CrossMark

# organic compounds

# 2-Chloro-N-(4-methoxybenzoyl)benzene-sulfonamide

S Sreenivasa,[a] B. S. Palakshamurthy,[b] K. J. Pampa,[c] N. K. Lokanath[d] and P. A. Suchetan[e]*

[a]Department of Studies and Research in Chemistry, Tumkur University, Tumkur, Karnataka 572 103, India, [b]Department of Studies and Research in Physics, U.C.S., Tumkur University, Tumkur, Karnataka 572 103, India, [c]Department of Studies in Microbiology, University of Mysore, Manasagangotri, Mysore, India, [d]Department of Studies in Physics, University of Mysore, Manasagangotri, Mysore, India, and [e]Department of Studies and Research in Chemistry, U.C.S., Tumkur University, Tumkur, Karnataka 572 103, India
Correspondence e-mail: pasuchetan@yahoo.co.in

In the title compound, $C_{14}H_{12}ClNO_4S$, the dihedral angle between the aromatic rings is 82.07 (1)° and the dihedral angle between the planes defined by the S—N—C=O fragment and the sulfonyl benzene ring is 82.46 (3)°. In the crystal, the molecules are linked into $C(4)$ chains running along [001] by strong N—H···O hydrogen bonds. A C—H···O interaction reinforces the [001] chains: its graph-set symbol is $C(7)$. The chains are cross-linked into (100) sheets by further C—H···O interactions as $C(6)$ chains along [001]. The structure also features weak $\pi$–$\pi$ stacking interactions [centroid–centroid distances = 3.577 (1) and 3.8016 (1) Å].

## Related literature

For related structures see: Gowda *et al.* (2010*a*,*b*); Suchetan *et al.* (2011*a*,*b*).
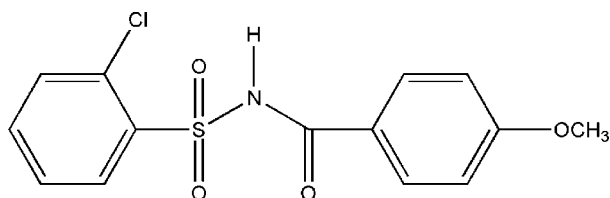
## Experimental

### Crystal data

| | |
|---|---|
| $C_{14}H_{12}ClNO_4S$ | $V$ = 1494.2 (4) Å$^3$ |
| $M_r$ = 325.76 | $Z$ = 4 |
| Monoclinic, $P2_1/c$ | Cu $K\alpha$ radiation |
| $a$ = 14.5293 (19) Å | $\mu$ = 3.71 mm$^{-1}$ |
| $b$ = 10.6225 (14) Å | $T$ = 293 K |
| $c$ = 9.6918 (14) Å | $0.44 \times 0.35 \times 0.26$ mm |
| $\beta$ = 92.695 (5)° | |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 17846 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | 2449 independent reflections |
| $T_{min}$ = 0.263, $T_{max}$ = 0.381 | 2295 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.058 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.063 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.163 | |
| $S$ = 1.11 | $\Delta\rho_{max}$ = 0.52 e Å$^{-3}$ |
| 2449 reflections | $\Delta\rho_{min}$ = −0.37 e Å$^{-3}$ |
| 195 parameters | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2$^i$ | 0.81 (3) | 2.09 (3) | 2.872 (3) | 172 (3) |
| C3—H3···O1$^{ii}$ | 0.93 | 2.57 | 3.370 (4) | 144 |
| C9—H9···O2$^i$ | 0.93 | 2.48 | 3.288 (3) | 145 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus*; 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*.

## References

Bruker (2009). *APEX2, SADABS, and SAINT-Plus.* Bruker AXS Inc., Madison, Wisconsin, USA.
Gowda, B. T., Foro, S., Suchetan, P. A. & Fuess, H. (2010*a*). *Acta Cryst.* E**66**, o794.
Gowda, B. T., Foro, S., Suchetan, P. A. & Fuess, H. (2010*b*). *Acta Cryst.* E**66**, o1466.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Suchetan, P. A., Foro, S. & Gowda, B. T. (2011*a*). *Acta Cryst.* E**67**, o146.
Suchetan, P. A., Foro, S. & Gowda, B. T. (2011*b*). *Acta Cryst.* E**67**, o930.

# supporting information

## 2-Chloro-*N*-(4-methoxybenzoyl)benzenesulfonamide

### S Sreenivasa, B. S. Palakshamurthy, K. J. Pampa, N. K. Lokanath and P. A. Suchetan

### S1. Introduction

As a part of our continued structural studies of N-(aroyl)-arylsulfonamides (Suchetan *et al.*, 2011*a*, 2011*b*; Gowda *et al.*, 2010*a*, 2010*b*), we report here the crystal structure of the title compound (I) (Fig 1).

### S2. Experimental

#### S2.1. Synthesis and crystallization

The title compound (I) was prepared by refluxing a mixture of 4-methoxybenzoic acid, 2-chlorobenzenesulfonamide and phosphorous oxychloride (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: 445 K).

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

#### S2.2. 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).

### S3. Results and discussion

In I, the dihedral angle between the two aromatic rings is 82.07 (1)°. Compared to this, the dihedral angle is 73.3 (1)° in N-(benzoyl)-2-chlorobenzenesulfonamide (II, Gowda *et al.*, 2010*a*), 85.7 (1)° in N-(4-chlorobenzoyl)-2-chlorobenzene-sulfonamide (III, Suchetan *et al.*, 2011*a*), 89.1 (2)° in N-(4-methylbenzoyl)-2-chlorobenzenesulfonamide (IV, Gowda *et al.*, 2010*b*) and 85.4 (1)° in N-(4-nitrobenzoyl)-2-chlorobenzenesulfonamide (V, Suchetan *et al.*, 2011*b*). This shows that introducing a substituent into the para position of the benzoyl ring of II correlates with a increase of the dihedral angle between the aromatic rings. Further, 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 ring being 82.46 (3)°.

In the crystal structure, the molecules are linked into C(4) chains running along [001] through strong N1—H1⋯O2 hydrogen bonds (Figure 2). The molecules are further linked into one another through C3—H3⋯O1 (Figure 3) and C9—H9⋯O2 (Figure 4) interactions into C(6) and C(7) chains running along [001]. The structure is further stabilized by two alternate π-π interactions, Cg(methoxyphenyl)-Cg(methoxyphenyl) and Cg(chlorophenyl)-Cg(chlorophenyl) distances being respectively 3.577 (1)Å and 3.8016 (1)Å.
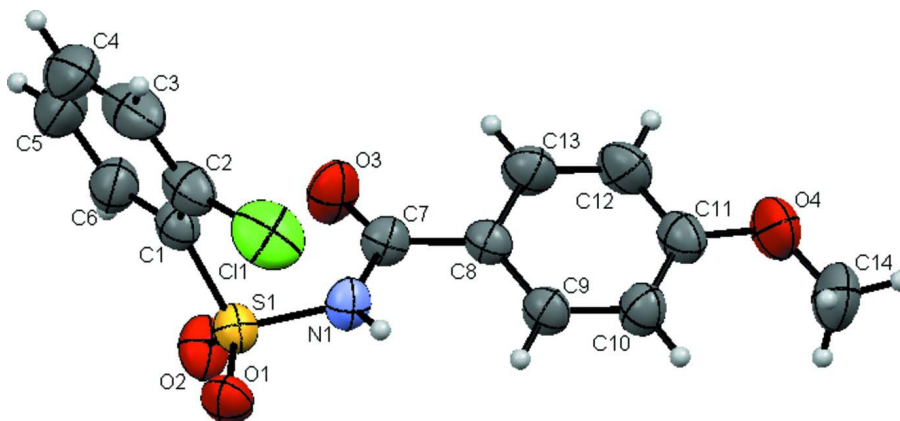
**Figure 1**

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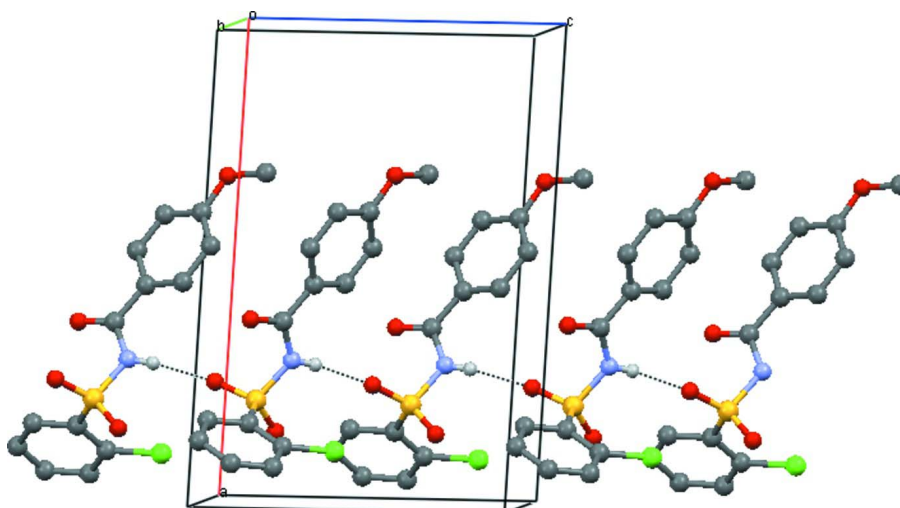


**Figure 2**
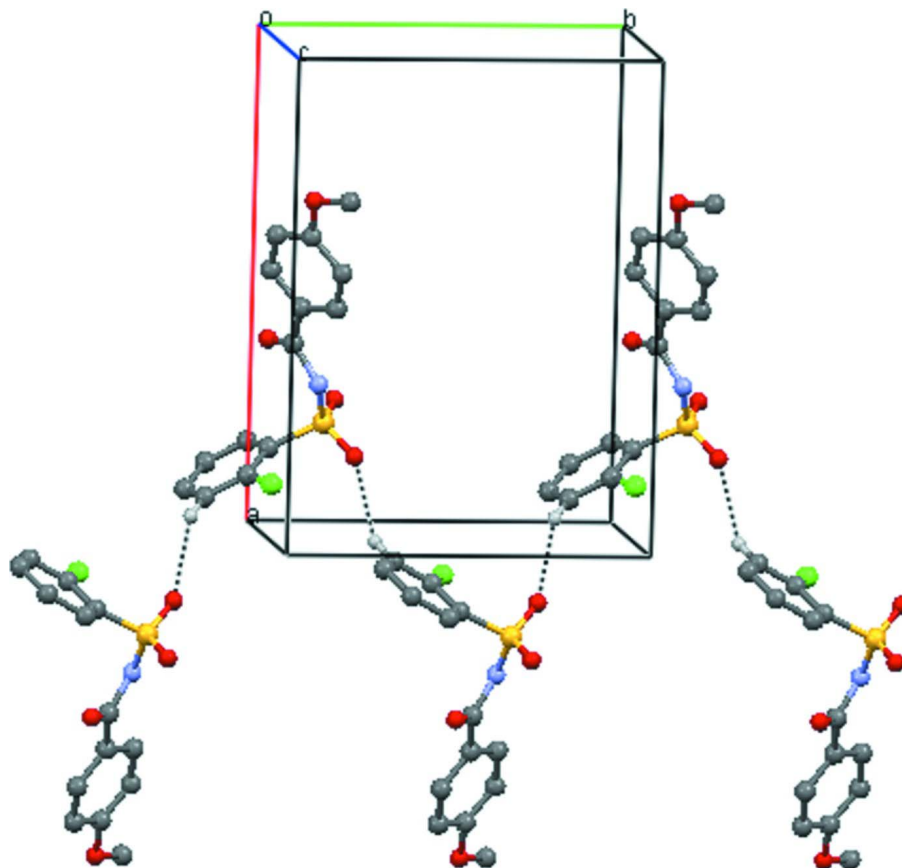
Formation of C(4) chains through N—H⋯O hydrogen bonds.

**Figure 3**

Formation of C(6) chains through C3—H3···O1 interactions running along [001].
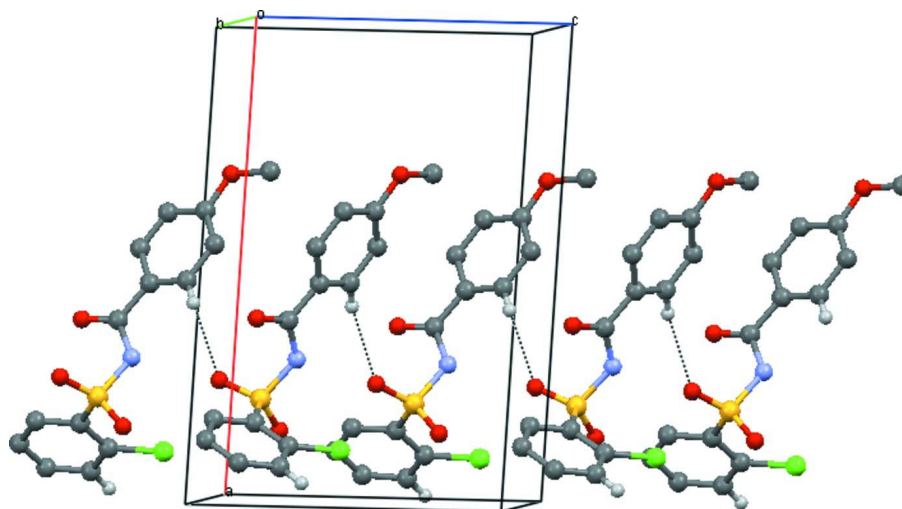


**Figure 4**

Formation of C(7) chains through C9—H9···O2 interactions running along [001].
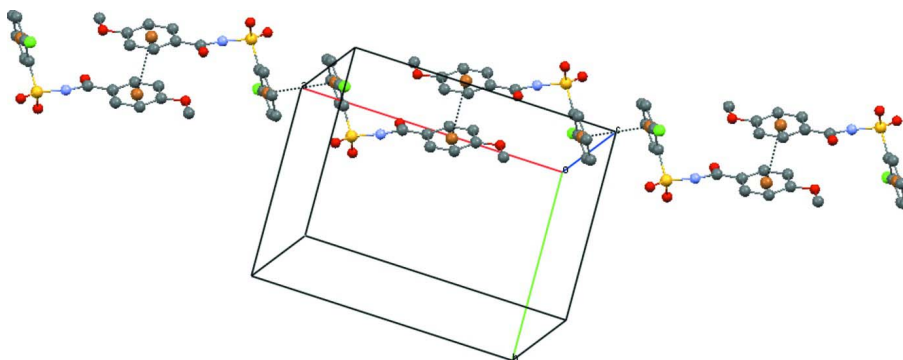
**Figure 5**

$\pi$-$\pi$ stacking interactions observed in the crystal structure of I.

**2-Chloro-*N*-(4-methoxybenzoyl)benzenesulfonamide**

*Crystal data*

| | |
|---|---|
| $C_{14}H_{12}ClNO_4S$ | Prism |
| $M_r = 325.76$ | $D_x = 1.448$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Melting point: 445 K |
| Hall symbol: -P 2ybc | Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å |
| $a = 14.5293$ (19) Å | Cell parameters from 25 reflections |
| $b = 10.6225$ (14) Å | $\theta = 3.0$–$64.6°$ |
| $c = 9.6918$ (14) Å | $\mu = 3.71$ mm$^{-1}$ |
| $\beta = 92.695$ (5)° | $T = 293$ K |
| $V = 1494.2$ (4) Å$^3$ | Prism, colourless |
| $Z = 4$ | $0.44 \times 0.35 \times 0.26$ mm |
| $F(000) = 672$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 17846 measured reflections |
| Radiation source: fine-focus sealed tube | 2449 independent reflections |
| Graphite monochromator | 2295 reflections with $I > 2\sigma(I)$ |
| phi and $\varphi$ scans | $R_{int} = 0.058$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $\theta_{max} = 64.6°$, $\theta_{min} = 3.0°$ |
| | $h = -16 \rightarrow 16$ |
| | $k = -12 \rightarrow 12$ |
| $T_{min} = 0.263$, $T_{max} = 0.381$ | $l = -11 \rightarrow 9$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.063$ | |
| $wR(F^2) = 0.163$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.11$ | |
| 2449 reflections | $w = 1/[\sigma^2(F_o^2) + (0.109P)^2 + 0.3886P]$ |
| 195 parameters | where $P = (F_o^2 + 2F_c^2)/3$ |
| 0 restraints | $(\Delta/\sigma)_{max} < 0.001$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{max} = 0.52$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.37$ e Å$^{-3}$ |

*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$^2$)*

|  | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| H1 | 0.718 (2) | 0.192 (3) | 0.295 (4) | 0.066 (10)* |
| S1 | 0.79503 (4) | 0.19067 (5) | 0.11546 (6) | 0.0448 (3) |
| Cl1 | 0.90252 (7) | 0.02535 (9) | 0.35628 (9) | 0.0882 (4) |
| O1 | 0.85786 (12) | 0.27002 (19) | 0.1915 (2) | 0.0592 (5) |
| O2 | 0.75657 (13) | 0.2343 (2) | −0.01265 (19) | 0.0645 (5) |
| O4 | 0.32115 (14) | 0.1078 (2) | 0.5017 (3) | 0.0826 (7) |
| C9 | 0.54708 (16) | 0.1902 (2) | 0.3736 (3) | 0.0497 (6) |
| H9 | 0.5956 | 0.2456 | 0.3921 | 0.060* |
| C8 | 0.55277 (15) | 0.1039 (2) | 0.2671 (2) | 0.0439 (5) |
| C7 | 0.63122 (16) | 0.0964 (2) | 0.1759 (2) | 0.0467 (6) |
| N1 | 0.71064 (13) | 0.1640 (2) | 0.2183 (2) | 0.0482 (5) |
| O3 | 0.62999 (14) | 0.0385 (2) | 0.0682 (2) | 0.0705 (6) |
| C10 | 0.47035 (18) | 0.1952 (3) | 0.4531 (3) | 0.0562 (7) |
| H10 | 0.4673 | 0.2543 | 0.5235 | 0.067* |
| C13 | 0.47841 (19) | 0.0229 (3) | 0.2399 (3) | 0.0603 (7) |
| H13 | 0.4801 | −0.0340 | 0.1671 | 0.072* |
| C1 | 0.84769 (15) | 0.0440 (2) | 0.0838 (3) | 0.0485 (6) |
| C11 | 0.39843 (17) | 0.1122 (3) | 0.4276 (3) | 0.0565 (6) |
| C2 | 0.89668 (17) | −0.0230 (3) | 0.1868 (3) | 0.0604 (7) |
| C12 | 0.4026 (2) | 0.0265 (3) | 0.3197 (4) | 0.0679 (8) |
| H12 | 0.3539 | −0.0287 | 0.3013 | 0.081* |
| C3 | 0.9432 (2) | −0.1334 (3) | 0.1497 (5) | 0.0842 (12) |
| H3 | 0.9776 | −0.1787 | 0.2160 | 0.101* |
| C6 | 0.8439 (2) | 0.0008 (3) | −0.0515 (3) | 0.0638 (7) |
| H6 | 0.8105 | 0.0453 | −0.1195 | 0.077* |
| C4 | 0.9373 (3) | −0.1740 (3) | 0.0131 (5) | 0.0893 (12) |
| H4 | 0.9668 | −0.2481 | −0.0107 | 0.107* |
| C5 | 0.8897 (3) | −0.1082 (4) | −0.0854 (5) | 0.0851 (11) |
| H5 | 0.8877 | −0.1362 | −0.1765 | 0.102* |
| C14 | 0.3152 (3) | 0.1932 (4) | 0.6139 (5) | 0.0940 (13) |
| H14A | 0.3676 | 0.1823 | 0.6768 | 0.141* |
| H14B | 0.2598 | 0.1771 | 0.6612 | 0.141* |
| H14C | 0.3141 | 0.2780 | 0.5795 | 0.141* |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0411 (4) | 0.0523 (4) | 0.0410 (4) | 0.0020 (2) | 0.0010 (3) | 0.0046 (2) |
| Cl1 | 0.0929 (6) | 0.0998 (7) | 0.0690 (6) | −0.0016 (5) | −0.0274 (4) | 0.0253 (4) |
| O1 | 0.0552 (10) | 0.0589 (10) | 0.0636 (12) | −0.0150 (8) | 0.0034 (8) | −0.0062 (8) |
| O2 | 0.0623 (11) | 0.0852 (13) | 0.0459 (10) | 0.0168 (10) | 0.0013 (8) | 0.0179 (9) |
| O4 | 0.0488 (11) | 0.0906 (16) | 0.1105 (19) | −0.0120 (10) | 0.0257 (11) | −0.0087 (13) |
| C9 | 0.0382 (12) | 0.0555 (14) | 0.0552 (15) | −0.0069 (9) | −0.0011 (10) | −0.0066 (10) |
| C8 | 0.0404 (11) | 0.0450 (12) | 0.0459 (12) | −0.0027 (9) | −0.0037 (9) | 0.0013 (10) |
| C7 | 0.0436 (12) | 0.0541 (13) | 0.0418 (13) | 0.0007 (10) | −0.0048 (9) | −0.0023 (10) |
| N1 | 0.0421 (10) | 0.0628 (12) | 0.0394 (12) | −0.0026 (9) | −0.0010 (8) | −0.0064 (10) |
| O3 | 0.0594 (11) | 0.0961 (15) | 0.0557 (12) | −0.0101 (10) | 0.0010 (9) | −0.0290 (11) |
| C10 | 0.0429 (13) | 0.0642 (16) | 0.0616 (16) | −0.0030 (10) | 0.0047 (11) | −0.0110 (12) |
| C13 | 0.0529 (14) | 0.0595 (15) | 0.0681 (17) | −0.0110 (12) | −0.0015 (12) | −0.0141 (13) |
| C1 | 0.0368 (11) | 0.0534 (13) | 0.0555 (14) | −0.0019 (9) | 0.0043 (10) | 0.0023 (11) |
| C11 | 0.0406 (12) | 0.0594 (15) | 0.0697 (17) | −0.0029 (11) | 0.0055 (11) | 0.0053 (13) |
| C2 | 0.0396 (12) | 0.0604 (16) | 0.0806 (19) | −0.0003 (11) | −0.0018 (12) | 0.0167 (13) |
| C12 | 0.0467 (14) | 0.0664 (17) | 0.091 (2) | −0.0180 (12) | 0.0039 (13) | −0.0085 (15) |
| C3 | 0.0488 (15) | 0.0647 (19) | 0.139 (4) | 0.0075 (13) | 0.0061 (18) | 0.030 (2) |
| C6 | 0.0598 (15) | 0.0699 (17) | 0.0627 (17) | −0.0006 (13) | 0.0115 (13) | −0.0087 (14) |
| C4 | 0.072 (2) | 0.066 (2) | 0.133 (4) | 0.0070 (16) | 0.032 (2) | −0.012 (2) |
| C5 | 0.081 (2) | 0.077 (2) | 0.100 (3) | −0.0035 (18) | 0.030 (2) | −0.025 (2) |
| C14 | 0.0640 (19) | 0.103 (3) | 0.119 (3) | 0.0030 (18) | 0.041 (2) | −0.016 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O2 | 1.4154 (19) | C13—C12 | 1.375 (4) |
| S1—O1 | 1.4227 (19) | C13—H13 | 0.9300 |
| S1—N1 | 1.641 (2) | C1—C6 | 1.387 (4) |
| S1—C1 | 1.769 (3) | C1—C2 | 1.394 (4) |
| Cl1—C2 | 1.720 (3) | C11—C12 | 1.390 (5) |
| O4—C11 | 1.362 (3) | C2—C3 | 1.408 (5) |
| O4—C14 | 1.422 (5) | C12—H12 | 0.9300 |
| C9—C10 | 1.385 (4) | C3—C4 | 1.391 (6) |
| C9—C8 | 1.386 (4) | C3—H3 | 0.9300 |
| C9—H9 | 0.9300 | C6—C5 | 1.383 (5) |
| C8—C13 | 1.396 (3) | C6—H6 | 0.9300 |
| C8—C7 | 1.477 (3) | C4—C5 | 1.348 (6) |
| C7—O3 | 1.211 (3) | C4—H4 | 0.9300 |
| C7—N1 | 1.404 (3) | C5—H5 | 0.9300 |
| N1—H1 | 0.80 (4) | C14—H14A | 0.9600 |
| C10—C11 | 1.381 (4) | C14—H14B | 0.9600 |
| C10—H10 | 0.9300 | C14—H14C | 0.9600 |
| | | | |
| O2—S1—O1 | 118.55 (13) | O4—C11—C10 | 124.3 (3) |
| O2—S1—N1 | 108.28 (11) | O4—C11—C12 | 116.2 (2) |
| O1—S1—N1 | 105.51 (11) | C10—C11—C12 | 119.6 (2) |

| | | | |
|---|---|---|---|
| O2—S1—C1 | 106.98 (13) | C1—C2—C3 | 118.5 (3) |
| O1—S1—C1 | 109.85 (12) | C1—C2—Cl1 | 122.2 (2) |
| N1—S1—C1 | 107.16 (11) | C3—C2—Cl1 | 119.3 (3) |
| C11—O4—C14 | 117.6 (2) | C13—C12—C11 | 120.4 (2) |
| C10—C9—C8 | 121.2 (2) | C13—C12—H12 | 119.8 |
| C10—C9—H9 | 119.4 | C11—C12—H12 | 119.8 |
| C8—C9—H9 | 119.4 | C4—C3—C2 | 119.5 (3) |
| C9—C8—C13 | 118.4 (2) | C4—C3—H3 | 120.2 |
| C9—C8—C7 | 123.8 (2) | C2—C3—H3 | 120.2 |
| C13—C8—C7 | 117.8 (2) | C5—C6—C1 | 120.3 (3) |
| O3—C7—N1 | 119.4 (2) | C5—C6—H6 | 119.9 |
| O3—C7—C8 | 124.2 (2) | C1—C6—H6 | 119.9 |
| N1—C7—C8 | 116.4 (2) | C5—C4—C3 | 121.3 (3) |
| C7—N1—S1 | 122.55 (18) | C5—C4—H4 | 119.4 |
| C7—N1—H1 | 122 (2) | C3—C4—H4 | 119.4 |
| S1—N1—H1 | 115 (2) | C4—C5—C6 | 120.1 (4) |
| C11—C10—C9 | 119.9 (2) | C4—C5—H5 | 119.9 |
| C11—C10—H10 | 120.1 | C6—C5—H5 | 119.9 |
| C9—C10—H10 | 120.1 | O4—C14—H14A | 109.5 |
| C12—C13—C8 | 120.6 (3) | O4—C14—H14B | 109.5 |
| C12—C13—H13 | 119.7 | H14A—C14—H14B | 109.5 |
| C8—C13—H13 | 119.7 | O4—C14—H14C | 109.5 |
| C6—C1—C2 | 120.3 (3) | H14A—C14—H14C | 109.5 |
| C6—C1—S1 | 117.2 (2) | H14B—C14—H14C | 109.5 |
| C2—C1—S1 | 122.4 (2) | | |
| | | | |
| C10—C9—C8—C13 | 1.0 (4) | N1—S1—C1—C2 | −67.4 (2) |
| C10—C9—C8—C7 | 178.0 (2) | C14—O4—C11—C10 | −1.0 (5) |
| C9—C8—C7—O3 | −165.9 (3) | C14—O4—C11—C12 | 179.3 (3) |
| C13—C8—C7—O3 | 11.1 (4) | C9—C10—C11—O4 | 178.5 (3) |
| C9—C8—C7—N1 | 12.8 (3) | C9—C10—C11—C12 | −1.8 (4) |
| C13—C8—C7—N1 | −170.2 (2) | C6—C1—C2—C3 | 1.1 (4) |
| O3—C7—N1—S1 | 12.0 (3) | S1—C1—C2—C3 | −174.5 (2) |
| C8—C7—N1—S1 | −166.74 (17) | C6—C1—C2—Cl1 | −179.3 (2) |
| O2—S1—N1—C7 | 47.2 (2) | S1—C1—C2—Cl1 | 5.1 (3) |
| O1—S1—N1—C7 | 175.11 (19) | C8—C13—C12—C11 | 0.9 (5) |
| C1—S1—N1—C7 | −67.9 (2) | O4—C11—C12—C13 | −179.3 (3) |
| C8—C9—C10—C11 | 0.8 (4) | C10—C11—C12—C13 | 0.9 (5) |
| C9—C8—C13—C12 | −1.9 (4) | C1—C2—C3—C4 | −1.5 (4) |
| C7—C8—C13—C12 | −179.0 (3) | Cl1—C2—C3—C4 | 178.9 (3) |
| O2—S1—C1—C6 | 0.9 (2) | C2—C1—C6—C5 | −0.8 (4) |
| O1—S1—C1—C6 | −129.0 (2) | S1—C1—C6—C5 | 175.0 (2) |
| N1—S1—C1—C6 | 116.9 (2) | C2—C3—C4—C5 | 1.6 (5) |
| O2—S1—C1—C2 | 176.7 (2) | C3—C4—C5—C6 | −1.3 (6) |
| O1—S1—C1—C2 | 46.8 (2) | C1—C6—C5—C4 | 0.9 (5) |

*Hydrogen-bond geometry (Å, º)*

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2[i] | 0.81 (3) | 2.09 (3) | 2.872 (3) | 172 (3) |
| C3—H3···O1[ii] | 0.93 | 2.57 | 3.370 (4) | 144 |
| C9—H9···O2[i] | 0.93 | 2.48 | 3.288 (3) | 145 |

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