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N-(2,4-Dimethylphenyl)benzenesulfonamide

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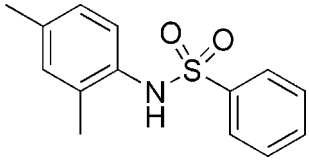
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.122; data-to-parameter ratio = 16.2.

The molecules of the title compound, $C_{14}H_{15}NO_2S$, are linked into centrosymmetric dimers *via* N—H···O hydrogen bonds. The packing is influenced by π–π stacking interactions [centroid-to-centroid separation = 3.780 (5) Å].

Related literature

For the structure of 4-methyl-*N*-(3-nitrophenyl)benzenesulfonamide, see: Xing *et al.* (2006).



Experimental

Crystal data

$C_{14}H_{15}NO_2S$
M_r = 261.33
Monoclinic, $P2_1/n$
a = 7.999 (3) Å
b = 11.073 (4) Å
c = 15.116 (5) Å
β = 96.822 (6)°
V = 1329.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.950, T_{max} = 0.963
7489 measured reflections
2721 independent reflections
2098 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.122
S = 1.05
2721 reflections
168 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.890 (9)	2.086 (11)	2.967 (2)	170 (2)

Symmetry code: (i) $-x, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: HB2495).

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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Xing, J.-D., Bai, G.-Y., Zeng, T. & Li, J.-S. (2006). *Acta Cryst.* E**62**, o79–o80.

  doi:10.1107/S160053680703677X

supplementary materials

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N-(2,4-Dimethylphenyl)benzenesulfonamide

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Comment

In the molecular structure of (I), Fig. 1, the N lone electron pair weakly conjugates the xylene ring due to the strong electron-withdrawing capability of benzenesulfonyl group. The sligtly long C7—N1 [1.435 (2) Å] bond length and selected torsion angles (Table 1) support this. Thus, the amide has a pyramidal arrangement of bonds around nitrogen, but the pyramid is somewhat shallower than expected for pure sp^3 hybridization. The xylene ring has an angle of 59.40 (10) ° with the phenyl ring.

In the crystal of (I), a strong self-complimentary N—H···O interaction (Table 2) links the molecules into centrosymmetric dimers, which extend along the a axle to form a 1-D chain. Aromatic π-π stacking [centroid separation = 3.780 (5) Å] between the xylene and phenyl ring link the 1-D chains.

Experimental

A solution of benzenesulfonyl chloride in CH_2Cl_2 was added dropwise to a mixture of 2,4-xylidine and triethylamine in CH_2Cl_2 at room temperature with stirring. The reaction mixture continued stirring overnight. The resulting solid was purified by recrystallization from methanol. Colourless blocks of (I) were grown by natural evaporation of a methanolic solution.

Refinement

The N-bound H atom was refined freely while the other H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

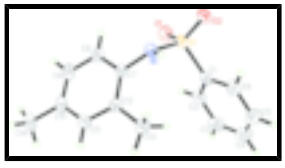

Fig. 1. (*a*). The molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids for the non-hydrogen atoms.

N-(2,4-Dimethylphenyl)benzenesulfonamide

Crystal data

$C_{14}H_{15}NO_2S$	F_{000} = 552
M_r = 261.33	D_x = 1.306 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å

Hall symbol: -P 2yn	Cell parameters from 2927 reflections
a = 7.999 (3) Å	θ = 2.8–26.4º
b = 11.073 (4) Å	μ = 0.24 mm^{-1}
c = 15.116 (5) Å	T = 294 (2) K
β = 96.822 (6)º	Block, colorless
V = 1329.4 (8) $Å^3$	0.22 × 0.20 × 0.16 mm
Z = 4	

Data collection

Bruker SMART 1K CCD diffractometer	2721 independent reflections
Radiation source: fine-focus sealed tube	2098 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 294(2) K	θ_{max} = 26.5º
ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 10$
T_{min} = 0.950, T_{max} = 0.963	$k = -13 \rightarrow 13$
7489 measured reflections	$l = -17 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.122	$w = 1/[\sigma^2(F_o^2) + (0.0618P)^2 + 0.376P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
2721 reflections	$\Delta\rho_{max}$ = 0.25 e $Å^{-3}$
168 parameters	$\Delta\rho_{min}$ = −0.34 e $Å^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
S1	0.15860 (6)	0.57386 (4)	0.39513 (3)	0.04420 (18)
O1	0.30915 (19)	0.58332 (14)	0.35412 (10)	0.0574 (4)
C12	0.2428 (2)	0.81756 (17)	0.56051 (12)	0.0415 (4)
N1	0.2010 (2)	0.61330 (15)	0.49881 (11)	0.0439 (4)
C1	0.0102 (3)	0.67673 (17)	0.34296 (12)	0.0454 (5)
O2	0.07517 (19)	0.45924 (13)	0.39753 (10)	0.0561 (4)
C7	0.3079 (2)	0.71364 (17)	0.52683 (12)	0.0383 (4)
C10	0.5276 (3)	0.8957 (2)	0.59282 (13)	0.0512 (5)
C8	0.4797 (3)	0.7013 (2)	0.52497 (14)	0.0508 (5)
H8	0.5226	0.6314	0.5020	0.061*
C6	−0.1581 (3)	0.6618 (2)	0.35252 (15)	0.0567 (6)
H6	−0.1931	0.5977	0.3856	0.068*
C11	0.3553 (3)	0.90632 (18)	0.59333 (13)	0.0488 (5)
H11	0.3133	0.9762	0.6168	0.059*
C14	0.6440 (3)	0.9943 (2)	0.63106 (16)	0.0699 (7)
H14A	0.6496	0.9937	0.6948	0.105*
H14B	0.6023	1.0711	0.6086	0.105*
H14C	0.7545	0.9810	0.6141	0.105*
C13	0.0571 (3)	0.8347 (2)	0.56425 (17)	0.0614 (6)
H13A	0.0373	0.9138	0.5869	0.092*
H13B	0.0175	0.7749	0.6028	0.092*
H13C	−0.0021	0.8264	0.5055	0.092*
C2	0.0635 (3)	0.7724 (2)	0.29396 (14)	0.0569 (6)
H2	0.1769	0.7819	0.2876	0.068*
C9	0.5866 (3)	0.7923 (2)	0.55703 (15)	0.0579 (6)
H9	0.7016	0.7837	0.5545	0.070*
C4	−0.2212 (4)	0.8378 (2)	0.26392 (16)	0.0714 (7)
H4	−0.2999	0.8921	0.2368	0.086*
C3	−0.0537 (4)	0.8530 (2)	0.25501 (15)	0.0703 (7)
H3	−0.0195	0.9180	0.2226	0.084*
C5	−0.2736 (3)	0.7434 (3)	0.31242 (17)	0.0700 (7)
H5	−0.3873	0.7342	0.3183	0.084*
H1A	0.114 (2)	0.601 (2)	0.5296 (13)	0.055 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0455 (3)	0.0408 (3)	0.0471 (3)	−0.0071 (2)	0.0086 (2)	−0.0059 (2)
O1	0.0510 (9)	0.0677 (10)	0.0562 (9)	−0.0066 (7)	0.0170 (7)	−0.0124 (7)
C12	0.0383 (10)	0.0443 (11)	0.0423 (10)	−0.0015 (8)	0.0057 (8)	0.0033 (8)
N1	0.0439 (9)	0.0438 (9)	0.0446 (9)	−0.0084 (7)	0.0075 (7)	0.0005 (7)
C1	0.0552 (12)	0.0427 (11)	0.0380 (10)	−0.0072 (9)	0.0042 (9)	−0.0062 (8)
O2	0.0623 (9)	0.0397 (8)	0.0666 (10)	−0.0096 (7)	0.0087 (7)	−0.0071 (7)
C7	0.0377 (10)	0.0417 (10)	0.0349 (9)	−0.0049 (8)	0.0018 (7)	0.0032 (8)

C10	0.0493 (12)	0.0627 (14)	0.0409 (11)	−0.0179 (10)	0.0021 (9)	0.0024 (9)
C8	0.0400 (11)	0.0572 (13)	0.0552 (12)	0.0036 (9)	0.0060 (9)	−0.0056 (10)
C6	0.0536 (13)	0.0626 (14)	0.0542 (13)	−0.0001 (11)	0.0081 (10)	0.0031 (10)
C11	0.0560 (13)	0.0441 (11)	0.0462 (11)	−0.0051 (9)	0.0053 (9)	−0.0026 (9)
C14	0.0701 (16)	0.0786 (18)	0.0583 (14)	−0.0342 (13)	−0.0034 (12)	−0.0022 (12)
C13	0.0439 (12)	0.0566 (14)	0.0841 (17)	0.0048 (10)	0.0094 (11)	−0.0084 (12)
C2	0.0717 (15)	0.0492 (12)	0.0495 (12)	−0.0151 (11)	0.0057 (11)	−0.0032 (10)
C9	0.0352 (11)	0.0788 (16)	0.0597 (13)	−0.0094 (10)	0.0050 (9)	−0.0050 (12)
C4	0.096 (2)	0.0631 (16)	0.0518 (14)	0.0215 (14)	−0.0051 (13)	−0.0043 (12)
C3	0.113 (2)	0.0462 (13)	0.0500 (13)	−0.0051 (14)	0.0040 (14)	0.0024 (10)
C5	0.0628 (15)	0.0838 (18)	0.0623 (15)	0.0133 (13)	0.0034 (12)	−0.0026 (13)

Geometric parameters (Å, °)

S1—O1	1.4223 (15)	C6—C5	1.379 (3)
S1—O2	1.4364 (15)	C6—H6	0.9300
S1—N1	1.6234 (18)	C11—H11	0.9300
S1—C1	1.763 (2)	C14—H14A	0.9600
C12—C11	1.384 (3)	C14—H14B	0.9600
C12—C7	1.385 (3)	C14—H14C	0.9600
C12—C13	1.506 (3)	C13—H13A	0.9600
N1—C7	1.435 (2)	C13—H13B	0.9600
N1—H1A	0.890 (9)	C13—H13C	0.9600
C1—C6	1.380 (3)	C2—C3	1.375 (4)
C1—C2	1.389 (3)	C2—H2	0.9300
C7—C8	1.385 (3)	C9—H9	0.9300
C10—C9	1.375 (3)	C4—C5	1.371 (4)
C10—C11	1.384 (3)	C4—C3	1.372 (4)
C10—C14	1.505 (3)	C4—H4	0.9300
C8—C9	1.372 (3)	C3—H3	0.9300
C8—H8	0.9300	C5—H5	0.9300
O1—S1—O2	119.74 (9)	C12—C11—H11	118.5
O1—S1—N1	108.09 (9)	C10—C14—H14A	109.5
O2—S1—N1	104.94 (9)	C10—C14—H14B	109.5
O1—S1—C1	108.52 (10)	H14A—C14—H14B	109.5
O2—S1—C1	106.98 (10)	C10—C14—H14C	109.5
N1—S1—C1	108.09 (9)	H14A—C14—H14C	109.5
C11—C12—C7	117.73 (18)	H14B—C14—H14C	109.5
C11—C12—C13	119.96 (18)	C12—C13—H13A	109.5
C7—C12—C13	122.30 (17)	C12—C13—H13B	109.5
C7—N1—S1	122.83 (13)	H13A—C13—H13B	109.5
C7—N1—H1A	116.1 (14)	C12—C13—H13C	109.5
S1—N1—H1A	112.1 (15)	H13A—C13—H13C	109.5
C6—C1—C2	120.8 (2)	H13B—C13—H13C	109.5
C6—C1—S1	119.29 (16)	C3—C2—C1	119.1 (2)
C2—C1—S1	119.90 (17)	C3—C2—H2	120.4
C12—C7—C8	120.45 (18)	C1—C2—H2	120.4
C12—C7—N1	121.03 (17)	C8—C9—C10	121.5 (2)
C8—C7—N1	118.39 (18)	C8—C9—H9	119.3

C9—C10—C11	117.50 (19)	C10—C9—H9	119.3
C9—C10—C14	122.0 (2)	C5—C4—C3	120.6 (2)
C11—C10—C14	120.5 (2)	C5—C4—H4	119.7
C9—C8—C7	119.9 (2)	C3—C4—H4	119.7
C9—C8—H8	120.0	C4—C3—C2	120.1 (2)
C7—C8—H8	120.0	C4—C3—H3	119.9
C5—C6—C1	119.1 (2)	C2—C3—H3	119.9
C5—C6—H6	120.5	C4—C5—C6	120.2 (3)
C1—C6—H6	120.5	C4—C5—H5	119.9
C10—C11—C12	122.91 (19)	C6—C5—H5	119.9
C10—C11—H11	118.5		
O1—S1—N1—C7	41.07 (18)	N1—C7—C8—C9	−175.53 (19)
O2—S1—N1—C7	169.91 (15)	C2—C1—C6—C5	0.2 (3)
C1—S1—N1—C7	−76.20 (17)	S1—C1—C6—C5	179.27 (18)
O1—S1—C1—C6	161.79 (16)	C9—C10—C11—C12	0.6 (3)
O2—S1—C1—C6	31.31 (19)	C14—C10—C11—C12	−178.8 (2)
N1—S1—C1—C6	−81.22 (18)	C7—C12—C11—C10	0.7 (3)
O1—S1—C1—C2	−19.14 (19)	C13—C12—C11—C10	179.29 (19)
O2—S1—C1—C2	−149.61 (16)	C6—C1—C2—C3	0.2 (3)
N1—S1—C1—C2	97.85 (17)	S1—C1—C2—C3	−178.86 (16)
C11—C12—C7—C8	−1.2 (3)	C7—C8—C9—C10	1.2 (3)
C13—C12—C7—C8	−179.7 (2)	C11—C10—C9—C8	−1.6 (3)
C11—C12—C7—N1	174.51 (17)	C14—C10—C9—C8	177.9 (2)
C13—C12—C7—N1	−4.0 (3)	C5—C4—C3—C2	0.8 (4)
S1—N1—C7—C12	110.71 (19)	C1—C2—C3—C4	−0.7 (3)
S1—N1—C7—C8	−73.5 (2)	C3—C4—C5—C6	−0.4 (4)
C12—C7—C8—C9	0.3 (3)	C1—C6—C5—C4	−0.1 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2^{i}	0.890 (9)	2.086 (11)	2.967 (2)	170 (2)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1.

Fig. 1