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N-(3-Nitrophenyl)methanesulfonamide

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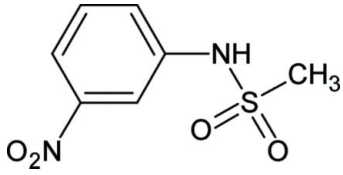
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.105; data-to-parameter ratio = 11.3.

The conformation of the N—H bond is *anti* to the *m*-nitro substituent in the structure of the title compound, $C_7H_8N_2O_4S$. The molecules are linked into centrosymmetric dimers through an N—H···O hydrogen bond.

Related literature

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



Experimental

Crystal data

$C_7H_8N_2O_4S$
M_r = 216.21
Triclinic, $P\overline{1}$
a = 6.959 (1) Å
b = 8.207 (1) Å
c = 8.759 (1) Å
α = 96.93 (1)°
β = 111.05 (1)°
γ = 99.78 (1)°
V = 451.02 (10) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 3.18 mm^{-1}
T = 299 (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2782 measured reflections
1611 independent reflections
1427 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
3 standard reflections
frequency: 120 min
intensity decay: 5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.105
S = 1.08
1611 reflections
143 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5*N*···O3^{i}	0.849 (10)	2.203 (16)	2.984 (2)	153 (3)

Symmetry code: (i) $-x+1, -y+2, -z+1$.

Data collection: *CAD-4-PC* (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: BT2328).

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supplementary materials

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N-(3-Nitrophenyl)methanesulfonamide

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Comment

Methanesulfonanilides are of interest due to their distinct chemical and physical properties. The alkyl sulfonanilido 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 would be of extreme interest in formulating an explanation of their biological activity similar to phenolic derivatives. The biological activity is thought to be due to the hydrogen of the phenyl N—H portion of the sulfonanilide molecules as it can align itself, in relation to a receptor site . Thus the structural studies of sulfonanilides are of interest. In the present work, the structure of *N*-(3-nitrophenyl)-methanesulfonamde (3NPMSA) has been determined to explore the substituent effects of polar groups on the structures of anilides and sulfonanilides as part of a study on the systematization of the crystal structures of this class of compounds in general (Gowda *et al.*, 2000; Gowda *et al.*, 2007*a*,b,c). In the structure of 3NPMSA the conformation of the N—H bond is anti to the meta-nitro substituent (Fig.1). The amide hydrogen is thus available to a receptor molecule during biological activity. Selected geometric parameters are shown in Table 1. The molecules are linked into centrosymmetric dimers (Fig. 2) through a N—H···O hydrogen bond (Table 2).

Experimental

The title compound was prepared according to a literature method (Jayalakshmi & Gowda, 2004). The purity of the compound was checked by determining its melting point. It was characterised by recording its infrared and NMR spectra (Jayalakshmi & Gowda, 2004). Single crystals of the title compound were

obtained from an ethanolic solution and used for X-ray diffraction studied at room temperature.

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (CH aromatic) or 0.96 Å (CH_3) with U_{iso}(H) = 1.2 U_{eq}(C) or U_{iso}(H) = 1.5 U_{eq}(C_{methyl}). The coordinates of the H atom bonded to N were refined with a distance restraint [N–H = 0.86 (1) Å] and U_{iso}(H) = 1.2 U_{eq}(N).

Figures

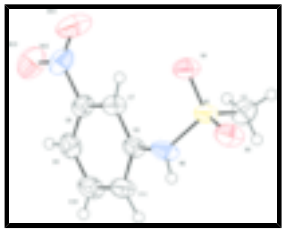

Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

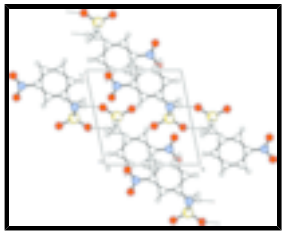

Fig. 2. Packing diagram viewed down the axis b

N-(3-nitrophenyl)methanesulfonamide

Crystal data

$C_7H_8N_2O_4S$	$Z = 2$
$M_r = 216.21$	$F_{000} = 224$
Triclinic, $P\overline{1}$	$D_x = 1.592$ Mg m^{-3}
Hall symbol: -P 1	Cu $K\alpha$ radiation $\lambda = 1.54180$ Å
$a = 6.959$ (1) Å	Cell parameters from 25 reflections
$b = 8.207$ (1) Å	$\theta = 5.5$–25.3º
$c = 8.759$ (1) Å	$\mu = 3.18$ mm^{-1}
$\alpha = 96.93$ (1)º	$T = 299$ (2) K
$\beta = 111.05$ (1)º	Prism, orange
$\gamma = 99.78$ (1)º	0.25 × 0.20 × 0.20 mm
$V = 451.02$ (10) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.071$
Radiation source: fine-focus sealed tube	$\theta_{max} = 66.9$º
Monochromator: graphite	$\theta_{min} = 5.5$º
$T = 299$(2) K	$h = -8 \rightarrow 8$
ω/2θ scans	$k = -9 \rightarrow 5$
Absorption correction: none	$l = -10 \rightarrow 10$
2782 measured reflections	3 standard reflections
1611 independent reflections	every 120 min
1427 reflections with $I > 2\sigma(I)$	intensity decay: 5%

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.0989P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.042$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.105$	$\Delta\rho_{max} = 0.49$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.49$ e Å^{-3}

1611 reflections

143 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

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

Extinction coefficient: 0.091 (5)

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	0.0954 (4)	0.8080 (3)	0.6291 (3)	0.0525 (6)
H1A	0.1469	0.9231	0.6882	0.063*
H1B	0.1232	0.7341	0.7074	0.063*
H1C	−0.0542	0.7869	0.5660	0.063*
C6	0.5674 (3)	0.7198 (2)	0.7373 (2)	0.0362 (4)
C7	0.5029 (3)	0.5475 (3)	0.7208 (2)	0.0390 (4)
H7	0.398 (4)	0.479 (3)	0.622 (3)	0.047*
C8	0.6099 (3)	0.4749 (2)	0.8503 (2)	0.0386 (4)
C9	0.7761 (3)	0.5638 (3)	0.9932 (3)	0.0447 (5)
H9	0.838 (4)	0.505 (4)	1.075 (3)	0.054*
C10	0.8369 (3)	0.7366 (3)	1.0067 (3)	0.0501 (5)
H10	0.947 (4)	0.796 (4)	1.100 (4)	0.060*
C11	0.7328 (3)	0.8137 (3)	0.8807 (3)	0.0456 (5)
H11	0.770 (4)	0.938 (4)	0.890 (3)	0.055*
N5	0.4746 (3)	0.8055 (2)	0.6095 (2)	0.0478 (5)
H5N	0.539 (4)	0.9067 (17)	0.621 (3)	0.057*
N12	0.5437 (3)	0.2912 (2)	0.8337 (2)	0.0515 (5)
O3	0.2113 (2)	0.8999 (2)	0.39469 (18)	0.0530 (4)
O4	0.1475 (2)	0.59956 (19)	0.41044 (18)	0.0507 (4)
O13	0.6464 (3)	0.2257 (2)	0.9437 (3)	0.0758 (6)
O14	0.3897 (4)	0.2133 (2)	0.7117 (2)	0.0742 (6)
S2	0.22342 (7)	0.77189 (6)	0.49366 (5)	0.0378 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0592 (13)	0.0449 (12)	0.0550 (12)	0.0107 (10)	0.0241 (10)	0.0113 (10)
C6	0.0321 (9)	0.0376 (10)	0.0367 (9)	0.0036 (7)	0.0118 (7)	0.0111 (8)
C7	0.0412 (10)	0.0353 (10)	0.0350 (9)	0.0021 (8)	0.0117 (8)	0.0062 (8)
C8	0.0439 (10)	0.0349 (10)	0.0435 (10)	0.0106 (8)	0.0225 (8)	0.0115 (8)
C9	0.0390 (10)	0.0542 (12)	0.0437 (11)	0.0151 (9)	0.0142 (8)	0.0192 (9)
C10	0.0378 (10)	0.0538 (13)	0.0434 (11)	0.0019 (9)	0.0022 (9)	0.0091 (10)
C11	0.0384 (10)	0.0386 (11)	0.0479 (11)	−0.0021 (8)	0.0075 (8)	0.0095 (9)
N5	0.0372 (9)	0.0424 (9)	0.0494 (10)	−0.0069 (7)	0.0029 (7)	0.0230 (8)
N12	0.0689 (12)	0.0380 (10)	0.0583 (11)	0.0180 (9)	0.0324 (10)	0.0162 (9)
O3	0.0497 (8)	0.0513 (9)	0.0454 (8)	−0.0002 (7)	0.0041 (6)	0.0257 (7)
O4	0.0506 (8)	0.0392 (8)	0.0468 (8)	−0.0013 (6)	0.0087 (6)	0.0006 (7)
O13	0.0925 (14)	0.0541 (11)	0.0904 (14)	0.0316 (10)	0.0319 (12)	0.0393 (11)
O14	0.1008 (15)	0.0382 (9)	0.0638 (11)	−0.0025 (9)	0.0188 (10)	0.0045 (8)
S2	0.0367 (3)	0.0330 (3)	0.0339 (3)	−0.00126 (19)	0.0055 (2)	0.00977 (19)

Geometric parameters (Å, °)

C1—S2	1.747 (2)	C9—C10	1.387 (3)
C1—H1A	0.9600	C9—H9	0.93 (3)
C1—H1B	0.9600	C10—C11	1.376 (3)
C1—H1C	0.9600	C10—H10	0.91 (3)
C6—C7	1.382 (3)	C11—H11	1.00 (3)
C6—C11	1.387 (3)	N5—S2	1.6293 (17)
C6—N5	1.411 (2)	N5—H5N	0.849 (10)
C7—C8	1.380 (3)	N12—O14	1.216 (3)
C7—H7	0.94 (3)	N12—O13	1.221 (3)
C8—C9	1.375 (3)	O3—S2	1.4351 (15)
C8—N12	1.472 (3)	O4—S2	1.4254 (15)
S2—C1—H1A	109.5	C11—C10—C9	120.5 (2)
S2—C1—H1B	109.5	C11—C10—H10	121.6 (19)
H1A—C1—H1B	109.5	C9—C10—H10	117.9 (19)
S2—C1—H1C	109.5	C10—C11—C6	120.6 (2)
H1A—C1—H1C	109.5	C10—C11—H11	121.9 (15)
H1B—C1—H1C	109.5	C6—C11—H11	117.4 (15)
C7—C6—C11	120.16 (19)	C6—N5—S2	126.27 (13)
C7—C6—N5	122.12 (17)	C6—N5—H5N	116.1 (19)
C11—C6—N5	117.69 (18)	S2—N5—H5N	111.8 (19)
C8—C7—C6	117.54 (18)	O14—N12—O13	123.6 (2)
C8—C7—H7	120.1 (15)	O14—N12—C8	118.38 (19)
C6—C7—H7	122.1 (15)	O13—N12—C8	118.0 (2)
C9—C8—C7	123.82 (19)	O4—S2—O3	118.55 (9)
C9—C8—N12	118.12 (19)	O4—S2—N5	109.14 (10)
C7—C8—N12	118.06 (19)	O3—S2—N5	104.09 (9)
C8—C9—C10	117.39 (19)	O4—S2—C1	108.26 (10)

C8—C9—H9	118.3 (16)	O3—S2—C1	109.55 (12)
C10—C9—H9	124.3 (16)	N5—S2—C1	106.62 (11)
C11—C6—C7—C8	−0.6 (3)	C7—C6—N5—S2	41.2 (3)
N5—C6—C7—C8	177.35 (18)	C11—C6—N5—S2	−140.83 (19)
C6—C7—C8—C9	−0.2 (3)	C9—C8—N12—O14	176.1 (2)
C6—C7—C8—N12	−179.54 (17)	C7—C8—N12—O14	−4.6 (3)
C7—C8—C9—C10	0.5 (3)	C9—C8—N12—O13	−3.6 (3)
N12—C8—C9—C10	179.83 (19)	C7—C8—N12—O13	175.7 (2)
C8—C9—C10—C11	0.0 (4)	C6—N5—S2—O4	−57.2 (2)
C9—C10—C11—C6	−0.8 (4)	C6—N5—S2—O3	175.34 (19)
C7—C6—C11—C10	1.1 (3)	C6—N5—S2—C1	59.6 (2)
N5—C6—C11—C10	−176.9 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···O3^{i}	0.849 (10)	2.203 (16)	2.984 (2)	153 (3)

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1.

Fig. 1

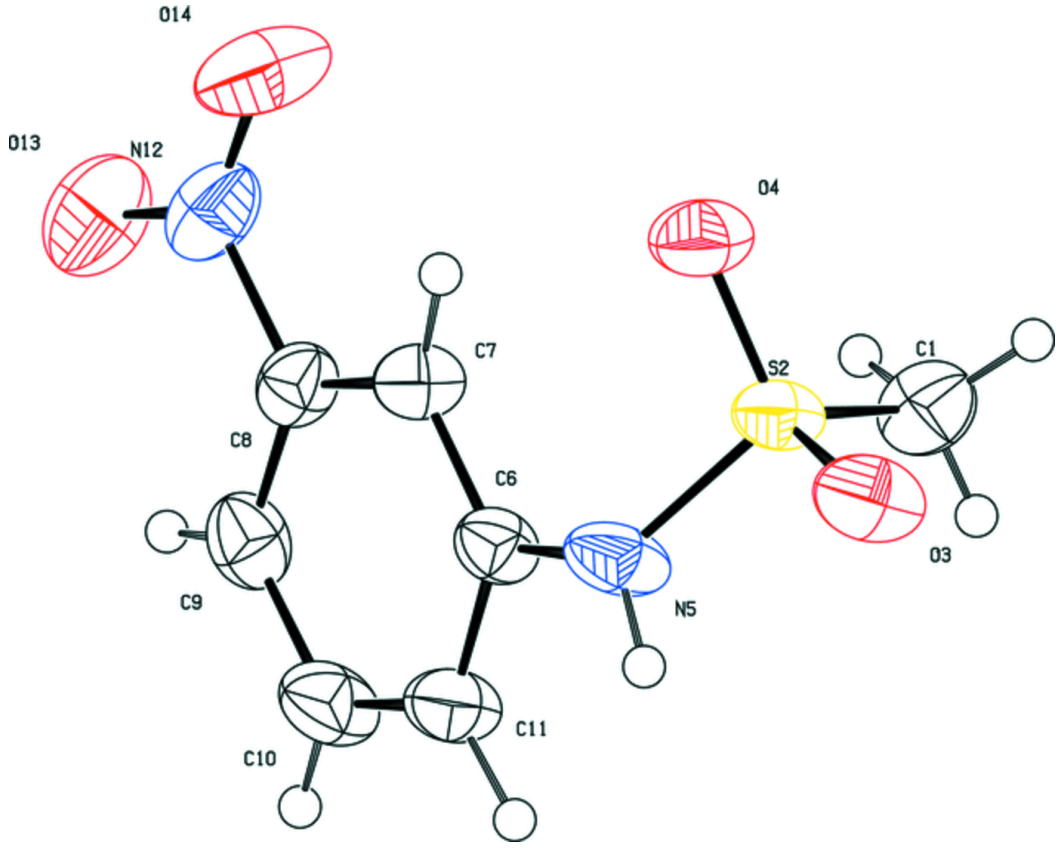

Fig. 2