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# Crystal structures of 4-methoxy-N-(4-methylphenyl)benzenesulfonamide and N-(4-fluorophenyl)-4-methoxybenzenesulfonamide

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Crystal structures of two N-(aryl)arylsulfonamides, namely, 4-methoxy-N-(4-methylphenyl)benzenesulfonamide, $C_{14}H_{15}NO_3S$, (I), and N-(4-fluorophenyl)-4-methoxybenzenesulfonamide, $C_{13}H_{12}FNO_3S$, (II), were determined and analyzed. In (I), the benzenesulfonamide ring is disordered over two orientations, in a 0.516 (7):0.484 (7) ratio, which are inclined to each other at 28.0 (1)°. In (I), the major component of the sulfonyl benzene ring and the aniline ring form a dihedral angle of 63.36 (19)°, while in (II), the planes of the two benzene rings form a dihedral angle of 44.26 (13)°. In the crystal structure of (I), N—H···O hydrogen bonds form infinite C(4) chains extended in [010], and intermolecular C—H···$\pi_{aryl}$ interactions link these chains into layers parallel to the ab plane. The crystal structure of (II) features N—H···O hydrogen bonds forming infinite one dimensional C(4) chains along [001]. Further, a pair of C—H···O intermolecular interactions consolidate the crystal packing of (II) into a three-dimensional supramolecular architecture.

## 1. Chemical context

Sulfonamide drugs were the first among the chemotherapeutic agents to be used for curing and preventing bacterial infection in human beings (Shiva Prasad et al., 2011). They play a vital role as a key constituent in a number of biologically active molecules. Up to now, sulfonamides have been known to exhibit a wide variety of biological activities, such as antibacterial (Subhakara Reddy et al., 2012; Himel et al., 1971), antifungal (Hanafy et al., 2007), antiinflamatory (Kuçukguzel et al., 2013), antitumor (Ghorab et al., 2011), anticancer (Mansour et al., 2011), anti-HIV (Sahu et al., 2007) and anti-tubercular activities (Vora & Mehta, 2012). In recent years, extensive research studies have been carried out on the synthesis and evaluation of pharmacological activities of molecules containing the sulfonamide moiety for different activities, and have been reported to be important pharmacophores (Mohan et al., 2013).

With these considerations in mind and based on our structural study of N-(4-substituted-phenyl)-4-methoxybenzenesulfonamides (Vinola et al., 2015), we report herein the crystal structures of 4-methoxy-N-(4-methylphenyl)benzenesulfonamide, (I), and N-(4-fluorophenyl)-4-methoxybenzenesulfonamide, (II).

## 2. Structural commentary

In (I) (Fig. 1), the benzenesulfonamide ring is disordered due to rotation across the $C_{ar}$—$S(O_2)$ bond over two orientations,
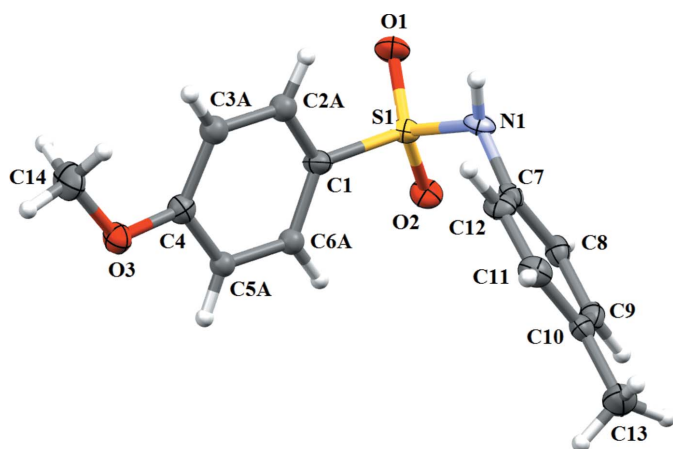


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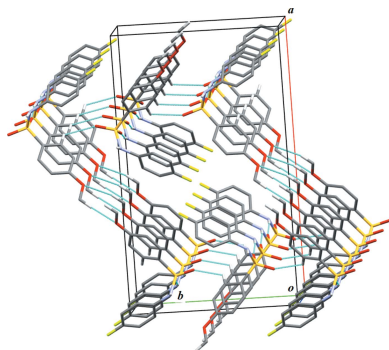
**Figure 1**
A view of (I), showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. Only the major component of the disordered benzene ring is shown.

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

$Cg$ is the centroid of the C7–C12 ring.

| $D-\mathrm{H}\cdots A$ | $D-\mathrm{H}$ | $\mathrm{H}\cdots A$ | $D\cdots A$ | $D-\mathrm{H}\cdots A$ |
|---|---|---|---|---|
| N1—H1···O2[i] | 0.89 (1) | 2.13 (1) | 3.010 (2) | 170 (2) |
| C14—H14B···$Cg$[ii] | 0.96 | 2.70 | 3.541 (2) | 146 |
| C9—H9···$Cg$[iii] | 0.93 | 2.87 | 3.560 (2) | 132 |

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

**Table 2**
Hydrogen-bond geometry (Å, °) for (II).

| $D-\mathrm{H}\cdots A$ | $D-\mathrm{H}$ | $\mathrm{H}\cdots A$ | $D\cdots A$ | $D-\mathrm{H}\cdots A$ |
|---|---|---|---|---|
| N1—H1···O2[i] | 0.90 (1) | 2.06 (1) | 2.951 (3) | 171 (3) |
| C6—H6···O1[ii] | 0.93 | 2.55 | 3.192 (3) | 127 |
| C13—H13B···O3[iii] | 0.96 | 2.60 | 3.468 (3) | 151 |

Symmetry codes: (i) $x, y, z+1$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+1, -y, z+\frac{1}{2}$.

with atoms C2, C3, C5 and C6 occupying two positions with a 0.516 (7):0.484 (7) ratio. The dihedral angle between the two parts of disordered benzene ring, *i.e.* C1/C2A/C3A/C4/C5A/C6A and C1/C2B/C3B/C4/C5B/C6B, is 28.0 (1)°. The dihedral angle between the sulfonyl benzene ring (considering the major component) and the aniline ring is 63.36 (19)°, and the N—C bond in the C—SO$_2$—NH—C segment has a *gauche* torsion with respect to the S=O bonds. Further, the molecule is twisted at the S—N bond, with a C1—S1—N1—C7 torsion angle of 66.33 (19)°. The methoxy group in the sulfonyl-benzene ring is in the same plane as that of the major component of the disordered sulfonylbenzene ring, the torsion angle C5A—C4—O3—C14 being −176.2 (4)°, while it deviates slightly from planarity with respect to the minor component, the C5B—C4—O3—C14 torsion angle being 165.9 (4)°.

In (II) (Fig. 2), the dihedral angle between the two benzene rings of 44.26 (13)° is less than that observed in (I), and the N—C bond in the C—SO$_2$—NH—C segment has a *gauche* torsion with respect to the S=O bonds. Further, the molecule
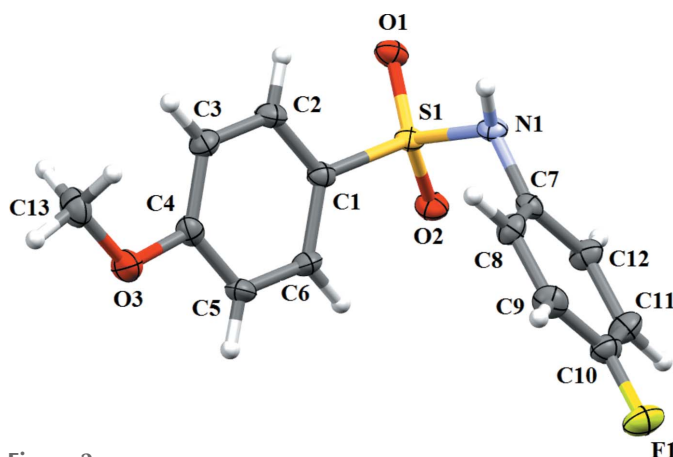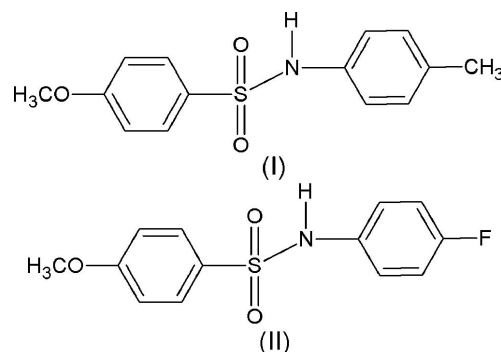
is twisted at the S—N bond, with a C1—S1—N1—C7 torsion angle of 68.4 (2)°. Similar to (I), the methoxy group in the sulfonylbenzene ring is in the same plane as that of the sulfonylbenzene ring, the C5—C4—O3—C13 torsion angle being 177.0 (2)°.



**3. Supramolecular features**

In the crystal structure of (I), N1—H1···O2 hydrogen bonds (Table 1) link the molecules into infinite one-dimensional *C*(4) chains along [010]. Neighbouring *C*(4) chains are inter-



**Figure 3**
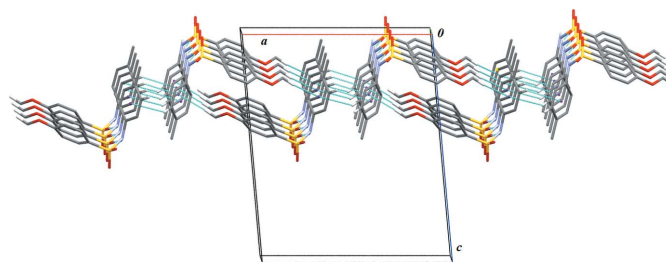A portion of the crystal packing of (I), viewed approximately along [010] and showing intermolecular hydrogen bonds as thin blue lines. Only the major component of the disordered benzene ring is shown. H atoms not involved in hydrogen bonding have been omitted for clarity.

**Figure 2**
A view of (II), showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

**Table 3**
Experimental details.

| | (I) | (II) |
|---|---|---|
| **Crystal data** | | |
| Chemical formula | $C_{14}H_{15}NO_3S$ | $C_{13}H_{12}FNO_3S$ |
| $M_r$ | 277.33 | 281.30 |
| Crystal system, space group | Monoclinic, $P2_1/c$ | Orthorhombic, $Pna2_1$ |
| Temperature (K) | 296 | 296 |
| $a, b, c$ (Å) | 14.5604 (5), 5.2459 (2), 17.6094 (6) | 20.2188 (13), 12.1199 (8), 5.1770 (3) |
| $\alpha, \beta, \gamma$ (°) | 90, 95.205 (2), 90 | 90, 90, 90 |
| $V$ (Å$^3$) | 1339.50 (8) | 1268.62 (14) |
| $Z$ | 4 | 4 |
| Radiation type | Cu $K\alpha$ | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 2.19 | 2.44 |
| Crystal size (mm) | $0.33 \times 0.27 \times 0.21$ | $0.32 \times 0.27 \times 0.22$ |
| | | |
| **Data collection** | | |
| Diffractometer | Bruker APEXII | Bruker APEXII |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2009) | Multi-scan (*SADABS*; Bruker, 2009) |
| $T_{min}, T_{max}$ | 0.517, 0.632 | 0.481, 0.585 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 7071, 2139, 2047 | 5438, 1830, 1784 |
| $R_{int}$ | 0.042 | 0.037 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.583 | 0.583 |
| | | |
| **Refinement** | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.048, 0.145, 1.12 | 0.034, 0.100, 1.09 |
| No. of reflections | 2139 | 1830 |
| No. of parameters | 175 | 177 |
| No. of restraints | 19 | 2 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}, \Delta\rho_{min}$ (e Å$^{-3}$) | 0.45, −0.43 | 0.30, −0.35 |
| Absolute structure | – | Flack (1983), 973 Friedel pairs |
| Absolute structure parameter | – | 0.08 (2) |

Computer programs: *APEX2*, *SAINT-Plus* and *XPREP* (Bruker, 2009), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

connected *via* C—H···$\pi_{aryl}$ interactions (Table 1) into layers (Fig. 3) parallel to the *ab* plane.

The crystal structure of (II) features N1—H1···O2 hydrogen bonds (Fig. 4 and Table 2), forming infinite one-dimensional $C(4)$ chains along [001]. Further, weak intermolecular C—H···O interactions (Table 2) consolidate the crystal packing of (II), leading to a three-dimensional supramolecular architecture (Fig. 5).

## 4. Database survey

Three *N*-(4-substituted-phenyl)-4-methoxybenzenesulfonamides (Vinola *et al.*, 2015), namely, 4-methoxy-*N*-(phenyl)benzenesulfonamide, (III), 4-methoxy-*N*-(4-methoxyphenyl)benzenesulfonamide, (IV), and *N*-(4-chlorophenyl)-4-methoxybenzenesulfonamide, (V), have been reported previously. Compounds (IV) and (V) crystallize in monoclinic syngony, while compound (III) crystallizes in orthorhombic syngony. The dihedral angles between the two benzene rings in (III), (IV) and (V) are 55.1 (1), 56.3 (1) and 42.6 (1)°, respectively. Comparison of the dihedral angles between the two benzene rings in (I)–(V) shows that, when an electron-donating substituent is introduced into the *para* position of the aniline ring of (I) it results in a slight increase in the dihedral angle, whereas, when an electron-withdrawing substituent is

introduced it decreases the dihedral angle. Further, the molecules of (III), (IV) and (V) are twisted at the S—N bond, with
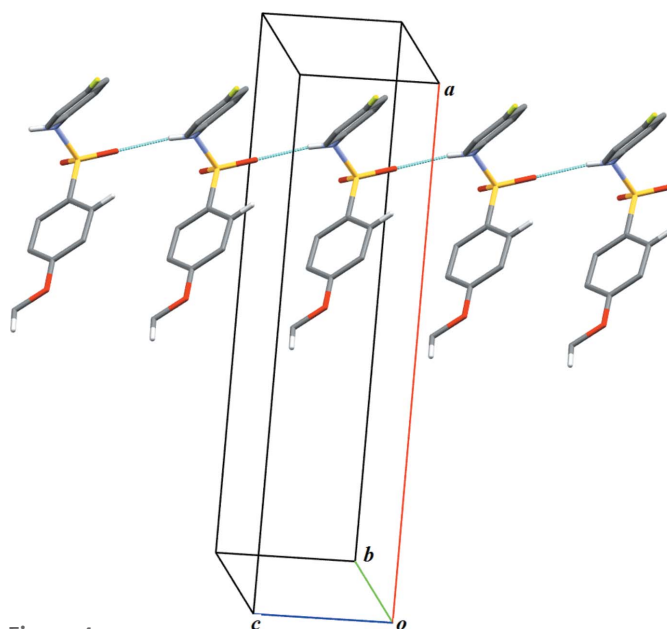


**Figure 4**
An N—H···O hydrogen-bonded (thin blue lines) chain of molecules in the crystal structure of (II).
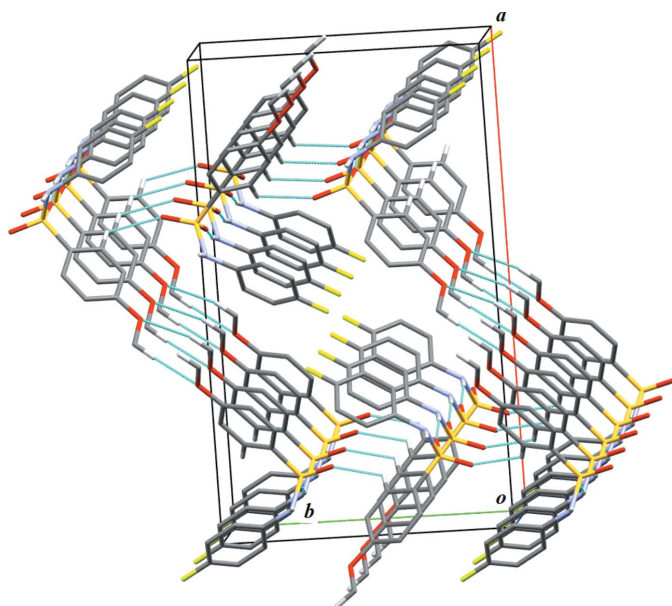
**Figure 5**
A portion of the crystal packing of (II). Thin blue lines denote intermolecular C—H···O hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted for clarity.

C1—S1—N1—C7 torsion angles of −72.9 (1), 66.2 (1) and 72.5 (1)°, respectively. These values are similar to those observed in (I) and (II).

Comparison of the crystal structures (I) and (V) shows that the effect of introducing an electron-donating substituent into the *para* position of the aniline ring of (I) is quite different than that due to electron-withdrawing substituents. The crystal structure of (III) features N—H···O hydrogen bonds that form *C*(4) chains, and thus, the supramolecular architecture is one-dimensional. In (IV), one N—H···O hydrogen bond and two alternating C—H···$\pi_{aryl}$ (centroid of aniline ring) interactions direct a two-dimensional architecture. This is quite similar to the crystal structure of (I). Thus, the methyl and methoxy groups on the aniline ring have similar influence on the crystal structures of these compounds. However, the crystal structures of (II) and (V) are very different. The crystal structure of (V) features N—H···O hydrogen bonds that form *C*(4) chains. Further, (V) does not feature any structure-directing intermolecular interactions, and thus, the structure is one-dimensional. In contrast to this, the crystal structure of (II) features an N—H···O and two C—H···O interactions, leading to a three-dimensional architecture. Thus, the Cl and F atoms on the aniline ring have very different influences on the crystal structures of these compounds.

## 5. Synthesis and crystallization

Compounds (I) and (II) were prepared according to the literature method of Vinola *et al.* (2015). The purity of the compounds were checked by determining the melting points. Single crystals used for X-ray diffraction studies were obtained by slow evaporation of ethanol solutions of the compounds at room temperature.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The amino H atoms were located in a difference map and were refined isotropically with the bond-length restraint N—H = 0.90 (1) Å. To improve considerably the values of *R*1, *wR*2, and *S* (goodness-of-fit), a partially obscured reflection (*i.e.* 100) was omitted from the final refinement of (I). The two parts (*A* and *B*) of the disordered benzenesulfonyl ring in (I) were restrained to be planar (FLAT instruction), and thus, the r.m.s. deviations (considering non-H atoms) observed for the planes defining the two rings are 0.047 (1) (major-component ring *A*) and 0.054 (1) Å (minor-component ring *B*). The disordered atoms (C2, C3, C5 and C6) in both components were isotropically refined, and the C—C bond lengths were restrained to 1.391 (1) Å.

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# supporting information

## Crystal structures of 4-methoxy-*N*-(4-methylphenyl)benzenesulfonamide and *N*-(4-fluorophenyl)-4-methoxybenzenesulfonamide

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**Computing details**

For both compounds, 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).

**(I) 4-Methoxy-*N*-(4-methylphenyl)benzenesulfonamide**

*Crystal data*

| | |
|---|---|
| $C_{14}H_{15}NO_3S$ | Prism |
| $M_r = 277.33$ | $D_x = 1.375$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å |
| $a = 14.5604 (5)$ Å | Cell parameters from 178 reflections |
| $b = 5.2459 (2)$ Å | $\theta = 5.0–64.1°$ |
| $c = 17.6094 (6)$ Å | $\mu = 2.19$ mm$^{-1}$ |
| $\beta = 95.205 (2)°$ | $T = 296$ K |
| $V = 1339.50 (8)$ Å$^3$ | Prism, colourless |
| $Z = 4$ | $0.33 \times 0.27 \times 0.21$ mm |
| $F(000) = 584$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII diffractometer | 2139 independent reflections |
| Radiation source: fine-focus sealed tube | 2047 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.042$ |
| phi and $\varphi$ scans | $\theta_{max} = 64.1°$, $\theta_{min} = 5.0°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $h = -16 \rightarrow 16$ |
| | $k = -5 \rightarrow 6$ |
| | $l = -20 \rightarrow 20$ |
| $T_{min} = 0.517$, $T_{max} = 0.632$ | 1 standard reflections every 1 reflections |
| 7071 measured reflections | intensity decay: 0.1% |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | |
| $wR(F^2) = 0.145$ | |
| $S = 1.12$ | Hydrogen site location: inferred from neighbouring sites |
| 2139 reflections | |
| 175 parameters | H atoms treated by a mixture of independent and constrained refinement |
| 19 restraints | |

$w = 1/[\sigma^2(F_o^2) + (0.095P)^2 + 0.6515P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.45$ e Å$^{-3}$
$\Delta\rho_{min} = -0.43$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| H1 | 0.7020 (19) | 0.376 (2) | 0.4174 (15) | 0.033 (7)* | |
| C1 | 0.87525 (15) | 0.0577 (4) | 0.41335 (12) | 0.0223 (5) | |
| C2A | 0.9220 (3) | 0.2925 (9) | 0.4259 (2) | 0.0227 (12)* | 0.516 (7) |
| H2A | 0.8960 | 0.4215 | 0.4532 | 0.027* | 0.516 (7) |
| C3A | 1.0070 (3) | 0.3298 (9) | 0.3973 (3) | 0.0243 (12)* | 0.516 (7) |
| H3A | 1.0392 | 0.4819 | 0.4057 | 0.029* | 0.516 (7) |
| C2B | 0.9452 (3) | 0.1901 (9) | 0.4561 (3) | 0.0230 (13)* | 0.484 (7) |
| H2B | 0.9355 | 0.2534 | 0.5040 | 0.028* | 0.484 (7) |
| C3B | 1.0299 (3) | 0.2268 (10) | 0.4262 (3) | 0.0231 (13)* | 0.484 (7) |
| H3B | 1.0768 | 0.3160 | 0.4540 | 0.028* | 0.484 (7) |
| C4 | 1.04337 (15) | 0.1285 (4) | 0.35455 (12) | 0.0226 (5) | |
| C5A | 0.9913 (3) | −0.0795 (10) | 0.3344 (3) | 0.0190 (14)* | 0.516 (7) |
| H5A | 1.0125 | −0.1992 | 0.3011 | 0.023* | 0.516 (7) |
| C6A | 0.9068 (4) | −0.1143 (11) | 0.3631 (3) | 0.0199 (16)* | 0.516 (7) |
| H6A | 0.8710 | −0.2557 | 0.3483 | 0.024* | 0.516 (7) |
| C5B | 0.9778 (4) | −0.0372 (12) | 0.3192 (4) | 0.0215 (16)* | 0.484 (7) |
| H5B | 0.9903 | −0.1226 | 0.2750 | 0.026* | 0.484 (7) |
| C6B | 0.8942 (4) | −0.0756 (12) | 0.3492 (3) | 0.0191 (17)* | 0.484 (7) |
| H6B | 0.8514 | −0.1900 | 0.3264 | 0.023* | 0.484 (7) |
| S1 | 0.76759 (3) | 0.02277 (10) | 0.45066 (3) | 0.0195 (3) | |
| O3 | 1.12308 (11) | 0.1523 (3) | 0.32071 (9) | 0.0257 (4) | |
| O1 | 0.77618 (12) | 0.1184 (3) | 0.52696 (8) | 0.0288 (4) | |
| O2 | 0.73662 (11) | −0.2332 (3) | 0.43553 (9) | 0.0239 (4) | |
| N1 | 0.69436 (13) | 0.2136 (3) | 0.40319 (10) | 0.0209 (5) | |
| C10 | 0.60286 (15) | 0.1132 (4) | 0.16969 (13) | 0.0233 (5) | |
| C7 | 0.66683 (14) | 0.1726 (4) | 0.32369 (12) | 0.0190 (5) | |
| C11 | 0.66087 (17) | 0.3146 (5) | 0.19337 (13) | 0.0269 (5) | |
| H11 | 0.6785 | 0.4311 | 0.1576 | 0.032* | |
| C9 | 0.57863 (15) | −0.0581 (5) | 0.22474 (14) | 0.0251 (5) | |
| H9 | 0.5409 | −0.1957 | 0.2099 | 0.030* | |
| C14 | 1.18279 (18) | 0.3601 (5) | 0.34384 (17) | 0.0401 (7) | |
| H14A | 1.1496 | 0.5177 | 0.3367 | 0.060* | |

| | | | | |
|------|-----------|-----------|-------------|-----------|
| H14B | 1.2345 | 0.3610 | 0.3137 | 0.060* |
| H14C | 1.2043 | 0.3410 | 0.3967 | 0.060* |
| C8 | 0.60898 (15) | −0.0295 (4) | 0.30080 (13) | 0.0219 (5) |
| H8 | 0.5908 | −0.1449 | 0.3366 | 0.026* |
| C12 | 0.69271 (16) | 0.3439 (4) | 0.26919 (12) | 0.0236 (5) |
| H12 | 0.7317 | 0.4791 | 0.2839 | 0.028* |
| C13 | 0.56880 (18) | 0.0780 (6) | 0.08674 (14) | 0.0363 (6) |
| H13A | 0.6139 | −0.0147 | 0.0614 | 0.054* |
| H13B | 0.5589 | 0.2417 | 0.0631 | 0.054* |
| H13C | 0.5119 | −0.0155 | 0.0831 | 0.054* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|-----|------------|------------|------------|-------------|-------------|-------------|
| C1 | 0.0253 (12) | 0.0218 (12) | 0.0201 (11) | −0.0001 (10) | 0.0032 (9) | −0.0043 (9) |
| C4 | 0.0233 (11) | 0.0225 (12) | 0.0222 (11) | 0.0006 (9) | 0.0021 (9) | 0.0015 (9) |
| S1 | 0.0239 (4) | 0.0169 (4) | 0.0181 (4) | −0.0004 (2) | 0.0046 (2) | −0.00107 (18) |
| O3 | 0.0223 (8) | 0.0264 (9) | 0.0290 (8) | −0.0022 (7) | 0.0056 (7) | 0.0003 (7) |
| O1 | 0.0336 (9) | 0.0348 (10) | 0.0187 (8) | 0.0010 (8) | 0.0062 (7) | −0.0046 (7) |
| O2 | 0.0294 (9) | 0.0151 (8) | 0.0277 (8) | −0.0003 (7) | 0.0046 (7) | 0.0038 (6) |
| N1 | 0.0286 (10) | 0.0129 (10) | 0.0220 (10) | 0.0015 (8) | 0.0061 (8) | −0.0028 (7) |
| C10 | 0.0199 (11) | 0.0249 (13) | 0.0254 (12) | 0.0060 (9) | 0.0027 (9) | −0.0035 (9) |
| C7 | 0.0186 (11) | 0.0154 (11) | 0.0236 (11) | 0.0038 (8) | 0.0046 (9) | −0.0017 (8) |
| C11 | 0.0322 (13) | 0.0231 (12) | 0.0258 (12) | 0.0017 (10) | 0.0060 (10) | 0.0025 (9) |
| C9 | 0.0187 (11) | 0.0223 (12) | 0.0339 (13) | −0.0017 (10) | 0.0008 (9) | −0.0041 (10) |
| C14 | 0.0262 (13) | 0.0385 (15) | 0.0570 (18) | −0.0111 (12) | 0.0118 (12) | −0.0074 (13) |
| C8 | 0.0177 (11) | 0.0179 (11) | 0.0305 (13) | −0.0004 (9) | 0.0042 (9) | 0.0032 (9) |
| C12 | 0.0294 (12) | 0.0145 (11) | 0.0274 (12) | −0.0036 (9) | 0.0051 (9) | −0.0021 (9) |
| C13 | 0.0329 (14) | 0.0476 (17) | 0.0281 (13) | 0.0003 (13) | 0.0019 (11) | −0.0059 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---------|-----------|---------|------------|
| C1—C6A | 1.371 (5) | S1—O2 | 1.4340 (17) |
| C1—C6B | 1.378 (5) | S1—N1 | 1.6360 (19) |
| C1—C2B | 1.395 (5) | O3—C14 | 1.430 (3) |
| C1—C2A | 1.415 (5) | N1—C7 | 1.437 (3) |
| C1—S1 | 1.763 (2) | N1—H1 | 0.893 (10) |
| C2A—C3A | 1.391 (5) | C10—C9 | 1.391 (3) |
| C2A—H2A | 0.9300 | C10—C11 | 1.393 (3) |
| C3A—C4 | 1.426 (5) | C10—C13 | 1.511 (3) |
| C3A—H3A | 0.9300 | C7—C8 | 1.391 (3) |
| C2B—C3B | 1.397 (6) | C7—C12 | 1.392 (3) |
| C2B—H2B | 0.9300 | C11—C12 | 1.382 (3) |
| C3B—C4 | 1.394 (5) | C11—H11 | 0.9300 |
| C3B—H3B | 0.9300 | C9—C8 | 1.380 (3) |
| C4—C5A | 1.358 (5) | C9—H9 | 0.9300 |
| C4—O3 | 1.358 (3) | C14—H14A | 0.9600 |
| C4—C5B | 1.395 (5) | C14—H14B | 0.9600 |

| | | | |
|---|---|---|---|
| C5A—C6A | 1.385 (6) | C14—H14C | 0.9600 |
| C5A—H5A | 0.9300 | C8—H8 | 0.9300 |
| C6A—H6A | 0.9300 | C12—H12 | 0.9300 |
| C5B—C6B | 1.385 (6) | C13—H13A | 0.9600 |
| C5B—H5B | 0.9300 | C13—H13B | 0.9600 |
| C6B—H6B | 0.9300 | C13—H13C | 0.9600 |
| S1—O1 | 1.4291 (16) | | |
| | | | |
| C6A—C1—C2B | 113.9 (3) | O1—S1—O2 | 120.18 (10) |
| C6B—C1—C2B | 120.3 (3) | O1—S1—N1 | 105.25 (10) |
| C6A—C1—C2A | 119.3 (3) | O2—S1—N1 | 107.39 (9) |
| C6B—C1—C2A | 116.1 (3) | O1—S1—C1 | 107.99 (10) |
| C6A—C1—S1 | 122.2 (3) | O2—S1—C1 | 107.66 (10) |
| C6B—C1—S1 | 120.2 (3) | N1—S1—C1 | 107.83 (10) |
| C2B—C1—S1 | 118.7 (2) | C4—O3—C14 | 117.83 (18) |
| C2A—C1—S1 | 117.6 (2) | C7—N1—S1 | 121.15 (14) |
| C3A—C2A—C1 | 119.8 (4) | C7—N1—H1 | 115.7 (17) |
| C3A—C2A—H2A | 120.1 | S1—N1—H1 | 112.5 (18) |
| C1—C2A—H2A | 120.1 | C9—C10—C11 | 117.8 (2) |
| C2A—C3A—C4 | 118.1 (4) | C9—C10—C13 | 120.9 (2) |
| C2A—C3A—H3A | 120.9 | C11—C10—C13 | 121.3 (2) |
| C4—C3A—H3A | 120.9 | C8—C7—C12 | 119.2 (2) |
| C1—C2B—C3B | 119.5 (4) | C8—C7—N1 | 120.31 (19) |
| C1—C2B—H2B | 120.3 | C12—C7—N1 | 120.4 (2) |
| C3B—C2B—H2B | 120.3 | C12—C11—C10 | 121.0 (2) |
| C4—C3B—C2B | 119.4 (4) | C12—C11—H11 | 119.5 |
| C4—C3B—H3B | 120.3 | C10—C11—H11 | 119.5 |
| C2B—C3B—H3B | 120.3 | C8—C9—C10 | 121.8 (2) |
| C5A—C4—O3 | 116.0 (3) | C8—C9—H9 | 119.1 |
| C5A—C4—C3B | 114.4 (3) | C10—C9—H9 | 119.1 |
| O3—C4—C3B | 124.1 (3) | O3—C14—H14A | 109.5 |
| O3—C4—C5B | 116.0 (3) | O3—C14—H14B | 109.5 |
| C3B—C4—C5B | 119.2 (3) | H14A—C14—H14B | 109.5 |
| C5A—C4—C3A | 120.5 (3) | O3—C14—H14C | 109.5 |
| O3—C4—C3A | 122.4 (2) | H14A—C14—H14C | 109.5 |
| C5B—C4—C3A | 115.1 (3) | H14B—C14—H14C | 109.5 |
| C4—C5A—C6A | 120.3 (4) | C9—C8—C7 | 119.8 (2) |
| C4—C5A—H5A | 119.9 | C9—C8—H8 | 120.1 |
| C6A—C5A—H5A | 119.9 | C7—C8—H8 | 120.1 |
| C1—C6A—C5A | 120.6 (4) | C11—C12—C7 | 120.4 (2) |
| C1—C6A—H6A | 119.7 | C11—C12—H12 | 119.8 |
| C5A—C6A—H6A | 119.7 | C7—C12—H12 | 119.8 |
| C6B—C5B—C4 | 120.7 (5) | C10—C13—H13A | 109.5 |
| C6B—C5B—H5B | 119.7 | C10—C13—H13B | 109.5 |
| C4—C5B—H5B | 119.7 | H13A—C13—H13B | 109.5 |
| C1—C6B—C5B | 119.2 (5) | C10—C13—H13C | 109.5 |
| C1—C6B—H6B | 120.4 | H13A—C13—H13C | 109.5 |
| C5B—C6B—H6B | 120.4 | H13B—C13—H13C | 109.5 |

| | | | |
|---|---|---|---|
| C6A—C1—C2A—C3A | −10.4 (6) | S1—C1—C6B—C5B | 177.4 (5) |
| C6B—C1—C2A—C3A | −26.8 (6) | C4—C5B—C6B—C1 | 1.9 (9) |
| C2B—C1—C2A—C3A | 79.3 (5) | C6A—C1—S1—O1 | 145.9 (4) |
| S1—C1—C2A—C3A | −179.7 (3) | C6B—C1—S1—O1 | 163.2 (4) |
| C1—C2A—C3A—C4 | 1.2 (6) | C2B—C1—S1—O1 | −7.0 (3) |
| C6A—C1—C2B—C3B | 27.0 (6) | C2A—C1—S1—O1 | −45.0 (3) |
| C6B—C1—C2B—C3B | 11.9 (6) | C6A—C1—S1—O2 | 14.8 (4) |
| C2A—C1—C2B—C3B | −80.4 (5) | C6B—C1—S1—O2 | 32.1 (4) |
| S1—C1—C2B—C3B | −177.9 (3) | C2B—C1—S1—O2 | −138.2 (3) |
| C1—C2B—C3B—C4 | −0.6 (6) | C2A—C1—S1—O2 | −176.2 (3) |
| C2B—C3B—C4—C5A | −27.1 (6) | C6A—C1—S1—N1 | −100.8 (4) |
| C2B—C3B—C4—O3 | −179.6 (3) | C6B—C1—S1—N1 | −83.5 (4) |
| C2B—C3B—C4—C5B | −9.8 (6) | C2B—C1—S1—N1 | 106.3 (3) |
| C2B—C3B—C4—C3A | 82.0 (6) | C2A—C1—S1—N1 | 68.2 (3) |
| C2A—C3A—C4—C5A | 8.2 (6) | C5A—C4—O3—C14 | −176.2 (4) |
| C2A—C3A—C4—O3 | 176.2 (3) | C3B—C4—O3—C14 | −24.1 (4) |
| C2A—C3A—C4—C3B | −80.1 (6) | C5B—C4—O3—C14 | 165.9 (4) |
| C2A—C3A—C4—C5B | 25.4 (6) | C3A—C4—O3—C14 | 15.3 (4) |
| O3—C4—C5A—C6A | −177.0 (4) | O1—S1—N1—C7 | −178.58 (16) |
| C3B—C4—C5A—C6A | 28.1 (7) | O2—S1—N1—C7 | −49.43 (18) |
| C5B—C4—C5A—C6A | −82.9 (14) | C1—S1—N1—C7 | 66.33 (19) |
| C3A—C4—C5A—C6A | −8.3 (7) | S1—N1—C7—C8 | 71.9 (2) |
| C6B—C1—C6A—C5A | 92.3 (16) | S1—N1—C7—C12 | −112.4 (2) |
| C2B—C1—C6A—C5A | −26.5 (7) | C9—C10—C11—C12 | −0.5 (3) |
| C2A—C1—C6A—C5A | 10.5 (7) | C13—C10—C11—C12 | −179.2 (2) |
| S1—C1—C6A—C5A | 179.3 (4) | C11—C10—C9—C8 | 1.3 (3) |
| C4—C5A—C6A—C1 | −1.2 (8) | C13—C10—C9—C8 | 180.0 (2) |
| C5A—C4—C5B—C6B | 86.0 (14) | C10—C9—C8—C7 | −1.2 (3) |
| O3—C4—C5B—C6B | 179.8 (5) | C12—C7—C8—C9 | 0.4 (3) |
| C3B—C4—C5B—C6B | 9.2 (8) | N1—C7—C8—C9 | 176.2 (2) |
| C3A—C4—C5B—C6B | −27.4 (7) | C10—C11—C12—C7 | −0.3 (3) |
| C6A—C1—C6B—C5B | −80.7 (16) | C8—C7—C12—C11 | 0.4 (3) |
| C2B—C1—C6B—C5B | −12.5 (8) | N1—C7—C12—C11 | −175.4 (2) |
| C2A—C1—C6B—C5B | 25.2 (8) | | |

*Hydrogen-bond geometry (Å, º)*

Cg is the centroid of the C7–C12 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O2[i] | 0.89 (1) | 2.13 (1) | 3.010 (2) | 170 (2) |
| C14—H14*B*···*Cg*[ii] | 0.96 | 2.70 | 3.541 (2) | 146 |
| C9—H9···*Cg*[iii] | 0.93 | 2.87 | 3.560 (2) | 132 |

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

**(II)** *N*-(4-Fluorophenyl)-4-methoxybenzenesulfonamide

*Crystal data*

| | |
|---|---|
| $C_{13}H_{12}FNO_3S$ | Prism |
| $M_r = 281.30$ | $D_x = 1.473$ Mg m$^{-3}$ |
| Orthorhombic, $Pna2_1$ | Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å |
| Hall symbol: P 2c -2n | Cell parameters from 143 reflections |
| $a = 20.2188$ (13) Å | $\theta = 4.3–64.1°$ |
| $b = 12.1199$ (8) Å | $\mu = 2.44$ mm$^{-1}$ |
| $c = 5.1770$ (3) Å | $T = 296$ K |
| $V = 1268.62$ (14) Å$^3$ | Prism, colourless |
| $Z = 4$ | $0.32 \times 0.27 \times 0.22$ mm |
| $F(000) = 584$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII diffractometer | 1830 independent reflections |
| Radiation source: fine-focus sealed tube | 1784 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.037$ |
| phi and $\varphi$ scans | $\theta_{max} = 64.1°$, $\theta_{min} = 4.3°$ |
| Absorption correction: multi-scan | $h = -22 \rightarrow 23$ |
| (*SADABS*; Bruker, 2009) | $k = -13 \rightarrow 14$ |
| $T_{min} = 0.481$, $T_{max} = 0.585$ | $l = -5 \rightarrow 5$ |
| 5438 measured reflections | 1 standard reflections every 1 reflections |
| | intensity decay: 0.1% |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.100$ | |
| $S = 1.09$ | $w = 1/[\sigma^2(F_o^2) + (0.0719P)^2]$ |
| 1830 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 177 parameters | $(\Delta/\sigma)_{max} = 0.001$ |
| 2 restraints | $\Delta\rho_{max} = 0.30$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{min} = -0.35$ e Å$^{-3}$ |
| | Absolute structure: Flack (1983), 973 Friedel pairs |
| Secondary atom site location: difference Fourier map | Absolute structure parameter: 0.08 (2) |

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.77164 (2) | 0.42206 (4) | 0.40154 (13) | 0.0172 (2) |
| F1 | 0.96703 (8) | −0.00461 (12) | 0.4446 (3) | 0.0328 (4) |

| | | | | |
|---|---|---|---|---|
| O1 | 0.75213 (8) | 0.53031 (14) | 0.4790 (4) | 0.0229 (4) |
| O2 | 0.79392 (9) | 0.40209 (15) | 0.1426 (4) | 0.0234 (4) |
| O3 | 0.56267 (8) | 0.10112 (16) | 0.6458 (4) | 0.0289 (5) |
| N1 | 0.83314 (9) | 0.38833 (18) | 0.5945 (4) | 0.0179 (5) |
| C10 | 0.93385 (12) | 0.0915 (2) | 0.4822 (6) | 0.0245 (6) |
| C6 | 0.70105 (11) | 0.2317 (2) | 0.3318 (5) | 0.0224 (6) |
| H6 | 0.7303 | 0.2162 | 0.1979 | 0.027* |
| C8 | 0.85326 (11) | 0.1947 (2) | 0.7108 (5) | 0.0229 (6) |
| H8 | 0.8215 | 0.2003 | 0.8401 | 0.028* |
| C7 | 0.86643 (11) | 0.2844 (2) | 0.5534 (5) | 0.0181 (5) |
| C4 | 0.60893 (10) | 0.1812 (2) | 0.5970 (6) | 0.0216 (6) |
| C2 | 0.66316 (11) | 0.3540 (2) | 0.6686 (6) | 0.0221 (5) |
| H2 | 0.6672 | 0.4199 | 0.7591 | 0.027* |
| C5 | 0.65224 (10) | 0.15819 (19) | 0.3967 (6) | 0.0234 (5) |
| H5 | 0.6482 | 0.0924 | 0.3056 | 0.028* |
| C11 | 0.94793 (12) | 0.1792 (2) | 0.3219 (6) | 0.0277 (6) |
| H11 | 0.9794 | 0.1731 | 0.1917 | 0.033* |
| C12 | 0.91355 (11) | 0.2773 (2) | 0.3611 (5) | 0.0240 (6) |
| H12 | 0.9224 | 0.3382 | 0.2575 | 0.029* |
| C3 | 0.61372 (11) | 0.2795 (2) | 0.7337 (5) | 0.0234 (6) |
| H3 | 0.5843 | 0.2952 | 0.8667 | 0.028* |
| C1 | 0.70619 (12) | 0.3303 (2) | 0.4696 (5) | 0.0186 (5) |
| C13 | 0.51905 (13) | 0.1183 (2) | 0.8577 (6) | 0.0330 (7) |
| H13A | 0.5443 | 0.1268 | 1.0134 | 0.049* |
| H13B | 0.4901 | 0.0560 | 0.8745 | 0.049* |
| H13C | 0.4933 | 0.1837 | 0.8281 | 0.049* |
| C9 | 0.88759 (13) | 0.0962 (2) | 0.6755 (6) | 0.0261 (6) |
| H9 | 0.8794 | 0.0353 | 0.7801 | 0.031* |
| H1 | 0.8245 (14) | 0.399 (2) | 0.763 (2) | 0.023 (8)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0222 (3) | 0.0161 (3) | 0.0134 (3) | −0.0004 (2) | −0.0004 (2) | −0.0003 (2) |
| F1 | 0.0403 (8) | 0.0248 (8) | 0.0333 (10) | 0.0127 (6) | 0.0008 (8) | −0.0014 (8) |
| O1 | 0.0286 (8) | 0.0160 (9) | 0.0241 (10) | 0.0003 (7) | −0.0029 (7) | −0.0009 (7) |
| O2 | 0.0280 (9) | 0.0249 (10) | 0.0172 (10) | −0.0017 (8) | 0.0010 (8) | −0.0009 (8) |
| O3 | 0.0258 (9) | 0.0260 (10) | 0.0349 (13) | −0.0065 (8) | 0.0066 (9) | −0.0040 (9) |
| N1 | 0.0228 (9) | 0.0193 (11) | 0.0117 (11) | −0.0006 (8) | 0.0019 (9) | −0.0019 (9) |
| C10 | 0.0262 (12) | 0.0222 (14) | 0.0251 (15) | 0.0056 (11) | −0.0031 (11) | −0.0029 (11) |
| C6 | 0.0239 (11) | 0.0208 (13) | 0.0225 (15) | 0.0030 (10) | 0.0038 (10) | −0.0064 (11) |
| C8 | 0.0221 (10) | 0.0265 (15) | 0.0202 (14) | 0.0010 (10) | 0.0050 (10) | 0.0016 (11) |
| C7 | 0.0202 (11) | 0.0186 (13) | 0.0155 (13) | −0.0019 (10) | −0.0016 (9) | −0.0015 (10) |
| C4 | 0.0201 (11) | 0.0181 (13) | 0.0265 (14) | −0.0009 (9) | −0.0039 (11) | 0.0023 (11) |
| C2 | 0.0268 (12) | 0.0202 (13) | 0.0193 (13) | −0.0003 (10) | −0.0019 (10) | −0.0052 (11) |
| C5 | 0.0258 (11) | 0.0183 (12) | 0.0261 (14) | −0.0003 (9) | −0.0027 (11) | −0.0081 (13) |
| C11 | 0.0279 (11) | 0.0306 (15) | 0.0246 (17) | 0.0054 (12) | 0.0065 (11) | −0.0005 (12) |
| C12 | 0.0275 (11) | 0.0227 (12) | 0.0218 (14) | 0.0003 (10) | 0.0065 (11) | 0.0023 (11) |

| | | | | | |
|---|---|---|---|---|---|
| C3 | 0.0234 (11) | 0.0268 (14) | 0.0201 (14) | −0.0002 (11) | 0.0034 (10) | −0.0032 (11) |
| C1 | 0.0212 (11) | 0.0182 (12) | 0.0162 (12) | 0.0018 (10) | −0.0026 (9) | −0.0010 (10) |
| C13 | 0.0272 (12) | 0.0401 (15) | 0.0316 (17) | −0.0092 (12) | 0.0027 (12) | 0.0013 (14) |
| C9 | 0.0316 (13) | 0.0208 (14) | 0.0260 (16) | −0.0008 (11) | −0.0004 (12) | 0.0050 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O1 | 1.4275 (18) | C8—H8 | 0.9300 |
| S1—O2 | 1.435 (2) | C7—C12 | 1.380 (3) |
| S1—N1 | 1.647 (2) | C4—C5 | 1.385 (4) |
| S1—C1 | 1.764 (2) | C4—C3 | 1.390 (4) |
| F1—C10 | 1.358 (3) | C2—C1 | 1.378 (4) |
| O3—C4 | 1.371 (3) | C2—C3 | 1.388 (4) |
| O3—C13 | 1.423 (3) | C2—H2 | 0.9300 |
| N1—C7 | 1.444 (3) | C5—H5 | 0.9300 |
| N1—H1 | 0.898 (10) | C11—C12 | 1.392 (4) |
| C10—C9 | 1.371 (4) | C11—H11 | 0.9300 |
| C10—C11 | 1.378 (4) | C12—H12 | 0.9300 |
| C6—C5 | 1.372 (3) | C3—H3 | 0.9300 |
| C6—C1 | 1.395 (3) | C13—H13A | 0.9600 |
| C6—H6 | 0.9300 | C13—H13B | 0.9600 |
| C8—C7 | 1.385 (4) | C13—H13C | 0.9600 |
| C8—C9 | 1.394 (4) | C9—H9 | 0.9300 |
| | | | |
| O1—S1—O2 | 120.28 (11) | C1—C2—H2 | 120.0 |
| O1—S1—N1 | 105.44 (11) | C3—C2—H2 | 120.0 |
| O2—S1—N1 | 106.74 (11) | C6—C5—C4 | 120.5 (2) |
| O1—S1—C1 | 108.44 (11) | C6—C5—H5 | 119.8 |
| O2—S1—C1 | 108.41 (11) | C4—C5—H5 | 119.8 |
| N1—S1—C1 | 106.77 (11) | C10—C11—C12 | 117.9 (2) |
| C4—O3—C13 | 117.5 (2) | C10—C11—H11 | 121.1 |
| C7—N1—S1 | 118.62 (16) | C12—C11—H11 | 121.1 |
| C7—N1—H1 | 111.3 (19) | C7—C12—C11 | 120.2 (2) |
| S1—N1—H1 | 113.8 (19) | C7—C12—H12 | 119.9 |
| F1—C10—C9 | 118.5 (2) | C11—C12—H12 | 119.9 |
| F1—C10—C11 | 118.3 (2) | C2—C3—C4 | 118.9 (2) |
| C9—C10—C11 | 123.3 (2) | C2—C3—H3 | 120.5 |
| C5—C6—C1 | 119.0 (2) | C4—C3—H3 | 120.5 |
| C5—C6—H6 | 120.5 | C2—C1—C6 | 120.9 (2) |
| C1—C6—H6 | 120.5 | C2—C1—S1 | 119.40 (19) |
| C7—C8—C9 | 120.0 (2) | C6—C1—S1 | 119.56 (19) |
| C7—C8—H8 | 120.0 | O3—C13—H13A | 109.5 |
| C9—C8—H8 | 120.0 | O3—C13—H13B | 109.5 |
| C12—C7—C8 | 120.5 (2) | H13A—C13—H13B | 109.5 |
| C12—C7—N1 | 118.9 (2) | O3—C13—H13C | 109.5 |
| C8—C7—N1 | 120.5 (2) | H13A—C13—H13C | 109.5 |
| O3—C4—C5 | 115.2 (2) | H13B—C13—H13C | 109.5 |
| O3—C4—C3 | 124.1 (2) | C10—C9—C8 | 118.1 (3) |

| | | | |
|---|---|---|---|
| C5—C4—C3 | 120.7 (2) | C10—C9—H9 | 121.0 |
| C1—C2—C3 | 120.0 (2) | C8—C9—H9 | 121.0 |
| | | | |
| O1—S1—N1—C7 | −176.37 (18) | C1—C2—C3—C4 | 0.5 (4) |
| O2—S1—N1—C7 | −47.4 (2) | O3—C4—C3—C2 | 179.3 (2) |
| C1—S1—N1—C7 | 68.4 (2) | C5—C4—C3—C2 | −0.8 (4) |
| C9—C8—C7—C12 | −0.1 (4) | C3—C2—C1—C6 | −0.2 (4) |
| C9—C8—C7—N1 | −177.5 (2) | C3—C2—C1—S1 | −176.4 (2) |
| S1—N1—C7—C12 | 80.1 (3) | C5—C6—C1—C2 | 0.1 (4) |
| S1—N1—C7—C8 | −102.5 (2) | C5—C6—C1—S1 | 176.26 (19) |
| C13—O3—C4—C5 | 177.0 (2) | O1—S1—C1—C2 | −27.8 (2) |
| C13—O3—C4—C3 | −3.0 (4) | O2—S1—C1—C2 | −159.9 (2) |
| C1—C6—C5—C4 | −0.3 (4) | N1—S1—C1—C2 | 85.4 (2) |
| O3—C4—C5—C6 | −179.4 (2) | O1—S1—C1—C6 | 156.0 (2) |
| C3—C4—C5—C6 | 0.7 (4) | O2—S1—C1—C6 | 23.8 (2) |
| F1—C10—C11—C12 | 179.8 (2) | N1—S1—C1—C6 | −90.8 (2) |
| C9—C10—C11—C12 | 0.5 (4) | F1—C10—C9—C8 | −179.3 (2) |
| C8—C7—C12—C11 | 0.6 (4) | C11—C10—C9—C8 | 0.0 (4) |
| N1—C7—C12—C11 | 178.0 (2) | C7—C8—C9—C10 | −0.2 (4) |
| C10—C11—C12—C7 | −0.8 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O2[i] | 0.90 (1) | 2.06 (1) | 2.951 (3) | 171 (3) |
| C6—H6···O1[ii] | 0.93 | 2.55 | 3.192 (3) | 127 |
| C13—H13*B*···O3[iii] | 0.96 | 2.60 | 3.468 (3) | 151 |

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) −*x*+3/2, *y*−1/2, *z*−1/2; (iii) −*x*+1, −*y*, *z*+1/2.