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N-(4-Chlorophenyl)-2,4-dimethylbenzenesulfonamide

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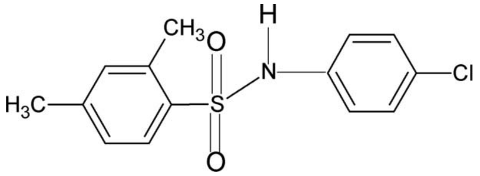
Key indicators: single-crystal X-ray study; *T* = 293 K; mean σ(C–C) = 0.004 Å; *R* factor = 0.049; *wR* factor = 0.121; data-to-parameter ratio = 16.6.

Molecules of the title compound, $C_{14}H_{14}ClNO_2S$, are bent at the S atom with a $C-SO_2-NH-C$ torsion angle of 57.7 (2)°. The benzene rings are rotated relative to each other by 68.1 (1)°. In the crystal, N—H···O(S) hydrogen bonds pack the molecules into infinite chains parallel to the *b* axis.

Related literature

For the hydrogen-bonding preferences of sulfonamides, see: Adsmond & Grant (2001). For studies on the effects of substituents on the structures and other aspects of *N*-(aryl)-amides, see: Arjunan *et al.* (2004); Gowda *et al.* (1999); for *N*-(aryl)-methanesulfonamides, see: Gowda *et al.* (2007); and for *N*-(aryl)-arylsulfonamides, see: Gelbrich *et al.* (2007); Gowda *et al.* (2010); Perlovich *et al.* (2006); Shakuntala *et al.* (2011). For the preparation of the title compound, see: Savitha & Gowda (2006).



Experimental

Crystal data

$C_{14}H_{14}ClNO_2S$
M_r = 295.77
Monoclinic, $P2_1/c$
a = 9.1093 (8) Å
b = 9.9106 (9) Å
c = 16.142 (1) Å
β = 96.505 (9)°
V = 1447.9 (2) Å^3
Z = 4
Mo *K*α radiation
μ = 0.41 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.888, T_{max} = 0.961
5342 measured reflections
2934 independent reflections
2219 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.121
S = 1.08
2934 reflections
177 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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}	0.83 (2)	2.08 (2)	2.891 (4)	166 (3)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); 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: BT5589).

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supplementary materials

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N-(4-Chlorophenyl)-2,4-dimethylbenzenesulfonamide

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Comment

The amide and sulfonamide moieties are the constituents of many biologically significant compounds. The hydrogen bonding preferences of sulfonamides have been investigated (Adsmond & Grant, 2001). As part of our work on the substituent effects on the structures and other aspects of *N*-(aryl)-amides (Arjunan *et al.*, 2004; Gowda *et al.*, 1999), *N*-(aryl)-methanesulfonamides (Gowda *et al.*, 2007) and *N*-(aryl)-arylsulfonamides (Gowda *et al.*, 2010; Shakuntala *et al.*, 2011), in the present work, the crystal structure of *N*-(4-chlorophenyl)-2,4-dimethylbenzenesulfonamide (I) has been determined (Fig. 1). The N—C bond in the C—SO_2—NH—C segment has *gauche* torsions with respect to the S═O bonds. The molecule is bent at the S atom with the C1—SO_2—NH—C7 torsion angle of 57.7 (2)°, compared to the values of -54.9 (2)° in *N*-(2-chlorophenyl)- 2,4-dimethylbenzenesulfonamide (II)(Gowda *et al.*, 2010) and 44.6 (2)° in *N*-(3-chlorophenyl)-2,4-dimethylbenzenesulfonamide (III) (Shakuntala *et al.*, 2011).

The two benzene rings in (I) are tilted relative to each other by 68.1 (1)°, compared to the value of 66.2 (1)° (II) and 75.7 (1)° in (III). The other bond parameters in (I) are similar to those observed in (II), (III) and other aryl sulfonamides (Perlovich *et al.*, 2006; Gelbrich *et al.*, 2007).

The crystal packing of molecules in (I) *via* N—H···O(S) hydrogen bonds (Table 1) is shown in Fig.2.

Experimental

The solution of 1,3-xylene (1,3-dimethylbenzene) (10 ml) in chloroform (40 ml) was treated dropwise with chlorosulfonic acid (25 ml) at 0 ° C. After the initial evolution of hydrogen chloride subsided, the reaction mixture was brought to room temperature and poured into crushed ice in a beaker. The chloroform layer was separated, washed with cold water and allowed to evaporate slowly. The residual 2,4-dimethylbenzenesulfonylchloride was treated with 4-chloroaniline in the stoichiometric ratio and boiled for ten minutes. The reaction mixture was then cooled to room temperature and added to ice cold water (100 cc). The resultant solid *N*-(4-chlorophenyl)-2,4-dimethylbenzenesulfonamide was filtered under suction and washed thoroughly with cold water. It was then recrystallized to constant melting point from dilute ethanol. The purity of the compound was checked and characterized by recording its infrared and NMR spectra (Savitha & Gowda, 2006).

The prism like colourless single crystals used in X-ray diffraction studies were grown in ethanolic solution by a slow evaporation at room temperature.

Refinement

The H atom of the NH group was located in a difference map and later restrained to the distance N—H = 0.86 (2) Å. The other H atoms were positioned with idealized geometry using a riding model with the aromatic C—H = 0.93Å and methyl C—H = 0.96 Å and with isotropic displacement parameters set at $1.2U_{eq}$(C-aromatic, N) and $1.5U_{eq}$(C-methyl).

Figures

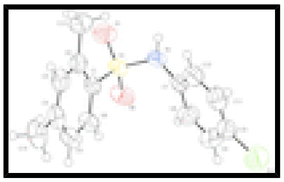

Fig. 1. Molecular structure of (I), showing the atom labelling scheme and displacement ellipsoids are drawn at the 50% probability level.

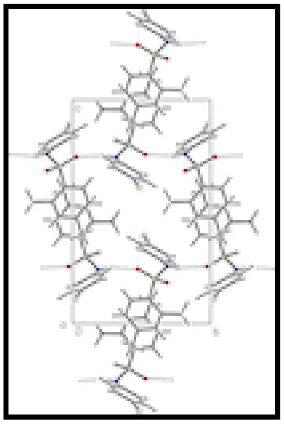

Fig. 2. Molecular packing of (I) with hydrogen bonding shown as dashed lines.

N-(4-Chlorophenyl)-2,4-dimethylbenzenesulfonamide

Crystal data

$C_{14}H_{14}ClNO_2S$	$F(000) = 616$
$M_r = 295.77$	$D_x = 1.357$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2044 reflections
$a = 9.1093$ (8) Å	$\theta = 2.5$–27.7°
$b = 9.9106$ (9) Å	$\mu = 0.41$ mm^{-1}
$c = 16.142$ (1) Å	$T = 293$ K
$\beta = 96.505$ (9)°	Prism, colourless
$V = 1447.9$ (2) Å^3	0.30 × 0.20 × 0.10 mm
$Z = 4$	

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector	2934 independent reflections
Radiation source: fine-focus sealed tube	2219 reflections with $I > 2\sigma(I)$
graphite	$R_{\text{int}} = 0.013$
Rotation method data acquisition using ω and φ scans	$\theta_{\text{max}} = 26.4°$, $\theta_{\text{min}} = 2.5°$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)	$h = -7 \rightarrow 11$
$T_{\text{min}} = 0.888$, $T_{\text{max}} = 0.961$	$k = -8 \rightarrow 12$
5342 measured reflections	$l = -20 \rightarrow 19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.049$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.121$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.08$	$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.9349P]$ where $P = (F_o^2 + 2F_c^2)/3$
2934 reflections	$(\Delta/\sigma)_{max} = 0.002$
177 parameters	$\Delta\rho_{max} = 0.28$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.32$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > \sigma(F^2)$ 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	0.6057 (3)	0.0526 (2)	0.39055 (15)	0.0469 (6)
C2	0.6430 (3)	0.1450 (3)	0.45485 (16)	0.0542 (6)
C3	0.7412 (3)	0.1003 (3)	0.52140 (17)	0.0641 (7)
H3	0.7676	0.1602	0.5649	0.077*
C4	0.8019 (3)	−0.0276 (3)	0.52681 (17)	0.0618 (7)
C5	0.7618 (3)	−0.1160 (3)	0.46227 (19)	0.0643 (7)
H5	0.8004	−0.2029	0.4644	0.077*
C6	0.6650 (3)	−0.0771 (3)	0.39452 (18)	0.0575 (7)
H6	0.6392	−0.1377	0.3513	0.069*
C7	0.7258 (3)	0.1399 (2)	0.21393 (14)	0.0458 (6)
C8	0.7325 (4)	0.0198 (3)	0.1716 (2)	0.0709 (8)
H8	0.6500	−0.0361	0.1639	0.085*
C9	0.8622 (4)	−0.0178 (3)	0.1404 (2)	0.0817 (10)
H9	0.8674	−0.0994	0.1125	0.098*
C10	0.9820 (4)	0.0654 (3)	0.15092 (19)	0.0696 (8)
C11	0.9774 (3)	0.1839 (3)	0.19339 (18)	0.0685 (8)
H11	1.0600	0.2396	0.2006	0.082*

C12	0.8494 (3)	0.2206 (3)	0.22558 (16)	0.0587 (7)
H12	0.8465	0.3006	0.2554	0.070*
C13	0.5833 (4)	0.2867 (3)	0.4561 (2)	0.0760 (9)
H13A	0.4795	0.2838	0.4616	0.091*
H13B	0.5985	0.3316	0.4050	0.091*
H13C	0.6338	0.3351	0.5023	0.091*
C14	0.9094 (4)	−0.0683 (4)	0.6002 (2)	0.0841 (10)
H14A	0.8563	−0.1060	0.6428	0.101*
H14B	0.9637	0.0094	0.6218	0.101*
H14C	0.9766	−0.1344	0.5829	0.101*
N1	0.5919 (2)	0.1852 (2)	0.24225 (13)	0.0504 (5)
H1N	0.587 (3)	0.2672 (18)	0.2515 (16)	0.061*
O1	0.3758 (2)	0.18577 (19)	0.31728 (13)	0.0667 (5)
O2	0.4524 (2)	−0.02597 (17)	0.25512 (12)	0.0638 (5)
Cl1	1.14202 (12)	0.01793 (12)	0.10872 (7)	0.1119 (4)
S1	0.49106 (7)	0.09643 (6)	0.29924 (4)	0.04969 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0499 (14)	0.0414 (12)	0.0497 (14)	−0.0080 (10)	0.0070 (11)	0.0040 (11)
C2	0.0632 (16)	0.0511 (14)	0.0504 (14)	−0.0098 (12)	0.0154 (12)	−0.0028 (12)
C3	0.0742 (18)	0.073 (2)	0.0456 (14)	−0.0171 (16)	0.0078 (13)	−0.0035 (14)
C4	0.0549 (16)	0.078 (2)	0.0523 (15)	−0.0122 (15)	0.0074 (12)	0.0172 (15)
C5	0.0646 (17)	0.0546 (16)	0.0729 (19)	0.0027 (14)	0.0044 (14)	0.0148 (15)
C6	0.0664 (17)	0.0424 (14)	0.0621 (16)	−0.0032 (12)	0.0006 (13)	0.0024 (12)
C7	0.0602 (15)	0.0353 (12)	0.0405 (12)	0.0029 (11)	0.0000 (11)	0.0061 (10)
C8	0.079 (2)	0.0476 (16)	0.088 (2)	−0.0072 (14)	0.0195 (17)	−0.0116 (15)
C9	0.104 (3)	0.0538 (18)	0.092 (2)	0.0131 (18)	0.032 (2)	−0.0058 (17)
C10	0.0696 (19)	0.076 (2)	0.0644 (18)	0.0251 (17)	0.0137 (15)	0.0246 (16)
C11	0.0613 (18)	0.081 (2)	0.0620 (17)	−0.0025 (16)	0.0021 (14)	0.0097 (16)
C12	0.0706 (18)	0.0540 (16)	0.0496 (15)	−0.0057 (14)	−0.0011 (13)	−0.0013 (12)
C13	0.100 (2)	0.0541 (18)	0.074 (2)	−0.0043 (16)	0.0123 (18)	−0.0156 (15)
C14	0.0680 (19)	0.114 (3)	0.0679 (19)	−0.0132 (19)	−0.0022 (16)	0.0274 (19)
N1	0.0649 (13)	0.0290 (10)	0.0575 (13)	0.0021 (10)	0.0074 (10)	0.0023 (9)
O1	0.0522 (11)	0.0563 (11)	0.0919 (14)	0.0044 (9)	0.0100 (10)	0.0039 (10)
O2	0.0695 (12)	0.0422 (10)	0.0751 (13)	−0.0126 (9)	−0.0118 (10)	−0.0014 (9)
Cl1	0.0955 (7)	0.1262 (9)	0.1214 (8)	0.0489 (6)	0.0447 (6)	0.0358 (7)
S1	0.0499 (3)	0.0361 (3)	0.0616 (4)	−0.0040 (3)	−0.0001 (3)	0.0016 (3)

Geometric parameters (Å, °)

C1—C6	1.392 (4)	C9—C10	1.363 (5)
C1—C2	1.397 (4)	C9—H9	0.9300
C1—S1	1.762 (3)	C10—C11	1.363 (5)
C2—C3	1.390 (4)	C10—Cl1	1.742 (3)
C2—C13	1.508 (4)	C11—C12	1.378 (4)
C3—C4	1.382 (4)	C11—H11	0.9300
C3—H3	0.9300	C12—H12	0.9300

C4—C5	1.378 (4)	C13—H13A	0.9600
C4—C14	1.504 (4)	C13—H13B	0.9600
C5—C6	1.380 (4)	C13—H13C	0.9600
C5—H5	0.9300	C14—H14A	0.9600
C6—H6	0.9300	C14—H14B	0.9600
C7—C12	1.377 (4)	C14—H14C	0.9600
C7—C8	1.377 (4)	N1—S1	1.630 (2)
C7—N1	1.423 (3)	N1—H1N	0.828 (17)
C8—C9	1.387 (4)	O1—S1	1.429 (2)
C8—H8	0.9300	O2—S1	1.430 (2)

C6—C1—C2	120.7 (2)	C11—C10—Cl1	120.3 (3)
C6—C1—S1	117.1 (2)	C10—C11—C12	119.5 (3)
C2—C1—S1	122.1 (2)	C10—C11—H11	120.2
C3—C2—C1	116.5 (3)	C12—C11—H11	120.2
C3—C2—C13	119.2 (3)	C7—C12—C11	120.6 (3)
C1—C2—C13	124.2 (3)	C7—C12—H12	119.7
C4—C3—C2	124.0 (3)	C11—C12—H12	119.7
C4—C3—H3	118.0	C2—C13—H13A	109.5
C2—C3—H3	118.0	C2—C13—H13B	109.5
C5—C4—C3	117.7 (3)	H13A—C13—H13B	109.5
C5—C4—C14	121.2 (3)	C2—C13—H13C	109.5
C3—C4—C14	121.1 (3)	H13A—C13—H13C	109.5
C4—C5—C6	120.8 (3)	H13B—C13—H13C	109.5
C4—C5—H5	119.6	C4—C14—H14A	109.5
C6—C5—H5	119.6	C4—C14—H14B	109.5
C5—C6—C1	120.3 (3)	H14A—C14—H14B	109.5
C5—C6—H6	119.9	C4—C14—H14C	109.5
C1—C6—H6	119.9	H14A—C14—H14C	109.5
C12—C7—C8	119.2 (3)	H14B—C14—H14C	109.5
C12—C7—N1	119.4 (2)	C7—N1—S1	124.70 (17)
C8—C7—N1	121.4 (2)	C7—N1—H1N	115.6 (19)
C7—C8—C9	120.0 (3)	S1—N1—H1N	112.6 (19)
C7—C8—H8	120.0	O1—S1—O2	118.81 (12)
C9—C8—H8	120.0	O1—S1—N1	104.76 (12)
C10—C9—C8	119.7 (3)	O2—S1—N1	107.43 (12)
C10—C9—H9	120.2	O1—S1—C1	111.24 (12)
C8—C9—H9	120.2	O2—S1—C1	107.25 (12)
C9—C10—C11	120.9 (3)	N1—S1—C1	106.67 (11)
C9—C10—Cl1	118.8 (3)		

C6—C1—C2—C3	0.2 (4)	C8—C9—C10—Cl1	−178.3 (3)
S1—C1—C2—C3	−176.34 (19)	C9—C10—C11—C12	−0.5 (4)
C6—C1—C2—C13	−179.5 (3)	Cl1—C10—C11—C12	179.3 (2)
S1—C1—C2—C13	4.0 (4)	C8—C7—C12—C11	1.8 (4)
C1—C2—C3—C4	0.0 (4)	N1—C7—C12—C11	−175.2 (2)
C13—C2—C3—C4	179.7 (3)	C10—C11—C12—C7	−1.2 (4)
C2—C3—C4—C5	−0.3 (4)	C12—C7—N1—S1	−130.2 (2)
C2—C3—C4—C14	179.1 (3)	C8—C7—N1—S1	52.9 (3)
C3—C4—C5—C6	0.4 (4)	C7—N1—S1—O1	175.7 (2)

C14—C4—C5—C6	−178.9 (3)	C7—N1—S1—O2	−57.0 (2)
C4—C5—C6—C1	−0.3 (4)	C7—N1—S1—C1	57.7 (2)
C2—C1—C6—C5	0.0 (4)	C6—C1—S1—O1	146.0 (2)
S1—C1—C6—C5	176.6 (2)	C2—C1—S1—O1	−37.4 (2)
C12—C7—C8—C9	−0.8 (4)	C6—C1—S1—O2	14.5 (2)
N1—C7—C8—C9	176.1 (3)	C2—C1—S1—O2	−168.8 (2)
C7—C8—C9—C10	−0.9 (5)	C6—C1—S1—N1	−100.3 (2)
C8—C9—C10—C11	1.5 (5)	C2—C1—S1—N1	76.3 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O2^{i}	0.83 (2)	2.08 (2)	2.891 (4)	166 (3)

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

Fig. 1

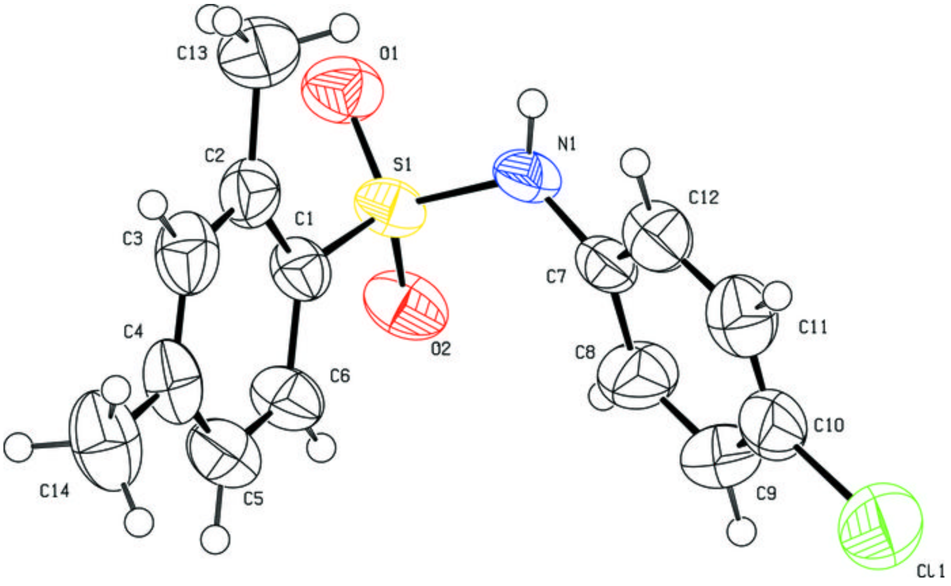

Fig. 2