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N-(3-Methylbenzoyl)-2-nitrobenzene-sulfonamide

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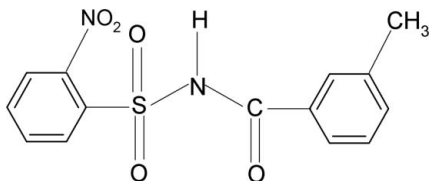
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.044; wR factor = 0.124; data-to-parameter ratio = 14.5.

In the title compound, $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_5\text{S}$, the conformation between the N—H group and the *ortho*-nitro group in the sulfonyl benzene ring is *syn* and that between the C=O and *meta*-methyl groups in the benzoyl ring is *anti*. The molecule is twisted at the S—N bond with a torsion angle of $64.3(2)^\circ$. The dihedral angle between the sulfonyl benzene ring and the —SO₂—NH—C—O segment is $75.73(7)^\circ$ and that between the sulfonyl and benzoyl benzene rings is $89.5(1)^\circ$. The crystal structure features inversion-related dimers linked by pairs of N—H···O(S) hydrogen bonds.

Related literature

For studies, including by our group, on the effects of substituents on the structures and other aspects of *N*-(aryl)-amides, see: Bowes *et al.* (2003); Gowda *et al.* (1999, 2003), on *N*-(aryl)-methanesulfonamides, see: Gowda *et al.* (2007), on *N*-(aryl)-arylsulfonamides, see: Shetty & Gowda (2005), on *N*-(substitutedbenzoyl)-arylsulfonamides, see: Suchetan *et al.* (2012), on *N*-chloroarylamides, see: Jyothi & Gowda (2004) and on *N*-bromoarylsulfonamides, see: Usha & Gowda (2006).



Experimental

Crystal data

 $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_5\text{S}$ $M_r = 320.32$ Orthorhombic, *Pbca* $a = 12.227(1)$ Å $b = 12.854(1)$ Å $c = 18.317(2)$ Å $V = 2878.8(5)$ Å³ $Z = 8$ Mo $K\alpha$ radiation $\mu = 0.25$ mm⁻¹ $T = 293$ K $0.48 \times 0.44 \times 0.32$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector

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

Diffraction, 2009)

 $T_{\min} = 0.889$, $T_{\max} = 0.924$

7423 measured reflections

2936 independent reflections

2306 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.019$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.044$ $wR(F^2) = 0.124$ $S = 1.04$

2936 reflections

203 parameters

1 restraint

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.38$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.33$ e Å⁻³

Table 1

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—H1N···O2 ⁱ	0.85 (2)	2.43 (2)	3.232 (3)	157 (2)

Symmetry code: (i) $-x, -y, -z + 1$.

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: BQ2333).

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supporting information

Acta Cryst. (2012). E68, o462 [doi:10.1107/S160053681200164X]

***N*-(3-Methylbenzoyl)-2-nitrobenzenesulfonamide**

P. A. Suchetan, Sabine Foro and B. Thimme Gowda

S1. Comment

Diaryl acylsulfonamides are known as potent antitumor agents. As part of our studies on the substituent effects on the structures and other aspects of *N*-(aryl)-amides (Bowes *et al.*, 2003; Gowda *et al.*, 1999, 2003), *N*-(aryl)-methanesulfonamides (Gowda *et al.*, 2007), *N*-(aryl)-arylsulfonamides (Shetty & Gowda, 2005); *N*-(substitutedbenzoyl)-arylsulfonamides (Suchetan *et al.*, 2012); *N*-chloroarylsulfonamides (Jyothi & Gowda, 2004) and *N*-bromoarylsulfonamides (Usha & Gowda, 2006), in the present work, the crystal structure of *N*-(3-methylbenzoyl)-2-nitrobenzenesulfonamide (I) has been determined (Fig.1).

The conformation between the N—H and C=O bonds in the C—SO₂—NH—C(O) segment is *anti* and the N—C bond in the segment has *gauche* torsion with respect to the S=O bonds (Fig.1), similar to that observed in *N*-(2-chlorobenzoyl)-2-nitrobenzenesulfonamide (II)(Suchetan *et al.*, 2012). In (I), the conformation between the N—H bond and the *ortho*-nitro group in the sulfonyl benzene ring is *syn*, similar to that observed in (II). Further, the conformation of the C=O is *anti* to the *meta*-methyl group in the benzoyl ring, similar to that observed between the C=O and the *ortho*-Cl atom in (II).

The molecule is twisted at the S—N bond with the torsional angle of 64.32 (20)°, compared to the value of -59.68 (17)° in (II).

The dihedral angle between the sulfonyl benzene ring and the —SO₂—NH—C—O segment is 75.7 (1)°, compared to the value of 77.5 (1)° in (II). Furthermore, the dihedral angle between the sulfonyl and the benzoyl benzene rings is 89.5 (1)°, compared to the value of 71.2 (1)° in (II).

In the crystal, the intermolecular N—H···O (S) hydrogen bonds (Table 1) link the molecules into dimeric chains. Part of the crystal structure is shown in Fig. 2.

S2. Experimental

The title compound was prepared by refluxing a mixture of *m*-methylbenzoic acid (0.02 mole), 2-nitrobenzenesulfonamide (0.02 mole) and excess phosphorous oxychloride for 3 h on a water bath. The resultant mixture was cooled and poured into crushed ice. The solid, *N*-(3-methylbenzoyl)-2-nitrobenzenesulfonamide, 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.

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

S3. Refinement

The H atom of the NH group was located in a difference map and later restrained to N—H = 0.86 (2) %Å. The other H atoms were positioned with idealized geometry using a riding model with the aromatic C—H = 0.93 Å and the methyl C

—H = 0.93 Å. All H atoms were refined with isotropic displacement parameters set at 1.2 U_{eq} (C-aromatic, N) and 1.5 U_{eq} (C-methyl).

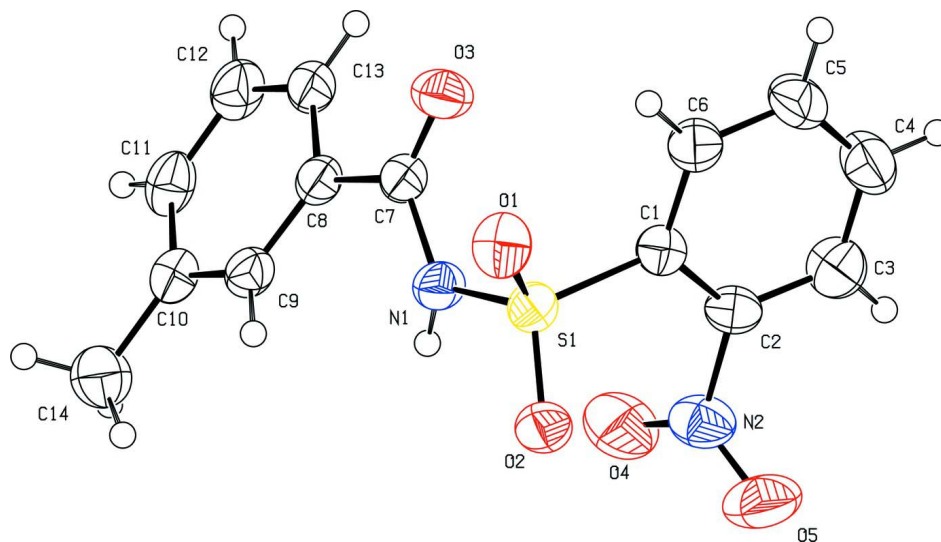
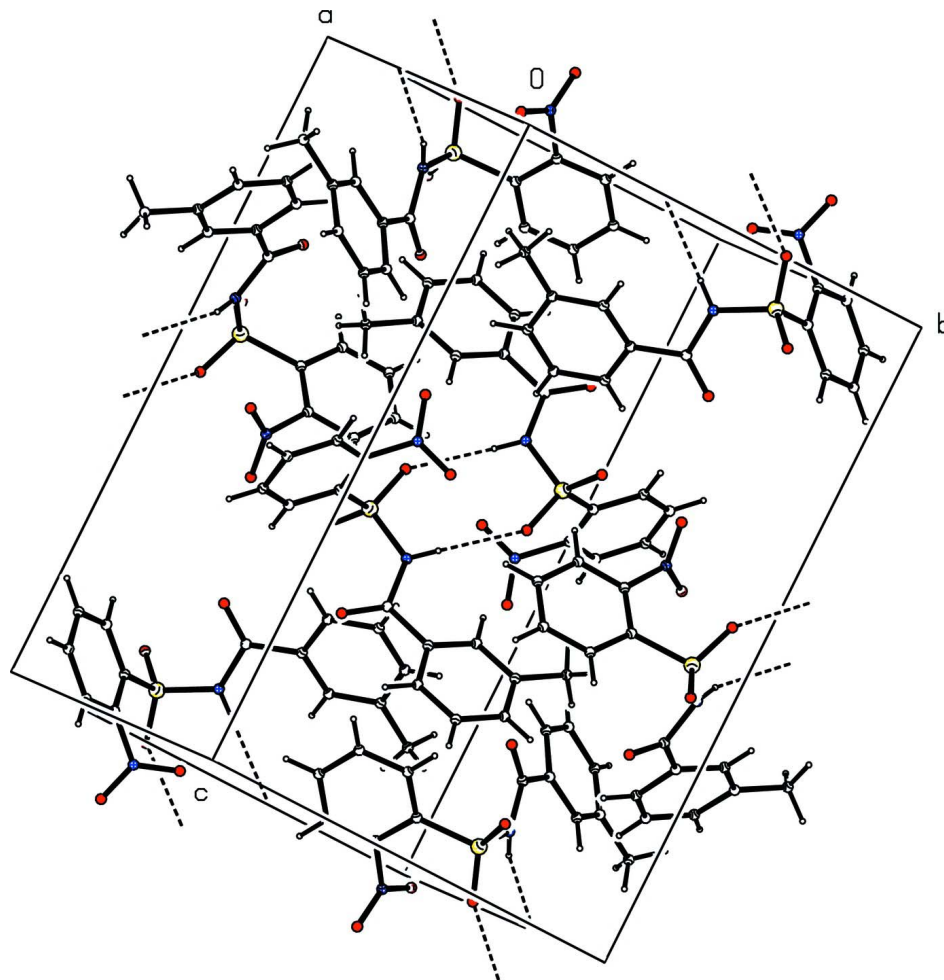


Figure 1

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

**Figure 2**

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

***N*-(3-Methylbenzoyl)-2-nitrobenzenesulfonamide**

Crystal data

$C_{14}H_{12}N_2O_5S$

$M_r = 320.32$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 12.227$ (1) Å

$b = 12.854$ (1) Å

$c = 18.317$ (2) Å

$V = 2878.8$ (5) Å³

$Z = 8$

$F(000) = 1328$

$D_x = 1.478$ Mg m⁻³

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

Cell parameters from 2012 reflections

$\theta = 2.6$ – 27.8°

$\mu = 0.25$ mm⁻¹

$T = 293$ K

Prism, colorless

$0.48 \times 0.44 \times 0.32$ mm

Data collection

Oxford Diffraction Xcalibur

diffractometer with a Sapphire CCD detector

Radiation source: fine-focus sealed tube

Graphite monochromator

Rotation method data acquisition using ω scans

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2009)

$T_{\min} = 0.889$, $T_{\max} = 0.924$

7423 measured reflections

2936 independent reflections

2306 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$
 $\theta_{\text{max}} = 26.4^\circ$, $\theta_{\text{min}} = 2.6^\circ$

$h = -15 \rightarrow 8$
 $k = -8 \rightarrow 16$
 $l = -21 \rightarrow 22$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.124$
 $S = 1.04$
 2936 reflections
 203 parameters
 1 restraint
 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
 $w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 1.5722P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.38 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.33 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	-0.01166 (16)	0.27278 (16)	0.42995 (11)	0.0350 (5)
C2	-0.08805 (18)	0.29514 (18)	0.48387 (12)	0.0388 (5)
C3	-0.1383 (2)	0.3902 (2)	0.48790 (14)	0.0527 (6)
H3	-0.1875	0.4044	0.5253	0.063*
C4	-0.1152 (2)	0.4641 (2)	0.43633 (15)	0.0570 (7)
H4	-0.1501	0.5283	0.4381	0.068*
C5	-0.0406 (2)	0.4437 (2)	0.38192 (15)	0.0555 (7)
H5	-0.0253	0.4942	0.3470	0.067*
C6	0.0114 (2)	0.34880 (18)	0.37891 (13)	0.0458 (6)
H6	0.0624	0.3358	0.3423	0.055*
C7	-0.04990 (18)	0.07627 (17)	0.31441 (11)	0.0374 (5)
C8	-0.12208 (17)	-0.00987 (17)	0.29044 (11)	0.0360 (5)
C9	-0.12101 (18)	-0.10611 (17)	0.32424 (11)	0.0382 (5)
H9	-0.0711	-0.1183	0.3616	0.046*
C10	-0.19217 (19)	-0.18475 (18)	0.30397 (12)	0.0410 (5)
C11	-0.2658 (2)	-0.16427 (19)	0.24824 (13)	0.0478 (6)
H11	-0.3160	-0.2150	0.2345	0.057*
C12	-0.2657 (2)	-0.0692 (2)	0.21280 (13)	0.0508 (6)
H12	-0.3144	-0.0575	0.1747	0.061*

C13	-0.19427 (19)	0.00806 (19)	0.23328 (12)	0.0439 (5)
H13	-0.1943	0.0717	0.2091	0.053*
C14	-0.1881 (2)	-0.2872 (2)	0.34183 (15)	0.0585 (7)
H14A	-0.1384	-0.2832	0.3823	0.070*
H14B	-0.1636	-0.3397	0.3083	0.070*
H14C	-0.2598	-0.3048	0.3593	0.070*
N1	-0.01587 (16)	0.06904 (15)	0.38733 (10)	0.0396 (4)
H1N	-0.0492 (18)	0.0295 (18)	0.4169 (12)	0.048*
N2	-0.11943 (17)	0.21727 (18)	0.53943 (12)	0.0520 (5)
O1	0.15719 (13)	0.17155 (13)	0.38424 (9)	0.0509 (4)
O2	0.07425 (14)	0.11701 (13)	0.50054 (9)	0.0467 (4)
O3	-0.02247 (15)	0.14867 (13)	0.27686 (9)	0.0522 (4)
O4	-0.1626 (2)	0.13838 (17)	0.51818 (12)	0.0779 (6)
O5	-0.10064 (18)	0.23912 (19)	0.60303 (10)	0.0743 (6)
S1	0.06292 (4)	0.15463 (4)	0.42754 (3)	0.03641 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0315 (10)	0.0356 (11)	0.0379 (10)	-0.0050 (9)	-0.0016 (8)	0.0003 (9)
C2	0.0348 (11)	0.0432 (12)	0.0383 (11)	-0.0042 (10)	0.0017 (9)	0.0074 (10)
C3	0.0457 (14)	0.0565 (15)	0.0558 (14)	0.0051 (12)	0.0116 (11)	0.0021 (12)
C4	0.0618 (17)	0.0420 (14)	0.0672 (16)	0.0094 (13)	0.0066 (13)	0.0048 (12)
C5	0.0707 (17)	0.0399 (13)	0.0559 (14)	-0.0009 (13)	0.0121 (13)	0.0125 (12)
C6	0.0521 (14)	0.0427 (13)	0.0427 (12)	-0.0032 (11)	0.0105 (10)	0.0024 (10)
C7	0.0424 (12)	0.0369 (11)	0.0328 (10)	0.0049 (10)	-0.0020 (9)	-0.0024 (9)
C8	0.0386 (11)	0.0380 (11)	0.0315 (10)	0.0037 (10)	-0.0018 (8)	-0.0051 (9)
C9	0.0399 (12)	0.0415 (12)	0.0331 (10)	0.0026 (10)	-0.0059 (9)	-0.0043 (9)
C10	0.0441 (12)	0.0414 (12)	0.0374 (11)	-0.0008 (10)	0.0012 (9)	-0.0078 (10)
C11	0.0454 (13)	0.0486 (13)	0.0492 (13)	-0.0030 (11)	-0.0073 (10)	-0.0171 (11)
C12	0.0526 (15)	0.0542 (15)	0.0457 (12)	0.0088 (12)	-0.0184 (11)	-0.0125 (12)
C13	0.0545 (14)	0.0402 (12)	0.0371 (11)	0.0100 (11)	-0.0077 (10)	-0.0051 (10)
C14	0.0701 (17)	0.0478 (14)	0.0577 (15)	-0.0141 (13)	-0.0055 (13)	-0.0004 (13)
N1	0.0475 (11)	0.0375 (10)	0.0337 (9)	-0.0093 (9)	-0.0039 (8)	0.0002 (8)
N2	0.0445 (12)	0.0611 (14)	0.0505 (12)	0.0044 (11)	0.0119 (9)	0.0157 (11)
O1	0.0370 (9)	0.0558 (10)	0.0600 (10)	-0.0012 (8)	0.0064 (8)	-0.0048 (8)
O2	0.0538 (10)	0.0472 (9)	0.0392 (8)	0.0012 (8)	-0.0141 (7)	0.0009 (7)
O3	0.0684 (11)	0.0454 (9)	0.0428 (9)	-0.0089 (9)	-0.0063 (8)	0.0099 (8)
O4	0.0936 (16)	0.0595 (13)	0.0806 (14)	-0.0224 (12)	0.0100 (12)	0.0177 (11)
O5	0.0813 (14)	0.0986 (17)	0.0429 (10)	0.0126 (13)	0.0139 (10)	0.0159 (11)
S1	0.0352 (3)	0.0378 (3)	0.0362 (3)	-0.0018 (2)	-0.0033 (2)	-0.0015 (2)

Geometric parameters (Å, °)

C1—C6	1.381 (3)	C9—H9	0.9300
C1—C2	1.389 (3)	C10—C11	1.386 (3)
C1—S1	1.772 (2)	C10—C14	1.489 (4)
C2—C3	1.369 (3)	C11—C12	1.384 (4)

C2—N2	1.478 (3)	C11—H11	0.9300
C3—C4	1.369 (4)	C12—C13	1.374 (3)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.376 (4)	C13—H13	0.9300
C4—H4	0.9300	C14—H14A	0.9600
C5—C6	1.376 (3)	C14—H14B	0.9600
C5—H5	0.9300	C14—H14C	0.9600
C6—H6	0.9300	N1—S1	1.6374 (19)
C7—O3	1.205 (3)	N1—H1N	0.847 (16)
C7—N1	1.402 (3)	N2—O4	1.208 (3)
C7—C8	1.482 (3)	N2—O5	1.220 (3)
C8—C9	1.383 (3)	O1—S1	1.4159 (17)
C8—C13	1.389 (3)	O2—S1	1.4288 (16)
C9—C10	1.384 (3)		
C6—C1—C2	118.2 (2)	C11—C10—C14	122.2 (2)
C6—C1—S1	118.96 (17)	C12—C11—C10	120.8 (2)
C2—C1—S1	122.75 (16)	C12—C11—H11	119.6
C3—C2—C1	121.6 (2)	C10—C11—H11	119.6
C3—C2—N2	116.8 (2)	C13—C12—C11	120.7 (2)
C1—C2—N2	121.6 (2)	C13—C12—H12	119.6
C4—C3—C2	119.3 (2)	C11—C12—H12	119.6
C4—C3—H3	120.3	C12—C13—C8	119.3 (2)
C2—C3—H3	120.3	C12—C13—H13	120.3
C3—C4—C5	120.3 (2)	C8—C13—H13	120.3
C3—C4—H4	119.9	C10—C14—H14A	109.5
C5—C4—H4	119.9	C10—C14—H14B	109.5
C4—C5—C6	120.3 (2)	H14A—C14—H14B	109.5
C4—C5—H5	119.9	C10—C14—H14C	109.5
C6—C5—H5	119.9	H14A—C14—H14C	109.5
C5—C6—C1	120.3 (2)	H14B—C14—H14C	109.5
C5—C6—H6	119.8	C7—N1—S1	123.95 (16)
C1—C6—H6	119.8	C7—N1—H1N	120.4 (17)
O3—C7—N1	120.8 (2)	S1—N1—H1N	113.5 (17)
O3—C7—C8	125.01 (19)	O4—N2—O5	125.7 (2)
N1—C7—C8	114.15 (19)	O4—N2—C2	117.4 (2)
C9—C8—C13	119.5 (2)	O5—N2—C2	116.9 (2)
C9—C8—C7	121.99 (18)	O1—S1—O2	119.82 (11)
C13—C8—C7	118.5 (2)	O1—S1—N1	109.29 (10)
C8—C9—C10	121.8 (2)	O2—S1—N1	104.51 (10)
C8—C9—H9	119.1	O1—S1—C1	107.53 (10)
C10—C9—H9	119.1	O2—S1—C1	108.46 (10)
C9—C10—C11	117.8 (2)	N1—S1—C1	106.52 (10)
C9—C10—C14	120.0 (2)		
C6—C1—C2—C3	-1.2 (3)	C14—C10—C11—C12	-178.3 (2)
S1—C1—C2—C3	174.72 (19)	C10—C11—C12—C13	-1.7 (4)
C6—C1—C2—N2	178.5 (2)	C11—C12—C13—C8	-0.3 (4)

S1—C1—C2—N2	-5.6 (3)	C9—C8—C13—C12	2.0 (3)
C1—C2—C3—C4	2.0 (4)	C7—C8—C13—C12	-176.7 (2)
N2—C2—C3—C4	-177.7 (2)	O3—C7—N1—S1	-0.6 (3)
C2—C3—C4—C5	-1.4 (4)	C8—C7—N1—S1	-179.30 (15)
C3—C4—C5—C6	0.0 (4)	C3—C2—N2—O4	117.3 (3)
C4—C5—C6—C1	0.7 (4)	C1—C2—N2—O4	-62.4 (3)
C2—C1—C6—C5	-0.1 (3)	C3—C2—N2—O5	-61.8 (3)
S1—C1—C6—C5	-176.2 (2)	C1—C2—N2—O5	118.5 (3)
O3—C7—C8—C9	157.0 (2)	C7—N1—S1—O1	-51.6 (2)
N1—C7—C8—C9	-24.3 (3)	C7—N1—S1—O2	179.02 (18)
O3—C7—C8—C13	-24.3 (3)	C7—N1—S1—C1	64.3 (2)
N1—C7—C8—C13	154.3 (2)	C6—C1—S1—O1	16.5 (2)
C13—C8—C9—C10	-1.7 (3)	C2—C1—S1—O1	-159.39 (18)
C7—C8—C9—C10	176.87 (19)	C6—C1—S1—O2	147.47 (18)
C8—C9—C10—C11	-0.2 (3)	C2—C1—S1—O2	-28.4 (2)
C8—C9—C10—C14	180.0 (2)	C6—C1—S1—N1	-100.53 (19)
C9—C10—C11—C12	1.9 (3)	C2—C1—S1—N1	83.54 (19)

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—H1N...O2 ⁱ	0.85 (2)	2.43 (2)	3.232 (3)	157 (2)

Symmetry code: (i) $-x, -y, -z+1$.