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Crystal structures of isomeric 3,5-dichloro-*N*-(2,3-dimethylphenyl)benzenesulfonamide, 3,5-dichloro-*N*-(2,6-dimethylphenyl)benzenesulfonamide and 3,5-dichloro-*N*-(3,5-dimethylphenyl)benzenesulfonamide

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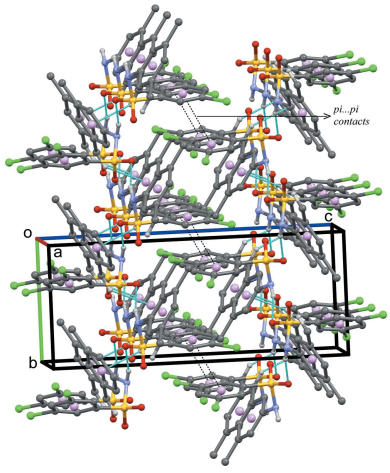
The crystal structures of three isomeric compounds of formula $C_{14}H_{13}Cl_2NO_2S$, namely 3,5-dichloro-*N*-(2,3-dimethylphenyl)-benzenesulfonamide (I), 3,5-dichloro-*N*-(2,6-dimethylphenyl)benzenesulfonamide (II) and 3,5-dichloro-*N*-(3,5-dimethylphenyl)benzenesulfonamide (III) are described. The molecules of all the three compounds are U-shaped with the two aromatic rings inclined at 41.3 (6)° in (I), 42.1 (2)° in (II) and 54.4 (3)° in (III). The molecular conformation of (II) is stabilized by intramolecular C—H···O hydrogen bonds and C—H···π interactions. The crystal structure of (I) features N—H···O hydrogen-bonded $R_2^2(8)$ loops interconnected *via* *C*(7) chains of C—H···O interactions, forming a three-dimensional architecture. The structure also features π–π interactions [$Cg\cdots Cg$ = 3.6970 (14) Å]. In (II), N—H···O hydrogen-bonded $R_2^2(8)$ loops are interconnected *via* π–π interactions [intercentroid distance = 3.606 (3) Å] to form a one-dimensional architecture running parallel to the *a* axis. In (III), adjacent *C*(4) chains of N—H···O hydrogen-bonded molecules running parallel to [010] are connected *via* C—H···π interactions, forming sheets parallel to the *ab* plane. Neighbouring sheets are linked *via* offset π–π interactions [intercentroid distance = 3.8303 (16) Å] to form a three-dimensional architecture.

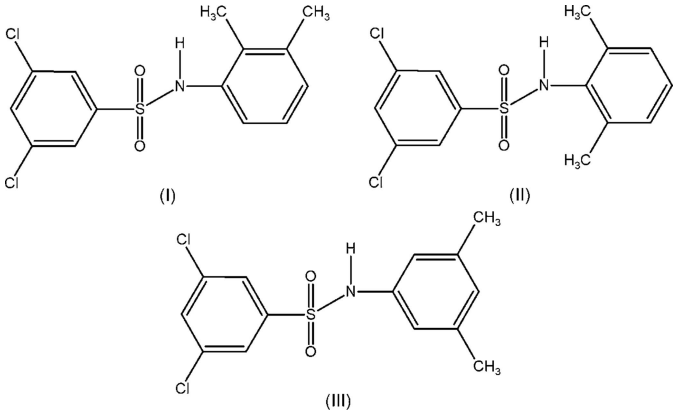
1. Chemical context

Sulfonamide drugs were the first chemotherapeutic agents to be used for curing and preventing bacterial infection in human beings (Shiva Prasad *et al.*, 2011). They play a vital role as key constituents in a number of biologically active molecules and are known to exhibit a wide variety of biological activities, such as antibacterial (Subhakara Reddy *et al.*, 2012; Himel *et al.*, 1971), antifungal (Hanafy *et al.*, 2007), anti-inflammatory (Küçükgüzel *et al.*, 2013), antitumor (Ghorab *et al.*, 2011), anticancer (Al-Said *et al.*, 2011), anti-HIV (Sahu *et al.*, 2007) and antitubercular activities (Vora & Mehta, 2012). In recent years, extensive research studies have been carried out on the synthesis and evaluation of the pharmacological properties of molecules containing the sulfonamide moiety, which have been reported to be important pharmacophores (Mohan *et al.*, 2013).

With these considerations in mind and based on our structural study of 3,5-dichloro-*N*-(substitutedphenyl)-benzenesulfonamides (Shakuntala, Naveen *et al.*, 2017;



Shakuntala, Lokanath *et al.*, 2017), we report herein the crystal structures of three isomers, *viz.* 3,5-dichloro-*N*-(2,3-dimethylphenyl)-benzenesulfonamide (I), 3,5-dichloro-*N*-(2,6-dimethylphenyl)benzenesulfonamide (II) and 3,5-dichloro-*N*-(3,5-dimethylphenyl)benzenesulfonamide (III).



2. Structural commentary

The molecule of (I) (Fig. 1) is U-shaped, with the sulfonylbenzene ring and the aniline ring inclined by 41.3 (6)°. The N—C bond in the C–SO_2–NH–C segment has a *gauche* torsion with respect to the S=O bonds, and the molecule is twisted at the S—N bond, with a C1—S1—N1—C7 torsion angle of 60.9 (2)°.

In the U-shaped molecules of (II) (Fig. 2), the dihedral angle between the sulfonylbenzene ring and the aniline ring is 42.1 (2)°. The molecule is twisted at the S—N bond, with a C1—S1—N1—C7 torsion angle of 69.8 (3)°. The molecular conformation of (II) is stabilized by an intramolecular C—H···O hydrogen bond and a C—H···π interaction (Table 2). The N—C bond in the C–SO_2–NH–C segment has a *gauche* torsion with respect to the S=O bonds.

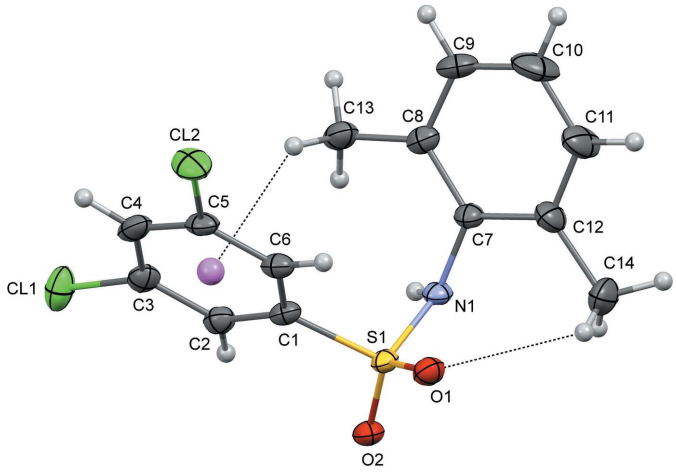


Figure 2
The molecular structure of (II) with displacement ellipsoids drawn at the 50% probability level. Intramolecular C—H···O and C—H···π hydrogen interactions are shown as dotted lines.

The molecule of (III) (Fig. 3) is also U-shaped, with the sulfonylbenzene ring tilted at an angle of 54.4 (3)° with respect to the aniline ring. The N—C bond in the C–SO_2–NH–C segment has a *gauche* torsion with respect to the S=O bonds, and the molecule is twisted at the S—N bond, with a C1—S1—N1—C7 torsion angle of 71.3 (2)°.

3. Supramolecular features

The crystal structure of (I) features inversion-related dimers linked by N1—H1···O2^{i} hydrogen bonds forming $R_2^2(8)$ loops (Fig. 4, Table 1). The $R_2^2(8)$ loops are interconnected *via* $C(7)$ chains of C4—H4···O1^{ii} intermolecular interactions, forming a three-dimensional supramolecular architecture. The structure also features π–π interactions involving the benzenesulfonyl ring and the aniline ring as illustrated in Fig. 4 [$Cg1\cdots Cg2^{iii}$ = 3.6970 (14) Å; $Cg1$ and $Cg2$ are the centroids

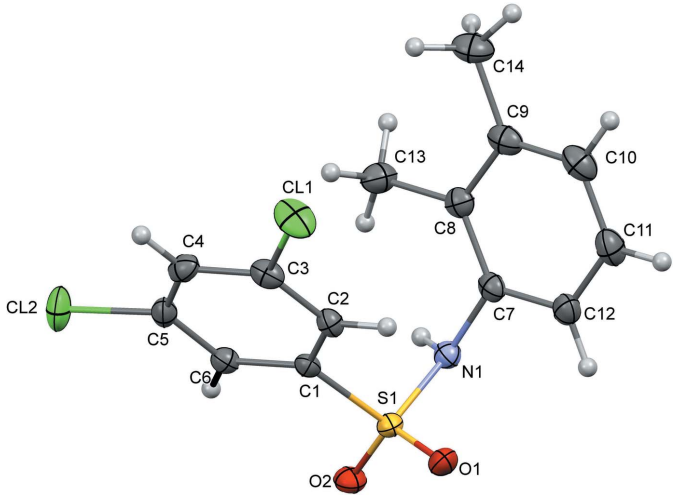


Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level.

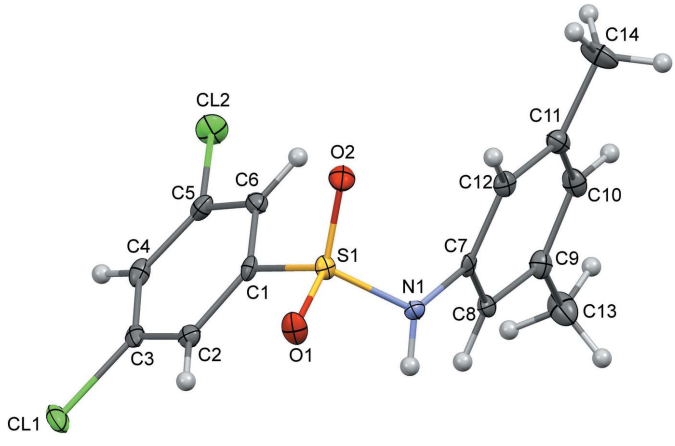


Figure 3
The molecular structure of (III) with displacement ellipsoids drawn at the 50% probability level.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.14	2.9590	159
C4—H4···O1^{ii}	0.95	2.41	3.332 (3)	164

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

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14*C*···O1	0.98	2.53	3.139 (8)	120
N1—H1···O2^{i}	0.85 (4)	2.12 (4)	2.937 (5)	160 (4)
C13—H13*A*···*Cg*1	0.98	2.67	3.493 (5)	142

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

of the C1–C6 and C7–C12 rings, respectively; symmetry code: (iii) $\frac{3}{2}-x, -\frac{1}{2}+y, \frac{3}{2}-z$].

In (II), N1—H1···O2^{i} hydrogen-bonded $R_2^2(8)$ loops (Fig. 5, Table 2) are connected *via* π–π interactions involving inversion-related benzenesulfonyl rings, forming a one-dimensional architecture running parallel to the *a* axis, as shown in Fig. 5 [*Cg*1···*Cg*1^{ii} = 3.606 (3) Å; *Cg*1 is the centroid of the C1–C6 ring; symmetry code: (ii) $2-x, 1-y, -z$].

In the crystal structure of (III), the molecules are interlinked *via* N1—H1···O1^{i} hydrogen bonds (Fig. 6, Table 3) to form *C*(4) chains running parallel to [010]. Adjacent chains are

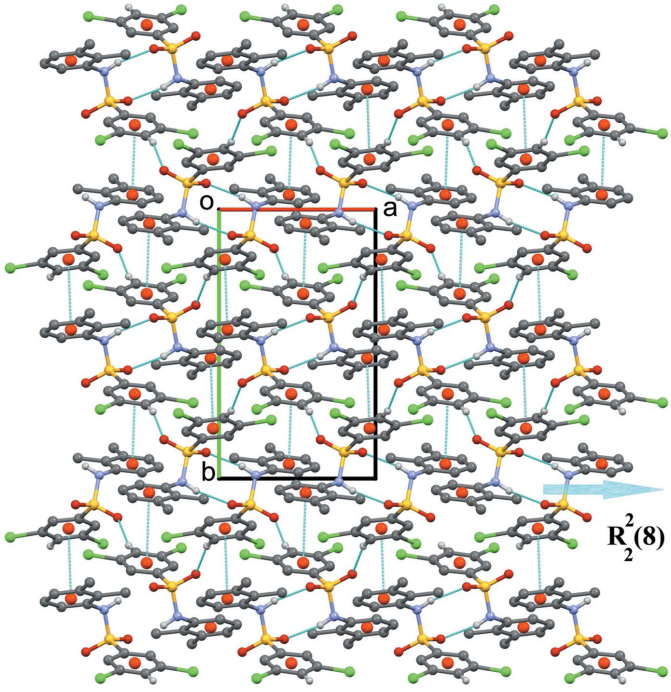


Figure 4
The three-dimensional supramolecular architecture of (I) viewed along the *c* axis. The N—H···O and C—H···O hydrogen bonds and π–π interactions are shown as thin blue dotted lines. H atoms not involved in hydrogen bonding are omitted for clarity.

Table 3
Hydrogen-bond geometry (Å, °) for (III).

*Cg*2 is the centroid of the aniline ring C7–C12

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.87	2.13	2.9848	167
C14—H14*B*···*Cg*2^{ii}	0.98	2.86	3.5135	124

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$.

connected by C14—H14*B*···π interactions involving the aniline ring, forming two-dimensional sheets parallel to the *ab* plane. Neighbouring sheets are further linked *via* offset π–π interactions involving inversion-related benzenesulfonyl rings, forming a three dimensional architecture as as illustrated in Fig. 7 [*Cg*1···*Cg*1^{i} = 3.8303 (16) Å, interplanar distance = 3.3874 (11) Å, slippage 1.788 (3) Å; *Cg*1 is the centroid of the C1–C6 ring; symmetry code: (iii) $1-x, -y, -z$].

4. Database survey

Two 3,5-dichloro-*N*-(substitutedphenyl)-benzenesulfonamides, namely 3,5-dichloro-*N*-(4-methylphenyl)benzenesulfonamide [Shakuntala, Naveen *et al.*, 2017, (IV)] and 3,5-dichloro-*N*-(2,4-dichlorophenyl)benzenesulfonamide [Shakuntala, Lokanath *et al.*, 2017, (V)], have been reported previously. The molecules of both (IV) and (V) are U-shaped

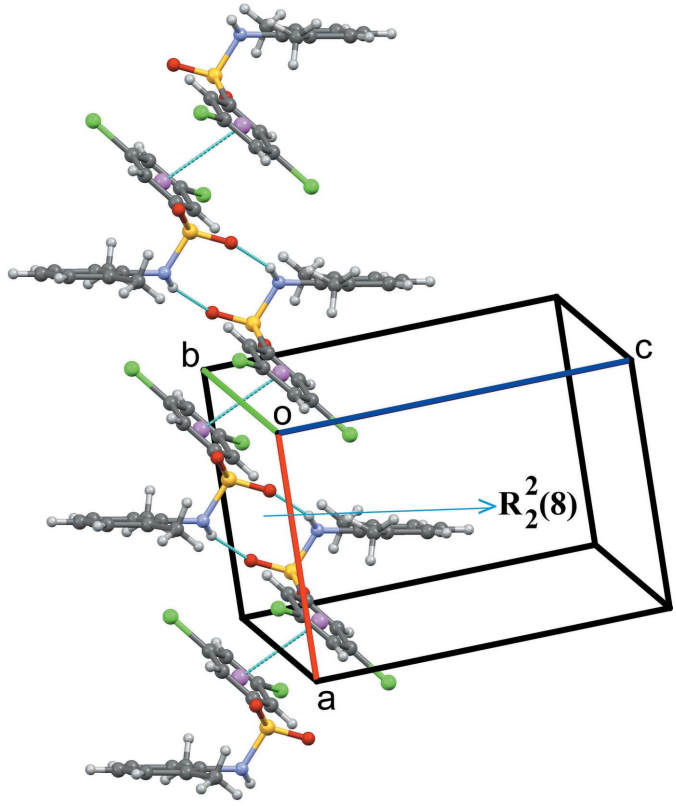


Figure 5
Partial crystal packing of (II) showing the formation of a one-dimensional architecture through N—H···O hydrogen bonds and π–π interactions (thin blue dotted lines).

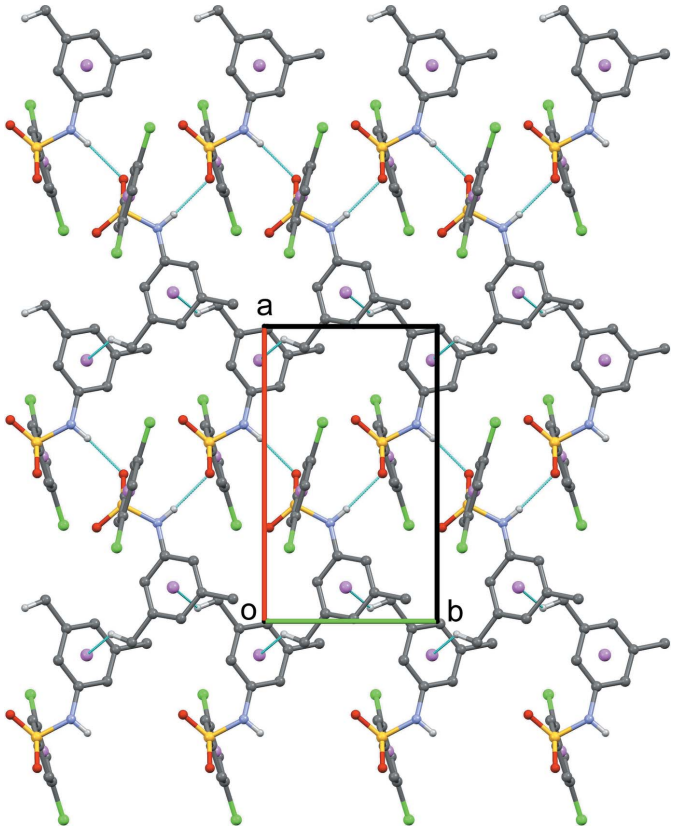


Figure 6
Partial crystal packing of (III) viewed down the *c* axis displaying two-dimensional sheets. Thin blue dotted lines denote N—H···O hydrogen bonds and C—H···π interactions. H atoms not involved in hydrogen bonding are omitted for clarity.

with the central C–S–N–C segment having a torsion angle of 67.2 (4)° in (IV) and 58.7 (3)° in (V). The dihedral angle between the benzene rings is 57.0 (2)° in (IV) and 40.23 (2)° in (V). The crystal structure of (IV) displays a three-dimensional supramolecular structure constructed *via* N—H···O and C—H···O hydrogen bonds and C—H···π interactions, whereas in (V) the three-dimensional supramolecular architecture is built through N—H···O and C—H···O hydrogen bonds, Cl···Cl contacts and π–π interactions.

5. Synthesis and crystallization

The title compounds were prepared according to a literature method (Rodrigues *et al.*, 2015). The purities of all the compounds were checked by determining their melting points. Colourless prismatic single crystals suitable for X-ray diffraction studies were obtained by slow evaporation of ethanolic solutions of the compounds at room temperature.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 4. The amino H atoms were located in difference-Fourier maps and refined isotropically with the N—H bond length restrained to be 0.88 (2) Å. All other H atoms were positioned geometrically and refined as riding with C—H = 0.95–0.98 Å and U_{iso}(H) = 1.2 or 1.5U_{eq}(C). A rotating model was applied to the methyl groups. To improve considerably the values of *R*1, *wR*2, and *S* (goodness-of-fit), a low-angle reflection partially obscured by the beam-stop (100) was omitted from the final refinement of (III).

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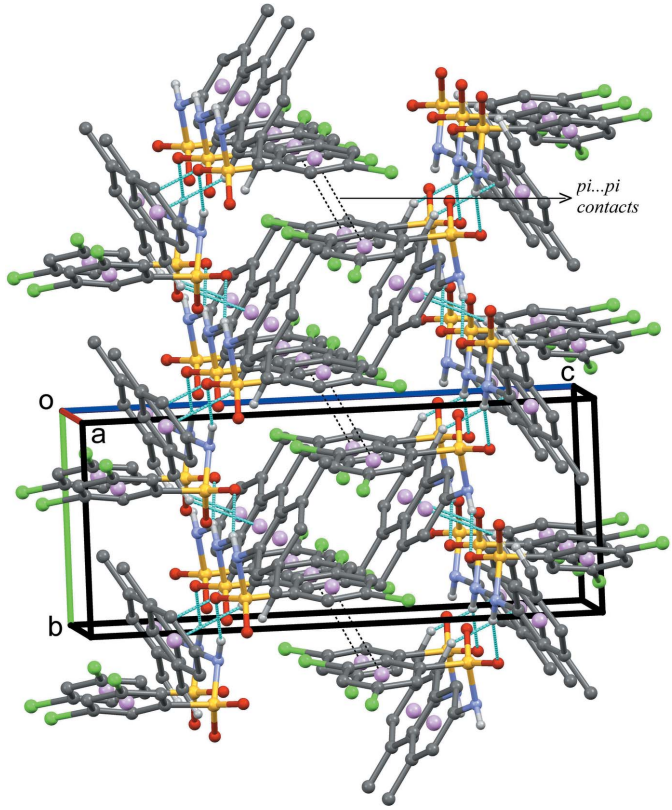

Figure 7
Crystal packing of (III) viewed approximately along the *a* axis, showing the π–π interactions (black dotted lines) between adjacent sheets. For clarity, only H atoms involved in N—H···O hydrogen bonds and C—H···π interactions (thin blue dotted lines) are included.

Table 4
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$C_{14}H_{13}Cl_2NO_2S$	$C_{14}H_{13}Cl_2NO_2S$	$C_{14}H_{13}Cl_2NO_2S$
M_r	330.21	330.21	330.21
Crystal system, space group	Monoclinic, $P2_1/n$	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/c$
Temperature (K)	100	100	100
a, b, c (Å)	8.2223 (3), 14.1546 (5), 12.7933 (4)	8.4817 (15), 8.6149 (15), 12.167 (2)	12.2268 (6), 7.0399 (3), 17.3130 (8)
α, β, γ (°)	90, 91.188 (1), 90	109.875 (5), 91.900 (5), 114.190 (5)	90, 100.409 (1), 90
V (Å^3)	1488.61 (9)	747.1 (2)	1465.70 (12)
Z	4	2	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	5.24	5.22	5.32
Crystal size (mm)	0.28 × 0.25 × 0.22	0.29 × 0.26 × 0.22	0.27 × 0.24 × 0.21
Data collection			
Diffractometer	Bruker APEXII CCD area detector	Bruker APEXII CCD area detector	Bruker APEXII CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)	Multi-scan (*SADABS*; Bruker, 2009)	Multi-scan (*SADABS*; Bruker,2009)
T_{min}, T_{max}	0.288, 0.316	0.275, 0.317	0.297, 0.327
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10308, 2440, 2347	6977, 2400, 1960	11468, 2412, 2374
R_{int}	0.053	0.124	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.584	0.581	0.585
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.162, 1.07	0.074, 0.233, 1.02	0.058, 0.152, 0.99
No. of reflections	2440	2400	2412
No. of parameters	187	187	187
No. of restraints	1	1	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.64, −0.63	0.99, −0.60	0.82, −0.88

Computer programs: *APEX2*, *SAINT-Plus* and *XPREP* (Bruker, 2009), *SHELXT* 2016/4 (Sheldrick, 2015*a*), *SHELXL2016/4* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2008).

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supporting information

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Crystal structures of isomeric 3,5-dichloro-*N*-(2,3-dimethylphenyl)benzenesulfonamide, 3,5-dichloro-*N*-(2,6-dimethylphenyl)benzenesulfonamide and 3,5-dichloro-*N*-(3,5-dimethylphenyl)benzenesulfonamide

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Computing details

Data collection: *APEX2* (Bruker, 2009) for (I); APEXII (Bruker, 2009) for (II), (III). For all compounds, cell refinement: *APEX2* (Bruker, 2009) and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* (Bruker, 2009) and *XPREP* (Bruker, 2009); program(s) used to solve structure: SHELXT 2016/4 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016/4* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2016/4* (Sheldrick, 2015b).

(I) 3,5-Dichloro-*N*-(2,3-dimethylphenyl)benzenesulfonamide

Crystal data

$C_{14}H_{13}Cl_2NO_2S$
M_r = 330.21
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 8.2223 (3) Å
b = 14.1546 (5) Å
c = 12.7933 (4) Å
β = 91.188 (1)°
V = 1488.61 (9) Å^3
Z = 4
F(000) = 680

Prism
D_x = 1.473 Mg m^{-3}
Melting point: 431 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 144 reflections
θ = 6.2–64.2°
μ = 5.24 mm^{-1}
T = 100 K
Prism, colourless
0.28 × 0.25 × 0.22 mm

Data collection

Bruker APEXII CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.288, T_{max} = 0.316

10308 measured reflections
2440 independent reflections
2347 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 64.2°, θ_{min} = 6.2°
h = −9→9
k = −16→15
l = −14→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.162
S = 1.07

2440 reflections
187 parameters
1 restraint
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1235P)^2 + 0.7281P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6064 (3)	0.35091 (16)	0.66816 (18)	0.0170 (5)
C2	0.7069 (3)	0.32517 (16)	0.75161 (18)	0.0189 (5)
H2	0.821571	0.332433	0.748662	0.023*
C3	0.6346 (3)	0.28862 (18)	0.83908 (19)	0.0222 (6)
C4	0.4689 (3)	0.27523 (17)	0.84477 (19)	0.0230 (6)
H4	0.421903	0.248689	0.905281	0.028*
C5	0.3733 (3)	0.30179 (17)	0.7592 (2)	0.0214 (6)
C6	0.4380 (3)	0.34137 (16)	0.67041 (19)	0.0191 (5)
H6	0.370447	0.361192	0.613395	0.023*
C7	0.8409 (3)	0.53406 (16)	0.67541 (19)	0.0200 (5)
C8	0.7774 (3)	0.56423 (17)	0.7703 (2)	0.0214 (6)
C9	0.8878 (3)	0.58319 (17)	0.8534 (2)	0.0255 (6)
C10	1.0528 (3)	0.57152 (19)	0.8392 (2)	0.0299 (6)
H10	1.126374	0.583905	0.895815	0.036*
C11	1.1130 (3)	0.5422 (2)	0.7444 (2)	0.0294 (6)
H11	1.226895	0.535041	0.736077	0.035*
C12	1.0071 (3)	0.52333 (18)	0.6620 (2)	0.0249 (6)
H12	1.047530	0.503204	0.596579	0.030*
C13	0.5980 (3)	0.5761 (2)	0.7852 (2)	0.0291 (6)
H13A	0.542286	0.578976	0.716866	0.044*
H13B	0.578180	0.634742	0.823689	0.044*
H13C	0.556474	0.522395	0.824971	0.044*
C14	0.8264 (4)	0.6143 (2)	0.9586 (2)	0.0349 (7)
H14A	0.918902	0.623555	1.007098	0.052*
H14B	0.754217	0.565655	0.986298	0.052*
H14C	0.766435	0.673737	0.950595	0.052*
N1	0.7344 (3)	0.51231 (14)	0.58726 (16)	0.0194 (5)
O1	0.8517 (2)	0.35517 (12)	0.54650 (13)	0.0237 (4)
O2	0.5832 (2)	0.40294 (13)	0.47232 (14)	0.0241 (4)
S1	0.69924 (7)	0.40208 (4)	0.55760 (4)	0.0177 (3)
CL1	0.75874 (9)	0.25743 (5)	0.94545 (5)	0.0355 (3)
CL2	0.16538 (7)	0.28217 (5)	0.76316 (6)	0.0356 (3)
H1	0.647 (3)	0.5457 (18)	0.585 (2)	0.017 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0190 (12)	0.0141 (11)	0.0178 (11)	−0.0010 (8)	0.0013 (9)	−0.0029 (9)
C2	0.0169 (12)	0.0171 (12)	0.0225 (12)	−0.0005 (9)	−0.0019 (9)	−0.0001 (9)
C3	0.0289 (14)	0.0171 (12)	0.0202 (13)	0.0006 (10)	−0.0053 (10)	0.0011 (9)
C4	0.0305 (15)	0.0193 (12)	0.0195 (13)	−0.0011 (10)	0.0068 (11)	0.0018 (10)
C5	0.0170 (12)	0.0185 (12)	0.0288 (13)	−0.0018 (9)	0.0041 (10)	−0.0033 (10)
C6	0.0191 (12)	0.0184 (12)	0.0196 (12)	0.0006 (9)	−0.0019 (10)	−0.0019 (9)
C7	0.0242 (13)	0.0164 (12)	0.0194 (12)	−0.0042 (9)	−0.0008 (10)	0.0030 (9)
C8	0.0254 (13)	0.0159 (12)	0.0229 (13)	0.0000 (10)	0.0012 (10)	0.0023 (9)
C9	0.0360 (15)	0.0178 (13)	0.0224 (14)	−0.0012 (10)	−0.0033 (11)	0.0012 (9)
C10	0.0322 (15)	0.0249 (14)	0.0322 (15)	−0.0020 (11)	−0.0100 (12)	0.0009 (11)
C11	0.0212 (13)	0.0273 (14)	0.0395 (16)	−0.0026 (10)	−0.0032 (12)	−0.0011 (12)
C12	0.0243 (13)	0.0208 (13)	0.0296 (14)	−0.0044 (10)	0.0044 (10)	−0.0020 (10)
C13	0.0300 (15)	0.0337 (15)	0.0235 (14)	0.0046 (11)	0.0012 (11)	−0.0033 (11)
C14	0.0444 (18)	0.0376 (17)	0.0225 (14)	0.0008 (13)	−0.0048 (13)	−0.0040 (12)
N1	0.0201 (11)	0.0197 (11)	0.0183 (10)	−0.0014 (8)	0.0001 (8)	0.0010 (8)
O1	0.0220 (9)	0.0251 (10)	0.0243 (9)	−0.0009 (7)	0.0067 (7)	−0.0038 (7)
O2	0.0294 (10)	0.0275 (10)	0.0153 (9)	−0.0031 (7)	−0.0014 (7)	−0.0009 (7)
S1	0.0193 (4)	0.0196 (4)	0.0144 (4)	−0.0022 (2)	0.0020 (3)	−0.0011 (2)
CL1	0.0443 (5)	0.0343 (5)	0.0270 (5)	−0.0034 (3)	−0.0159 (3)	0.0102 (3)
CL2	0.0172 (4)	0.0395 (5)	0.0504 (5)	−0.0054 (2)	0.0073 (3)	0.0049 (3)

Geometric parameters (Å, º)

C1—C2	1.385 (3)	C9—C10	1.382 (4)
C1—C6	1.392 (3)	C9—C14	1.512 (4)
C1—S1	1.776 (2)	C10—C11	1.384 (4)
C2—C3	1.379 (4)	C10—H10	0.9500
C2—H2	0.9500	C11—C12	1.380 (4)
C3—C4	1.379 (4)	C11—H11	0.9500
C3—CL1	1.741 (3)	C12—H12	0.9500
C4—C5	1.387 (4)	C13—H13A	0.9800
C4—H4	0.9500	C13—H13B	0.9800
C5—C6	1.383 (3)	C13—H13C	0.9800
C5—CL2	1.734 (2)	C14—H14A	0.9800
C6—H6	0.9500	C14—H14B	0.9800
C7—C12	1.390 (4)	C14—H14C	0.9800
C7—C8	1.398 (4)	N1—S1	1.630 (2)
C7—N1	1.446 (3)	N1—H1	0.862 (17)
C8—C9	1.410 (4)	O1—S1	1.4285 (18)
C8—C13	1.501 (4)	O2—S1	1.4346 (19)
C2—C1—C6	122.4 (2)	C11—C10—H10	119.3
C2—C1—S1	117.50 (17)	C12—C11—C10	119.8 (2)
C6—C1—S1	120.02 (18)	C12—C11—H11	120.1
C3—C2—C1	117.6 (2)	C10—C11—H11	120.1

C3—C2—H2	121.2	C11—C12—C7	119.4 (2)
C1—C2—H2	121.2	C11—C12—H12	120.3
C2—C3—C4	122.5 (2)	C7—C12—H12	120.3
C2—C3—CL1	118.3 (2)	C8—C13—H13A	109.5
C4—C3—CL1	119.19 (19)	C8—C13—H13B	109.5
C3—C4—C5	117.8 (2)	H13A—C13—H13B	109.5
C3—C4—H4	121.1	C8—C13—H13C	109.5
C5—C4—H4	121.1	H13A—C13—H13C	109.5
C6—C5—C4	122.4 (2)	H13B—C13—H13C	109.5
C6—C5—CL2	119.05 (19)	C9—C14—H14A	109.5
C4—C5—CL2	118.49 (19)	C9—C14—H14B	109.5
C5—C6—C1	117.1 (2)	H14A—C14—H14B	109.5
C5—C6—H6	121.4	C9—C14—H14C	109.5
C1—C6—H6	121.4	H14A—C14—H14C	109.5
C12—C7—C8	121.8 (2)	H14B—C14—H14C	109.5
C12—C7—N1	117.5 (2)	C7—N1—S1	119.12 (16)
C8—C7—N1	120.7 (2)	C7—N1—H1	113.9 (19)
C7—C8—C9	117.8 (2)	S1—N1—H1	111.8 (19)
C7—C8—C13	122.1 (2)	O1—S1—O2	119.99 (11)
C9—C8—C13	120.1 (2)	O1—S1—N1	108.44 (11)
C10—C9—C8	119.8 (2)	O2—S1—N1	106.30 (11)
C10—C9—C14	119.9 (3)	O1—S1—C1	106.41 (11)
C8—C9—C14	120.3 (2)	O2—S1—C1	108.61 (11)
C9—C10—C11	121.4 (3)	N1—S1—C1	106.38 (10)
C9—C10—H10	119.3		

C6—C1—C2—C3	0.2 (3)	C13—C8—C9—C14	0.9 (4)
S1—C1—C2—C3	177.68 (17)	C8—C9—C10—C11	0.5 (4)
C1—C2—C3—C4	1.5 (4)	C14—C9—C10—C11	179.3 (3)
C1—C2—C3—CL1	−179.10 (18)	C9—C10—C11—C12	−0.5 (4)
C2—C3—C4—C5	−1.3 (4)	C10—C11—C12—C7	0.0 (4)
CL1—C3—C4—C5	179.28 (19)	C8—C7—C12—C11	0.5 (4)
C3—C4—C5—C6	−0.6 (4)	N1—C7—C12—C11	−179.2 (2)
C3—C4—C5—CL2	178.04 (19)	C12—C7—N1—S1	76.0 (3)
C4—C5—C6—C1	2.2 (4)	C8—C7—N1—S1	−103.7 (2)
CL2—C5—C6—C1	−176.42 (17)	C7—N1—S1—O1	−53.25 (19)
C2—C1—C6—C5	−2.0 (3)	C7—N1—S1—O2	176.48 (17)
S1—C1—C6—C5	−179.40 (17)	C7—N1—S1—C1	60.9 (2)
C12—C7—C8—C9	−0.4 (4)	C2—C1—S1—O1	36.2 (2)
N1—C7—C8—C9	179.3 (2)	C6—C1—S1—O1	−146.31 (18)
C12—C7—C8—C13	179.9 (2)	C2—C1—S1—O2	166.63 (17)
N1—C7—C8—C13	−0.4 (4)	C6—C1—S1—O2	−15.9 (2)
C7—C8—C9—C10	−0.1 (4)	C2—C1—S1—N1	−79.3 (2)
C13—C8—C9—C10	179.6 (2)	C6—C1—S1—N1	98.2 (2)
C7—C8—C9—C14	−178.8 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.14	2.9590	159
C4—H4···O1^{ii}	0.95	2.41	3.332 (3)	164

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

(II) 3,5-Dichloro-*N*-(2,6-dimethylphenyl)benzenesulfonamide

Crystal data

$C_{14}H_{13}Cl_2NO_2S$
M_r = 330.21
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.4817 (15) Å
b = 8.6149 (15) Å
c = 12.167 (2) Å
α = 109.875 (5)°
β = 91.900 (5)°
γ = 114.190 (5)°
V = 747.1 (2) Å^3
Z = 2
F(000) = 340
Prism
D_x = 1.468 Mg m^{-3}
Melting point: 445 K
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 127 reflections
θ = 7.7–63.7°
μ = 5.22 mm^{-1}
T = 100 K
Prism, colourless
0.29 × 0.26 × 0.22 mm

Data collection

Bruker APEXII CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and *φ* scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.275, T_{max} = 0.317
6977 measured reflections
2400 independent reflections
1960 reflections with $I > 2\sigma(I)$
R_{int} = 0.124
θ_{max} = 63.7°, θ_{min} = 7.7°
h = −9→9
k = −9→9
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.233
S = 1.02
2400 reflections
187 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1757P)^2 + 0.6254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8417 (4)	0.5358 (5)	0.1002 (4)	0.0203 (9)

C2	0.7459 (5)	0.3554 (5)	0.0217 (4)	0.0241 (10)
H2	0.644651	0.320522	−0.034335	0.029*
C3	0.8001 (5)	0.2253 (6)	0.0260 (4)	0.0249 (10)
C4	0.9467 (5)	0.2750 (6)	0.1103 (4)	0.0293 (11)
H4	0.981555	0.185462	0.115199	0.035*
C5	1.0386 (5)	0.4578 (6)	0.1860 (4)	0.0244 (9)
C6	0.9904 (5)	0.5912 (6)	0.1831 (4)	0.0238 (10)
H6	1.056523	0.716677	0.235918	0.029*
C7	0.6763 (5)	0.7502 (5)	0.3150 (4)	0.0211 (9)
C8	0.6651 (5)	0.6237 (6)	0.3668 (4)	0.0236 (9)
C9	0.7175 (5)	0.6907 (7)	0.4904 (5)	0.0317 (10)
H9	0.712684	0.607766	0.526909	0.038*
C10	0.7765 (7)	0.8761 (8)	0.5608 (5)	0.0444 (13)
H10	0.813297	0.919881	0.644715	0.053*
C11	0.7815 (7)	0.9971 (7)	0.5082 (5)	0.0438 (13)
H11	0.821341	1.123758	0.557153	0.053*
C12	0.7300 (6)	0.9386 (6)	0.3863 (4)	0.0316 (10)
C13	0.5959 (5)	0.4220 (6)	0.2945 (4)	0.0310 (11)
H13A	0.693639	0.395208	0.269174	0.046*
H13B	0.509594	0.386272	0.223963	0.046*
H13C	0.539097	0.352168	0.342708	0.046*
C14	0.7304 (8)	1.0734 (7)	0.3333 (6)	0.0472 (14)
H14A	0.728356	1.180297	0.395426	0.071*
H14B	0.626024	1.013250	0.269485	0.071*
H14C	0.837145	1.114337	0.300552	0.071*
N1	0.6231 (4)	0.6893 (4)	0.1889 (3)	0.0201 (8)
O1	0.9163 (3)	0.8797 (4)	0.1562 (3)	0.0251 (7)
O2	0.6731 (3)	0.6436 (4)	−0.0152 (3)	0.0230 (7)
S1	0.76785 (10)	0.70217 (12)	0.10237 (9)	0.0183 (4)
CL1	0.68515 (13)	−0.00070 (13)	−0.07437 (12)	0.0365 (4)
CL2	1.22462 (13)	0.52449 (17)	0.28944 (10)	0.0372 (4)
H1	0.529 (4)	0.590 (4)	0.154 (4)	0.029 (13)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0210 (17)	0.0232 (19)	0.021 (2)	0.0095 (15)	0.0048 (14)	0.0138 (18)
C2	0.0242 (19)	0.028 (2)	0.026 (3)	0.0125 (17)	0.0086 (16)	0.015 (2)
C3	0.0255 (19)	0.025 (2)	0.030 (3)	0.0108 (16)	0.0127 (17)	0.017 (2)
C4	0.036 (2)	0.037 (2)	0.036 (3)	0.0227 (19)	0.018 (2)	0.028 (2)
C5	0.0274 (19)	0.036 (2)	0.020 (3)	0.0176 (17)	0.0061 (16)	0.017 (2)
C6	0.0248 (19)	0.031 (2)	0.021 (3)	0.0132 (17)	0.0061 (16)	0.0152 (19)
C7	0.0243 (18)	0.023 (2)	0.017 (2)	0.0111 (15)	0.0018 (14)	0.0093 (18)
C8	0.0214 (18)	0.027 (2)	0.027 (3)	0.0112 (16)	0.0060 (15)	0.0163 (19)
C9	0.036 (2)	0.039 (2)	0.028 (3)	0.0152 (19)	0.0064 (17)	0.024 (2)
C10	0.054 (3)	0.047 (3)	0.016 (3)	0.009 (2)	0.002 (2)	0.011 (2)
C11	0.071 (3)	0.025 (2)	0.019 (3)	0.012 (2)	0.004 (2)	0.003 (2)
C12	0.046 (2)	0.026 (2)	0.018 (3)	0.0152 (18)	0.0054 (17)	0.0052 (19)

C13	0.037 (2)	0.037 (2)	0.035 (3)	0.0208 (19)	0.0160 (18)	0.025 (2)
C14	0.084 (4)	0.028 (2)	0.038 (4)	0.032 (2)	0.014 (3)	0.014 (2)
N1	0.0240 (16)	0.0213 (17)	0.014 (2)	0.0091 (14)	0.0001 (13)	0.0080 (15)
O1	0.0289 (14)	0.0217 (14)	0.0246 (19)	0.0094 (12)	0.0039 (11)	0.0114 (13)
O2	0.0277 (13)	0.0266 (15)	0.0197 (19)	0.0136 (11)	0.0048 (11)	0.0128 (13)
S1	0.0223 (6)	0.0178 (6)	0.0160 (7)	0.0090 (4)	0.0011 (4)	0.0080 (5)
CL1	0.0340 (6)	0.0203 (6)	0.0533 (10)	0.0120 (5)	0.0106 (5)	0.0121 (6)
CL2	0.0392 (7)	0.0598 (8)	0.0266 (8)	0.0335 (6)	0.0034 (5)	0.0189 (6)

Geometric parameters (Å, º)

C1—C2	1.375 (6)	C9—C10	1.386 (8)
C1—C6	1.389 (6)	C9—H9	0.9500
C1—S1	1.777 (4)	C10—C11	1.385 (8)
C2—C3	1.390 (6)	C10—H10	0.9500
C2—H2	0.9500	C11—C12	1.383 (7)
C3—C4	1.401 (6)	C11—H11	0.9500
C3—CL1	1.726 (4)	C12—C14	1.506 (7)
C4—C5	1.377 (6)	C13—H13A	0.9800
C4—H4	0.9500	C13—H13B	0.9800
C5—C6	1.379 (6)	C13—H13C	0.9800
C5—CL2	1.743 (4)	C14—H14A	0.9800
C6—H6	0.9500	C14—H14B	0.9800
C7—C8	1.407 (6)	C14—H14C	0.9800
C7—C12	1.417 (6)	N1—S1	1.638 (3)
C7—N1	1.430 (5)	N1—H1	0.85 (2)
C8—C9	1.395 (6)	O1—S1	1.428 (3)
C8—C13	1.493 (6)	O2—S1	1.431 (3)
C2—C1—C6	122.0 (4)	C11—C10—H10	120.2
C2—C1—S1	119.5 (3)	C12—C11—C10	121.8 (5)
C6—C1—S1	118.3 (3)	C12—C11—H11	119.1
C1—C2—C3	118.7 (4)	C10—C11—H11	119.1
C1—C2—H2	120.7	C11—C12—C7	117.9 (5)
C3—C2—H2	120.7	C11—C12—C14	120.1 (4)
C2—C3—C4	120.9 (4)	C7—C12—C14	122.0 (4)
C2—C3—CL1	119.4 (3)	C8—C13—H13A	109.5
C4—C3—CL1	119.6 (3)	C8—C13—H13B	109.5
C5—C4—C3	117.8 (4)	H13A—C13—H13B	109.5
C5—C4—H4	121.1	C8—C13—H13C	109.5
C3—C4—H4	121.1	H13A—C13—H13C	109.5
C6—C5—C4	122.8 (4)	H13B—C13—H13C	109.5
C6—C5—CL2	118.4 (3)	C12—C14—H14A	109.5
C4—C5—CL2	118.8 (3)	C12—C14—H14B	109.5
C5—C6—C1	117.6 (4)	H14A—C14—H14B	109.5
C5—C6—H6	121.2	C12—C14—H14C	109.5
C1—C6—H6	121.2	H14A—C14—H14C	109.5
C8—C7—C12	121.2 (4)	H14B—C14—H14C	109.5

C8—C7—N1	120.7 (4)	C7—N1—S1	120.9 (2)
C12—C7—N1	118.0 (4)	C7—N1—H1	118 (4)
C9—C8—C7	118.2 (4)	S1—N1—H1	109 (3)
C9—C8—C13	119.6 (4)	O1—S1—O2	120.06 (18)
C7—C8—C13	122.2 (4)	O1—S1—N1	108.41 (17)
C10—C9—C8	121.2 (5)	O2—S1—N1	106.27 (16)
C10—C9—H9	119.4	O1—S1—C1	107.28 (17)
C8—C9—H9	119.4	O2—S1—C1	107.33 (18)
C9—C10—C11	119.6 (5)	N1—S1—C1	106.81 (17)
C9—C10—H10	120.2		

C6—C1—C2—C3	0.1 (6)	C9—C10—C11—C12	−0.4 (8)
S1—C1—C2—C3	−176.4 (3)	C10—C11—C12—C7	−1.9 (8)
C1—C2—C3—C4	1.6 (6)	C10—C11—C12—C14	177.5 (5)
C1—C2—C3—CL1	−178.3 (3)	C8—C7—C12—C11	3.8 (6)
C2—C3—C4—C5	−2.2 (6)	N1—C7—C12—C11	180.0 (4)
CL1—C3—C4—C5	177.7 (3)	C8—C7—C12—C14	−175.5 (4)
C3—C4—C5—C6	1.1 (6)	N1—C7—C12—C14	0.7 (6)
C3—C4—C5—CL2	−178.5 (3)	C8—C7—N1—S1	−96.3 (4)
C4—C5—C6—C1	0.5 (6)	C12—C7—N1—S1	87.5 (4)
CL2—C5—C6—C1	−179.9 (3)	C7—N1—S1—O1	−45.5 (3)
C2—C1—C6—C5	−1.1 (6)	C7—N1—S1—O2	−175.8 (3)
S1—C1—C6—C5	175.4 (3)	C7—N1—S1—C1	69.8 (3)
C12—C7—C8—C9	−3.4 (5)	C2—C1—S1—O1	−159.3 (3)
N1—C7—C8—C9	−179.5 (3)	C6—C1—S1—O1	24.1 (4)
C12—C7—C8—C13	175.3 (4)	C2—C1—S1—O2	−29.0 (4)
N1—C7—C8—C13	−0.8 (5)	C6—C1—S1—O2	154.4 (3)
C7—C8—C9—C10	1.0 (6)	C2—C1—S1—N1	84.6 (4)
C13—C8—C9—C10	−177.7 (4)	C6—C1—S1—N1	−92.0 (3)
C8—C9—C10—C11	0.9 (7)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14*C*···O1	0.98	2.53	3.139 (8)	120
N1—H1···O2^{i}	0.85 (4)	2.12 (4)	2.937 (5)	160 (4)
C13—H13*A*···*Cg*1	0.98	2.67	3.493 (5)	142

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

(III) 3,5-dichloro-*N*-(3,5-dimethylphenyl)benzenesulfonamide

Crystal data

$C_{14}H_{13}Cl_2NO_2S$	*c* = 17.3130 (8) Å
M_r = 330.21	*β* = 100.409 (1)°
Monoclinic, $P2_1/c$	*V* = 1465.70 (12) Å^3
Hall symbol: -P 2ybc	*Z* = 4
a = 12.2268 (6) Å	*F*(000) = 680
b = 7.0399 (3) Å	Prism

D_x = 1.496 Mg m^{-3}
Melting point: 462 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 128 reflections
θ = 6.8–64.4°

μ = 5.32 mm^{-1}
T = 100 K
Prism, colourless
0.27 × 0.24 × 0.21 mm

Data collection

Bruker APEXII CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (SADABS; Bruker,2009)
T_{min} = 0.297, T_{max} = 0.327

11468 measured reflections
2412 independent reflections
2374 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 64.4°, θ_{min} = 6.8°
h = −14→14
k = −8→7
l = −19→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.152
S = 0.99
2412 reflections
187 parameters
1 restraint

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1156P)^2 + 2.094P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.4234 (2)	0.1933 (4)	0.62264 (15)	0.0107 (6)
C2	0.5280 (2)	0.2511 (4)	0.61112 (15)	0.0120 (6)
H2	0.586016	0.277777	0.654187	0.014*
C3	0.5443 (2)	0.2682 (4)	0.53442 (15)	0.0120 (6)
C4	0.4606 (2)	0.2341 (4)	0.47057 (15)	0.0138 (6)
H4	0.473647	0.246812	0.418356	0.017*
C5	0.3574 (2)	0.1810 (4)	0.48539 (16)	0.0133 (6)
C6	0.3366 (2)	0.1572 (4)	0.56068 (16)	0.0128 (6)
H6	0.265674	0.117738	0.569706	0.015*
C7	0.2216 (2)	0.4234 (4)	0.69407 (14)	0.0108 (6)
C8	0.2040 (2)	0.5888 (4)	0.64942 (15)	0.0126 (6)
H8	0.264930	0.668527	0.644084	0.015*
C9	0.0966 (2)	0.6368 (4)	0.61262 (16)	0.0146 (6)
C10	0.0089 (2)	0.5168 (4)	0.62049 (15)	0.0161 (6)
H10	−0.063981	0.547186	0.593959	0.019*
C11	0.0254 (2)	0.3533 (4)	0.66637 (16)	0.0144 (6)
C12	0.1329 (2)	0.3073 (4)	0.70360 (15)	0.0124 (6)

H12	0.145662	0.196778	0.735448	0.015*
C13	0.0756 (3)	0.8176 (4)	0.5651 (2)	0.0242 (7)
H13A	−0.000712	0.816863	0.535489	0.036*
H13B	0.127963	0.825736	0.528605	0.036*
H13C	0.085778	0.927260	0.600562	0.036*
C14	−0.0718 (2)	0.2318 (5)	0.67730 (18)	0.0244 (7)
H14A	−0.117650	0.300752	0.708934	0.037*
H14B	−0.044640	0.113872	0.704178	0.037*
H14C	−0.116566	0.201609	0.625895	0.037*
N1	0.33273 (18)	0.3807 (3)	0.73296 (12)	0.0111 (5)
O1	0.49846 (16)	0.1842 (3)	0.77286 (11)	0.0169 (5)
O2	0.31742 (16)	0.0286 (3)	0.72152 (11)	0.0159 (5)
S1	0.39385 (5)	0.18095 (9)	0.71907 (3)	0.0102 (3)
CL1	0.67420 (5)	0.33657 (9)	0.51672 (4)	0.0189 (3)
CL2	0.24931 (6)	0.14477 (11)	0.40666 (4)	0.0212 (3)
H1	0.379 (3)	0.475 (4)	0.739 (2)	0.027 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0138 (14)	0.0084 (12)	0.0104 (13)	0.0043 (10)	0.0040 (10)	0.0001 (9)
C2	0.0122 (13)	0.0108 (14)	0.0122 (13)	0.0013 (10)	0.0003 (10)	0.0004 (10)
C3	0.0135 (13)	0.0064 (13)	0.0175 (14)	0.0022 (10)	0.0066 (11)	0.0016 (10)
C4	0.0214 (14)	0.0108 (13)	0.0105 (13)	0.0039 (11)	0.0067 (11)	0.0022 (10)
C5	0.0161 (14)	0.0116 (14)	0.0111 (14)	0.0037 (10)	−0.0010 (11)	−0.0026 (10)
C6	0.0122 (13)	0.0117 (13)	0.0153 (14)	−0.0003 (9)	0.0043 (11)	0.0001 (10)
C7	0.0122 (13)	0.0148 (14)	0.0060 (11)	0.0012 (10)	0.0036 (10)	−0.0044 (10)
C8	0.0132 (13)	0.0133 (13)	0.0131 (13)	−0.0017 (10)	0.0071 (10)	−0.0018 (10)
C9	0.0170 (14)	0.0159 (14)	0.0116 (13)	0.0027 (11)	0.0044 (11)	0.0020 (10)
C10	0.0122 (13)	0.0231 (15)	0.0124 (13)	0.0024 (11)	0.0004 (10)	0.0007 (11)
C11	0.0137 (14)	0.0188 (14)	0.0109 (13)	−0.0026 (11)	0.0027 (11)	−0.0014 (10)
C12	0.0142 (13)	0.0157 (14)	0.0072 (12)	0.0007 (10)	0.0019 (10)	0.0006 (10)
C13	0.0195 (15)	0.0220 (16)	0.0321 (18)	0.0041 (12)	0.0072 (13)	0.0111 (13)
C14	0.0128 (13)	0.0310 (17)	0.0271 (16)	−0.0065 (13)	−0.0021 (12)	0.0065 (13)
N1	0.0103 (11)	0.0123 (12)	0.0108 (11)	−0.0017 (9)	0.0021 (9)	−0.0031 (9)
O1	0.0134 (10)	0.0264 (11)	0.0097 (10)	0.0052 (8)	−0.0014 (8)	0.0020 (8)
O2	0.0191 (10)	0.0123 (10)	0.0179 (10)	−0.0004 (8)	0.0072 (8)	0.0037 (7)
S1	0.0103 (4)	0.0134 (4)	0.0068 (4)	0.0015 (2)	0.0015 (3)	0.0016 (2)
CL1	0.0142 (4)	0.0199 (4)	0.0255 (5)	−0.0004 (2)	0.0112 (3)	0.0027 (2)
CL2	0.0202 (4)	0.0311 (5)	0.0103 (4)	−0.0013 (3)	−0.0029 (3)	−0.0028 (3)

Geometric parameters (Å, º)

C1—C6	1.389 (4)	C9—C10	1.391 (4)
C1—C2	1.391 (4)	C9—C13	1.512 (4)
C1—S1	1.773 (3)	C10—C11	1.393 (4)
C2—C3	1.383 (4)	C10—H10	0.9500
C2—H2	0.9500	C11—C12	1.394 (4)

C3—C4	1.385 (4)	C11—C14	1.504 (4)
C3—CL1	1.739 (3)	C12—H12	0.9500
C4—C5	1.385 (4)	C13—H13A	0.9800
C4—H4	0.9500	C13—H13B	0.9800
C5—C6	1.382 (4)	C13—H13C	0.9800
C5—CL2	1.737 (3)	C14—H14A	0.9800
C6—H6	0.9500	C14—H14B	0.9800
C7—C12	1.392 (4)	C14—H14C	0.9800
C7—C8	1.393 (4)	N1—S1	1.631 (2)
C7—N1	1.435 (3)	N1—H1	0.869 (19)
C8—C9	1.394 (4)	O1—S1	1.440 (2)
C8—H8	0.9500	O2—S1	1.428 (2)

C6—C1—C2	122.5 (2)	C11—C10—H10	119.2
C6—C1—S1	117.4 (2)	C10—C11—C12	118.9 (3)
C2—C1—S1	119.9 (2)	C10—C11—C14	120.3 (3)
C3—C2—C1	117.3 (2)	C12—C11—C14	120.7 (3)
C3—C2—H2	121.4	C7—C12—C11	119.9 (2)
C1—C2—H2	121.4	C7—C12—H12	120.0
C4—C3—C2	122.6 (2)	C11—C12—H12	120.0
C4—C3—CL1	118.27 (19)	C9—C13—H13A	109.5
C2—C3—CL1	119.2 (2)	C9—C13—H13B	109.5
C3—C4—C5	117.7 (2)	H13A—C13—H13B	109.5
C3—C4—H4	121.1	C9—C13—H13C	109.5
C5—C4—H4	121.1	H13A—C13—H13C	109.5
C6—C5—C4	122.4 (3)	H13B—C13—H13C	109.5
C6—C5—CL2	118.6 (2)	C11—C14—H14A	109.5
C4—C5—CL2	118.9 (2)	C11—C14—H14B	109.5
C5—C6—C1	117.5 (3)	H14A—C14—H14B	109.5
C5—C6—H6	121.3	C11—C14—H14C	109.5
C1—C6—H6	121.3	H14A—C14—H14C	109.5
C12—C7—C8	120.8 (2)	H14B—C14—H14C	109.5
C12—C7—N1	120.9 (2)	C7—N1—S1	122.12 (18)
C8—C7—N1	118.3 (2)	C7—N1—H1	116 (2)
C7—C8—C9	119.7 (2)	S1—N1—H1	112 (2)
C7—C8—H8	120.2	O2—S1—O1	120.14 (12)
C9—C8—H8	120.2	O2—S1—N1	108.89 (11)
C10—C9—C8	119.2 (2)	O1—S1—N1	105.56 (11)
C10—C9—C13	120.4 (3)	O2—S1—C1	108.09 (12)
C8—C9—C13	120.4 (3)	O1—S1—C1	107.45 (12)
C9—C10—C11	121.5 (2)	N1—S1—C1	105.85 (11)
C9—C10—H10	119.2		

C6—C1—C2—C3	−1.3 (4)	C9—C10—C11—C12	−1.5 (4)
S1—C1—C2—C3	−176.48 (19)	C9—C10—C11—C14	176.7 (3)
C1—C2—C3—C4	1.4 (4)	C8—C7—C12—C11	1.9 (4)
C1—C2—C3—CL1	−179.05 (19)	N1—C7—C12—C11	178.9 (2)
C2—C3—C4—C5	0.0 (4)	C10—C11—C12—C7	−0.5 (4)

CL1—C3—C4—C5	−179.60 (19)	C14—C11—C12—C7	−178.7 (2)
C3—C4—C5—C6	−1.5 (4)	C12—C7—N1—S1	59.0 (3)
C3—C4—C5—CL2	177.90 (19)	C8—C7—N1—S1	−123.9 (2)
C4—C5—C6—C1	1.5 (4)	C7—N1—S1—O2	−44.7 (2)
CL2—C5—C6—C1	−177.86 (19)	C7—N1—S1—O1	−174.93 (19)
C2—C1—C6—C5	−0.1 (4)	C7—N1—S1—C1	71.3 (2)
S1—C1—C6—C5	175.20 (19)	C6—C1—S1—O2	37.4 (2)
C12—C7—C8—C9	−1.2 (4)	C2—C1—S1—O2	−147.2 (2)
N1—C7—C8—C9	−178.3 (2)	C6—C1—S1—O1	168.42 (19)
C7—C8—C9—C10	−0.7 (4)	C2—C1—S1—O1	−16.2 (2)
C7—C8—C9—C13	178.9 (2)	C6—C1—S1—N1	−79.1 (2)
C8—C9—C10—C11	2.1 (4)	C2—C1—S1—N1	96.2 (2)
C13—C9—C10—C11	−177.5 (3)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the aniline ring C7–C12

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.87	2.13	2.9848	167
C14—H14*B*···*Cg*2^{ii}	0.98	2.86	3.5135	124

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) −*x*, *y*+1/2, −*z*+1/2.