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N-(4-Fluorophenyl)methanesulfonamide

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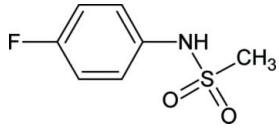
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.010 Å; R factor = 0.097; wR factor = 0.262; data-to-parameter ratio = 15.7.

The structure of the title compound (4FPMSA), $C_7H_8FNO_2S$, closely resembles those of *N*-phenylmethanesulfonamde (PMSA) and other alkyl sulfonanilides. The substitution of either the fluoro, bromo or nitro group at the *para* position of PMSA does not change the space group, unlike in the case of *meta* substitutions in PMSA. The geometric parameters in PMSA, 4FPMSA, 4BPMSA and 4NPMSA are similar except for some difference in the angle S2—N5—C6 and some torsional angles. As in other alkyl sulfonanilides, the amide hydrogen sits alone on one side of the plane of the benzene ring, while the whole methanesulfonyl group is on the opposite side of the plane. It is thus available to a receptor molecule during biological activity. The molecules in the title compound are packed into a layer structure in the *a*-axis direction *via* N—H···O hydrogen bonds [H···O = 2.08 (2), N···O = 2.911 (6) Å and N—H···O = 164 (6)°].

Related literature

For related literature, see: Gowda *et al.* (2007*a*,*b*,*c*); Jayalakshmi & Gowda (2004); Klug (1968); Clark & Reid (1995).



Experimental

Crystal data

$C_7H_8FNO_2S$
M_r = 189.20
Monoclinic, $P2_1/c$
a = 17.272 (3) Å
b = 5.059 (1) Å
c = 10.140 (2) Å
β = 101.65 (1)°
V = 867.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 293 (2) K
0.50 × 0.48 × 0.03 mm

Data collection

Oxford Diffraction Xcalibur Diffractometer with Sapphire CCD detector
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
T_{min} = 0.852, T_{max} = 0.988
4986 measured reflections
1757 independent reflections
1471 reflections with $I > 2\sigma(I)$
R_{int} = 0.087

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.098
$wR(F^2)$ = 0.262
S = 1.20
1757 reflections
112 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 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}	0.859 (10)	2.08 (2)	2.911 (6)	164 (6)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2004); 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* (Sheldrick, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2011).

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supplementary materials

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N-(4-Fluorophenyl)methanesulfonamide

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Comment

The stereochemistry of biologically significant alkyl sulfonanilides, particularly in the vicinity of the phenyl–NH portion is of interest as it helps in explaining their biological activity. In the present work, the structure of *N*-(4-fluorophenyl)-methanesulfonamde (4FPMSA) has been determined (Fig. 1) to explore the substituent effects on the structures of sulphonanilides (Gowda *et al.*, 2007*a*-*c*). The substitution of either the fluoro or nitro group at the *para* position of *N*- (phenyl)-methanesulfonamde (PMSA),(Klug, 1968) does not change the space group (Gowda *et al.*, 2007*a*), unlike in the case of *meta* substitutions in PMSA (Gowda *et al.*, 2007*b,c*). The bond parameters in PMSA, 4FPMSA and *N*-(4-nitrophenyl)-methanesulfonamde (4NPMSA)are similar except some changes in the angle, S2N5C6: 120.0 (1)° (PMSA); 120.2 (3)° (4FPMSA) and 128.1 (3)° (4NPMSA), respectively, and in torsional angles, C1—S2—N5—C6, S2—N5—C6—C7, S2—N5—C6—C11: 62.2 (2)°, 75.5 (2)°, -106.6 (2)° (PMSA); -70.7 (4)°, 102.8 (5)°, -78.1 (6)° (4FPMSA) & -67.2 (4)°, -21.5 (6)%, 158.9 (4)° (4NPMSA), respectively. The amide hydrogen sits 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 that observed in other alkyl sulfonanilides (Gowda *et al.*, 2007*a*-*c*). It is thus available to a receptor molecule during its biological activity. The molecules in the title compound are packed into layer structure (Fig. 2) in the direction of *a* axis *via* N—H···O hydrogen bonds(Table 1).

Experimental

The title compound was prepared according to the literature method (Jayalakshmi & Gowda, 2004). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Jayalakshmi & Gowda, 2004). Single crystals of the title compound were obtained from a slow evaporation of its ethanolic solution and used for X-ray diffraction studies at room temperature.

Refinement

The H atom of the NH group was located in a diffrerence map and its position refined. The carbon-bound H atoms were positioned with idealized geometry and refined using a riding model with C—H = 0.93 Å (CH aromatic) or 0.96 Å (CH_3). Isotropic displacement parameters for all H atoms were set equal to $1.2U_{eq}$ (parent atom).

Figures

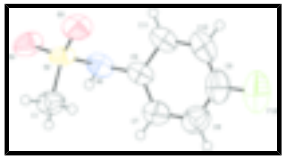

Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

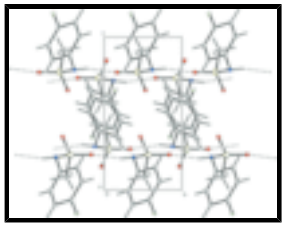

Fig. 2. Hydrogen bonding in the title compound. Hydrogen bonds are shown as dashed lines.

N-(4-Fluorophenyl)methanesulfonamide

Crystal data

$C_7H_8FNO_2S$	F_{000} = 392
M_r = 189.20	D_x = 1.448 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2243 reflections
a = 17.272 (3) Å	θ = 3.6–22.0º
b = 5.059 (1) Å	μ = 0.35 mm^{-1}
c = 10.140 (2) Å	T = 293 (2) K
β = 101.65 (1)º	Plate, colourless
V = 867.8 (3) Å^3	0.50 × 0.48 × 0.03 mm
Z = 4	

Data collection

Oxford Diffraction Xcalibur Diffractometer with Sapphire CCD detector	1757 independent reflections
Radiation source: fine-focus sealed tube	1471 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.087
T = 301(2) K	θ_{max} = 26.4º
Rotation method data acquisition using ω scans	θ_{min} = 4.1º
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2004)	h = −21→21
T_{min} = 0.852, T_{max} = 0.988	k = −6→6
4986 measured reflections	l = −7→12

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.098	$w = 1/[\sigma^2(F_o^2) + (0.1115P)^2 + 1.0115P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.262	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.20	$\Delta\rho_{max}$ = 0.50 e Å^{-3}
1757 reflections	$\Delta\rho_{min}$ = −0.54 e Å^{-3}

112 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Extinction correction: none

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	0.5825 (4)	0.0142 (13)	0.4135 (6)	0.0720 (16)
H1A	0.5800	−0.1721	0.4302	0.086*
H1B	0.5303	0.0880	0.3990	0.086*
H1C	0.6152	0.0981	0.4898	0.086*
C6	0.7729 (3)	−0.0529 (9)	0.3838 (5)	0.0558 (13)
C7	0.7940 (4)	−0.1872 (12)	0.5050 (6)	0.0697 (15)
H7	0.7612	−0.3199	0.5258	0.084*
C8	0.8630 (4)	−0.1275 (15)	0.5955 (7)	0.0833 (19)
H8	0.8784	−0.2233	0.6748	0.100*
C9	0.9079 (4)	0.0773 (16)	0.5645 (8)	0.084 (2)
C10	0.8894 (4)	0.2161 (14)	0.4461 (8)	0.0833 (19)
H10	0.9224	0.3510	0.4283	0.100*
C11	0.8209 (4)	0.1538 (12)	0.3523 (7)	0.0716 (16)
H11	0.8073	0.2459	0.2716	0.086*
N5	0.7032 (3)	−0.1189 (9)	0.2855 (5)	0.0605 (12)
H5N	0.683 (3)	−0.271 (6)	0.294 (6)	0.073*
O3	0.6484 (3)	0.3356 (7)	0.2684 (4)	0.0803 (13)
O4	0.5695 (3)	−0.0318 (8)	0.1535 (4)	0.0776 (13)
F12	0.9756 (3)	0.1488 (12)	0.6532 (6)	0.1259 (18)
S2	0.62315 (9)	0.0664 (2)	0.26953 (12)	0.0555 (5)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.082 (4)	0.076 (4)	0.063 (3)	0.015 (3)	0.029 (3)	0.007 (3)
C6	0.070 (3)	0.040 (3)	0.064 (3)	−0.002 (2)	0.032 (3)	−0.009 (2)
C7	0.079 (4)	0.061 (4)	0.073 (4)	0.000 (3)	0.026 (3)	0.004 (3)
C8	0.089 (5)	0.089 (5)	0.073 (4)	0.013 (4)	0.019 (4)	0.002 (3)

C9	0.062 (4)	0.096 (5)	0.094 (5)	0.010 (3)	0.017 (3)	−0.030 (4)
C10	0.068 (4)	0.077 (4)	0.113 (5)	−0.011 (3)	0.036 (4)	−0.018 (4)
C11	0.076 (4)	0.063 (4)	0.083 (4)	−0.014 (3)	0.034 (3)	−0.002 (3)
N5	0.079 (3)	0.041 (2)	0.069 (3)	−0.008 (2)	0.031 (2)	−0.010 (2)
O3	0.107 (3)	0.0325 (19)	0.096 (3)	−0.012 (2)	0.008 (3)	0.0096 (19)
O4	0.112 (3)	0.063 (3)	0.049 (2)	−0.018 (2)	−0.004 (2)	−0.0031 (17)
F12	0.077 (3)	0.160 (5)	0.132 (4)	0.001 (3)	0.002 (3)	−0.043 (3)
S2	0.0833 (10)	0.0364 (7)	0.0463 (7)	−0.0082 (6)	0.0115 (6)	0.0026 (5)

Geometric parameters (Å, °)

C1—S2	1.763 (5)	C8—H8	0.9300
C1—H1A	0.9600	C9—C10	1.371 (10)
C1—H1B	0.9600	C9—F12	1.372 (8)
C1—H1C	0.9600	C10—C11	1.397 (9)
C6—C7	1.387 (8)	C10—H10	0.9300
C6—C11	1.410 (7)	C11—H11	0.9300
C6—N5	1.439 (7)	N5—S2	1.651 (5)
C7—C8	1.383 (9)	N5—H5N	0.859 (10)
C7—H7	0.9300	O3—S2	1.431 (4)
C8—C9	1.368 (10)	O4—S2	1.432 (4)
S2—C1—H1A	109.5	C10—C9—F12	117.1 (7)
S2—C1—H1B	109.5	C9—C10—C11	119.7 (6)
H1A—C1—H1B	109.5	C9—C10—H10	120.1
S2—C1—H1C	109.5	C11—C10—H10	120.1
H1A—C1—H1C	109.5	C10—C11—C6	118.0 (6)
H1B—C1—H1C	109.5	C10—C11—H11	121.0
C7—C6—C11	120.2 (6)	C6—C11—H11	121.0
C7—C6—N5	122.3 (5)	C6—N5—S2	120.2 (3)
C11—C6—N5	117.6 (5)	C6—N5—H5N	116 (4)
C8—C7—C6	121.2 (6)	S2—N5—H5N	100 (4)
C8—C7—H7	119.4	O3—S2—O4	118.2 (3)
C6—C7—H7	119.4	O3—S2—N5	106.9 (3)
C9—C8—C7	117.7 (7)	O4—S2—N5	105.9 (3)
C9—C8—H8	121.1	O3—S2—C1	108.8 (3)
C7—C8—H8	121.1	O4—S2—C1	109.2 (3)
C8—C9—C10	123.2 (7)	N5—S2—C1	107.4 (3)
C8—C9—F12	119.7 (8)		
C11—C6—C7—C8	−1.8 (9)	C7—C6—C11—C10	0.2 (8)
N5—C6—C7—C8	177.3 (5)	N5—C6—C11—C10	−178.8 (5)
C6—C7—C8—C9	3.1 (9)	C7—C6—N5—S2	102.8 (5)
C7—C8—C9—C10	−3.1 (10)	C11—C6—N5—S2	−78.1 (6)
C7—C8—C9—F12	178.0 (5)	C6—N5—S2—O3	45.9 (4)
C8—C9—C10—C11	1.6 (10)	C6—N5—S2—O4	172.7 (4)
F12—C9—C10—C11	−179.4 (5)	C6—N5—S2—C1	−70.7 (4)
C9—C10—C11—C6	−0.1 (9)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···O3^{i}	0.859 (10)	2.08 (2)	2.911 (6)	164 (6)

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1

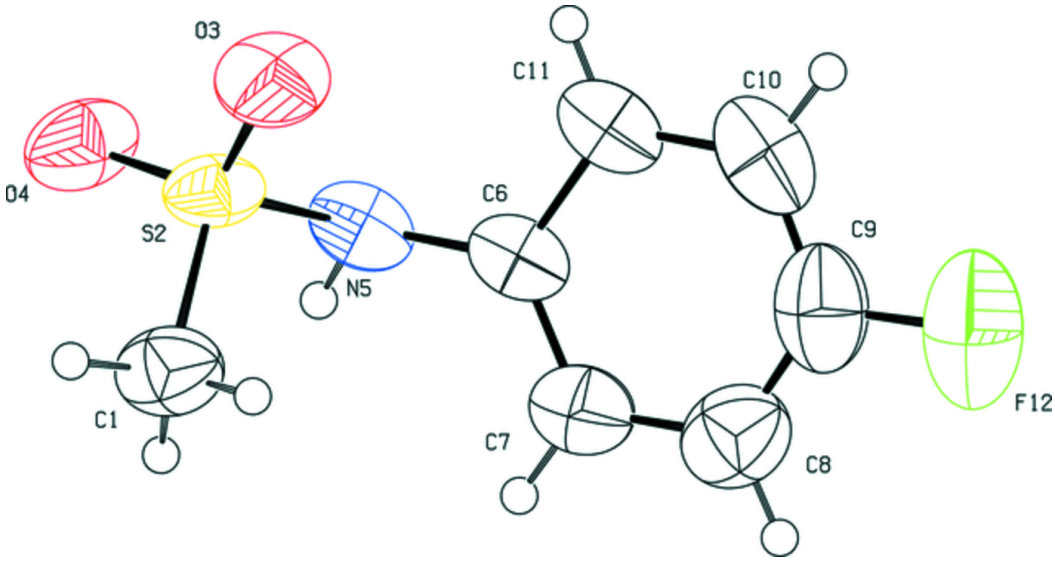

Fig. 2