

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

4-Chloro-*N*-(3,5-dichlorophenyl)-2-methylbenzenesulfonamideVinola Z. Rodrigues,<sup>a</sup> Sabine Foro,<sup>b</sup> B. Thimme Gowda<sup>a\*</sup> and K. Shakuntala<sup>a</sup>

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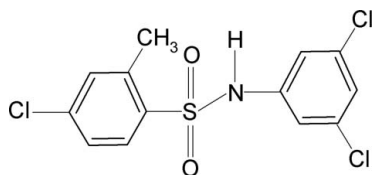
Received 19 October 2011; accepted 19 October 2011

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.140; data-to-parameter ratio = 17.0.

In the title compound,  $\text{C}_{13}\text{H}_{10}\text{Cl}_3\text{NO}_2\text{S}$ , torsion angle of the  $\text{C}-\text{SO}_2-\text{NH}-\text{C}$  group in the molecule is  $-58.57$  (26)°. The sulfonyl and aniline benzene rings are tilted relative to each other by 84.2 (1)°. The crystal structure features inversion-related dimers linked by pairs of  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds.

## Related literature

For the preparation of the title compound, see: Savitha & Gowda (2006). For the hydrogen-bonding preferences of sulfonamides, see: Adsmund & Grant (2001). For studies of the effects of substituents on the structure and other aspects of *N*-(aryl)amides, see: Gowda *et al.* (2000); of *N*-(aryl)methanesulfonamides, see: Gowda *et al.* (2007); of *N*-(aryl)arylsulfonamides, see: Gelbrich *et al.* (2007); Perlovich *et al.* (2006); Rodrigues *et al.* (2011); Shetty & Gowda (2005); and of *N*-(chloro)arylsulfonamides, see: Gowda *et al.* (2004).



## Experimental

## Crystal data

$\text{C}_{13}\text{H}_{10}\text{Cl}_3\text{NO}_2\text{S}$   
 $M_r = 350.63$   
Triclinic,  $P\bar{1}$   
 $a = 7.9638$  (8) Å

$b = 8.8494$  (9) Å  
 $c = 11.649$  (1) Å  
 $\alpha = 97.002$  (8)°  
 $\beta = 102.726$  (9)°

$\gamma = 100.408$  (9)°  
 $V = 776.35$  (13) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation

$\mu = 0.72$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.44 \times 0.42 \times 0.36$  mm

## Data collection

Oxford Xcalibur diffractometer  
with a Sapphire CCD detector  
Absorption correction: multi-scan  
(*CrysAlis RED*; Oxford  
Diffraction, 2009)  
 $T_{\min} = 0.742$ ,  $T_{\max} = 0.781$

5369 measured reflections  
3137 independent reflections  
2649 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.009$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.140$   
 $S = 1.06$   
3137 reflections  
185 parameters  
1 restraint

H atoms treated by a mixture of  
independent and constrained  
refinement  
 $\Delta\rho_{\text{max}} = 0.44$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.47$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O1}^i$	0.83 (2)	2.06 (2)	2.884 (3)	172 (3)

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

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*.

VZR thanks the University Grants Commission, Government of India, New Delhi, for the award of an RFSMS fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5682).

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## supporting information

*Acta Cryst.* (2011). E67, o3066 [doi:10.1107/S1600536811043327]

## 4-Chloro-*N*-(3,5-dichlorophenyl)-2-methylbenzenesulfonamide

Vinola Z. Rodrigues, Sabine Foro, B. Thimme Gowda and K. Shakuntala

### S1. Comment

The sulfonamide moiety is a constituent of many biologically significant compounds. The hydrogen bonding preferences of sulfonamides have been investigated (Admond & Grant, 2001). As part of our studies on the effects of substituents on the structures and other aspects of *N*-(aryl)-amides (Gowda *et al.*, 2000), *N*-(aryl)-methanesulfonamides (Gowda *et al.*, 2007), *N*-(aryl)-arylsulfonamides (Rodrigues *et al.*, 2011; Shetty & Gowda, 2005) and *N*-(chloro)-arylsulfonamides (Gowda *et al.*, 2004), in the present work, the crystal structure of 4-Chloro-2-methyl-*N*-(3,5-dichlorophenyl)benzenesulfonamide (I) has been determined (Fig. 1).

In (I), the conformation of the N—C bond in the C—SO<sub>2</sub>—NH—C segment has *trans* and *gauche* torsion angles with the S=O bonds. Further, the N—H bond is *syn* to the *ortho*-methyl group in the sulfonyl benzene ring and to one of the *meta*-Cl atoms in the anilino ring of (I).

The molecule is bent at the S atom with the C—SO<sub>2</sub>—NH—C torsion angle of -58.57 (26)°, compared to the value of -49.42 (23)° in 4-Chloro-2-methyl-*N*-(3,4-dichlorophenyl)benzenesulfonamide (II) (Rodrigues *et al.*, 2011).

The sulfonyl and the aniline benzene rings are tilted relative to each other by 84.2 (1)°, compared to the value of 54.6 (1)° in (II).

The other bond parameters in (I) are similar to those observed in (II) and other aryl sulfonamides (Perlovich *et al.*, 2006; Gelbrich *et al.*, 2007).

In the crystal, the intermolecular N—H···O hydrogen bonds (Table 1) link the molecules into dimeric chains. Part of the crystal structure is shown in Fig. 2.

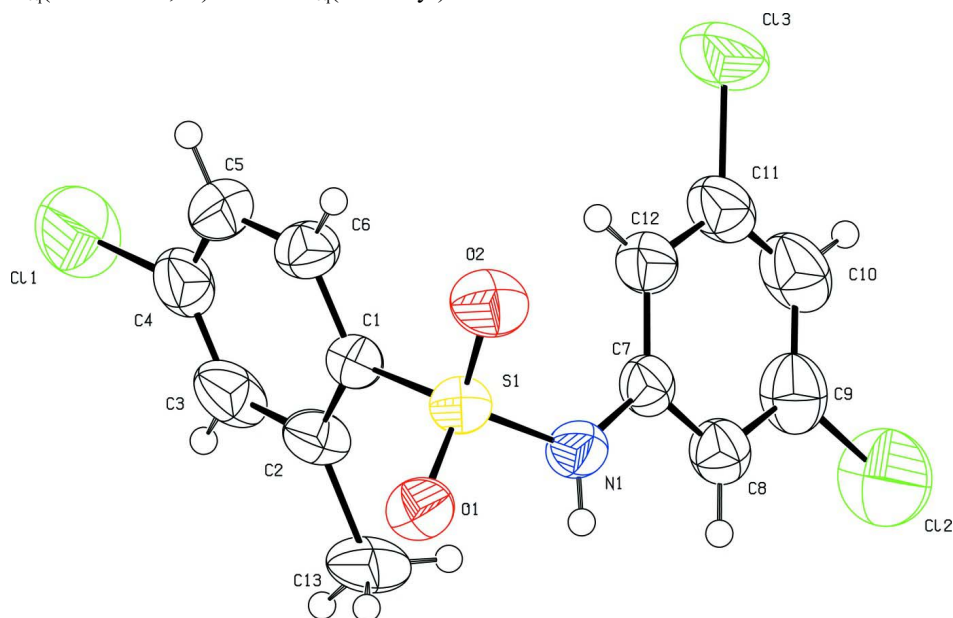
### S2. Experimental

The solution of *m*-chlorotoluene (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-methyl-4-chlorobenzenesulfonylchloride was treated with 3,5-dichlorolaniline in the stoichiometric ratio and boiled for 10 min. The reaction mixture was then cooled to room temperature and added to ice cold water (100 ml). The resultant solid 4-chloro-*N*-(3,5-dichlorophenyl)-2-methylbenzenesulfonamide 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).

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

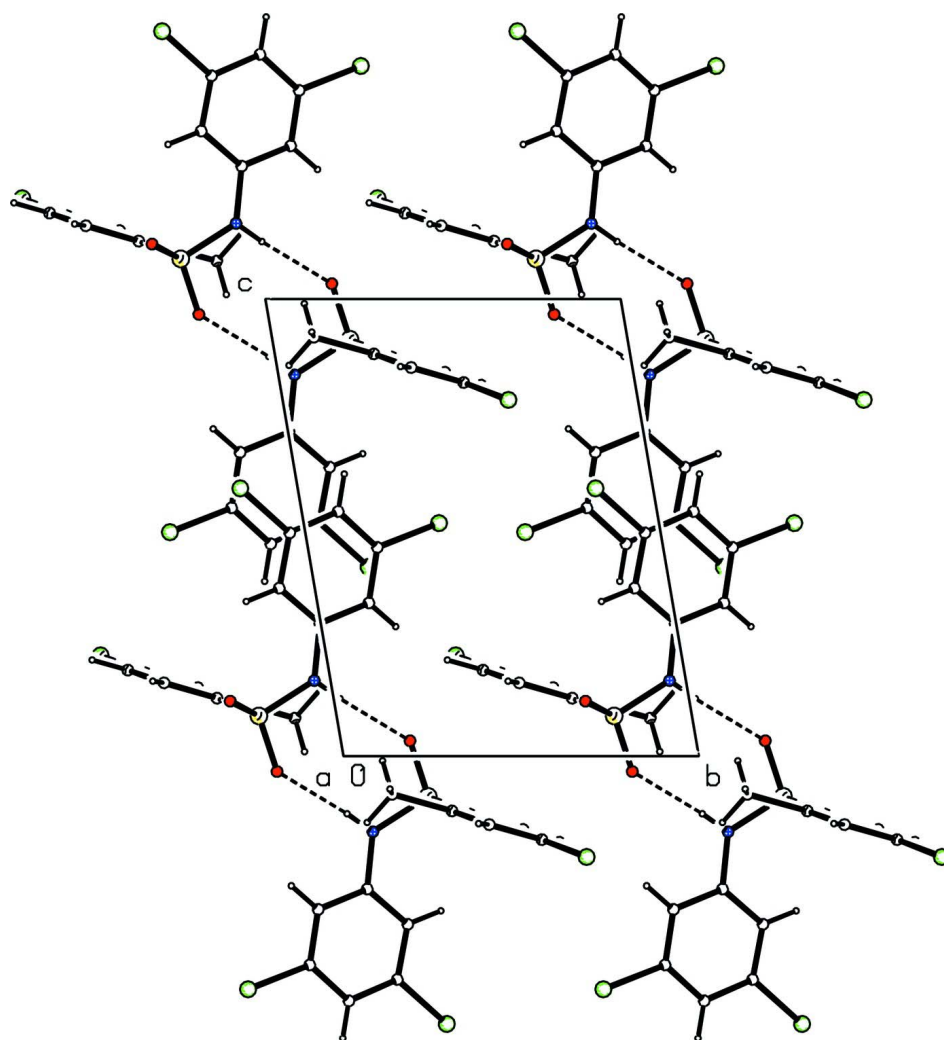
### S3. Refinement

The H atom of the NH group was located in a difference map and its coordinates were refined with the N—H distance restrained to 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. All H atoms were refined with isotropic displacement parameters  $U_{\text{iso}}(\text{H})$  set to  $1.2U_{\text{eq}}(\text{C aromatic, N})$  and  $1.5U_{\text{eq}}(\text{C methyl})$ .



**Figure 1**

Molecular structure of the title compound, showing the atom labelling scheme and displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**

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

#### 4-Chloro-*N*-(3,5-dichlorophenyl)-2-methylbenzenesulfonamide

##### Crystal data

$C_{13}H_{10}Cl_3NO_2S$

$M_r = 350.63$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.9638\ (8)\ \text{\AA}$

$b = 8.8494\ (9)\ \text{\AA}$

$c = 11.649\ (1)\ \text{\AA}$

$\alpha = 97.002\ (8)^\circ$

$\beta = 102.726\ (9)^\circ$

$\gamma = 100.408\ (9)^\circ$

$V = 776.35\ (13)\ \text{\AA}^3$

$Z = 2$

$F(000) = 356$

$D_x = 1.500\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3195 reflections

$\theta = 3.2\text{--}27.7^\circ$

$\mu = 0.72\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, colourless

$0.44 \times 0.42 \times 0.36\ \text{mm}$

*Data collection*

Oxford Xcalibur  
diffractometer with a Sapphire CCD detector  
Radiation source: fine-focus sealed tube  
Graphite monochromator  
rotation method data acquisition using  $\omega$  scans  
Absorption correction: multi-scan  
(*CrysAlis RED*; Oxford Diffraction, 2009)  
 $T_{\min} = 0.742$ ,  $T_{\max} = 0.781$

5369 measured reflections  
3137 independent reflections  
2649 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.009$   
 $\theta_{\max} = 26.4^\circ$ ,  $\theta_{\min} = 3.2^\circ$   
 $h = -9 \rightarrow 9$   
 $k = -11 \rightarrow 6$   
 $l = -14 \rightarrow 13$

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.140$   
 $S = 1.06$   
3137 reflections  
185 parameters  
1 restraint  
Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map  
Hydrogen site location: inferred from  
neighbouring sites  
H atoms treated by a mixture of independent  
and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0686P)^2 + 0.5149P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.44 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.47 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6313 (3)	0.3284 (3)	0.8732 (2)	0.0413 (5)
C2	0.7898 (3)	0.2789 (3)	0.8801 (2)	0.0520 (6)
C3	0.9242 (4)	0.3774 (4)	0.8502 (3)	0.0671 (8)
H3	1.0310	0.3479	0.8525	0.080*
C4	0.9016 (4)	0.5179 (4)	0.8174 (3)	0.0660 (8)
C5	0.7472 (4)	0.5659 (3)	0.8117 (3)	0.0643 (8)
H5	0.7342	0.6614	0.7895	0.077*
C6	0.6109 (4)	0.4700 (3)	0.8396 (2)	0.0523 (6)
H6	0.5043	0.5006	0.8359	0.063*
C7	0.3567 (3)	0.0027 (3)	0.7092 (2)	0.0473 (6)
C8	0.3722 (4)	-0.1450 (3)	0.6648 (2)	0.0549 (6)
H8	0.4155	-0.2093	0.7163	0.066*
C9	0.3226 (5)	-0.1955 (4)	0.5433 (3)	0.0707 (8)
C10	0.2603 (5)	-0.1027 (5)	0.4647 (3)	0.0769 (10)
H10	0.2280	-0.1379	0.3827	0.092*

C11	0.2473 (4)	0.0441 (4)	0.5115 (3)	0.0667 (8)
C12	0.2941 (4)	0.0998 (3)	0.6324 (2)	0.0570 (7)
H12	0.2841	0.1995	0.6617	0.068*
C13	0.8193 (4)	0.1183 (4)	0.9168 (3)	0.0657 (8)
H13A	0.7491	0.0347	0.8550	0.079*
H13B	0.7852	0.1076	0.9900	0.079*
H13C	0.9415	0.1148	0.9278	0.079*
N1	0.4035 (3)	0.0459 (3)	0.83447 (19)	0.0530 (5)
H1N	0.440 (4)	-0.018 (3)	0.874 (3)	0.064*
O1	0.5024 (3)	0.1945 (2)	1.03359 (15)	0.0547 (5)
O2	0.3065 (3)	0.2924 (3)	0.8798 (2)	0.0652 (5)
Cl1	1.07180 (15)	0.63564 (18)	0.77947 (12)	0.1240 (5)
Cl2	0.3407 (2)	-0.38086 (15)	0.49006 (10)	0.1233 (5)
Cl3	0.16476 (15)	0.16169 (14)	0.41414 (9)	0.1002 (4)
S1	0.45050 (8)	0.21891 (7)	0.91211 (5)	0.04505 (19)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0421 (12)	0.0438 (12)	0.0388 (11)	0.0124 (9)	0.0091 (9)	0.0067 (9)
C2	0.0455 (13)	0.0640 (16)	0.0511 (14)	0.0199 (12)	0.0100 (11)	0.0186 (12)
C3	0.0386 (13)	0.099 (2)	0.0649 (18)	0.0144 (14)	0.0081 (12)	0.0280 (17)
C4	0.0526 (16)	0.081 (2)	0.0532 (15)	-0.0097 (14)	0.0028 (12)	0.0232 (14)
C5	0.0736 (19)	0.0516 (16)	0.0627 (17)	0.0044 (14)	0.0087 (14)	0.0187 (13)
C6	0.0579 (15)	0.0477 (14)	0.0540 (14)	0.0182 (12)	0.0128 (12)	0.0104 (11)
C7	0.0420 (12)	0.0527 (14)	0.0440 (12)	0.0003 (10)	0.0105 (10)	0.0107 (10)
C8	0.0544 (15)	0.0579 (15)	0.0492 (14)	0.0075 (12)	0.0113 (11)	0.0066 (12)
C9	0.077 (2)	0.072 (2)	0.0558 (17)	0.0080 (16)	0.0166 (15)	-0.0060 (15)
C10	0.079 (2)	0.100 (3)	0.0421 (15)	0.0053 (19)	0.0079 (14)	0.0072 (16)
C11	0.0576 (17)	0.086 (2)	0.0512 (15)	0.0018 (15)	0.0064 (13)	0.0256 (15)
C12	0.0555 (15)	0.0586 (16)	0.0530 (15)	0.0050 (12)	0.0076 (12)	0.0154 (12)
C13	0.0505 (15)	0.082 (2)	0.085 (2)	0.0451 (15)	0.0225 (14)	0.0335 (16)
N1	0.0683 (14)	0.0466 (12)	0.0415 (11)	0.0092 (10)	0.0088 (10)	0.0104 (9)
O1	0.0713 (12)	0.0540 (10)	0.0429 (9)	0.0162 (9)	0.0200 (8)	0.0084 (8)
O2	0.0515 (11)	0.0776 (14)	0.0795 (14)	0.0308 (10)	0.0258 (10)	0.0203 (11)
Cl1	0.0745 (6)	0.1562 (12)	0.1290 (10)	-0.0240 (7)	0.0142 (6)	0.0702 (9)
Cl2	0.1735 (13)	0.0994 (8)	0.0837 (7)	0.0466 (8)	0.0144 (7)	-0.0283 (6)
Cl3	0.1019 (7)	0.1234 (9)	0.0713 (6)	0.0149 (6)	0.0016 (5)	0.0515 (6)
S1	0.0460 (3)	0.0480 (3)	0.0460 (3)	0.0156 (2)	0.0163 (2)	0.0092 (2)

*Geometric parameters (Å, °)*

C1—C6	1.383 (3)	C8—H8	0.9300
C1—C2	1.399 (3)	C9—C10	1.375 (5)
C1—S1	1.763 (2)	C9—Cl2	1.725 (4)
C2—C3	1.388 (4)	C10—C11	1.377 (5)
C2—C13	1.575 (4)	C10—H10	0.9300
C3—C4	1.376 (5)	C11—C12	1.377 (4)

C3—H3	0.9300	C11—C13	1.734 (3)
C4—C5	1.362 (5)	C12—H12	0.9300
C4—C11	1.727 (3)	C13—H13A	0.9600
C5—C6	1.376 (4)	C13—H13B	0.9600
C5—H5	0.9300	C13—H13C	0.9600
C6—H6	0.9300	N1—S1	1.615 (2)
C7—C8	1.383 (4)	N1—H1N	0.825 (17)
C7—C12	1.391 (4)	O1—S1	1.4384 (19)
C7—N1	1.410 (3)	O2—S1	1.4206 (19)
C8—C9	1.376 (4)		
C6—C1—C2	121.3 (2)	C8—C9—C12	118.2 (3)
C6—C1—S1	116.38 (19)	C9—C10—C11	117.7 (3)
C2—C1—S1	122.24 (19)	C9—C10—H10	121.2
C3—C2—C1	116.9 (2)	C11—C10—H10	121.2
C3—C2—C13	119.8 (2)	C10—C11—C12	122.6 (3)
C1—C2—C13	123.3 (2)	C10—C11—C13	118.5 (2)
C4—C3—C2	121.0 (3)	C12—C11—C13	118.9 (3)
C4—C3—H3	119.5	C11—C12—C7	118.0 (3)
C2—C3—H3	119.5	C11—C12—H12	121.0
C5—C4—C3	121.8 (3)	C7—C12—H12	121.0
C5—C4—C11	118.9 (3)	C2—C13—H13A	109.5
C3—C4—C11	119.3 (3)	C2—C13—H13B	109.5
C4—C5—C6	118.6 (3)	H13A—C13—H13B	109.5
C4—C5—H5	120.7	C2—C13—H13C	109.5
C6—C5—H5	120.7	H13A—C13—H13C	109.5
C5—C6—C1	120.5 (3)	H13B—C13—H13C	109.5
C5—C6—H6	119.8	C7—N1—S1	128.18 (19)
C1—C6—H6	119.8	C7—N1—H1N	117 (2)
C8—C7—C12	120.6 (2)	S1—N1—H1N	112 (2)
C8—C7—N1	116.5 (2)	O2—S1—O1	118.37 (12)
C12—C7—N1	122.8 (3)	O2—S1—N1	109.26 (13)
C9—C8—C7	119.0 (3)	O1—S1—N1	104.09 (11)
C9—C8—H8	120.5	O2—S1—C1	107.01 (12)
C7—C8—H8	120.5	O1—S1—C1	109.78 (11)
C10—C9—C8	122.0 (3)	N1—S1—C1	107.94 (12)
C10—C9—C12	119.8 (3)		
C6—C1—C2—C3	-0.8 (4)	C12—C9—C10—C11	179.7 (3)
S1—C1—C2—C3	-178.2 (2)	C9—C10—C11—C12	0.1 (5)
C6—C1—C2—C13	-179.5 (3)	C9—C10—C11—C13	-178.7 (3)
S1—C1—C2—C13	3.1 (4)	C10—C11—C12—C7	0.0 (5)
C1—C2—C3—C4	1.0 (4)	C13—C11—C12—C7	178.7 (2)
C13—C2—C3—C4	179.7 (3)	C8—C7—C12—C11	0.4 (4)
C2—C3—C4—C5	-0.6 (5)	N1—C7—C12—C11	-178.1 (2)
C2—C3—C4—C11	-179.3 (2)	C8—C7—N1—S1	161.9 (2)
C3—C4—C5—C6	-0.1 (5)	C12—C7—N1—S1	-19.5 (4)
C11—C4—C5—C6	178.6 (2)	C7—N1—S1—O2	57.5 (3)

C4—C5—C6—C1	0.3 (4)	C7—N1—S1—O1	-175.2 (2)
C2—C1—C6—C5	0.2 (4)	C7—N1—S1—C1	-58.6 (3)
S1—C1—C6—C5	177.7 (2)	C6—C1—S1—O2	9.9 (2)
C12—C7—C8—C9	-0.8 (4)	C2—C1—S1—O2	-172.5 (2)
N1—C7—C8—C9	177.8 (3)	C6—C1—S1—O1	-119.7 (2)
C7—C8—C9—C10	0.9 (5)	C2—C1—S1—O1	57.8 (2)
C7—C8—C9—C12	-179.3 (2)	C6—C1—S1—N1	127.4 (2)
C8—C9—C10—C11	-0.5 (5)	C2—C1—S1—N1	-55.0 (2)

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N1—H1N...O1 <sup>i</sup>	0.83 (2)	2.06 (2)	2.884 (3)	172 (3)

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