

N-(3,5-Dichlorophenyl)-2,4-dimethylbenzenesulfonamide

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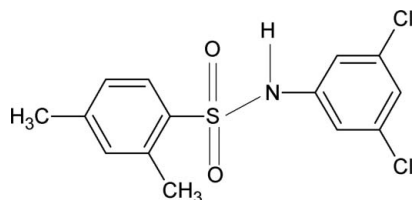
Received 1 April 2010; accepted 12 April 2010

Key indicators: single-crystal X-ray study; $T = 299$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.053; wR factor = 0.189; data-to-parameter ratio = 14.4.

In the crystal structure of the title compound, $\text{C}_{14}\text{H}_{13}\text{Cl}_2\text{NO}_2\text{S}$, the conformation of the $\text{N}-\text{C}$ bond in the $\text{C}-\text{SO}_2-\text{NH}-\text{C}$ segment has *gauche* torsions with respect to the $\text{S}=\text{O}$ bonds. The molecule is bent at the N atom, with an $\text{C}-\text{SO}_2-\text{NH}-\text{C}$ torsion angle of -54.9 (3°). The two benzene rings are tilted relative to each other by 82.3 (2°). The molecules are linked into centrosymmetric $R_2^2(8)$ motifs by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds and $\text{C}-\text{H}\cdots\pi$ interactions along $[100]$.

Related literature

For the preparation of the compound, see: Savitha & Gowda (2006). For our study of the effect of substituents on the structures of *N*-(aryl)arylsulfonamides, see: Gowda *et al.* (2008, 2009*a,b*). For related structures, see: Gelbrich *et al.* (2007); Perlovich *et al.* (2006). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{13}\text{Cl}_2\text{NO}_2\text{S}$
 $M_r = 330.21$
Monoclinic, $C2/c$

$a = 23.085$ (3) Å
 $b = 8.113$ (2) Å
 $c = 16.503$ (3) Å

$\beta = 102.03$ (2°)
 $V = 3022.9$ (10) Å³
 $Z = 8$
Cu $K\alpha$ radiation

$\mu = 5.16$ mm⁻¹
 $T = 299$ K
 $0.55 \times 0.45 \times 0.38$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.164$, $T_{\max} = 0.245$
7561 measured reflections

2690 independent reflections
2340 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.089$
3 standard reflections every 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.189$
 $S = 1.14$
2690 reflections
187 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.56$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.46$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$Cg1$ is the centroid of the $\text{C}1-\text{C}6$ ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N}1-\text{H}1\text{N}\cdots\text{O}1^i$	0.86 (4)	2.05 (5)	2.900 (4)	168 (4)
$\text{C}10-\text{H}10\cdots Cg1^{ii}$	0.93	2.92	3.834 (4)	168

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

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2275).

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supplementary materials

Acta Cryst. (2010). E66, o1090 [doi:10.1107/S1600536810013504]

***N*-(3,5-Dichlorophenyl)-2,4-dimethylbenzenesulfonamide**

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Comment

As part of a study of substituent effects on the structures of *N*-(aryl)arylsulfonamides (Gowda *et al.*, 2008; 2009*a,b*), we report here the crystal structure of the title compound (I), (Fig. 1). The conformation of the N—C bond in the C—SO₂—NH—C segment of the structure has gauche torsions with respect to the S=O bonds. The molecule is bent at the *N* atom with the C1—SO₂—NH—C7 torsion angle of -54.9 (3)°, compared to the values of 46.1 (3)° (glide image of molecule 1) and 47.7 (3)° (molecule 2) in the two independent molecules of 2,4-dimethyl-*N*-(phenyl)benzenesulfonamide (II) (Gowda *et al.*, 2009*a*), -68.1 (3)° in *N*-(3,5-dichlorophenyl)benzenesulfonamide (III) (Gowda *et al.*, 2008); 53.9 (2)° in 2,4-dimethyl-*N*-(3,5-dimethylphenyl)-benzenesulfonamide (IV) (Gowda *et al.*, 2009*b*) and -69.7 (2)° in 2,4-dimethyl-*N*-(3,4-dichlorophenyl)benzenesulfonamide (V) (Gowda *et al.*, 2009*b*).

The two benzene rings in (I) are tilted relative to each other by 82.3 (1)°, compared to the values of 67.5 (1)° (molecule 1) and 72.9 (1)° (molecule 2) in the two independent molecules of (II), 57.0 (1)° in (III), 82.1 (1)° in (IV) and 82.4 (1)° in (V). The other atomic parameters in (I) are similar to those observed in (II), (III), (IV), (V) and other aryl sulfonamides (Perlovich *et al.*, 2006; Gelbrich *et al.*, 2007) as representative examples. The molecules are linked into centrosymmetric R₂²(8) motifs by N—H···O hydrogen bonds and C—H···π interactions along [1 0 0] (Bernstein *et al.*, 1995), Fig. 2.

Experimental

The solution of 1,3-xylene (1,3-dimethylbenzene) (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 2,4-dimethylbenzenesulfonylchloride was treated with 3,5-dichloroaniline in the stoichiometric ratio and boiled for ten minutes. The reaction mixture was then cooled to room temperature and added to ice cold water (100 ml). The resultant solid 2,4-dimethyl-*N*-(3,5-dichlorophenyl)benzenesulfonamide 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).

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

Refinement

The H atom of the NH group was located in a difference map and its position refined with N—H = 0.86 (4) Å. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.96 Å. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

Figures

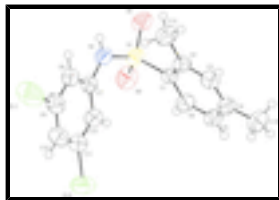


Fig. 1. Molecular structure of the title compound, showing the atom labelling scheme. The displacement ellipsoids are drawn at the 50% probability level. The H atoms are represented as small spheres of arbitrary radii.

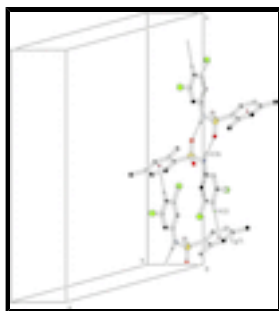


Fig. 2. Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

N-(3,5-Dichlorophenyl)-2,4-dimethylbenzenesulfonamide

Crystal data

$C_{14}H_{13}Cl_2NO_2S$

$M_r = 330.21$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 23.085\ (3)\ \text{\AA}$

$b = 8.113\ (2)\ \text{\AA}$

$c = 16.503\ (3)\ \text{\AA}$

$\beta = 102.03\ (2)^\circ$

$V = 3022.9\ (10)\ \text{\AA}^3$

$Z = 8$

$F(000) = 1360$

$D_x = 1.451\ \text{Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54180\ \text{\AA}$

Cell parameters from 25 reflections

$\theta = 5.5\text{--}18.6^\circ$

$\mu = 5.16\ \text{mm}^{-1}$

$T = 299\ \text{K}$

Prism, colourless

$0.55 \times 0.45 \times 0.38\ \text{mm}$

Data collection

Enraf-Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube
graphite

$\omega/2\theta$ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{\min} = 0.164$, $T_{\max} = 0.245$

7561 measured reflections

2690 independent reflections

2340 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.089$

$\theta_{\max} = 66.9^\circ$, $\theta_{\min} = 3.9^\circ$

$h = -15 \rightarrow 27$

$k = -9 \rightarrow 9$

$l = -19 \rightarrow 19$

3 standard reflections every 120 min

intensity decay: 1.0%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.189$	$w = 1/[\sigma^2(F_o^2) + (0.1031P)^2 + 3.0862P]$
$S = 1.14$	where $P = (F_o^2 + 2F_c^2)/3$
2690 reflections	$(\Delta/\sigma)_{\max} = 0.006$
187 parameters	$\Delta\rho_{\max} = 0.56 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -0.46 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1+0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.00090 (16)

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.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.43013 (12)	0.1399 (3)	0.15596 (17)	0.0411 (6)
C2	0.44290 (12)	0.2976 (4)	0.13142 (18)	0.0442 (6)
C3	0.43210 (14)	0.4268 (4)	0.1793 (2)	0.0509 (7)
H3	0.4397	0.5330	0.1631	0.061*
C4	0.41035 (13)	0.4069 (4)	0.2511 (2)	0.0507 (7)
C5	0.39736 (14)	0.2499 (4)	0.27317 (19)	0.0541 (8)
H5	0.3822	0.2338	0.3205	0.065*
C6	0.40659 (14)	0.1169 (4)	0.22618 (19)	0.0505 (7)
H6	0.3971	0.0114	0.2412	0.061*
C7	0.35181 (14)	0.0098 (4)	-0.0243 (2)	0.0479 (7)
C8	0.33700 (14)	0.0724 (4)	-0.1038 (2)	0.0537 (8)
H8	0.3663	0.0948	-0.1332	0.064*
C9	0.27851 (16)	0.1011 (5)	-0.1390 (2)	0.0653 (9)
C10	0.23406 (16)	0.0720 (6)	-0.0964 (3)	0.0728 (11)
H10	0.1946	0.0926	-0.1205	0.087*

supplementary materials

C11	0.24997 (17)	0.0121 (5)	-0.0178 (3)	0.0658 (10)
C12	0.30817 (16)	-0.0218 (5)	0.0207 (2)	0.0594 (9)
H12	0.3176	-0.0639	0.0742	0.071*
C13	0.46692 (19)	0.3326 (5)	0.0555 (2)	0.0657 (10)
H13A	0.4371	0.3088	0.0070	0.079*
H13B	0.5010	0.2648	0.0557	0.079*
H13C	0.4780	0.4466	0.0551	0.079*
C14	0.4006 (2)	0.5542 (5)	0.3010 (3)	0.0769 (12)
H14A	0.3644	0.6078	0.2751	0.092*
H14B	0.4331	0.6296	0.3040	0.092*
H14C	0.3982	0.5200	0.3558	0.092*
Cl1	0.26077 (5)	0.1724 (2)	-0.23956 (8)	0.1056 (6)
Cl2	0.19530 (5)	-0.0269 (2)	0.03757 (9)	0.1007 (5)
N1	0.41245 (12)	-0.0223 (4)	0.00734 (18)	0.0542 (7)
H1N	0.4333 (19)	0.011 (5)	-0.027 (3)	0.065*
O1	0.50684 (10)	-0.0457 (3)	0.10170 (15)	0.0615 (7)
O2	0.41982 (13)	-0.1739 (3)	0.13907 (17)	0.0680 (7)
S1	0.44494 (3)	-0.03942 (9)	0.10412 (5)	0.0485 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0405 (13)	0.0437 (14)	0.0396 (13)	0.0051 (11)	0.0094 (11)	0.0025 (11)
C2	0.0423 (14)	0.0489 (15)	0.0427 (14)	0.0023 (12)	0.0115 (11)	0.0066 (12)
C3	0.0515 (16)	0.0429 (15)	0.0588 (18)	0.0019 (13)	0.0128 (14)	0.0043 (13)
C4	0.0469 (15)	0.0571 (18)	0.0489 (16)	0.0066 (13)	0.0117 (13)	-0.0040 (14)
C5	0.0572 (17)	0.0655 (19)	0.0440 (15)	0.0038 (15)	0.0207 (13)	0.0031 (14)
C6	0.0584 (17)	0.0503 (16)	0.0460 (16)	0.0012 (13)	0.0181 (13)	0.0088 (13)
C7	0.0446 (15)	0.0497 (15)	0.0491 (16)	0.0012 (12)	0.0092 (12)	-0.0122 (13)
C8	0.0481 (16)	0.0595 (18)	0.0534 (18)	0.0003 (14)	0.0105 (13)	-0.0058 (14)
C9	0.0530 (18)	0.079 (2)	0.059 (2)	-0.0018 (17)	-0.0004 (15)	-0.0007 (18)
C10	0.0436 (17)	0.094 (3)	0.076 (3)	0.0021 (18)	0.0022 (17)	-0.010 (2)
C11	0.0499 (18)	0.081 (2)	0.069 (2)	-0.0055 (17)	0.0176 (17)	-0.0172 (19)
C12	0.0541 (18)	0.072 (2)	0.0534 (19)	-0.0005 (15)	0.0141 (15)	-0.0095 (15)
C13	0.085 (2)	0.062 (2)	0.059 (2)	-0.0049 (18)	0.0346 (19)	0.0102 (16)
C14	0.090 (3)	0.071 (3)	0.075 (3)	0.010 (2)	0.028 (2)	-0.0170 (19)
Cl1	0.0679 (7)	0.1625 (14)	0.0765 (7)	-0.0020 (7)	-0.0073 (5)	0.0331 (8)
Cl2	0.0616 (6)	0.1549 (13)	0.0940 (9)	-0.0108 (6)	0.0353 (6)	-0.0121 (8)
N1	0.0481 (14)	0.0703 (18)	0.0441 (14)	0.0076 (12)	0.0096 (12)	-0.0056 (12)
O1	0.0525 (13)	0.0771 (17)	0.0535 (13)	0.0247 (11)	0.0077 (10)	-0.0028 (11)
O2	0.0908 (18)	0.0436 (12)	0.0717 (16)	0.0060 (12)	0.0214 (14)	0.0064 (11)
S1	0.0521 (5)	0.0462 (5)	0.0475 (5)	0.0114 (3)	0.0106 (3)	0.0007 (3)

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

C1—C6	1.391 (4)	C9—C10	1.379 (6)
C1—C2	1.392 (4)	C9—C11	1.725 (4)
C1—S1	1.757 (3)	C10—C11	1.362 (6)
C2—C3	1.366 (4)	C10—H10	0.9300

C2—C13	1.500 (4)	C11—C12	1.389 (5)
C3—C4	1.389 (5)	C11—Cl2	1.735 (4)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.375 (5)	C13—H13A	0.9600
C4—C14	1.495 (5)	C13—H13B	0.9600
C5—C6	1.371 (5)	C13—H13C	0.9600
C5—H5	0.9300	C14—H14A	0.9600
C6—H6	0.9300	C14—H14B	0.9600
C7—C8	1.381 (5)	C14—H14C	0.9600
C7—C12	1.394 (5)	N1—S1	1.623 (3)
C7—N1	1.413 (4)	N1—H1N	0.86 (4)
C8—C9	1.374 (5)	O1—S1	1.439 (2)
C8—H8	0.9300	O2—S1	1.414 (3)
C6—C1—C2	120.6 (3)	C9—C10—H10	121.2
C6—C1—S1	116.4 (2)	C10—C11—C12	123.3 (4)
C2—C1—S1	123.0 (2)	C10—C11—Cl2	119.0 (3)
C3—C2—C1	117.5 (3)	C12—C11—Cl2	117.6 (3)
C3—C2—C13	118.8 (3)	C11—C12—C7	117.2 (4)
C1—C2—C13	123.7 (3)	C11—C12—H12	121.4
C2—C3—C4	123.1 (3)	C7—C12—H12	121.4
C2—C3—H3	118.5	C2—C13—H13A	109.5
C4—C3—H3	118.5	C2—C13—H13B	109.5
C5—C4—C3	118.1 (3)	H13A—C13—H13B	109.5
C5—C4—C14	121.9 (3)	C2—C13—H13C	109.5
C3—C4—C14	120.0 (3)	H13A—C13—H13C	109.5
C6—C5—C4	120.7 (3)	H13B—C13—H13C	109.5
C6—C5—H5	119.6	C4—C14—H14A	109.5
C4—C5—H5	119.6	C4—C14—H14B	109.5
C5—C6—C1	120.0 (3)	H14A—C14—H14B	109.5
C5—C6—H6	120.0	C4—C14—H14C	109.5
C1—C6—H6	120.0	H14A—C14—H14C	109.5
C8—C7—C12	120.7 (3)	H14B—C14—H14C	109.5
C8—C7—N1	116.7 (3)	C7—N1—S1	126.8 (2)
C12—C7—N1	122.6 (3)	C7—N1—H1N	110 (3)
C9—C8—C7	119.4 (3)	S1—N1—H1N	118 (3)
C9—C8—H8	120.3	O2—S1—O1	118.57 (16)
C7—C8—H8	120.3	O2—S1—N1	108.85 (17)
C8—C9—C10	121.7 (4)	O1—S1—N1	103.52 (15)
C8—C9—C11	118.6 (3)	O2—S1—C1	107.61 (14)
C10—C9—C11	119.7 (3)	O1—S1—C1	109.74 (14)
C11—C10—C9	117.7 (3)	N1—S1—C1	108.13 (14)
C11—C10—H10	121.2		
C6—C1—C2—C3	0.8 (4)	C11—C9—C10—C11	178.5 (3)
S1—C1—C2—C3	-176.7 (2)	C9—C10—C11—C12	-0.5 (7)
C6—C1—C2—C13	-178.5 (3)	C9—C10—C11—Cl2	-179.7 (3)
S1—C1—C2—C13	4.0 (4)	C10—C11—C12—C7	0.7 (6)
C1—C2—C3—C4	1.3 (5)	Cl2—C11—C12—C7	180.0 (3)
C13—C2—C3—C4	-179.5 (3)	C8—C7—C12—C11	0.0 (5)

supplementary materials

C2—C3—C4—C5	-2.2 (5)	N1—C7—C12—C11	-178.8 (3)
C2—C3—C4—C14	179.0 (3)	C8—C7—N1—S1	159.3 (3)
C3—C4—C5—C6	1.0 (5)	C12—C7—N1—S1	-21.8 (5)
C14—C4—C5—C6	179.9 (3)	C7—N1—S1—O2	61.7 (3)
C4—C5—C6—C1	0.9 (5)	C7—N1—S1—O1	-171.3 (3)
C2—C1—C6—C5	-1.9 (5)	C7—N1—S1—C1	-54.9 (3)
S1—C1—C6—C5	175.8 (2)	C6—C1—S1—O2	9.6 (3)
C12—C7—C8—C9	-1.0 (5)	C2—C1—S1—O2	-172.8 (3)
N1—C7—C8—C9	177.9 (3)	C6—C1—S1—O1	-120.7 (3)
C7—C8—C9—C10	1.3 (6)	C2—C1—S1—O1	56.9 (3)
C7—C8—C9—C11	-177.8 (3)	C6—C1—S1—N1	127.0 (2)
C8—C9—C10—C11	-0.5 (7)	C2—C1—S1—N1	-55.4 (3)

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

Cg1 is the centroid of the C1—C6 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1N \cdots O1 ⁱ	0.86 (4)	2.05 (5)	2.900 (4)	168 (4)
C10—H10 \cdots Cg1 ⁱⁱ	0.93	2.92	3.834 (4)	168

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

Fig. 1

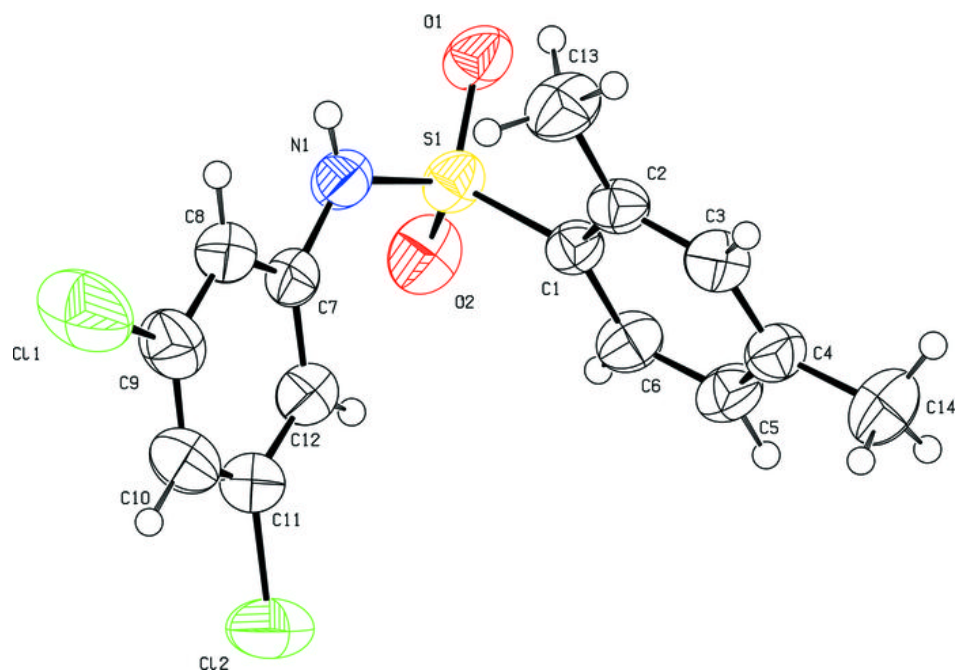


Fig. 2

