Table 2. *Bond lengths* (Å) *for non-hydrogen atoms*
(estimated standard deviations in parentheses)

C(1)—C(2)	1·529 (6)	C(9)—C(11)	1·326 (4)
C(1)—C(10)	1·540 (5)	C(10)—C(19)	1·551 (5)
C(2)—C(3)	1·504 (7)	C(11)—C(12)	1·491 (5)
C(3)—C(4)	1·447 (5)	C(12)—C(13)	1·532 (4)
C(3)—O(3)	1·219 (5)	C(13)—C(14)	1·543 (4)
C(4)—C(5)	1·331 (5)	C(13)—C(17)	1·517 (4)
C(5)—C(6)	1·502 (5)	C(13)—C(18)	1·547 (4)
C(5)—C(10)	1·530 (4)	C(14)—C(15)	1·527 (4)
C(6)—C(7)	1·519 (5)	C(15)—C(16)	1·498 (5)
C(7)—C(8)	1·522 (4)	C(15)—O(15)	1·209 (4)
C(8)—C(9)	1·519 (4)	C(17)—O(17A)	1·194 (4)
C(8)—C(14)	1·542 (4)	C(17)—O(17B)	1·329 (4)
C(9)—C(10)	1·534 (4)	O(17B)—C(20)	1·452 (4)

Table 3. *Bond angles* (°) *for non-hydrogen atoms*
(estimated standard deviations in parentheses)

C(2)—C(1)—C(10)	113·2 (3)	C(5)—C(10)—C(19)	106·8 (3)
C(1)—C(2)—C(3)	109·9 (4)	C(1)—C(10)—C(19)	110·4 (3)
C(2)—C(3)—C(4)	114·5 (3)	C(9)—C(11)—C(12)	126·3 (3)
C(2)—C(3)—O(3)	122·4 (4)	C(11)—C(12)—C(13)	113·0 (3)
C(4)—C(3)—O(3)	123·0 (4)	C(12)—C(13)—C(14)	110·7 (2)
C(3)—C(4)—C(5)	125·4 (4)	C(12)—C(13)—C(17)	111·3 (2)
C(4)—C(5)—C(6)	121·4 (3)	C(12)—C(13)—C(18)	109·9 (3)
C(4)—C(5)—C(10)	122·1 (3)	C(14)—C(13)—C(17)	108·8 (2)
C(10)—C(5)—C(6)	116·5 (3)	C(14)—C(13)—C(18)	109·9 (2)
C(5)—C(6)—C(7)	114·8 (3)	C(17)—C(13)—C(18)	106·1 (3)
C(6)—C(7)—C(8)	111·8 (3)	C(13)—C(14)—C(8)	111·6 (2)
C(7)—C(8)—C(9)	110·7 (2)	C(13)—C(14)—C(15)	113·1 (2)
C(7)—C(8)—C(14)	113·7 (3)	C(8)—C(14)—C(15)	111·6 (2)
C(9)—C(8)—C(14)	112·6 (2)	C(14)—C(15)—C(16)	118·2 (3)
C(8)—C(9)—C(10)	117·5 (2)	C(14)—C(15)—O(15)	121·9 (3)
C(8)—C(9)—C(11)	120·8 (3)	O(15)—C(15)—C(16)	119·9 (3)
C(10)—C(9)—C(11)	121·6 (3)	C(13)—C(17)—O(17A)	124·7 (3)
C(9)—C(10)—C(5)	110·6 (2)	C(13)—C(17)—O(17B)	112·6 (3)
C(9)—C(10)—C(1)	109·3 (3)	O(17A)—C(17)—O(17B)	122·6 (3)
C(9)—C(10)—C(19)	109·6 (3)	C(17)—O(17B)—C(20)	117·2 (3)
C(5)—C(10)—C(1)	110·3 (3)		

compound C(9) is sp^2 hybridized which gives rise to a shortening of the adjacent bonds [C(9)—C(10), 1·534(4); C(9)—C(8), 1·519(4) Å] and an increase in the bond angles around C(9).

The C(3)—C(4) bond distance of 1·447 (5) Å is short for a formal single bond, but both C(3) and C(4) are involved in π bonding and the torsion angle defined by O(3), C(3), C(4), C(5) is −172·0° which would indicate some delocalization of the π system along C(3)—C(4). The review by Duax *et al.* corroborates a shorter C(3)—C(4) bond distance in similar compounds, but gives a mean value of 1·455 (3) Å which is a less marked contraction than in compound (I). However, thermal parameters for the atoms in ring A of our structure are noticeably higher than those for the remainder of the structure, and this will also cause some foreshortening of bond lengths.

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Refinement of the Structure of *N*-(2-Hydroxyethyl)taurine

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Abstract. $C_4H_{11}NO_4S$, $M_r = 169·2$, orthorhombic, *Pbca*, $a = 9·675$ (3), $b = 11·636$ (4), $c = 12·752$ (6) Å, $V = 1435·6$ Å³, $Z = 8$, $D_m = 1·560$, $D_c = 1·566$ Mg m^{-3}, μ(Mo $K\alpha$) = 0·403 mm^{-1}. $R = 0·036$ for 2114 reflections. Crystals consist of $HOCH_2CH_2NH_2^+$-$CH_2CH_2SO_3^-$ zwitterions connected by hydrogen bonds of 2·731 (2), 2·812 (2) and 2·855 (2) Å. Torsion angles S—C—C—N and N—C—C—O are 176·1 (1) and −58·7 (2)°.

Introduction. The structure of the title compound obtained on the basis of film data with an anisotropic refinement of the non-hydrogen atoms ($R = 0·120$) was reported by Galešić, Herceg, Matković, Šljukić, Trupčević & Zelenko (1974). In the present work diffractometer data are used, H atom positions determined and more precise bond lengths and angles reported.

Intensities were collected from a crystal ground to a

sphere of radius 0·21 mm on a Philips PW 1100 four-circle diffractometer with Mo $K\alpha$ radiation and the θ–2θ scanning technique with a scan range of 1·6° and a scan rate of 0·04° s^{-1}. The cell parameters, determined from diffractometer data, differ by 0·045 Å in b and less than 0·010 Å in a and c from the cell dimensions cited previously (Galešić *et al.*, 1974). Absent reflections 0kl, $k \neq 2n$; $h0l$, $l \neq 2n$ and $hk0$, $h \neq 2n$ confirmed space group *Pbca*. Reflections were measured up to sin $\theta/\lambda = 0\cdot81$ Å^{-1} and 2214 unique reflections were recorded; 97 of them with $I < 2\sigma(I)$ were classified as unobserved. Corrections were made for Lorentz and polarization factors. The previous coordinates of the non-hydrogen atoms (Galešić *et al.*, 1974) were used as input data. H atoms were located from a difference map. Isotropic least-squares refinement of the non-hydrogen atoms gave an R of 0·085 and with H atoms included an R of 0·070. The final R of 0·036 was obtained by full-matrix refinement with anisotropic thermal parameters for the non-hydrogen and isotropic for the H atoms. The refinement was performed varying separately the non-hydrogen and H atoms.* Three reflections, 102, 202 and 302, with observed (calculated) structure factors 34·3 (89·0), 8·1 (42·2) and 32·1 (77·9) respectively, were rejected from

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35452 (23 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

the final cycles. These reflections were classified as wrong; their observed structure factors (80·4, 58·1 and 85·8), determined in the previous work (Galešić *et al.*, 1974), were in much better agreement. The scattering factors of Cromer & Mann (1968) were used for the non-hydrogen and those of Stewart, Davidson & Simpson (1965) for the H atoms. Calculations were performed with the XRAY system (Stewart, Kruger, Ammon, Dickinson & Hall, 1972) and the *ORFFE* 3 program (Busing, Martin & Levy, 1971). The final atomic coordinates are listed in Table 1. All parameter shifts in the final cycle were <0·1σ. Calculations were performed on a Univac 1110 computer at the University of Zagreb.

Discussion. Fig. 1 shows a schematic drawing of the molecule with bond lengths and angles. It is evident that the molecule is a zwitterion, $\text{HOCH}_2\text{CH}_2\text{-}$ $\text{NH}_3^+\text{CH}_2\text{CH}_2\text{SO}_3^-$. The present results and those previously published (Galešić *et al.*, 1974) are in agreement. The largest differences in the bond lengths are 0·017 for C(2)—N, 0·016 for C(4)—O(4) and 0·010 Å for S—C(1), while other differences are <0·005 Å. The differences in angles are <0·7°. The torsion angles between S and N along C(1)—C(2) and between N and O(4) along C(3)—C(4) are 176·1 (1) and −58·7 (2)°. S—O lengths are proportional to the strengths of hydrogen bonds in which these O atoms are engaged as acceptors. Hydrogen bonding (Table 2,

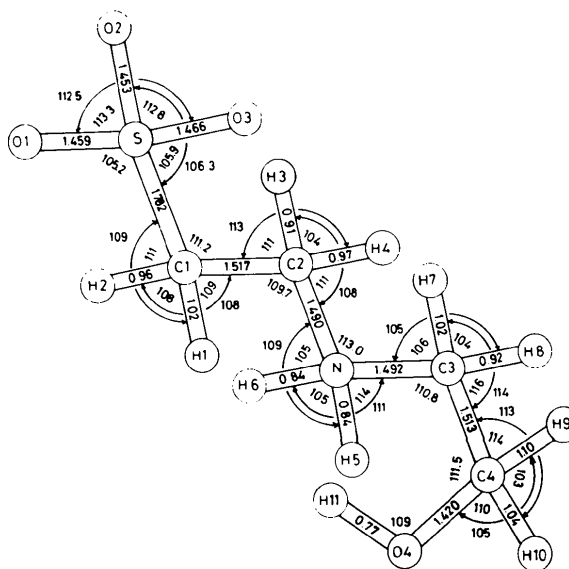Table 1. *Fractional positional parameters* ($\times 10^4$; $\times 10^5$ *for* S; $\times 10^3$ *for* H) *and isotropic temperature factors* (Å^2)

The equivalent isotropic temperature factors for the non-hydrogen atoms were computed using the expression

$$B_{\text{eq}} = \tfrac{8}{3}\pi^2 (U_{11} + U_{22} + U_{33}).$$

	x	y	z	B
S	12518 (5)	16961 (4)	2359 (4)	1·70 (2)
O(1)	795 (2)	1834 (1)	−848 (1)	2·45 (6)
O(2)	2239 (2)	768 (1)	374 (1)	2·61 (7)
O(3)	94 (2)	1634 (2)	975 (1)	2·88 (7)
O(4)	5863 (2)	5306 (1)	2585 (1)	2·58 (6)
N	3459 (2)	4050 (1)	1882 (1)	1·66 (6)
C(1)	2151 (2)	2990 (2)	542 (2)	1·85 (6)
C(2)	2628 (2)	2996 (2)	1675 (1)	1·80 (6)
C(3)	3819 (2)	4195 (2)	3012 (1)	2·08 (7)
C(4)	4626 (2)	5293 (2)	3184 (2)	2·32 (8)
H(1)	151 (3)	367 (2)	41 (2)	2·2 (6)
H(2)	295 (3)	307 (2)	10 (2)	3·2 (6)
H(3)	316 (2)	237 (2)	182 (2)	1·9 (5)
H(4)	187 (3)	293 (2)	217 (2)	2·8 (6)
H(5)	305 (3)	462 (2)	163 (2)	3·2 (6)
H(6)	417 (3)	397 (2)	152 (2)	2·8 (6)
H(7)	435 (2)	347 (2)	322 (2)	2·0 (5)
H(8)	300 (3)	413 (2)	337 (2)	3·0 (6)
H(9)	495 (3)	543 (2)	400 (2)	3·9 (6)
H(10)	405 (3)	603 (2)	302 (2)	2·6 (6)
H(11)	572 (4)	558 (3)	205 (3)	5·8 (9)

Fig. 1. Atomic numbering with bond lengths (Å) and angles (°). The angles designated by arrows are shown outside the arrows. The e.s.d.'s range from 0·002 to 0·003 Å for lengths involving non-hydrogen atoms and from 0·02 to 0·03 Å for those involving H. E.s.d.'s for the angles range from 0·1 to 0·2° for those involving non-hydrogen atoms only and from 1 to 3° for angles involving H.

Table 2. *Geometry of the hydrogen bonds*

D	H	A	$D \cdots A$ (Å)	$D-H$ (Å)	$H \cdots A$ (Å)	$D-H \cdots A$ (°)
O(4)	H(11)	O(3a)	2·731 (2)	0·77 (3)	2·00 (4)	160 (4)
N	H(5)	O(2a)	2·855 (2)	0·84 (3)	2·10 (3)	149 (3)
N	H(5)	O(4b)	2·984 (2)	0·84 (3)	2·47 (3)*	120 (2)
N	H(6)	O(1c)	2·812 (2)	0·84 (3)	2·02 (3)	158 (2)

The symmetry operations are: (a) $\frac{1}{2} - x$, $\frac{1}{2} + y$, z; (b) $-\frac{1}{2} + x$, y, $\frac{1}{2} - z$; (c) $\frac{1}{2} + x$, $\frac{1}{2} - y$, $-z$.
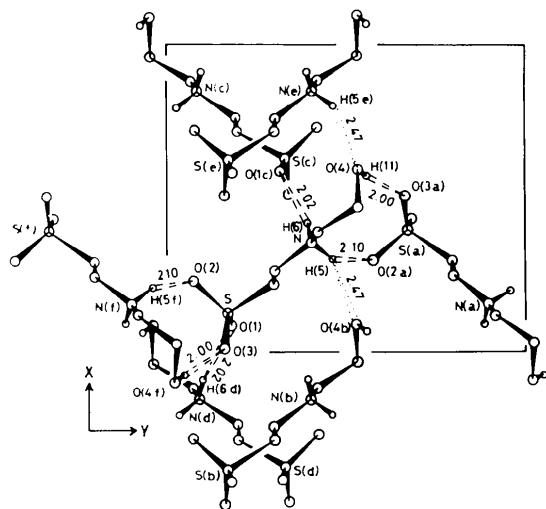
* Weak hydrogen contact.

Fig. 2. The hydrogen-bonding scheme presented as a projection of seven zwitterions along |001|. Dashed lines denote hydrogen bonds and dotted lines weak hydrogen contacts. Small letters indicate symmetry operations: (a) $\frac{1}{2} - x$, $\frac{1}{2} + y$, z; (b) $-\frac{1}{2} + x$, y, $\frac{1}{2} - z$; (c) $\frac{1}{2} + x$, $\frac{1}{2} - y$, $-z$; (d) $-\frac{1}{2} + x$, $\frac{1}{2} - y$, $-z$; (e) $\frac{1}{2} + x$, y, $\frac{1}{2} - z$; (f) $\frac{1}{2} - x$, $-\frac{1}{2} + y$, z.

Fig. 2) is realized by H(5), H(6) and H(11). It appears that H(5) also participates in an additional weak hydrogen contact to O(4b) which cannot be characterized as a bifurcated hydrogen bond since the separation of H(5) and the O(4) atom from a neighbouring molecule (denoted by an asterisk in Table 2) exceeds the sum of the van der Waals radii and the corresponding angle is 120 (2)° (Olovsson & Jönsson,

1976). Zwitterions are connected along b through H(11) and H(5) hydrogen bonds, with $O \cdots H$ separations of 2·00 and 2·10 Å, and form nine-membered rings. Hydrogen bonds through H(6) with $O \cdots H$ separations of 2·02 Å together with the weak contacts through H(5) with $O \cdots H$ separations of 2·47 Å connect zwitterions along a. Each zwitterion is connected to four others by three pairs of hydrogen bonds and to two others by one pair of weak hydrogen contacts. The largest difference in hydrogen-bond lengths compared with previous results (Galešić *et al.*, 1974) is 0·015 Å for the $O(4) \cdots O(5)$ hydrogen bond; the other differences are <0·010 Å. The determination of H atom positions precludes the existence of a bifurcated hydrogen bond which was assumed in the previous paper.

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