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# *N*-(2,5-Dimethylphenyl)-2-nitrobenzenesulfonamide

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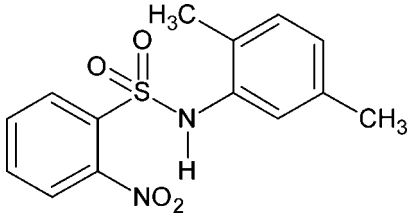
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.042; $wR$ factor = 0.108; data-to-parameter ratio = 15.7.

In the crystal structure of the title compound, $C_{14}H_{14}N_2O_4S$, the N—H bond is *syn* to the *ortho*-nitro group in the sulfonyl benzene ring and *anti* to the *ortho*- and *syn* to the *meta*-methyl groups in the aniline ring. The molecule is twisted at the S—N bond with a torsion angle of 71.41 (18)°. The dihedral angle between the planes of the benzene rings is 51.07 (8)°. In the crystal, pairs of N—H···$O_{sulfonamide}$ hydrogen bonds link the molecules into inversion dimers.

## Related literature

For studies on the effects of substituents on the structures and other aspects of *N*-arylsulfonamides, see: Chaithanya *et al.* (2012); Gowda *et al.* (2002) and of *N*-chloroarylsulfonamides, see: Gowda & Shetty (2004); Shetty & Gowda (2004).




## Experimental

### Crystal data

$C_{14}H_{14}N_2O_4S$
$M_r$ = 306.33
Triclinic, $P\overline{1}$
$a$ = 8.1987 (7) Å
$b$ = 9.6729 (9) Å
$c$ = 9.9328 (9) Å
$\alpha$ = 84.386 (9)°
$\beta$ = 72.096 (8)°
$\gamma$ = 89.239 (9)°
$V$ = 745.86 (12) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.23 mm$^{-1}$
$T$ = 293 K
0.36 × 0.24 × 0.16 mm

### Data collection

Oxford Diffraction Xcaliburdiffractometer with Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
$T_{min}$ = 0.921, $T_{max}$ = 0.964
4954 measured reflections
3027 independent reflections
2629 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.011

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.108
$S$ = 1.14
3027 reflections
193 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*···O2$^{i}$ | 0.82 (2) | 2.27 (2) | 3.023 (2) | 152 (2) |

Symmetry code: (i) $-x, -y, -z+2$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); 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: RZ5026).

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# supporting information

*Acta Cryst.* (2012). E**68**, o3426 [doi:10.1107/S1600536812047630]

## *N*-(2,5-Dimethylphenyl)-2-nitrobenzenesulfonamide

**U. Chaithanya, Sabine Foro and B. Thimme Gowda**

### S1. Comment

As a part of studying the effect of substituents on the structures and other aspects of *N*-arylsulfonamides (Chaithanya *et al.*, 2012; Gowda *et al.*, 2002) and *N*-chloroarylsulfonamides (Gowda & Shetty, 2004; Shetty & Gowda, 2004), in the present work, the crystal structure of *N*-(2,5-dimethylphenyl)-2-nitrobenzene- sulfonamide (I) has been determined (Fig. 1). The conformation of the N—H bond is *syn* to the *ortho*-nitro group in the sulfonyl benzene ring and *anti* to the *ortho*-methyl and *syn* to the *meta*-methyl groups in the anilino ring, compared to the *anti* conformation observed between the N—H bond and both the *ortho*- and *meta*-methyl groups in the anilino ring observed in *N*-(2,3-dimethylphenyl)-2-nitrobenzene- sulfonamide (II) (Chaithanya *et al.*, 2012).

The molecules in (I) are twisted at the S—N bond with the torsional angle of 71.41 (18)°, compared to the values of -60.37 (30) and 58.81 (34)° in the two independent molecules of (II).

The dihedral angle between the sulfonyl and the anilino rings is 51.07 (8)°, compared to the values of 53.67 (8) and 56.99 (9)° in the two molecules of (II).

The amide H-atom showed the intermolecular H-bonding with the sulfonyl oxygen atom of the other molecule, generating inversion dimers (Table 1, Fig. 2.)

In the crystal structure, N1—H1N···O2(S) intermolecular hydrogen bonds link the molecules into inversion dimers (Table 1, Fig. 2.)

### S2. Experimental

The title compound was prepared by treating 2-nitrobenzenesulfonyl- chloride with 2,5-dimethylaniline in the stoichiometric ratio and boiling the reaction mixture for 15 minutes. The reaction mixture was then cooled to room temperature and added to ice cold water (100 ml). The resultant solid *N*-(2,5-dimethylphenyl)-2-nitrobenzenesulfonamide was filtered under suction and washed thoroughly with cold water and dilute HCl to remove the excess sulfonyl-chloride and aniline, respectively. It was then recrystallized to constant melting point from dilute ethanol. The purity of the compound was checked and characterized by its infrared spectra.

Prism like light brown single crystals of the title compound used in X-ray diffraction studies were grown in ethanolic solution by slow evaporation of the solvent at room temperature.

### S3. Refinement

H atoms bonded to C were positioned with idealized geometry using a riding model with the aromatic C—H = 0.93 Å, methyl C—H = 0.96 Å. The amino H atoms were freely refined with the N—H distance restrained to 0.86 (2) 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) of the parent atom.

The (0 1 1) reflection is probably affected by the beamstop and was omitted from the refinement.

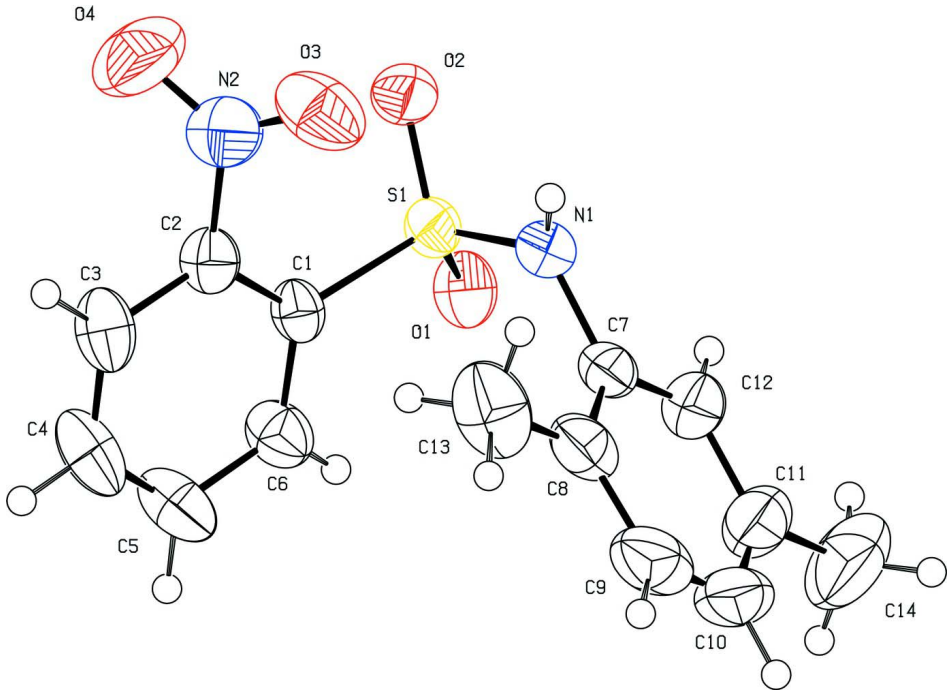


**Figure 1**

Molecular structure of the title compound, showing the atom labelling scheme and with displacement ellipsoids drawn at the 50% probability level.

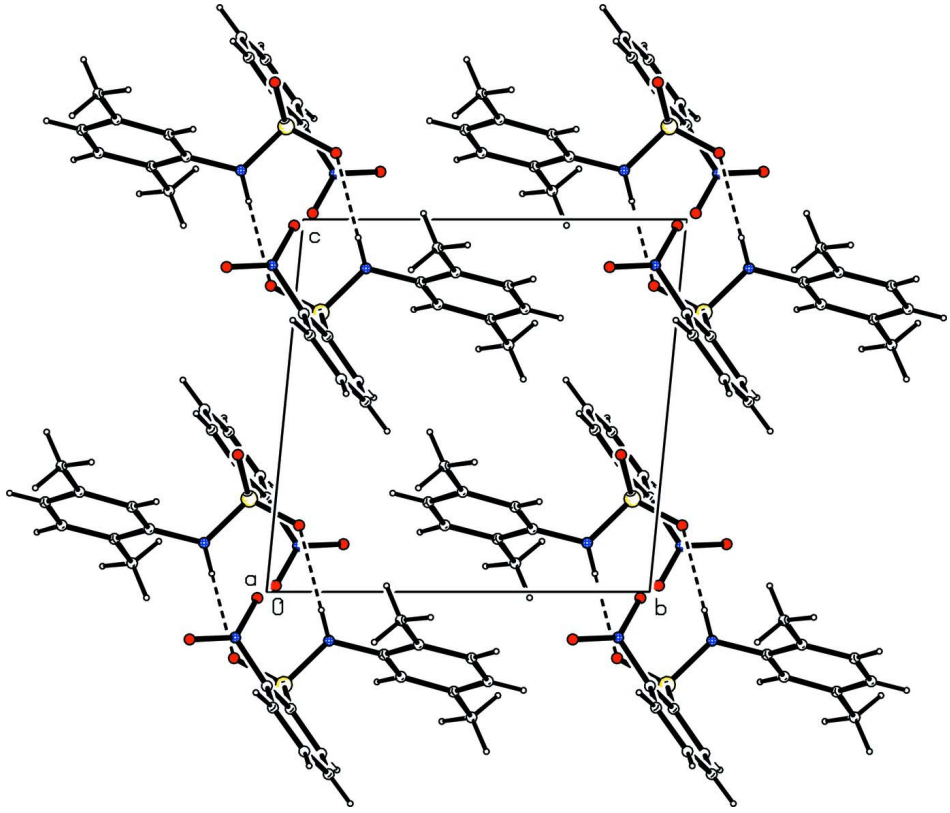


**Figure 2**

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

### *N*-(2,5-Dimethylphenyl)-2-nitrobenzenesulfonamide

*Crystal data*

$C_{14}H_{14}N_2O_4S$
$M_r = 306.33$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.1987\ (7)$ Å
$b = 9.6729\ (9)$ Å
$c = 9.9328\ (9)$ Å
$\alpha = 84.386\ (9)°$
$\beta = 72.096\ (8)°$
$\gamma = 89.239\ (9)°$
$V = 745.86\ (12)$ Å$^3$
$Z = 2$
$F(000) = 320$
$D_x = 1.364$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3120 reflections
$\theta = 2.6–27.8°$
$\mu = 0.23$ mm$^{-1}$
$T = 293$ K
Prism, light brown
0.36 × 0.24 × 0.16 mm

*Data collection*

Oxford Diffraction Xcaliburdiffractometer with Sapphire CCD
Radiation source: fine-focus sealed tube
Graphite monochromator
Rotation method data acquisition using $\omega$ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
$T_{min} = 0.921$, $T_{max} = 0.964$
4954 measured reflections
3027 independent reflections
2629 reflections with $I > 2\sigma(I)$
$R_{int} = 0.011$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.6°$
$h = -10\rightarrow10$
$k = -12\rightarrow11$
$l = -12\rightarrow10$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.108$
$S = 1.14$
3027 reflections
193 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
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 0.3685P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ e Å$^{-3}$

*Special details*

**Experimental**. Absorption correction: 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 | 0.3540 (2) | 0.0929 (2) | 0.6857 (2) | 0.0387 (4) |
| C2 | 0.4684 (2) | 0.0253 (2) | 0.7467 (2) | 0.0433 (4) |
| C3 | 0.6437 (3) | 0.0467 (3) | 0.6890 (3) | 0.0561 (6) |
| H3 | 0.7187 | −0.0016 | 0.7294 | 0.067* |
| C4 | 0.7051 (3) | 0.1400 (3) | 0.5713 (3) | 0.0657 (7) |
| H4 | 0.8226 | 0.1564 | 0.5326 | 0.079* |
| C5 | 0.5947 (3) | 0.2092 (3) | 0.5104 (3) | 0.0657 (7) |
| H5 | 0.6376 | 0.2732 | 0.4313 | 0.079* |
| C6 | 0.4199 (3) | 0.1846 (2) | 0.5655 (2) | 0.0525 (5) |
| H6 | 0.3462 | 0.2299 | 0.5216 | 0.063* |
| C7 | 0.0552 (3) | 0.3225 (2) | 0.8314 (2) | 0.0448 (5) |
| C8 | 0.1732 (3) | 0.4106 (2) | 0.8577 (2) | 0.0567 (6) |
| C9 | 0.1583 (4) | 0.5520 (3) | 0.8214 (3) | 0.0760 (8) |
| H9 | 0.2318 | 0.6147 | 0.8398 | 0.091* |
| C10 | 0.0386 (4) | 0.6010 (3) | 0.7595 (3) | 0.0772 (9) |
| H10 | 0.0348 | 0.6961 | 0.7352 | 0.093* |
| C11 | −0.0768 (4) | 0.5141 (3) | 0.7317 (3) | 0.0701 (7) |
| C12 | −0.0680 (3) | 0.3728 (2) | 0.7717 (2) | 0.0546 (5) |
| H12 | −0.1464 | 0.3114 | 0.7580 | 0.065* |
| C13 | 0.3075 (4) | 0.3582 (3) | 0.9231 (3) | 0.0808 (9) |
| H13A | 0.3794 | 0.2942 | 0.8642 | 0.121* |
| H13B | 0.2531 | 0.3118 | 1.0159 | 0.121* |

| | | | | |
|---|---|---|---|---|
| H13C | 0.3759 | 0.4350 | 0.9310 | 0.121* |
| C14 | −0.2091 (5) | 0.5675 (4) | 0.6626 (4) | 0.1074 (12) |
| H14A | −0.1524 | 0.6151 | 0.5709 | 0.161* |
| H14B | −0.2833 | 0.6304 | 0.7213 | 0.161* |
| H14C | −0.2756 | 0.4907 | 0.6518 | 0.161* |
| N1 | 0.0568 (2) | 0.17583 (17) | 0.86856 (18) | 0.0440 (4) |
| H1N | 0.054 (3) | 0.147 (2) | 0.9500 (18) | 0.053* |
| N2 | 0.4089 (3) | −0.0701 (2) | 0.8773 (2) | 0.0605 (5) |
| O1 | 0.06849 (18) | 0.11008 (16) | 0.63232 (16) | 0.0524 (4) |
| O2 | 0.09053 (18) | −0.06778 (14) | 0.82168 (17) | 0.0530 (4) |
| O3 | 0.3174 (2) | −0.0226 (2) | 0.98338 (19) | 0.0766 (6) |
| O4 | 0.4595 (3) | −0.1884 (2) | 0.8720 (3) | 0.1039 (8) |
| S1 | 0.12780 (6) | 0.06923 (5) | 0.75061 (5) | 0.04028 (15) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0295 (9) | 0.0461 (10) | 0.0427 (10) | 0.0008 (7) | −0.0130 (8) | −0.0090 (8) |
| C2 | 0.0392 (10) | 0.0489 (11) | 0.0462 (11) | 0.0018 (8) | −0.0184 (8) | −0.0087 (9) |
| C3 | 0.0352 (10) | 0.0803 (16) | 0.0610 (14) | 0.0081 (10) | −0.0235 (10) | −0.0184 (12) |
| C4 | 0.0340 (11) | 0.107 (2) | 0.0540 (13) | −0.0084 (12) | −0.0080 (10) | −0.0155 (13) |
| C5 | 0.0470 (12) | 0.0948 (19) | 0.0483 (13) | −0.0161 (12) | −0.0074 (10) | 0.0054 (12) |
| C6 | 0.0427 (11) | 0.0664 (14) | 0.0482 (12) | −0.0028 (10) | −0.0159 (9) | 0.0026 (10) |
| C7 | 0.0419 (10) | 0.0408 (10) | 0.0425 (10) | −0.0039 (8) | 0.0003 (8) | −0.0034 (8) |
| C8 | 0.0508 (12) | 0.0569 (13) | 0.0516 (12) | −0.0120 (10) | 0.0032 (10) | −0.0149 (10) |
| C9 | 0.0778 (18) | 0.0586 (16) | 0.0737 (18) | −0.0236 (14) | 0.0073 (15) | −0.0178 (13) |
| C10 | 0.099 (2) | 0.0401 (13) | 0.0682 (17) | −0.0027 (14) | 0.0094 (16) | −0.0016 (12) |
| C11 | 0.0859 (19) | 0.0550 (15) | 0.0579 (14) | 0.0203 (13) | −0.0073 (13) | −0.0015 (11) |
| C12 | 0.0560 (13) | 0.0474 (12) | 0.0562 (13) | 0.0057 (10) | −0.0110 (10) | −0.0070 (10) |
| C13 | 0.0585 (15) | 0.101 (2) | 0.090 (2) | −0.0091 (14) | −0.0240 (14) | −0.0389 (17) |
| C14 | 0.136 (3) | 0.085 (2) | 0.100 (3) | 0.050 (2) | −0.041 (2) | 0.0008 (19) |
| N1 | 0.0415 (9) | 0.0426 (9) | 0.0433 (9) | −0.0010 (7) | −0.0078 (7) | 0.0007 (7) |
| N2 | 0.0507 (11) | 0.0670 (13) | 0.0716 (14) | −0.0038 (9) | −0.0350 (11) | 0.0086 (10) |
| O1 | 0.0400 (7) | 0.0664 (10) | 0.0586 (9) | 0.0051 (7) | −0.0254 (7) | −0.0112 (7) |
| O2 | 0.0451 (8) | 0.0412 (8) | 0.0708 (10) | −0.0064 (6) | −0.0158 (7) | −0.0025 (7) |
| O3 | 0.0671 (11) | 0.1086 (16) | 0.0516 (10) | −0.0154 (10) | −0.0196 (9) | 0.0114 (10) |
| O4 | 0.1010 (17) | 0.0670 (13) | 0.147 (2) | 0.0127 (12) | −0.0545 (16) | 0.0241 (13) |
| S1 | 0.0304 (2) | 0.0421 (3) | 0.0500 (3) | −0.00165 (17) | −0.01472 (19) | −0.0047 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.383 (3) | C9—H9 | 0.9300 |
| C1—C2 | 1.389 (3) | C10—C11 | 1.380 (4) |
| C1—S1 | 1.7764 (18) | C10—H10 | 0.9300 |
| C2—C3 | 1.384 (3) | C11—C12 | 1.392 (3) |
| C2—N2 | 1.470 (3) | C11—C14 | 1.512 (4) |
| C3—C4 | 1.371 (4) | C12—H12 | 0.9300 |
| C3—H3 | 0.9300 | C13—H13A | 0.9600 |

| | | | |
|---|---|---|---|
| C4—C5 | 1.369 (4) | C13—H13B | 0.9600 |
| C4—H4 | 0.9300 | C13—H13C | 0.9600 |
| C5—C6 | 1.383 (3) | C14—H14A | 0.9600 |
| C5—H5 | 0.9300 | C14—H14B | 0.9600 |
| C6—H6 | 0.9300 | C14—H14C | 0.9600 |
| C7—C12 | 1.382 (3) | N1—S1 | 1.6049 (18) |
| C7—C8 | 1.397 (3) | N1—H1N | 0.823 (16) |
| C7—N1 | 1.431 (3) | N2—O4 | 1.213 (3) |
| C8—C9 | 1.393 (4) | N2—O3 | 1.218 (3) |
| C8—C13 | 1.500 (4) | O1—S1 | 1.4242 (15) |
| C9—C10 | 1.367 (5) | O2—S1 | 1.4295 (15) |

| | | | |
|---|---|---|---|
| C6—C1—C2 | 118.12 (18) | C10—C11—C12 | 116.9 (3) |
| C6—C1—S1 | 117.31 (15) | C10—C11—C14 | 122.5 (3) |
| C2—C1—S1 | 124.57 (15) | C12—C11—C14 | 120.6 (3) |
| C3—C2—C1 | 121.6 (2) | C7—C12—C11 | 121.1 (2) |
| C3—C2—N2 | 116.78 (18) | C7—C12—H12 | 119.4 |
| C1—C2—N2 | 121.63 (18) | C11—C12—H12 | 119.4 |
| C4—C3—C2 | 119.0 (2) | C8—C13—H13A | 109.5 |
| C4—C3—H3 | 120.5 | C8—C13—H13B | 109.5 |
| C2—C3—H3 | 120.5 | H13A—C13—H13B | 109.5 |
| C5—C4—C3 | 120.4 (2) | C8—C13—H13C | 109.5 |
| C5—C4—H4 | 119.8 | H13A—C13—H13C | 109.5 |
| C3—C4—H4 | 119.8 | H13B—C13—H13C | 109.5 |
| C4—C5—C6 | 120.5 (2) | C11—C14—H14A | 109.5 |
| C4—C5—H5 | 119.7 | C11—C14—H14B | 109.5 |
| C6—C5—H5 | 119.7 | H14A—C14—H14B | 109.5 |
| C5—C6—C1 | 120.3 (2) | C11—C14—H14C | 109.5 |
| C5—C6—H6 | 119.9 | H14A—C14—H14C | 109.5 |
| C1—C6—H6 | 119.9 | H14B—C14—H14C | 109.5 |
| C12—C7—C8 | 121.8 (2) | C7—N1—S1 | 121.88 (14) |
| C12—C7—N1 | 117.78 (19) | C7—N1—H1N | 119.0 (17) |
| C8—C7—N1 | 120.4 (2) | S1—N1—H1N | 115.8 (17) |
| C9—C8—C7 | 116.1 (2) | O4—N2—O3 | 125.3 (2) |
| C9—C8—C13 | 121.2 (2) | O4—N2—C2 | 117.4 (2) |
| C7—C8—C13 | 122.6 (2) | O3—N2—C2 | 117.3 (2) |
| C10—C9—C8 | 121.9 (3) | O1—S1—O2 | 119.85 (9) |
| C10—C9—H9 | 119.1 | O1—S1—N1 | 108.74 (9) |
| C8—C9—H9 | 119.1 | O2—S1—N1 | 107.05 (9) |
| C9—C10—C11 | 122.1 (2) | O1—S1—C1 | 105.37 (9) |
| C9—C10—H10 | 118.9 | O2—S1—C1 | 108.28 (9) |
| C11—C10—H10 | 118.9 | N1—S1—C1 | 106.93 (9) |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.9 (3) | C8—C7—C12—C11 | 1.7 (3) |
| S1—C1—C2—C3 | 178.74 (16) | N1—C7—C12—C11 | −179.5 (2) |
| C6—C1—C2—N2 | 177.9 (2) | C10—C11—C12—C7 | −2.4 (4) |
| S1—C1—C2—N2 | −2.5 (3) | C14—C11—C12—C7 | 178.3 (2) |
| C1—C2—C3—C4 | 2.1 (3) | C12—C7—N1—S1 | 75.0 (2) |

| | | | |
|---|---|---|---|
| N2—C2—C3—C4 | −176.8 (2) | C8—C7—N1—S1 | −106.1 (2) |
| C2—C3—C4—C5 | −1.2 (4) | C3—C2—N2—O4 | −59.0 (3) |
| C3—C4—C5—C6 | −0.8 (4) | C1—C2—N2—O4 | 122.2 (2) |
| C4—C5—C6—C1 | 2.0 (4) | C3—C2—N2—O3 | 118.6 (2) |
| C2—C1—C6—C5 | −1.2 (3) | C1—C2—N2—O3 | −60.2 (3) |
| S1—C1—C6—C5 | 179.19 (19) | C7—N1—S1—O1 | −41.91 (18) |
| C12—C7—C8—C9 | 0.5 (3) | C7—N1—S1—O2 | −172.73 (15) |
| N1—C7—C8—C9 | −178.28 (19) | C7—N1—S1—C1 | 71.41 (18) |
| C12—C7—C8—C13 | 179.7 (2) | C6—C1—S1—O1 | 22.19 (19) |
| N1—C7—C8—C13 | 0.9 (3) | C2—C1—S1—O1 | −157.44 (17) |
| C7—C8—C9—C10 | −2.0 (4) | C6—C1—S1—O2 | 151.56 (17) |
| C13—C8—C9—C10 | 178.8 (2) | C2—C1—S1—O2 | −28.1 (2) |
| C8—C9—C10—C11 | 1.3 (4) | C6—C1—S1—N1 | −93.39 (18) |
| C9—C10—C11—C12 | 0.9 (4) | C2—C1—S1—N1 | 86.97 (18) |
| C9—C10—C11—C14 | −179.7 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*···O2$^{i}$ | 0.82 (2) | 2.27 (2) | 3.023 (2) | 152 (2) |

Symmetry code: (i) −*x*, −*y*, −*z*+2.