organic compounds

1-Hydroxyethyl-2-methyl-5-nitro-imidazolium 3-carboxy-4-hydroxy-benzenesulfonate

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Cocrystallization of 1-hydroxyethyl-2-methyl-5-nitroimidazole (metronidazole) and 5-sulfosalicylic acid (5-H_2SSA) from methanol solution yields the title salt, $C_6H_{10}N_3O_3^+ \cdot C_7H_5O_6S^-$. In the crystal structure, the ions are linked by a combination of intermolecular O—H···O, N—H···O and C—H···O hydrogen bonds, forming a three-dimensional framework. The hydroxyl group of the cation is disordered over two sites in a 0.860 (4):0.140 (4) ratio.

Related literature

For related literature, see: Athar *et al.* (2005); Bharti *et al.* (2002); Castelli *et al.* (2000); Cohen-Jonathan *et al.* (2001); Crozet *et al.* (2002); Galván-Tejada *et al.* (2002); Hodgkiss (1998); Kennedy *et al.* (2006); Meng *et al.* (2007); Skupin *et al.* (1997); Wu *et al.* (2003).

Experimental

Crystal data

$C_6H_{10}N_3O_3^+ \cdot C_7H_5O_6S^-$	V = 1602.9 (6) Å^3
M_r = 389.34	Z = 4
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
a = 8.8438 (3) Å	μ = 0.26 mm^{-1}
b = 13.0249 (4) Å	T = 294 (2) K
c = 14.148 (5) Å	$0.35 \times 0.26 \times 0.20$ mm
β = 100.413 (1)°	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	17399 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)	3503 independent reflections
T_{min} = 0.904, T_{max} = 0.950	3156 reflections with $I > 2\sigma(I)$
	R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.118	
S = 1.06	$\Delta\rho_{max}$ = 0.32 e Å^{-3}
3503 reflections	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
262 parameters	
4 restraints	

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2	0.83 (3)	1.86 (3)	2.618 (2)	151 (3)
N2—H2···O6	0.81 (2)	1.97 (2)	2.7557 (19)	163 (2)
C13—H13D···O7^i	0.97	2.46	3.280 (3)	142
C11—H11C···O4^{ii}	0.96	2.55	3.457 (3)	157
O9—H9A···O5^{iii}	0.82 (1)	2.129 (13)	2.940 (2)	170 (4)
O9′—H9′···O2^{iv}	0.82 (1)	2.258 (13)	2.830 (2)	127 (2)
O1—H1···O4^v	0.86 (3)	1.73 (3)	2.5801 (19)	171 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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, 2003); software used to prepare material for publication: *PLATON*.

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supporting information

1-Hydroxyethyl-2-methyl-5-nitroimidazolium 3-carboxy-4-hydroxybenzene-sulfonate

Bo Yang

S1. Comment

1-Hydroxyethyl-2-methyl-5-nitrimidazole (metronidazole) is often used in the treatment of anaerobic protozoan and bacterial infections (Castelli *et al.*, 2000; Cohen-Jonathan *et al.*, 2001; Hodgkiss *et al.*, 1998). However, the low solubility in water makes its absorption in human body much less than expected. Recently, many efforts have been devoted to developing some new substitutes for the medicine, *i.e.* i) metal-organic coordination compounds (Kennedy *et al.*, 2006; Galván-Tejada *et al.*, 2002; Athar *et al.*, 2005; Bharti *et al.*, 2002; Wu *et al.*, 2003), ii) organic substitute derivatives (Crozet *et al.*, 2002, Skupin *et al.*, 1997) and iii) pharmaceutical co-crystals. In this paper, we report the 1:1 molecular adduct formed by metronidazole 5-sulfosalicylic acid (5-H_2SSA), (I).

In (I), the H atom is transferred from the sulfonic acid group to the imidazole N atom (Fig.1) forming an 1:1 organic adduct, which is similar to the analogous organic adducts reported (Meng *et al.*, 2007). The hydroxyl O atom is disordered at two sites with occupancy being 0.86 (1)/0.14 (1) for the major and minor components, respectively.

In the crystal packing, the component ions are linked by a combination of O—H⋯O, N—H⋯O and C—H⋯O hydrogen bonds (Table 1), forming a three-dimensional network (Fig.2). There are no other interactions (*e.g.* C—H⋯π and π-π) observed in the crystal structure by using *PLATON* (Spek, 2003).

S2. Experimental

All the reagents and solvents were used as obtained without further purification. Equivalent molar amount of metronidazole and 5-sulfosalicylic acid dihydrate were dissolved in methanol (10 ml). The mixture was stirred for ten minutes at 300 K and then filtered. Block colorless crystals of (I) suitable for single-crystal X-ray diffraction analysis were grown by slow evaporation of the solution at the bottom of the vessel in two days.

S3. Refinement

H atoms bonded to C atoms were positioned geometrically [C–H = 0.93Å (aromatic), 0.97(methylene) and 0.96(methyl)] and refined in riding modes [$U_{iso}(H) = 1.2U_{eq}$(aromatic and methylene C) and $1.5U{\sim}eq{\sim}$(methyl C]. H atoms bonded to N and O atoms were found in Fourier difference maps with the constraints of N—H = 0.86 (2) Å,*O*—H = 0.82 (2) Å, and $U_{iso}(H) = 1.2U_{eq}(N)$ or $1.5U_{eq}(O)$]. The hydroxyl O atom is disordered at two sites with the occupancy being 0.86 (1):0.14 (1) for the major and minor components, respectively.
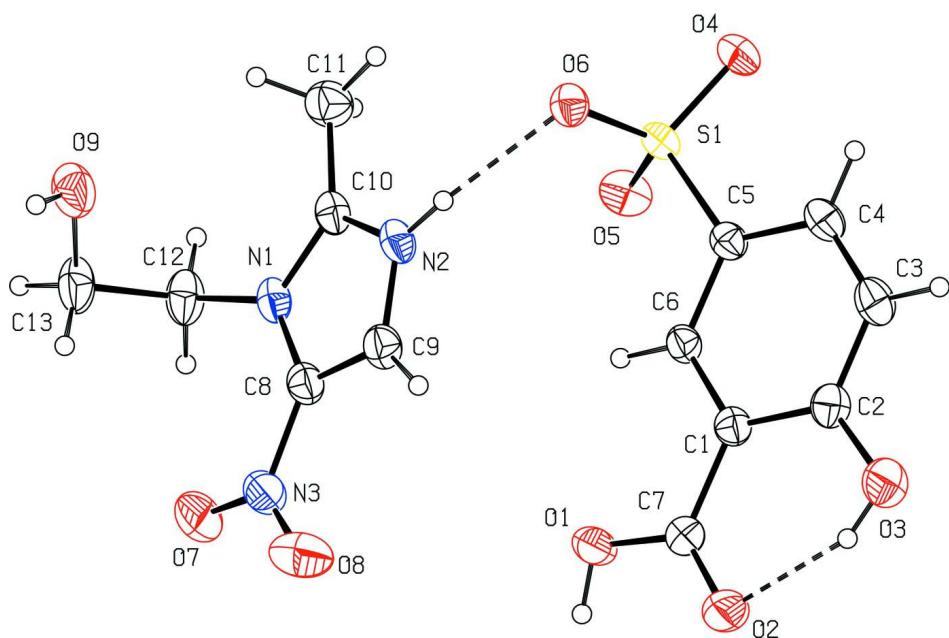
Figure 1

Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H-bonds are shown in dashed lines.
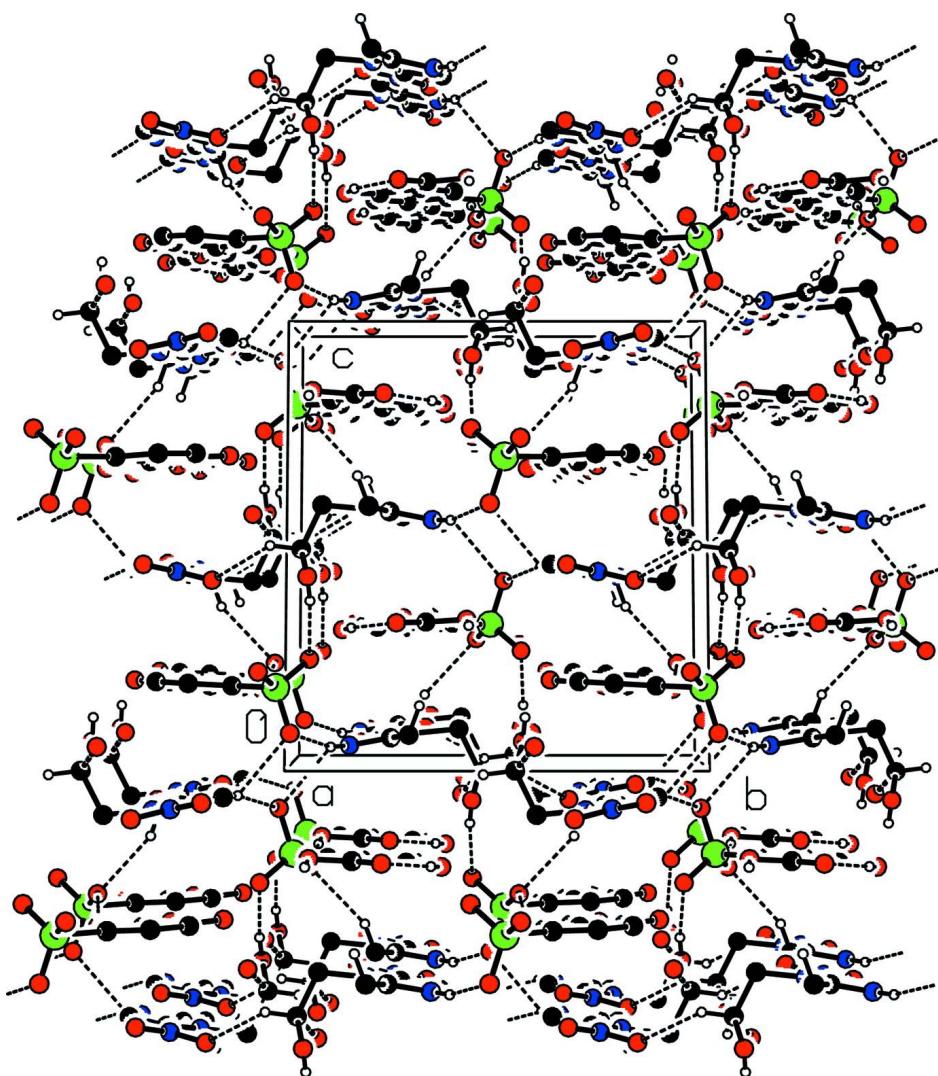
Figure 2

Part of the crystal structure of (I), showing the formation of the three-dimensional framework structure. Hydrogen bonds are shown as dashed lines. For the sake of clarity, H atoms not involved in the motif have been omitted from the drawing.

1-Hydroxyethyl-2-methyl-5-nitroimidazolium 3-carboxy-4-hydroxybenzenesulfonate

Crystal data
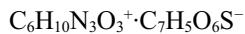
$C_6H_{10}N_3O_3^+ \cdot C_7H_5O_6S^-$	$F(000) = 808$
$M_r = 389.34$	$D_x = 1.613$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 9747 reflections
$a = 8.8438$ (3) Å	$\theta = 2.5$–$28.2°$
$b = 13.0249$ (4) Å	$\mu = 0.26$ mm^{-1}
$c = 14.148$ (5) Å	$T = 294$ K
$\beta = 100.413$ (1)°	Block, colorless
$V = 1602.9$ (6) Å^3	$0.35 \times 0.26 \times 0.20$ mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	17399 measured reflections
Radiation source: fine focus sealed Siemens Mo tube	3503 independent reflections
	3156 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.020$
0.3° wide ω exposures scans	$\theta_{max} = 27.0°$, $\theta_{min} = 2.1°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)	$h = -11 \rightarrow 11$
	$k = -16 \rightarrow 16$
$T_{min} = 0.905$, $T_{max} = 0.950$	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.118$	
$S = 1.07$	H atoms treated by a mixture of independent and constrained refinement
3503 reflections	
262 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0695P)^2 + 0.4716P]$ where $P = (F_o^2 + 2F_c^2)/3$
4 restraints	
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} < 0.001$
	$\Delta\rho_{max} = 0.32$ e Å^{-3}
	$\Delta\rho_{min} = -0.31$ e Å^{-3}

Special details

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}	Occ. (<1)
C1	0.26714 (18)	0.68882 (13)	0.68052 (11)	0.0389 (3)	
C2	0.3234 (2)	0.78986 (13)	0.68903 (12)	0.0441 (4)	
C3	0.4814 (2)	0.80629 (14)	0.69525 (14)	0.0520 (4)	
H3	0.5198	0.8729	0.7007	0.062*	
C4	0.5807 (2)	0.72533 (14)	0.69348 (13)	0.0462 (4)	
H4	0.6851	0.7376	0.6965	0.055*	
C5	0.52498 (18)	0.62468 (13)	0.68713 (11)	0.0380 (3)	
C6	0.36914 (18)	0.60747 (13)	0.68103 (11)	0.0380 (3)	
H6	0.3320	0.5405	0.6772	0.046*	
C7	0.1012 (2)	0.67003 (14)	0.67435 (13)	0.0433 (4)	
C8	0.1649 (2)	0.27776 (14)	0.56001 (12)	0.0443 (4)	
C9	0.2283 (2)	0.36913 (14)	0.54592 (13)	0.0474 (4)	
H9	0.1782	0.4318	0.5342	0.057*	
C10	0.41167 (19)	0.25196 (13)	0.56990 (11)	0.0405 (4)	
C11	0.5662 (2)	0.20700 (17)	0.58081 (16)	0.0591 (5)	

H11A	0.6376	0.2584	0.5680	0.089*	
H11B	0.5650	0.1512	0.5363	0.089*	
H11C	0.5969	0.1820	0.6452	0.089*	
C12	0.2655 (3)	0.09157 (14)	0.58498 (13)	0.0546 (5)	
H12A	0.1935	0.0764	0.6273	0.065*	
H12B	0.3647	0.0633	0.6137	0.065*	
C13	0.2110 (3)	0.04186 (16)	0.48829 (16)	0.0625 (6)	
H13A	0.2000	−0.0315	0.4965	0.075*	0.860 (4)
H13B	0.1113	0.0694	0.4597	0.075*	0.860 (4)
H13C	0.2960	0.0404	0.4535	0.075*	0.140 (4)
H13D	0.1834	−0.0288	0.4987	0.075*	0.140 (4)
N1	0.27916 (17)	0.20437 (10)	0.57531 (10)	0.0415 (3)	
N2	0.38028 (18)	0.35061 (12)	0.55237 (11)	0.0441 (3)	
H2	0.447 (3)	0.3933 (19)	0.5509 (15)	0.055 (6)*	
N3	0.0052 (2)	0.26065 (16)	0.56153 (12)	0.0582 (4)	
O1	0.06220 (15)	0.57238 (10)	0.66817 (11)	0.0551 (4)	
H1	−0.029 (3)	0.567 (2)	0.6806 (19)	0.083*	
O2	0.00803 (16)	0.73868 (11)	0.67490 (13)	0.0644 (4)	
O3	0.23266 (19)	0.87220 (10)	0.69337 (12)	0.0612 (4)	
H3A	0.144 (4)	0.849 (3)	0.688 (2)	0.092*	
O4	0.80111 (14)	0.55223 (12)	0.72322 (11)	0.0577 (4)	
O5	0.59335 (15)	0.44064 (11)	0.74685 (10)	0.0552 (4)	
O6	0.62653 (14)	0.48356 (9)	0.58626 (9)	0.0447 (3)	
O7	−0.0358 (2)	0.17473 (15)	0.58045 (15)	0.0874 (6)	
O8	−0.0796 (2)	0.33520 (18)	0.54514 (15)	0.0865 (6)	
O9	0.3138 (2)	0.06004 (17)	0.42931 (13)	0.0725 (7)	0.860 (4)
H9A	0.260 (4)	0.065 (3)	0.3759 (14)	0.109*	0.860 (4)
O9′	0.1003 (12)	0.0853 (9)	0.4339 (7)	0.066 (4)	0.140 (4)
H9′	0.13 (3)	0.135 (12)	0.408 (15)	0.099*	0.140 (4)
S1	0.64580 (4)	0.51687 (3)	0.68609 (3)	0.03782 (14)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0401 (8)	0.0393 (8)	0.0371 (8)	−0.0030 (7)	0.0064 (6)	−0.0011 (6)
C2	0.0514 (10)	0.0369 (8)	0.0437 (9)	−0.0007 (7)	0.0078 (7)	0.0033 (7)
C3	0.0565 (11)	0.0377 (9)	0.0610 (11)	−0.0127 (8)	0.0084 (9)	0.0039 (8)
C4	0.0425 (9)	0.0445 (9)	0.0514 (10)	−0.0126 (7)	0.0077 (7)	0.0038 (7)
C5	0.0367 (8)	0.0395 (8)	0.0381 (8)	−0.0048 (6)	0.0070 (6)	0.0012 (6)
C6	0.0380 (8)	0.0358 (8)	0.0404 (8)	−0.0065 (6)	0.0075 (6)	−0.0027 (6)
C7	0.0412 (8)	0.0417 (9)	0.0472 (9)	0.0003 (7)	0.0088 (7)	−0.0034 (7)
C8	0.0451 (9)	0.0486 (10)	0.0391 (8)	−0.0103 (7)	0.0073 (7)	−0.0059 (7)
C9	0.0491 (9)	0.0401 (9)	0.0517 (10)	−0.0048 (7)	0.0058 (8)	−0.0027 (7)
C10	0.0464 (9)	0.0394 (8)	0.0343 (8)	−0.0087 (7)	0.0036 (6)	−0.0016 (6)
C11	0.0510 (10)	0.0617 (12)	0.0620 (12)	0.0035 (9)	0.0035 (9)	0.0017 (10)
C12	0.0836 (14)	0.0359 (9)	0.0447 (9)	−0.0151 (9)	0.0128 (9)	0.0021 (7)
C13	0.0888 (16)	0.0447 (10)	0.0561 (12)	−0.0255 (11)	0.0188 (11)	−0.0107 (9)
N1	0.0520 (8)	0.0365 (7)	0.0351 (7)	−0.0120 (6)	0.0060 (6)	−0.0017 (5)

N2	0.0465 (8)	0.0371 (7)	0.0480 (8)	−0.0133 (6)	0.0066 (6)	−0.0014 (6)
N3	0.0501 (9)	0.0760 (12)	0.0500 (9)	−0.0176 (9)	0.0134 (7)	−0.0135 (8)
O1	0.0359 (6)	0.0428 (7)	0.0875 (10)	−0.0024 (5)	0.0135 (6)	−0.0028 (6)
O2	0.0482 (7)	0.0479 (8)	0.0985 (12)	0.0063 (6)	0.0172 (7)	−0.0104 (7)
O3	0.0614 (8)	0.0360 (7)	0.0852 (11)	0.0023 (6)	0.0104 (8)	0.0021 (7)
O4	0.0333 (6)	0.0637 (9)	0.0728 (9)	−0.0072 (6)	0.0014 (6)	−0.0126 (7)
O5	0.0534 (7)	0.0544 (8)	0.0578 (8)	0.0007 (6)	0.0105 (6)	0.0214 (6)
O6	0.0486 (7)	0.0396 (6)	0.0456 (7)	−0.0045 (5)	0.0079 (5)	−0.0006 (5)
O7	0.0759 (11)	0.0821 (12)	0.1140 (15)	−0.0409 (10)	0.0429 (10)	−0.0266 (11)
O8	0.0517 (9)	0.1110 (16)	0.0978 (13)	0.0069 (10)	0.0161 (9)	0.0071 (11)
O9	0.0805 (13)	0.0892 (14)	0.0503 (10)	−0.0317 (11)	0.0186 (9)	−0.0189 (9)
O9′	0.082 (8)	0.066 (7)	0.047 (6)	0.001 (6)	0.006 (5)	−0.013 (5)
S1	0.0307 (2)	0.0400 (2)	0.0417 (2)	−0.00536 (14)	0.00351 (15)	0.00333 (15)

Geometric parameters (Å, º)

C1—C6	1.391 (2)	C11—H11B	0.9600
C1—C2	1.405 (2)	C11—H11C	0.9600
C1—C7	1.475 (2)	C12—N1	1.482 (2)
C2—O3	1.348 (2)	C12—C13	1.512 (3)
C2—C3	1.400 (3)	C12—H12A	0.9700
C3—C4	1.376 (3)	C12—H12B	0.9700
C3—H3	0.9300	C13—O9′	1.265 (8)
C4—C5	1.398 (2)	C13—O9	1.361 (3)
C4—H4	0.9300	C13—H13A	0.9700
C5—C6	1.384 (2)	C13—H13B	0.9700
C5—S1	1.7662 (17)	C13—H13C	0.9700
C6—H6	0.9300	C13—H13D	0.9700
C7—O2	1.217 (2)	N2—H2	0.81 (2)
C7—O1	1.317 (2)	N3—O7	1.221 (3)
C8—C9	1.346 (2)	N3—O8	1.223 (3)
C8—N1	1.379 (2)	O1—H1	0.86 (3)
C8—N3	1.434 (2)	O3—H3A	0.83 (3)
C9—N2	1.352 (2)	O4—S1	1.4539 (12)
C9—H9	0.9300	O5—S1	1.4437 (13)
C10—N2	1.328 (2)	O6—S1	1.4579 (14)
C10—N1	1.340 (2)	O9—H13C	0.4764
C10—C11	1.469 (3)	O9—H9A	0.82 (1)
C11—H11A	0.9600	O9′—H9′	0.82 (1)
C6—C1—C2	119.60 (15)	C13—C12—H12B	109.4
C6—C1—C7	120.76 (15)	H12A—C12—H12B	108.0
C2—C1—C7	119.61 (15)	O9′—C13—O9	94.5 (6)
O3—C2—C3	118.11 (16)	O9′—C13—C12	116.4 (5)
O3—C2—C1	123.01 (16)	O9—C13—C12	109.93 (18)
C3—C2—C1	118.87 (16)	O9′—C13—H13A	115.5
C4—C3—C2	120.97 (16)	O9—C13—H13A	109.7
C4—C3—H3	119.5	C12—C13—H13A	109.7

C2—C3—H3	119.5	O9—C13—H13B	109.7
C3—C4—C5	120.09 (16)	C12—C13—H13B	109.7
C3—C4—H4	120.0	H13A—C13—H13B	108.2
C5—C4—H4	120.0	O9′—C13—H13C	106.6
C6—C5—C4	119.46 (16)	C12—C13—H13C	108.5
C6—C5—S1	117.90 (12)	H13A—C13—H13C	98.3
C4—C5—S1	122.63 (13)	H13B—C13—H13C	121.6
C5—C6—C1	120.98 (15)	O9′—C13—H13D	109.2
C5—C6—H6	119.5	O9—C13—H13D	118.2
C1—C6—H6	119.5	C12—C13—H13D	108.4
O2—C7—O1	122.75 (17)	H13B—C13—H13D	100.4
O2—C7—C1	123.05 (17)	H13C—C13—H13D	107.4
O1—C7—C1	114.20 (15)	C10—N1—C8	107.09 (14)
C9—C8—N1	108.85 (15)	C10—N1—C12	123.38 (16)
C9—C8—N3	125.28 (18)	C8—N1—C12	129.19 (16)
N1—C8—N3	125.85 (17)	C10—N2—C9	110.91 (15)
C8—C9—N2	105.54 (16)	C10—N2—H2	122.7 (16)
C8—C9—H9	127.2	C9—N2—H2	126.1 (16)
N2—C9—H9	127.2	O7—N3—O8	124.99 (19)
N2—C10—N1	107.62 (16)	O7—N3—C8	118.5 (2)
N2—C10—C11	124.35 (17)	O8—N3—C8	116.46 (19)
N1—C10—C11	128.03 (17)	C7—O1—H1	108 (2)
C10—C11—H11A	109.5	C2—O3—H3A	105 (2)
C10—C11—H11B	109.5	C13—O9—H9A	104 (3)
H11A—C11—H11B	109.5	H13C—O9—H9A	119.2
C10—C11—H11C	109.5	C13—O9′—H9′	109 (10)
H11A—C11—H11C	109.5	O5—S1—O4	112.76 (9)
H11B—C11—H11C	109.5	O5—S1—O6	112.23 (8)
N1—C12—C13	111.03 (16)	O4—S1—O6	112.44 (8)
N1—C12—H12A	109.4	O5—S1—C5	106.37 (8)
C13—C12—H12A	109.4	O4—S1—C5	106.18 (8)
N1—C12—H12B	109.4	O6—S1—C5	106.24 (7)
C6—C1—C2—O3	−176.99 (16)	C11—C10—N1—C8	−179.79 (17)
C7—C1—C2—O3	1.0 (3)	N2—C10—N1—C12	174.03 (15)
C6—C1—C2—C3	1.7 (2)	C11—C10—N1—C12	−6.0 (3)
C7—C1—C2—C3	179.71 (16)	C9—C8—N1—C10	−0.29 (19)
O3—C2—C3—C4	178.52 (17)	N3—C8—N1—C10	−178.63 (16)
C1—C2—C3—C4	−0.2 (3)	C9—C8—N1—C12	−173.61 (17)
C2—C3—C4—C5	−1.2 (3)	N3—C8—N1—C12	8.0 (3)
C3—C4—C5—C6	1.1 (3)	C13—C12—N1—C10	−96.5 (2)
C3—C4—C5—S1	−179.15 (14)	C13—C12—N1—C8	75.8 (2)
C4—C5—C6—C1	0.4 (2)	N1—C10—N2—C9	−0.10 (19)
S1—C5—C6—C1	−179.38 (12)	C11—C10—N2—C9	179.92 (17)
C2—C1—C6—C5	−1.8 (2)	C8—C9—N2—C10	−0.1 (2)
C7—C1—C6—C5	−179.78 (15)	C9—C8—N3—O7	−175.94 (19)
C6—C1—C7—O2	179.04 (18)	N1—C8—N3—O7	2.1 (3)
C2—C1—C7—O2	1.1 (3)	C9—C8—N3—O8	2.8 (3)

C6—C1—C7—O1	−1.0 (2)	N1—C8—N3—O8	−179.15 (17)
C2—C1—C7—O1	−178.93 (16)	C6—C5—S1—O5	−42.03 (15)
N1—C8—C9—N2	0.23 (19)	C4—C5—S1—O5	138.20 (15)
N3—C8—C9—N2	178.58 (16)	C6—C5—S1—O4	−162.37 (13)
N1—C12—C13—O9′	−44.9 (7)	C4—C5—S1—O4	17.86 (17)
N1—C12—C13—O9	61.0 (3)	C6—C5—S1—O6	77.73 (14)
N2—C10—N1—C8	0.23 (18)	C4—C5—S1—O6	−102.04 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O2	0.83 (3)	1.86 (3)	2.618 (2)	151 (3)
N2—H2···O6	0.81 (2)	1.97 (2)	2.7557 (19)	163 (2)
C13—H13*D*···O7[i]	0.97	2.46	3.280 (3)	142
C11—H11*C*···O4[ii]	0.96	2.55	3.457 (3)	157
O9—H9*A*···O5[iii]	0.82 (1)	2.13 (1)	2.940 (2)	170 (4)
O9′—H9′···O2[iv]	0.82 (1)	2.26 (1)	2.830 (2)	127 (2)
O1—H1···O4[v]	0.86 (3)	1.73 (3)	2.5801 (19)	171 (3)

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