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N-(4-Nitrophenyl)methanesulfonamide

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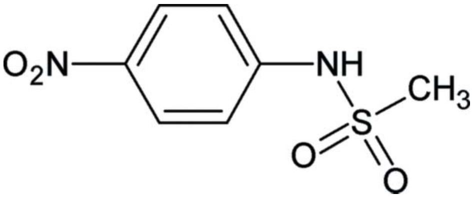
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.007 Å; R factor = 0.060; wR factor = 0.182; data-to-parameter ratio = 12.8.

The structure of the title compound (4NPMSA), $C_7H_8N_2O_4S$, closely resembles those of *N*-phenylmethanesulfonamide (PMSA) and *N*-(3-nitrophenyl)methanesulfonamide (4NPMSA), with slightly different geometric parameters. The substitution of a nitro group at the *para* position of PMSA does not change the space group, unlike the case of *meta* substitution (3NPMSA), where it changes from monoclinic $P2_1/c$ to triclinic $P\bar{1}$ [Gowda, Foro & Fuess (2007*c*). *Acta Cryst.* E**63**, o2337]. The N—H H atom and the methylsulfonyl group are *trans* to one another across the plane of the benzene ring. Thus, the amide H atom is available to a receptor molecule during biological activity. An N—H···O hydrogen bond links the molecules into centrosymmetric dimers.

Related literature

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



Experimental

Crystal data

$C_7H_8N_2O_4S$
M_r = 216.21
Monoclinic, $P2_1/c$
a = 10.879 (2) Å
b = 10.336 (2) Å
c = 8.715 (1) Å
β = 110.13 (1)°
V = 920.1 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 3.12 mm^{-1}
T = 299 (2) K
0.17 × 0.15 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.547, T_{max} = 0.778 (expected range = 0.640–0.911)
1780 measured reflections
1642 independent reflections
1149 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
3 standard reflections frequency: 120 min intensity decay: 3.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.182
S = 1.09
1642 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5N···O3^{i}	0.86	2.07	2.914 (5)	168

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2006).

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supplementary materials

Acta Cryst. (2007). E**63**, o2339 [**doi:10.1107/S160053680701598X**]

N-(4-Nitrophenyl)methanesulfonamide

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Comment

The alkyl sulfonanilide moiety is an important constituent of many biologically significant compounds. The stereochemistry of these molecules, particularly in the vicinity of the phenyl-N—H portion, is of interest in explaining their biological activity. This biological activity is thought to be due to the H atom of the phenyl N—H portion of the sulfonanilide molecules, as it can align itself in relation to a receptor site. Therefore, structural studies of sulfonanilides are of interest. In the present work, the structure of the title compound (4NPMSA) has been determined to explore the substituent effects of polar groups on the structures of anilides and sulfonanilides (Gowda *et al.*, 2007a,b; Gowda *et al.*, 2000; Gowda, Kozisek *et al.*, 2007).

The substitution of a nitro group at the *para* position of *N*-(phenyl)methanesulfonamide (PMSA) does not change the space group, unlike in the case of *meta* substitution (3NPMSA), where it changes from monoclinic P21/c (Klug, 1968) to triclinic $P\overline{1}$ (Gowda *et al.*, 2007c).

The N—H H atom projects alone on one side of the plane of the phenyl group, while the whole methanesulfonyl group is on the opposite side of the plane (Fig. 1), similar to what was observed in PMSA (Klug, 1968) and 3NPMSA (Gowda *et al.*, 2007c). The amide H atom is thus available to a receptor molecule during biological activity.

An N—H···O hydrogen bond links the molecules of (I) into centrosymmetric dimers (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 $1.5U_{eq}(CH_3)$.

Figures

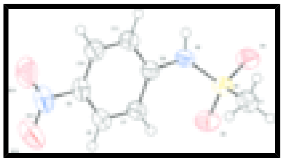
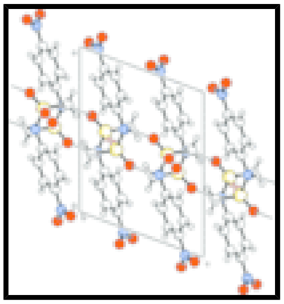


Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as small spheres of arbitrary radii.

Fig. 2. A packing diagram, viewed down the axis b



N-(4-Nitrophenyl)methanesulfonamide

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$C_7H_8N_2O_4S$

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Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.879$ (2) Å

$b = 10.336$ (2) Å

$c = 8.715$ (1) Å

$\beta = 110.13$ (1)°

$V = 920.1$ (3) Å^3

$Z = 4$

$F_{000} = 448$

$D_x = 1.561$ Mg m^{-3}

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

Cell parameters from 25 reflections

$\theta = 4.3$–24.4°

$\mu = 3.12$ mm^{-1}

$T = 299$ (2) K

Laminar, grey

0.17 × 0.15 × 0.03 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
(North *et al.*, 1968)

$T_{min} = 0.547$, $T_{max} = 0.778$

1780 measured reflections

1642 independent reflections

1149 reflections with $I > 2\sigma(I)$

$R_{int} = 0.035$

$\theta_{max} = 66.9$°

$\theta_{min} = 4.3$°

$h = -12\rightarrow12$

$k = -12\rightarrow1$

$l = -10\rightarrow0$

3 standard reflections

every 120 min

intensity decay: 3.5%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.060$

$wR(F^2) = 0.182$

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1074P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.56$ e Å^{-3}

$S = 1.09$

1642 reflections

128 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$\Delta\rho_{\min} = -0.61$ e Å^{-3}

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

Extinction coefficient: 0.0089 (16)

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*	$U_{\text{iso}}*/U_{\text{eq}}$
C1	0.6245 (5)	0.4037 (5)	0.4016 (5)	0.0484 (12)
H1A	0.5738	0.3869	0.4705	0.058*
H1B	0.6365	0.4953	0.3951	0.058*
H1C	0.7083	0.3624	0.4465	0.058*
C6	0.2974 (4)	0.4055 (4)	0.1995 (5)	0.0383 (10)
C7	0.2810 (5)	0.2996 (4)	0.2895 (6)	0.0454 (11)
H7	0.3418	0.2326	0.3160	0.054*
C8	0.1728 (5)	0.2953 (5)	0.3392 (6)	0.0486 (12)
H8	0.1603	0.2248	0.3985	0.058*
C9	0.0845 (4)	0.3948 (5)	0.3008 (6)	0.0467 (12)
C10	0.1012 (5)	0.5004 (5)	0.2138 (6)	0.0521 (12)
H10	0.0406	0.5675	0.1892	0.063*
C11	0.2070 (4)	0.5065 (5)	0.1636 (6)	0.0473 (11)
H11	0.2187	0.5781	0.1055	0.057*
N5	0.4013 (4)	0.4164 (4)	0.1407 (5)	0.0429 (9)
H5N	0.3894	0.4683	0.0598	0.051*
N12	−0.0295 (4)	0.3886 (5)	0.3520 (6)	0.0596 (12)
O3	0.6074 (3)	0.3835 (3)	0.0984 (4)	0.0535 (9)
O4	0.5206 (4)	0.2075 (3)	0.2198 (4)	0.0534 (9)
O13	−0.0451 (4)	0.2933 (4)	0.4271 (6)	0.0816 (14)
O14	−0.1055 (4)	0.4809 (5)	0.3203 (6)	0.0847 (14)
S2	0.54234 (11)	0.34283 (10)	0.20640 (13)	0.0386 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.053 (3)	0.055 (3)	0.040 (3)	−0.008 (2)	0.019 (2)	−0.003 (2)
C6	0.039 (2)	0.037 (2)	0.036 (2)	−0.0042 (18)	0.0099 (19)	−0.0023 (18)
C7	0.044 (3)	0.039 (2)	0.056 (3)	0.001 (2)	0.020 (2)	0.008 (2)
C8	0.044 (3)	0.048 (3)	0.057 (3)	−0.008 (2)	0.021 (2)	0.003 (2)
C9	0.037 (2)	0.050 (3)	0.055 (3)	−0.008 (2)	0.017 (2)	−0.009 (2)
C10	0.045 (2)	0.044 (3)	0.069 (3)	0.004 (2)	0.021 (2)	0.005 (2)
C11	0.045 (2)	0.037 (2)	0.059 (3)	0.000 (2)	0.018 (2)	0.008 (2)
N5	0.045 (2)	0.042 (2)	0.046 (2)	0.0050 (17)	0.0208 (18)	0.0135 (17)
N12	0.048 (2)	0.062 (3)	0.074 (3)	−0.015 (2)	0.026 (2)	−0.016 (2)
O3	0.058 (2)	0.065 (2)	0.0493 (19)	0.0109 (17)	0.0337 (17)	0.0111 (16)
O4	0.070 (2)	0.0342 (17)	0.057 (2)	0.0042 (16)	0.0222 (18)	−0.0036 (15)
O13	0.086 (3)	0.066 (3)	0.117 (4)	−0.018 (2)	0.066 (3)	−0.004 (3)
O14	0.051 (2)	0.085 (3)	0.129 (4)	0.006 (2)	0.045 (3)	−0.003 (3)
S2	0.0457 (6)	0.0369 (6)	0.0377 (6)	0.0035 (5)	0.0202 (4)	0.0006 (5)

Geometric parameters (Å, °)

C1—S2	1.744 (5)	C9—C10	1.377 (7)
C1—H1A	0.9600	C9—N12	1.457 (6)
C1—H1B	0.9600	C10—C11	1.366 (6)
C1—H1C	0.9600	C10—H10	0.9300
C6—C11	1.394 (6)	C11—H11	0.9300
C6—C7	1.394 (6)	N5—S2	1.629 (4)
C6—N5	1.398 (5)	N5—H5N	0.8600
C7—C8	1.388 (7)	N12—O13	1.226 (6)
C7—H7	0.9300	N12—O14	1.230 (6)
C8—C9	1.368 (7)	O3—S2	1.422 (3)
C8—H8	0.9300	O4—S2	1.431 (3)
S2—C1—H1A	109.5	C11—C10—C9	119.9 (5)
S2—C1—H1B	109.5	C11—C10—H10	120.0
H1A—C1—H1B	109.5	C9—C10—H10	120.0
S2—C1—H1C	109.5	C10—C11—C6	120.0 (4)
H1A—C1—H1C	109.5	C10—C11—H11	120.0
H1B—C1—H1C	109.5	C6—C11—H11	120.0
C11—C6—C7	119.9 (4)	C6—N5—S2	128.1 (3)
C11—C6—N5	117.1 (4)	C6—N5—H5N	116.0
C7—C6—N5	123.1 (4)	S2—N5—H5N	116.0
C8—C7—C6	119.2 (4)	O13—N12—O14	122.5 (5)
C8—C7—H7	120.4	O13—N12—C9	119.2 (5)
C6—C7—H7	120.4	O14—N12—C9	118.3 (5)
C9—C8—C7	119.9 (5)	O3—S2—O4	118.5 (2)
C9—C8—H8	120.0	O3—S2—N5	104.6 (2)
C7—C8—H8	120.0	O4—S2—N5	108.9 (2)
C8—C9—C10	121.1 (5)	O3—S2—C1	109.5 (2)

C8—C9—N12	119.5 (5)	O4—S2—C1	108.5 (2)
C10—C9—N12	119.4 (5)	N5—S2—C1	106.2 (2)

C11—C6—C7—C8	1.3 (7)	C11—C6—N5—S2	158.9 (4)
N5—C6—C7—C8	−178.2 (4)	C7—C6—N5—S2	−21.5 (6)
C6—C7—C8—C9	−0.6 (7)	C8—C9—N12—O13	−0.9 (7)
C7—C8—C9—C10	−0.3 (8)	C10—C9—N12—O13	178.7 (5)
C7—C8—C9—N12	179.3 (4)	C8—C9—N12—O14	177.9 (5)
C8—C9—C10—C11	0.4 (8)	C10—C9—N12—O14	−2.4 (7)
N12—C9—C10—C11	−179.3 (5)	C6—N5—S2—O3	177.0 (4)
C9—C10—C11—C6	0.4 (8)	C6—N5—S2—O4	49.4 (4)
C7—C6—C11—C10	−1.3 (7)	C6—N5—S2—C1	−67.2 (4)
N5—C6—C11—C10	178.3 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···O3^{i}	0.86	2.07	2.914 (5)	168

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

Fig. 1

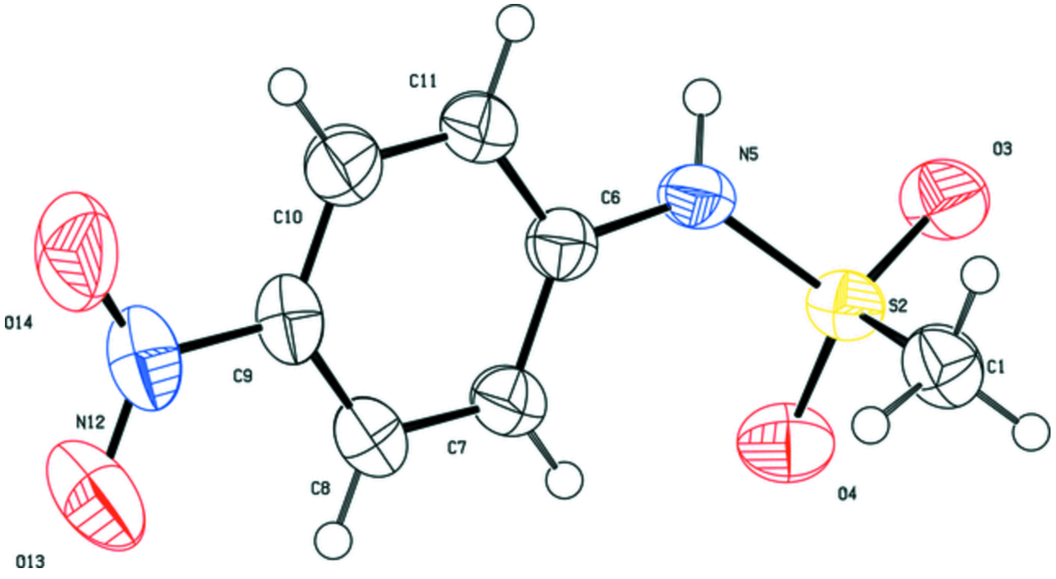

Fig. 2