Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 2,6-Dimethylpyridinium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

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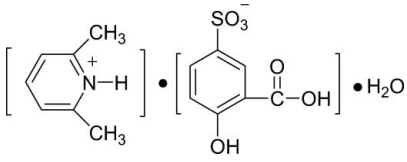
Received 5 November 2007; accepted 18 November 2007

Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.033; $wR$ factor = 0.110; data-to-parameter ratio = 12.5.

The asymmetric unit of the title compound, $C_7H_{10}N^+\cdot C_7H_5O_6S^-\cdot H_2O$, contains one 2,6-dimethylpyridinium cation, one 3-carboxy-4-hydroxybenzenesulfonate anion and one water molecule. Intermolecular O—H···O, O—H···S and N—H···O hydrogen bonds, and $\pi$–$\pi$ interactions between the benzene and pyridine rings of neighboring ions [centroid-to-centroid distance = 3.6706 (12) Å], generate a three-dimensional hydrogen-bonded framework structure.

## Related literature

For related literature, see: Smith *et al.* (2007).



## Experimental

### Crystal data

$C_7H_{10}N^+\cdot C_7H_5O_6S^-\cdot H_2O$
$M_r$ = 343.35
Monoclinic, $P2_1/n$
$a$ = 8.8340 (13) Å
$b$ = 14.840 (2) Å
$c$ = 12.2062 (17) Å
$\beta$ = 97.057 (2)°
$V$ = 1588.1 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.24 mm$^{-1}$
$T$ = 294 (2) K
0.26 × 0.24 × 0.20 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.940, $T_{max}$ = 0.954
8045 measured reflections
2810 independent reflections
2331 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.110
$S$ = 0.99
2810 reflections
225 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H4···O2$^{i}$ | 0.82 | 1.91 | 2.7006 (18) | 160 |
| O4—H4···S1$^{i}$ | 0.82 | 2.81 | 3.4464 (15) | 136 |
| N1—H1$A$···O7$^{ii}$ | 0.90 (1) | 1.85 (1) | 2.748 (2) | 175 (2) |
| O7—H7$A$···O1$^{iii}$ | 0.86 (1) | 2.03 (1) | 2.884 (2) | 173 (3) |
| O7—H7$B$···O3$^{iv}$ | 0.86 (1) | 1.93 (1) | 2.787 (2) | 173 (3) |
| O6—H6···O5 | 0.82 | 1.93 | 2.647 (2) | 145 |

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

The authors are grateful for the financial support of Tianjin Polytechnic University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2511).

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  doi:10.1107/S1600536807060400 

# supplementary materials

*Acta Cryst.* (2007). E**63**, o4900 [ **doi:10.1107/S1600536807060400** ]

# 2,6-Dimethylpyridinium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

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## Comment

5-Sulfosalicylic acid (SSA) has six potential donor sites in the three substituent groups (the sulfonic acid, the carboxylic acid and the phenolic groups), and it gives mono-, di- and trianionic ligand species through deprotonation. The presence of numerous oxygen atoms in the substituent groups usually results in hydrogen-bonding associations, and the self-assembly process of crystallization often requires the incorporation of water molecules in the structures (Smith *et al.* 2007). We report here the crystal structure of the title compound.

The asymmetric unit of the title compound contains one 2,6-dimethyl pyridinium cation, one 3-carboxyl-4-hydroxyl-benzenesulfonate anion and one water molecule (Fig. 1). The bond distances and angles in the cationic and anionic species are normal. An intramolecular O6—H6···O5 hydrogen bond is observed. The molecular packing (Fig. 2) is stabilized by intermolecular O—H···O, O—H···S and N—H···O hydrogen bonds (Table 1), and π-π interactions between the benzene and pyridine rings of the neighboring ions [centroid-to-centroid distance is 3.6706 (12) Å]. These interactions generate a three-dimensional hydrogen-bonded framework structure.

## Experimental

2-Hydroxy-5-sulfobenzoic acid (2.18 g, 10 mmol), 2,6-dimethylpyridine (1.07 g, 10 mmol) and $H_2O$ (20 ml) were loaded into a 50 ml roundbottom flask, and heated to dissolve the solid. Crystals of the title compound were obtained by slow evaporation of the deionic $H_2O$ solution.

## Refinement

The H atoms of the water molecule, and the N-bound H atom H atom were located in a difference Fourier map, and refined with the O—H and N—H distance restraints of 0.86 (1) and 0.90 (1) Å, respectively. All other H atoms were positioned geometrically [O—H = 0.82 Å (hydroxyl), C—H = 0.93 Å (aromatic) and 0.96 Å (methyl)] and refined using a riding model, with $U_{iso}$(H) = 1.5$U_{eq}$(carrier) for hydroxyl and methyl H atoms and 1.2$U_{eq}$(C) for other H atoms.

## Figures

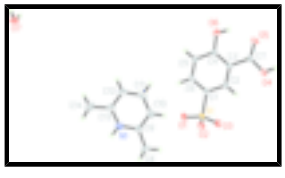

Fig. 1. The asymmteric unit of title compound. Displacement ellipsoids are drawn at the 30% probability level.

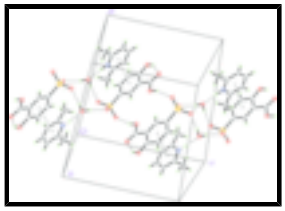

Fig. 2. Part of the crystal packing of the title compound. π-π interactions, O—H···O and N—H···O hydrogen bonds are shown as dashed lines.

### 2,6-Dimethylpyridinium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

*Crystal data*

| | |
|---|---|
| $C_7H_{10}N^+·C_7H_5O_6S^−·H_2O$ | $F_{000}$ = 720 |
| $M_r$ = 343.35 | $D_x$ = 1.436 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 4380 reflections |
| $a$ = 8.8340 (13) Å | θ = 2.7–26.4º |
| $b$ = 14.840 (2) Å | μ = 0.24 mm$^{-1}$ |
| $c$ = 12.2062 (17) Å | $T$ = 294 (2) K |
| β = 97.057 (2)º | Block, colourless |
| $V$ = 1588.1 (4) Å$^3$ | 0.26 × 0.24 × 0.20 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 2810 independent reflections |
| Radiation source: fine-focus sealed tube | 2331 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.027 |
| $T$ = 294(2) K | $\theta_{max}$ = 25.0º |
| φ and ω scans | $\theta_{min}$ = 2.2º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −9→10 |
| $T_{min}$ = 0.940, $T_{max}$ = 0.954 | $k$ = −17→11 |
| 8045 measured reflections | $l$ = −14→14 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.033 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.110 | $w = 1/[\sigma^2(F_o^2) + (0.0735P)^2 + 0.3819P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 0.99 | $(\Delta/\sigma)_{max}$ = 0.003 |
| 2810 reflections | $\Delta\rho_{max}$ = 0.21 e Å$^{-3}$ |

| | |
|---|---|
| 225 parameters | $\Delta\rho_{min} = -0.31$ e Å$^{-3}$ |
| 4 restraints | Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.088 (5) |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.19980 (5) | 0.97070 (3) | 0.73325 (3) | 0.03601 (19) |
| O1 | 0.24931 (16) | 0.93374 (10) | 0.63251 (11) | 0.0483 (4) |
| O2 | 0.32890 (14) | 0.99904 (9) | 0.81389 (11) | 0.0456 (4) |
| O3 | 0.08412 (16) | 1.04152 (9) | 0.71330 (12) | 0.0515 (4) |
| O4 | −0.21320 (16) | 0.93634 (9) | 1.00700 (12) | 0.0481 (4) |
| H4 | −0.2600 | 0.9446 | 1.0601 | 0.072* |
| O5 | −0.23614 (17) | 0.79077 (9) | 1.05258 (12) | 0.0513 (4) |
| O6 | −0.08353 (17) | 0.66773 (9) | 0.95369 (12) | 0.0507 (4) |
| H6 | −0.1434 | 0.6857 | 0.9951 | 0.076* |
| N1 | 0.76930 (17) | 0.80636 (10) | 0.61307 (13) | 0.0399 (4) |
| C1 | 0.10902 (18) | 0.88043 (11) | 0.79670 (13) | 0.0309 (4) |
| C2 | 0.00140 (18) | 0.89931 (11) | 0.86792 (13) | 0.0308 (4) |
| H2 | −0.0255 | 0.9588 | 0.8797 | 0.037* |
| C3 | −0.06686 (18) | 0.82946 (11) | 0.92206 (13) | 0.0310 (4) |
| C4 | −0.0247 (2) | 0.73902 (11) | 0.90409 (14) | 0.0351 (4) |
| C5 | 0.0842 (2) | 0.72112 (12) | 0.83225 (15) | 0.0407 (4) |
| H5 | 0.1127 | 0.6619 | 0.8205 | 0.049* |
| C6 | 0.1497 (2) | 0.79065 (12) | 0.77869 (14) | 0.0372 (4) |
| H6A | 0.2208 | 0.7778 | 0.7307 | 0.045* |
| C7 | −0.18011 (19) | 0.84923 (12) | 0.99981 (14) | 0.0347 (4) |
| C8 | 0.6895 (3) | 0.96258 (14) | 0.6310 (2) | 0.0643 (6) |
| H8A | 0.7911 | 0.9842 | 0.6532 | 0.096* |
| H8B | 0.6186 | 0.9965 | 0.6683 | 0.096* |
| H8C | 0.6650 | 0.9697 | 0.5527 | 0.096* |
| C9 | 0.6800 (2) | 0.86485 (13) | 0.66063 (16) | 0.0434 (5) |
| C10 | 0.5833 (2) | 0.83132 (16) | 0.73238 (19) | 0.0551 (6) |
| H10 | 0.5226 | 0.8701 | 0.7680 | 0.066* |
| C11 | 0.5786 (2) | 0.73910 (18) | 0.7501 (2) | 0.0645 (7) |

| | | | | |
|---|---|---|---|---|
| H11 | 0.5138 | 0.7158 | 0.7976 | 0.077* |
| C12 | 0.6690 (3) | 0.68186 (16) | 0.6981 (2) | 0.0599 (6) |
| H12 | 0.6635 | 0.6201 | 0.7096 | 0.072* |
| C13 | 0.7683 (2) | 0.71537 (13) | 0.62877 (16) | 0.0449 (5) |
| C14 | 0.8735 (3) | 0.65944 (15) | 0.5681 (2) | 0.0632 (6) |
| H14A | 0.8272 | 0.6493 | 0.4939 | 0.095* |
| H14B | 0.8921 | 0.6027 | 0.6050 | 0.095* |
| H14C | 0.9684 | 0.6908 | 0.5669 | 0.095* |
| O7 | 1.01536 (19) | 0.12730 (11) | 0.51013 (13) | 0.0578 (4) |
| H1A | 0.836 (2) | 0.8274 (15) | 0.5687 (15) | 0.059 (7)* |
| H7A | 0.9323 (19) | 0.1105 (17) | 0.4717 (16) | 0.079 (9)* |
| H7B | 1.038 (3) | 0.0964 (16) | 0.5696 (14) | 0.079 (9)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0364 (3) | 0.0391 (3) | 0.0354 (3) | 0.00222 (17) | 0.01625 (19) | 0.00305 (18) |
| O1 | 0.0522 (8) | 0.0591 (9) | 0.0381 (7) | 0.0007 (7) | 0.0232 (6) | −0.0004 (6) |
| O2 | 0.0414 (7) | 0.0505 (8) | 0.0474 (8) | −0.0074 (6) | 0.0152 (6) | −0.0069 (6) |
| O3 | 0.0534 (8) | 0.0476 (8) | 0.0579 (9) | 0.0147 (6) | 0.0241 (7) | 0.0182 (7) |
| O4 | 0.0560 (9) | 0.0419 (8) | 0.0524 (8) | −0.0009 (6) | 0.0314 (7) | −0.0035 (6) |
| O5 | 0.0579 (9) | 0.0465 (8) | 0.0549 (8) | −0.0069 (7) | 0.0294 (7) | 0.0069 (7) |
| O6 | 0.0649 (9) | 0.0343 (7) | 0.0563 (9) | −0.0062 (6) | 0.0211 (7) | 0.0038 (6) |
| N1 | 0.0381 (8) | 0.0388 (9) | 0.0415 (9) | −0.0063 (7) | 0.0002 (7) | 0.0063 (7) |
| C1 | 0.0293 (8) | 0.0371 (9) | 0.0269 (8) | 0.0008 (7) | 0.0061 (7) | −0.0006 (7) |
| C2 | 0.0314 (8) | 0.0315 (9) | 0.0303 (9) | 0.0011 (7) | 0.0063 (7) | −0.0008 (7) |
| C3 | 0.0299 (8) | 0.0346 (9) | 0.0284 (8) | −0.0019 (7) | 0.0031 (7) | −0.0013 (7) |
| C4 | 0.0378 (9) | 0.0330 (9) | 0.0340 (9) | −0.0043 (7) | 0.0025 (7) | 0.0002 (7) |
| C5 | 0.0471 (10) | 0.0314 (9) | 0.0440 (10) | 0.0050 (8) | 0.0078 (8) | −0.0056 (8) |
| C6 | 0.0359 (9) | 0.0428 (10) | 0.0340 (9) | 0.0048 (8) | 0.0093 (7) | −0.0063 (8) |
| C7 | 0.0326 (9) | 0.0386 (9) | 0.0338 (9) | −0.0041 (7) | 0.0076 (7) | −0.0009 (7) |
| C8 | 0.0694 (15) | 0.0409 (12) | 0.0827 (17) | 0.0032 (10) | 0.0094 (13) | 0.0018 (11) |
| C9 | 0.0366 (10) | 0.0448 (11) | 0.0473 (11) | −0.0013 (8) | −0.0017 (8) | 0.0038 (8) |
| C10 | 0.0365 (10) | 0.0680 (15) | 0.0606 (13) | 0.0019 (10) | 0.0057 (9) | 0.0082 (11) |
| C11 | 0.0412 (11) | 0.0811 (17) | 0.0718 (15) | −0.0072 (11) | 0.0091 (11) | 0.0309 (13) |
| C12 | 0.0489 (12) | 0.0477 (12) | 0.0794 (16) | −0.0120 (10) | −0.0066 (11) | 0.0247 (11) |
| C13 | 0.0410 (10) | 0.0384 (10) | 0.0511 (11) | −0.0048 (8) | −0.0116 (9) | 0.0044 (9) |
| C14 | 0.0650 (14) | 0.0471 (12) | 0.0733 (15) | 0.0041 (11) | −0.0087 (12) | −0.0101 (11) |
| O7 | 0.0619 (10) | 0.0654 (10) | 0.0469 (9) | −0.0062 (8) | 0.0093 (8) | 0.0132 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—O1 | 1.4616 (13) | C5—H5 | 0.93 |
| S1—O3 | 1.4652 (14) | C6—H6A | 0.93 |
| S1—O2 | 1.4733 (14) | C8—C9 | 1.500 (3) |
| S1—C1 | 1.7861 (17) | C8—H8A | 0.96 |
| O4—C7 | 1.331 (2) | C8—H8B | 0.96 |
| O4—H4 | 0.82 | C8—H8C | 0.96 |
| O5—C7 | 1.221 (2) | C9—C10 | 1.388 (3) |

| | | | |
|---|---|---|---|
| O6—C4 | 1.354 (2) | C10—C11 | 1.387 (3) |
| O6—H6 | 0.82 | C10—H10 | 0.93 |
| N1—C9 | 1.351 (3) | C11—C12 | 1.374 (4) |
| N1—C13 | 1.364 (2) | C11—H11 | 0.93 |
| N1—H1A | 0.904 (10) | C12—C13 | 1.384 (3) |
| C1—C2 | 1.393 (2) | C12—H12 | 0.93 |
| C1—C6 | 1.404 (2) | C13—C14 | 1.506 (3) |
| C2—C3 | 1.405 (2) | C14—H14A | 0.96 |
| C2—H2 | 0.93 | C14—H14B | 0.96 |
| C3—C4 | 1.417 (2) | C14—H14C | 0.96 |
| C3—C7 | 1.490 (2) | O7—H7A | 0.858 (9) |
| C4—C5 | 1.405 (3) | O7—H7B | 0.861 (9) |
| C5—C6 | 1.385 (3) | | |
| O1—S1—O3 | 113.83 (8) | O5—C7—C3 | 122.91 (16) |
| O1—S1—O2 | 112.46 (8) | O4—C7—C3 | 113.79 (15) |
| O3—S1—O2 | 111.91 (9) | C9—C8—H8A | 109.5 |
| O1—S1—C1 | 106.26 (8) | C9—C8—H8B | 109.5 |
| O3—S1—C1 | 105.60 (8) | H8A—C8—H8B | 109.5 |
| O2—S1—C1 | 106.04 (8) | C9—C8—H8C | 109.5 |
| C7—O4—H4 | 109.5 | H8A—C8—H8C | 109.5 |
| C4—O6—H6 | 109.5 | H8B—C8—H8C | 109.5 |
| C9—N1—C13 | 124.16 (17) | N1—C9—C10 | 118.54 (19) |
| C9—N1—H1A | 119.6 (15) | N1—C9—C8 | 117.70 (19) |
| C13—N1—H1A | 116.2 (15) | C10—C9—C8 | 123.7 (2) |
| C2—C1—C6 | 119.71 (16) | C11—C10—C9 | 119.0 (2) |
| C2—C1—S1 | 119.80 (13) | C11—C10—H10 | 120.5 |
| C6—C1—S1 | 120.44 (13) | C9—C10—H10 | 120.5 |
| C1—C2—C3 | 120.70 (16) | C12—C11—C10 | 120.5 (2) |
| C1—C2—H2 | 119.6 | C12—C11—H11 | 119.7 |
| C3—C2—H2 | 119.6 | C10—C11—H11 | 119.7 |
| C2—C3—C4 | 119.34 (15) | C11—C12—C13 | 120.6 (2) |
| C2—C3—C7 | 121.00 (15) | C11—C12—H12 | 119.7 |
| C4—C3—C7 | 119.65 (15) | C13—C12—H12 | 119.7 |
| O6—C4—C5 | 117.47 (16) | N1—C13—C12 | 117.2 (2) |
| O6—C4—C3 | 123.25 (16) | N1—C13—C14 | 117.49 (19) |
| C5—C4—C3 | 119.27 (16) | C12—C13—C14 | 125.3 (2) |
| C6—C5—C4 | 120.76 (16) | C13—C14—H14A | 109.5 |
| C6—C5—H5 | 119.6 | C13—C14—H14B | 109.5 |
| C4—C5—H5 | 119.6 | H14A—C14—H14B | 109.5 |
| C5—C6—C1 | 120.21 (16) | C13—C14—H14C | 109.5 |
| C5—C6—H6A | 119.9 | H14A—C14—H14C | 109.5 |
| C1—C6—H6A | 119.9 | H14B—C14—H14C | 109.5 |
| O5—C7—O4 | 123.29 (16) | H7A—O7—H7B | 113.5 (15) |
| O1—S1—C1—C2 | −155.64 (13) | C2—C1—C6—C5 | −0.6 (3) |
| O3—S1—C1—C2 | −34.41 (16) | S1—C1—C6—C5 | 176.90 (13) |
| O2—S1—C1—C2 | 84.50 (15) | C2—C3—C7—O5 | −176.23 (16) |
| O1—S1—C1—C6 | 26.86 (16) | C4—C3—C7—O5 | 2.4 (3) |
| O3—S1—C1—C6 | 148.08 (15) | C2—C3—C7—O4 | 3.2 (2) |

| | | | |
|---|---|---|---|
| O2—S1—C1—C6 | −93.01 (15) | C4—C3—C7—O4 | −178.16 (15) |
| C6—C1—C2—C3 | 0.1 (2) | C13—N1—C9—C10 | 1.7 (3) |
| S1—C1—C2—C3 | −177.46 (12) | C13—N1—C9—C8 | −177.32 (18) |
| C1—C2—C3—C4 | 0.3 (2) | N1—C9—C10—C11 | −1.8 (3) |
| C1—C2—C3—C7 | 178.96 (15) | C8—C9—C10—C11 | 177.1 (2) |
| C2—C3—C4—O6 | 179.29 (16) | C9—C10—C11—C12 | 0.4 (3) |
| C7—C3—C4—O6 | 0.6 (2) | C10—C11—C12—C13 | 1.2 (4) |
| C2—C3—C4—C5 | −0.1 (2) | C9—N1—C13—C12 | −0.1 (3) |
| C7—C3—C4—C5 | −178.82 (16) | C9—N1—C13—C14 | 179.10 (17) |
| O6—C4—C5—C6 | −179.86 (16) | C11—C12—C13—N1 | −1.4 (3) |
| C3—C4—C5—C6 | −0.4 (3) | C11—C12—C13—C14 | 179.5 (2) |
| C4—C5—C6—C1 | 0.8 (3) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H4···O2$^{i}$ | 0.82 | 1.91 | 2.7006 (18) | 160 |
| O4—H4···S1$^{i}$ | 0.82 | 2.81 | 3.4464 (15) | 136 |
| N1—H1A···O7$^{ii}$ | 0.90 (1) | 1.85 (1) | 2.748 (2) | 175 (2) |
| O7—H7A···O1$^{iii}$ | 0.86 (1) | 2.03 (1) | 2.884 (2) | 173 (3) |
| O7—H7B···O3$^{iv}$ | 0.86 (1) | 1.93 (1) | 2.787 (2) | 173 (3) |
| O6—H6···O5 | 0.82 | 1.93 | 2.647 (2) | 145 |

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

**Fig. 1**

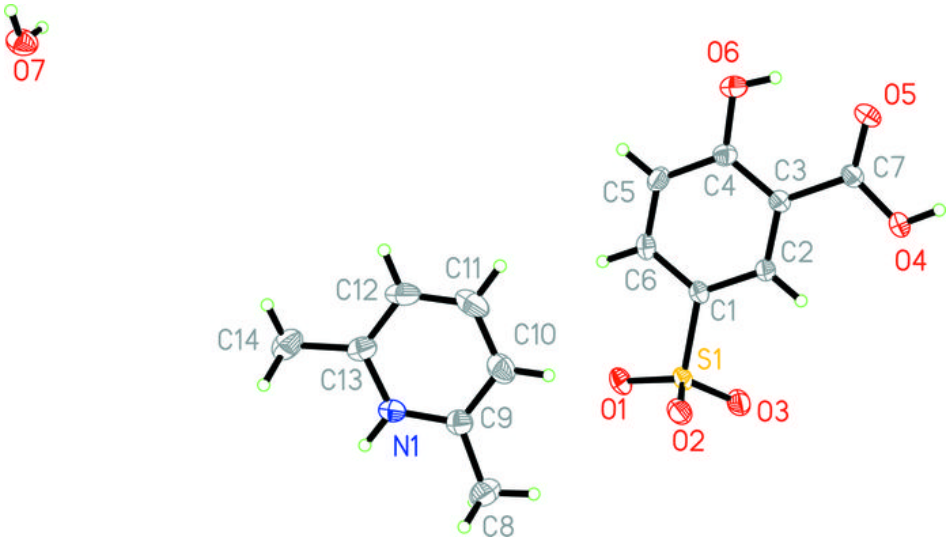
O7
O6
O5
C7
C3
C4
C5
C2
O4
C6
C1
S1
O1
O2
O3
C11
C12
C10
C14
C13
C9
N1
C8

**Fig. 2**