

2-(2-Pyridylmethylammonio)ethanesulfonate
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In the crystal structure of the title compound, $C_8H_{12}N_2O_3S \cdot 2H_2O$ (HPMT·2H₂O), the organic molecule is a zwitterion. The crystal packing is determined by intermolecular hydrogen bonds with participation of water molecules, both as donors (O—H···O) and as acceptors (N⁺—H···O).

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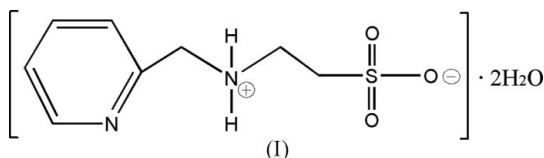
Key indicators

Single-crystal X-ray study
 $T = 273$ K
 Mean $\sigma(C-C) = 0.003$ Å
 R factor = 0.037
 wR factor = 0.099
 Data-to-parameter ratio = 13.2

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

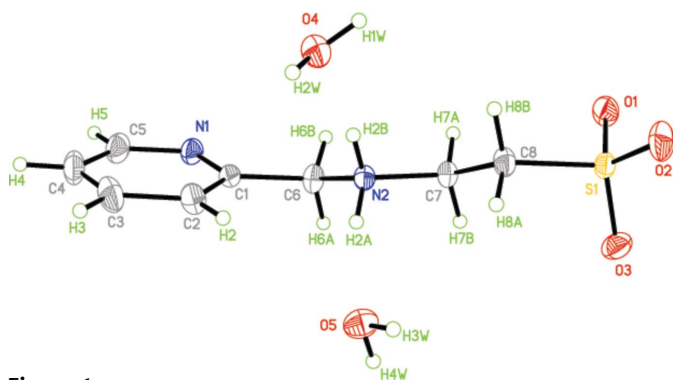
Comment

Recently, a number of Schiff base complexes derived from taurine have been reported (Jiang *et al.*, 2004, 2006; Li *et al.*, 2005, 2006; Zeng *et al.*, 2003; Zhang *et al.*, 2005). The design and synthesis of novel coordination complexes have attracted more attention (Subramanian & Zaworotko, 1995) because of their applications in many fields (Zhao *et al.*, 2001). Taurine, an amino acid containing sulfur, is indispensable to humans and has important physiological functions. However, there have been no reports on the crystal structures of the corresponding free Schiff base ligands so far; one of the reasons might be that it is difficult to crystallize them. In this paper, we report the crystal structure of the title compound, (I) (Fig. 1). The H atom of the sulfonic acid group is transferred to the amino N atom, forming the zwitterionic amino acid. This structure is similar to that of *N*-(2-hydroxybenzyl)glycine (Beltran *et al.*, 2001) and *N*-(2-pyridylmethyl)iminodiacetic acid hemihydrate (Choquesillo-Lazarte *et al.*, 2002), where the H atom of the carboxyl group is transferred to the amino N atom. The bond length and angles (Table 1) deviate slightly from those of the mononuclear Co^{II} complex (Li *et al.*, 2006), perhaps as a result of chelation in the latter. Both water molecules are involved in hydrogen bonds as donors and acceptors, whereas ammonium acts as a double donor and pyridine N as a single acceptor (Table 1 and Fig. 2).



Experimental

The reduced Schiff base *N*-(2-pyridylmethyl)taurine, the trivial name of the title organic compound (HPMT) was prepared according to the method of Li *et al.* (2006). HPMT (1.0 mmol) was dissolved in a water–methanol mixture (1:1 *v/v*, 10 ml) and then stirred at room temperature for 1 h. After filtration, the filtrate was left to stand at room temperature. Colourless block-shaped crystals were obtained in a yield of 50% after several days. Analysis, found: C 38.01, H 6.30, N


Figure 1

Molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

11.13, S 12.70%; $C_8H_{16}N_2O_5S$ requires: C 38.05, H 6.34, N 11.10, S 12.68. IR (KBr, ν , cm^{-1}): 783.3 [$\gamma(C=C-H)$], 758.8 (γCH_2); 1200.5, 1171.3, 1056.1 (νSO_3^-); 1645.7, 1598.5 ($\nu C=C+C=N$); 3365.3 ($\nu N-H$); 3462.5 ($\nu O-H$)

Crystal data

$C_8H_{12}N_2O_5S \cdot 2H_2O$
 $M_r = 252.29$
 Monoclinic, $P2_1/c$
 $a = 7.810$ (6) Å
 $b = 5.942$ (5) Å
 $c = 25.443$ (19) Å
 $\beta = 90.801$ (9)°
 $V = 1180.7$ (15) Å³

$Z = 4$
 $D_x = 1.419$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.28$ mm⁻¹
 $T = 273$ (2) K
 Block, colourless
 $0.39 \times 0.23 \times 0.22$ mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.898$, $T_{max} = 0.940$

4345 measured reflections
 2125 independent reflections
 1812 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.019$
 $\theta_{max} = 25.5^\circ$

Refinement

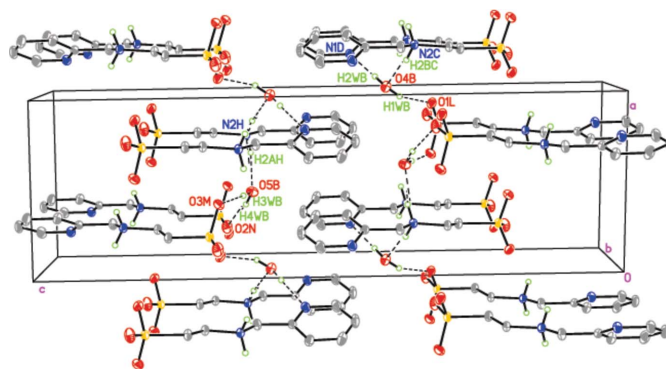
Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.099$
 $S = 1.07$
 2125 reflections
 161 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 0.3057P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.27$ e Å⁻³
 $\Delta\rho_{min} = -0.46$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

| | | | |
|----------|-------------|----------|-------------|
| S1–O1 | 1.4492 (16) | N2–C7 | 1.503 (2) |
| S1–O2 | 1.4528 (18) | C1–C2 | 1.386 (3) |
| S1–O3 | 1.4608 (17) | C1–C6 | 1.516 (3) |
| S1–C8 | 1.780 (2) | C2–C3 | 1.387 (3) |
| N1–C1 | 1.341 (3) | C3–C4 | 1.373 (4) |
| N1–C5 | 1.348 (3) | C4–C5 | 1.373 (3) |
| N2–C6 | 1.487 (3) | C7–C8 | 1.515 (3) |
| O1–S1–O2 | 112.42 (10) | C2–C1–C6 | 124.52 (17) |
| O1–S1–O3 | 112.51 (11) | N2–C6–C1 | 113.63 (15) |
| O2–S1–O3 | 113.22 (10) | N2–C7–C8 | 109.98 (15) |
| C6–N2–C7 | 111.90 (14) | C7–C8–S1 | 111.38 (13) |
| N1–C1–C6 | 113.20 (16) | | |


Figure 2

The crystal packing of (I), showing hydrogen bonds as dashed lines. For the sake of clarity, H atoms on C atoms have been omitted.

Table 2

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|----------------------------|------------|--------------|--------------|----------------|
| O5–H4W...O2 ⁱ | 0.856 (10) | 1.955 (11) | 2.802 (3) | 170 (3) |
| O5–H3W...O3 ⁱⁱ | 0.855 (10) | 1.978 (10) | 2.831 (3) | 175 (3) |
| O4–H2W...N1 ⁱⁱⁱ | 0.855 (10) | 1.998 (10) | 2.852 (3) | 178 (3) |
| O4–H1W...O1 ^{iv} | 0.856 (10) | 2.038 (15) | 2.847 (2) | 158 (3) |
| N2–H2B...O4 | 0.90 | 1.86 | 2.751 (3) | 171 |
| N2–H2A...O5 | 0.90 | 1.89 | 2.778 (3) | 168 |

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

The H atoms bonded to C and N atoms were positioned geometrically with C–H distance 0.93–0.97 Å and N–H distances of 0.900 Å, and treated as riding atoms, with $U_{iso}(H) = 1.2U_{eq}(C,N)$. The H atoms on O atoms were located in a difference Fourier map and their positional and isotropic displacement parameters were refined; the applied restraints of the O–H distances were 0.855–0.856 Å.

Data collection: APEXII (Bruker, 2004); cell refinement: APEXII; data reduction: SAINT (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2004); software used to prepare material for publication: SHELXTL.

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