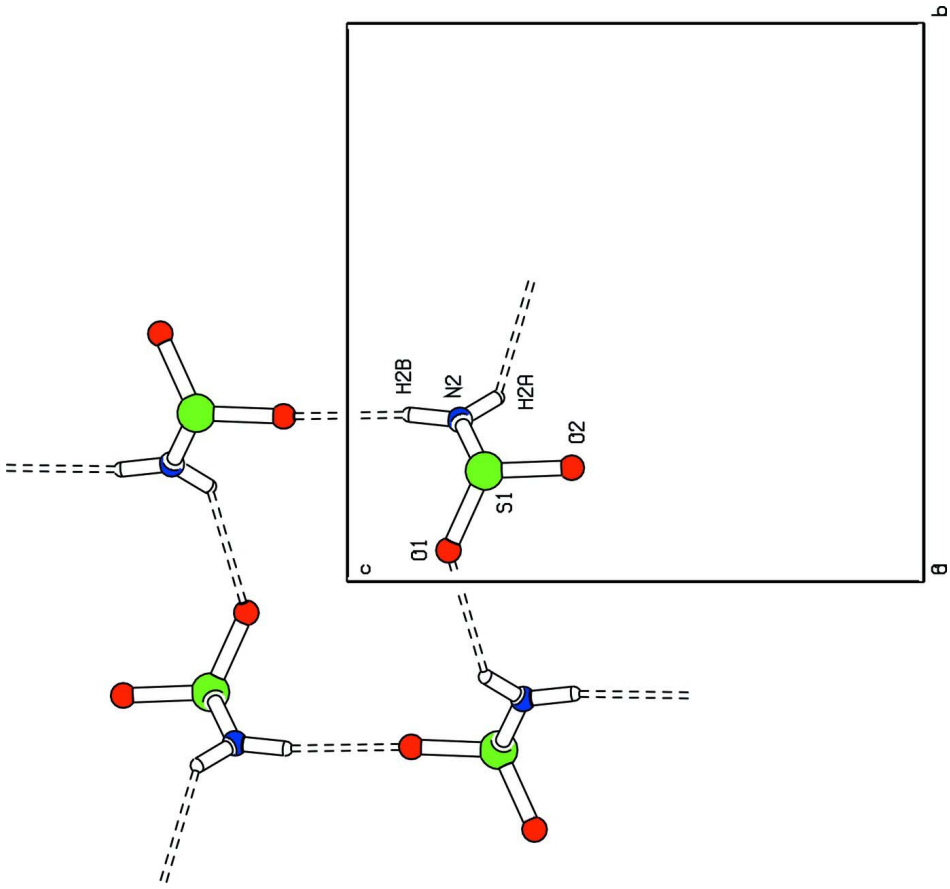

Figure 2

A portion of the packing diagram for (I) showing graph-set motif $R^4_4(16)$ ring. For the sake clarity the atoms not involved in the motif shown have been omitted Symmetry codes: (i) x, -y+1/2, z+1/2; (ii)-x,y+1/2,-z+3/2.

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c = 10.408 (5) Å
β = 114.689 (6)°
V = 854.4 (7) Å^3
Z = 4
$F(000)$ = 392
D_x = 1.448 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3354 reflections
θ = 2.2–28.2°
μ = 0.34 mm^{-1}
T = 273 K
Block, colorless
0.16 × 0.13 × 0.10 mm

Data collection

Bruker SMART 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} = 0.948, T_{max} = 0.967
4115 measured reflections
1449 independent reflections
1338 reflections with $I > 2\sigma(I)$

R_{int} = 0.017
θ_{max} = 25.1°, θ_{min} = 3.1°
h = −11→11
k = −10→10
l = −12→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.132
S = 1.10
1449 reflections
110 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
$w = 1/[\sigma^2(F_o^2) + (0.0721P)^2 + 0.701P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.047 (9)

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	0.13944 (9)	0.19821 (9)	0.76214 (8)	0.0361 (4)
O1	0.1511 (3)	0.0560 (3)	0.8246 (3)	0.0533 (8)
O2	0.0800 (3)	0.2040 (4)	0.6109 (3)	0.0603 (9)
N1	0.2315 (4)	0.5060 (4)	0.6773 (4)	0.0604 (10)
H1A	0.2566	0.5867	0.6510	0.073*
H1B	0.1391	0.4815	0.6450	0.073*
N2	0.0260 (3)	0.2896 (3)	0.8048 (3)	0.0412 (7)
H2A	−0.0514	0.3293	0.7402	0.049*
H2B	0.0426	0.2990	0.8924	0.049*
C1	0.3488 (4)	0.4078 (4)	0.7793 (3)	0.0357 (7)
C2	0.3186 (3)	0.2754 (4)	0.8318 (3)	0.0342 (7)
C3	0.4324 (4)	0.1967 (4)	0.9361 (4)	0.0396 (8)
H3	0.4098	0.1121	0.9727	0.048*
C4	0.5787 (4)	0.2433 (4)	0.9859 (4)	0.0443 (9)
H4	0.6543	0.1920	1.0571	0.053*
C5	0.6107 (3)	0.3669 (4)	0.9282 (4)	0.0417 (8)
C6	0.4979 (4)	0.4501 (4)	0.8300 (4)	0.0406 (8)
H6	0.5221	0.5362	0.7969	0.049*
C7	0.7610 (3)	0.4151 (5)	0.9737 (4)	0.0497 (9)
H7A	0.7795	0.4947	1.0389	0.074*

H7B	0.7771	0.4471	0.8933	0.074*
H7C	0.8276	0.3360	1.0193	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0355 (6)	0.0364 (6)	0.0356 (6)	−0.0058 (3)	0.0140 (4)	−0.0071 (3)
O1	0.0470 (15)	0.0348 (14)	0.0722 (18)	−0.0059 (11)	0.0191 (13)	−0.0030 (12)
O2	0.0540 (16)	0.086 (2)	0.0376 (14)	−0.0211 (14)	0.0163 (12)	−0.0185 (13)
N1	0.056 (2)	0.063 (2)	0.062 (2)	0.0026 (16)	0.0245 (17)	0.0197 (17)
N2	0.0373 (16)	0.0455 (17)	0.0419 (15)	0.0014 (12)	0.0174 (13)	0.0004 (12)
C1	0.0368 (16)	0.0390 (17)	0.0348 (15)	0.0007 (13)	0.0184 (13)	−0.0019 (13)
C2	0.0329 (16)	0.0357 (16)	0.0352 (16)	−0.0012 (12)	0.0155 (13)	−0.0053 (12)
C3	0.0414 (18)	0.0327 (17)	0.0435 (18)	0.0024 (13)	0.0165 (15)	0.0001 (13)
C4	0.0360 (18)	0.0431 (19)	0.0474 (19)	0.0067 (14)	0.0109 (15)	−0.0027 (16)
C5	0.0313 (17)	0.047 (2)	0.0467 (18)	−0.0029 (14)	0.0165 (14)	−0.0113 (15)
C6	0.0395 (17)	0.0420 (18)	0.0443 (18)	−0.0051 (14)	0.0213 (15)	−0.0005 (15)
C7	0.0246 (16)	0.058 (2)	0.062 (2)	−0.0056 (15)	0.0139 (16)	−0.0010 (18)

Geometric parameters (Å, º)

S1—O2	1.433 (3)	C2—C3	1.393 (5)
S1—O1	1.438 (3)	C3—C4	1.383 (5)
S1—N2	1.602 (3)	C3—H3	0.9300
S1—C2	1.756 (3)	C4—C5	1.378 (6)
N1—C1	1.500 (5)	C4—H4	0.9300
N1—H1A	0.8600	C5—C6	1.383 (5)
N1—H1B	0.8600	C5—C7	1.426 (4)
N2—H2A	0.8600	C6—H6	0.9300
N2—H2B	0.8600	C7—H7A	0.9600
C1—C6	1.395 (5)	C7—H7B	0.9600
C1—C2	1.412 (5)	C7—H7C	0.9600
O2—S1—O1	116.68 (18)	C4—C3—C2	120.6 (3)
O2—S1—N2	105.80 (18)	C4—C3—H3	119.7
O1—S1—N2	106.29 (16)	C2—C3—H3	119.7
O2—S1—C2	108.58 (16)	C5—C4—C3	118.9 (3)
O1—S1—C2	107.49 (16)	C5—C4—H4	120.5
N2—S1—C2	112.08 (16)	C3—C4—H4	120.5
C1—N1—H1A	120.0	C4—C5—C6	120.9 (3)
C1—N1—H1B	120.0	C4—C5—C7	120.3 (3)
H1A—N1—H1B	120.0	C6—C5—C7	118.7 (4)
S1—N2—H2A	120.0	C5—C6—C1	121.5 (3)
S1—N2—H2B	120.0	C5—C6—H6	119.2
H2A—N2—H2B	120.0	C1—C6—H6	119.2
C6—C1—C2	116.9 (3)	C5—C7—H7A	109.5
C6—C1—N1	118.9 (3)	C5—C7—H7B	109.5
C2—C1—N1	124.3 (3)	H7A—C7—H7B	109.5

C3—C2—C1	120.9 (3)	C5—C7—H7C	109.5
C3—C2—S1	117.4 (3)	H7A—C7—H7C	109.5
C1—C2—S1	121.6 (3)	H7B—C7—H7C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···O2^{i}	0.86	2.15	3.003 (4)	174
N2—H2*A*···O1^{ii}	0.86	2.27	2.975 (4)	139
N1—H1*B*···O2	0.86	2.60	3.080 (5)	117

Symmetry codes: (i) x, $-y+1/2$, $z+1/2$; (ii) $-x$, $y+1/2$, $-z+3/2$.