Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

N-(2-Methylphenyl)methanesulfonamide

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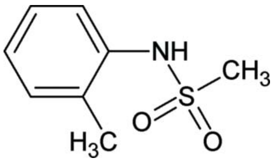
Received 1 April 2007; accepted 2 April 2007

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.098; data-to-parameter ratio = 11.2.

The conformation of the N—H bond in the structure of the title compound (2MPMSA), $C_8H_{11}NO_2S$, is *syn* to the *ortho*-methyl substituent, in contrast with the *anti* conformation observed for the *meta*-methyl-substituted compound (3MPMSA). The *ortho* substitution of the methyl group in *N*-phenylmethanesulfonamde (PMSA) changes its space group from monoclinic $P2_1/c$ to triclinic $P\overline{1}$, compared with the change from monoclinic $P2_1/c$ to orthorhombic *Pccn* on *meta*-substitution. The bond parameters in PMSA, 2MPMSA and 3MPMSA are similar, except for the torsion angles involving the S—N bond. The N—H H atom alone lies on one side of the plane of the phenyl group, while the whole methanesulfonyl group is on the opposite side of the plane, similar to what was observed in PMSA and 3MPMSA. Thus, the amide H atom is available to a receptor molecule during biological activity. The molecules of the title compound form centrosymmetric dimers *via* an N—H···O(sulfonyl) hydrogen bond.

Related literature

For related literature, see: Gowda *et al.* (2007*a*,*b*,*c*,*d*); Gowda, Kozisek *et al.* (2007); Gowda *et al.* (2000); Jayalakshmi & Gowda (2004); Klug (1968).



Experimental

Crystal data

$C_8H_{11}NO_2S$
M_r = 185.24
Triclinic, $P\overline{1}$
a = 5.719 (1) Å
b = 9.041 (1) Å
c = 9.225 (2) Å
α = 79.53 (1)°
β = 87.360 (1)°
γ = 74.440 (10)°
V = 451.85 (14) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 2.87 mm^{-1}
T = 299 (2) K
0.13 × 0.13 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min}$ = 0.731, $T_{\max}$ = 0.789
1713 measured reflections
1606 independent reflections
1259 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.036
3 standard reflections
frequency: 120 min
intensity decay: 1.8%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.098
S = 1.08
1606 reflections
143 parameters
1 restraint
Only H-atom coordinates refined
$\Delta\rho_{\max}$ = 0.17 e Å^{-3}
$\Delta\rho_{\min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5N···O3$^{\rm i}$	0.848 (10)	2.104 (12)	2.943 (3)	170 (3)

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

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, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

BTG gratefully thanks the Alexander von Humboldt Foundation, Bonn, Germany, for an extension of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2008).

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doi:10.1107/S1600536807016273

supplementary materials

Acta Cryst. (2007). E**63**, o2340 [**doi:10.1107/S1600536807016273**]

N-(2-Methylphenyl)methanesulfonamide

B. T. Gowda, **S. Foro** and **H. Fuess**

Comment

The biological activity of alkyl sulfonanilides is thought to be due to the H atom of the phenyl N—H portion of the sulfonanilide molecule, as it can align itself in relation to a receptor site. Therefore, the structural studies of sulfonanilides are of interest. In the present work, the structure of *N*-(2-methylphenyl)methanesulfonamde (2MPMSA), (I), has been determined to explore the substituent effects on the solid-state structures of anilides and sulfonanilides (Gowda *et al.*, 2007*a*,*b*,*c*,*d*; Gowda, Kozisek *et al.*, 2007; Gowda *et al.*, 2000).

The conformation of the N—H bond in the structure of 2MPMSA is *syn* to the *ortho*-methyl substituent (Fig. 1), in contrast with the anti conformation observed for the *meta*-methyl-substituted compound (3MPMSA) (Gowda *et al.*, 2007*c*). The *ortho*-substitution of the methyl group in *N*-(phenyl)methanesulfonamde (PMSA) changes its space group from monoclinic $P2_1/c$ (Klug, 1968) to triclinic $P\bar{1}$, compared with the change from monoclinic $P2_1/c$ to orthorhombic Pccn on *meta*-methyl substitution (Gowda *et al.*, 2007*c*).

The bond parameters in PMSA (Klug, 1968), 2MPMSA and 3MPMSA (Gowda *et al.*, 2007*c*) are similar except for the torsion angles C1—S2—N5—C6, S2—N5—C6—C7, S2—N5—C6—C11, which have the following values: 62.2 (2), 75.5 (2) and -106.6 (2)°, respectively, in PMSA; -64.5 (2), 117.1 (2) and -65.3 (3)°, respectively, in 2MPMSA; 57.9 (3), 68.1 (4) and -114.3 (3)°, respectively, in 3MPMSA. The data included for PMSA are the values determined under the present conditions as the literature values were determined in [Meaning not clear. Text missing?] (Klug, 1968).

The N—H H atom lies alone on one side of the plane of the phenyl group, while

the whole methanesulfonyl group is on the opposite side of the plane, similar to what was observed in PMSA and 3MPMSA. Thus, the amide H atom is available to

a receptor molecule during biological activity.

The molecules in the title compound form centrosymmetric dimers *via* an N5—H5N···O3(1 - *x*,-*y*, 1 - *z*) hydrogen bond (Table 1 and Fig. 2).

Experimental

The title compound was prepared according to the literature method of Jayalakshmi & Gowda (2004). The purity of the compound was checked by determining its melting point. It was characterized by recording its IR and NMR

spectra (Jayalakshmi & Gowda, 2004). Single crystals of the title compound were obtained by slow evaporation of an ethanolic solution and used for X-ray diffraction studied at room temperature.

Refinement

All H atoms attached to C and N atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å (CH aromatic) or 0.96 Å (CH_3) and N—H = 0.86 Å, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$ or $1.5U_{eq}(C)$ for methyl H. [This does not match the data in the CIF, where coordinates have been refined - please provide correct text]

Figures

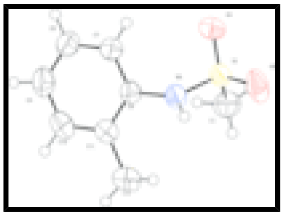

Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented as small spheres of arbitrary radii.

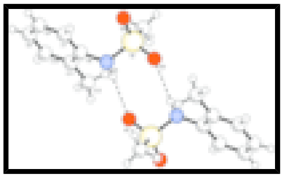

Fig. 2. The hydrogen bonding in the title compound. Hydrogen bonds are shown as dashed lines.

N-(2-Methylphenyl)methanesulfonamide

Crystal data

$C_8H_{11}NO_2S$

$M_r = 185.24$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 5.7190 (10)$ Å

$b = 9.0410 (10)$ Å

$c = 9.225 (2)$ Å

$\alpha = 79.530 (10)°$

$\beta = 87.360 (10)°$

$\gamma = 74.440 (10)°$

$V = 451.85 (14)$ Å^3

$Z = 2$

$F_{000} = 196$

$D_x = 1.361$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.54180$ Å

Cell parameters from 25 reflections

$\theta = 7.7–23.7°$

$\mu = 2.87$ mm^{-1}

$T = 299 (2)$ K

Block, grey

0.13 × 0.13 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 299(2)$ K

$\omega/2\theta$ scans

Absorption correction: ψ scan

$R_{int} = 0.036$

$\theta_{max} = 66.9°$

$\theta_{min} = 4.9°$

$h = -6\rightarrow6$

$k = -10\rightarrow10$

$l = 0\rightarrow10$

(North *et al.*, 1968)

$T_{min} = 0.731$, $T_{max} = 0.789$

1713 measured reflections

1606 independent reflections

1259 reflections with $I > 2\sigma(I)$

3 standard reflections

every 120 min

intensity decay: 1.8%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.098$

$S = 1.08$

1606 reflections

143 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2 + 0.0954P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.17$ e Å^{-3}

$\Delta\rho_{min} = -0.26$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0117 (14)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.2073 (7)	0.0168 (4)	0.1937 (4)	0.0679 (9)
H1A	0.265 (6)	−0.052 (4)	0.124 (4)	0.081*
H1B	0.142 (6)	−0.028 (4)	0.276 (4)	0.081*
H1C	0.094 (6)	0.114 (4)	0.145 (4)	0.081*
C6	0.1994 (4)	0.3574 (3)	0.2840 (3)	0.0404 (5)
C7	0.2887 (5)	0.4558 (3)	0.1760 (3)	0.0511 (7)
H7	0.447 (5)	0.424 (3)	0.142 (3)	0.061*
C8	0.1438 (6)	0.6009 (3)	0.1180 (3)	0.0623 (8)
H8	0.207 (5)	0.668 (4)	0.042 (3)	0.075*
C9	−0.0875 (6)	0.6489 (4)	0.1688 (3)	0.0648 (8)

H9	−0.194 (6)	0.749 (4)	0.136 (3)	0.078*
C10	−0.1738 (5)	0.5531 (4)	0.2789 (3)	0.0589 (7)
H10	−0.331 (6)	0.586 (4)	0.316 (3)	0.071*
C11	−0.0351 (4)	0.4046 (3)	0.3388 (3)	0.0445 (6)
C12	−0.1334 (6)	0.3018 (4)	0.4577 (4)	0.0625 (8)
H12A	−0.128 (6)	0.210 (4)	0.430 (4)	0.075*
H12B	−0.042 (6)	0.279 (4)	0.546 (4)	0.075*
H12C	−0.289 (6)	0.348 (4)	0.476 (3)	0.075*
N5	0.3555 (4)	0.2077 (2)	0.3434 (2)	0.0468 (5)
H5N	0.348 (5)	0.164 (3)	0.4324 (15)	0.056*
O3	0.6064 (4)	−0.0557 (2)	0.3450 (2)	0.0789 (7)
O4	0.5642 (4)	0.1338 (2)	0.1154 (2)	0.0607 (5)
S2	0.45723 (12)	0.07166 (7)	0.24662 (7)	0.0469 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.081 (2)	0.066 (2)	0.067 (2)	−0.0319 (18)	0.0114 (18)	−0.0207 (17)
C6	0.0437 (13)	0.0398 (12)	0.0373 (12)	−0.0079 (10)	−0.0027 (10)	−0.0098 (10)
C7	0.0554 (16)	0.0479 (14)	0.0484 (15)	−0.0124 (12)	0.0083 (13)	−0.0083 (12)
C8	0.083 (2)	0.0462 (15)	0.0524 (17)	−0.0124 (15)	0.0093 (15)	−0.0053 (13)
C9	0.079 (2)	0.0470 (16)	0.0564 (17)	0.0033 (15)	−0.0053 (16)	−0.0070 (14)
C10	0.0462 (16)	0.0626 (18)	0.0629 (18)	−0.0006 (13)	−0.0016 (13)	−0.0190 (15)
C11	0.0422 (14)	0.0506 (14)	0.0420 (13)	−0.0117 (11)	−0.0021 (10)	−0.0123 (11)
C12	0.0543 (18)	0.073 (2)	0.0635 (19)	−0.0230 (16)	0.0117 (15)	−0.0131 (17)
N5	0.0536 (13)	0.0458 (12)	0.0336 (11)	−0.0021 (10)	−0.0019 (9)	−0.0041 (9)
O3	0.0951 (16)	0.0603 (12)	0.0507 (12)	0.0292 (11)	−0.0059 (11)	−0.0045 (10)
O4	0.0651 (12)	0.0637 (12)	0.0509 (11)	−0.0162 (10)	0.0203 (9)	−0.0105 (9)
S2	0.0516 (4)	0.0431 (4)	0.0376 (3)	−0.0008 (3)	0.0031 (2)	−0.0037 (2)

Geometric parameters (Å, °)

C1—S2	1.749 (4)	C9—H9	0.95 (3)
C1—H1A	0.96 (3)	C10—C11	1.392 (4)
C1—H1B	0.91 (3)	C10—H10	0.94 (3)
C1—H1C	0.99 (3)	C11—C12	1.495 (4)
C6—C7	1.386 (3)	C12—H12A	0.90 (3)
C6—C11	1.395 (3)	C12—H12B	0.95 (3)
C6—N5	1.434 (3)	C12—H12C	0.90 (3)
C7—C8	1.377 (4)	N5—S2	1.617 (2)
C7—H7	0.93 (3)	N5—H5N	0.848 (10)
C8—C9	1.366 (4)	O3—S2	1.4286 (19)
C8—H8	0.96 (3)	O4—S2	1.4225 (19)
C9—C10	1.374 (4)		

S2—C1—H1A	107 (2)	C11—C10—H10	117.6 (19)
S2—C1—H1B	108 (2)	C10—C11—C6	116.9 (2)
H1A—C1—H1B	114 (3)	C10—C11—C12	121.2 (3)
S2—C1—H1C	106 (2)	C6—C11—C12	121.9 (2)

H1A—C1—H1C	110 (3)	C11—C12—H12A	111 (2)
H1B—C1—H1C	112 (3)	C11—C12—H12B	112 (2)
C7—C6—C11	120.9 (2)	H12A—C12—H12B	107 (3)
C7—C6—N5	118.9 (2)	C11—C12—H12C	110 (2)
C11—C6—N5	120.1 (2)	H12A—C12—H12C	108 (3)
C8—C7—C6	120.2 (3)	H12B—C12—H12C	109 (3)
C8—C7—H7	119.5 (18)	C6—N5—S2	123.02 (16)
C6—C7—H7	120.3 (18)	C6—N5—H5N	122.6 (19)
C9—C8—C7	119.9 (3)	S2—N5—H5N	108 (2)
C9—C8—H8	120.6 (19)	O4—S2—O3	118.19 (13)
C7—C8—H8	119.5 (19)	O4—S2—N5	109.11 (12)
C8—C9—C10	119.9 (3)	O3—S2—N5	105.40 (12)
C8—C9—H9	123.7 (19)	O4—S2—C1	107.17 (15)
C10—C9—H9	116 (2)	O3—S2—C1	109.20 (17)
C9—C10—C11	122.1 (3)	N5—S2—C1	107.33 (15)
C9—C10—H10	120.3 (19)		

C11—C6—C7—C8	−1.8 (4)	N5—C6—C11—C10	178.2 (2)
N5—C6—C7—C8	−179.3 (2)	C7—C6—C11—C12	−178.6 (3)
C6—C7—C8—C9	1.0 (5)	N5—C6—C11—C12	−1.1 (4)
C7—C8—C9—C10	0.9 (5)	C7—C6—N5—S2	−65.4 (3)
C8—C9—C10—C11	−2.0 (5)	C11—C6—N5—S2	117.1 (2)
C9—C10—C11—C6	1.2 (4)	C6—N5—S2—O4	51.3 (2)
C9—C10—C11—C12	−179.5 (3)	C6—N5—S2—O3	179.2 (2)
C7—C6—C11—C10	0.7 (4)	C6—N5—S2—C1	−64.5 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···O3^{i}	0.848 (10)	2.104 (12)	2.943 (3)	170 (3)

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

Fig. 1

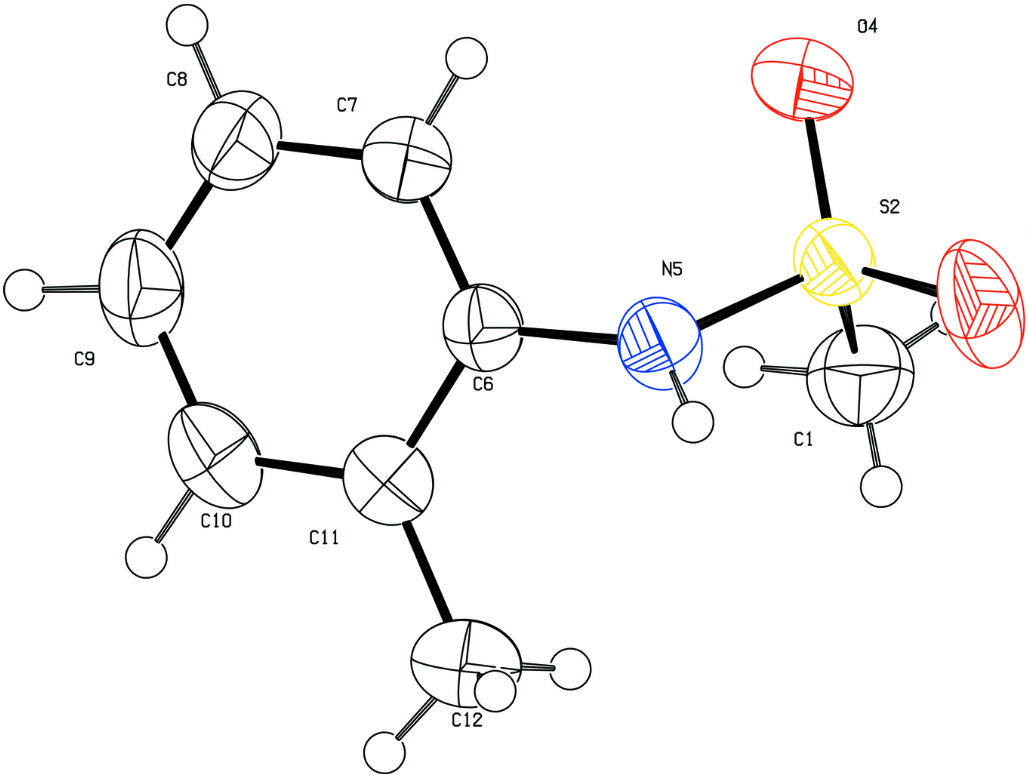

Fig. 2