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## Structure Reports

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**N-(4-Methylphenylsulfonyl)-3-nitrobenzamide**S. Sreenivasa,<sup>a</sup> M. S. Nanjundaswamy,<sup>b</sup> A. G. Sudha,<sup>c</sup>  
K. J. Pampa,<sup>d</sup> N. K. Lokanath<sup>e</sup> and P. A. Suchetan<sup>f\*</sup>

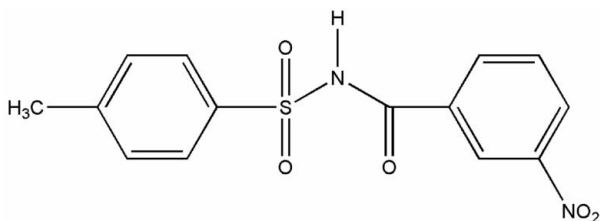
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.039;  $wR$  factor = 0.114; data-to-parameter ratio = 11.7.

In the title compound,  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_5\text{S}$ , the dihedral angle between the aromatic rings is  $86.29(1)^\circ$  and the conformation between the  $\text{C}=\text{O}$  bond of the amide group and the *meta*- $\text{NO}_2$  group is *syn*. The  $\text{C}-\text{S}-\text{N}-\text{C}$  torsion angle is  $-65.87(19)^\circ$  and the molecule has an L-shaped conformation. In the crystal, the molecules are connected into inversion dimers through pairs of  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds and  $\text{C}-\text{H}\cdots\text{O}$  interactions forming  $R_2^2(8)$  and  $R_2^2(14)$  loops, respectively. The dimers are connected by further  $\text{C}-\text{H}\cdots\text{O}$  interactions, thereby forming (100) sheets.

## Related literature

For related structures see: Suchetan *et al.* (2010, 2011, 2012).

## Experimental

## Crystal data

 $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_5\text{S}$  $M_r = 320.32$ 

Monoclinic,  $P2_1/c$   
 $a = 4.9736(5)$  Å  
 $b = 23.245(2)$  Å  
 $c = 12.7197(11)$  Å  
 $\beta = 100.820(4)^\circ$   
 $V = 1444.4(2)$  Å<sup>3</sup>

$Z = 4$   
Cu  $K\alpha$  radiation  
 $\mu = 2.24$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.39 \times 0.29 \times 0.20$  mm

## Data collection

Bruker APEXII diffractometer  
Absorption correction: multi-scan  
(SADABS; Bruker, 2009)  
 $T_{\min} = 0.481$ ,  $T_{\max} = 0.638$

12115 measured reflections  
2378 independent reflections  
2053 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.035$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$   
 $wR(F^2) = 0.114$   
 $S = 1.06$   
2378 reflections  
204 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.23$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{HN1}\cdots\text{O2}^i$	0.80 (3)	2.14 (3)	2.927 (3)	167
$\text{C13}-\text{H13}\cdots\text{O2}^i$	0.93	2.59	3.333 (3)	137
$\text{C3}-\text{H3}\cdots\text{O4}^{ii}$	0.93	2.58	3.459 (3)	155

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

Data collection: APEX2 (Bruker, 2009); cell refinement: APEX2 and SAINT-Plus (Bruker, 2009); data reduction: SAINT-Plus and XPREP (Bruker, 2009); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: SHELXL97.

The authors acknowledge the IOE X-ray diffractometer facility, University of Mysore, Mysore, for the data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7184).

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## supplementary materials

*Acta Cryst.* (2014). E70, o191 [doi:10.1107/S1600536814001317]

## N-(4-Methylphenylsulfonyl)-3-nitrobenzamide

S. Sreenivasa, M. S. Nanjundaswamy, A. G. Sudha, K. J. Pampa, N. K. Lokanath and P. A. Suchetan

### 1. Introduction

As a part of our continued efforts to study the crystal structures of N-(aroyl)-arylsulfonamides (Suchetan *et al.*, 2010, 2011, 2012), we report here the crystal structure of the title compound (I) (Fig 1).

### 2. Experimental

#### 2.1. Synthesis and crystallization

The title compound (I) was prepared by refluxing a mixture of 3-nitrobenzoic acid, 4-methylbenzenesulfonamide and phosphorous oxychloride ( $\text{POCl}_3$ ) for 2 h on a water bath. The resultant mixture was cooled and poured into ice cold water. The solid obtained was filtered and washed thoroughly with water and then dissolved in sodium bicarbonate solution. The compound was later reprecipitated by acidifying the filtered solution with dilute HCl. The compound obtained was filtered and later dried (Melting point: 459 K).

Colorless prisms of (I) were obtained from a slow evaporation of its aqueous methanolic solution at room temperature.

#### 2.2. Refinement

The H atom of the NH group was located in a difference map and later refined freely. 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 1.2–1.5 times of the  $U_{eq}$  of the parent atom).

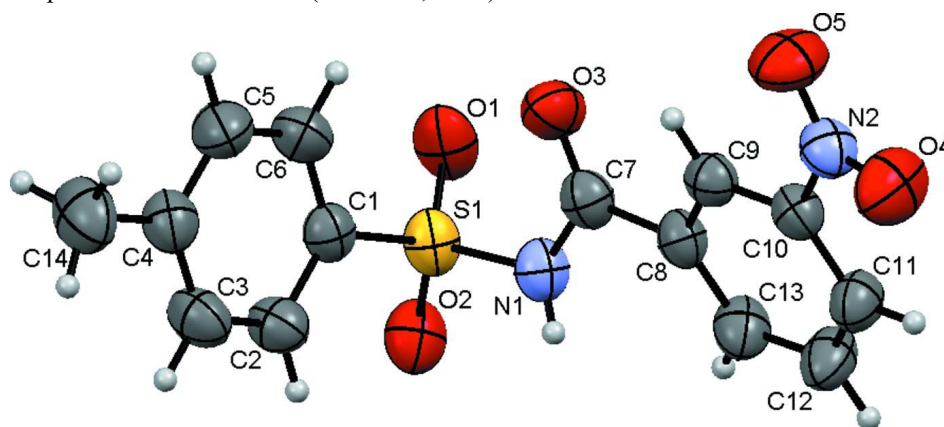
### 3. Results and discussion

In I, the dihedral angle between the two aromatic rings is 86.29 (1)°. Compared to this, the dihedral angle is 79.4 (1)° in N-(4-methylphenylsulfonyl)-benzamide (II) (Suchetan *et al.*, 2010), 89.8 (1)° in N-(4-methylphenylsulfonyl)-4-nitrobenzamide (III) (Suchetan *et al.*, 2011) and 86.9 (2)° in N-(phenylsulfonyl)-3-nitrobenzamide (IV) (Suchetan *et al.*, 2012). Thus, introducing a nitro group into the benzoyl ring results in an increase of the dihedral angle between the aromatic rings. The conformation between the N—H bond and the *meta*-NO<sub>2</sub> group is *anti* in contrast to the *syn* conformation observed in IV (Suchetan *et al.*, 2012). The molecule is twisted at the S atom, the dihedral angle between the planes defined by the S—N—C=O segment in the central chain and the sulfonyl benzene rings being 79.16 (1)°.

In the crystal structure, the molecules are connected into inversion dimers through N1—HN1 $\cdots$ O2 hydrogen bonds (Table 1, Figure 2) and C13—H13 $\cdots$ O2 interactions forming R<sub>2</sub><sup>2</sup>(8) and R<sub>2</sub><sup>2</sup>(14) ring motifs respectively. These dimers are further connected into C(12) chains through C3—H3 $\cdots$ O4 interactions forming sheets (Figure 2).

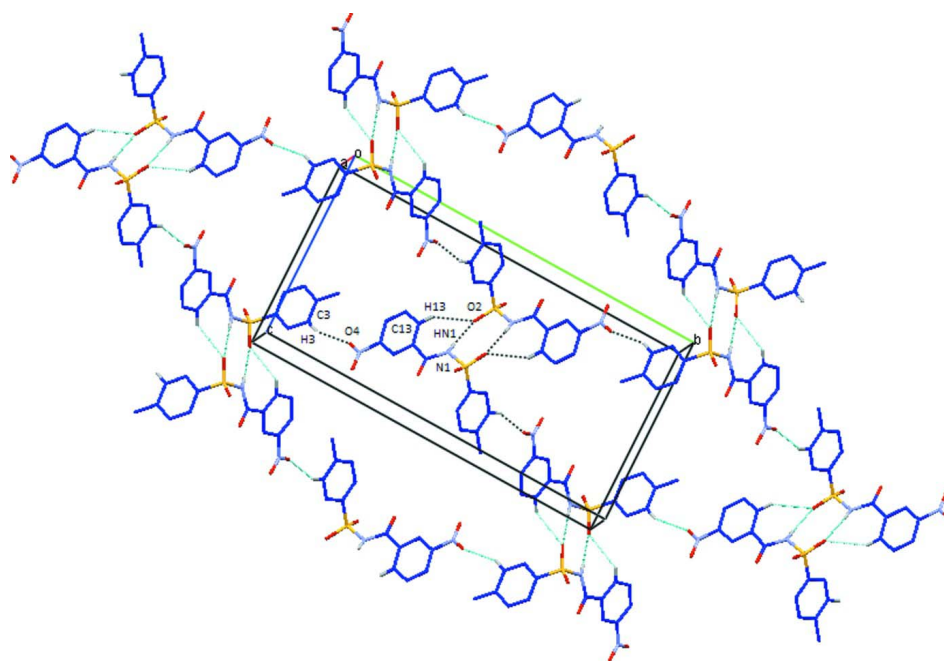
**Computing details**

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).



**Figure 1**

Molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level.



**Figure 2**

Formation of sheets in the crystal structure.

***N*-(4-Methylphenylsulfonyl)-3-nitrobenzamide**

*Crystal data*

$C_{14}H_{12}N_2O_5S$   
 $M_r = 320.32$

Monoclinic,  $P2_1/c$   
 Hall symbol: -P 2ybc

$a = 4.9736$  (5) Å  
 $b = 23.245$  (2) Å  
 $c = 12.7197$  (11) Å  
 $\beta = 100.820$  (4)°  
 $V = 1444.4$  (2) Å<sup>3</sup>  
 $Z = 4$   
 $F(000) = 664$   
 Prism  
 $D_x = 1.473$  Mg m<sup>-3</sup>

Melting point: 459 K  
 Cu  $K\alpha$  radiation,  $\lambda = 1.54178$  Å  
 Cell parameters from 1127 reflections  
 $\theta = 3.8$ – $64.5$ °  
 $\mu = 2.24$  mm<sup>-1</sup>  
 $T = 293$  K  
 Prism, colourless  
 $0.39 \times 0.29 \times 0.20$  mm

*Data collection*

Bruker APEXII  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 phi and  $\varphi$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2009)  
 $T_{\min} = 0.481$ ,  $T_{\max} = 0.638$   
 12115 measured reflections

2378 independent reflections  
 2053 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.035$   
 $\theta_{\max} = 64.5$ °,  $\theta_{\min} = 3.8$ °  
 $h = -5 \rightarrow 4$   
 $k = -26 \rightarrow 26$   
 $l = -14 \rightarrow 14$   
 2 standard reflections every 1 reflections  
 intensity decay: 1%

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.039$   
 $wR(F^2) = 0.114$   
 $S = 1.06$   
 2378 reflections  
 204 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

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  
 $w = 1/[\sigma^2(F_o^2) + (0.0621P)^2 + 0.3691P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.23$  e Å<sup>-3</sup>

*Special details*

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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  $F^2 > 2\sigma(F^2)$  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<sup>2</sup>)*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	1.10155 (10)	0.50190 (2)	0.32699 (4)	0.0546 (2)
C8	0.6073 (4)	0.63811 (8)	0.33442 (15)	0.0481 (5)
C9	0.4226 (4)	0.66836 (8)	0.25927 (16)	0.0481 (5)
H9	0.4108	0.6615	0.1865	0.058*
O2	1.1994 (3)	0.47252 (7)	0.42557 (13)	0.0667 (4)
N2	0.0629 (4)	0.74082 (8)	0.21424 (15)	0.0570 (4)
O1	1.2908 (3)	0.52526 (7)	0.26821 (15)	0.0720 (5)

N1	0.9164 (4)	0.55519 (7)	0.36288 (16)	0.0534 (4)
C10	0.2572 (4)	0.70859 (8)	0.29425 (15)	0.0471 (5)
O3	0.8066 (3)	0.59550 (7)	0.19878 (13)	0.0695 (5)
O4	-0.1159 (4)	0.76822 (9)	0.24399 (15)	0.0891 (6)
O5	0.0900 (4)	0.73809 (9)	0.12131 (13)	0.0853 (6)
C4	0.4935 (5)	0.38740 (9)	0.11605 (18)	0.0593 (5)
C3	0.5450 (5)	0.38158 (10)	0.22531 (18)	0.0646 (6)
H3	0.4508	0.3537	0.2563	0.077*
C7	0.7819 (4)	0.59512 (9)	0.29113 (17)	0.0518 (5)
C5	0.6344 (5)	0.42936 (10)	0.07092 (18)	0.0680 (6)
H5	0.6014	0.4341	-0.0030	0.082*
C11	0.2669 (5)	0.71991 (9)	0.40117 (17)	0.0583 (5)
H11	0.1494	0.7467	0.4229	0.070*
C1	0.8710 (4)	0.45716 (8)	0.24416 (16)	0.0490 (5)
C6	0.8239 (5)	0.46431 (10)	0.13467 (19)	0.0630 (6)
H6	0.9182	0.4923	0.1039	0.076*
C13	0.6243 (5)	0.64965 (9)	0.44227 (17)	0.0602 (6)
H13	0.7500	0.6298	0.4928	0.072*
C2	0.7316 (5)	0.41580 (10)	0.29029 (17)	0.0588 (5)
H2	0.7635	0.4111	0.3642	0.071*
C12	0.4558 (5)	0.69042 (10)	0.47530 (18)	0.0669 (6)
H12	0.4696	0.6981	0.5479	0.080*
C14	0.2854 (6)	0.34997 (12)	0.0463 (2)	0.0845 (8)
H14A	0.1814	0.3292	0.0903	0.127*
H14B	0.3776	0.3232	0.0078	0.127*
H14C	0.1647	0.3736	-0.0035	0.127*
HN1	0.860 (5)	0.5495 (10)	0.417 (2)	0.062 (8)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0368 (3)	0.0518 (3)	0.0732 (4)	0.0021 (2)	0.0053 (2)	-0.0047 (2)
C8	0.0445 (11)	0.0416 (10)	0.0566 (11)	-0.0023 (8)	0.0052 (9)	-0.0015 (8)
C9	0.0469 (11)	0.0478 (11)	0.0488 (10)	-0.0051 (9)	0.0071 (8)	-0.0001 (8)
O2	0.0538 (9)	0.0660 (10)	0.0726 (10)	0.0159 (7)	-0.0079 (7)	-0.0034 (8)
N2	0.0582 (11)	0.0534 (10)	0.0563 (11)	0.0032 (9)	0.0024 (8)	0.0041 (8)
O1	0.0428 (8)	0.0662 (10)	0.1106 (13)	-0.0065 (7)	0.0238 (8)	-0.0066 (9)
N1	0.0444 (10)	0.0513 (10)	0.0627 (11)	0.0046 (8)	0.0053 (8)	-0.0017 (8)
C10	0.0458 (11)	0.0423 (10)	0.0508 (11)	-0.0017 (8)	0.0027 (8)	0.0028 (8)
O3	0.0759 (11)	0.0679 (10)	0.0705 (11)	0.0121 (8)	0.0292 (8)	0.0079 (8)
O4	0.0871 (13)	0.0949 (14)	0.0821 (12)	0.0449 (11)	0.0077 (10)	0.0063 (10)
O5	0.0957 (14)	0.1043 (14)	0.0529 (10)	0.0235 (11)	0.0063 (9)	0.0148 (9)
C4	0.0611 (13)	0.0514 (12)	0.0619 (13)	0.0011 (10)	0.0025 (10)	-0.0020 (10)
C3	0.0647 (14)	0.0599 (13)	0.0669 (14)	-0.0144 (11)	0.0066 (11)	0.0075 (11)
C7	0.0448 (11)	0.0488 (11)	0.0612 (13)	-0.0026 (9)	0.0084 (9)	-0.0004 (9)
C5	0.0866 (17)	0.0651 (14)	0.0516 (12)	-0.0038 (12)	0.0111 (11)	-0.0008 (10)
C11	0.0665 (14)	0.0519 (11)	0.0551 (12)	0.0116 (10)	0.0082 (10)	-0.0036 (9)
C1	0.0414 (11)	0.0471 (10)	0.0587 (12)	0.0034 (8)	0.0100 (8)	-0.0014 (9)
C6	0.0686 (15)	0.0589 (13)	0.0647 (13)	-0.0080 (11)	0.0207 (11)	0.0028 (10)
C13	0.0670 (14)	0.0536 (12)	0.0540 (12)	0.0093 (10)	-0.0041 (10)	0.0001 (9)

C2	0.0591 (13)	0.0605 (13)	0.0546 (12)	-0.0081 (10)	0.0054 (10)	0.0051 (10)
C12	0.0871 (17)	0.0623 (14)	0.0471 (11)	0.0166 (12)	0.0017 (11)	-0.0057 (10)
C14	0.096 (2)	0.0701 (16)	0.0780 (17)	-0.0173 (14)	-0.0082 (14)	-0.0066 (13)

*Geometric parameters (Å, °)*

S1—O1	1.4156 (17)	C4—C14	1.507 (3)
S1—O2	1.4305 (16)	C3—C2	1.375 (3)
S1—N1	1.6580 (18)	C3—H3	0.9300
S1—C1	1.747 (2)	C5—C6	1.385 (3)
C8—C13	1.385 (3)	C5—H5	0.9300
C8—C9	1.386 (3)	C11—C12	1.382 (3)
C8—C7	1.495 (3)	C11—H11	0.9300
C9—C10	1.373 (3)	C1—C6	1.378 (3)
C9—H9	0.9300	C1—C2	1.379 (3)
N2—O4	1.211 (2)	C6—H6	0.9300
N2—O5	1.216 (2)	C13—C12	1.382 (3)
N2—C10	1.470 (3)	C13—H13	0.9300
N1—C7	1.383 (3)	C2—H2	0.9300
N1—HN1	0.80 (2)	C12—H12	0.9300
C10—C11	1.377 (3)	C14—H14A	0.9600
O3—C7	1.204 (3)	C14—H14B	0.9600
C4—C3	1.372 (3)	C14—H14C	0.9600
C4—C5	1.387 (3)		
O1—S1—O2	119.71 (11)	N1—C7—C8	116.62 (19)
O1—S1—N1	108.51 (10)	C6—C5—C4	120.8 (2)
O2—S1—N1	103.33 (10)	C6—C5—H5	119.6
O1—S1—C1	109.63 (10)	C4—C5—H5	119.6
O2—S1—C1	108.74 (10)	C10—C11—C12	118.2 (2)
N1—S1—C1	105.96 (9)	C10—C11—H11	120.9
C13—C8—C9	119.62 (18)	C12—C11—H11	120.9
C13—C8—C7	124.23 (18)	C6—C1—C2	120.7 (2)
C9—C8—C7	116.14 (18)	C6—C1—S1	120.36 (16)
C10—C9—C8	118.78 (18)	C2—C1—S1	118.94 (16)
C10—C9—H9	120.6	C1—C6—C5	119.3 (2)
C8—C9—H9	120.6	C1—C6—H6	120.4
O4—N2—O5	123.57 (19)	C5—C6—H6	120.4
O4—N2—C10	118.53 (19)	C12—C13—C8	120.42 (19)
O5—N2—C10	117.89 (18)	C12—C13—H13	119.8
C7—N1—S1	123.00 (17)	C8—C13—H13	119.8
C7—N1—HN1	118.4 (18)	C3—C2—C1	119.0 (2)
S1—N1—HN1	114.5 (17)	C3—C2—H2	120.5
C9—C10—C11	122.56 (18)	C1—C2—H2	120.5
C9—C10—N2	118.58 (17)	C11—C12—C13	120.4 (2)
C11—C10—N2	118.86 (18)	C11—C12—H12	119.8
C3—C4—C5	118.4 (2)	C13—C12—H12	119.8
C3—C4—C14	121.1 (2)	C4—C14—H14A	109.5
C5—C4—C14	120.5 (2)	C4—C14—H14B	109.5
C4—C3—C2	121.9 (2)	H14A—C14—H14B	109.5

C4—C3—H3	119.0	C4—C14—H14C	109.5
C2—C3—H3	119.0	H14A—C14—H14C	109.5
O3—C7—N1	121.6 (2)	H14B—C14—H14C	109.5
O3—C7—C8	121.82 (19)		
C13—C8—C9—C10	-1.0 (3)	C14—C4—C5—C6	179.3 (2)
C7—C8—C9—C10	-179.78 (17)	C9—C10—C11—C12	1.7 (3)
O1—S1—N1—C7	51.79 (19)	N2—C10—C11—C12	-178.2 (2)
O2—S1—N1—C7	179.85 (17)	O1—S1—C1—C6	-23.4 (2)
C1—S1—N1—C7	-65.87 (19)	O2—S1—C1—C6	-155.95 (17)
C8—C9—C10—C11	-0.3 (3)	N1—S1—C1—C6	93.55 (19)
C8—C9—C10—N2	179.61 (17)	O1—S1—C1—C2	158.45 (17)
O4—N2—C10—C9	166.6 (2)	O2—S1—C1—C2	25.9 (2)
O5—N2—C10—C9	-12.9 (3)	N1—S1—C1—C2	-84.63 (19)
O4—N2—C10—C11	-13.5 (3)	C2—C1—C6—C5	-0.1 (3)
O5—N2—C10—C11	167.0 (2)	S1—C1—C6—C5	-178.20 (18)
C5—C4—C3—C2	-0.3 (4)	C4—C5—C6—C1	-0.2 (4)
C14—C4—C3—C2	-179.2 (2)	C9—C8—C13—C12	1.0 (3)
S1—N1—C7—O3	-4.9 (3)	C7—C8—C13—C12	179.6 (2)
S1—N1—C7—C8	175.83 (14)	C4—C3—C2—C1	0.0 (4)
C13—C8—C7—O3	-162.5 (2)	C6—C1—C2—C3	0.2 (3)
C9—C8—C7—O3	16.1 (3)	S1—C1—C2—C3	178.32 (18)
C13—C8—C7—N1	16.8 (3)	C10—C11—C12—C13	-1.7 (4)
C9—C8—C7—N1	-164.58 (18)	C8—C13—C12—C11	0.4 (4)
C3—C4—C5—C6	0.4 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—HM1...O2 <sup>i</sup>	0.80 (3)	2.14 (3)	2.927 (3)	167
C13—H13...O2 <sup>i</sup>	0.93	2.59	3.333 (3)	137
C3—H3...O4 <sup>ii</sup>	0.93	2.58	3.459 (3)	155

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