such as the lack of cysteic acid decarboxylase in some animals known to produce taurine, indicates, however, that taurine might be formed in another manner. Its possible formation from 1-amino-2-mercapto ethane will be investigated by means of this compound labelled with radioactive sulfur.

The syntheses of taurine described in the literature have been critically studied and found unsuitable for its labelling with radioactive sulfur [3-12]. We therefore have worked out the following synthesis, which has been found suitable for semi-micro work and which gives an overall yield of approximately 50 per cent from the sulfur of thiocyanate.

The conversion of labelled sulfate to thiocyanate may be performed according to Wood (1947) [13]. The thiocyanate is reacted with 1-benzoylamino-2-brom ethane. The latter is prepared by benzoylating the hydrobromide of 1-amino-2-brom ethane in dry pyridine. The reaction

$$SCN^- + C_6H_5CONHCH_2CH_2Br = Br^- + \\ + C_6H_5CONHCH_2CH_2SCN$$

proceeds smoothly in 100 per cent ethanol at 50 degrees C with an average yield of 90 per cent. The resultant 1-benzoylamino-2-thiocyanate of ethane melts after recrystallisation from aqueous ethanol at 80° C (uncorr.) and forms small, white crystalline needles.

On hydrolysis of the 1-benzoylamino-2-thiocyanate of ethane with 2 eqv. of potassium hydroxyde and the simultaneous oxidation of the mercaptan formed to the disulfide by bubbling air through the alcoholic solution, the dibenzoyl-cystamine of m.p. 132.5° C (uncorr.) is formed in almost quantitative yield. This is hydrolyzed to cystamine by boiling with 22 per cent hydrochloric acid, and can be either reduced to the hydrochloride of 1-amino-2-mercapto ethane, or oxidized according to Schöberl [14] to taurine in about 60 per cent yield. The taurine separates on the addition of ethanol to the aqueous solution as typical crystalline needles of m. p. 228—230° C.

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The Structure of Acetaldehyde-ammonia, and a Note on its Anhydrous Form

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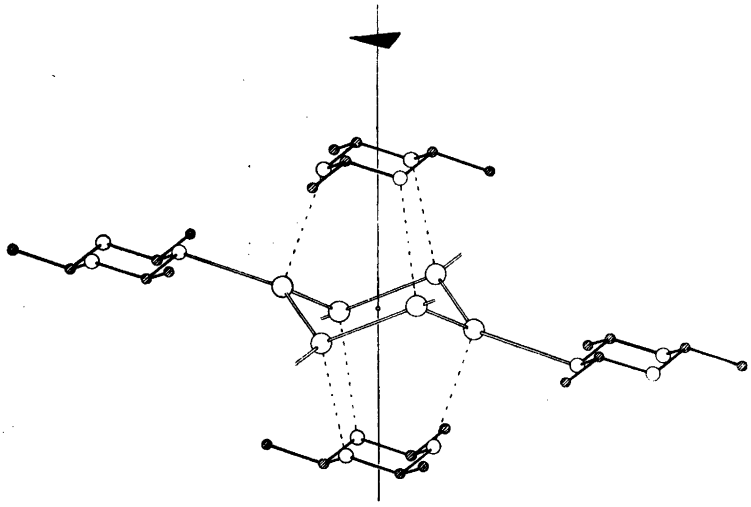
Acetaldehyde-ammonia (m. p. 94—96° C) crystallizes in the rhombohedral space group $D_{3d}^5 - R\bar{3}m$. [1, 2]. The hexagonal lattice constants as determined by the author are: $a = 11.29$ Å, $c = 15.86$ Å. There are 18 units of $CH_3 \cdot CHO \cdot NH_3$ in the hexagonal unit cell. The 18-fold position of this space group is a special one, involving a symmetry plane, whereas the 6-fold position requires the point symmetry $C_{3v}-3m$.

According to an X-ray investigation carried out by Moerman [2] the solid com-



O N C

Fig. 1.

pound is a trihydrate of 2,4,6-trimethyl-hexahydro-1,3,5-triazine, in correspondence with the view of Delépine [3]. However, the intensity material employed by Moerman was rather poor, and a re-investigation has therefore been carried out.

As a first trial a structure was considered based on the following principles: The main part is a hydrogenated triazine ring in the "chair" form with tetrahedral valency angles throughout as in an ideal *cyclo*hexane ring. One methyl group is bonded to each carbon atom of the ring in $\varkappa$ position. The C—N and C—C bond lengths are assumed to be 1.47 Å and 1.54 Å, respectively.

This molecule is placed with the center of the ring in the 6-fold position, the coordinates of which are (0, 0, z). All carbon and nitrogen atoms have then to lie in symmetry planes intersecting at 60°. The oxygen atoms of the water molecules must also be placed in these symmetry planes.

Consideration of ($hk0$) reflexions gives the distance of the oxygen atoms from the threefold axis, whereas the z parameters are determined by means of the ($0kl$) reflexions. A satisfactory correspondence between observed and calculated intensities was obtained with the following relationship between hydrogenated triazine rings and the water molecules: Between each nitrogen atom of the ring and one oxygen atom a hydrogen bond is established, having a direction corresponding to a $\varkappa$ bond in *cyclo*hexane and a length of 2.91 Å. The center of the ring has a z parameter equal to 0.26. As a result of this another hydrogen bond is established between nitrogen and oxygen atoms, hav-

ing a length of 3.18 Å and making an angle of about 20° with the threefold axis. Further, six oxygen atoms are linked together by means of hydrogen bonds, all having the length of 2.71 Å. An oxygen ring in the "chair" form of the *cyclo*hexane type is thus formed. The center of this ring coincides with a symmetry center of the lattice.

In Moerman's structure the methyl groups are situated nearly in ε position to the carbon atoms of the ring. Further, his parameters lead to a covalent C—C distance of 2.08 Å and a van der Waals' distance between two methyl groups of 2.67 Å. The hydrogen bond lengths between nitrogen and oxygen atoms are 2.67 Å and between two oxygen atoms 3.36 Å.

All these values differ greatly from those obtained in the present investigation. Here, all intensities of reflexions obtainable with Cu-K radiation were estimated and a Fourier section in the plane $y = -x$ was carried through. Only small deviations from the ideal structure pictured above were observed. A complete account of the analysis will be given shortly.

Fig. 1 gives a picture of the structure. The central ring is that formed by six oxygen atoms. Of neighbouring hydrogenated triazine rings two have their centers on the threefold axis, and six are arranged trigonally around the axis. Of these last rings only two are drawn. Covalent bonds are represented by heavy lines, hydrogen bonds of normal length by double lines and the longer hydrogen bonds by broken lines. Hydrogen atoms are altogether omitted from the Figure.

If acetaldehyde-ammonia is left for some hours in a vacuum desiccator containing sulfuric acid or even calcium chloride, it loses water and small apparently cubic crystals are obtained. Delépine analyzed this compound and found it to have the composition $(C_2H_5N)_x$.

Examinations carried out by means of a polarizing microscope and X-rays showed that the crystals are really cubic with a lattice constant $a = 14.56$ Å. Some freshly prepared crystals were observed to have very nearly the same density as quinoline ($d = 1.093$). The number of molecules of the form $C_6H_{15}N_3$ is therefore equal to *sixteen*.

Systematic absences of reflexions lead unambigously to the space group T_h^6-Pa3. In this space group the general position is a 24-fold one, but there is an 8-fold special position involving a threefold axis.

It is therefore possible to place two substituted triazine rings with their centers in two eightfold positions. This conclusion strongly supports the view of Delépine that the triazine rings of the acetaldehyde-ammonia structure are left intact when the water molecules are removed.

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