

Diisopropylammonium benzenesulfonate

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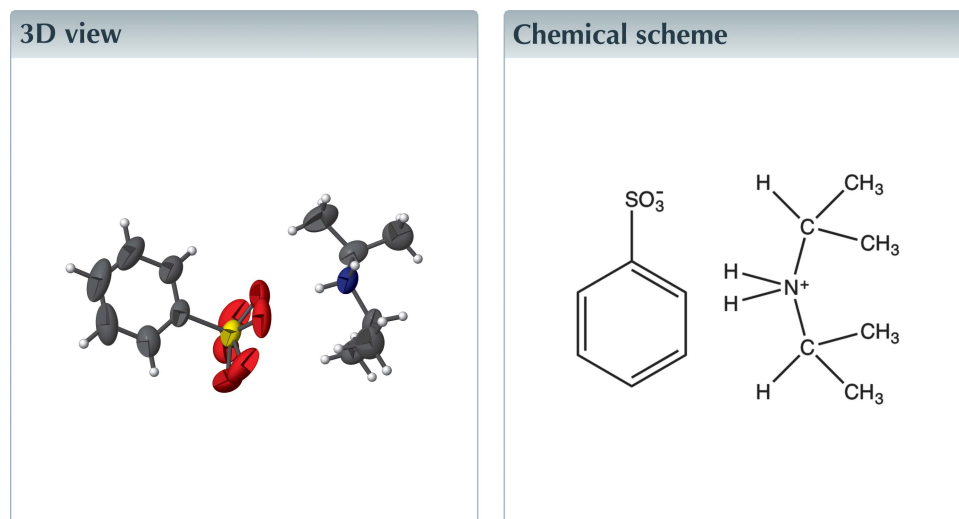
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In the anion of the title molecular salt, $C_6H_5O_3S^-$, the O atoms of the sulfonate group is rotationally disordered over two sets of sites in a 0.711 (9):0.289 (9) ratio. The extended structure displays N—H···O hydrogen bonds between the cation and anion, which results in infinite chains propagating parallel to [010]. The chains are linked by weak C—H···O interactions, yielding a two-dimensional network.



Structure description

Ammonium salts of phenylsulfonic acid have been reported by several groups (Lee *et al.*, 2015; Skořepová *et al.*, 2017; Karak *et al.*, 2017). We have now reacted phenylsulfonic acid with diisopropylamine, which yielded crystals of the title molecular salt.

The asymmetric unit is comprised of one diisopropylammonium cation and one phenyl sulfonate anion (Fig. 1): the oxygen atoms of the sulfonate group are rotationally disordered over two orientations in a 0.711 (9):0.289 (9) ratio. The C—C and C—N bonds in the cation are similar to those reported previously for diisopropylammonium-containing compounds (Sarr *et al.*, 2012; Lin *et al.*, 2017).

In the extended structure, the cations and anions are linked *via* N—H···O hydrogen bonds (Table 1) giving rise to [010] chains. These chains are in turn linked through weak C—H···O interactions, leading to a layered structure (Fig. 2).

Synthesis and crystallization

Phenylsulfonic acid (5.0 g; 3.0 mmol) was reacted with diisopropylamine (3.0 g; 3.0 mmol) in ethanol (50 ml). Slow solvent evaporation at room temperature yielded colourless blocks of the title compound after a week.

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–H1A···O1 ⁱ | 0.86 (2) | 2.06 (2) | 2.893 (4) | 165.0 (19) |
| N1–H1A···O1A ⁱ | 0.86 (2) | 1.85 (2) | 2.684 (6) | 163 (2) |
| N1–H1B···O2 | 0.91 (2) | 1.90 (3) | 2.782 (4) | 162 (2) |
| N1–H1B···O2A | 0.91 (2) | 2.05 (3) | 2.946 (9) | 167 (2) |
| C8–H8A···O2 | 0.98 | 2.45 | 3.246 (5) | 138 |
| C9–H9A···O1 ⁱ | 0.98 | 2.54 | 3.313 (4) | 136 |
| C11–H11B···O3 ⁱⁱ | 0.98 | 2.57 | 3.493 (4) | 157 |

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

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. During the early stages of the refinement, rotational disorder of the oxygen atoms of the sulfonate group was detected. The disorder was modelled using two sets of sites, which refined to occupancies of 0.711 (9):0.289 (9).

Funding information

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Table 2
Experimental details.

| | |
|---|--|
| Crystal data | |
| Chemical formula | $C_6H_{16}N^+ \cdot C_6H_5O_3S^-$ |
| <i>M_r</i> | 259.36 |
| Crystal system, space group | Monoclinic, <i>P2₁/c</i> |
| Temperature (K) | 200 |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 11.7370 (13), 8.8719 (8), 14.3722 (16) |
| β (°) | 106.616 (3) |
| <i>V</i> (Å ³) | 1434.1 (3) |
| <i>Z</i> | 4 |
| Radiation type | Mo <i>K</i> α |
| μ (mm ⁻¹) | 0.22 |
| Crystal size (mm) | 0.60 × 0.45 × 0.35 |
| Data collection | |
| Diffractometer | Bruker X2S Benchtop |
| Absorption correction | Multi-scan (<i>SADABS</i> ; Bruker, 2016) |
| <i>T_{min}</i> , <i>T_{max}</i> | 0.38, 0.93 |
| No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections | 11569, 2910, 2104 |
| <i>R_{int}</i> | 0.106 |
| (<i>sin</i> θ / λ) _{max} (Å ⁻¹) | 0.625 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i> | 0.050, 0.152, 1.05 |
| No. of reflections | 2910 |
| No. of parameters | 195 |
| No. of restraints | 3 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³) | 0.26, -0.34 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

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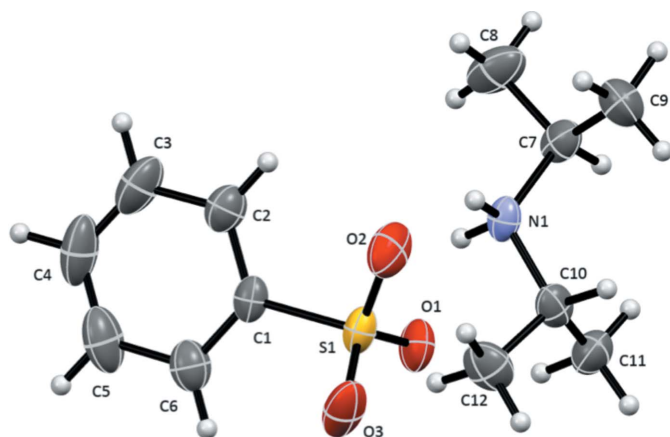


Figure 1
View of the title molecular salt showing anisotropic displacement parameters for non-H atoms drawn at the 30% probability level. Only the major disorder component of the sulfonate group is shown.

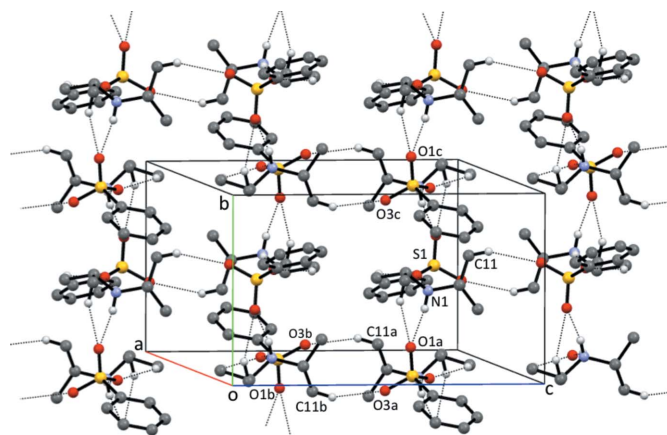


Figure 2
Partial packing diagram showing the hydrogen-bonding interactions. Only H atoms involved in the intermolecular interactions are shown. Symmetry codes: (a) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (b) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (c) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$.

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full crystallographic data

IUCrData (2018). 3, x180876 [https://doi.org/10.1107/S2414314618008763]

Diisopropylammonium benzenesulfonate

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Diisopropylammonium bis(propan-2-yl)azanium

Crystal data

$C_6H_{16}N^+ \cdot C_6H_5O_3S^-$

$M_r = 259.36$

Monoclinic, $P2_1/c$

$a = 11.7370$ (13) Å

$b = 8.8719$ (8) Å

$c = 14.3722$ (16) Å

$\beta = 106.616$ (3)°

$V = 1434.1$ (3) Å³

$Z = 4$

$F(000) = 560$

$D_x = 1.201$ Mg m⁻³

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

Cell parameters from 4767 reflections

$\theta = 2.7\text{--}25.1^\circ$

$\mu = 0.22$ mm⁻¹

$T = 200$ K

Block, colorless

$0.60 \times 0.45 \times 0.35$ mm

Data collection

Bruker X2S Benchtop
diffractometer

Radiation source: sealed microfocus tube

Detector resolution: 8.3330 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2016)

$T_{\min} = 0.38$, $T_{\max} = 0.93$

11569 measured reflections

2910 independent reflections

2104 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.106$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 2.7^\circ$

$h = -14 \rightarrow 14$

$k = -10 \rightarrow 10$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.152$

$S = 1.05$

2910 reflections

195 parameters

3 restraints

Primary atom site location: structure-invariant

direct methods

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.288P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.26$ e Å⁻³

$\Delta\rho_{\min} = -0.34$ e Å⁻³

Extinction correction: SHELXL2014

(Sheldrick, 2015)

Extinction coefficient: 0.0085 (18)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All hydrogen atoms were observed in difference Fourier maps. The H atoms were refined using a riding model with C—H distances of 0.98 Å for the methyl carbon atoms and 0.95 Å for the phenyl carbon atoms. The methyl C—H hydrogen atom isotropic displacement parameters were set using the approximation $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ and the phenyl hydrogen-atom isotropic displacement parameters were set using the approximation $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The hydrogen atoms bonded to the nitrogen atom were refined freely, including isotropic displacement parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|--------------|-------------|--------------|----------------------------------|-----------|
| S1 | 0.71911 (5) | 0.49488 (6) | 0.84523 (4) | 0.0597 (2) | |
| O1 | 0.7417 (3) | 0.6492 (3) | 0.8574 (3) | 0.0749 (12) | 0.711 (9) |
| O2 | 0.6149 (3) | 0.4620 (6) | 0.7613 (3) | 0.0911 (15) | 0.711 (9) |
| O3 | 0.7116 (4) | 0.4164 (4) | 0.9309 (3) | 0.0989 (19) | 0.711 (9) |
| O1A | 0.6956 (12) | 0.6349 (8) | 0.7859 (11) | 0.102 (4) | 0.289 (9) |
| O2A | 0.6285 (6) | 0.3979 (7) | 0.8244 (11) | 0.087 (4) | 0.289 (9) |
| O3A | 0.7621 (8) | 0.5452 (19) | 0.9473 (6) | 0.131 (7) | 0.289 (9) |
| N1 | 0.37129 (18) | 0.4253 (2) | 0.72964 (14) | 0.0541 (5) | |
| H1A | 0.3478 (19) | 0.335 (3) | 0.7122 (14) | 0.059 (6)* | |
| H1B | 0.452 (2) | 0.422 (3) | 0.7500 (16) | 0.071 (7)* | |
| C1 | 0.84060 (18) | 0.4120 (2) | 0.81419 (16) | 0.0532 (5) | |
| C2 | 0.8331 (2) | 0.3820 (3) | 0.71892 (19) | 0.0742 (7) | |
| H2 | 0.7635 | 0.4086 | 0.669 | 0.089* | |
| C3 | 0.9270 (3) | 0.3130 (4) | 0.6959 (3) | 0.1026 (10) | |
| H3 | 0.9213 | 0.2918 | 0.6299 | 0.123* | |
| C4 | 1.0259 (3) | 0.2755 (4) | 0.7654 (3) | 0.1098 (12) | |
| H4 | 1.0894 | 0.227 | 0.7485 | 0.132* | |
| C5 | 1.0359 (2) | 0.3064 (4) | 0.8596 (3) | 0.1040 (11) | |
| H5 | 1.107 | 0.2812 | 0.9084 | 0.125* | |
| C6 | 0.9420 (2) | 0.3753 (3) | 0.8858 (2) | 0.0769 (7) | |
| H6 | 0.9485 | 0.3963 | 0.952 | 0.092* | |
| C7 | 0.3239 (3) | 0.5281 (2) | 0.64440 (17) | 0.0660 (7) | |
| H7 | 0.3422 | 0.6346 | 0.6664 | 0.079* | |
| C8 | 0.3885 (3) | 0.4913 (3) | 0.5695 (2) | 0.1053 (11) | |
| H8A | 0.4745 | 0.4962 | 0.5999 | 0.158* | |
| H8B | 0.3659 | 0.5643 | 0.5162 | 0.158* | |
| H8C | 0.3667 | 0.3896 | 0.544 | 0.158* | |
| C9 | 0.1911 (3) | 0.5110 (4) | 0.6045 (2) | 0.0968 (10) | |
| H9A | 0.1719 | 0.4063 | 0.5843 | 0.145* | |
| H9B | 0.1618 | 0.5778 | 0.5484 | 0.145* | |
| H9C | 0.1532 | 0.5378 | 0.6548 | 0.145* | |
| C10 | 0.3368 (2) | 0.4608 (3) | 0.82055 (16) | 0.0628 (6) | |
| H10 | 0.2486 | 0.4748 | 0.8028 | 0.075* | |
| C11 | 0.3956 (3) | 0.6040 (3) | 0.86640 (18) | 0.0797 (8) | |
| H11A | 0.4819 | 0.5894 | 0.8886 | 0.119* | |
| H11B | 0.3666 | 0.6301 | 0.9219 | 0.119* | |
| H11C | 0.3766 | 0.6857 | 0.8186 | 0.119* | |
| C12 | 0.3702 (3) | 0.3269 (3) | 0.8884 (2) | 0.0883 (8) | |
| H12A | 0.4564 | 0.3115 | 0.906 | 0.132* | |

| | | | | |
|------|--------|--------|--------|--------|
| H12B | 0.3297 | 0.2366 | 0.8559 | 0.132* |
| H12C | 0.3461 | 0.3462 | 0.9473 | 0.132* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| S1 | 0.0560 (4) | 0.0497 (4) | 0.0838 (4) | 0.0034 (2) | 0.0366 (3) | -0.0044 (2) |
| O1 | 0.0762 (18) | 0.0450 (13) | 0.106 (3) | 0.0086 (11) | 0.0297 (18) | -0.0087 (14) |
| O2 | 0.0475 (15) | 0.110 (3) | 0.119 (3) | -0.0055 (16) | 0.0300 (18) | -0.035 (2) |
| O3 | 0.134 (4) | 0.082 (2) | 0.118 (3) | 0.024 (2) | 0.095 (3) | 0.022 (2) |
| O1A | 0.140 (9) | 0.042 (4) | 0.149 (10) | 0.042 (5) | 0.082 (8) | 0.031 (5) |
| O2A | 0.048 (4) | 0.046 (4) | 0.177 (13) | -0.001 (3) | 0.050 (6) | -0.011 (5) |
| O3A | 0.098 (6) | 0.224 (18) | 0.075 (5) | 0.015 (7) | 0.031 (4) | -0.046 (7) |
| N1 | 0.0545 (11) | 0.0392 (10) | 0.0768 (12) | 0.0004 (9) | 0.0318 (9) | 0.0019 (8) |
| C1 | 0.0482 (11) | 0.0393 (10) | 0.0803 (13) | -0.0035 (8) | 0.0318 (10) | 0.0005 (9) |
| C2 | 0.0680 (15) | 0.0794 (16) | 0.0849 (16) | 0.0017 (13) | 0.0374 (13) | -0.0044 (13) |
| C3 | 0.107 (2) | 0.104 (2) | 0.127 (3) | 0.001 (2) | 0.081 (2) | -0.0199 (19) |
| C4 | 0.090 (2) | 0.082 (2) | 0.189 (4) | 0.0177 (17) | 0.090 (3) | 0.007 (2) |
| C5 | 0.0518 (15) | 0.097 (2) | 0.165 (3) | 0.0134 (15) | 0.0345 (19) | 0.028 (2) |
| C6 | 0.0588 (14) | 0.0732 (15) | 0.0996 (18) | 0.0020 (12) | 0.0241 (14) | 0.0064 (13) |
| C7 | 0.102 (2) | 0.0376 (10) | 0.0683 (14) | 0.0005 (11) | 0.0403 (14) | 0.0031 (9) |
| C8 | 0.154 (3) | 0.098 (2) | 0.086 (2) | -0.014 (2) | 0.069 (2) | -0.0031 (15) |
| C9 | 0.098 (2) | 0.099 (2) | 0.0853 (19) | 0.0297 (17) | 0.0137 (18) | 0.0179 (15) |
| C10 | 0.0497 (12) | 0.0769 (14) | 0.0711 (13) | 0.0092 (11) | 0.0319 (11) | 0.0153 (11) |
| C11 | 0.093 (2) | 0.0788 (16) | 0.0755 (16) | 0.0141 (14) | 0.0369 (14) | -0.0058 (12) |
| C12 | 0.0853 (18) | 0.0942 (19) | 0.0882 (17) | 0.0015 (16) | 0.0293 (15) | 0.0330 (15) |

Geometric parameters (Å, °)

| | | | |
|--------|-----------|----------|-----------|
| S1—O2A | 1.334 (6) | C5—H5 | 0.95 |
| S1—O1 | 1.396 (3) | C6—H6 | 0.95 |
| S1—O3 | 1.439 (3) | C7—C9 | 1.507 (4) |
| S1—O3A | 1.478 (7) | C7—C8 | 1.519 (3) |
| S1—O2 | 1.481 (3) | C7—H7 | 1.0 |
| S1—O1A | 1.487 (7) | C8—H8A | 0.98 |
| S1—C1 | 1.771 (2) | C8—H8B | 0.98 |
| N1—C7 | 1.501 (3) | C8—H8C | 0.98 |
| N1—C10 | 1.508 (3) | C9—H9A | 0.98 |
| N1—H1A | 0.86 (2) | C9—H9B | 0.98 |
| N1—H1B | 0.91 (2) | C9—H9C | 0.98 |
| C1—C6 | 1.372 (3) | C10—C11 | 1.504 (3) |
| C1—C2 | 1.373 (3) | C10—C12 | 1.516 (3) |
| C2—C3 | 1.381 (4) | C10—H10 | 1.0 |
| C2—H2 | 0.95 | C11—H11A | 0.98 |
| C3—C4 | 1.339 (5) | C11—H11B | 0.98 |
| C3—H3 | 0.95 | C11—H11C | 0.98 |
| C4—C5 | 1.354 (5) | C12—H12A | 0.98 |
| C4—H4 | 0.95 | C12—H12B | 0.98 |

| | | | |
|--------------|-------------|---------------|-------------|
| C5—C6 | 1.403 (4) | C12—H12C | 0.98 |
| O1—S1—O3 | 115.1 (2) | N1—C7—C9 | 110.5 (2) |
| O2A—S1—O3A | 116.2 (6) | N1—C7—C8 | 107.7 (2) |
| O1—S1—O2 | 112.2 (2) | C9—C7—C8 | 112.3 (2) |
| O3—S1—O2 | 111.3 (2) | N1—C7—H7 | 108.7 |
| O2A—S1—O1A | 113.9 (6) | C9—C7—H7 | 108.7 |
| O3A—S1—O1A | 105.8 (6) | C8—C7—H7 | 108.7 |
| O2A—S1—C1 | 108.8 (3) | C7—C8—H8A | 109.5 |
| O1—S1—C1 | 107.50 (14) | C7—C8—H8B | 109.5 |
| O3—S1—C1 | 105.38 (14) | H8A—C8—H8B | 109.5 |
| O3A—S1—C1 | 107.7 (4) | C7—C8—H8C | 109.5 |
| O2—S1—C1 | 104.49 (14) | H8A—C8—H8C | 109.5 |
| O1A—S1—C1 | 103.5 (3) | H8B—C8—H8C | 109.5 |
| C7—N1—C10 | 116.82 (17) | C7—C9—H9A | 109.5 |
| C7—N1—H1A | 108.3 (14) | C7—C9—H9B | 109.5 |
| C10—N1—H1A | 107.7 (14) | H9A—C9—H9B | 109.5 |
| C7—N1—H1B | 112.8 (15) | C7—C9—H9C | 109.5 |
| C10—N1—H1B | 104.0 (15) | H9A—C9—H9C | 109.5 |
| H1A—N1—H1B | 107 (2) | H9B—C9—H9C | 109.5 |
| C6—C1—C2 | 119.8 (2) | C11—C10—N1 | 110.68 (18) |
| C6—C1—S1 | 119.83 (19) | C11—C10—C12 | 112.2 (2) |
| C2—C1—S1 | 120.32 (18) | N1—C10—C12 | 108.0 (2) |
| C1—C2—C3 | 119.8 (3) | C11—C10—H10 | 108.6 |
| C1—C2—H2 | 120.1 | N1—C10—H10 | 108.6 |
| C3—C2—H2 | 120.1 | C12—C10—H10 | 108.6 |
| C4—C3—C2 | 120.8 (3) | C10—C11—H11A | 109.5 |
| C4—C3—H3 | 119.6 | C10—C11—H11B | 109.5 |
| C2—C3—H3 | 119.6 | H11A—C11—H11B | 109.5 |
| C3—C4—C5 | 120.3 (3) | C10—C11—H11C | 109.5 |
| C3—C4—H4 | 119.9 | H11A—C11—H11C | 109.5 |
| C5—C4—H4 | 119.9 | H11B—C11—H11C | 109.5 |
| C4—C5—C6 | 120.5 (3) | C10—C12—H12A | 109.5 |
| C4—C5—H5 | 119.8 | C10—C12—H12B | 109.5 |
| C6—C5—H5 | 119.8 | H12A—C12—H12B | 109.5 |
| C1—C6—C5 | 118.8 (3) | C10—C12—H12C | 109.5 |
| C1—C6—H6 | 120.6 | H12A—C12—H12C | 109.5 |
| C5—C6—H6 | 120.6 | H12B—C12—H12C | 109.5 |
| O2A—S1—C1—C6 | -112.9 (7) | C6—C1—C2—C3 | 1.0 (4) |
| O1—S1—C1—C6 | 82.8 (3) | S1—C1—C2—C3 | -178.0 (2) |
| O3—S1—C1—C6 | -40.4 (3) | C1—C2—C3—C4 | -0.3 (5) |
| O3A—S1—C1—C6 | 13.9 (7) | C2—C3—C4—C5 | -0.7 (5) |
| O2—S1—C1—C6 | -157.8 (3) | C3—C4—C5—C6 | 1.2 (5) |
| O1A—S1—C1—C6 | 125.6 (7) | C2—C1—C6—C5 | -0.5 (4) |
| O2A—S1—C1—C2 | 66.0 (7) | S1—C1—C6—C5 | 178.4 (2) |
| O1—S1—C1—C2 | -98.3 (3) | C4—C5—C6—C1 | -0.6 (4) |
| O3—S1—C1—C2 | 138.5 (3) | C10—N1—C7—C9 | -68.0 (3) |

| | | | |
|--------------|------------|---------------|-----------|
| O3A—S1—C1—C2 | -167.2 (7) | C10—N1—C7—C8 | 168.9 (2) |
| O2—S1—C1—C2 | 21.1 (3) | C7—N1—C10—C11 | -69.1 (3) |
| O1A—S1—C1—C2 | -55.4 (7) | C7—N1—C10—C12 | 167.7 (2) |

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—H1A...O1 ⁱ | 0.86 (2) | 2.06 (2) | 2.893 (4) | 165.0 (19) |
| N1—H1A...O1A ⁱ | 0.86 (2) | 1.85 (2) | 2.684 (6) | 163 (2) |
| N1—H1B...O2 | 0.91 (2) | 1.90 (3) | 2.782 (4) | 162 (2) |
| N1—H1B...O2A | 0.91 (2) | 2.05 (3) | 2.946 (9) | 167 (2) |
| C8—H8A...O2 | 0.98 | 2.45 | 3.246 (5) | 138 |
| C9—H9A...O1 ⁱ | 0.98 | 2.54 | 3.313 (4) | 136 |
| C11—H11B...O3 ⁱⁱ | 0.98 | 2.57 | 3.493 (4) | 157 |
| C7—H7...O2A ⁱⁱⁱ | 1.0 | 2.36 | 3.336 (8) | 166 |
| C12—H12B...O1A ⁱ | 0.98 | 2.17 | 2.944 (11) | 135 |
| C12—H12C...O3A ⁱⁱ | 0.98 | 2.44 | 3.371 (8) | 159 |

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