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Carl Henrik Görbitz,[a]* Kristian Prydz[b] and Sigurd Ugland[a]

[a]Department of Chemistry, University of Oslo, PO Box 1033 Blindern, N-0315 Oslo, Norway, and [b]Department of Biochemistry, University of Oslo, PO Box 1041 Blindern, N-0315 Oslo, Norway
Correspondence e-mail: c.h.gorbitz@kjemi.uio.no

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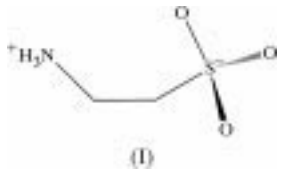
The structure of taurine (2-aminoethanesulfonic acid), $C_2H_7NO_3S$, has been redetermined at 150 K, and is compared with the structures of glycine and β-alanine which, like taurine, are enzymatically conjugated with bile acids.

Comment

Bile acids are conjugated with glycine and taurine, (I), to become more water soluble, which facilitates secretion. This enzymatic activity seems to have a bimodal localization in rat liver with different Kms for glycine and taurine, but competition experiments indicate that the same enzymes are able to catalyse conjugation both with glycine and taurine (Kase & Björkhem, 1989). Furthermore, β-alanine (3-aminopropanoic acid, not to be misinterpreted as a second polymorph of L-alanine) is also a substrate. This makes a structural comparison of these three amino acids interesting. The strucure of taurine was first presented by Okaya (1966). We report here a more accurate low-temperature study.



(I)

Glycine has been crystallized in three polymorphic forms, α-glycine (Jönnson & Kvick, 1972), β-glycine (Iitaka, 1960) and γ-glycine (Kvick *et al.*, 1980) with different hydrogen-bond patterns. The structure of α-glycine (Jönnson & Kvick, 1972) is very similar to the structure of β-alanine (Jose & Pant, 1965; Papavinasam *et al.*, 1986) in that amino acid dimers (with centers of symmetry) connected by two hydrogen bonds occur in both structures. The corresponding first-level graph-sets (Etter, 1990; Bernstein *et al.*, 1995) are $R^2_2(10)$ and $R^2_2(12)$, respectively. The conformation at the central C—C bond in β-alanine is *gauche* [N—C—C—C = 83.2 (2)°, Papavinasam *et al.*, 1986]. A *gauche* orientation is found also for taurine with N1—C2—C1—S1 = 70.96 (5)°. In addition to a weak intramolecular contact between the amino- and sulfonic acid groups [graph-set S(6)], the hydrogen-bond pattern again incorporates the centrosymmetric $R^2_2(12)$ motif, involving not just one, but two different neighboring molecules resulting in formation of hydrogen-bonded ribbons along the *a* axis. In summary, the structures of glycine (in the α-modification, Jönnson & Kvick, 1972), β-alanine (Papavinasam *et al.*, 1986) and taurine show several common features. In particular, the tendency of these molecules to form hydrogen-bonded ring systems may be important for substrate specificity when conjugation with bile acids occurs.

Experimental

Taurine was purchased from Sigma. The crystals were obtained by diffusion of 2-propanol into 50 µl of an aqueous solution containing about 2.0 mg of the acid.

Crystal data

$C_2H_7NO_3S$
M_r = 125.15
Monoclinic, $P2_1/c$
a = 5.2729 (1) Å
b = 11.6565 (3) Å
c = 7.8383 (2) Å
β = 94.011 (1)°
V = 480.59 (2) Å^3
Z = 4
D_x = 1.730 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2830 reflections
θ = 3.5–40.0°
μ = 0.563 mm^{-1}
T = 150 (2) K
Block, colourless
0.60 × 0.45 × 0.40 mm

Data collection

Siemens SMART CCD diffractometer
Sets of exposures each taken over 0.6° ω rotation scans
Absorption correction: empirical (SADABS; Sheldrick, 1996)
T_{min} = 0.755, T_{max} = 0.844
7640 measured reflections
2891 independent reflections
2736 reflections with $I > 2\sigma(I)$
R_{int} = 0.0273
θ_{max} = 40.26°
$h = -9 \rightarrow 8$
$k = -21 \rightarrow 20$
$l = -14 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.075
S = 1.126
2891 reflections
93 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.0602P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.526 e Å^{-3}
$\Delta\rho_{min}$ = −0.417 e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.133 (10)

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.4543 (5)	S1—C1	1.7842 (6)
S1—O2	1.4690 (5)	N1—C2	1.4911 (7)
S1—O3	1.4699 (4)	C1—C2	1.5249 (8)
O1—S1—C1	106.95 (3)	C2—C1—S1	112.61 (4)
O2—S1—C1	105.71 (3)	N1—C2—C1	112.28 (4)
O3—S1—C1	105.85 (3)		
O1—S1—C1—C2	179.69 (4)	S1—C1—C2—N1	70.96 (5)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.790 (14)	2.416 (15)	2.924 (1)	123.2 (13)
N1—H1···O3^{i}	0.790 (14)	2.386 (15)	3.000 (1)	135.5 (13)
N1—H1···O2^{i}	0.790 (14)	2.543 (14)	3.218 (1)	144.3 (14)
N1—H2···O2^{ii}	0.812 (15)	1.991 (15)	2.789 (1)	167.1 (15)
N1—H3···O3^{iii}	0.811 (15)	2.112 (14)	2.879 (1)	157.8 (14)

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

The data collection nominally covered over a hemisphere of reciprocal space by a combination of five sets of exposures; two with the detector set at $2\theta = 30^\circ$ and three with $2\theta = 55^\circ$. Each set had a different φ angle for the crystal and each exposure covered 0.6° in ω. The crystal-to-detector distance was 4.97 cm. Coverage of the unique set is over 99% complete to at least 70° in 2θ. H atoms were refined isotropically.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997).

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