organic compounds

2-Methylimidazolium 3-carboxy-4-hydroxybenzenesulfonate dihydrate

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The asymmetric unit of the title structure, $C_4H_7N_2^+\cdot C_7H_5O_6S^-\cdot 2H_2O$, consists of one 2-methylimidazolium cation, one sulfosalicylate anion and two water molecules. Hydrogen bonds and π–π stacking interactions [$Cg1\cdots Cg2 = 3.958$ (2) and 3.781 (2) Å, where $Cg1$ and $Cg2$ are the centroids of the benzene and imadazole rings, respectively] link molecules into a three-dimensional framework.

Related literature

For related literature, see: Bernstein *et al.* (1995); Fan *et al.* (2005); Muthiah *et al.* (2003); Smith (2005); Smith *et al.* (2004, 2005*a*, 2005*b*, 2006); Smith, Wermuth & Healy (2005); Wang & Wei (2007).
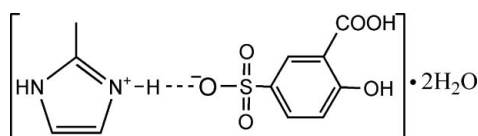
Experimental

Crystal data

$C_4H_7N_2^+\cdot C_7H_5O_6S^-\cdot 2H_2O$	$V = 1510.09$ (13) Å^3
$M_r = 336.32$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 6.9050$ (3) Å	$\mu = 0.26$ mm^{-1}
$b = 13.9594$ (7) Å	$T = 295$ (2) K
$c = 15.6665$ (8) Å	$0.40 \times 0.12 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	17325 measured reflections
	3511 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	3149 reflections with $I > 2\sigma(I)$
$T_{min} = 0.904$, $T_{max} = 0.965$	$R_{int} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$	$\Delta\rho_{max} = 0.30$ e Å^{-3}
$wR(F^2) = 0.133$	$\Delta\rho_{min} = -0.44$ e Å^{-3}
$S = 1.11$	Absolute structure: Flack (1983), with 1145 Friedel pairs
3511 reflections	Flack parameter: -0.02 (11)
224 parameters	
H atoms treated by a mixture of independent and constrained refinement	

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

$D—\text{H}\cdots A$	$D—\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D—\text{H}\cdots A$
O8—H8$A\cdots$O6	0.75 (5)	2.22 (6)	2.881 (4)	147 (6)
O7—H7$A\cdots$O4	0.79 (6)	1.99 (7)	2.781 (4)	180 (7)
O3—H3$A\cdots$O2	0.87 (4)	1.87 (5)	2.619 (3)	144 (4)
N1—H1$B\cdots$O4	0.79 (4)	2.02 (4)	2.806 (3)	171 (4)
C10—H10$\cdots$O1^i	0.93	2.38	3.286 (3)	166
C9—H9$\cdots$O6^i	0.93	2.37	3.290 (3)	172
O7—H7$B\cdots$O5^{ii}	0.77 (4)	1.99 (4)	2.758 (4)	174 (4)
O3—H3$A\cdots$O5^{iii}	0.87 (4)	2.45 (4)	2.970 (3)	119 (4)
N2—H2$A\cdots$O8^{iv}	0.83 (4)	1.94 (4)	2.745 (3)	162 (3)
O8—H8$B\cdots$O2^v	0.78 (6)	2.12 (6)	2.875 (4)	164 (6)
O1—H1$A\cdots$O7^v	0.83 (5)	1.72 (5)	2.539 (3)	167 (5)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2478).

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supplementary materials

2-Methylimidazolium 3-carboxy-4-hydroxybenzenesulfonate dihydrate

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Comment

3-carboxy-4-hydroxybenzenesulfonic acid (5-sulfosalicylic acid, 5-SSA) is a strong organic acid (pK_{a1}= 0.30) which can readily release its sulfonic proton when reacting with most Lewis bases (Smith *et al.*, 2004; Smith *et al.*, 2005*a*,*b*; Smith, Wermuth & Healy, 2005; Smith, 2005; Smith *et al.*, 2006; Muthiah *et al.*, 2003; Fan, *et al.*, 2005; Wang & Wei, 2007). Furthermore, with deprotonation of the sulfonate group, the three O atoms together with additional carboxylic acid and phenol functional groups can provide diverse hydrogen-bonding associations, enhancing the potential for self-assembly. As part of our research program to gain more insight into hydrogen bonding interactions involving 5-SSA, we report here the molecular and supramolecular structure of 2-methyl-imidazolium 3-carboxy-4-hydroxybenzenesulfonate dihydrate.

The asymmetric unit contains one 2-methyl-imidazolium cation, one sulfosalicylate anion and two water molecules (Fig. 1). As expected, the proton was released from the sulfonic group to the imidazole N atom. The hydroxyl O3 atom forms an intramolecular hydrogen bond to carboxyl O2 atom. Apart from this feature, no other unremarkable bond distances and bond angles are present.

In the supramolecular structure, by a combination of X–H⋯O (X= C, N and O) hydrogen bonds and π-π stacking interactions a three-dimensional framework is formed which can be readily analysed and described in terms of simple substructures generated by each of the individual intermolecular interactions.

Firstly, the water O7 atoms at (x, y, z) acts as hydrogen-bonding donor, *via*. H7A and H7B, to the sulfonate O4 at (x, y, z) and O5 at($-1 + x$, y, z), respectively, so producing by translation a one-dimensional $C^2_1(6)$ (Bernstein *et al.*, 1995) chain running parallel to the [100] direction (Fig.2). Similarly, the other two H-bonds involving water atom O8 gives rise to another chain running parallel to [100] direction, but this time generated by the 2_1 screw axis along (x, 3/4, 1/2) (Fig.3). The combination of the four hydrogen bonds and O1–H1A⋯O7 (Table 1) generates a one-dimensional ladder-like chain (Fig.4) running parallel to the [100] direction.

Secondly, the N1 and N2 atoms in 2-methyl-imidazolium at (x, y, z) act as hydrogen-bonding donors, to the sulfonate O4 at(x, y, z) and water O8 atoms at ($-1/2 + x$,3/2 $- y$, 2 $- z$), respectively, linking the adjacent ladder-like chains into a two-dimensional network running parallel to the (100) direction. These 2-D networks are joined by intermolecular O3–H3A⋯O5, C9–H9⋯O6, C10–H10⋯O1 hydrogen bonds and π-π stacking interactions between the symmetry-related phenyl and imidazole rings, so forming a complex three-dimensional framework (Fig. 5). In more detail, the centroids distances between aromatic rings at (x, y, z) and imidazole rings at (1/2 $- x$, 1 $- y$, $-1/2 + z$) and (3/2 $- x$, 1 $- y$, $-1/2 + z$) are 3.958 (2) and 3.781 (2) Å, respectively; the mean corresponding interplanar distances are 3.411 and 3.458 Å, respectively, which indicates the existence of the π-π interactions.

supplementary materials

Experimental

All the reagents and solvents were used as obtained without further purification. Equivalent molar amount of 2-methyl-imidazole (0.2 mmol, 16.2 mg) and 5-sulfosalicylic acid dihydrate (0.2 mmol, 50.8 g) were dissolved in 95% methanol (10 ml). The mixture was stirred for ten minutes at ambient temperature. The resulting clear solution was kept in air for several days. 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.

Refinement

All the H atoms bonded to carbon atoms were located at the geometrical positions [C–H =0.96 Å (methyl) or 0.93 Å (aromatic), and $U_{iso}(H) = 1.5U_{eq}$ (methyl) or $1.2U_{eq}$ (aromatic). H atoms attached to N and O atoms were located from the difference maps with the N–H and O–H distances refined freely and their U_{iso} values set 1.5 or 1.2 times of their carrier atoms. The title compound is almost certainly racemic in solution but has spontaneously racemized upon crystallization. The absolute configuration of the molecules in the crystal selected was readily determined; but this configuration has no chemical significance.
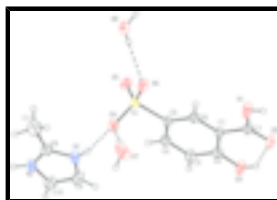
Figures

Fig. 1. Molecular structure showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonding are shown as dashed lines.
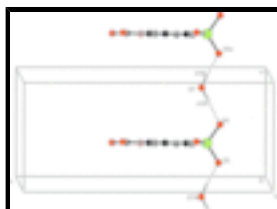

Fig. 2. Part of the crystal structure showing the formation of the one-dimensional chain by 5-SSA anions and water O7 solvent molecules. Hydrogen bonding are shown as dashed lines. For the sake of clarity, the cations and water O8 molecules and H atoms not involved in the motif have been omitted. Atoms marked with sign '#' and '$' are at the symmetry postion of $(-1 + x, y, z)$ and $(1 + x, y, z)$, respectively.

Fig. 3. Part of the crystal structure showing the formation of the other one-dimensional chain by 5-SSA anions and water O7 solvent molecules. Hydrogen bonding are shown as dashed lines. For the sake of clarity, the cations and water O7 molecules and H atoms not involved in the motif have been omitted. Atoms marked with sign '#' and '$' are at the symmetry postion of $(1/2 + x, 3/2 - y, 1 - z)$ and $(-1/2 + x, 3/2 - y, 1 - z)$, respectively.
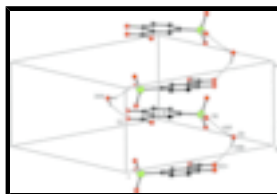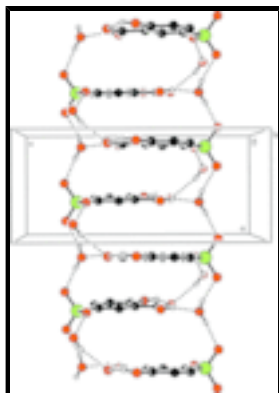
Fig. 4. Part of the crystal structure showing the formation of the one-dimensional network. Hydrogen bonding are shown as dashed lines. For the sake of clarity, the cations and H atoms not involved in the motif have been omitted.
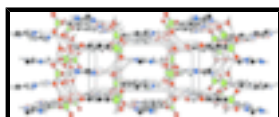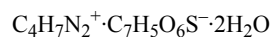

Fig. 5. Part of the crystal structure showing the formation of the three-dimensional network. Hydrogen bonding are shown as dashed lines. For the sake of clarity, H atoms not involved in the motif have been omitted.

2-Methylimidazolium 3-carboxy-4-hydroxybenzenesulfonate dihydrate

Crystal data

$C_4H_7N_2^+ \cdot C_7H_5O_6S^- \cdot 2H_2O$	$F_{000} = 704$
$M_r = 336.32$	$D_x = 1.479$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 5849 reflections
$a = 6.9050\ (3)$ Å	$\theta = 2.9$–26.9º
$b = 13.9594\ (7)$ Å	$\mu = 0.26$ mm^{-1}
$c = 15.6665\ (8)$ Å	$T = 295\ (2)$ K
$V = 1510.09\ (13)$ Å^3	Block, colorless
$Z = 4$	$0.40 \times 0.12 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3511 independent reflections
Radiation source: fine focus sealed Siemens Mo tube	3149 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.034$
$T = 295(2)$ K	$\theta_{max} = 28.0$º
0.3° wide ω exposures scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{min} = 0.904$, $T_{max} = 0.965$	$k = -18 \rightarrow 18$
17325 measured reflections	$l = -19 \rightarrow 20$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0695P)^2 + 0.4997P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.133$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.11$	$\Delta\rho_{max} = 0.30$ e Å^{-3}
3511 reflections	$\Delta\rho_{min} = -0.43$ e Å^{-3}
224 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1145 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.02 (11)

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 $F^2 > 2\text{sigma}(F^2)$ 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	$U_{iso}*/U_{eq}$
C1	0.6301 (4)	0.56571 (18)	0.51991 (15)	0.0326 (5)
C2	0.6179 (4)	0.46797 (18)	0.53943 (17)	0.0377 (6)
C3	0.6186 (5)	0.43870 (19)	0.62482 (17)	0.0433 (7)
H3	0.6116	0.3739	0.6381	0.052*
C4	0.6297 (5)	0.50491 (19)	0.68880 (16)	0.0407 (6)
H4	0.6311	0.4848	0.7454	0.049*
C5	0.6390 (4)	0.60271 (17)	0.66999 (14)	0.0330 (5)
C6	0.6403 (5)	0.63214 (18)	0.58583 (15)	0.0355 (5)
H6	0.6481	0.6971	0.5731	0.043*
C7	0.6311 (5)	0.59695 (17)	0.42940 (15)	0.0368 (6)
C8	0.3965 (4)	0.5708 (2)	1.01344 (19)	0.0417 (7)
C9	0.3869 (5)	0.4361 (2)	0.9403 (2)	0.0485 (7)
H9	0.3896	0.3930	0.8951	0.058*
C10	0.3641 (5)	0.4153 (2)	1.0228 (2)	0.0483 (7)
H10	0.3458	0.3546	1.0459	0.058*
C11	0.4109 (7)	0.6736 (2)	1.0360 (3)	0.0728 (11)
H11A	0.3304	0.6866	1.0846	0.109*
H11B	0.3686	0.7118	0.9885	0.109*
H11C	0.5429	0.6890	1.0494	0.109*
N1	0.4055 (4)	0.53398 (18)	0.93551 (15)	0.0449 (6)
H1B	0.424 (6)	0.567 (3)	0.895 (2)	0.054*

N2	0.3727 (4)	0.49894 (17)	1.06694 (15)	0.0413 (5)
H2A	0.348 (5)	0.501 (2)	1.119 (2)	0.050*
O1	0.6397 (5)	0.68944 (14)	0.41822 (12)	0.0607 (7)
H1A	0.627 (7)	0.705 (3)	0.367 (3)	0.091*
O2	0.6238 (4)	0.54015 (13)	0.37059 (11)	0.0491 (5)
O3	0.6085 (4)	0.39857 (14)	0.48008 (13)	0.0527 (6)
H3A	0.593 (7)	0.426 (3)	0.431 (3)	0.079*
O4	0.4787 (3)	0.66868 (15)	0.80653 (12)	0.0488 (6)
O5	0.8265 (3)	0.66487 (17)	0.80139 (13)	0.0524 (6)
O6	0.6494 (4)	0.78034 (14)	0.71641 (12)	0.0522 (6)
O7	0.1513 (5)	0.7529 (3)	0.73539 (18)	0.0801 (10)
H7A	0.245 (9)	0.729 (4)	0.755 (4)	0.120*
O8	0.8383 (5)	0.9568 (2)	0.76303 (15)	0.0656 (7)
H8B	0.930 (8)	0.961 (4)	0.734 (4)	0.098*
H8A	0.832 (9)	0.904 (4)	0.756 (4)	0.098*
S1	0.65096 (11)	0.68606 (4)	0.75465 (4)	0.03738 (18)
H7B	0.056 (6)	0.730 (3)	0.751 (3)	0.056*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0433 (14)	0.0313 (12)	0.0232 (11)	0.0000 (12)	0.0005 (11)	0.0025 (9)
C2	0.0498 (16)	0.0298 (12)	0.0336 (13)	0.0021 (12)	0.0011 (12)	−0.0002 (10)
C3	0.0661 (19)	0.0279 (12)	0.0359 (13)	0.0000 (13)	0.0026 (14)	0.0061 (10)
C4	0.0574 (17)	0.0363 (13)	0.0283 (12)	0.0003 (14)	−0.0005 (13)	0.0088 (10)
C5	0.0447 (14)	0.0320 (12)	0.0223 (10)	0.0003 (12)	−0.0010 (11)	−0.0001 (9)
C6	0.0489 (15)	0.0297 (11)	0.0279 (11)	−0.0010 (12)	0.0015 (12)	0.0033 (9)
C7	0.0533 (16)	0.0290 (12)	0.0280 (12)	0.0014 (12)	−0.0005 (13)	−0.0001 (9)
C8	0.0487 (17)	0.0346 (14)	0.0419 (15)	0.0035 (12)	0.0056 (13)	−0.0021 (11)
C9	0.0600 (19)	0.0390 (14)	0.0464 (16)	0.0040 (14)	−0.0048 (16)	−0.0125 (12)
C10	0.0606 (19)	0.0306 (13)	0.0536 (17)	−0.0030 (14)	−0.0047 (16)	0.0026 (11)
C11	0.100 (3)	0.0357 (17)	0.083 (3)	0.0018 (19)	0.016 (2)	−0.0102 (17)
N1	0.0622 (16)	0.0417 (13)	0.0307 (12)	0.0059 (12)	0.0029 (11)	0.0056 (10)
N2	0.0526 (14)	0.0420 (12)	0.0295 (11)	0.0021 (12)	−0.0021 (11)	−0.0001 (9)
O1	0.123 (2)	0.0329 (10)	0.0264 (9)	0.0013 (14)	0.0010 (13)	0.0041 (8)
O2	0.0850 (16)	0.0363 (10)	0.0260 (9)	0.0076 (11)	−0.0047 (11)	−0.0040 (7)
O3	0.0954 (18)	0.0300 (10)	0.0328 (10)	−0.0021 (11)	−0.0009 (12)	−0.0034 (8)
O4	0.0681 (14)	0.0471 (13)	0.0311 (10)	0.0020 (10)	0.0097 (10)	0.0041 (9)
O5	0.0618 (14)	0.0579 (14)	0.0375 (11)	−0.0119 (11)	−0.0131 (10)	0.0042 (9)
O6	0.0949 (17)	0.0314 (10)	0.0302 (9)	−0.0062 (11)	−0.0018 (12)	0.0028 (7)
O7	0.0634 (16)	0.115 (2)	0.0615 (17)	−0.0039 (18)	−0.0015 (16)	0.0513 (16)
O8	0.0788 (17)	0.0787 (17)	0.0394 (12)	−0.0074 (16)	0.0121 (13)	−0.0131 (12)
S1	0.0579 (4)	0.0336 (3)	0.0206 (3)	−0.0040 (3)	−0.0010 (3)	0.0020 (2)

Geometric parameters (Å, °)

C1—C6	1.390 (3)	C9—N1	1.374 (4)
C1—C2	1.401 (4)	C9—H9	0.9300
C1—C7	1.484 (3)	C10—N2	1.358 (4)

C2—O3	1.344 (3)	C10—H10	0.9300
C2—C3	1.399 (4)	C11—H11A	0.9600
C3—C4	1.366 (4)	C11—H11B	0.9600
C3—H3	0.9300	C11—H11C	0.9600
C4—C5	1.398 (3)	N1—H1B	0.79 (4)
C4—H4	0.9300	N2—H2A	0.83 (4)
C5—C6	1.381 (3)	O1—H1A	0.83 (5)
C5—S1	1.766 (2)	O3—H3A	0.87 (4)
C6—H6	0.9300	O4—S1	1.461 (2)
C7—O2	1.216 (3)	O5—S1	1.447 (2)
C7—O1	1.304 (3)	O6—S1	1.446 (2)
C8—N2	1.317 (4)	O7—H7A	0.79 (6)
C8—N1	1.326 (4)	O7—H7B	0.77 (4)
C8—C11	1.481 (4)	O8—H8B	0.78 (6)
C9—C10	1.334 (5)	O8—H8A	0.75 (5)
C6—C1—C2	119.4 (2)	C9—C10—N2	107.5 (3)
C6—C1—C7	120.9 (2)	C9—C10—H10	126.3
C2—C1—C7	119.7 (2)	N2—C10—H10	126.3
O3—C2—C3	116.8 (2)	C8—C11—H11A	109.5
O3—C2—C1	123.6 (2)	C8—C11—H11B	109.5
C3—C2—C1	119.5 (2)	H11A—C11—H11B	109.5
C4—C3—C2	120.3 (2)	C8—C11—H11C	109.5
C4—C3—H3	119.9	H11A—C11—H11C	109.5
C2—C3—H3	119.9	H11B—C11—H11C	109.5
C3—C4—C5	120.6 (2)	C8—N1—C9	109.3 (3)
C3—C4—H4	119.7	C8—N1—H1B	121 (3)
C5—C4—H4	119.7	C9—N1—H1B	130 (3)
C6—C5—C4	119.5 (2)	C8—N2—C10	109.6 (2)
C6—C5—S1	121.37 (19)	C8—N2—H2A	128 (2)
C4—C5—S1	119.15 (18)	C10—N2—H2A	122 (2)
C5—C6—C1	120.7 (2)	C7—O1—H1A	112 (3)
C5—C6—H6	119.6	C2—O3—H3A	108 (3)
C1—C6—H6	119.6	S1—O4—H1B	130.6 (11)
O2—C7—O1	123.0 (2)	H7A—O7—H7B	113 (5)
O2—C7—C1	122.1 (2)	H8B—O8—H8A	92 (5)
O1—C7—C1	114.8 (2)	O6—S1—O5	113.71 (15)
N2—C8—N1	107.3 (2)	O6—S1—O4	112.05 (14)
N2—C8—C11	126.4 (3)	O5—S1—O4	111.51 (12)
N1—C8—C11	126.3 (3)	O6—S1—C5	106.75 (11)
C10—C9—N1	106.3 (3)	O5—S1—C5	106.53 (14)
C10—C9—H9	126.8	O4—S1—C5	105.68 (13)
N1—C9—H9	126.8		
C6—C1—C2—O3	−179.6 (3)	N1—C9—C10—N2	−1.1 (4)
C7—C1—C2—O3	0.6 (5)	N2—C8—N1—C9	0.0 (4)
C6—C1—C2—C3	−0.8 (5)	C11—C8—N1—C9	179.9 (3)
C7—C1—C2—C3	179.5 (3)	C10—C9—N1—C8	0.8 (4)
O3—C2—C3—C4	179.4 (3)	N1—C8—N2—C10	−0.7 (4)
C1—C2—C3—C4	0.5 (5)	C11—C8—N2—C10	179.4 (4)

C2—C3—C4—C5	0.5 (5)	C9—C10—N2—C8	1.2 (4)
C3—C4—C5—C6	−1.1 (5)	H1B—O4—S1—O6	−164.3 (14)
C3—C4—C5—S1	179.4 (3)	H1B—O4—S1—O5	−35.6 (14)
C4—C5—C6—C1	0.8 (5)	H1B—O4—S1—C5	79.8 (14)
S1—C5—C6—C1	−179.8 (2)	C6—C5—S1—O6	3.4 (3)
C2—C1—C6—C5	0.1 (5)	C4—C5—S1—O6	−177.2 (3)
C7—C1—C6—C5	179.9 (3)	C6—C5—S1—O5	−118.5 (3)
C6—C1—C7—O2	179.4 (3)	C4—C5—S1—O5	60.9 (3)
C2—C1—C7—O2	−0.8 (5)	C6—C5—S1—O4	122.8 (3)
C6—C1—C7—O1	−0.8 (4)	C4—C5—S1—O4	−57.8 (3)
C2—C1—C7—O1	178.9 (3)		

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O8—H8A⋯O6	0.75 (5)	2.22 (6)	2.881 (4)	147 (6)
O7—H7A⋯O4	0.79 (6)	1.99 (7)	2.781 (4)	180 (7)
O3—H3A⋯O2	0.87 (4)	1.87 (5)	2.619 (3)	144 (4)
N1—H1B⋯O4	0.79 (4)	2.02 (4)	2.806 (3)	171 (4)
C10—H10⋯O1[i]	0.93	2.38	3.286 (3)	166
C9—H9⋯O6[i]	0.93	2.37	3.290 (3)	172
O7—H7B⋯O5[ii]	0.77 (4)	1.99 (4)	2.758 (4)	174 (4)
O3—H3A⋯O5[iii]	0.87 (4)	2.45 (4)	2.970 (3)	119 (4)
N2—H2A⋯O8[iv]	0.83 (4)	1.94 (4)	2.745 (3)	162 (3)
O8—H8B⋯O2[v]	0.78 (6)	2.12 (6)	2.875 (4)	164 (6)
O1—H1A⋯O7[v]	0.83 (5)	1.72 (5)	2.539 (3)	167 (5)

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

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5