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

**P. A. Suchetan,[a] Sabine Foro[b] and B. Thimme Gowda[a]***

[a]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, and [b]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany
Correspondence e-mail: gowdabt@yahoo.com

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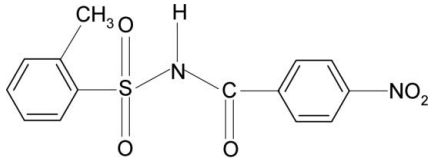
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.009 Å; $R$ factor = 0.058; $wR$ factor = 0.146; data-to-parameter ratio = 9.4.

In the title compound, $C_{14}H_{12}N_2O_5S$, the conformation of the N—C bond in the C—$SO_2$—NH—C(O) segment has *gauche* torsions with respect to the S=O bonds. The molecule is twisted at the S atom, the C—S($O_2$)—NH—C(O) torsion angle being 61.8 (5)°. The dihedral angle between the sulfonyl benzene ring and the —$SO_2$—NH—C—O segment is 86.8 (2)° and that between the sulfonyl and the benzoyl benzene rings is 83.8 (2)°. In the crystal, molecules are linked into zigzag chains along the *a* axis *via* N—H···O hydrogen bonds.

## Related literature

For our study of the effect of substituents on the structures of *N*-(aryl)-amides, see: Gowda *et al.* (2000), on the structures of *N*-(aryl)-methanesulfonamides, see: Gowda *et al.* (2007) and on the structures of *N*-(*p*-substituted-benzoyl)-*p*-substituted-benzenesulfonamides, see: Suchetan *et al.* (2010, 2011).




## Experimental

### Crystal data

$C_{14}H_{12}N_2O_5S$
$M_r$ = 320.32
Monoclinic, $P2_1$
$a$ = 11.088 (2) Å
$b$ = 5.3490 (7) Å
$c$ = 12.344 (2) Å
$\beta$ = 104.45 (2)°
$V$ = 709.0 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.26 mm$^{-1}$
$T$ = 293 K
0.36 × 0.14 × 0.08 mm

### Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
$T_{min}$ = 0.914, $T_{max}$ = 0.980
2485 measured reflections
1912 independent reflections
1701 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.146
$S$ = 1.22
1912 reflections
203 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.49 e Å$^{-3}$
Absolute structure: Flack (1983), 295 Friedel pairs
Flack parameter: 0.2 (2)

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*···O2$^{i}$ | 0.87 (3) | 2.12 (4) | 2.992 (6) | 174 (5) |

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

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: BQ2287).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o929 [ **doi:10.1107/S1600536811009846** ]

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

**P. A. Suchetan, S. Foro and B. T. Gowda**

## 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.*, 2000, 2007; Suchetan *et al.*, 2010, 2011), the structure of 2-methyl-*N*-(4-nitrobenzoyl)-benzenesulfonamide (I) has been determined (Fig.1). The conformation of the N—C bond in the C—$SO_2$—NH—C(O) segment has *gauche* torsions with respect to the S═O bonds. Further, the N—H bond in the C—$SO_2$—NH—C(O) segment is *anti* to the C=O bond, similar to those observed in 2-methyl-*N*-(4-chlorobenzoyl)-benzenesulfonamide (II) (Suchetan *et al.*, 2010) and 4-Methyl-*N*-(4-nitrobenzoyl)- benzenesulfonamide (III) (Suchetan *et al.*, 2011).

The molecules are twisted at the *S* atoms with the C—S($O_2$)—NH—C(O) torsional angle of 61.8 (5)°, compared to the values of -54.2 (2)° and 63.8 (2)°, in the two independent molecules of (II) and 58.7 (3)° in (III).

The dihedral angle between the sulfonyl benzene ring and the —$SO_2$—NH—C—O segment is 86.8 (2)°, compared to the values of 85.0 (1)° (molecule 1) & 87.0 (1)° (molecule 2) in (II) and 81.5 (2)° in (III).

The dihedral angle between the sulfonyl and the benzoyl benzene rings is 83.8 (2)°, compared to the values of 89.4 (1)° (molecule 1) and 82.1 (1)° (molecule 2) in (II) and 89.8 (1)° in (III).

The packing of molecules in the crystal linked by of N—H···O hydrogen bonds (Table 1) is shown in Fig. 2.

## Experimental

The title compound was prepared by refluxing a mixture of 4-nitrobenzoic acid, 2-methylbenzenesulfonamide and phosphorous oxychloride for 3 h 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.

Rod like colorless single crystals of the title compound used in x-ray diffraction studies were obtained by slow evaporation of its 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 (4) 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

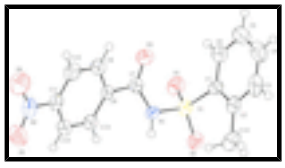

Fig. 1. Molecular structure of the title compound, showing the atom labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

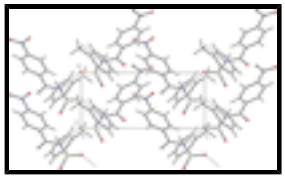

Fig. 2. Molecular packing in the title compound. Hydrogen bonds are shown as dashed lines.

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

*Crystal data*

| | |
|---|---|
| $C_{14}H_{12}N_2O_5S$ | $F(000) = 332$ |
| $M_r = 320.32$ | $D_x = 1.501$ Mg m$^{-3}$ |
| Monoclinic, $P2_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2yb | Cell parameters from 1591 reflections |
| $a = 11.088$ (2) Å | $\theta = 2.9$–$28.0°$ |
| $b = 5.3490$ (7) Å | $\mu = 0.26$ mm$^{-1}$ |
| $c = 12.344$ (2) Å | $T = 293$ K |
| $\beta = 104.45$ (2)° | Rod, colorless |
| $V = 709.0$ (2) Å$^3$ | 0.36 × 0.14 × 0.08 mm |
| $Z = 2$ | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector | 1912 independent reflections |
| Radiation source: fine-focus sealed tube | 1701 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.031$ |
| Rotation method data acquisition using ω and φ scans | $\theta_{max} = 26.4°$, $\theta_{min} = 2.9°$ |
| Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009) | $h = -11 \rightarrow 13$ |
| $T_{min} = 0.914$, $T_{max} = 0.980$ | $k = -6 \rightarrow 2$ |
| 2485 measured reflections | $l = -15 \rightarrow 5$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.058$ | H atoms treated by a mixture of independent and constrained refinement |

| | |
|---|---|
| $wR(F^2) = 0.146$ | $w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 1.1687P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.22$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 1912 reflections | $\Delta\rho_{max} = 0.40$ e Å$^{-3}$ |
| 203 parameters | $\Delta\rho_{min} = -0.49$ e Å$^{-3}$ |
| 2 restraints | Absolute structure: Flack (1983), 295 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.2 (2) |

*Special details*

**Experimental**. CrysAlis RED (Oxford Diffraction, 2009) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.7626 (5) | 0.1060 (12) | 0.1331 (4) | 0.0342 (12) |
| C2 | 0.6994 (5) | 0.3107 (13) | 0.0729 (5) | 0.0423 (14) |
| C3 | 0.5918 (6) | 0.3851 (16) | 0.1032 (6) | 0.0584 (19) |
| H3 | 0.5454 | 0.5171 | 0.0649 | 0.070* |
| C4 | 0.5522 (6) | 0.2708 (18) | 0.1870 (6) | 0.064 (2) |
| H4 | 0.4819 | 0.3312 | 0.2066 | 0.076* |
| C5 | 0.6146 (6) | 0.0673 (17) | 0.2430 (6) | 0.062 (2) |
| H5 | 0.5852 | −0.0150 | 0.2977 | 0.075* |
| C6 | 0.7216 (5) | −0.0105 (17) | 0.2157 (4) | 0.0472 (14) |
| H6 | 0.7666 | −0.1440 | 0.2540 | 0.057* |
| C7 | 1.0346 (5) | 0.2574 (12) | 0.2879 (4) | 0.0366 (13) |
| C8 | 1.1292 (4) | 0.4580 (11) | 0.3348 (4) | 0.0328 (14) |
| C9 | 1.1242 (5) | 0.5551 (15) | 0.4365 (4) | 0.0476 (18) |
| H9 | 1.0667 | 0.4932 | 0.4732 | 0.057* |
| C10 | 1.2052 (6) | 0.7466 (14) | 0.4848 (5) | 0.0488 (16) |
| H10 | 1.2013 | 0.8180 | 0.5526 | 0.059* |
| C11 | 1.2906 (5) | 0.8261 (13) | 0.4292 (5) | 0.0409 (14) |
| C12 | 1.2986 (5) | 0.7304 (14) | 0.3293 (5) | 0.0464 (16) |
| H12 | 1.3574 | 0.7902 | 0.2936 | 0.056* |
| C13 | 1.2161 (5) | 0.5394 (15) | 0.2817 (4) | 0.0451 (17) |
| H13 | 1.2205 | 0.4681 | 0.2140 | 0.054* |
| C14 | 0.7364 (6) | 0.4421 (13) | −0.0192 (5) | 0.0554 (18) |

| | | | | |
|---|---|---|---|---|
| H14A | 0.7156 | 0.3408 | −0.0855 | 0.067* |
| H14B | 0.8245 | 0.4721 | 0.0015 | 0.067* |
| H14C | 0.6929 | 0.5986 | −0.0335 | 0.067* |
| N1 | 1.0112 (4) | 0.2138 (9) | 0.1743 (3) | 0.0319 (10) |
| H1N | 1.031 (5) | 0.298 (11) | 0.121 (4) | 0.038* |
| N2 | 1.3751 (4) | 1.0337 (13) | 0.4783 (4) | 0.0491 (13) |
| O1 | 0.9359 (4) | −0.2274 (9) | 0.1691 (3) | 0.0492 (11) |
| O2 | 0.9059 (3) | 0.0189 (10) | −0.0029 (3) | 0.0428 (9) |
| O3 | 0.9818 (4) | 0.1447 (10) | 0.3468 (3) | 0.0539 (13) |
| O4 | 1.3758 (5) | 1.0989 (12) | 0.5732 (4) | 0.0753 (16) |
| O5 | 1.4394 (4) | 1.1259 (11) | 0.4219 (4) | 0.0690 (15) |
| S1 | 0.90691 (11) | 0.0026 (3) | 0.11283 (10) | 0.0351 (3) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.037 (3) | 0.039 (3) | 0.026 (2) | −0.002 (3) | 0.0066 (19) | −0.006 (2) |
| C2 | 0.039 (3) | 0.043 (4) | 0.040 (3) | −0.004 (3) | 0.000 (2) | −0.005 (3) |
| C3 | 0.037 (3) | 0.062 (5) | 0.068 (4) | 0.008 (3) | −0.003 (3) | −0.009 (4) |
| C4 | 0.044 (3) | 0.082 (6) | 0.068 (5) | −0.008 (4) | 0.021 (3) | −0.025 (5) |
| C5 | 0.051 (3) | 0.081 (7) | 0.059 (4) | −0.015 (4) | 0.021 (3) | −0.003 (4) |
| C6 | 0.042 (3) | 0.054 (4) | 0.044 (3) | −0.006 (4) | 0.007 (2) | −0.001 (4) |
| C7 | 0.031 (3) | 0.041 (4) | 0.036 (3) | 0.001 (3) | 0.005 (2) | 0.005 (3) |
| C8 | 0.027 (2) | 0.039 (4) | 0.031 (2) | 0.001 (2) | 0.0022 (18) | 0.005 (2) |
| C9 | 0.038 (3) | 0.068 (6) | 0.036 (3) | −0.006 (3) | 0.008 (2) | −0.002 (3) |
| C10 | 0.050 (3) | 0.053 (4) | 0.041 (3) | 0.001 (3) | 0.007 (3) | −0.011 (3) |
| C11 | 0.031 (3) | 0.044 (4) | 0.041 (3) | 0.004 (3) | −0.002 (2) | 0.004 (3) |
| C12 | 0.035 (3) | 0.061 (5) | 0.043 (3) | −0.010 (3) | 0.008 (2) | 0.000 (3) |
| C13 | 0.038 (3) | 0.065 (5) | 0.031 (2) | −0.008 (3) | 0.006 (2) | −0.005 (3) |
| C14 | 0.064 (4) | 0.044 (5) | 0.052 (3) | 0.007 (3) | 0.001 (3) | 0.005 (3) |
| N1 | 0.036 (2) | 0.032 (3) | 0.026 (2) | −0.004 (2) | 0.0047 (17) | 0.0006 (19) |
| N2 | 0.036 (2) | 0.046 (4) | 0.057 (3) | 0.003 (3) | −0.002 (2) | −0.006 (3) |
| O1 | 0.052 (2) | 0.039 (3) | 0.052 (2) | 0.007 (2) | 0.0060 (19) | 0.006 (2) |
| O2 | 0.0432 (19) | 0.047 (3) | 0.0359 (17) | 0.002 (2) | 0.0052 (14) | −0.006 (2) |
| O3 | 0.054 (2) | 0.066 (3) | 0.040 (2) | −0.015 (2) | 0.0095 (18) | 0.003 (2) |
| O4 | 0.083 (4) | 0.079 (4) | 0.059 (3) | −0.020 (3) | 0.010 (2) | −0.027 (3) |
| O5 | 0.053 (3) | 0.070 (4) | 0.083 (3) | −0.020 (3) | 0.015 (2) | −0.002 (3) |
| S1 | 0.0365 (6) | 0.0337 (7) | 0.0330 (6) | 0.0020 (7) | 0.0043 (4) | −0.0006 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.366 (8) | C9—H9 | 0.9300 |
| C1—C2 | 1.408 (9) | C10—C11 | 1.369 (9) |
| C1—S1 | 1.769 (5) | C10—H10 | 0.9300 |
| C2—C3 | 1.395 (9) | C11—C12 | 1.359 (8) |
| C2—C14 | 1.479 (8) | C11—N2 | 1.481 (9) |
| C3—C4 | 1.365 (10) | C12—C13 | 1.399 (9) |
| C3—H3 | 0.9300 | C12—H12 | 0.9300 |
| C4—C5 | 1.380 (12) | C13—H13 | 0.9300 |

| | | | |
|---|---|---|---|
| C4—H4 | 0.9300 | C14—H14A | 0.9600 |
| C5—C6 | 1.377 (8) | C14—H14B | 0.9600 |
| C5—H5 | 0.9300 | C14—H14C | 0.9600 |
| C6—H6 | 0.9300 | N1—S1 | 1.659 (5) |
| C7—O3 | 1.202 (6) | N1—H1N | 0.87 (3) |
| C7—N1 | 1.381 (6) | N2—O5 | 1.219 (7) |
| C7—C8 | 1.511 (8) | N2—O4 | 1.220 (6) |
| C8—C13 | 1.366 (7) | O1—S1 | 1.410 (5) |
| C8—C9 | 1.371 (7) | O2—S1 | 1.428 (3) |
| C9—C10 | 1.395 (9) | | |
| C6—C1—C2 | 122.3 (5) | C9—C10—H10 | 121.1 |
| C6—C1—S1 | 116.4 (5) | C12—C11—C10 | 123.3 (6) |
| C2—C1—S1 | 121.1 (4) | C12—C11—N2 | 118.4 (5) |
| C3—C2—C1 | 115.2 (6) | C10—C11—N2 | 118.3 (5) |
| C3—C2—C14 | 119.4 (6) | C11—C12—C13 | 118.2 (6) |
| C1—C2—C14 | 125.4 (5) | C11—C12—H12 | 120.9 |
| C4—C3—C2 | 122.3 (7) | C13—C12—H12 | 120.9 |
| C4—C3—H3 | 118.9 | C8—C13—C12 | 119.8 (5) |
| C2—C3—H3 | 118.9 | C8—C13—H13 | 120.1 |
| C3—C4—C5 | 121.2 (7) | C12—C13—H13 | 120.1 |
| C3—C4—H4 | 119.4 | C2—C14—H14A | 109.5 |
| C5—C4—H4 | 119.4 | C2—C14—H14B | 109.5 |
| C6—C5—C4 | 118.0 (7) | H14A—C14—H14B | 109.5 |
| C6—C5—H5 | 121.0 | C2—C14—H14C | 109.5 |
| C4—C5—H5 | 121.0 | H14A—C14—H14C | 109.5 |
| C1—C6—C5 | 120.9 (7) | H14B—C14—H14C | 109.5 |
| C1—C6—H6 | 119.6 | C7—N1—S1 | 120.8 (4) |
| C5—C6—H6 | 119.6 | C7—N1—H1N | 132 (4) |
| O3—C7—N1 | 122.2 (5) | S1—N1—H1N | 106 (4) |
| O3—C7—C8 | 121.4 (5) | O5—N2—O4 | 124.6 (6) |
| N1—C7—C8 | 116.5 (4) | O5—N2—C11 | 118.0 (5) |
| C13—C8—C9 | 120.9 (5) | O4—N2—C11 | 117.3 (5) |
| C13—C8—C7 | 123.2 (5) | O1—S1—O2 | 119.3 (3) |
| C9—C8—C7 | 115.9 (5) | O1—S1—N1 | 108.8 (3) |
| C8—C9—C10 | 120.1 (5) | O2—S1—N1 | 104.3 (2) |
| C8—C9—H9 | 120.0 | O1—S1—C1 | 107.9 (3) |
| C10—C9—H9 | 120.0 | O2—S1—C1 | 109.9 (2) |
| C11—C10—C9 | 117.8 (6) | N1—S1—C1 | 105.9 (3) |
| C11—C10—H10 | 121.1 | | |
| C6—C1—C2—C3 | −0.3 (8) | C10—C11—C12—C13 | −0.6 (10) |
| S1—C1—C2—C3 | −175.1 (5) | N2—C11—C12—C13 | −178.1 (5) |
| C6—C1—C2—C14 | −178.4 (6) | C9—C8—C13—C12 | −2.2 (9) |
| S1—C1—C2—C14 | 6.7 (8) | C7—C8—C13—C12 | 178.4 (6) |
| C1—C2—C3—C4 | 1.4 (10) | C11—C12—C13—C8 | 1.2 (9) |
| C14—C2—C3—C4 | 179.6 (6) | O3—C7—N1—S1 | 0.5 (8) |
| C2—C3—C4—C5 | −2.8 (11) | C8—C7—N1—S1 | −178.6 (4) |
| C3—C4—C5—C6 | 3.0 (11) | C12—C11—N2—O5 | 7.1 (8) |
| C2—C1—C6—C5 | 0.7 (9) | C10—C11—N2—O5 | −170.5 (6) |

| | | | |
|---|---|---|---|
| S1—C1—C6—C5 | 175.7 (5) | C12—C11—N2—O4 | −172.3 (6) |
| C4—C5—C6—C1 | −1.9 (10) | C10—C11—N2—O4 | 10.1 (9) |
| O3—C7—C8—C13 | 160.5 (6) | C7—N1—S1—O1 | −53.9 (5) |
| N1—C7—C8—C13 | −20.4 (8) | C7—N1—S1—O2 | 177.8 (4) |
| O3—C7—C8—C9 | −18.9 (9) | C7—N1—S1—C1 | 61.8 (5) |
| N1—C7—C8—C9 | 160.3 (5) | C6—C1—S1—O1 | 14.8 (5) |
| C13—C8—C9—C10 | 2.6 (9) | C2—C1—S1—O1 | −170.0 (4) |
| C7—C8—C9—C10 | −178.0 (5) | C6—C1—S1—O2 | 146.4 (5) |
| C8—C9—C10—C11 | −2.0 (10) | C2—C1—S1—O2 | −38.4 (6) |
| C9—C10—C11—C12 | 1.0 (10) | C6—C1—S1—N1 | −101.5 (5) |
| C9—C10—C11—N2 | 178.5 (6) | C2—C1—S1—N1 | 73.6 (5) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1N···O2$^{i}$ | 0.87 (3) | 2.12 (4) | 2.992 (6) | 174 (5) |

Symmetry codes: (i) −*x*+2, *y*+1/2, −*z*.

**Fig. 1**

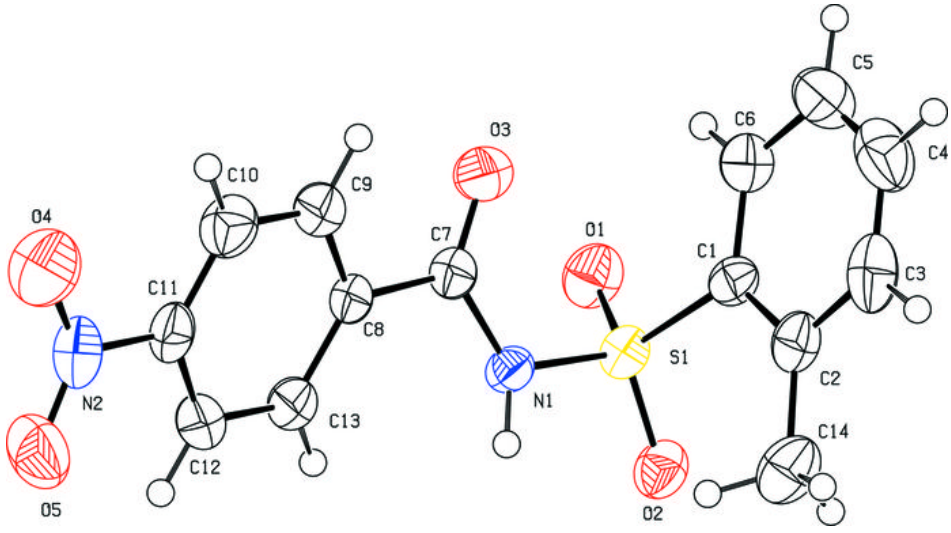

**Fig. 2**