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N-(2-Methoxyphenyl)-4-methylbenzenesulfonamide

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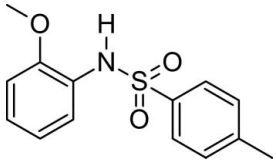
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.050; wR factor = 0.143; data-to-parameter ratio = 19.4.

In the title compound, $C_{14}H_{15}NO_3S$, the geometry around the S atom of the SO_2 group is distorted tetrahedral. The methoxy- and methyl-substituted aromatic rings are oriented at a dihedral angle of 71.39 (9)°. Intermolecular N—H···O hydrogen bonds form inversion dimers, which stabilize the crystal structure.

Related literature

For the antimicrobial activity of sulfonamide compounds, see: Gao & Pederson (2005). For a related thiazine molecule, see: Arshad *et al.* (2010). For a related structure, see: Aziz-ur-Rehman *et al.* (2010). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{14}H_{15}NO_3S$
M_r = 277.33
Orthorhombic, *Pbca*
a = 12.7395 (9) Å
b = 11.4906 (6) Å
c = 18.6968 (10) Å
V = 2736.9 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 296 K
0.42 × 0.33 × 0.21 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.906, T_{max} = 0.951
13798 measured reflections
3376 independent reflections
1313 reflections with $I > 2\sigma(I)$
R_{int} = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.143
S = 0.91
3376 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O2^{i}	0.84	2.35	3.112 (3)	151

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5047).

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supporting information

Acta Cryst. (2010). E**66**, o2976 [https://doi.org/10.1107/S1600536810042984]

N-(2-Methoxyphenyl)-4-methylbenzenesulfonamide

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S1. Comment

Sulfonamide compounds are well known as antimicrobial agents (Gao & Pederson, 2005). The structure reported here is a precursor used in the synthesis of thiazine heterocycles (Arshad *et al.*, 2010).

The bond lengths and angles in the title compound are similar to those observed in the recently published *N*-(2-methoxyphenyl)benzenesulfonamide (II) (Aziz-ur-Rehman *et al.*, 2010). The two aromatic rings (C1/C2/C3/C4/C5/C6) and C7/C8/C9/C10/C11/C12) are oriented at dihedral angles of 71.39 (0.09)° unlike the dihedral angles observed for the two independent molecules in II. Similarly the torsion angle C—S—N(H)—C is -56.5 (3) compared with 67.25 (15)° in molecule A and -81.17 (16)° in molecule B of (II). Inversion related intermolecular N—H···O hydrogen bonds form dimers and generate an eight-membered $R_2^2(8)$ ring motif (Bernstein *et al.*, 1995) Table. 1, Fig. 2.

S2. Experimental

A mixture of *para* toluenesulfonyl chloride (0.00104 mol; 0.200 g), *o*-anisidine (0.00104 mol; 0.128 g), was stirred in 10–15 ml of distilled water, while maintaining pH of the reaction mixture at 8–10 using 3% sodium carbonate. The progress of the reaction was checked by TLC. On completion of reaction the precipitates obtained were filtered, washed with water and finally dried. Suitable crystals for X-Ray analysis were grown from DCM (dichloromethane) by slow evaporation.

S3. Refinement

All the C—H and H-atoms were positioned with idealized geometry with C—H = 0.93 Å for aromatic C—H = 0.96 Å and were refined using a riding model with U_{iso}(H) = 1.2 U_{eq}(C) for aromatic, with U_{iso}(H) = 1.5 U_{eq}(C) for methyl. The N–H H atom was fixed in its found position with U_{iso}(H) = 1.2 U_{eq}(N).

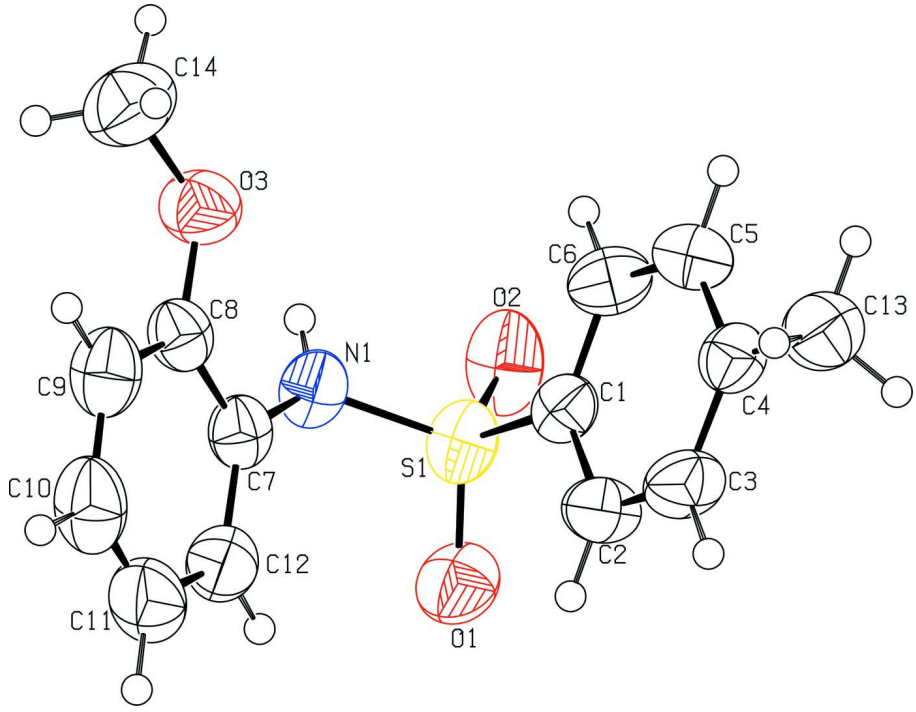

Figure 1

The molecular structure of (I) showing 50% displacement ellipsoids.

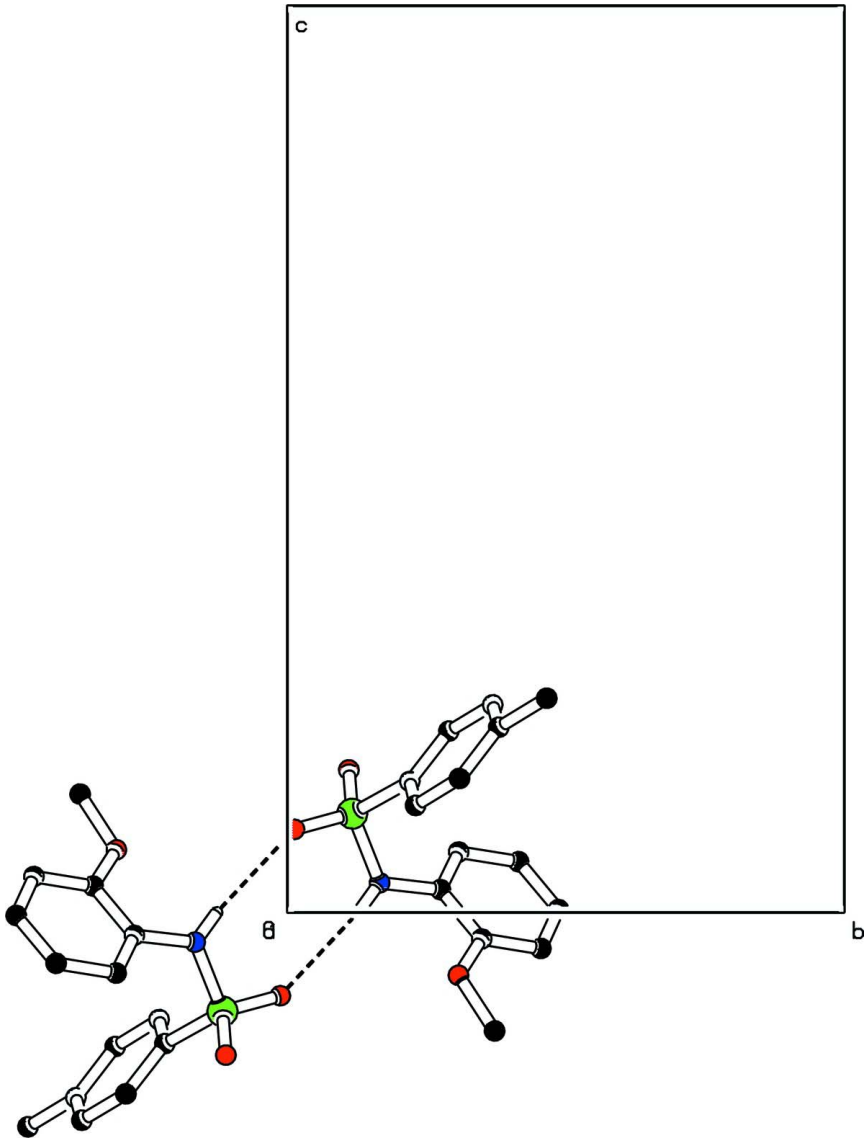

Figure 2

Inversion dimers formed through N—H···O hydrogen bonds drawn as dashed lines.

N-(2-Methoxyphenyl)-4-methylbenzenesulfonamide

Crystal data

$C_{14}H_{15}NO_3S$
$M_r = 277.33$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.7395\ (9)$ Å
$b = 11.4906\ (6)$ Å
$c = 18.6968\ (10)$ Å
$V = 2736.9\ (3)$ Å^3
$Z = 8$

$F(000) = 1168$
$D_x = 1.346$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1013 reflections
$\theta = 3.2–19.2°$
$\mu = 0.24$ mm^{-1}
$T = 296$ K
Needle, light brown
0.42 × 0.33 × 0.21 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.906, T_{max} = 0.951
13798 measured reflections
3376 independent reflections
1313 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
θ_{max} = 28.3°, θ_{min} = 3.2°
h = −16→10
k = −11→15
l = −24→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.143
S = 0.91
3376 reflections
174 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
S1	0.51740 (7)	0.61649 (6)	0.39096 (4)	0.0571 (3)
O1	0.60405 (18)	0.61039 (18)	0.34278 (11)	0.0706 (7)
N1	0.55946 (19)	0.6656 (2)	0.46723 (12)	0.0529 (7)
C1	0.4303 (2)	0.7199 (2)	0.35541 (14)	0.0465 (7)
O2	0.46120 (19)	0.51265 (17)	0.40827 (11)	0.0751 (7)
C2	0.4619 (3)	0.7899 (3)	0.30004 (16)	0.0584 (8)
H2	0.5298	0.7842	0.2822	0.070*
O3	0.49484 (18)	0.80720 (18)	0.56921 (11)	0.0662 (6)
C3	0.3924 (3)	0.8688 (3)	0.27103 (16)	0.0607 (9)
H3	0.4146	0.9162	0.2337	0.073*
C4	0.2908 (3)	0.8796 (2)	0.29578 (15)	0.0510 (8)
C5	0.2613 (3)	0.8091 (3)	0.35213 (17)	0.0598 (9)
H5	0.1935	0.8150	0.3703	0.072*
H1N	0.5306	0.6270	0.4999	0.072*
C6	0.3298 (3)	0.7303 (3)	0.38188 (16)	0.0610 (9)
H6	0.3082	0.6839	0.4199	0.073*

C7	0.6101 (2)	0.7748 (2)	0.47481 (15)	0.0481 (8)
C8	0.5756 (2)	0.8488 (2)	0.52917 (16)	0.0491 (8)
C9	0.6239 (3)	0.9550 (3)	0.53963 (18)	0.0650 (9)
H9	0.6006	1.0047	0.5755	0.078*
C10	0.7065 (3)	0.9868 (3)	0.4967 (2)	0.0742 (11)
H10	0.7391	1.0583	0.5038	0.089*
C11	0.7412 (3)	0.9152 (3)	0.4440 (2)	0.0766 (11)
H11	0.7969	0.9380	0.4151	0.092*
C12	0.6934 (3)	0.8076 (3)	0.43331 (16)	0.0629 (9)
H12	0.7182	0.7579	0.3979	0.075*
C13	0.2160 (3)	0.9656 (3)	0.26372 (17)	0.0697 (10)
H13A	0.2137	0.9552	0.2128	0.105*
H13B	0.2391	1.0432	0.2745	0.105*
H13C	0.1472	0.9536	0.2833	0.105*
C14	0.4637 (3)	0.8720 (3)	0.63051 (18)	0.0889 (12)
H14A	0.4396	0.9476	0.6159	0.133*
H14B	0.5224	0.8804	0.6623	0.133*
H14C	0.4079	0.8318	0.6547	0.133*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0728 (6)	0.0410 (5)	0.0575 (5)	0.0023 (4)	−0.0082 (5)	−0.0047 (4)
O1	0.0764 (17)	0.0696 (16)	0.0659 (14)	0.0201 (12)	0.0028 (13)	−0.0123 (12)
N1	0.0685 (19)	0.0410 (14)	0.0491 (14)	−0.0108 (13)	−0.0068 (13)	0.0069 (12)
C1	0.057 (2)	0.0393 (17)	0.0436 (16)	−0.0066 (15)	0.0000 (15)	−0.0013 (14)
O2	0.104 (2)	0.0370 (12)	0.0845 (16)	−0.0171 (12)	−0.0261 (14)	0.0047 (11)
C2	0.051 (2)	0.064 (2)	0.0603 (19)	0.0033 (17)	0.0091 (17)	0.0070 (17)
O3	0.0647 (17)	0.0638 (14)	0.0700 (14)	−0.0036 (12)	0.0084 (12)	−0.0086 (12)
C3	0.067 (2)	0.064 (2)	0.0515 (19)	0.0029 (19)	0.0090 (18)	0.0179 (17)
C4	0.056 (2)	0.0500 (19)	0.0469 (18)	0.0010 (16)	−0.0005 (16)	−0.0061 (16)
C5	0.051 (2)	0.063 (2)	0.065 (2)	−0.0016 (17)	0.0114 (17)	0.0007 (18)
C6	0.070 (3)	0.057 (2)	0.0552 (19)	−0.0038 (18)	0.0124 (19)	0.0129 (17)
C7	0.052 (2)	0.0433 (18)	0.0492 (18)	−0.0005 (16)	−0.0084 (16)	0.0078 (15)
C8	0.047 (2)	0.046 (2)	0.0543 (18)	−0.0001 (16)	−0.0065 (16)	0.0053 (15)
C9	0.078 (3)	0.050 (2)	0.066 (2)	−0.007 (2)	−0.014 (2)	−0.0039 (18)
C10	0.084 (3)	0.060 (2)	0.079 (2)	−0.024 (2)	−0.022 (2)	0.010 (2)
C11	0.072 (3)	0.086 (3)	0.072 (3)	−0.028 (2)	−0.007 (2)	0.020 (2)
C12	0.065 (2)	0.069 (2)	0.055 (2)	−0.0093 (19)	−0.0024 (18)	0.0010 (18)
C13	0.068 (3)	0.075 (2)	0.066 (2)	0.015 (2)	0.0018 (19)	0.0041 (18)
C14	0.098 (3)	0.100 (3)	0.069 (2)	0.005 (2)	0.012 (2)	−0.011 (2)

Geometric parameters (Å, º)

S1—O1	1.426 (2)	C6—H6	0.9300
S1—O2	1.429 (2)	C7—C12	1.368 (4)
S1—N1	1.625 (2)	C7—C8	1.396 (4)
S1—C1	1.756 (3)	C8—C9	1.381 (4)

N1—C7	1.418 (3)	C9—C10	1.373 (5)
N1—H1N	0.8394	C9—H9	0.9300
C1—C2	1.371 (4)	C10—C11	1.357 (5)
C1—C6	1.378 (4)	C10—H10	0.9300
C2—C3	1.378 (4)	C11—C12	1.393 (4)
C2—H2	0.9300	C11—H11	0.9300
O3—C8	1.359 (3)	C12—H12	0.9300
O3—C14	1.424 (3)	C13—H13A	0.9600
C3—C4	1.379 (4)	C13—H13B	0.9600
C3—H3	0.9300	C13—H13C	0.9600
C4—C5	1.382 (4)	C14—H14A	0.9600
C4—C13	1.498 (4)	C14—H14B	0.9600
C5—C6	1.375 (4)	C14—H14C	0.9600
C5—H5	0.9300		

O1—S1—O2	119.32 (14)	C12—C7—N1	122.7 (3)
O1—S1—N1	108.43 (13)	C8—C7—N1	117.9 (3)
O2—S1—N1	104.86 (12)	O3—C8—C9	124.8 (3)
O1—S1—C1	106.45 (14)	O3—C8—C7	115.1 (3)
O2—S1—C1	109.52 (15)	C9—C8—C7	120.1 (3)
N1—S1—C1	107.79 (13)	C10—C9—C8	119.6 (3)
C7—N1—S1	123.03 (19)	C10—C9—H9	120.2
C7—N1—H1N	126.5	C8—C9—H9	120.2
S1—N1—H1N	108.1	C11—C10—C9	120.9 (3)
C2—C1—C6	119.5 (3)	C11—C10—H10	119.6
C2—C1—S1	119.8 (3)	C9—C10—H10	119.6
C6—C1—S1	120.6 (2)	C10—C11—C12	120.0 (4)
C1—C2—C3	119.7 (3)	C10—C11—H11	120.0
C1—C2—H2	120.2	C12—C11—H11	120.0
C3—C2—H2	120.2	C7—C12—C11	120.1 (3)
C8—O3—C14	118.1 (3)	C7—C12—H12	119.9
C2—C3—C4	122.0 (3)	C11—C12—H12	119.9
C2—C3—H3	119.0	C4—C13—H13A	109.5
C4—C3—H3	119.0	C4—C13—H13B	109.5
C3—C4—C5	117.3 (3)	H13A—C13—H13B	109.5
C3—C4—C13	121.4 (3)	C4—C13—H13C	109.5
C5—C4—C13	121.2 (3)	H13A—C13—H13C	109.5
C6—C5—C4	121.4 (3)	H13B—C13—H13C	109.5
C6—C5—H5	119.3	O3—C14—H14A	109.5
C4—C5—H5	119.3	O3—C14—H14B	109.5
C5—C6—C1	120.1 (3)	H14A—C14—H14B	109.5
C5—C6—H6	120.0	O3—C14—H14C	109.5
C1—C6—H6	120.0	H14A—C14—H14C	109.5
C12—C7—C8	119.3 (3)	H14B—C14—H14C	109.5

O1—S1—N1—C7	58.3 (3)	C2—C1—C6—C5	1.0 (5)
O2—S1—N1—C7	−173.2 (2)	S1—C1—C6—C5	−178.0 (2)
C1—S1—N1—C7	−56.5 (3)	S1—N1—C7—C12	−51.4 (4)

O1—S1—C1—C2	−11.4 (3)	S1—N1—C7—C8	131.6 (2)
O2—S1—C1—C2	−141.7 (2)	C14—O3—C8—C9	−6.2 (4)
N1—S1—C1—C2	104.7 (2)	C14—O3—C8—C7	173.0 (3)
O1—S1—C1—C6	167.6 (2)	C12—C7—C8—O3	−177.7 (3)
O2—S1—C1—C6	37.3 (3)	N1—C7—C8—O3	−0.6 (4)
N1—S1—C1—C6	−76.3 (3)	C12—C7—C8—C9	1.5 (4)
C6—C1—C2—C3	−0.7 (4)	N1—C7—C8—C9	178.6 (3)
S1—C1—C2—C3	178.3 (2)	O3—C8—C9—C10	178.5 (3)
C1—C2—C3—C4	−0.3 (5)	C7—C8—C9—C10	−0.6 (5)
C2—C3—C4—C5	1.0 (5)	C8—C9—C10—C11	0.1 (5)
C2—C3—C4—C13	−179.9 (3)	C9—C10—C11—C12	−0.5 (6)
C3—C4—C5—C6	−0.7 (5)	C8—C7—C12—C11	−1.8 (5)
C13—C4—C5—C6	−179.8 (3)	N1—C7—C12—C11	−178.9 (3)
C4—C5—C6—C1	−0.3 (5)	C10—C11—C12—C7	1.3 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O2^{i}	0.84	2.35	3.112 (3)	151

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