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N-(6-Chloropyridazin-3-yl)-4-methylbenzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.159
Data-to-parameter ratio = 20.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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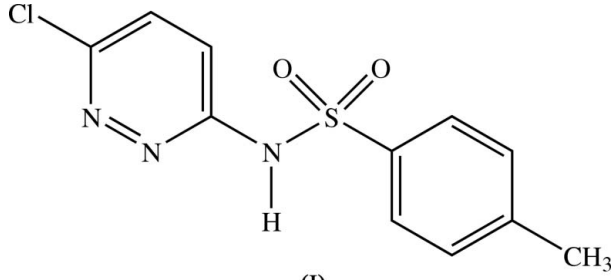
In the title compound, $C_{11}H_{10}ClN_3O_2S$, the pyridazine ring and the benzene ring adopt a distorted V configuration, forming a dihedral angle of 73.79 (11)°. The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds. Weak intramolecular C—H···O and intermolecular C—H···O and C—H···N interactions are also observed. The molecules are linked into one-dimensional chains along the *c* axis and these chains are interconnected, forming a two-dimensional network.

Comment

N-(6-Chloro-3-pyridazinyl)-4-methylbenzenesulfonamide, (I), is a synthetic antibacterial drug of the sulfanilamide family (Ciba Ltd, 1961). A number of sufanilamide drugs have been crystallographically characterized in recent decades (Acharya *et al.*, 1982; Adsmond & Grant, 2001; Basak *et al.*, 1983; Caira & Mohamed, 1992; Deo *et al.*, 1980; Joshi *et al.*, 1983). Some of them, *viz.* sulfamerazine and sulfamethazine, have been studied several times (Acharya *et al.*, 1982; Adsmond & Grant, 2001; Basak *et al.*, 1983; Caira *et al.*, 1992; Deo *et al.*, 1980). Recently, we reported the crystal structure of sulfachloropyridazine (Tan *et al.*, 2005) and we report here the structure of the title compound, (I), a chloropyridazine sulfonamide derivative.



(I)

Bond lengths and angles in (I) (Table 1) are in normal ranges (Allen *et al.*, 1987) and agree with the corresponding values found in sulfamerazine and sulfamethazine (Acharya *et al.*, 1982; Adsmond & Grant, 2001; Basak *et al.*, 1983; Caira *et al.*, 1992; Deo *et al.*, 1980; Tan *et al.*, 2005). S—C is a single bond (Tan *et al.*, 2005), but shorter than those found in the metal sulfadiazinate complexes [1.746 (4) or 1.768 (5) Å; Garcia-Raso *et al.*, 1997; Yuan *et al.*, 2001]; it therefore appears that there is no extension of the benzene-ring electron delocalization to the S atom. The S—O bond lengths are very similar and comparable to those found in free sulfadiazine (Joshi *et al.*, 1983) and sulfachloropyridazine (Tan *et al.*, 2005).

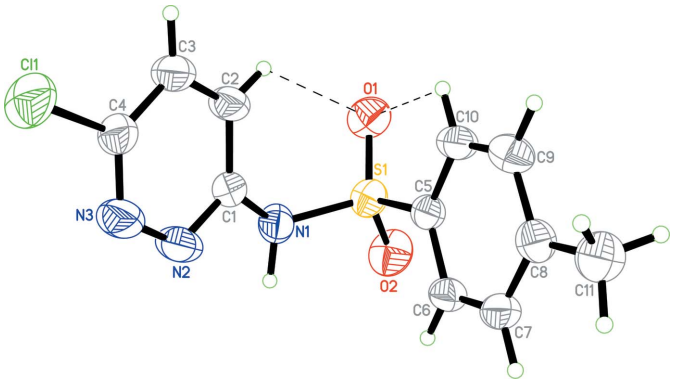


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Intramolecular hydrogen bonds are shown as dashed lines.

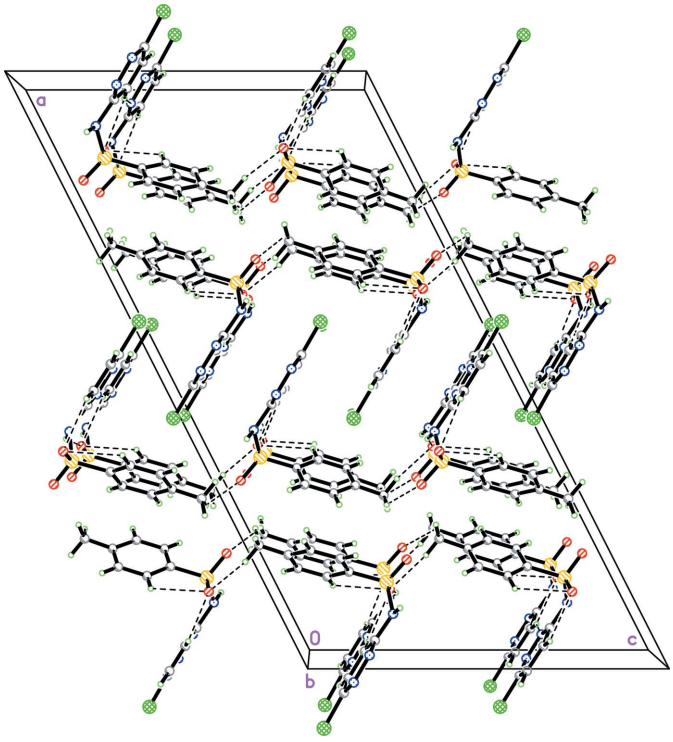


Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

The heterocyclic ring geometry in (I) is comparable to that found for free pyridazine (Blake & Rankin, 1991). The pyridazine and benzene rings form a distorted V configuration indicated by the torsion angle C5—S1—N1—C1 of 54.74 (18)°; the dihedral angle between these two rings is 73.79 (11)°, which is smaller than in sulfachloropyridazine [82.86 (6)°; Tan *et al.*, 2005].

Weak intramolecular C2—H2*A*···O1 and C10—H10*A*···O1 interactions (Table 2) generate $R_2^1(6)$ and $R_2^1(5)$ motifs, respectively (Bernstein, *et al.*, 1995). The intermolecular hydrogen bond N1—H1*N*1···O1(x, 1 + y, z), involves the sulfonamide NH group and sulfonamide O atom. Molecules are linked into one-dimensional chains along the *c* axis through weak C—H···O interactions (Fig. 2 and Table 2). These chains are linked together through further weak C—H···O interactions (Table 2), forming a two-dimensional network. A C—H···π interaction is also observed (Table 2, *Cg* is the centroid of the benzene ring).

Experimental

N-(6-Chloropyridazin-3-yl)-4-methylbenzenesulfonamide (0.2 mmol) and $Zn(CH_3COO)_2$ (0.5 mmol) were placed in a Pyrex tube. After addition of EtOH (1.0 ml) and H_2O (0.5 ml), the tube was frozen with liquid N_2, evacuated and sealed with a torch. The tube was heated at 343 K for 1 d to give light-yellow rod-shaped crystals of (I) in a 46% yield.

Crystal data

$C_{11}H_{10}ClN_3O_2S$
M_r = 283.74
Monoclinic, $C2/c$
a = 29.8577 (4) Å
b = 5.6198 (1) Å
c = 16.1140 (2) Å
β = 116.892 (1)°
V = 2411.45 (7) Å^3
Z = 8
D_x = 1.563 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 297 (2) K
Rod, light yellow
0.50 × 0.33 × 0.27 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.792, T_{max} = 0.881
19119 measured reflections
3507 independent reflections
2965 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 30.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.159
S = 1.05
3507 reflections
168 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0966P)^2 + 1.8315P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.4258 (17)	N1—C1	1.406 (2)
S1—O2	1.4345 (15)	N2—C1	1.317 (3)
S1—N1	1.6592 (18)	N2—N3	1.341 (3)
S1—C5	1.7373 (19)	N3—C4	1.304 (3)
Cl1—C4	1.731 (2)		
O1—S1—O2	118.62 (10)	O2—S1—C5	109.91 (10)
O1—S1—N1	108.07 (10)	N1—S1—C5	106.41 (9)
O2—S1—N1	104.04 (10)	C1—N1—S1	122.74 (13)
O1—S1—C5	109.04 (10)		
O1—S1—N1—C1	−62.25 (19)	N1—S1—C5—C10	−105.64 (16)
O2—S1—N1—C1	170.81 (17)	O1—S1—C5—C6	−170.73 (14)
C5—S1—N1—C1	54.74 (18)	O2—S1—C5—C6	−39.13 (18)
S1—N1—C1—C2	42.5 (3)	N1—S1—C5—C6	72.93 (16)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O1^{i}	0.98 (3)	2.44 (3)	3.336 (2)	153 (2)
C2—H2*A*···O1	0.93	2.48	3.086 (3)	123
C2—H2*A*···N2^{ii}	0.93	2.41	3.264 (2)	152
C10—H10*A*···O1	0.93	2.57	2.929 (3)	104
C11—H11*A*···O1^{iii}	0.96	2.46	3.370 (3)	158
C11—H11*C*···O2^{iv}	0.96	2.48	3.109 (3)	123
C7—H7*A*···*Cg*1^{v}	0.93	2.81	3.467 (2)	128

Symmetry codes: (i) $x, y+1, z$; (ii) $x, y-1, z$; (iii) $x, -y, z-\frac{1}{2}$; (iv) $x, -y+1, z-\frac{1}{2}$; (v) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$. *Cg* is the centroid of the benzene ring.

The H atom bound to atom N1 was located in a difference Fourier map and refined isotropically. The remainding H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.98 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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