

N-(2-Acetylphenyl)benzenesulfonamide

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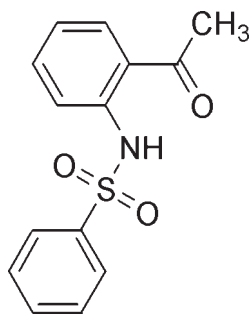
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.045; wR factor = 0.142; data-to-parameter ratio = 29.5.

In the title compound, $\text{C}_{14}\text{H}_{13}\text{NO}_3\text{S}$, the phenyl ring makes a dihedral angle of $81.5(1)^\circ$ with the benzene ring. The molecular structure is stabilized by an intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond and weak $\text{C}-\text{H}\cdots\text{O}$ interactions. In the crystal structure, molecules are linked by weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For the biological activity of benzenesulfonamide derivatives, see: Badr (2008); Hanafy *et al.* (2007); Yang *et al.* (2002). For related structures, see: Chakkaravarthi *et al.* (2007); Li & Yang (2006). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{13}\text{NO}_3\text{S}$
 $M_r = 275.31$
Triclinic, $P\bar{1}$

$a = 7.9909(3)$ Å
 $b = 8.6860(4)$ Å
 $c = 10.0701(4)$ Å

$\alpha = 88.016(2)^\circ$
 $\beta = 68.673(3)^\circ$
 $\gamma = 83.424(2)^\circ$
 $V = 646.79(5)$ Å³
 $Z = 2$

Mo $K\alpha$ radiation
 $\mu = 0.25$ mm⁻¹
 $T = 295$ K
 $0.24 \times 0.20 \times 0.20$ mm

Data collection

Bruker Kappa APEX2 diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.942$, $T_{\max} = 0.951$

18690 measured reflections
5104 independent reflections
3886 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.142$
 $S = 1.03$
5104 reflections

173 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.41$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O3}$	0.86	2.03	2.596 (2)	123
$\text{C2}-\text{H2}\cdots\text{O1}$	0.93	2.52	2.893 (2)	104
$\text{C12}-\text{H12}\cdots\text{O1}$	0.93	2.40	3.057 (2)	128
$\text{C11}-\text{H11}\cdots\text{O1}^{\text{i}}$	0.93	2.51	3.380 (2)	156
$\text{C14}-\text{H14C}\cdots\text{Cg1}^{\text{ii}}$	0.96	2.96	3.763 (2)	142

Symmetry codes: (i) $-x, -y + 2, -z$; (ii) $-x + 1, -y + 1, -z$. Cg1 is the centroid of the benzene C7–C12 ring.

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; 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.

The authors wish to acknowledge IIT, Madras for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2453).

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supplementary materials

Acta Cryst. (2009). E65, o2241 [doi:10.1107/S1600536809033273]

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Comment

The benzenesulfonamide derivatives are known to exhibit antitumor (Yang *et al.*, 2002), anti-bacterial (Badr, 2008) and anti-fungal (Hanafy *et al.*, 2007) activities. The geometric parameters in (I) (Fig. 1) agree with the reported values of similar structures (Chakkaravarthi *et al.*, 2007; Li & Yang, 2006).

The phenyl ring C1—C6 makes the dihedral angle of 81.5 (1)° with the benzene ring C7—C12. A distorted tetrahedral geometry [O1—S1—N1 109.49 (6)° and O2—S1—N1 104.32 (6)°] is observed around the S1 atom. The molecular structure is stabilized by weak intramolecular C—H···O and N—H···O interactions and the molecules are linked by weak intermolecular C—H···O and C—H··· π interactions (Fig. 2 & Table 1). The intramolecular N1—H1···O3 interaction generates a six-membered ring, with graph-set motif S(6) and the intermolecular C11—H11···O1 interaction generates a fourteen membered ring, with graph-set motif $R_2^2(14)$.

Experimental

To a stirred solution of 1-(2-aminophenyl)ethanone (3.0 g, 22.19 mmol) in dry DCM (50 ml) at room temperature, pyridine (1.75 g, 22.12 mmol) was slowly added. After 10 min, PhSO₂Cl (4.71 g, 26.61 mmol) was added and stirred at room temperature for 15 h. Then the reaction mixture was poured over crushed ice containing conc. HCl (10 ml), work up of the reaction followed by recrystallization from CDCl₃ gave the compound.

Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic C—H, N—H = 0.86 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for N—H, and C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for CH₃.

Figures

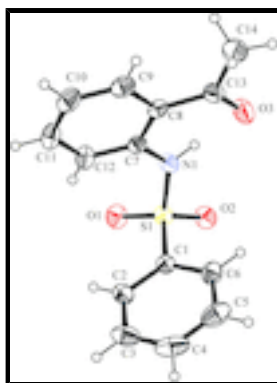


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

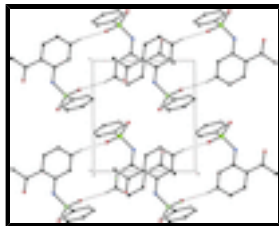


Fig. 2. The packing of (I), viewed down the a axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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Crystal data

$C_{14}H_{13}NO_3S$

$M_r = 275.31$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.9909$ (3) Å

$b = 8.6860$ (4) Å

$c = 10.0701$ (4) Å

$\alpha = 88.016$ (2)°

$\beta = 68.673$ (3)°

$\gamma = 83.424$ (2)°

$V = 646.79$ (5) Å³

$Z = 2$

$F_{000} = 288$

$D_x = 1.414$ Mg m⁻³

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

Cell parameters from 8349 reflections

$\theta = 2.2$ – 33.4 °

$\mu = 0.25$ mm⁻¹

$T = 295$ K

Block, colourless

$0.24 \times 0.20 \times 0.20$ mm

Data collection

Bruker Kappa APEX2
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 295$ K

ω and φ scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.942$, $T_{\max} = 0.951$

18690 measured reflections

5104 independent reflections

3886 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\max} = 33.6$ °

$\theta_{\min} = 2.2$ °

$h = -12 \rightarrow 12$

$k = -13 \rightarrow 13$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.142$

$S = 1.03$

5104 reflections

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0792P)^2 + 0.0784P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.35$ e Å⁻³

173 parameters

$$\Delta\rho_{\min} = -0.41 \text{ e } \text{\AA}^{-3}$$

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.21195 (4)	0.73664 (3)	-0.31916 (3)	0.04029 (10)
O1	0.07767 (14)	0.86458 (13)	-0.26435 (13)	0.0585 (3)
O2	0.21545 (16)	0.65492 (13)	-0.44094 (11)	0.0551 (3)
O3	0.3126 (2)	0.31720 (13)	-0.18266 (13)	0.0665 (3)
N1	0.18906 (16)	0.60455 (13)	-0.19706 (11)	0.0434 (2)
H1	0.1726	0.5138	-0.2181	0.052*
C1	0.42453 (17)	0.80008 (14)	-0.35373 (12)	0.0382 (2)
C2	0.4361 (2)	0.95013 (16)	-0.31914 (15)	0.0486 (3)
H2	0.3324	1.0179	-0.2762	0.058*
C3	0.6061 (3)	0.9970 (2)	-0.35014 (18)	0.0661 (5)
H3	0.6175	1.0975	-0.3282	0.079*
C4	0.7578 (3)	0.8955 (3)	-0.4131 (2)	0.0755 (6)
H4	0.8714	0.9279	-0.4334	0.091*
C5	0.7442 (2)	0.7457 (3)	-0.4469 (2)	0.0717 (5)
H5	0.8481	0.6780	-0.4893	0.086*
C6	0.5762 (2)	0.69662 (19)	-0.41754 (16)	0.0528 (3)
H6	0.5653	0.5963	-0.4401	0.063*
C7	0.19359 (15)	0.62435 (14)	-0.06059 (12)	0.0378 (2)
C8	0.24861 (16)	0.49460 (15)	0.00745 (12)	0.0396 (2)
C9	0.2463 (2)	0.51504 (19)	0.14513 (14)	0.0522 (3)
H9	0.2818	0.4304	0.1916	0.063*
C10	0.1932 (2)	0.6560 (2)	0.21426 (16)	0.0603 (4)
H10	0.1927	0.6662	0.3060	0.072*
C11	0.1410 (2)	0.7816 (2)	0.14616 (17)	0.0626 (4)
H11	0.1061	0.8776	0.1920	0.075*
C12	0.1396 (2)	0.76713 (18)	0.01025 (16)	0.0523 (3)
H12	0.1025	0.8529	-0.0341	0.063*
C13	0.30558 (19)	0.34007 (16)	-0.06119 (15)	0.0468 (3)
C14	0.3558 (3)	0.2063 (2)	0.0194 (2)	0.0679 (5)
H14A	0.3861	0.1139	-0.0380	0.102*
H14B	0.2557	0.1924	0.1059	0.102*
H14C	0.4581	0.2265	0.0420	0.102*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.04233 (17)	0.04223 (16)	0.04242 (17)	-0.00101 (11)	-0.02377 (13)	0.00144 (11)
O1	0.0481 (5)	0.0583 (6)	0.0696 (7)	0.0125 (4)	-0.0272 (5)	0.0008 (5)
O2	0.0710 (7)	0.0605 (6)	0.0490 (5)	-0.0116 (5)	-0.0384 (5)	0.0009 (4)
O3	0.1044 (10)	0.0446 (5)	0.0568 (6)	-0.0009 (6)	-0.0384 (6)	-0.0043 (4)
N1	0.0550 (6)	0.0410 (5)	0.0411 (5)	-0.0103 (4)	-0.0243 (5)	0.0022 (4)

supplementary materials

C1	0.0429 (6)	0.0398 (5)	0.0355 (5)	-0.0036 (4)	-0.0189 (4)	0.0031 (4)
C2	0.0650 (8)	0.0437 (6)	0.0444 (6)	-0.0105 (6)	-0.0276 (6)	0.0039 (5)
C3	0.0859 (12)	0.0725 (10)	0.0590 (9)	-0.0414 (10)	-0.0410 (9)	0.0211 (8)
C4	0.0614 (10)	0.1176 (17)	0.0625 (10)	-0.0449 (11)	-0.0334 (8)	0.0380 (11)
C5	0.0411 (7)	0.1059 (15)	0.0622 (10)	-0.0024 (8)	-0.0149 (7)	0.0170 (10)
C6	0.0467 (7)	0.0562 (8)	0.0530 (7)	0.0033 (6)	-0.0174 (6)	-0.0028 (6)
C7	0.0331 (5)	0.0453 (6)	0.0352 (5)	-0.0070 (4)	-0.0118 (4)	0.0001 (4)
C8	0.0355 (5)	0.0482 (6)	0.0352 (5)	-0.0092 (4)	-0.0119 (4)	0.0043 (4)
C9	0.0548 (8)	0.0672 (9)	0.0376 (6)	-0.0123 (7)	-0.0193 (5)	0.0081 (6)
C10	0.0634 (9)	0.0818 (11)	0.0365 (6)	-0.0114 (8)	-0.0174 (6)	-0.0065 (7)
C11	0.0681 (10)	0.0686 (10)	0.0477 (8)	0.0010 (8)	-0.0175 (7)	-0.0198 (7)
C12	0.0559 (8)	0.0520 (7)	0.0486 (7)	0.0032 (6)	-0.0202 (6)	-0.0078 (6)
C13	0.0494 (7)	0.0433 (6)	0.0473 (7)	-0.0069 (5)	-0.0171 (5)	0.0061 (5)
C14	0.0797 (12)	0.0559 (9)	0.0628 (10)	0.0037 (8)	-0.0240 (8)	0.0138 (7)

Geometric parameters (Å, °)

S1—O1	1.4246 (11)	C6—H6	0.9300
S1—O2	1.4280 (10)	C7—C12	1.3957 (19)
S1—N1	1.6274 (11)	C7—C8	1.4090 (17)
S1—C1	1.7555 (13)	C8—C9	1.3969 (17)
O3—C13	1.2260 (17)	C8—C13	1.4772 (19)
N1—C7	1.4049 (15)	C9—C10	1.374 (2)
N1—H1	0.8597	C9—H9	0.9300
C1—C2	1.3824 (18)	C10—C11	1.374 (3)
C1—C6	1.3834 (19)	C10—H10	0.9300
C2—C3	1.385 (2)	C11—C12	1.383 (2)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.373 (3)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.495 (2)
C4—C5	1.382 (3)	C14—H14A	0.9600
C4—H4	0.9300	C14—H14B	0.9600
C5—C6	1.380 (2)	C14—H14C	0.9600
C5—H5	0.9300		
O1—S1—O2	118.85 (7)	C12—C7—N1	121.74 (12)
O1—S1—N1	109.49 (6)	C12—C7—C8	119.64 (12)
O2—S1—N1	104.32 (6)	N1—C7—C8	118.58 (11)
O1—S1—C1	108.17 (7)	C9—C8—C7	117.87 (12)
O2—S1—C1	109.31 (6)	C9—C8—C13	119.87 (12)
N1—S1—C1	105.96 (6)	C7—C8—C13	122.26 (11)
C7—N1—S1	126.34 (9)	C10—C9—C8	122.23 (14)
C7—N1—H1	116.8	C10—C9—H9	118.9
S1—N1—H1	116.8	C8—C9—H9	118.9
C2—C1—C6	122.22 (13)	C11—C10—C9	119.21 (14)
C2—C1—S1	119.85 (11)	C11—C10—H10	120.4
C6—C1—S1	117.93 (10)	C9—C10—H10	120.4
C1—C2—C3	118.27 (15)	C10—C11—C12	120.77 (15)
C1—C2—H2	120.9	C10—C11—H11	119.6
C3—C2—H2	120.9	C12—C11—H11	119.6

C4—C3—C2	120.15 (16)	C11—C12—C7	120.27 (15)
C4—C3—H3	119.9	C11—C12—H12	119.9
C2—C3—H3	119.9	C7—C12—H12	119.9
C3—C4—C5	120.96 (15)	O3—C13—C8	122.15 (12)
C3—C4—H4	119.5	O3—C13—C14	118.48 (14)
C5—C4—H4	119.5	C8—C13—C14	119.37 (13)
C6—C5—C4	119.90 (18)	C13—C14—H14A	109.5
C6—C5—H5	120.0	C13—C14—H14B	109.5
C4—C5—H5	120.0	H14A—C14—H14B	109.5
C5—C6—C1	118.50 (16)	C13—C14—H14C	109.5
C5—C6—H6	120.7	H14A—C14—H14C	109.5
C1—C6—H6	120.7	H14B—C14—H14C	109.5
O1—S1—N1—C7	-57.47 (12)	S1—N1—C7—C12	29.02 (17)
O2—S1—N1—C7	174.32 (11)	S1—N1—C7—C8	-153.13 (10)
C1—S1—N1—C7	58.98 (12)	C12—C7—C8—C9	0.11 (18)
O1—S1—C1—C2	3.58 (12)	N1—C7—C8—C9	-177.78 (11)
O2—S1—C1—C2	134.36 (10)	C12—C7—C8—C13	179.40 (12)
N1—S1—C1—C2	-113.75 (10)	N1—C7—C8—C13	1.50 (17)
O1—S1—C1—C6	-175.46 (10)	C7—C8—C9—C10	-0.2 (2)
O2—S1—C1—C6	-44.68 (12)	C13—C8—C9—C10	-179.52 (14)
N1—S1—C1—C6	67.21 (11)	C8—C9—C10—C11	-0.2 (2)
C6—C1—C2—C3	0.07 (19)	C9—C10—C11—C12	0.7 (3)
S1—C1—C2—C3	-178.93 (10)	C10—C11—C12—C7	-0.8 (3)
C1—C2—C3—C4	-0.2 (2)	N1—C7—C12—C11	178.19 (13)
C2—C3—C4—C5	0.1 (2)	C8—C7—C12—C11	0.4 (2)
C3—C4—C5—C6	0.2 (3)	C9—C8—C13—O3	-178.77 (14)
C4—C5—C6—C1	-0.3 (2)	C7—C8—C13—O3	2.0 (2)
C2—C1—C6—C5	0.2 (2)	C9—C8—C13—C14	1.5 (2)
S1—C1—C6—C5	179.21 (12)	C7—C8—C13—C14	-177.78 (14)

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1 \cdots O3	0.86	2.03	2.596 (2)	123
C2—H2 \cdots O1	0.93	2.52	2.893 (2)	104
C12—H12 \cdots O1	0.93	2.40	3.057 (2)	128
C11—H11 \cdots O1 ⁱ	0.93	2.51	3.380 (2)	156
C14—H14C \cdots Cg1 ⁱⁱ	0.96	2.96	3.763 (2)	142

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

Fig. 1

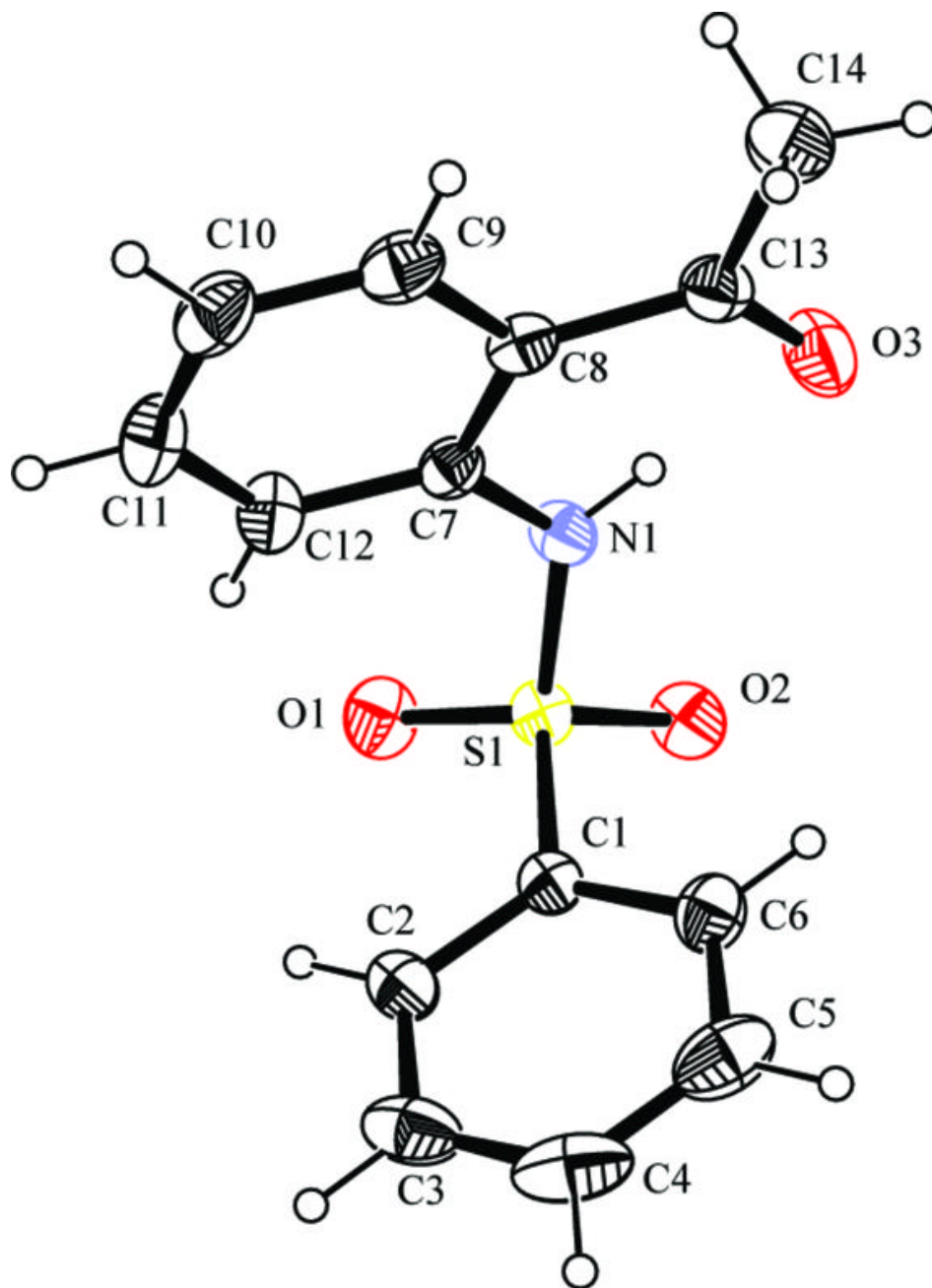


Fig. 2

