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2,5-Dichloro-*N*-(4-methoxyphenyl)-benzensulfonamide

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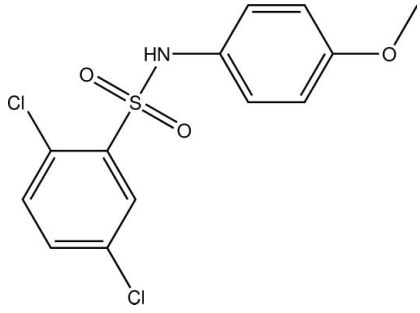
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.108; data-to-parameter ratio = 18.6.

In the title compound, $C_{13}H_{11}Cl_2NO_3S$, the dihedral angle between the benzene rings is 74.37 (3)°. In the crystal, intermolecular N—H···O hydrogen bonds link the molecules into chains along the *b* axis.

Related literature

For our previous studies on sulfonamide derivatives, see: Khan *et al.* (2010); Sharif *et al.* (2010). For background to the pharmacological uses of sulfonamides, see: Korolkovas (1988); Mandell & Sande (1992).



Experimental

Crystal data

$C_{13}H_{11}Cl_2NO_3S$
M_r = 332.19
Monoclinic, $P2_1/c$
a = 13.1599 (4) Å
b = 7.8179 (2) Å
c = 14.4830 (5) Å
β = 110.566 (1)°
V = 1395.09 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.62 mm^{-1}
T = 296 K
0.25 × 0.17 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
13132 measured reflections
3456 independent reflections
2690 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.108
S = 1.06
3456 reflections
186 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N12—H12···O19^{i}	0.78 (2)	2.50 (3)	3.267 (2)	168 (2)

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

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); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2254).

References

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Khan, I. U., Akkurt, M., Sharif, S. & Ahmad, W. (2010). *Acta Cryst.* E**66**, o3053.
Korolkovas, A. (1988). *Essentials of Medicinal Chemistry*, 2nd ed., pp. 699–716. New York: Wiley.
Mandell, G. L. & Sande, M. A. (1992). *Goodman and Gilman, The Pharmacological Basis of Therapeutics 2*, edited by A. Gilman, T. W. Rall, A. S. Nies & P. Taylor, 8th ed., pp. 1047–1057. Singapore: McGraw-Hill.
Sharif, S., Iqbal, H., Khan, I. U., John, P. & Tiekink, E. R. T. (2010). *Acta Cryst.* E**66**, o1288.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2011). E**67**, o369 [**doi:10.1107/S1600536811000936**]

2,5-Dichloro-*N*-(4-methoxyphenyl)benzensulfonamide

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Comment

In continuation of our studies of sulfonamides synthesis (Khan *et al.*, 2010; Sharif *et al.*, 2010), of interest owing to their biological properties (Korolkovas, 1988; Mandell & Sande, 1992). Herein, the crystal structure of (I) is described

In the title compound (I), (Fig. 1), the 4-methoxyphenyl moiety is almost planar with r.m.s. deviation of 0.018 Å from the corresponding least-squares plane defined by the nine constituent atoms. The dihedral angle between the benzene rings is 74.37 (3) °. In the crystal, intermolecular N—H···O hydrogen bonds link the molecules into chains along the *b* axis (Table 1, Fig. 2).

Experimental

To *para*-anisidine (123 mg, 1 mmol) in distilled water (10 ml) was added 2,5-dichloro benzene sulfonyl chloride (0.245 mg, 1 mmol) with stirring at room temperature while maintaining the pH = 8 using 3% sodium carbonate. The progress of the reaction was monitored by TLC. The precipitate formed in this way was washed with water, dried and crystallized from methanol.

Refinement

The H atom of the NH group was located in a difference Fourier map and refined freely. The remaining H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.96 Å, and with U_{iso}(H) = 1.2U_{eq} (C) for aromatic and 1.5U_{eq}(C) for methyl H atoms.

Figures

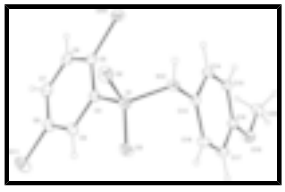

Fig. 1. The molecular structure of (I) showing the atom-numbering scheme and 30% probability ellipsoids.

Fig. 2. Part of the crystal structure of (I), showing chain of molecules linked by intermolecular N—H···O hydrogen bonds (dashed lines) along the *b* axis.

2,5-Dichloro-*N*-(4-methoxyphenyl)benzensulfonamide

Crystal data

$C_{13}H_{11}Cl_2NO_3S$	$F(000) = 680$
$M_r = 332.19$	$D_x = 1.582$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 4792 reflections
$a = 13.1599$ (4) Å	$\theta = 2.9$–$28.0°$
$b = 7.8179$ (2) Å	$\mu = 0.62$ mm^{-1}
$c = 14.4830$ (5) Å	$T = 296$ K
$\beta = 110.566$ (1)°	Block, colourless
$V = 1395.09$ (7) Å^3	0.25 × 0.17 × 0.12 mm
$Z = 4$	

Data collection

Bruker APEXII CCD diffractometer	$R_{int} = 0.030$
φ and ω scans	$\theta_{max} = 28.3°$, $\theta_{min} = 3.0°$
13132 measured reflections	$h = -17\rightarrow17$
3456 independent reflections	$k = -10\rightarrow10$
2690 reflections with $I > 2\sigma(I)$	$l = -18\rightarrow19$

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.6614P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.108$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.46$ e Å^{-3}
3456 reflections	$\Delta\rho_{min} = -0.31$ e Å^{-3}
186 parameters	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}

S1	0.72780 (4)	0.85926 (6)	0.82650 (3)	0.03916 (14)
O2	0.73299 (14)	1.04147 (19)	0.82443 (12)	0.0552 (4)
O3	0.69500 (12)	0.7655 (2)	0.73648 (10)	0.0493 (4)
C4	0.85981 (16)	0.7804 (2)	0.89567 (14)	0.0369 (4)
C5	0.91579 (17)	0.8160 (3)	0.99528 (15)	0.0419 (4)
C6	1.02137 (18)	0.7615 (3)	1.03996 (17)	0.0509 (5)
H6	1.0576	0.7843	1.1065	0.061*
C7	1.07387 (19)	0.6737 (3)	0.98749 (18)	0.0539 (6)
H7	1.1455	0.6385	1.0176	0.065*
C8	1.01785 (18)	0.6389 (3)	0.88887 (17)	0.0485 (5)
C9	0.91210 (17)	0.6898 (3)	0.84328 (15)	0.0427 (4)
H9	0.8756	0.6635	0.7772	0.051*
Cl10	0.85599 (5)	0.93075 (8)	1.06480 (4)	0.05536 (17)
Cl11	1.08144 (6)	0.53037 (11)	0.82003 (6)	0.0786 (2)
N12	0.64500 (14)	0.8123 (2)	0.88365 (13)	0.0398 (4)
H12	0.6441 (19)	0.888 (3)	0.9181 (17)	0.046 (7)*
C13	0.63424 (15)	0.6413 (2)	0.91467 (13)	0.0350 (4)
C14	0.65129 (17)	0.6093 (3)	1.01225 (14)	0.0412 (4)
H14	0.6706	0.6986	1.0575	0.049*
C15	0.64003 (17)	0.4456 (3)	1.04402 (15)	0.0423 (5)
H15	0.6504	0.4257	1.11	0.051*
C16	0.61338 (16)	0.3123 (3)	0.97760 (15)	0.0405 (4)
C17	0.59349 (19)	0.3448 (3)	0.87865 (15)	0.0476 (5)
H17	0.5737	0.2557	0.8333	0.057*
C18	0.60287 (18)	0.5083 (3)	0.84720 (15)	0.0448 (5)
H18	0.5881	0.5295	0.7806	0.054*
O19	0.60296 (14)	0.1448 (2)	1.00210 (12)	0.0560 (4)
C20	0.6237 (2)	0.1095 (3)	1.10353 (19)	0.0610 (6)
H20A	0.6977	0.138	1.1414	0.091*
H20B	0.6117	−0.0098	1.1116	0.091*
H20C	0.5759	0.1765	1.126	0.091*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0448 (3)	0.0397 (3)	0.0347 (2)	0.0049 (2)	0.0162 (2)	0.00713 (19)
O2	0.0669 (10)	0.0399 (8)	0.0638 (10)	0.0066 (7)	0.0292 (9)	0.0140 (7)
O3	0.0502 (8)	0.0672 (10)	0.0303 (7)	0.0043 (7)	0.0137 (6)	0.0024 (7)
C4	0.0414 (10)	0.0341 (9)	0.0361 (9)	−0.0023 (8)	0.0147 (8)	0.0044 (7)
C5	0.0504 (11)	0.0387 (10)	0.0371 (10)	−0.0093 (9)	0.0158 (9)	0.0011 (8)
C6	0.0489 (12)	0.0532 (13)	0.0423 (11)	−0.0122 (10)	0.0056 (10)	0.0042 (10)
C7	0.0414 (11)	0.0580 (14)	0.0583 (14)	−0.0021 (10)	0.0128 (10)	0.0121 (11)
C8	0.0474 (12)	0.0490 (12)	0.0533 (12)	0.0055 (9)	0.0231 (10)	0.0097 (10)
C9	0.0471 (11)	0.0426 (11)	0.0404 (10)	0.0018 (9)	0.0178 (9)	0.0049 (8)
Cl10	0.0707 (4)	0.0531 (3)	0.0446 (3)	−0.0098 (3)	0.0231 (3)	−0.0122 (2)
Cl11	0.0661 (4)	0.1040 (6)	0.0740 (5)	0.0343 (4)	0.0349 (4)	0.0095 (4)
N12	0.0480 (10)	0.0371 (9)	0.0386 (9)	0.0037 (7)	0.0205 (8)	−0.0011 (7)
C13	0.0340 (9)	0.0368 (10)	0.0363 (9)	0.0017 (7)	0.0151 (8)	−0.0002 (8)

C14	0.0475 (11)	0.0427 (11)	0.0356 (10)	−0.0059 (8)	0.0175 (9)	−0.0070 (8)
C15	0.0475 (11)	0.0487 (12)	0.0332 (10)	−0.0065 (9)	0.0172 (9)	−0.0002 (8)
C16	0.0415 (10)	0.0391 (10)	0.0427 (11)	−0.0018 (8)	0.0171 (9)	0.0011 (8)
C17	0.0629 (13)	0.0414 (11)	0.0390 (11)	−0.0044 (9)	0.0185 (10)	−0.0090 (9)
C18	0.0574 (13)	0.0449 (11)	0.0312 (9)	−0.0003 (9)	0.0146 (9)	−0.0023 (8)
O19	0.0776 (11)	0.0403 (8)	0.0550 (9)	−0.0060 (7)	0.0290 (8)	0.0021 (7)
C20	0.0800 (17)	0.0519 (14)	0.0613 (15)	0.0073 (12)	0.0377 (13)	0.0149 (12)

Geometric parameters (Å, °)

S1—O3	1.4243 (15)	N12—H12	0.78 (2)
S1—O2	1.4269 (16)	C13—C14	1.374 (3)
S1—N12	1.6250 (17)	C13—C18	1.387 (3)
S1—C4	1.783 (2)	C14—C15	1.386 (3)
C4—C9	1.385 (3)	C14—H14	0.93
C4—C5	1.398 (3)	C15—C16	1.377 (3)
C5—C6	1.378 (3)	C15—H15	0.93
C5—Cl10	1.731 (2)	C16—O19	1.376 (2)
C6—C7	1.377 (3)	C16—C17	1.387 (3)
C6—H6	0.93	C17—C18	1.377 (3)
C7—C8	1.385 (3)	C17—H17	0.93
C7—H7	0.93	C18—H18	0.93
C8—C9	1.373 (3)	O19—C20	1.424 (3)
C8—Cl11	1.732 (2)	C20—H20A	0.96
C9—H9	0.93	C20—H20B	0.96
N12—C13	1.433 (3)	C20—H20C	0.96
O3—S1—O2	119.74 (10)	S1—N12—H12	108.5 (18)
O3—S1—N12	107.95 (10)	C14—C13—C18	119.27 (18)
O2—S1—N12	106.36 (10)	C14—C13—N12	119.59 (17)
O3—S1—C4	104.98 (9)	C18—C13—N12	121.09 (17)
O2—S1—C4	108.22 (10)	C13—C14—C15	120.78 (18)
N12—S1—C4	109.34 (9)	C13—C14—H14	119.6
C9—C4—C5	118.95 (19)	C15—C14—H14	119.6
C9—C4—S1	116.27 (15)	C16—C15—C14	119.84 (18)
C5—C4—S1	124.56 (16)	C16—C15—H15	120.1
C6—C5—C4	120.1 (2)	C14—C15—H15	120.1
C6—C5—Cl10	118.46 (17)	O19—C16—C15	124.31 (18)
C4—C5—Cl10	121.40 (16)	O19—C16—C17	116.17 (18)
C7—C6—C5	120.9 (2)	C15—C16—C17	119.51 (19)
C7—C6—H6	119.5	C18—C17—C16	120.37 (19)
C5—C6—H6	119.5	C18—C17—H17	119.8
C6—C7—C8	118.6 (2)	C16—C17—H17	119.8
C6—C7—H7	120.7	C17—C18—C13	120.14 (18)
C8—C7—H7	120.7	C17—C18—H18	119.9
C9—C8—C7	121.4 (2)	C13—C18—H18	119.9
C9—C8—Cl11	118.56 (18)	C16—O19—C20	116.76 (18)
C7—C8—Cl11	120.00 (18)	O19—C20—H20A	109.5
C8—C9—C4	120.0 (2)	O19—C20—H20B	109.5
C8—C9—H9	120	H20A—C20—H20B	109.5

C4—C9—H9	120	O19—C20—H20C	109.5
C13—N12—S1	121.87 (14)	H20A—C20—H20C	109.5
C13—N12—H12	119.1 (18)	H20B—C20—H20C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N12—H12···O19^{i}	0.78 (2)	2.50 (3)	3.267 (2)	168 (2)

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

Fig. 1

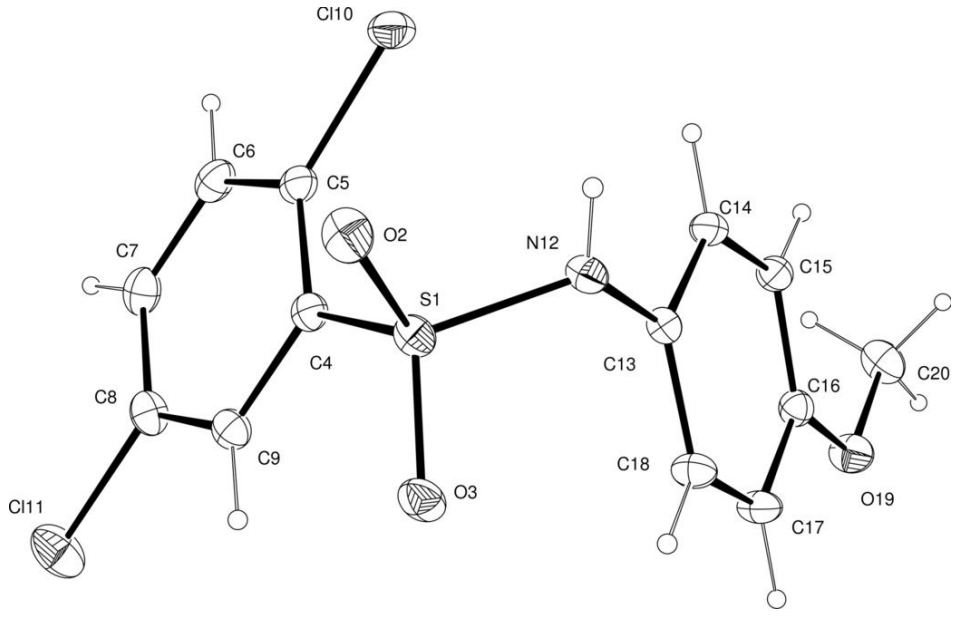
Cl10
C6
C5
O2
N12
C14
C7
S1
C15
C4
C13
C20
C8
C16
C9
C18
O3
O19
Cl11
C17

Fig. 2