

## 4-Methyl-*N*-(4-nitrobenzoyl)benzenesulfonamide

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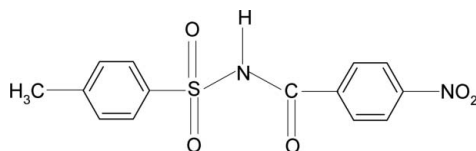
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.051;  $wR$  factor = 0.128; data-to-parameter ratio = 11.2.

In title compound,  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_5\text{S}$ , the dihedral angle between the sulfonyl benzene ring and the  $-\text{SO}_2-\text{NH}-\text{C}-\text{O}$  segment is  $81.5(2)^\circ$  and that between the sulfonyl and the benzoyl benzene rings is  $89.8(1)^\circ$ . In the crystal, molecules are linked into chains along the  $b$  axis via intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds.  $\text{C}-\text{H}\cdots\text{O}$  interactions are also observed.

### Related literature

For background to our study of the effect of substituents on the structures of methanesulfonamides, see: Gowda *et al.* (2007). For the effect of substituents on the structures of *N*-(aryl)-arylsulfonamides, see: Gowda *et al.* (2005). For the effect of substituents on the structures of *N*-(*p*-substituted benzoyl)-*p*-substituted benzenesulfonamides, see: Suchetan *et al.* (2010*a,b*).



### Experimental

#### Crystal data

$\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_5\text{S}$   
 $M_r = 320.32$   
 Monoclinic,  $P2_1$   
 $a = 11.722(3)$  Å  
 $b = 5.137(1)$  Å  
 $c = 12.488(3)$  Å  
 $\beta = 105.09(2)^\circ$

$V = 726.0(3)$  Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.25$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.40 \times 0.12 \times 0.08$  mm

#### Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector  
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford

Diffraction, 2009)  
 $T_{\min} = 0.907$ ,  $T_{\max} = 0.980$   
 2664 measured reflections  
 2265 independent reflections  
 1993 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$   
 $wR(F^2) = 0.128$   
 $S = 1.17$   
 2265 reflections  
 203 parameters  
 2 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.26$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.36$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), 605 Friedel pairs  
 Flack parameter:  $-0.05(14)$

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O2}^{\text{i}}$	0.85 (3)	2.22 (3)	3.054 (4)	164 (4)
$\text{N1}-\text{H1N}\cdots\text{O1}^{\text{ii}}$	0.85 (3)	2.54 (4)	2.944 (5)	110 (3)
$\text{C9}-\text{H9}\cdots\text{O3}^{\text{iii}}$	0.93	2.58	3.254 (5)	130
$\text{C13}-\text{H13}\cdots\text{O2}^{\text{i}}$	0.93	2.53	3.347 (5)	147

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2084).

### References

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**supplementary materials**

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## 4-Methyl-*N*-(4-nitrobenzoyl)benzenesulfonamide

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### Comment

The amide and sulfonamide moieties are important constituents of many biologically significant compounds. As a part of studying the effect of substituents on the structures of this class of compounds (Gowda *et al.*, 2005, 2007; Suchetan *et al.*, 2010*a,b*), the structure of 4-methyl-*N*-(4-nitrobenzoyl)-benzenesulfonamide (I) has been determined. The conformation of the N—H bond in the C—SO<sub>2</sub>—NH—C(O) segment is *anti* to the C=O bond (Fig.1), similar to those observed in *N*-(4-chlorobenzoyl)-4-methylbenzenesulfonamide (II) (Suchetan *et al.*, 2010*a*) and 4-methyl-*N*-(4-methylbenzoyl)-benzenesulfonamide (III) (Suchetan *et al.*, 2010*b*).

The molecules are twisted at the *S* atoms with the C—S(O<sub>2</sub>)—NH—C(O) torsional angle of 58.7 (3)°, compared to the values of 67.1 (2)° (molecule 1) and 67.7 (2)° (molecule 2) in (II) and 62.0 (2)° in (III).

The dihedral angle between the sulfonyl benzene ring and the —SO<sub>2</sub>—NH—C—O segment is 81.5 (2)°, compared to the values of 83.6 (1)° (molecule 1) and 81.0 (1)° (molecule 2) in (II) and 84.9 (1)° in (III).

The dihedral angle between the sulfonyl and the benzoyl benzene rings is 89.8 (1)°, compared to the values of 81.0 (1)° (molecule 1) and 76.3 (1)° (molecule 2) in (II) and 89.0 (1)° in (III).

In the crystal packing the molecules are linked by intermolecular N—H···O hydrogen bonds (Table 1, Fig. 2). Two C—H···O interactions are also observed.

### Experimental

The title compound was prepared by refluxing a mixture of 4-nitrobenzoic acid, 4-methylbenzenesulfonamide and phosphorous oxychloride for 3 hr on a water bath. The resultant mixture was cooled and poured into ice cold water. The solid obtained was filtered, washed thoroughly with water and then dissolved in sodium bicarbonate solution. The compound was later reprecipitated by acidifying the filtered solution with dilute HCl. It was filtered, dried and recrystallized.

The rod like colourless single crystals of the title compound used in X-ray diffraction studies were obtained by slow evaporation of a toluene solution at room temperature.

### Refinement

The H atom of the NH group was located in a difference map and later restrained to N—H = 0.86 (3) Å. The other H atoms were positioned with idealized geometry using a riding model with the aromatic C—H distance = 0.93 Å and methyl C—H = 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

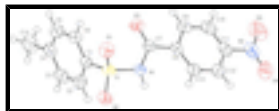


Fig. 1. Molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

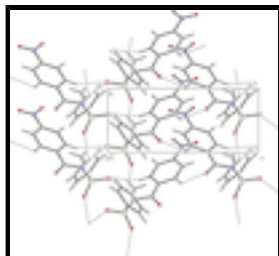


Fig. 2. Molecular packing in the title compound. Hydrogen bonds are shown as dashed lines.

## 4-Methyl-N-(4-nitrobenzoyl)benzenesulfonamide

### Crystal data

$C_{14}H_{12}N_2O_5S$

$M_r = 320.32$

Monoclinic,  $P2_1$

Hall symbol: P 2yb

$a = 11.722$  (3) Å

$b = 5.137$  (1) Å

$c = 12.488$  (3) Å

$\beta = 105.09$  (2)°

$V = 726.0$  (3) Å<sup>3</sup>

$Z = 2$

$F(000) = 332$

$D_x = 1.465$  Mg m<sup>-3</sup>

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

Cell parameters from 1463 reflections

$\theta = 2.8$ – $27.9$ °

$\mu = 0.25$  mm<sup>-1</sup>

$T = 293$  K

Rod, colourless

$0.40 \times 0.12 \times 0.08$  mm

### Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector

Radiation source: fine-focus sealed tube

graphite

Rotation method data acquisition using  $\omega$  and  $\varphi$  scans  $\theta_{\max} = 26.4$ °,  $\theta_{\min} = 2.8$ °

Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)

$T_{\min} = 0.907$ ,  $T_{\max} = 0.980$

2664 measured reflections

2265 independent reflections

1993 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$h = -13 \rightarrow 14$

$k = -4 \rightarrow 6$

$l = -15 \rightarrow 12$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

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

$wR(F^2) = 0.128$	$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.6019P]$
$S = 1.17$	where $P = (F_o^2 + 2F_c^2)/3$
2265 reflections	$(\Delta/\sigma)_{\max} = 0.001$
203 parameters	$\Delta\rho_{\max} = 0.26 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), <b>605 Friedel pairs</b> Flack parameter: $-0.05$ (14)

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2737 (4)	0.1687 (9)	0.1307 (3)	0.0362 (9)
C2	0.2176 (4)	0.3782 (10)	0.0686 (4)	0.0460 (11)
H2	0.2510	0.4608	0.0178	0.055*
C3	0.1097 (4)	0.4617 (11)	0.0842 (4)	0.0532 (13)
H3	0.0708	0.6011	0.0428	0.064*
C4	0.0597 (4)	0.3414 (10)	0.1600 (4)	0.0481 (12)
C5	0.1184 (4)	0.1350 (11)	0.2208 (4)	0.0522 (13)
H5	0.0853	0.0517	0.2716	0.063*
C6	0.2260 (4)	0.0498 (12)	0.2073 (3)	0.0438 (9)
H6	0.2655	-0.0871	0.2500	0.053*
C7	0.5340 (4)	0.3078 (9)	0.2885 (3)	0.0371 (10)
C8	0.6231 (3)	0.5138 (8)	0.3373 (3)	0.0343 (10)
C9	0.6277 (4)	0.5947 (12)	0.4452 (3)	0.0509 (12)
H9	0.5779	0.5190	0.4834	0.061*
C10	0.7056 (5)	0.7857 (11)	0.4949 (4)	0.0549 (14)
H10	0.7075	0.8438	0.5658	0.066*
C11	0.7808 (4)	0.8898 (10)	0.4380 (4)	0.0449 (11)
C12	0.7788 (4)	0.8124 (10)	0.3324 (4)	0.0499 (12)
H12	0.8301	0.8864	0.2953	0.060*
C13	0.6993 (4)	0.6224 (10)	0.2822 (3)	0.0469 (13)
H13	0.6972	0.5672	0.2108	0.056*
C14	-0.0577 (4)	0.4337 (15)	0.1747 (5)	0.0717 (17)
H14A	-0.1132	0.2924	0.1602	0.086*
H14B	-0.0869	0.5734	0.1238	0.086*

## supplementary materials

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H14C	-0.0476	0.4941	0.2493	0.086*
N1	0.5123 (3)	0.2647 (7)	0.1742 (3)	0.0329 (8)
H1N	0.525 (4)	0.377 (8)	0.129 (3)	0.039*
N2	0.8665 (4)	1.0941 (10)	0.4911 (3)	0.0568 (11)
O1	0.4318 (3)	-0.1903 (6)	0.1572 (3)	0.0502 (8)
O2	0.4040 (3)	0.0951 (7)	-0.0061 (2)	0.0487 (8)
O3	0.4829 (3)	0.1812 (7)	0.3440 (2)	0.0542 (9)
O4	0.9267 (4)	1.1940 (9)	0.4363 (4)	0.0806 (13)
O5	0.8702 (4)	1.1530 (10)	0.5865 (3)	0.0890 (15)
S1	0.40811 (9)	0.0583 (2)	0.10898 (7)	0.0359 (3)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.040 (2)	0.035 (2)	0.0326 (19)	0.0028 (19)	0.0070 (16)	-0.0031 (18)
C2	0.048 (3)	0.039 (3)	0.050 (3)	-0.002 (2)	0.013 (2)	0.001 (2)
C3	0.052 (3)	0.053 (3)	0.049 (3)	0.015 (2)	0.003 (2)	0.010 (2)
C4	0.041 (2)	0.061 (3)	0.038 (2)	0.003 (2)	0.0028 (19)	-0.006 (2)
C5	0.047 (2)	0.065 (4)	0.046 (2)	-0.002 (2)	0.0154 (19)	0.003 (2)
C6	0.048 (2)	0.045 (2)	0.0384 (19)	0.003 (3)	0.0112 (17)	0.005 (3)
C7	0.038 (2)	0.044 (3)	0.031 (2)	0.006 (2)	0.0105 (17)	0.0044 (19)
C8	0.0359 (19)	0.039 (3)	0.0254 (16)	0.0066 (19)	0.0035 (14)	-0.0010 (17)
C9	0.058 (3)	0.063 (4)	0.0313 (19)	-0.005 (3)	0.0122 (18)	0.000 (2)
C10	0.073 (3)	0.058 (4)	0.031 (2)	0.001 (3)	0.009 (2)	-0.007 (2)
C11	0.047 (2)	0.038 (3)	0.043 (2)	0.008 (2)	-0.001 (2)	0.002 (2)
C12	0.051 (3)	0.057 (3)	0.044 (2)	-0.011 (2)	0.015 (2)	-0.008 (2)
C13	0.047 (2)	0.063 (4)	0.0330 (19)	-0.005 (2)	0.0133 (18)	-0.008 (2)
C14	0.049 (3)	0.099 (5)	0.066 (3)	0.018 (3)	0.013 (3)	-0.001 (3)
N1	0.0442 (19)	0.030 (2)	0.0241 (16)	0.0003 (16)	0.0081 (14)	0.0031 (13)
N2	0.064 (2)	0.047 (3)	0.048 (2)	0.002 (2)	-0.0050 (18)	-0.005 (2)
O1	0.053 (2)	0.037 (2)	0.061 (2)	0.0047 (16)	0.0156 (15)	-0.0032 (15)
O2	0.0562 (17)	0.060 (2)	0.0305 (13)	-0.0034 (18)	0.0115 (12)	-0.0111 (16)
O3	0.062 (2)	0.069 (2)	0.0339 (15)	-0.0161 (19)	0.0162 (14)	0.0028 (16)
O4	0.080 (3)	0.077 (3)	0.074 (3)	-0.031 (3)	0.002 (2)	-0.004 (2)
O5	0.113 (3)	0.089 (4)	0.056 (2)	-0.019 (3)	0.006 (2)	-0.029 (2)
S1	0.0428 (5)	0.0325 (5)	0.0324 (4)	0.0018 (6)	0.0099 (4)	-0.0027 (5)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

C1—C6	1.371 (6)	C9—H9	0.9300
C1—C2	1.388 (6)	C10—C11	1.376 (7)
C1—S1	1.761 (4)	C10—H10	0.9300
C2—C3	1.396 (6)	C11—C12	1.372 (6)
C2—H2	0.9300	C11—N2	1.485 (6)
C3—C4	1.383 (7)	C12—C13	1.382 (6)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.379 (7)	C13—H13	0.9300
C4—C14	1.511 (7)	C14—H14A	0.9600
C5—C6	1.385 (6)	C14—H14B	0.9600

C5—H5	0.9300	C14—H14C	0.9600
C6—H6	0.9300	N1—S1	1.661 (4)
C7—O3	1.215 (5)	N1—H1N	0.85 (3)
C7—N1	1.401 (5)	N2—O4	1.217 (6)
C7—C8	1.500 (6)	N2—O5	1.219 (5)
C8—C13	1.379 (6)	O1—S1	1.409 (3)
C8—C9	1.398 (5)	O2—S1	1.438 (3)
C9—C10	1.374 (7)		
C6—C1—C2	121.0 (4)	C11—C10—H10	120.5
C6—C1—S1	120.5 (4)	C12—C11—C10	122.1 (5)
C2—C1—S1	118.4 (3)	C12—C11—N2	118.3 (4)
C1—C2—C3	118.3 (4)	C10—C11—N2	119.6 (4)
C1—C2—H2	120.8	C11—C12—C13	118.7 (4)
C3—C2—H2	120.8	C11—C12—H12	120.6
C4—C3—C2	121.3 (5)	C13—C12—H12	120.6
C4—C3—H3	119.4	C8—C13—C12	120.5 (4)
C2—C3—H3	119.4	C8—C13—H13	119.7
C5—C4—C3	118.7 (4)	C12—C13—H13	119.7
C5—C4—C14	121.0 (5)	C4—C14—H14A	109.5
C3—C4—C14	120.3 (5)	C4—C14—H14B	109.5
C4—C5—C6	121.1 (4)	H14A—C14—H14B	109.5
C4—C5—H5	119.5	C4—C14—H14C	109.5
C6—C5—H5	119.5	H14A—C14—H14C	109.5
C1—C6—C5	119.5 (5)	H14B—C14—H14C	109.5
C1—C6—H6	120.2	C7—N1—S1	121.0 (3)
C5—C6—H6	120.2	C7—N1—H1N	124 (3)
O3—C7—N1	120.7 (4)	S1—N1—H1N	110 (3)
O3—C7—C8	122.7 (4)	O4—N2—O5	124.5 (5)
N1—C7—C8	116.6 (3)	O4—N2—C11	118.1 (4)
C13—C8—C9	119.5 (4)	O5—N2—C11	117.4 (5)
C13—C8—C7	123.8 (3)	O1—S1—O2	119.9 (2)
C9—C8—C7	116.7 (4)	O1—S1—N1	109.32 (19)
C10—C9—C8	120.1 (4)	O2—S1—N1	103.62 (18)
C10—C9—H9	119.9	O1—S1—C1	108.1 (2)
C8—C9—H9	119.9	O2—S1—C1	108.24 (19)
C9—C10—C11	119.0 (4)	N1—S1—C1	106.99 (19)
C9—C10—H10	120.5		
C6—C1—C2—C3	-1.4 (7)	N2—C11—C12—C13	-180.0 (4)
S1—C1—C2—C3	178.6 (4)	C9—C8—C13—C12	-0.9 (7)
C1—C2—C3—C4	0.5 (7)	C7—C8—C13—C12	179.7 (4)
C2—C3—C4—C5	0.0 (7)	C11—C12—C13—C8	0.3 (7)
C2—C3—C4—C14	-179.4 (5)	O3—C7—N1—S1	5.4 (5)
C3—C4—C5—C6	0.5 (7)	C8—C7—N1—S1	-175.2 (3)
C14—C4—C5—C6	179.9 (5)	C12—C11—N2—O4	4.0 (7)
C2—C1—C6—C5	1.9 (7)	C10—C11—N2—O4	-175.5 (5)
S1—C1—C6—C5	-178.1 (4)	C12—C11—N2—O5	-177.1 (5)
C4—C5—C6—C1	-1.4 (7)	C10—C11—N2—O5	3.4 (7)
O3—C7—C8—C13	166.2 (4)	C7—N1—S1—O1	-58.2 (4)

## supplementary materials

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N1—C7—C8—C13	-13.2 (6)	C7—N1—S1—O2	172.9 (3)
O3—C7—C8—C9	-13.2 (6)	C7—N1—S1—C1	58.7 (3)
N1—C7—C8—C9	167.4 (4)	C6—C1—S1—O1	15.4 (4)
C13—C8—C9—C10	1.7 (7)	C2—C1—S1—O1	-164.7 (3)
C7—C8—C9—C10	-178.9 (4)	C6—C1—S1—O2	146.7 (4)
C8—C9—C10—C11	-1.9 (8)	C2—C1—S1—O2	-33.4 (4)
C9—C10—C11—C12	1.3 (8)	C6—C1—S1—N1	-102.2 (4)
C9—C10—C11—N2	-179.3 (4)	C2—C1—S1—N1	77.7 (4)
C10—C11—C12—C13	-0.5 (7)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1N $\cdots$ O2 <sup>i</sup>	0.85 (3)	2.22 (3)	3.054 (4)	164 (4)
N1—H1N $\cdots$ O1 <sup>ii</sup>	0.85 (3)	2.54 (4)	2.944 (5)	110 (3)
C9—H9 $\cdots$ O3 <sup>iii</sup>	0.93	2.58	3.254 (5)	130
C13—H13 $\cdots$ O2 <sup>i</sup>	0.93	2.53	3.347 (5)	147

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



Fig. 1

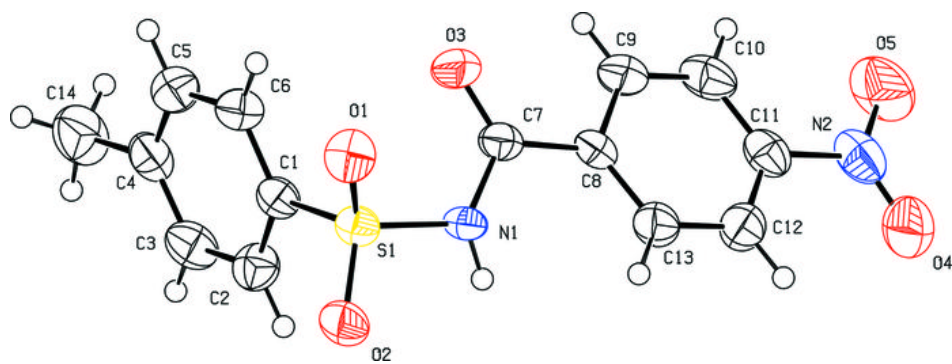


Fig. 2

