

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## Uronium 3-carboxy-4-hydroxybenzene-sulfonate

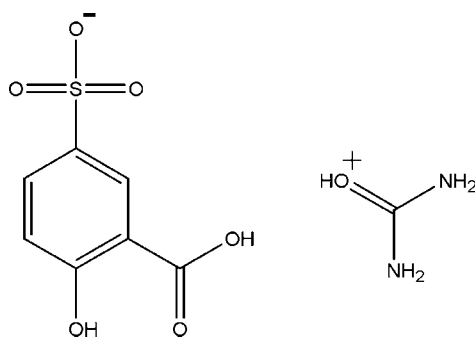
 A. Silambarasan,<sup>a</sup> M. Krishna Kumar,<sup>a</sup>  
 G. Chakkaravarthi,<sup>b\*</sup> R. Mohan Kumar<sup>a</sup> and  
 P. R. Umarani<sup>c\*</sup>
<sup>a</sup>Department of Physics, Presidency College, Chennai 600 005, India, <sup>b</sup>Department of Physics, CPCL Polytechnic College, Chennai 600 068, India, and <sup>c</sup>Kunthavai Naacchiyaar Govt. Arts College (W), Thanjavur 613 007, India  
 Correspondence e-mail: chakkaravarthi\_2005@yahoo.com, kan\_uma6@yahoo.com

Received 21 September 2013; accepted 25 October 2013

 Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.037;  $wR$  factor = 0.110; data-to-parameter ratio = 22.0.

 In the title compound,  $\text{CH}_5\text{N}_2\text{O}^+\cdot\text{C}_7\text{H}_5\text{O}_6\text{S}^-$ , the dihedral angle between the benzene ring and the mean plane of the uronium cation is  $76.02$  (8)°. The carboxyl group in the anion is twisted by  $1.47$  (9)° from the benzene ring. In the crystal, the cation is linked to the anion by weak  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds and  $\pi-\pi$  interactions [centroid-centroid distance =  $3.8859$  (8) Å], forming a three-dimensional network.

## Related literature

 For the biological activity of urea derivatives, see: Sliskovic *et al.* (1999); Furlong *et al.* (2000); Houghton *et al.* (1995). For related structures, see: Krishnakumar *et al.* (2012); Sudhahar *et al.* (2013); Worsham & Busing (1969); Nelyubina *et al.* (2007).


## Experimental

## Crystal data

 $\text{CH}_5\text{N}_2\text{O}^+\cdot\text{C}_7\text{H}_5\text{O}_6\text{S}^-$   
 $M_r = 278.24$   
 Triclinic,  $P1$   
 $a = 7.2248$  (4) Å

 $b = 8.7718$  (5) Å  
 $c = 10.1549$  (5) Å  
 $\alpha = 85.504$  (3)°  
 $\beta = 71.087$  (2)°

 $\gamma = 68.659$  (2)°  
 $V = 566.50$  (5) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation

 $\mu = 0.32$  mm<sup>-1</sup>  
 $T = 295$  K  
 $0.30 \times 0.24 \times 0.20$  mm

## Data collection

 Bruker APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2004)  
 $T_{\min} = 0.911$ ,  $T_{\max} = 0.939$ 

 14246 measured reflections  
 4079 independent reflections  
 3432 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.110$   
 $S = 1.05$   
 4079 reflections  
 185 parameters  
 7 restraints

 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.41$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.40$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O3}-\text{H3A}\cdots\text{O2}$	0.82 (1)	1.83 (1)	2.5966 (14)	154 (18)
$\text{O7}-\text{H7}\cdots\text{O6}$	0.82 (1)	1.85 (1)	2.6629 (14)	169 (18)
$\text{N1}-\text{H1A}\cdots\text{O4}$	0.84 (1)	1.96 (1)	2.7979 (16)	175 (16)
$\text{O1}-\text{H1}\cdots\text{O5}^{\text{i}}$	0.83 (1)	1.84 (1)	2.6511 (12)	167 (18)
$\text{N1}-\text{H1B}\cdots\text{O5}^{\text{ii}}$	0.85 (1)	1.95 (1)	2.7976 (16)	178 (15)
$\text{N2}-\text{H2B}\cdots\text{O6}^{\text{ii}}$	0.86 (1)	2.22 (1)	3.0712 (16)	172 (15)
$\text{N2}-\text{H2A}\cdots\text{O3}^{\text{iii}}$	0.85 (1)	2.19 (1)	3.0347 (16)	173 (15)

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; 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.

The authors thank the SAIF, IIT Madras, for the data collection. MKK thanks the Council of Scientific and Industrial Research, New Delhi, India, for providing financial support [project No. 03 (1200)/11/EMR-II].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2485).

## References

- Bruker (2004). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Furlong, E. T., Burkhardt, M. R., Gates, P. M., Werner, S. L. & Battaglin, W. A. (2000). *Sci. Total Environ.* **248**, 135–146.
- Houghton, P. J., Sosinski, J., Thakar, J. H., Border, G. B. & Grindey, G. B. (1995). *Biochem. Pharmacol.* **49**, 661–668.
- Krishnakumar, M., Sudhahar, S., Silambarasan, A., Chakkaravarthi, G. & Mohankumar, R. (2012). *Acta Cryst.* **E68**, o3268.
- Nelyubina, Y. V., Lyssenko, K. A., Golovanov, D. G. & Antipin, Yu. A. (2007). *CrystEngComm.* **9**, 991–996.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sliskovic, D. R., Krause, B. R. & Bocan, T. M. A. (1999). *Annu. Rep. Med. Chem.* **34**, 101–110.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Sudhahar, S., Krishnakumar, M., Sornamurthy, B. M., Chakkaravarthi, G. & Mohankumar, R. (2013). *Acta Cryst.* **E69**, o279.
- Worsham, J. E. & Busing, W. R. (1969). *Acta Cryst.* **B25**, 572–578.

## supplementary materials

*Acta Cryst.* (2013). E69, o1725 [doi:10.1107/S1600536813029474]

## Uronium 3-carboxy-4-hydroxybenzenesulfonate

A. Silambarasan, M. Krishna Kumar, G. Chakkaravarthi, R. Mohan Kumar and P. R. Umarani

### 1. Comment

Urea derivatives are known to exhibit anticholesterolemic, herbicidal and antitumor activities (Sliskovic *et al.*, 1999; Furlong *et al.*, 2000; Houghton *et al.*, 1995). Herein, we report the crystal structure of the title compound (I, Fig. 1). The asymmetric unit consists of one  $\text{CH}_5\text{N}_2\text{O}^+$  cation and one  $\text{C}_7\text{H}_5\text{O}_6\text{S}^-$  anion. In the title compound, the geometric parameters of the uronium cation (Worsham & Busing, 1969; Nelyubina *et al.*, 2007) and 3-carboxy-4-hydroxybenzenesulfonate anion (Krishnakumar *et al.*, 2012; Sudhahar *et al.*, 2013) are comparable with the reported structures.

The dihedral angle between the benzene ring and the mean plane of the uronium fragment is  $76.02(8)^\circ$ . In the anion, the carboxyl group makes the dihedral angle of  $1.47(9)^\circ$  with the benzene ring. In the molecular structure, cation and anion are linked by  $\text{O}—\text{H}\cdots\text{O}$  and  $\text{N}—\text{H}\cdots\text{O}$  hydrogen bonds, and the molecular conformation of the anion is controlled by weak  $\text{O}—\text{H}\cdots\text{O}$  hydrogen bond (Fig. 1). The crystal structure exhibits weak intermolecular  $\text{O}—\text{H}\cdots\text{O}$ ,  $\text{N}—\text{H}\cdots\text{O}$  (Table 1 and Fig. 2) and  $\pi\cdots\pi$  [ $\text{Cg1}\cdots\text{Cg1}^i$  distance:  $3.8859(8)$  Å; ( $i$ )  $x, 1-y, 1-z$ ; Cg1 is the centroid of the ring C1 $\cdots$ C6] interactions, to form a three dimensional network.

### 2. Experimental

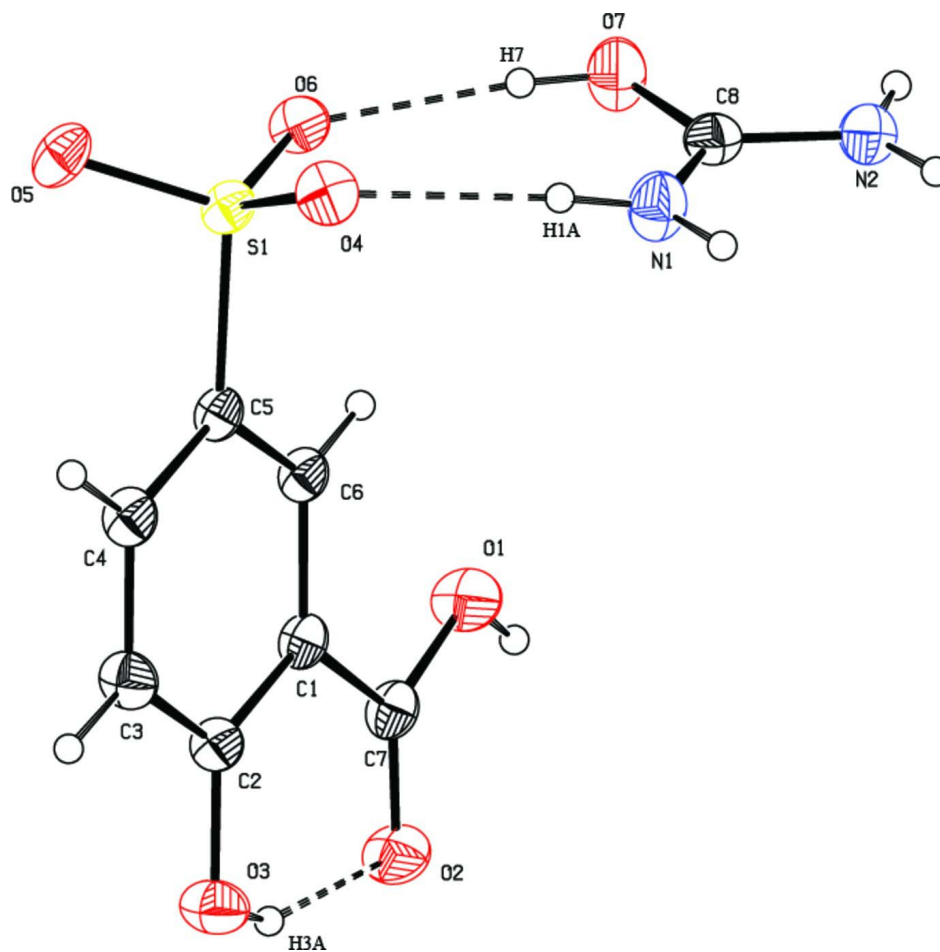
Urea ( $\text{CH}_4\text{N}_2\text{O}$ , 3.003 g) and 5-sulfosalicylic acid ( $\text{C}_7\text{H}_6\text{O}_6\text{S}$ , 12.711 g, 1:1 ratio) were mixed in water and the resulting solution was allowed for slow evaporation at room temperature. Good quality crystals, suitable for X-ray intensity data collection, were collected after 2 weeks.

### 3. Refinement

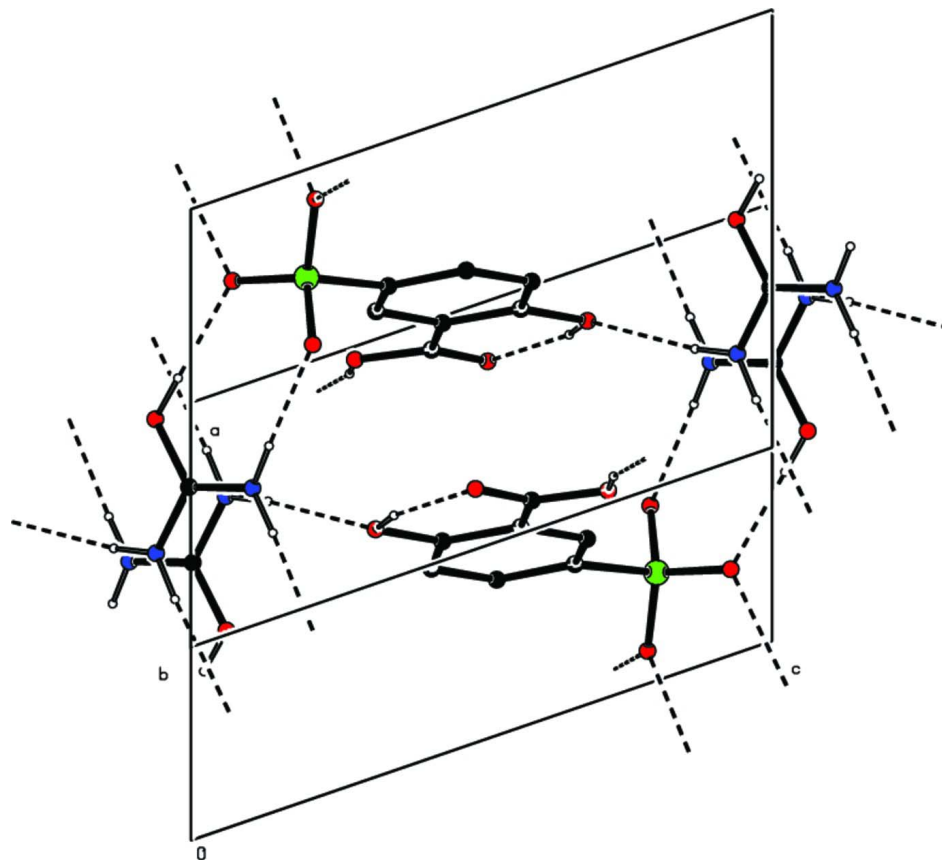
H atoms bonded to O and N heteroatoms were placed from difference maps and refined with free coordinates, although restrictions were applied on bond lengths:  $\text{N}—\text{H} = 0.86(1)$  Å and  $\text{O}—\text{H} = 0.82(1)$  Å. Isotropic displacement parameters for these H atoms were calculated as  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$  for  $\text{O}—\text{H}$  bonds and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$  for  $\text{N}—\text{H}$  bonds. H atoms for CH groups were positioned geometrically and refined using a riding model, with  $\text{C}—\text{H} = 0.93$  Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINTE* (Bruker, 2004); data reduction: *SAINTE* (Bruker, 2004); 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* (Sheldrick, 2008).

**Figure 1**

The molecular structure of (I), with 30% probability displacement ellipsoids for non-H atoms. Intramolecular hydrogen bonds are shown as dashed lines.



**Figure 2**

The packing of (I), viewed down *b* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

### Uronium 3-carboxy-4-hydroxybenzenesulfonate

#### Crystal data

$\text{CH}_5\text{N}_2\text{O}^+\cdot\text{C}_7\text{H}_5\text{O}_6\text{S}^-$

$M_r = 278.24$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.2248\ (4)\ \text{\AA}$

$b = 8.7718\ (5)\ \text{\AA}$

$c = 10.1549\ (5)\ \text{\AA}$

$\alpha = 85.504\ (3)^\circ$

$\beta = 71.087\ (2)^\circ$

$\gamma = 68.659\ (2)^\circ$

$V = 566.50\ (5)\ \text{\AA}^3$

$Z = 2$

$F(000) = 288$

$D_x = 1.631\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 7318 reflections

$\theta = 2.1\text{--}32.8^\circ$

$\mu = 0.32\ \text{mm}^{-1}$

$T = 295\ \text{K}$

Block, colourless

$0.30 \times 0.24 \times 0.20\ \text{mm}$

#### Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  and  $\varphi$  scan

Absorption correction: multi-scan

(*SADABS*; Bruker, 2004)

$T_{\min} = 0.911$ ,  $T_{\max} = 0.939$

14246 measured reflections

4079 independent reflections

3432 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$   
 $\theta_{\text{max}} = 33.6^\circ$ ,  $\theta_{\text{min}} = 2.1^\circ$   
 $h = -11 \rightarrow 11$

$k = -13 \rightarrow 13$   
 $l = -14 \rightarrow 15$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.110$   
 $S = 1.05$   
 4079 reflections  
 185 parameters  
 7 restraints  
 0 constraints  
 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.1089P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.41 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.40 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: *SHELXL97*,  
 $\text{Fc}^* = k\text{Fc}[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.105 (7)

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.22603 (17)	0.52320 (13)	0.56728 (12)	0.0301 (2)
C2	0.28443 (18)	0.45643 (14)	0.43261 (12)	0.0324 (2)
C3	0.3015 (2)	0.29542 (15)	0.41388 (13)	0.0376 (3)
H3	0.3363	0.2524	0.3246	0.045*
C4	0.26724 (19)	0.20039 (14)	0.52622 (13)	0.0347 (2)
H4	0.2801	0.0928	0.5132	0.042*
C5	0.21286 (17)	0.26557 (12)	0.66054 (12)	0.0288 (2)
C6	0.19033 (17)	0.42571 (13)	0.68131 (12)	0.0301 (2)
H6	0.1514	0.4687	0.7712	0.036*
C7	0.20231 (19)	0.69528 (14)	0.58615 (14)	0.0343 (2)
C8	0.5164 (2)	0.26399 (16)	1.00316 (13)	0.0378 (3)
N1	0.6134 (2)	0.16284 (17)	0.89415 (14)	0.0474 (3)
N2	0.6150 (2)	0.32507 (16)	1.05987 (13)	0.0431 (3)
O1	0.1437 (2)	0.74360 (11)	0.71788 (11)	0.0490 (3)
O2	0.23382 (18)	0.78366 (11)	0.48953 (11)	0.0473 (2)
O3	0.32586 (18)	0.54310 (12)	0.31773 (10)	0.0459 (2)
O4	0.39451 (15)	0.02256 (11)	0.79035 (11)	0.0417 (2)
O5	0.05090 (15)	0.05458 (11)	0.78561 (11)	0.0417 (2)
O6	0.08949 (15)	0.24191 (11)	0.92865 (9)	0.0380 (2)
O7	0.31385 (16)	0.31219 (15)	1.06119 (12)	0.0513 (3)
S1	0.18626 (4)	0.13680 (3)	0.80111 (3)	0.03090 (10)
H1A	0.551 (2)	0.1153 (18)	0.8654 (16)	0.037*
H1B	0.7463 (14)	0.1303 (19)	0.8589 (15)	0.037*
H2A	0.543 (2)	0.3875 (17)	1.1326 (12)	0.037*
H2B	0.7490 (14)	0.2929 (19)	1.0274 (16)	0.037*
H1	0.129 (3)	0.8404 (12)	0.7270 (18)	0.046*
H3A	0.303 (3)	0.6342 (14)	0.3493 (18)	0.046*
H7	0.253 (3)	0.278 (2)	1.0221 (17)	0.046*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0310 (5)	0.0228 (4)	0.0369 (6)	-0.0100 (4)	-0.0100 (4)	-0.0027 (4)
C2	0.0333 (5)	0.0287 (5)	0.0338 (6)	-0.0102 (4)	-0.0095 (4)	-0.0006 (4)
C3	0.0466 (6)	0.0317 (5)	0.0328 (6)	-0.0125 (5)	-0.0105 (5)	-0.0068 (4)
C4	0.0412 (6)	0.0245 (5)	0.0382 (6)	-0.0114 (4)	-0.0110 (5)	-0.0070 (4)
C5	0.0300 (4)	0.0222 (4)	0.0341 (5)	-0.0099 (4)	-0.0083 (4)	-0.0037 (4)
C6	0.0342 (5)	0.0237 (4)	0.0327 (5)	-0.0115 (4)	-0.0082 (4)	-0.0053 (4)
C7	0.0361 (5)	0.0244 (5)	0.0434 (6)	-0.0117 (4)	-0.0123 (5)	-0.0015 (4)
C8	0.0418 (6)	0.0372 (6)	0.0358 (6)	-0.0163 (5)	-0.0127 (5)	0.0067 (5)
N1	0.0385 (6)	0.0541 (7)	0.0480 (7)	-0.0165 (5)	-0.0089 (5)	-0.0101 (5)
N2	0.0458 (6)	0.0439 (6)	0.0433 (6)	-0.0191 (5)	-0.0152 (5)	0.0014 (5)
O1	0.0766 (7)	0.0265 (4)	0.0465 (5)	-0.0241 (5)	-0.0149 (5)	-0.0053 (4)
O2	0.0630 (6)	0.0306 (4)	0.0512 (6)	-0.0213 (4)	-0.0176 (5)	0.0064 (4)
O3	0.0634 (6)	0.0374 (5)	0.0356 (5)	-0.0196 (5)	-0.0130 (4)	0.0036 (4)
O4	0.0428 (5)	0.0284 (4)	0.0487 (5)	-0.0056 (4)	-0.0155 (4)	-0.0018 (4)
O5	0.0445 (5)	0.0310 (4)	0.0515 (5)	-0.0216 (4)	-0.0064 (4)	-0.0068 (4)
O6	0.0445 (5)	0.0331 (4)	0.0337 (4)	-0.0155 (4)	-0.0052 (3)	-0.0066 (3)
O7	0.0402 (5)	0.0632 (7)	0.0490 (6)	-0.0176 (5)	-0.0095 (4)	-0.0137 (5)
S1	0.03538 (15)	0.02207 (13)	0.03448 (16)	-0.01185 (10)	-0.00736 (11)	-0.00307 (9)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

C1—C6	1.3966 (16)	C8—O7	1.3029 (16)
C1—C2	1.4010 (16)	C8—N1	1.3047 (17)
C1—C7	1.4766 (15)	C8—N2	1.3104 (18)
C2—O3	1.3523 (15)	N1—H1A	0.841 (9)
C2—C3	1.3951 (17)	N1—H1B	0.852 (9)
C3—C4	1.3695 (18)	N2—H2A	0.850 (9)
C3—H3	0.9300	N2—H2B	0.858 (9)
C4—C5	1.3976 (15)	O1—H1	0.826 (9)
C4—H4	0.9300	O3—H3A	0.824 (9)
C5—C6	1.3791 (14)	O4—S1	1.4468 (10)
C5—S1	1.7544 (12)	O5—S1	1.4602 (9)
C6—H6	0.9300	O6—S1	1.4654 (9)
C7—O2	1.2165 (16)	O7—H7	0.821 (9)
C7—O1	1.3189 (16)		
C6—C1—C2	119.27 (10)	O1—C7—C1	113.41 (11)
C6—C1—C7	121.23 (10)	O7—C8—N1	121.64 (12)
C2—C1—C7	119.50 (11)	O7—C8—N2	115.88 (12)
O3—C2—C3	117.87 (11)	N1—C8—N2	122.48 (13)
O3—C2—C1	122.19 (10)	C8—N1—H1A	121.2 (11)
C3—C2—C1	119.95 (11)	C8—N1—H1B	120.5 (11)
C4—C3—C2	120.39 (11)	H1A—N1—H1B	117.5 (15)
C4—C3—H3	119.8	C8—N2—H2A	117.9 (11)
C2—C3—H3	119.8	C8—N2—H2B	118.8 (11)
C3—C4—C5	119.82 (10)	H2A—N2—H2B	123.0 (15)
C3—C4—H4	120.1	C7—O1—H1	112.4 (12)

C5—C4—H4	120.1	C2—O3—H3A	103.8 (13)
C6—C5—C4	120.59 (11)	C8—O7—H7	115.2 (13)
C6—C5—S1	120.71 (9)	O4—S1—O5	112.06 (6)
C4—C5—S1	118.63 (8)	O4—S1—O6	112.49 (6)
C5—C6—C1	119.95 (10)	O5—S1—O6	111.64 (5)
C5—C6—H6	120.0	O4—S1—C5	106.92 (6)
C1—C6—H6	120.0	O5—S1—C5	106.35 (6)
O2—C7—O1	123.37 (11)	O6—S1—C5	106.94 (5)
O2—C7—C1	123.22 (11)		
C6—C1—C2—O3	-178.47 (11)	C7—C1—C6—C5	179.73 (10)
C7—C1—C2—O3	1.84 (18)	C6—C1—C7—O2	179.30 (12)
C6—C1—C2—C3	1.51 (17)	C2—C1—C7—O2	-1.02 (18)
C7—C1—C2—C3	-178.18 (11)	C6—C1—C7—O1	-0.71 (16)
O3—C2—C3—C4	178.12 (12)	C2—C1—C7—O1	178.98 (11)
C1—C2—C3—C4	-1.86 (19)	C6—C5—S1—O4	-106.66 (10)
C2—C3—C4—C5	0.64 (19)	C4—C5—S1—O4	70.32 (10)
C3—C4—C5—C6	0.94 (18)	C6—C5—S1—O5	133.45 (9)
C3—C4—C5—S1	-176.05 (10)	C4—C5—S1—O5	-49.56 (10)
C4—C5—C6—C1	-1.28 (17)	C6—C5—S1—O6	14.04 (11)
S1—C5—C6—C1	175.65 (8)	C4—C5—S1—O6	-168.98 (9)
C2—C1—C6—C5	0.05 (17)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O3—H3A $\cdots$ O2	0.82 (1)	1.83 (1)	2.5966 (14)	154 (18)
O7—H7 $\cdots$ O6	0.82 (1)	1.85 (1)	2.6629 (14)	169 (18)
N1—H1A $\cdots$ O4	0.84 (1)	1.96 (1)	2.7979 (16)	175 (16)
O1—H1 $\cdots$ O5 <sup>i</sup>	0.83 (1)	1.84 (1)	2.6511 (12)	167 (18)
N1—H1B $\cdots$ O5 <sup>ii</sup>	0.85 (1)	1.95 (1)	2.7976 (16)	178 (15)
N2—H2B $\cdots$ O6 <sup>ii</sup>	0.86 (1)	2.22 (1)	3.0712 (16)	172 (15)
N2—H2A $\cdots$ O3 <sup>iii</sup>	0.85 (1)	2.19 (1)	3.0347 (16)	173 (15)

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