

Imidazolium 3-carboxy-4-hydroxy-benzenesulfonate

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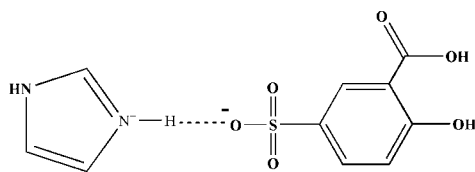
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 Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.056; wR factor = 0.169; data-to-parameter ratio = 13.9.

The asymmetric unit of the title structure, $\text{C}_3\text{H}_5\text{N}_2^+\cdot\text{C}_7\text{H}_5\text{O}_6\text{S}^-$, consists of an imidazolium cation and a sulfosalicylate anion connected *via* an $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond. In the crystal structure, intermolecular hydrogen bonds and $\pi-\pi$ stacking interactions [with centroid-centroid distances of 3.655 (2)–4.075 (2) Å] link the molecules into a three-dimensional framework.

Related literature

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



Experimental

Crystal data

 $\text{C}_3\text{H}_5\text{N}_2^+\cdot\text{C}_7\text{H}_5\text{O}_6\text{S}^-$
 $M_r = 286.26$

 Monoclinic, $P2_1/n$
 $a = 6.9486$ (5) Å

 $b = 14.5898$ (11) Å

 $c = 12.0504$ (9) Å

 $\beta = 104.220$ (1)°

 $V = 1184.22$ (15) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 0.30$ mm⁻¹
 $T = 294$ (2) K

 $0.10 \times 0.10 \times 0.08$ mm

Data collection

 Bruker SMART APEX CCD
area-detector diffractometer

 Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

 $T_{\min} = 0.969$, $T_{\max} = 0.971$

 12957 measured reflections
2575 independent reflections

 1805 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.169$
 $S = 1.07$

2575 reflections

185 parameters

 H atoms treated by a mixture of
independent and constrained
refinement

 $\Delta\rho_{\text{max}} = 0.65$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.41$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H3A}\cdots\text{O1}$	0.86 (4)	1.85 (4)	2.665 (3)	158 (3)
$\text{N1}-\text{H1A}\cdots\text{O4}$	0.87 (4)	1.89 (4)	2.720 (3)	159 (3)
$\text{C8}-\text{H8}\cdots\text{O3}^{\text{i}}$	0.93	2.39	3.206 (4)	147
$\text{C8}-\text{H8}\cdots\text{O5}^{\text{ii}}$	0.93	2.59	3.167 (4)	121
$\text{C4}-\text{H4}\cdots\text{O4}$	0.93	2.57	2.930 (3)	104
$\text{C6}-\text{H6}\cdots\text{O2}$	0.93	2.37	2.696 (3)	100
$\text{C10}-\text{H10}\cdots\text{O2}^{\text{iii}}$	0.93	2.49	3.293 (4)	144
$\text{C9}-\text{H9}\cdots\text{O6}^{\text{iii}}$	0.93	2.50	3.419 (4)	168
$\text{C4}-\text{H4}\cdots\text{O6}^{\text{iii}}$	0.93	2.58	3.310 (3)	136
$\text{O2}-\text{H2B}\cdots\text{O5}^{\text{iv}}$	0.87 (4)	1.67 (4)	2.536 (3)	174 (4)
$\text{N2}-\text{H2A}\cdots\text{O1}^{\text{v}}$	0.89 (4)	1.97 (4)	2.832 (3)	162 (3)

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2493).

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supplementary materials

Acta Cryst. (2007). E63, o4038 [doi:10.1107/S1600536807043826]

Imidazolium 3-carboxy-4-hydroxybenzenesulfonate

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Comment

5-sulfosalicylic acid (5-SSA) is a strong organic acid which can readily release its sulfonic proton when reacting with many Lewis bases. The crystals structures of a series of 5-SSA organic salts have been reported (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). More recently, two organic salts formed by 5-SSA and benzimidazole and 4-Methylimidazole have been reported (Wang & Wei, 2007; Hou, 2007). To further the research of analogous 5-SSA-containing organic adducts, we report here the crystal structure of imidazolium 3-carboxy-4-hydroxybenzenesulfonate (abbr. 5-SSA·Im).

The asymmetric unit consists of one imidazolium cation, one sulfosalicylate anion (Fig. 1). The sulfonic hydrogen atom has been transferred to the imine N atom. Unlike the reported analogs (Hou, 2007; Wang & Wei, 2007), in the title structure there are no solvent molecules in the crystal lattice. In the supramolecular structure, by a combination of N–H···O, O–H···O and C–H···O hydrogen bonds and π - π stacking interactions the ions are linked into a three-dimensional framework which can be easily discussed in terms of two types of simple substructures.

Firstly, by means of the series of H-bond interactions listed in table 1, 5-SSA anions and imidazole (abbr. Im) cations are interlinked into a two-dimensional network running parallel to the (101) direction (Fig.2). In addition to H-bonds interactions, the (101) network is consolidated by two intra-network π - π stacking interactions [$Cg1\cdots Cg1^{vii} = 4.075$ (2) Å and $Cg2\cdots Cg2^{ix} = 3.655$ (2) Å, symmetry code: (vii) $1 - x, 1 - y, 1 - z$; (ix) $1 - x, 2 - y, 1 - z$ where $Cg1$ and $Cg2$ are the centroids of the benzene and imidazole rings.]

Secondly, by the other two symmetry-related π - π stacking interactions between the adjacent network [$Cg1\cdots Cg1^{vi} = 3.874$ (2) Å and $Cg2\cdots Cg2^{viii} = 3.774$ (2) Å, symmetry code: (vi) $-x, 1 - y, 1 - z$; (viii) $-x, 2 - y, 1 - z$, where $Cg1$ and $Cg2$ are the centroids of the benzene and imidazole rings] the adjacent two-dimensional networks are interlinked into a three-dimensional network (Fig.3). It is noteworthy that in the supramolecular structure of the title compound the 5-SSA anions and Im cations are stacked homogeneously, *i.e.* 5-SSA anions stack only on top of 5-SSA anions, and Im anions stack only on top of Im anion. However, the stacks in the 4-Methyl dihydrate and benzimidazole trihydrate analogs reported by (Hou, 2007; Wang & Wei, 2007) are heterogeneous and homogeneous, respectively. Why and how the cations and water solvent molecules affect the stacking patterns is worthy of further study.

Experimental

Crystals of the title compound were unexpectedly obtained by mixing equimolar amount of 5-sulfosalicylic acid dihydrate (0.1 mmol, 25.4 mg), imidazole (0.1 mmol, 6.8 mg) and silver nitrate (0.1 mmol, 17.0 mg) in 10 ml water solvent sealed in a 25 ml Teflon-lined autoclave. The mixture was heated to 423 K and maintained for 140 h. After slowly cooling to room temperature with the rate of 10°/h, colorless crystals suitable for single-crystal X-ray diffraction analysis were obtained. The crystals were filtered and washed with distilled water and dried in air (Yield: 40%, 13.0 mg, based on the 1:1 organic salt.)

Refinement

H atoms bonded to carbon atoms were located at the geometrical positions with $C-H=0.93 \text{ \AA}$, and $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$. 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, respectively.

Figures

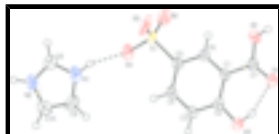


Fig. 1. Molecular structure, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

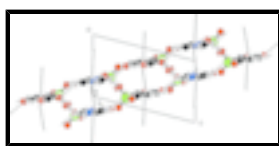


Fig. 2. Part of the crystal structure, showing the formation of the two-dimensional (101) network formed by 5-SSA anions and Im anions. Hydrogen bonds and $\pi-\pi$ stacking interactions are shown as dashed lines.

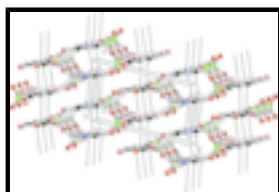
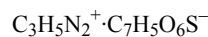


Fig. 3. Part of the crystal structure, showing the formation of the three-dimensional network formed by 5-SSA anions and Im anions. Hydrogen bonds and $\pi-\pi$ stacking interactions are shown as dashed lines.

Imidazolium 3-carboxy-4-hydroxybenzenesulfonate

Crystal data



$M_r = 286.26$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 6.9486 (5) \text{ \AA}$

$b = 14.5898 (11) \text{ \AA}$

$c = 12.0504 (9) \text{ \AA}$

$\beta = 104.220 (1)^\circ$

$V = 1184.22 (15) \text{ \AA}^3$

$Z = 4$

$F_{000} = 592$

$D_x = 1.606 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2471 reflections

$\theta = 2.2-24.7^\circ$

$\mu = 0.30 \text{ mm}^{-1}$

$T = 294 (2) \text{ K}$

Block, colorless

$0.10 \times 0.10 \times 0.08 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer

2575 independent reflections

Radiation source: fine focus sealed Siemens Mo tube

1805 reflections with $I > 2\sigma(I)$

Monochromator: graphite

$R_{\text{int}} = 0.049$

$T = 294(2) \text{ K}$

$\theta_{\text{max}} = 27.0^\circ$

0.3° wide ω exposures scans $\theta_{\min} = 2.2^\circ$
 Absorption correction: multi-scan $h = -8 \rightarrow 8$
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.969$, $T_{\max} = 0.971$ $k = -18 \rightarrow 18$
 12957 measured reflections $l = -15 \rightarrow 15$

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier map
 Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites
 $R[F^2 > 2\sigma(F^2)] = 0.057$ H atoms treated by a mixture of independent and constrained refinement
 $wR(F^2) = 0.169$ $w = 1/[\sigma^2(F_o^2) + (0.1041P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.07$ $(\Delta/\sigma)_{\max} < 0.001$
 2575 reflections $\Delta\rho_{\max} = 0.65 \text{ e } \text{Å}^{-3}$
 185 parameters $\Delta\rho_{\min} = -0.40 \text{ e } \text{Å}^{-3}$
 Primary atom site location: structure-invariant direct methods Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2333 (3)	0.47417 (16)	0.47446 (19)	0.0266 (5)
C2	0.3081 (4)	0.49675 (17)	0.58992 (19)	0.0305 (6)
C3	0.3199 (4)	0.58790 (17)	0.6234 (2)	0.0339 (6)
H3	0.3695	0.6029	0.7001	0.041*
C4	0.2586 (4)	0.65660 (17)	0.5438 (2)	0.0334 (6)
H4	0.2680	0.7176	0.5668	0.040*
C5	0.1832 (4)	0.63454 (16)	0.42953 (19)	0.0299 (6)
C6	0.1715 (4)	0.54408 (15)	0.39553 (19)	0.0285 (6)
H6	0.1216	0.5297	0.3187	0.034*
C7	0.2281 (4)	0.37808 (16)	0.4350 (2)	0.0311 (6)
C8	0.2003 (5)	1.0567 (2)	0.4116 (3)	0.0465 (7)
H8	0.1535	1.0663	0.3333	0.056*

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C9	0.2919 (4)	0.9900 (2)	0.5773 (3)	0.0513 (8)
H9	0.3198	0.9449	0.6336	0.062*
C10	0.3176 (5)	1.0799 (2)	0.5933 (3)	0.0539 (8)
H10	0.3656	1.1096	0.6629	0.065*
N1	0.2177 (4)	0.97671 (16)	0.4640 (2)	0.0453 (6)
H1A	0.188 (5)	0.928 (3)	0.422 (3)	0.068*
N2	0.2606 (4)	1.11996 (17)	0.4891 (2)	0.0486 (7)
H2A	0.266 (5)	1.180 (3)	0.477 (3)	0.073*
O1	0.2791 (3)	0.31374 (12)	0.50053 (15)	0.0416 (5)
O2	0.1645 (3)	0.36856 (13)	0.32466 (15)	0.0464 (6)
H2B	0.192 (5)	0.319 (3)	0.292 (3)	0.070*
O3	0.3731 (3)	0.43343 (14)	0.67244 (14)	0.0444 (6)
H3A	0.350 (5)	0.385 (3)	0.632 (3)	0.067*
O4	0.1132 (4)	0.80550 (13)	0.38169 (18)	0.0608 (7)
O5	0.2646 (5)	0.71675 (13)	0.2598 (2)	0.0731 (8)
O6	-0.0765 (4)	0.69516 (18)	0.2535 (2)	0.0870 (10)
S1	0.11344 (12)	0.72006 (4)	0.32363 (5)	0.0403 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0296 (14)	0.0194 (12)	0.0319 (12)	-0.0017 (10)	0.0096 (10)	-0.0019 (9)
C2	0.0358 (15)	0.0234 (12)	0.0314 (12)	-0.0011 (10)	0.0066 (10)	0.0029 (9)
C3	0.0442 (16)	0.0252 (13)	0.0318 (12)	-0.0033 (11)	0.0080 (11)	-0.0056 (10)
C4	0.0459 (17)	0.0190 (12)	0.0353 (12)	-0.0037 (11)	0.0100 (11)	-0.0048 (9)
C5	0.0375 (15)	0.0194 (12)	0.0337 (12)	-0.0016 (10)	0.0103 (11)	0.0007 (9)
C6	0.0388 (15)	0.0195 (12)	0.0262 (11)	-0.0008 (10)	0.0057 (10)	-0.0007 (8)
C7	0.0373 (15)	0.0212 (12)	0.0352 (13)	0.0032 (10)	0.0099 (11)	-0.0005 (9)
C8	0.059 (2)	0.0361 (16)	0.0417 (15)	-0.0014 (14)	0.0069 (14)	0.0025 (11)
C9	0.050 (2)	0.0452 (18)	0.0535 (17)	0.0016 (14)	0.0026 (14)	0.0190 (14)
C10	0.058 (2)	0.051 (2)	0.0468 (16)	-0.0051 (16)	0.0030 (15)	-0.0055 (14)
N1	0.0522 (16)	0.0236 (12)	0.0595 (15)	-0.0015 (11)	0.0125 (12)	-0.0062 (10)
N2	0.0590 (17)	0.0211 (12)	0.0619 (16)	-0.0022 (11)	0.0073 (13)	0.0006 (10)
O1	0.0604 (14)	0.0190 (9)	0.0433 (11)	0.0023 (8)	0.0088 (9)	0.0015 (7)
O2	0.0721 (15)	0.0243 (10)	0.0373 (11)	0.0076 (9)	0.0030 (10)	-0.0081 (7)
O3	0.0688 (15)	0.0251 (10)	0.0329 (10)	0.0013 (9)	0.0000 (10)	0.0044 (7)
O4	0.110 (2)	0.0157 (9)	0.0564 (13)	0.0093 (11)	0.0199 (13)	-0.0023 (8)
O5	0.136 (2)	0.0249 (11)	0.0788 (16)	0.0221 (12)	0.0651 (16)	0.0256 (10)
O6	0.104 (2)	0.0504 (16)	0.0761 (16)	-0.0188 (13)	-0.0361 (16)	0.0301 (12)
S1	0.0679 (6)	0.0144 (4)	0.0370 (4)	-0.0005 (3)	0.0100 (3)	0.0037 (2)

Geometric parameters (\AA , $^\circ$)

C1—C6	1.389 (3)	C8—N1	1.318 (4)
C1—C2	1.400 (3)	C8—H8	0.9300
C1—C7	1.478 (3)	C9—C10	1.332 (5)
C2—O3	1.351 (3)	C9—N1	1.350 (4)
C2—C3	1.386 (3)	C9—H9	0.9300
C3—C4	1.380 (3)	C10—N2	1.353 (4)

C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.386 (3)	N1—H1A	0.87 (4)
C4—H4	0.9300	N2—H2A	0.89 (4)
C5—C6	1.378 (3)	O2—H2B	0.87 (4)
C5—S1	1.765 (2)	O3—H3A	0.86 (4)
C6—H6	0.9300	O4—S1	1.4296 (19)
C7—O1	1.222 (3)	O5—S1	1.447 (3)
C7—O2	1.301 (3)	O6—S1	1.428 (3)
C8—N2	1.307 (4)		
C6—C1—C2	119.0 (2)	N2—C8—H8	126.1
C6—C1—C7	119.8 (2)	N1—C8—H8	126.1
C2—C1—C7	121.1 (2)	C10—C9—N1	107.0 (3)
O3—C2—C3	117.2 (2)	C10—C9—H9	126.5
O3—C2—C1	123.1 (2)	N1—C9—H9	126.5
C3—C2—C1	119.7 (2)	C9—C10—N2	107.0 (3)
C4—C3—C2	120.5 (2)	C9—C10—H10	126.5
C4—C3—H3	119.7	N2—C10—H10	126.5
C2—C3—H3	119.7	C8—N1—C9	109.0 (3)
C3—C4—C5	119.9 (2)	C8—N1—H1A	118 (2)
C3—C4—H4	120.0	C9—N1—H1A	133 (2)
C5—C4—H4	120.0	C8—N2—C10	109.1 (3)
C6—C5—C4	119.9 (2)	C8—N2—H2A	126 (2)
C6—C5—S1	118.44 (17)	C10—N2—H2A	124 (2)
C4—C5—S1	121.59 (19)	C7—O2—H2B	120 (2)
C5—C6—C1	120.9 (2)	C2—O3—H3A	100 (2)
C5—C6—H6	119.5	O6—S1—O4	113.53 (17)
C1—C6—H6	119.5	O6—S1—O5	111.29 (19)
O1—C7—O2	123.4 (2)	O4—S1—O5	112.18 (14)
O1—C7—C1	122.7 (2)	O6—S1—C5	107.30 (13)
O2—C7—C1	113.9 (2)	O4—S1—C5	107.19 (12)
N2—C8—N1	107.9 (3)	O5—S1—C5	104.74 (12)
C6—C1—C2—O3	-179.4 (2)	C2—C1—C7—O1	3.5 (4)
C7—C1—C2—O3	-2.3 (4)	C6—C1—C7—O2	0.6 (3)
C6—C1—C2—C3	-0.2 (4)	C2—C1—C7—O2	-176.5 (2)
C7—C1—C2—C3	176.9 (2)	N1—C9—C10—N2	-0.7 (4)
O3—C2—C3—C4	179.2 (2)	N2—C8—N1—C9	-0.4 (4)
C1—C2—C3—C4	0.0 (4)	C10—C9—N1—C8	0.7 (4)
C2—C3—C4—C5	0.5 (4)	N1—C8—N2—C10	-0.1 (4)
C3—C4—C5—C6	-0.7 (4)	C9—C10—N2—C8	0.5 (4)
C3—C4—C5—S1	-177.1 (2)	C6—C5—S1—O6	50.0 (3)
C4—C5—C6—C1	0.4 (4)	C4—C5—S1—O6	-133.5 (3)
S1—C5—C6—C1	176.93 (19)	C6—C5—S1—O4	172.3 (2)
C2—C1—C6—C5	0.0 (4)	C4—C5—S1—O4	-11.3 (3)
C7—C1—C6—C5	-177.1 (2)	C6—C5—S1—O5	-68.3 (2)
C6—C1—C7—O1	-179.4 (2)	C4—C5—S1—O5	108.1 (2)

Hydrogen-bond geometry (Å, °)

D—H...A	D—H	H...A	D...A	D—H...A
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supplementary materials

O3—H3A···O1	0.86 (4)	1.85 (4)	2.665 (3)	158 (3)
N1—H1A···O4	0.87 (4)	1.89 (4)	2.720 (3)	159 (3)
C8—H8···O3 ⁱ	0.93	2.39	3.206 (4)	147
C8—H8···O5 ⁱⁱ	0.93	2.59	3.167 (4)	121
C4—H4···O4	0.93	2.57	2.930 (3)	104
C6—H6···O2	0.93	2.37	2.696 (3)	100
C10—H10···O2 ⁱⁱⁱ	0.93	2.49	3.293 (4)	144
C9—H9···O6 ⁱⁱⁱ	0.93	2.50	3.419 (4)	168
C4—H4···O6 ⁱⁱⁱ	0.93	2.58	3.310 (3)	136
O2—H2B···O5 ^{iv}	0.87 (4)	1.67 (4)	2.536 (3)	174 (4)
N2—H2A···O1 ^v	0.89 (4)	1.97 (4)	2.832 (3)	162 (3)

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

Fig. 1

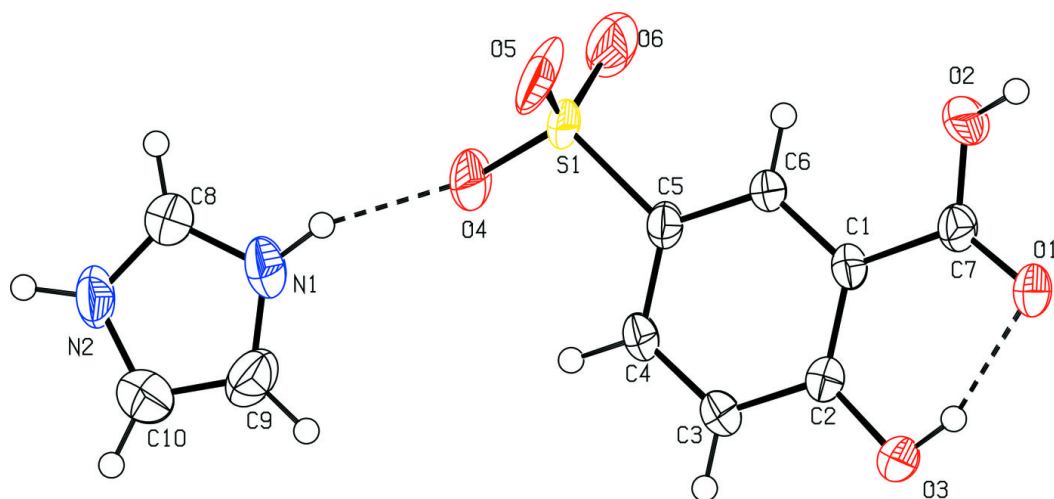


Fig. 2

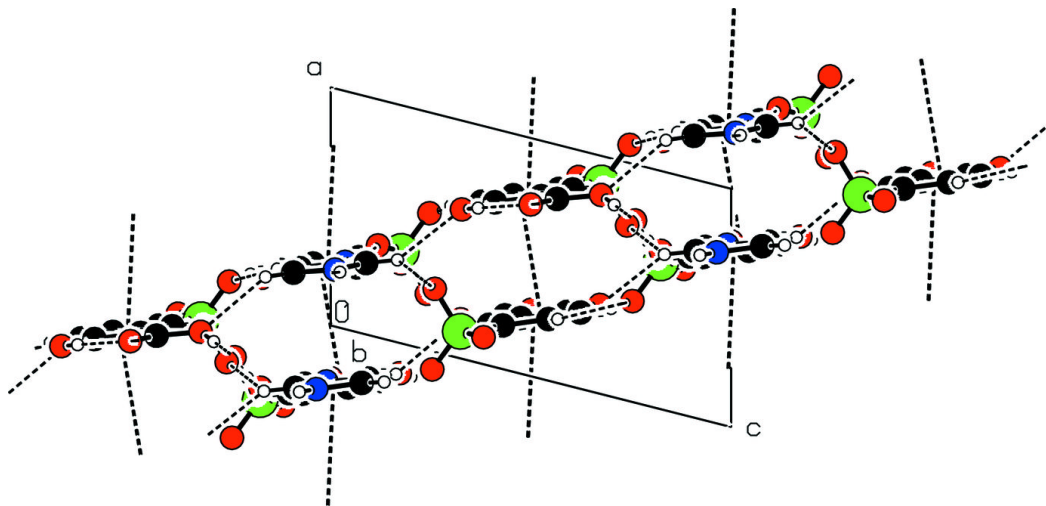


Fig. 3

