

N-(5-Chloro-2-methoxyphenyl)benzene-sulfonamide

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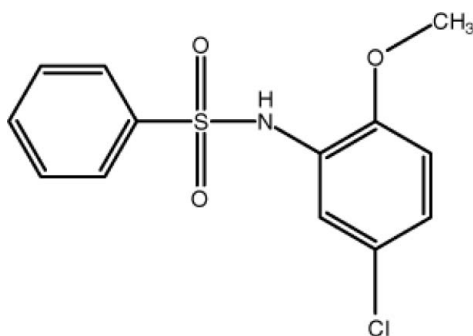
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.035; wR factor = 0.096; data-to-parameter ratio = 18.8.

In the title compound, $\text{C}_{13}\text{H}_{12}\text{ClNO}_3\text{S}$, the dihedral angle between the two aromatic rings is $73.94(9)^\circ$. An intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond occurs. In the crystal, intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds connect the molecules to centrosymmetric dimers, forming an $R_2^2(8)$ ring motif. The packing is consolidated by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and weak $\pi-\pi$ interactions [centroid-centroid distances = $3.81(3)$ and $3.81(3)$ Å].

Related literature

For the biological properties of sulfonamide derivatives, see: Berredjem *et al.* (2000); Lee & Lee (2002); Soledade *et al.* (2006); Xiao & Timberlake (2000). For related structures, see: Aziz-ur-Rehman *et al.* (2010*a,b*); Khan *et al.* (2010); Akkurt *et al.* (2010).



Experimental

Crystal data

$\text{C}_{13}\text{H}_{12}\text{ClNO}_3\text{S}$
 $M_r = 297.76$

Triclinic, $P\bar{1}$
 $a = 8.2201(2)$ Å

$b = 8.9395(2)$ Å
 $c = 10.5544(2)$ Å
 $\alpha = 77.206(1)^\circ$
 $\beta = 76.366(1)^\circ$
 $\gamma = 66.408(1)^\circ$
 $V = 683.65(3)$ Å³

$Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.43$ mm⁻¹
 $T = 296$ K
 $0.24 \times 0.16 \times 0.08$ mm

Data collection

Bruker APEXII CCD
diffractometer
12007 measured reflections

3333 independent reflections
2906 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.096$
 $S = 1.02$
3333 reflections
177 parameters
1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^{\text{i}}$	0.828 (16)	2.217 (16)	3.0096 (15)	160.2 (16)
$\text{C4}-\text{H4}\cdots\text{O2}^{\text{ii}}$	0.93	2.55	3.368 (3)	147
$\text{C8}-\text{H8}\cdots\text{O2}$	0.93	2.34	2.9491 (17)	123
$\text{C13}-\text{H13B}\cdots\text{O2}^{\text{iii}}$	0.96	2.48	3.362 (3)	153

Symmetry codes: (i) $-x, -y + 1, -z + 2$; (ii) $x + 1, y, z$; (iii) $x, y + 1, z$.

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) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5375).

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supplementary materials

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N-(5-Chloro-2-methoxyphenyl)benzenesulfonamide

Aziz-ur-Rehman, Shahzaman, M. Akkurt, M. A. Abbasi and I. U. Khan

Comment

Sulfonamide is found in a number of synthetic as well as natural compounds. These molecules possess many biological activities *e.g.*, herbicidal, anti-malarial, anti-convulsant and anti-hypertensive (Soledade *et al.*, 2006; Xiao & Timberlake, 2000; Berredjem *et al.*, 2000; Lee & Lee, 2002). In the present paper, the structure of *N*-(5-chloro-2-methoxyphenyl)benzenesulfonamide has been determined as part of a research program involving the synthesis and biological evaluation of sulfur-containing compounds.

In the title molecule (I), (Fig. 1), both sulfonamido-O atoms lie on the opposite side of the S-bound phenyl ring to the sulfonamido-N1 atom [the O1–S1–C1–C6, O2–S1–C1–C2 and N1–S1–C1–C2 torsion angles are $-34.32(13)$, $14.43(13)$ and $-101.83(12)^\circ$, respectively]. The dihedral angle formed between the phenyl (C1–C6) and benzene (C7–C12) rings in (I) is $73.94(9)^\circ$.

The molecules of (I) are dimerized due to the intermolecular N—H \cdots O hydrogen bonding (Table 1, Fig. 2) producing a $R_2^2(8)$ ring motif.

In addition, there are C—H \cdots O hydrogen bonds, as well as π – π interactions [$Cg1\cdots Cg1(1-x, -y, 2-z) = 3.8163(11) \text{ \AA}$ and $Cg2\cdots Cg2(-x, 1-y, 1-z) = 3.9472(12) \text{ \AA}$; where $Cg1$ and $Cg2$ are centroids of the phenyl and benzene rings (C1–C6 and C7–C12), respectively], between the aromatic rings of each dimer.

Experimental

A mixture benzenesulfonyl chloride (10.0 mmol; 1.45 ml), 5-chloro-2-methoxy aniline (10.0 mmol; 1.47 g), aqueous sodium carbonate (10%; 20.0 ml) and water (25 ml) was stirred for one and half hour at room temperature. The crude mixture was washed with water and dried. The product was dissolved in methanol and recrystallized by slow evaporation of the solvent, to generate colourless crystal of *N*-(5-chloro-2-methoxyphenyl)benzenesulfonamide in 71% yield.

Refinement

The amino H atom is located in a difference Fourier map and refined freely. The remaining H atoms were positioned geometrically (C—H = 0.93 and 0.96 \AA) and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

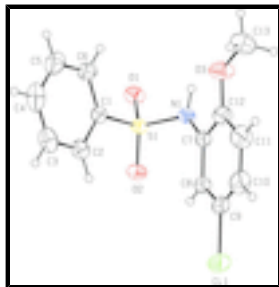


Fig. 1. The title molecule drawn with displacement ellipsoids drawn at the 30% probability level.

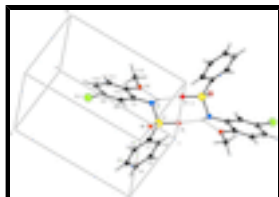


Fig. 2. View of the dimeric N—H...O interactions between two molecules in the unit cell.

N-(5-chloro-2-methoxyphenyl)benzenesulfonamide

Crystal data

$C_{13}H_{12}ClNO_3S$

$M_r = 297.76$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.2201$ (2) Å

$b = 8.9395$ (2) Å

$c = 10.5544$ (2) Å

$\alpha = 77.206$ (1)°

$\beta = 76.366$ (1)°

$\gamma = 66.408$ (1)°

$V = 683.65$ (3) Å³

$Z = 2$

$F(000) = 308$

$D_x = 1.446$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6946 reflections

$\theta = 2.5$ – 28.2 °

$\mu = 0.43$ mm⁻¹

$T = 296$ K

Prism, colourless

$0.24 \times 0.16 \times 0.08$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: sealed tube
graphite

φ and ω scans

12007 measured reflections

3333 independent reflections

2906 reflections with $I > 2\sigma(I)$

$R_{int} = 0.023$

$\theta_{max} = 28.3$ °, $\theta_{min} = 4.0$ °

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -14 \rightarrow 12$

Refinement

Refinement on F^2

Primary atom site location: structure-invariant direct
methods

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.035$$

$$wR(F^2) = 0.096$$

$$S = 1.01$$

3333 reflections

177 parameters

1 restraint

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

$$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.1401P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.29733 (8)	0.24190 (8)	0.34117 (5)	0.0934 (2)
S1	0.14406 (4)	0.27960 (4)	0.88801 (3)	0.0380 (1)
O1	0.03295 (14)	0.31471 (13)	1.01239 (9)	0.0510 (3)
O2	0.13974 (14)	0.15335 (13)	0.82861 (10)	0.0506 (3)
O3	0.1709 (2)	0.71184 (16)	0.69335 (12)	0.0734 (5)
N1	0.08081 (16)	0.45288 (14)	0.78854 (10)	0.0429 (3)
C1	0.36916 (18)	0.23297 (16)	0.90100 (12)	0.0398 (4)
C2	0.5039 (2)	0.11582 (19)	0.83059 (15)	0.0521 (5)
C3	0.6805 (2)	0.0782 (2)	0.8436 (2)	0.0696 (6)
C4	0.7178 (3)	0.1563 (3)	0.9253 (2)	0.0767 (7)
C5	0.5824 (3)	0.2731 (3)	0.9938 (2)	0.0731 (7)
C6	0.4049 (2)	0.3136 (2)	0.98279 (16)	0.0557 (5)
C7	0.16189 (18)	0.47011 (17)	0.65422 (12)	0.0422 (4)
C8	0.1896 (2)	0.35789 (19)	0.57270 (13)	0.0505 (4)
C9	0.2635 (2)	0.3861 (2)	0.44138 (15)	0.0616 (5)
C10	0.3044 (3)	0.5227 (3)	0.39090 (16)	0.0756 (7)
C11	0.2737 (3)	0.6360 (3)	0.47153 (17)	0.0739 (7)
C12	0.2046 (2)	0.6098 (2)	0.60401 (14)	0.0541 (5)
C13	0.1961 (3)	0.8625 (3)	0.6504 (3)	0.0875 (9)
H1	0.058 (2)	0.5318 (19)	0.8273 (16)	0.052 (4)*
H2	0.47690	0.06350	0.77580	0.0630*
H3	0.77380	0.00000	0.79700	0.0830*

supplementary materials

H4	0.83650	0.12960	0.93410	0.0920*
H5	0.61010	0.32540	1.04810	0.0880*
H6	0.31220	0.39270	1.02900	0.0670*
H8	0.15940	0.26520	0.60520	0.0600*
H10	0.35290	0.53940	0.30240	0.0910*
H11	0.29940	0.73070	0.43700	0.0890*
H13A	0.32050	0.84190	0.61440	0.1310*
H13B	0.16150	0.92250	0.72360	0.1310*
H13C	0.12340	0.92620	0.58390	0.1310*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1058 (4)	0.0954 (4)	0.0594 (3)	0.0032 (3)	-0.0179 (2)	-0.0448 (3)
S1	0.0403 (2)	0.0368 (2)	0.0370 (2)	-0.0163 (1)	0.0011 (1)	-0.0095 (1)
O1	0.0538 (6)	0.0510 (6)	0.0416 (5)	-0.0206 (5)	0.0098 (4)	-0.0100 (4)
O2	0.0566 (6)	0.0459 (5)	0.0577 (6)	-0.0253 (5)	-0.0063 (5)	-0.0146 (4)
O3	0.1093 (11)	0.0642 (8)	0.0596 (7)	-0.0505 (8)	0.0026 (7)	-0.0160 (6)
N1	0.0491 (6)	0.0385 (6)	0.0360 (5)	-0.0107 (5)	-0.0019 (4)	-0.0111 (4)
C1	0.0435 (7)	0.0381 (6)	0.0381 (6)	-0.0193 (5)	-0.0049 (5)	0.0003 (5)
C2	0.0465 (8)	0.0504 (8)	0.0515 (8)	-0.0145 (6)	-0.0008 (6)	-0.0058 (6)
C3	0.0437 (8)	0.0664 (11)	0.0793 (11)	-0.0144 (8)	0.0003 (8)	0.0052 (9)
C4	0.0524 (10)	0.0787 (13)	0.0975 (14)	-0.0378 (10)	-0.0255 (10)	0.0310 (11)
C5	0.0829 (13)	0.0731 (12)	0.0857 (13)	-0.0494 (11)	-0.0375 (11)	0.0098 (10)
C6	0.0643 (9)	0.0529 (8)	0.0591 (9)	-0.0286 (7)	-0.0153 (7)	-0.0068 (7)
C7	0.0419 (7)	0.0437 (7)	0.0351 (6)	-0.0092 (5)	-0.0058 (5)	-0.0073 (5)
C8	0.0535 (8)	0.0491 (8)	0.0420 (7)	-0.0073 (6)	-0.0100 (6)	-0.0131 (6)
C9	0.0611 (9)	0.0675 (10)	0.0397 (7)	0.0007 (8)	-0.0109 (6)	-0.0189 (7)
C10	0.0797 (12)	0.0875 (14)	0.0370 (7)	-0.0161 (10)	0.0030 (7)	-0.0062 (8)
C11	0.0871 (13)	0.0748 (12)	0.0503 (9)	-0.0341 (10)	0.0042 (8)	0.0014 (8)
C12	0.0602 (9)	0.0554 (9)	0.0442 (7)	-0.0219 (7)	-0.0022 (6)	-0.0080 (6)
C13	0.1028 (17)	0.0654 (12)	0.1064 (17)	-0.0453 (12)	-0.0112 (13)	-0.0149 (11)

Geometric parameters (\AA , $^\circ$)

Cl1—C9	1.7424 (17)	C7—C8	1.380 (2)
S1—O1	1.4296 (10)	C8—C9	1.387 (2)
S1—O2	1.4227 (12)	C9—C10	1.358 (3)
S1—N1	1.6323 (12)	C10—C11	1.375 (3)
S1—C1	1.7588 (16)	C11—C12	1.386 (2)
O3—C12	1.361 (2)	C2—H2	0.9300
O3—C13	1.404 (3)	C3—H3	0.9300
N1—C7	1.4205 (16)	C4—H4	0.9300
N1—H1	0.828 (16)	C5—H5	0.9300
C1—C2	1.380 (2)	C6—H6	0.9300
C1—C6	1.384 (2)	C8—H8	0.9300
C2—C3	1.386 (3)	C10—H10	0.9300
C3—C4	1.374 (3)	C11—H11	0.9300
C4—C5	1.370 (3)	C13—H13A	0.9600

C5—C6	1.383 (3)	C13—H13B	0.9600
C7—C12	1.391 (2)	C13—H13C	0.9600
C11...C6 ⁱ	3.6473 (17)	C7...C11 ⁱⁱⁱ	3.6152 (17)
C11...C2 ⁱⁱ	3.6292 (17)	C7...C9 ⁱⁱⁱ	3.520 (2)
C11...C7 ⁱⁱⁱ	3.6152 (17)	C8...C8 ⁱⁱⁱ	3.566 (2)
C11...H2 ⁱⁱ	2.9600	C8...O2	2.9491 (17)
C11...H13A ^{iv}	3.0500	C8...C9 ⁱⁱⁱ	3.524 (2)
S1...H8	2.9900	C9...C8 ⁱⁱⁱ	3.524 (2)
O1...N1 ^v	3.0096 (15)	C9...C7 ⁱⁱⁱ	3.520 (2)
O1...O1 ^v	3.0957 (15)	C13...O2 ^{xi}	3.362 (3)
O1...O3 ^v	3.1699 (16)	C3...H11 ^{iv}	3.0800
O2...C13 ^{vi}	3.362 (3)	C11...H13A	2.8100
O2...C4 ^{vii}	3.368 (3)	C11...H13C	2.7900
O2...C8	2.9491 (17)	C13...H11	2.5800
O2...C4 ^{viii}	3.382 (2)	H1...O3	2.241 (17)
O3...O1 ^v	3.1699 (16)	H1...O1 ^v	2.217 (16)
O3...N1	2.6284 (19)	H2...O2	2.5100
O1...H6	2.7000	H2...C11 ⁱⁱ	2.9600
O1...H1 ^v	2.217 (16)	H4...O2 ^{ix}	2.5500
O2...H13B ^{vi}	2.4800	H6...O1	2.7000
O2...H4 ^{vii}	2.5500	H8...S1	2.9900
O2...H8	2.3400	H8...O2	2.3400
O2...H2	2.5100	H11...C13	2.5800
O3...H1	2.241 (17)	H11...H13A	2.3700
N1...O3	2.6284 (19)	H11...H13C	2.3800
N1...O1 ^v	3.0096 (15)	H11...C3 ^{iv}	3.0800
C1...C3 ^{viii}	3.499 (2)	H13A...C11	2.8100
C2...C11 ⁱⁱ	3.6292 (17)	H13A...H11	2.3700
C3...C1 ^{viii}	3.499 (2)	H13A...C11 ^{iv}	3.0500
C4...O2 ^{ix}	3.368 (3)	H13B...O2 ^{xi}	2.4800
C4...O2 ^{viii}	3.382 (2)	H13C...C11	2.7900
C6...C11 ^x	3.6473 (17)	H13C...H11	2.3800
O1—S1—O2	118.95 (7)	C10—C11—C12	120.3 (2)
O1—S1—N1	105.06 (6)	C7—C12—C11	119.51 (16)
O1—S1—C1	109.15 (7)	O3—C12—C7	114.94 (13)
O2—S1—N1	108.21 (6)	O3—C12—C11	125.55 (17)
O2—S1—C1	107.73 (7)	C1—C2—H2	121.00
N1—S1—C1	107.19 (7)	C3—C2—H2	121.00
C12—O3—C13	119.30 (17)	C2—C3—H3	120.00
S1—N1—C7	122.57 (10)	C4—C3—H3	120.00
C7—N1—H1	115.2 (11)	C3—C4—H4	120.00
S1—N1—H1	110.4 (11)	C5—C4—H4	120.00
S1—C1—C6	118.85 (11)	C4—C5—H5	120.00
S1—C1—C2	118.88 (12)	C6—C5—H5	120.00

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C2—C1—C6	122.27 (16)	C1—C6—H6	121.00
C1—C2—C3	118.25 (15)	C5—C6—H6	121.00
C2—C3—C4	120.09 (18)	C7—C8—H8	121.00
C3—C4—C5	120.9 (2)	C9—C8—H8	121.00
C4—C5—C6	120.5 (2)	C9—C10—H10	120.00
C1—C6—C5	118.07 (17)	C11—C10—H10	120.00
N1—C7—C12	117.82 (12)	C10—C11—H11	120.00
N1—C7—C8	121.96 (13)	C12—C11—H11	120.00
C8—C7—C12	120.14 (12)	O3—C13—H13A	109.00
C7—C8—C9	118.69 (15)	O3—C13—H13B	109.00
C11—C9—C8	117.57 (13)	O3—C13—H13C	109.00
C8—C9—C10	121.73 (16)	H13A—C13—H13B	109.00
C11—C9—C10	120.68 (13)	H13A—C13—H13C	109.00
C9—C10—C11	119.57 (17)	H13B—C13—H13C	109.00
O1—S1—N1—C7	179.00 (12)	C1—C2—C3—C4	0.2 (3)
O2—S1—N1—C7	-52.96 (14)	C2—C3—C4—C5	-0.7 (3)
C1—S1—N1—C7	62.98 (14)	C3—C4—C5—C6	0.6 (3)
O1—S1—C1—C2	144.89 (11)	C4—C5—C6—C1	0.0 (3)
O2—S1—C1—C2	14.43 (13)	C12—C7—C8—C9	1.2 (2)
N1—S1—C1—C2	-101.83 (12)	N1—C7—C12—O3	3.1 (2)
O1—S1—C1—C6	-34.32 (13)	C8—C7—C12—O3	179.75 (16)
O2—S1—C1—C6	-164.78 (11)	C8—C7—C12—C11	0.5 (3)
N1—S1—C1—C6	78.96 (12)	N1—C7—C12—C11	-176.09 (18)
C13—O3—C12—C7	-175.04 (19)	N1—C7—C8—C9	177.65 (15)
C13—O3—C12—C11	4.1 (3)	C7—C8—C9—C10	-1.8 (3)
S1—N1—C7—C12	-135.26 (14)	C7—C8—C9—C11	179.83 (13)
S1—N1—C7—C8	48.2 (2)	C8—C9—C10—C11	0.6 (3)
C2—C1—C6—C5	-0.4 (2)	C11—C9—C10—C11	178.93 (19)
C6—C1—C2—C3	0.3 (2)	C9—C10—C11—C12	1.2 (4)
S1—C1—C2—C3	-178.87 (12)	C10—C11—C12—C7	-1.7 (3)
S1—C1—C6—C5	178.76 (14)	C10—C11—C12—O3	179.1 (2)

Symmetry codes: (i) $x, y, z-1$; (ii) $-x+1, -y, -z+1$; (iii) $-x, -y+1, -z+1$; (iv) $-x+1, -y+1, -z+1$; (v) $-x, -y+1, -z+2$; (vi) $x, y-1, z$; (vii) $x-1, y, z$; (viii) $-x+1, -y, -z+2$; (ix) $x+1, y, z$; (x) $x, y, z+1$; (xi) $x, y+1, z$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots O1 ^v	0.828 (16)	2.217 (16)	3.0096 (15)	160.2 (16)
C4—H4 \cdots O2 ^{ix}	0.93	2.55	3.368 (3)	147
C8—H8 \cdots O2	0.93	2.34	2.9491 (17)	123
C13—H13B \cdots O2 ^{xi}	0.96	2.48	3.362 (3)	153

Symmetry codes: (v) $-x, -y+1, -z+2$; (ix) $x+1, y, z$; (xi) $x, y+1, z$.

Fig. 1

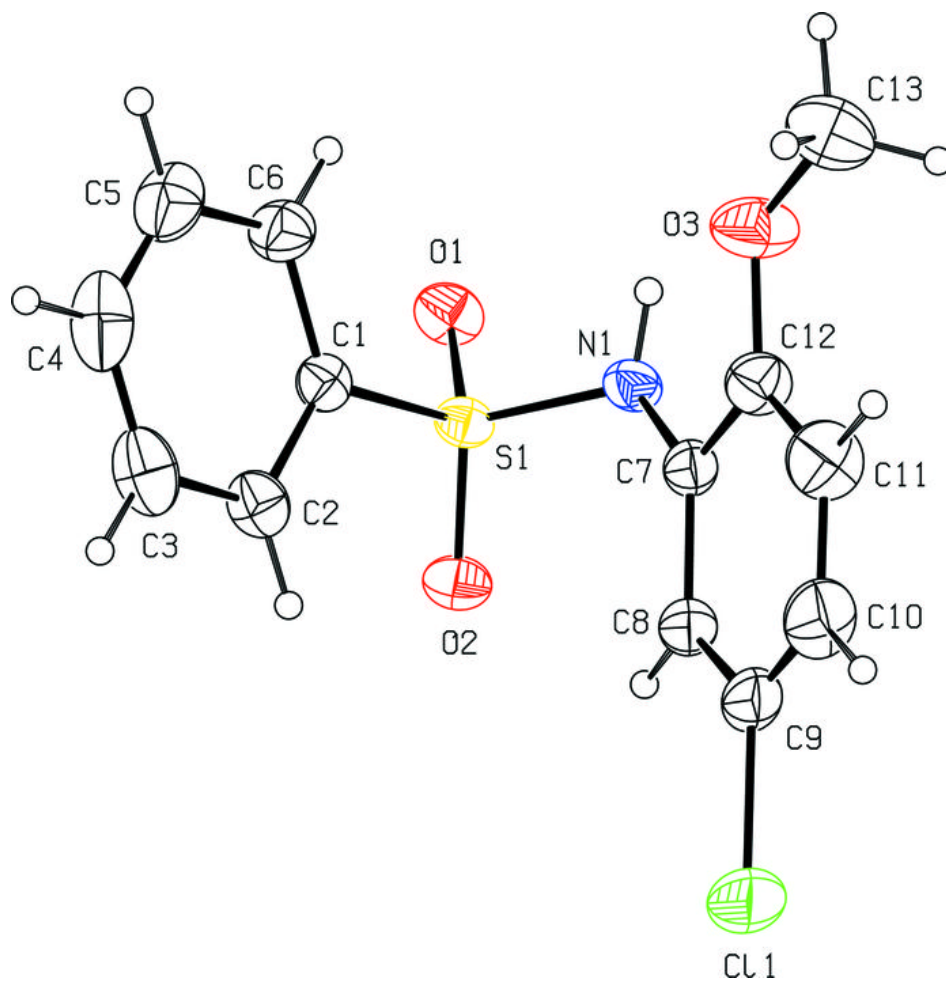


Fig. 2

