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4-Methyl-*N*-phenylbenzenesulfonamide

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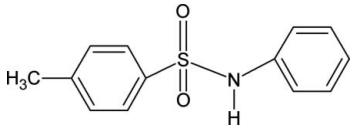
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.006 Å; R factor = 0.071; wR factor = 0.217; data-to-parameter ratio = 14.3.

In the title compound, $C_{13}H_{13}NO_2S$, the dihedral angle between the aromatic rings is 68.4 (1)°. In the crystal, the molecules are linked into inversion dimers by pairs of N—H···O hydrogen bonds. The unit cell of this compound was reported previously [Oh *et al.* (1985). *Chung. Kwa. Yong. (Chung. J. Sci.)*, **12**, 67] but no atomic coordinates were established in the earlier study.

Related literature

For related structures, see: Gelbrich *et al.* (2007); Gowda *et al.* (2005, 2009*a*,*b*); Gowda, Foro, Nirmala, Terao & Fuess (2009); Perlovich *et al.* (2006).



Experimental

Crystal data

$C_{13}H_{13}NO_2S$
M_r = 247.30
Monoclinic, $P2_1/c$
a = 8.770 (2) Å
b = 9.768 (2) Å
c = 16.234 (5) Å
β = 113.200 (2)°
V = 1278.2 (6) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.17 mm^{-1}
T = 299 K
0.55 × 0.50 × 0.40 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.336, T_{max} = 0.420
3091 measured reflections
2278 independent reflections
2041 reflections with $I > 2\sigma(I)$
R_{int} = 0.096
3 standard reflections
frequency: 120 min
intensity decay: 2.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.217
S = 1.10
2278 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.77 (4)	2.17 (5)	2.932 (4)	172 (4)

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

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2138).

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supporting information

Acta Cryst. (2009). E**65**, o1219 [doi:10.1107/S1600536809016377]

4-Methyl-*N*-phenylbenzenesulfonamide

B. Thimme Gowda, Sabine Foro, P. G. Nirmala, Hiromitsu Terao and Hartmut Fuess

S1. Comment

As part of a study of the effect of substituent on the crystal structures of *N*-(aryl)-arylsulfonamides (Gowda *et al.*, 2009*a, b, c*), in the present work, the structure of 4-methyl-*N*-(phenyl)- benzenesulfonamide (I) has been determined. The conformations of the N—C bond in the C—SO_2—NH—C segment of the structure are "*trans*" and "*gauche*" with respect to the S═O bonds (Fig. 1). The molecule is bent at the S atom with the C—SO_2—NH—C torsion angle of -51.6 (3)°. The two benzene rings in (I) are tilted relative to each other by 68.4 (1)°. The other bond parameters in (I) are similar to those observed in 2,4-dimethyl-*N*-(phenyl)-benzenesulfonamide (Gowda *et al.*, 2009 *a*), 4-chloro-2-methyl-*N*-(phenyl)-benzenesulfonamide (Gowda *et al.*, 2009 *b*), 4-methyl-*N*-(3,4-dimethylphenyl)- benzenesulfonamide (Gowda *et al.*, 2009 *c*)) and other aryl sulfonamides (Perlovich *et al.*, 2006; Gelbrich *et al.*, 2007). The N—H···O hydrogen bonds (Table 1) pack the molecules into column like chains in the direction of *a*- axis (Fig. 2).

S2. Experimental

The purity of the commercial sample was checked and characterized by recording its infrared and NMR spectra (Gowda *et al.*, 2005). The single crystals used in X-ray diffraction studies were grown in ethanolic solution by slow evaporation at room temperature.

S3. Refinement

The N-bound H atom was located in difference map and its positional parameters were refined freely [N—H = 0.77 (4) Å]. The other H atoms were positioned with idealized geometry using a riding model [C—H = 0.93–0.96 Å] with U_{iso}(H) = 1.2 U_{eq}(*N*)

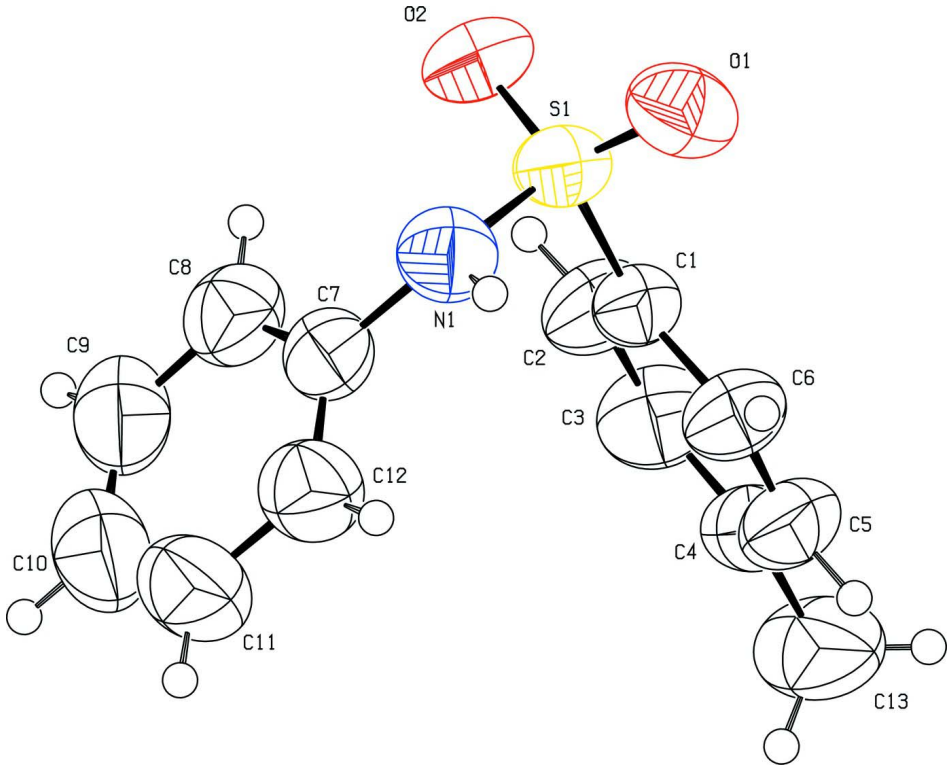

Figure 1

Molecular structure of (I), showing the atom labeling scheme and displacement ellipsoids drawn at the 50% probability level.

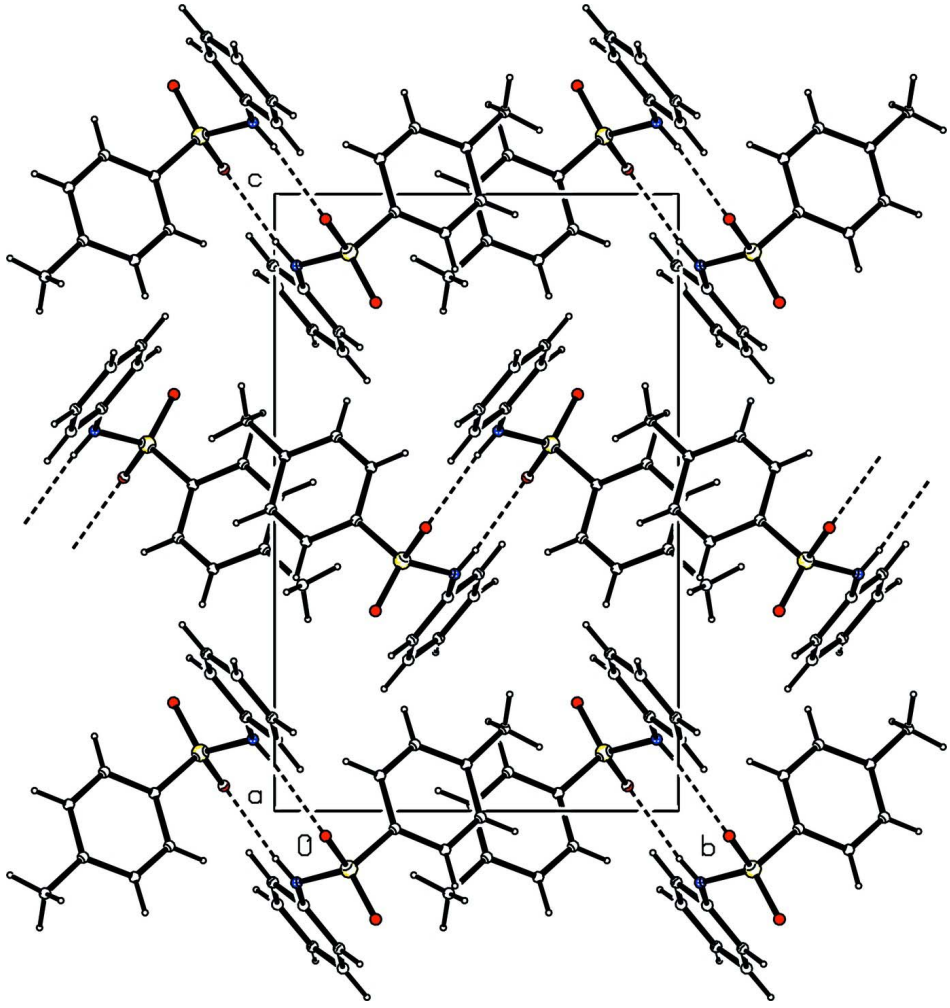

Figure 2

Molecular packing of (I) with hydrogen bonding shown as dashed lines.

4-Methyl-*N*-phenylbenzenesulfonamide

Crystal data

$C_{13}H_{13}NO_2S$
$M_r = 247.30$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.770\ (2)$ Å
$b = 9.768\ (2)$ Å
$c = 16.234\ (5)$ Å
$\beta = 113.200\ (2)°$
$V = 1278.2\ (6)$ Å^3
$Z = 4$
$F(000) = 520$
$D_x = 1.285$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 25 reflections
$\theta = 5.4–20.7°$
$\mu = 2.17$ mm^{-1}
$T = 299$ K
Prism, colourless
0.55 × 0.50 × 0.40 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans

Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.336, T_{max} = 0.420
3091 measured reflections
2278 independent reflections
2041 reflections with $I > 2\sigma(I)$
R_{int} = 0.096
θ_{max} = 66.9°, θ_{min} = 5.4°
h = −3→10
k = −11→0
l = −19→19
3 standard reflections every 120 min
intensity decay: 2.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.217
S = 1.10
2278 reflections
159 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1256P)^2 + 0.4489P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.023
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}
Extinction correction: (*SHELXL97*; Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.060 (5)

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}
C1	0.3623 (4)	0.2024 (3)	0.4713 (2)	0.0641 (7)
C2	0.2930 (5)	0.0780 (4)	0.4369 (2)	0.0810 (9)
H2	0.2768	0.0535	0.3787	0.097*
C3	0.2480 (5)	−0.0098 (4)	0.4897 (3)	0.0929 (11)
H3	0.2037	−0.0949	0.4670	0.112*
C4	0.2669 (4)	0.0254 (4)	0.5752 (3)	0.0866 (11)
C5	0.3360 (5)	0.1527 (5)	0.6073 (3)	0.0881 (11)
H5	0.3495	0.1790	0.6648	0.106*
C6	0.3838 (4)	0.2390 (4)	0.5571 (2)	0.0799 (9)
H6	0.4313	0.3230	0.5804	0.096*
C7	0.1172 (4)	0.4284 (3)	0.3472 (2)	0.0708 (8)
C8	0.0374 (5)	0.3408 (4)	0.2771 (3)	0.0855 (10)
H8	0.0972	0.2892	0.2519	0.103*
C9	−0.1321 (5)	0.3311 (5)	0.2450 (3)	0.0982 (13)
H9	−0.1867	0.2712	0.1981	0.118*
C10	−0.2223 (5)	0.4065 (6)	0.2800 (4)	0.1095 (16)
H10	−0.3372	0.3987	0.2570	0.131*

C11	−0.1428 (6)	0.4932 (6)	0.3488 (4)	0.1133 (16)
H11	−0.2042	0.5457	0.3725	0.136*
C12	0.0292 (5)	0.5048 (4)	0.3844 (3)	0.0899 (11)
H12	0.0833	0.5631	0.4324	0.108*
C13	0.2197 (7)	−0.0689 (6)	0.6336 (4)	0.1236 (18)
H13A	0.1824	−0.1544	0.6032	0.148*
H13B	0.1322	−0.0283	0.6468	0.148*
H13C	0.3142	−0.0845	0.6884	0.148*
N1	0.2939 (3)	0.4457 (3)	0.3838 (2)	0.0762 (8)
H1N	0.318 (5)	0.497 (5)	0.423 (3)	0.091*
O1	0.5798 (3)	0.3739 (3)	0.45932 (19)	0.0863 (8)
O2	0.4014 (3)	0.2496 (3)	0.32444 (16)	0.0858 (8)
S1	0.42133 (9)	0.31592 (8)	0.40573 (5)	0.0689 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0670 (15)	0.0712 (17)	0.0583 (16)	0.0062 (12)	0.0292 (13)	−0.0007 (13)
C2	0.104 (2)	0.077 (2)	0.071 (2)	−0.0127 (17)	0.0435 (18)	−0.0128 (16)
C3	0.111 (3)	0.077 (2)	0.103 (3)	−0.0077 (19)	0.055 (2)	0.001 (2)
C4	0.091 (2)	0.095 (2)	0.091 (2)	0.029 (2)	0.054 (2)	0.029 (2)
C5	0.103 (2)	0.106 (3)	0.066 (2)	0.017 (2)	0.0442 (18)	0.0030 (19)
C6	0.095 (2)	0.086 (2)	0.0664 (19)	0.0000 (17)	0.0399 (17)	−0.0132 (16)
C7	0.0718 (17)	0.0718 (18)	0.0711 (18)	−0.0004 (13)	0.0305 (14)	0.0198 (14)
C8	0.089 (2)	0.091 (2)	0.076 (2)	−0.0102 (18)	0.0330 (18)	0.0057 (18)
C9	0.084 (2)	0.106 (3)	0.090 (3)	−0.013 (2)	0.019 (2)	0.019 (2)
C10	0.079 (2)	0.121 (4)	0.114 (4)	−0.003 (2)	0.023 (2)	0.038 (3)
C11	0.094 (3)	0.127 (4)	0.128 (4)	0.030 (3)	0.054 (3)	0.028 (3)
C12	0.090 (2)	0.088 (2)	0.095 (3)	0.0093 (18)	0.0404 (19)	0.008 (2)
C13	0.143 (4)	0.120 (4)	0.140 (4)	0.033 (3)	0.090 (3)	0.052 (3)
N1	0.0754 (16)	0.0734 (17)	0.0824 (19)	−0.0075 (12)	0.0341 (14)	−0.0006 (13)
O1	0.0727 (13)	0.0901 (16)	0.1026 (18)	−0.0101 (11)	0.0414 (12)	−0.0152 (14)
O2	0.1054 (17)	0.0989 (18)	0.0709 (14)	−0.0013 (14)	0.0541 (13)	−0.0068 (12)
S1	0.0721 (6)	0.0749 (6)	0.0691 (6)	−0.0036 (3)	0.0379 (4)	−0.0048 (3)

Geometric parameters (Å, º)

C1—C2	1.374 (5)	C8—H8	0.9300
C1—C6	1.378 (4)	C9—C10	1.358 (7)
C1—S1	1.750 (3)	C9—H9	0.9300
C2—C3	1.375 (5)	C10—C11	1.355 (8)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.375 (6)	C11—C12	1.391 (6)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.392 (6)	C12—H12	0.9300
C4—C13	1.492 (5)	C13—H13A	0.9600
C5—C6	1.349 (5)	C13—H13B	0.9600
C5—H5	0.9300	C13—H13C	0.9600

C6—H6	0.9300	N1—S1	1.633 (3)
C7—C12	1.373 (5)	N1—H1N	0.77 (4)
C7—C8	1.375 (5)	O1—S1	1.434 (2)
C7—N1	1.434 (4)	O2—S1	1.418 (2)
C8—C9	1.371 (5)		

C2—C1—C6	120.1 (3)	C8—C9—H9	119.1
C2—C1—S1	120.2 (2)	C11—C10—C9	119.2 (4)
C6—C1—S1	119.7 (3)	C11—C10—H10	120.4
C1—C2—C3	119.2 (3)	C9—C10—H10	120.4
C1—C2—H2	120.4	C10—C11—C12	121.0 (5)
C3—C2—H2	120.4	C10—C11—H11	119.5
C2—C3—C4	121.5 (4)	C12—C11—H11	119.5
C2—C3—H3	119.2	C7—C12—C11	118.6 (4)
C4—C3—H3	119.2	C7—C12—H12	120.7
C3—C4—C5	117.6 (3)	C11—C12—H12	120.7
C3—C4—C13	122.3 (5)	C4—C13—H13A	109.5
C5—C4—C13	120.1 (4)	C4—C13—H13B	109.5
C6—C5—C4	121.7 (3)	H13A—C13—H13B	109.5
C6—C5—H5	119.2	C4—C13—H13C	109.5
C4—C5—H5	119.2	H13A—C13—H13C	109.5
C5—C6—C1	119.9 (4)	H13B—C13—H13C	109.5
C5—C6—H6	120.1	C7—N1—S1	122.3 (2)
C1—C6—H6	120.1	C7—N1—H1N	109 (3)
C12—C7—C8	120.7 (3)	S1—N1—H1N	113 (3)
C12—C7—N1	117.2 (3)	O2—S1—O1	118.69 (15)
C8—C7—N1	122.0 (3)	O2—S1—N1	109.20 (17)
C9—C8—C7	118.7 (4)	O1—S1—N1	104.00 (16)
C9—C8—H8	120.7	O2—S1—C1	108.57 (15)
C7—C8—H8	120.7	O1—S1—C1	109.23 (16)
C10—C9—C8	121.8 (5)	N1—S1—C1	106.47 (14)
C10—C9—H9	119.1		

C6—C1—C2—C3	−0.9 (5)	C8—C7—C12—C11	−0.9 (6)
S1—C1—C2—C3	179.8 (3)	N1—C7—C12—C11	178.3 (4)
C1—C2—C3—C4	1.6 (6)	C10—C11—C12—C7	1.3 (7)
C2—C3—C4—C5	−1.0 (6)	C12—C7—N1—S1	135.5 (3)
C2—C3—C4—C13	−179.6 (4)	C8—C7—N1—S1	−45.3 (4)
C3—C4—C5—C6	−0.3 (5)	C7—N1—S1—O2	65.5 (3)
C13—C4—C5—C6	178.3 (4)	C7—N1—S1—O1	−166.9 (3)
C4—C5—C6—C1	1.0 (6)	C7—N1—S1—C1	−51.6 (3)
C2—C1—C6—C5	−0.3 (5)	C2—C1—S1—O2	−6.3 (3)
S1—C1—C6—C5	178.9 (3)	C6—C1—S1—O2	174.5 (2)
C12—C7—C8—C9	−0.1 (5)	C2—C1—S1—O1	−137.1 (3)
N1—C7—C8—C9	−179.2 (3)	C6—C1—S1—O1	43.7 (3)
C7—C8—C9—C10	0.7 (6)	C2—C1—S1—N1	111.2 (3)
C8—C9—C10—C11	−0.4 (7)	C6—C1—S1—N1	−68.0 (3)
C9—C10—C11—C12	−0.6 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1^{i}	0.77 (4)	2.17 (5)	2.932 (4)	172 (4)

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