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4,6-Dimethylbenzene-1,3-disulfonamide

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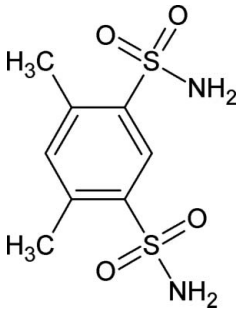
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.099; data-to-parameter ratio = 13.7.

The structure of the title compound, $C_8H_{12}N_2O_4S_2$, resembles those of other arylsulfonamides. The molecules in the title compound are packed into an infinite three-dimensional molecular network stabilized by hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2002, 2007*a*,*b*,*c*,*d*); Kumar *et al.* (1992).



Experimental

Crystal data

$C_8H_{12}N_2O_4S_2$
M_r = 264.32
Orthorhombic, *Pbca*
a = 14.4793 (2) Å
b = 8.0520 (1) Å
c = 19.1935 (4) Å
V = 2237.72 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 297 (2) K
0.31 × 0.18 × 0.14 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (Clark & Reid, 1995)
T_{min} = 0.868, T_{max} = 0.942
33751 measured reflections
2183 independent reflections
1693 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.099
S = 1.07
2183 reflections
159 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.829 (15)	2.269 (16)	3.050 (2)	157 (2)
N1—H1B···O2^{ii}	0.821 (15)	2.279 (17)	3.016 (2)	149 (2)
N2—H2A···O4^{iii}	0.830 (17)	2.062 (19)	2.848 (3)	158 (2)
N2—H2B···O1^{iv}	0.825 (17)	2.18 (2)	2.939 (2)	153 (2)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2140).

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supplementary materials

Acta Cryst. (2007). E**63**, o3361 [**doi:10.1107/S1600536807031297**]

4,6-Dimethylbenzene-1,3-disulfonamide

B. T. Gowda, K. S. Babitha, M. Tokarcík, J. Kozísek and H. Fuess

Comment

Arylsulfonamides and their N-halo compounds are of interest in synthetic, mechanistic, analytical and biological chemistry. In the present work, the structure of 4,6-dimethyl-benzene-1,3-disulfonamide has been determined to explore the effect of substituents on the solid state structures of sulfonamides and *N*-halo-arylsulfonamides (Gowda *et al.*, 2007*a*, *b*, *c*). The structure of the title compound (Fig. 1) resembles those of other arylsulfonamides (Gowda *et al.*, 2007*a*, *b*, *c*, *d*; Kumar *et al.*, 1992). It crystallizes in the orthorhombic space group Pbca, in contrast to the monoclinic space group $P2_1/c$ observed for both 3,4-dimethylbenzenesulfonamide (Gowda *et al.*, 2007*b*) and 3,4-dichlorobenzenesulfonamide (Gowda *et al.*, 2007*c*), and the triclinic space group P1 with 2-methyl-4-chloro-benzenesulfonamide (Gowda *et al.*, 2007*d*), and monoclinic space group *Pc* with the parent benzenesulfonamide (Gowda *et al.*, 2007*a*) and 4-methyl-benzenesulfonamide (Kumar *et al.*, 1992). The bond parameters are similar to those in other arylsulfonamides. The molecules in the title compound are packed into infinite 3-D molecular network stabilized by hydrogen bonding (Table 1 and Fig. 2).

Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2002). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra. Single crystals of the title compound were obtained from a slow evaporation of its ethanolic solution.

Refinement

H atoms of methyl groups and benzene ring were placed geometrically and refined using a riding model with C—H distances 0.96Å (methyl) and 0.93Å (ring). H atoms of amide groups were visible in the difference map and have been subsequently treated as riding with N—H bond length restrained to 0.83 (2) Å. All H atoms have isotropic thermal displacements with U_{iso}(H) = 1.5U_{eq}(C) for methyl and U_{iso}(H) = 1.2U_{eq}(C,*N*) for benzene and amide H atoms. No restraints were applied to non-hydrogen atoms.

Figures

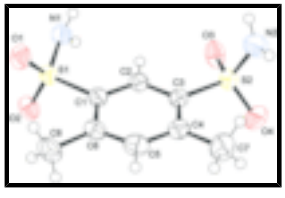

Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

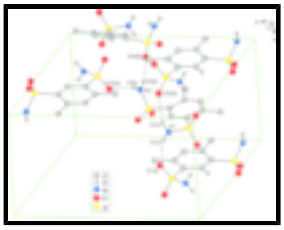

Fig. 2. Crystal structure of the title compound stabilized by hydrogen bonds N1—H1A···O1(i), N1—H1B···O2(ii), N2—H2A···O4(iii), N2—H2B···O1(iv). Symmetry codes: (i) −*x* + 1/2,*y* + 1/2,*z*; (ii) −*x* + 1/2,*y* − 1/2,*z*; (iii) −*x* + 1,*y* − 1/2,-*z* + 1/2; (iv) *x* + 1/2,-*y* + 1/2,-*z* + 1. H atoms not involved in hydrogen bonds have been omitted.

4,6-Dimethylbenzene-1,3-disulfonamide

Crystal data

$C_8H_{12}N_2O_4S_2$	F_{000} = 1104
M_r = 264.32	D_x = 1.569 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 14260 reflections
a = 14.4793 (2) Å	θ = 3.0–29.5º
b = 8.0520 (1) Å	μ = 0.48 mm^{-1}
c = 19.1935 (4) Å	*T* = 297 (2) K
V = 2237.72 (6) Å^3	Block, colourless
Z = 8	0.31 × 0.18 × 0.14 mm

Data collection

Oxford Diffraction Xcalibur diffractometer	1693 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 297(2) K	θ_{max} = 26.0º
φ scans, and ω scans with κ offsets	θ_{min} = 5.1º
Absorption correction: analytical (Clark & Reid, 1995)	*h* = −17→17
T_{min} = 0.868, T_{max} = 0.942	*k* = −9→9
33751 measured reflections	*l* = −23→23
2183 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.032	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.099	$w = 1/[\sigma^2(F_o^2) + (0.0661P)^2 + 0.0106P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.003
2183 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
159 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}

4 restraints
Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.23215 (12)	0.4353 (2)	0.44644 (10)	0.0325 (4)
C2	0.32502 (12)	0.4435 (2)	0.42955 (10)	0.0320 (4)
H2	0.3683	0.4692	0.4637	0.038*
C3	0.35327 (13)	0.4134 (2)	0.36175 (10)	0.0337 (4)
C4	0.28991 (14)	0.3696 (2)	0.30997 (11)	0.0421 (5)
C5	0.19745 (14)	0.3675 (3)	0.32909 (12)	0.0470 (5)
H5	0.1541	0.342	0.295	0.056*
C6	0.16569 (12)	0.4010 (2)	0.39580 (11)	0.0376 (5)
C7	0.31541 (17)	0.3244 (3)	0.23612 (12)	0.0656 (7)
H7A	0.3575	0.2323	0.2366	0.098*
H7B	0.3443	0.4179	0.214	0.098*
H7C	0.2607	0.2943	0.2109	0.098*
C8	0.06333 (14)	0.3980 (3)	0.41059 (13)	0.0535 (6)
H8A	0.0466	0.4947	0.437	0.08*
H8B	0.0484	0.3001	0.4368	0.08*
H8C	0.0299	0.3972	0.3674	0.08*
N1	0.28772 (11)	0.4730 (2)	0.58211 (9)	0.0397 (4)
H1A	0.3209 (14)	0.556 (2)	0.5760 (12)	0.048*
H1B	0.3178 (13)	0.387 (2)	0.5829 (12)	0.048*
N2	0.51984 (14)	0.2642 (3)	0.33063 (11)	0.0569 (5)
H2A	0.5078 (17)	0.213 (3)	0.2941 (11)	0.068*
H2B	0.5402 (18)	0.217 (3)	0.3656 (11)	0.068*
O1	0.14493 (9)	0.32605 (15)	0.55488 (7)	0.0451 (4)
O2	0.15455 (9)	0.62787 (16)	0.53936 (7)	0.0440 (4)
O3	0.51437 (10)	0.50240 (18)	0.40649 (8)	0.0507 (4)
O4	0.48035 (12)	0.5335 (2)	0.28186 (9)	0.0664 (5)
S1	0.19779 (3)	0.46871 (5)	0.53417 (2)	0.03266 (18)
S2	0.47313 (3)	0.43915 (6)	0.34460 (3)	0.03907 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0319 (10)	0.0292 (10)	0.0362 (11)	−0.0005 (7)	0.0009 (8)	0.0020 (8)
C2	0.0296 (10)	0.0330 (9)	0.0335 (11)	−0.0026 (7)	−0.0023 (8)	0.0013 (8)
C3	0.0324 (10)	0.0358 (10)	0.0329 (11)	0.0002 (8)	0.0003 (8)	0.0036 (8)
C4	0.0436 (11)	0.0496 (11)	0.0332 (11)	0.0054 (9)	−0.0055 (9)	0.0021 (9)
C5	0.0418 (12)	0.0534 (12)	0.0456 (13)	−0.0028 (9)	−0.0150 (10)	−0.0040 (10)
C6	0.0307 (10)	0.0364 (10)	0.0457 (13)	−0.0004 (8)	−0.0048 (9)	−0.0003 (9)
C7	0.0620 (15)	0.0968 (19)	0.0379 (13)	0.0059 (14)	−0.0054 (11)	−0.0141 (13)
C8	0.0317 (11)	0.0664 (14)	0.0623 (15)	−0.0024 (10)	−0.0058 (10)	−0.0029 (12)
N1	0.0381 (10)	0.0435 (10)	0.0376 (10)	−0.0002 (7)	0.0025 (8)	−0.0004 (8)
N2	0.0646 (13)	0.0638 (13)	0.0422 (12)	0.0225 (10)	−0.0098 (10)	−0.0131 (10)
O1	0.0397 (8)	0.0394 (8)	0.0562 (9)	−0.0069 (6)	0.0116 (7)	0.0065 (6)
O2	0.0384 (8)	0.0340 (7)	0.0595 (9)	0.0050 (6)	0.0051 (6)	−0.0057 (6)
O3	0.0345 (8)	0.0660 (9)	0.0516 (10)	−0.0064 (7)	0.0038 (7)	−0.0163 (8)
O4	0.0598 (10)	0.0812 (12)	0.0581 (11)	−0.0013 (8)	0.0130 (8)	0.0347 (9)
S1	0.0287 (3)	0.0316 (3)	0.0376 (3)	−0.00196 (18)	0.00553 (19)	−0.00020 (19)
S2	0.0347 (3)	0.0463 (3)	0.0362 (3)	0.0016 (2)	0.0054 (2)	0.0042 (2)

Geometric parameters (Å, °)

C1—C2	1.385 (2)	C7—H7C	0.96
C1—C6	1.395 (3)	C8—H8A	0.96
C1—S1	1.776 (2)	C8—H8B	0.96
C2—C3	1.386 (3)	C8—H8C	0.96
C2—H2	0.93	N1—S1	1.5949 (18)
C3—C4	1.398 (3)	N1—H1A	0.829 (15)
C3—S2	1.7785 (19)	N1—H1B	0.821 (15)
C4—C5	1.388 (3)	N2—S2	1.586 (2)
C4—C7	1.509 (3)	N2—H2A	0.830 (17)
C5—C6	1.387 (3)	N2—H2B	0.825 (17)
C5—H5	0.93	O1—S1	1.4364 (13)
C6—C8	1.509 (3)	O2—S1	1.4297 (13)
C7—H7A	0.96	O3—S2	1.4236 (15)
C7—H7B	0.96	O4—S2	1.4275 (16)
C2—C1—C6	121.07 (18)	C6—C8—H8A	109.5
C2—C1—S1	119.12 (15)	C6—C8—H8B	109.5
C6—C1—S1	119.81 (14)	H8A—C8—H8B	109.5
C1—C2—C3	119.88 (18)	C6—C8—H8C	109.5
C1—C2—H2	120.1	H8A—C8—H8C	109.5
C3—C2—H2	120.1	H8B—C8—H8C	109.5
C2—C3—C4	121.20 (18)	S1—N1—H1A	114.1 (16)
C2—C3—S2	116.20 (14)	S1—N1—H1B	115.1 (16)
C4—C3—S2	122.58 (15)	H1A—N1—H1B	112 (2)
C5—C4—C3	116.63 (19)	S2—N2—H2A	119.5 (18)
C5—C4—C7	118.76 (19)	S2—N2—H2B	114.9 (19)

C3—C4—C7	124.61 (19)	H2A—N2—H2B	122 (3)
C6—C5—C4	124.15 (18)	O2—S1—O1	117.66 (8)
C6—C5—H5	117.9	O2—S1—N1	107.33 (9)
C4—C5—H5	117.9	O1—S1—N1	107.02 (9)
C5—C6—C1	116.93 (17)	O2—S1—C1	108.94 (8)
C5—C6—C8	119.74 (18)	O1—S1—C1	106.88 (8)
C1—C6—C8	123.33 (18)	N1—S1—C1	108.76 (9)
C4—C7—H7A	109.5	O3—S2—O4	118.87 (10)
C4—C7—H7B	109.5	O3—S2—N2	106.27 (10)
H7A—C7—H7B	109.5	O4—S2—N2	107.38 (11)
C4—C7—H7C	109.5	O3—S2—C3	107.26 (9)
H7A—C7—H7C	109.5	O4—S2—C3	106.83 (9)
H7B—C7—H7C	109.5	N2—S2—C3	110.12 (10)
C6—C1—C2—C3	−1.6 (3)	C2—C1—C6—C8	−177.22 (18)
S1—C1—C2—C3	178.28 (12)	S1—C1—C6—C8	2.9 (3)
C1—C2—C3—C4	−1.9 (3)	C2—C1—S1—O2	106.92 (14)
C1—C2—C3—S2	176.44 (12)	C6—C1—S1—O2	−73.16 (15)
C2—C3—C4—C5	3.6 (3)	C2—C1—S1—O1	−124.98 (14)
S2—C3—C4—C5	−174.66 (15)	C6—C1—S1—O1	54.94 (16)
C2—C3—C4—C7	−176.00 (19)	C2—C1—S1—N1	−9.76 (16)
S2—C3—C4—C7	5.7 (3)	C6—C1—S1—N1	170.16 (15)
C3—C4—C5—C6	−1.9 (3)	C2—C3—S2—O3	−5.20 (16)
C7—C4—C5—C6	177.7 (2)	C4—C3—S2—O3	173.16 (16)
C4—C5—C6—C1	−1.4 (3)	C2—C3—S2—O4	−133.67 (15)
C4—C5—C6—C8	179.01 (19)	C4—C3—S2—O4	44.69 (19)
C2—C1—C6—C5	3.2 (3)	C2—C3—S2—N2	110.03 (16)
S1—C1—C6—C5	−176.68 (14)	C4—C3—S2—N2	−71.62 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.829 (15)	2.269 (16)	3.050 (2)	157 (2)
N1—H1B···O2^{ii}	0.821 (15)	2.279 (17)	3.016 (2)	149 (2)
N2—H2A···O4^{iii}	0.830 (17)	2.062 (19)	2.848 (3)	158 (2)
N2—H2B···O1^{iv}	0.825 (17)	2.18 (2)	2.939 (2)	153 (2)

Symmetry codes: (i) −*x*+1/2, *y*+1/2, *z*; (ii) −*x*+1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1/2, −*z*+1/2; (iv) *x*+1/2, −*y*+1/2, −*z*+1.

Fig. 1

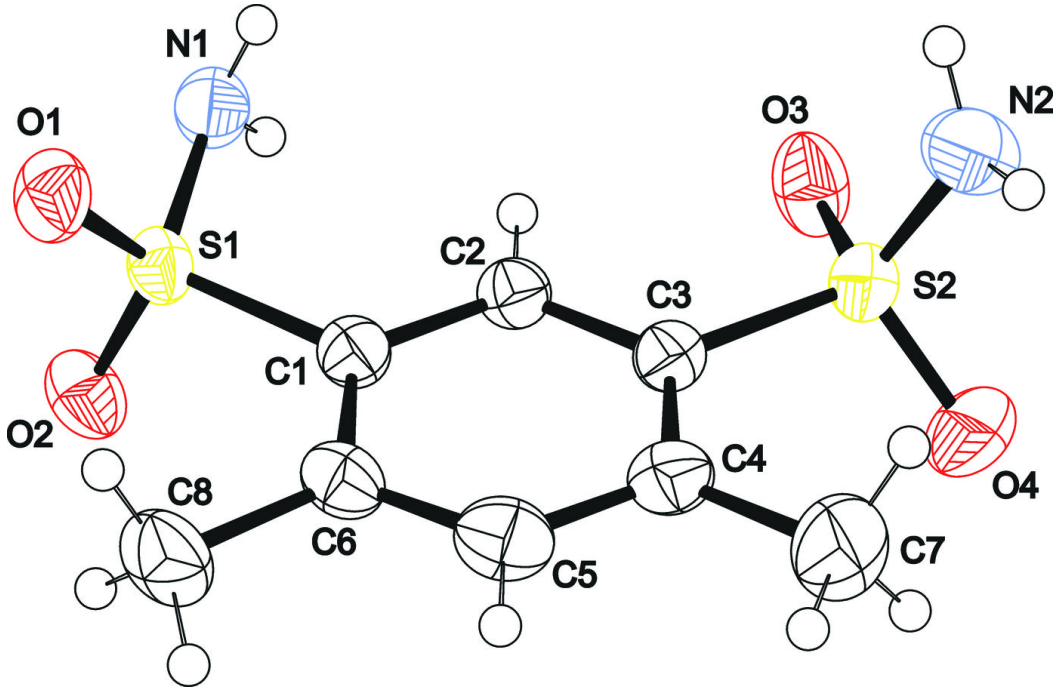

Fig. 2