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Preliminary Communication

Preparation and Crystal Data of *N*-(2-hydroxyethyl) taurine, $HOCH_2CH_2NHCH_2CH_2SO_3H$

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Taurine is a constituent of the bile acids. Since the knowledge of the crystal structure of taurine was important in understanding the biological role of the molecule, structural work on this compound was carried out by several authors[1–3]. The last study[3] has established that taurine possesses the zwitterion configuration with structural formula $NH_3^+—CH_2—CH_2—SO_3^-$.

Many taurine derivatives showed various biological activity. *N*-bis(2-chloroethyl) taurine[4] and *N*-bis(2-bromoethyl) taurine[5] were synthesized as potential agents against carcinoma. The synthesis of *N*-(2-hydroxyethyl) taurine is associated with a program to prepare derivatives of taurine as intermediates for further syntheses of compounds which could be of pharmaceutical interest.

SYNTHESIS

A mixture of sodium 2-bromoethanesulfonate (4 g, 0.019 mole), 2-aminoethanol (11.6 g, 0.19 mole), and 30 ml of water was heated at 150 °C for 3 h in a sealed tube. The volatile components were removed by vacuum distillation gradually increasing the temperature of the oil bath to 140—150 °C. The semi-solid residue was triturated with absolute ethanol until it solidified. The solid product was recrystallized from 70% ethanol. Yield 4 g (62.5%). Colorless crystals, m. p. 206—208 °C.

Anal. $C_4H_{11}NO_4S$ calc'd.: C 28.39; H 6.56; N 8.27; S 18.95%
found: C 28.28; H 6.35; N 8.40; S 19.07%

CRYSTAL DATA

The crystal data were obtained from oscillation and Weissenberg photographs using CuKα radiation. The crystals are orthorhombic with $a = 9.666$ (4), $b = 11.681$ (6), $c = 12.754$ (8) Å, $Z = 8$, space group is *Pbca* (No. 61). The density, $D_m = 1.560$ g cm^{-3}, determined pycnometrically using decalin as liquid, is in agreement with calculated, $D_x = 1.563$ g cm^{-3}.

The crystal structure analysis, which is still in progress, was solved by Patterson and three-dimensional electron density synthesis, followed by least-squares refinement. The present R-value is 13%, 1229 independent non-zero structure factors being used. The obtained distances are in good agreement with the structure of taurine[3]. The main difference between these two structures is the position of sulfur and nitrogen atoms regarding the central methylene linkage. In taurine they are in *gauche*[3], and in *N*-(2-hydroxyethyl) taurine, in *anti* position. The positions of hydrogen atoms were not detected

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with sufficient accuracy, but supposed, taking into account the bond lengths, the coordination of the surrounding atoms and Van der Waals contacts. On the basis of these considerations the correct formula of *N*-(2-hydroxyethyl) taurine is $HO—CH_2—CH_2—NH_2^+—CH_2—CH_2—SO_3^-$.

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IZVOD

Preparacija i kristalografski podaci za *N*-(2-hidroksietil) taurin, $HOCH_2CH_2NHCH_2CH_2SO_3H$

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Opisana je preparacija *N*-(2-hidroksietil) taurina. Kristalografski podaci jesu: $a = 9.666\ (4)$, $b = 11.681\ (4)$, $c = 12.754\ (8)$ Å; $Z = 8$, prostorna grupa je Pbca, a gustoća $D_m = 1.560\ gcm^{-3}$.

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