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# 2-Amino-3-methylpyridinium 2-amino-5-methylpyridinium sulfate monohydrate

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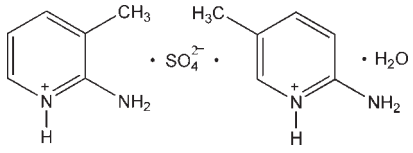
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.043; $wR$ factor = 0.129; data-to-parameter ratio = 13.4.

The asymmetric unit of the title compound, $2C_6H_9N_2^+\cdot SO_4^{2-}\cdot H_2O$, contains two isomeric protonated aminomethylpyridine cations, a sulfate anion and a solvent water molecule. The cations are in the iminium tautomeric form. In the crystal structure, intermolecular O—H···O, N—H···O and weak C—H···O hydrogen bonds link the components into a three-dimensional network. Additional stabilization is provided by weak $\pi$–$\pi$ stacking interactions, with centroid–centroid distances of 3.758 (2) and 3.774 (1) Å.

## Related literature

For related structures, see: Nahringbauer & Kvick (1977); Espenbetov *et al.* (1985); Jin *et al.* (2000, 2001, 2005); Luque *et al.* (1997). For studies on the tautomeric forms of 2-aminopyridine systems, see: Inuzuka & Fujimoto (1986, 1990); Ishikawa *et al.* (2002).



## Experimental

### Crystal data

$2C_6H_9N_2^+\cdot SO_4^{2-}\cdot H_2O$
$M_r$ = 332.39
Monoclinic, $P2_1/c$
$a$ = 8.4071 (7) Å
$b$ = 20.7654 (17) Å
$c$ = 9.3369 (8) Å
$\beta$ = 103.983 (1)°
$V$ = 1581.7 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.23 mm$^{-1}$
$T$ = 293 K
0.30 × 0.30 × 0.30 mm

### Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.908, $T_{max}$ = 0.923
8087 measured reflections
2780 independent reflections
2492 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.015

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.129
$S$ = 1.06
2780 reflections
207 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1 | 0.86 | 1.82 | 2.657 (2) | 164 |
| N2—H2*A*···O2 | 0.86 | 2.14 | 2.991 (3) | 170 |
| N3—H3···O3 | 0.86 | 1.93 | 2.781 (3) | 173 |
| N4—H4*A*···O1 | 0.86 | 2.02 | 2.826 (3) | 156 |
| N4—H4*B*···O5 | 0.86 | 2.07 | 2.857 (3) | 152 |
| C5—H5···O5 | 0.93 | 2.41 | 3.334 (3) | 171 |
| O5—H5*B*···O2$^{i}$ | 0.82 (3) | 2.03 (3) | 2.833 (3) | 167 (3) |
| O5—H5*A*···O3$^{ii}$ | 0.80 (2) | 2.10 (4) | 2.845 (3) | 157 (3) |
| C2—H2···O1$^{iii}$ | 0.93 | 2.41 | 3.334 (3) | 176 |
| N2—H2*B*···O4$^{iii}$ | 0.86 | 1.99 | 2.835 (3) | 168 |
| C11—H11···O3$^{iv}$ | 0.93 | 2.56 | 3.317 (3) | 138 |

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2943).

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# supplementary materials

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# 2-Amino-3-methylpyridinium 2-amino-5-methylpyridinium sulfate monohydrate

**J. Gong, G. Chen, S.-F. Ni, Y.-Y. Zhang and H.-B. Wang**

## Comment

We are not aware of any articles which report crystal structures containing different two pyridininium cations and a sulfate cation. We present the crystal structure of the title compound, (I), herein.

The asymmetric unit of the title compound (I) is shown in Fig. 1. Protonation of atom N1 of the 2-amino-5-methyl-pyridine and N3 of 2-amino-3-methyl-pyridine cation results in a widening of the C1—N1—C5 and C7—N3—C11 angles. These values can be compared to those of 117.5 (3)° in neutral 2-amino-5-methyl-pyridine (Nahringbauer & Kvick, 1977) and 118.0 (2)° in neutral 2-amino-3-methyl-pyridine (Espenbetov *et al.*, 1985). The C1-C5/N1 ring and C7-C11/N3 pyridinium rings are both essentially planar, with a maximum deviation from the mean plane of the rings of 0.024 (3)Å for atom N2 and 0.007 (3)Å for atom C9. The geometries of the two pyridinium rings are similar to those observed in other 2-aminopyridine structures (Luque *et al.*, 1997; Jin *et al.*, 2000,2001,2005) that are in the iminium tautomeric form (Inuzuka & Fujimoto, 1986,1990; Ishikawa *et al.*, 2002).

In the crystal structure, intermolecular O-H···O, N-H···O and weak C-H···O hydrogen bonds link the components of the structure into a three-dimensional network (Fig. 2). Additional stabilization is provided by weak π–π stacking interactions with centroid to centroid distances of 3.758 (2) and 3.774 (1)Å.

## Experimental

2-Amino-3-methyl-pyridine, 2-amino-5-methyl-pyridine and sulfuric acid were mixed in molar ratio 1:1:1 and dissolved in sufficient water. The solution was stirred and heated until a clear solution resulted. Colourless crystals of (I) were formed by gradual evaporation of excess water over a period of one week at 293 K.

## Refinement

H atoms of the water molecule were located in a differnce Fourier map, and were refined independently with isotropic displacement parameters. Other H atom were placed in calculated positions and allowed to ride on their parent atoms at distances of 0.93 Å for aromatic C atoms, 0.86 Å for amido and 0.96 Å for methyl with isotropic displacement parameters 1.2 times $U_{eq}$ of the parent atoms or 1.5 times $U_{eq}$ for methyl C atoms.

## Figures

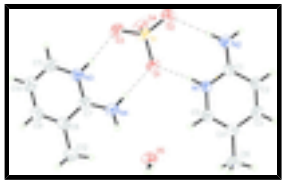

Fig. 1. The asymmetric unit of (I) showing 40% probabilty ellipsoids for non-hydrogen atoms. The dashed lines indicate hydrogen bonds.

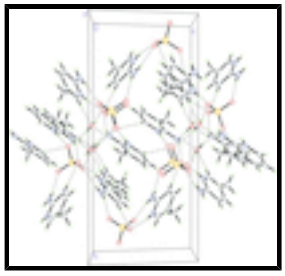

Fig. 2. Part of the crystal structure showing hydrogen bonds as dashed lines.

**2-Amino-3-methylpyridinium 2-amino-5-methylpyridinium sulfate monohydrate**

*Crystal data*

| | |
|---|---|
| $2C_6H_9N_2^+ \cdot SO_4^{2-} \cdot H_2O$ | $Z = 4$ |
| $M_r = 332.39$ | $F_{000} = 704.0$ |
| Monoclinic, $P2_1/c$ | $D_x = 1.396$ Mg m$^{-3}$ |
| Hall symbol: -P 2ybc | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 8.4071$ (7) Å | $\theta = 2.1$–$25.1^o$ |
| $b = 20.7654$ (17) Å | $\mu = 0.23$ mm$^{-1}$ |
| $c = 9.3369$ (8) Å | $T = 293$ K |
| $\beta = 103.983$ (1)$^o$ | Prism, colorless |
| $V = 1581.7$ (2) Å$^3$ | 0.30 × 0.30 × 0.30 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX area-detector diffractometer | 2780 independent reflections |
| Radiation source: fine-focus sealed tube | 2492 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.015$ |
| $T = 293$ K | $\theta_{max} = 25.0^o$ |
| φ and ω scan | $\theta_{min} = 2.0^o$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | $h = -10 \rightarrow 9$ |
| $T_{min} = 0.908$, $T_{max} = 0.923$ | $k = -24 \rightarrow 23$ |
| 8087 measured reflections | $l = -11 \rightarrow 10$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.043$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.129$ | $w = 1/[\sigma^2(F_o^2) + (0.0672P)^2 + 1.0523P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.06$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 2780 reflections | $\Delta\rho_{max} = 0.37$ e Å$^{-3}$ |

| | |
|---|---|
| 207 parameters | $\Delta\rho_{min} = -0.37$ e 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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| H5B | 0.897 (4) | 0.5692 (16) | 0.975 (4) | 0.072 (10)* |
| H5A | 0.873 (4) | 0.5243 (17) | 1.060 (4) | 0.076 (12)* |
| S1 | 0.13278 (6) | 0.60692 (2) | 0.79985 (6) | 0.03698 (19) |
| O1 | 0.3104 (2) | 0.60658 (8) | 0.8712 (2) | 0.0532 (5) |
| O2 | 0.0451 (2) | 0.63253 (9) | 0.9043 (2) | 0.0589 (5) |
| O3 | 0.08256 (19) | 0.53962 (8) | 0.76110 (18) | 0.0468 (4) |
| O4 | 0.1027 (3) | 0.64557 (10) | 0.6672 (2) | 0.0701 (6) |
| O5 | 0.8248 (2) | 0.55071 (10) | 1.0044 (2) | 0.0524 (5) |
| N1 | 0.4680 (2) | 0.67850 (8) | 1.09636 (19) | 0.0366 (4) |
| H1 | 0.4085 | 0.6519 | 1.0356 | 0.044* |
| N2 | 0.2340 (2) | 0.73695 (10) | 1.0919 (2) | 0.0537 (5) |
| H2A | 0.1785 | 0.7101 | 1.0292 | 0.064* |
| H2B | 0.1856 | 0.7691 | 1.1213 | 0.064* |
| N3 | 0.3036 (2) | 0.47027 (10) | 0.6431 (2) | 0.0439 (5) |
| H3 | 0.2413 | 0.4940 | 0.6818 | 0.053* |
| N4 | 0.5202 (3) | 0.50690 (11) | 0.8229 (2) | 0.0550 (6) |
| H4A | 0.4523 | 0.5294 | 0.8577 | 0.066* |
| H4B | 0.6232 | 0.5080 | 0.8647 | 0.066* |
| C1 | 0.3949 (3) | 0.72881 (11) | 1.1434 (2) | 0.0383 (5) |
| C2 | 0.4942 (3) | 0.77118 (11) | 1.2445 (3) | 0.0452 (5) |
| H2 | 0.4480 | 0.8064 | 1.2807 | 0.054* |
| C3 | 0.6580 (3) | 0.76018 (12) | 1.2886 (3) | 0.0489 (6) |
| H3A | 0.7229 | 0.7884 | 1.3552 | 0.059* |
| C4 | 0.7325 (3) | 0.70730 (12) | 1.2365 (3) | 0.0443 (5) |
| C5 | 0.6321 (3) | 0.66757 (11) | 1.1403 (2) | 0.0406 (5) |
| H5 | 0.6764 | 0.6320 | 1.1035 | 0.049* |
| C6 | 0.9147 (3) | 0.69585 (16) | 1.2847 (4) | 0.0686 (8) |
| H6A | 0.9644 | 0.7290 | 1.3526 | 0.103* |
| H6B | 0.9607 | 0.6966 | 1.2001 | 0.103* |
| H6C | 0.9350 | 0.6546 | 1.3322 | 0.103* |

| | | | | |
|---|---|---|---|---|
| C7 | 0.4663 (3) | 0.47068 (11) | 0.7055 (2) | 0.0409 (5) |
| C8 | 0.5701 (3) | 0.43135 (11) | 0.6419 (3) | 0.0443 (5) |
| C9 | 0.4968 (4) | 0.39642 (13) | 0.5209 (3) | 0.0584 (7) |
| H9 | 0.5618 | 0.3708 | 0.4764 | 0.070* |
| C10 | 0.3270 (4) | 0.39747 (14) | 0.4606 (3) | 0.0668 (8) |
| H10 | 0.2803 | 0.3727 | 0.3783 | 0.080* |
| C11 | 0.2333 (3) | 0.43492 (13) | 0.5239 (3) | 0.0553 (7) |
| H11 | 0.1205 | 0.4364 | 0.4856 | 0.066* |
| C12 | 0.7509 (3) | 0.42992 (14) | 0.7089 (3) | 0.0584 (7) |
| H12A | 0.7763 | 0.4577 | 0.7935 | 0.088* |
| H12B | 0.8083 | 0.4444 | 0.6376 | 0.088* |
| H12C | 0.7840 | 0.3867 | 0.7385 | 0.088* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0324 (3) | 0.0332 (3) | 0.0414 (3) | −0.0057 (2) | 0.0014 (2) | 0.0011 (2) |
| O1 | 0.0341 (9) | 0.0525 (10) | 0.0654 (11) | −0.0031 (7) | −0.0027 (8) | −0.0152 (8) |
| O2 | 0.0513 (11) | 0.0522 (11) | 0.0765 (12) | −0.0050 (8) | 0.0215 (9) | −0.0146 (9) |
| O3 | 0.0433 (9) | 0.0382 (9) | 0.0543 (10) | −0.0094 (7) | 0.0030 (7) | −0.0033 (7) |
| O4 | 0.0798 (14) | 0.0605 (12) | 0.0590 (12) | −0.0227 (10) | −0.0047 (10) | 0.0196 (9) |
| O5 | 0.0385 (10) | 0.0571 (11) | 0.0607 (12) | −0.0011 (9) | 0.0103 (9) | 0.0047 (9) |
| N1 | 0.0374 (10) | 0.0344 (9) | 0.0361 (9) | −0.0005 (7) | 0.0052 (7) | −0.0023 (7) |
| N2 | 0.0389 (11) | 0.0536 (12) | 0.0639 (14) | 0.0080 (9) | 0.0034 (10) | −0.0141 (10) |
| N3 | 0.0387 (10) | 0.0449 (11) | 0.0465 (11) | 0.0045 (8) | 0.0071 (8) | 0.0032 (9) |
| N4 | 0.0383 (11) | 0.0714 (15) | 0.0506 (12) | 0.0024 (10) | 0.0018 (9) | −0.0153 (11) |
| C1 | 0.0404 (12) | 0.0390 (12) | 0.0347 (11) | 0.0041 (9) | 0.0077 (9) | 0.0022 (9) |
| C2 | 0.0516 (14) | 0.0408 (12) | 0.0415 (12) | 0.0046 (10) | 0.0080 (10) | −0.0081 (10) |
| C3 | 0.0511 (14) | 0.0475 (14) | 0.0425 (13) | −0.0055 (11) | 0.0003 (11) | −0.0078 (10) |
| C4 | 0.0385 (12) | 0.0476 (13) | 0.0444 (12) | −0.0003 (10) | 0.0052 (10) | 0.0027 (10) |
| C5 | 0.0401 (12) | 0.0391 (12) | 0.0429 (12) | 0.0053 (9) | 0.0108 (10) | 0.0018 (9) |
| C6 | 0.0398 (14) | 0.077 (2) | 0.083 (2) | −0.0004 (13) | 0.0031 (13) | −0.0047 (17) |
| C7 | 0.0430 (12) | 0.0402 (12) | 0.0375 (11) | −0.0011 (9) | 0.0060 (9) | 0.0052 (9) |
| C8 | 0.0453 (13) | 0.0412 (12) | 0.0459 (12) | 0.0055 (10) | 0.0101 (10) | 0.0056 (10) |
| C9 | 0.0624 (17) | 0.0525 (15) | 0.0592 (16) | 0.0093 (12) | 0.0127 (13) | −0.0087 (12) |
| C10 | 0.0681 (19) | 0.0652 (18) | 0.0580 (17) | 0.0031 (14) | −0.0028 (14) | −0.0178 (14) |
| C11 | 0.0488 (14) | 0.0547 (15) | 0.0529 (15) | −0.0019 (12) | −0.0061 (12) | −0.0008 (12) |
| C12 | 0.0462 (14) | 0.0590 (16) | 0.0687 (17) | 0.0090 (12) | 0.0116 (13) | 0.0029 (13) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—O4 | 1.4460 (19) | C2—H2 | 0.9300 |
| S1—O2 | 1.4577 (19) | C3—C4 | 1.408 (3) |
| S1—O3 | 1.4792 (16) | C3—H3A | 0.9300 |
| S1—O1 | 1.4808 (17) | C4—C5 | 1.354 (3) |
| O5—H5B | 0.82 (4) | C4—C6 | 1.508 (3) |
| O5—H5A | 0.79 (4) | C5—H5 | 0.9300 |
| N1—C1 | 1.339 (3) | C6—H6A | 0.9600 |
| N1—C5 | 1.360 (3) | C6—H6B | 0.9600 |

| | | | |
|---|---|---|---|
| N1—H1 | 0.8600 | C6—H6C | 0.9600 |
| N2—C1 | 1.333 (3) | C7—C8 | 1.426 (3) |
| N2—H2A | 0.8600 | C8—C9 | 1.358 (4) |
| N2—H2B | 0.8600 | C8—C12 | 1.498 (3) |
| N3—C11 | 1.345 (3) | C9—C10 | 1.402 (4) |
| N3—C7 | 1.351 (3) | C9—H9 | 0.9300 |
| N3—H3 | 0.8600 | C10—C11 | 1.341 (4) |
| N4—C7 | 1.316 (3) | C10—H10 | 0.9300 |
| N4—H4A | 0.8600 | C11—H11 | 0.9300 |
| N4—H4B | 0.8600 | C12—H12A | 0.9600 |
| C1—C2 | 1.407 (3) | C12—H12B | 0.9600 |
| C2—C3 | 1.358 (3) | C12—H12C | 0.9600 |
| O4—S1—O2 | 111.00 (13) | C4—C5—N1 | 121.5 (2) |
| O4—S1—O3 | 109.53 (11) | C4—C5—H5 | 119.2 |
| O2—S1—O3 | 110.35 (10) | N1—C5—H5 | 119.2 |
| O4—S1—O1 | 109.70 (12) | C4—C6—H6A | 109.5 |
| O2—S1—O1 | 108.56 (11) | C4—C6—H6B | 109.5 |
| O3—S1—O1 | 107.63 (9) | H6A—C6—H6B | 109.5 |
| H5B—O5—H5A | 104 (3) | C4—C6—H6C | 109.5 |
| C1—N1—C5 | 122.93 (19) | H6A—C6—H6C | 109.5 |
| C1—N1—H1 | 118.5 | H6B—C6—H6C | 109.5 |
| C5—N1—H1 | 118.5 | N4—C7—N3 | 118.1 (2) |
| C1—N2—H2A | 120.0 | N4—C7—C8 | 123.5 (2) |
| C1—N2—H2B | 120.0 | N3—C7—C8 | 118.3 (2) |
| H2A—N2—H2B | 120.0 | C9—C8—C7 | 116.9 (2) |
| C11—N3—C7 | 123.8 (2) | C9—C8—C12 | 123.2 (2) |
| C11—N3—H3 | 118.1 | C7—C8—C12 | 119.9 (2) |
| C7—N3—H3 | 118.1 | C8—C9—C10 | 122.6 (3) |
| C7—N4—H4A | 120.0 | C8—C9—H9 | 118.7 |
| C7—N4—H4B | 120.0 | C10—C9—H9 | 118.7 |
| H4A—N4—H4B | 120.0 | C11—C10—C9 | 118.8 (3) |
| N2—C1—N1 | 119.1 (2) | C11—C10—H10 | 120.6 |
| N2—C1—C2 | 123.3 (2) | C9—C10—H10 | 120.6 |
| N1—C1—C2 | 117.6 (2) | C10—C11—N3 | 119.6 (2) |
| C3—C2—C1 | 119.5 (2) | C10—C11—H11 | 120.2 |
| C3—C2—H2 | 120.3 | N3—C11—H11 | 120.2 |
| C1—C2—H2 | 120.3 | C8—C12—H12A | 109.5 |
| C2—C3—C4 | 122.0 (2) | C8—C12—H12B | 109.5 |
| C2—C3—H3A | 119.0 | H12A—C12—H12B | 109.5 |
| C4—C3—H3A | 119.0 | C8—C12—H12C | 109.5 |
| C5—C4—C3 | 116.5 (2) | H12A—C12—H12C | 109.5 |
| C5—C4—C6 | 121.9 (2) | H12B—C12—H12C | 109.5 |
| C3—C4—C6 | 121.6 (2) | | |
| C5—N1—C1—N2 | 178.2 (2) | C11—N3—C7—C8 | −0.1 (3) |
| C5—N1—C1—C2 | −0.9 (3) | N4—C7—C8—C9 | 179.8 (2) |
| N2—C1—C2—C3 | −178.4 (2) | N3—C7—C8—C9 | 0.6 (3) |
| N1—C1—C2—C3 | 0.7 (3) | N4—C7—C8—C12 | −0.1 (4) |
| C1—C2—C3—C4 | −0.1 (4) | N3—C7—C8—C12 | −179.3 (2) |

| | | | |
|---|---|---|---|
| C2—C3—C4—C5 | −0.3 (4) | C7—C8—C9—C10 | −0.9 (4) |
| C2—C3—C4—C6 | 179.3 (2) | C12—C8—C9—C10 | 179.0 (3) |
| C3—C4—C5—N1 | 0.2 (3) | C8—C9—C10—C11 | 0.7 (5) |
| C6—C4—C5—N1 | −179.5 (2) | C9—C10—C11—N3 | −0.1 (4) |
| C1—N1—C5—C4 | 0.4 (3) | C7—N3—C11—C10 | −0.1 (4) |
| C11—N3—C7—N4 | −179.4 (2) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1 | 0.86 | 1.82 | 2.657 (2) | 164 |
| N2—H2A···O2 | 0.86 | 2.14 | 2.991 (3) | 170 |
| N3—H3···O3 | 0.86 | 1.93 | 2.781 (3) | 173 |
| N4—H4A···O1 | 0.86 | 2.02 | 2.826 (3) | 156 |
| N4—H4B···O5 | 0.86 | 2.07 | 2.857 (3) | 152 |
| C5—H5···O5 | 0.93 | 2.41 | 3.334 (3) | 171 |
| O5—H5B···O2$^{i}$ | 0.82 (3) | 2.03 (3) | 2.833 (3) | 167 (3) |
| O5—H5A···O3$^{ii}$ | 0.80 (2) | 2.10 (4) | 2.845 (3) | 157 (3) |
| C2—H2···O1$^{iii}$ | 0.93 | 2.41 | 3.334 (3) | 176 |
| N2—H2B···O4$^{iii}$ | 0.86 | 1.99 | 2.835 (3) | 168 |
| C11—H11···O3$^{iv}$ | 0.93 | 2.56 | 3.317 (3) | 138 |

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

**Fig. 1**

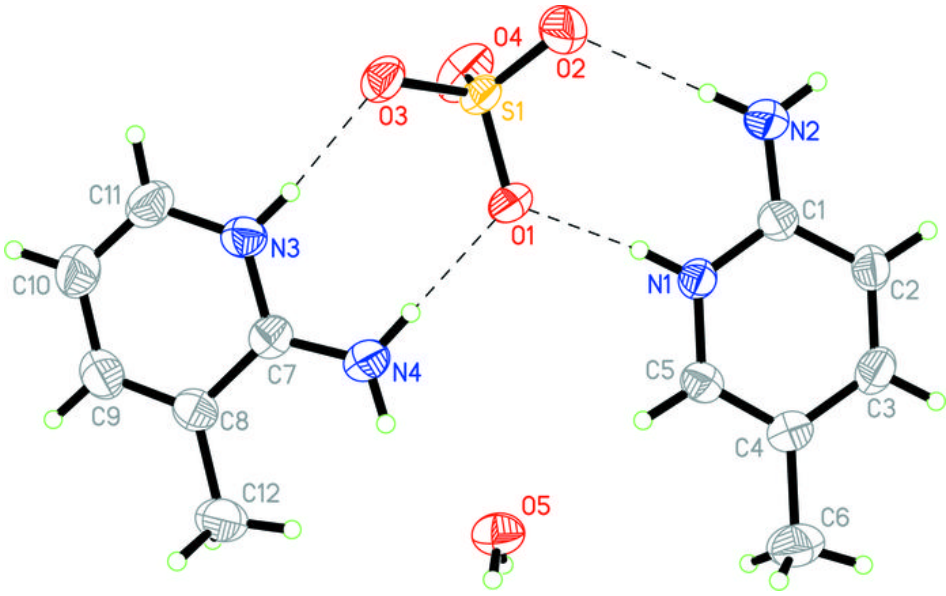

**Fig. 2**