THE CRYSTAL STRUCTURE OF DL-ORNITHINE HYDROBROMIDE*

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Introduction

THE investigation of the crystal structure of DL-Ornithine Hydrobromide, NH_2-CH_2-CH_2-CH_2-CH-COOH.HBr was undertaken as a part of the series of structure determinations of amino-acids and related compounds in this laboratory. This is a short preliminary report on the structure which has been established in all its essential details.

Experimental

Good crystals of DL-Ornithine Hydrobromide were obtained by a slow evaporation of an aqueous solution of the substance. Good single crystals for X-ray studies were really difficult to obtain. The crystals were found to be short needles with the a-axis as the needle axis. Crystallographic data[1] were collected using oscillation, Weissenberg and Buerger precession photographs with CuKα radiation. The crystal belongs to the monoclinic system with four molecules of ($C_5N_2O_2H_{12}$.HBr) in the unit cell of dimensions $a = 9{\cdot}39$ Å; $b = 7{\cdot}9$ Å; $c = 11{\cdot}66$ Å; $\beta = 109° 50'$. The systematic absences were 0 k 0, k odd absent and h 0 l, l odd absent and thus the space group was uniquely fixed as $P2_1/c$.

The three dimensional intensity data from zero to seven layers were collected along the a-axis. The intensities were collected using the multiple film technique and were estimated visually. The usual Lorentz and polarization corrections were applied and the intensities were reduced to the absolute scale by Wilson plots. No absorption corrections were made since the mean absorption factor for the crystal was small ($\mu r < 0{\cdot}75$).

Structure Determination

Initial work was started on the a-axis projection. The 'y' and 'z' co-ordinates of the heavy atom bromine were fixed from the a-axis projection Patterson. A weighted beta synthesis[2] was done for this projection and this broadly indicated the orientation of the molecule. However, it was decided to tackle the structure using the three dimensional data. After determining the third co-ordinate of the heavy atom from the h 0 l Patterson, a three dimensional Fourier map was computed with the bromine phases. A cut off was used in the above Fourier—namely reflections with $|F_0|/|F_c| > 4$ were omitted from the calculations.

The above map revealed all the atoms except one oxygen, which did not come up with enough strength. The position of this oxygen atom was fixed mainly from stereochemical considerations. The R-factor computed at this stage for all the 3 D reflections was found to be 27% and the data included all the unobserved reflections. Four cycles of Least squares refinement in stages reduced the R-factor to 13·5% for 1,330 reflections. The last cycle was done with the unobserved reflections having the scheme of weighting suggested by Hamilton[3] (1955). A few more cycles of refinement seem to be needed to reach the accuracy permissible by the data. The main features presented here, however, are not expected to be altered finally.

The co-ordinates of the atoms at the present stage of refinement are given in Table 1. The

Table I

Atom	x/a	y/b	z/c
Br (1)	0·4540	0·1279	0·1445
O (1)	0·0486	0·1312	0·1466
O (2)	0·9203	0·1310	0·2658
N (1)	0·2598	0·3354	0·3067
N (2)	0·1334	0·6768	0·5744
C (1)	0·0394	0·1551	0·2436
C (2)	0·1803	0·2159	0·3523
C (3)	0·2704	0·0635	0·4117
C (4)	0·1997	0·9538	0·4777
C (5)	0·2837	0·7933	0·5336

numbering of the various atoms is shown in Fig. 1 which also gives the projection of the molecule down the unique axis. The structure is stabilized by a system of six hydrogen bonds. The environment of the nitrogen shows that each nitrogen atom has three good neighbours to form three hydrogen bonds suggesting thereby that each nitrogen is most probably in an NH_3^+ configuration. This also indicates that the carbonyl group is of the form COO^-. However, detailed confirmation of these will become available after final refinements. The hydrogen bonding scheme is indicated in Fig. 1. Nitrogen (1) bonds with two bromines and one oxygen (3·45 Å, 3·44 Å, 2·85 Å) and Nitrogen (2) bonds with two oxygens and one

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bromine (2·90 Å, 2·81 Å, 3·33 Å). In addition Nitrogen (2) has an oxygen at 3·05 Å, which is a possible hydrogen bond distance. However, this would appear to be only a non-bonded interaction, since the angle C(5)-N(2)-O(2) = 167·6°, which is very unfavourable for a hydrogen bond. A detailed discussion of the structure will be reported in due course.

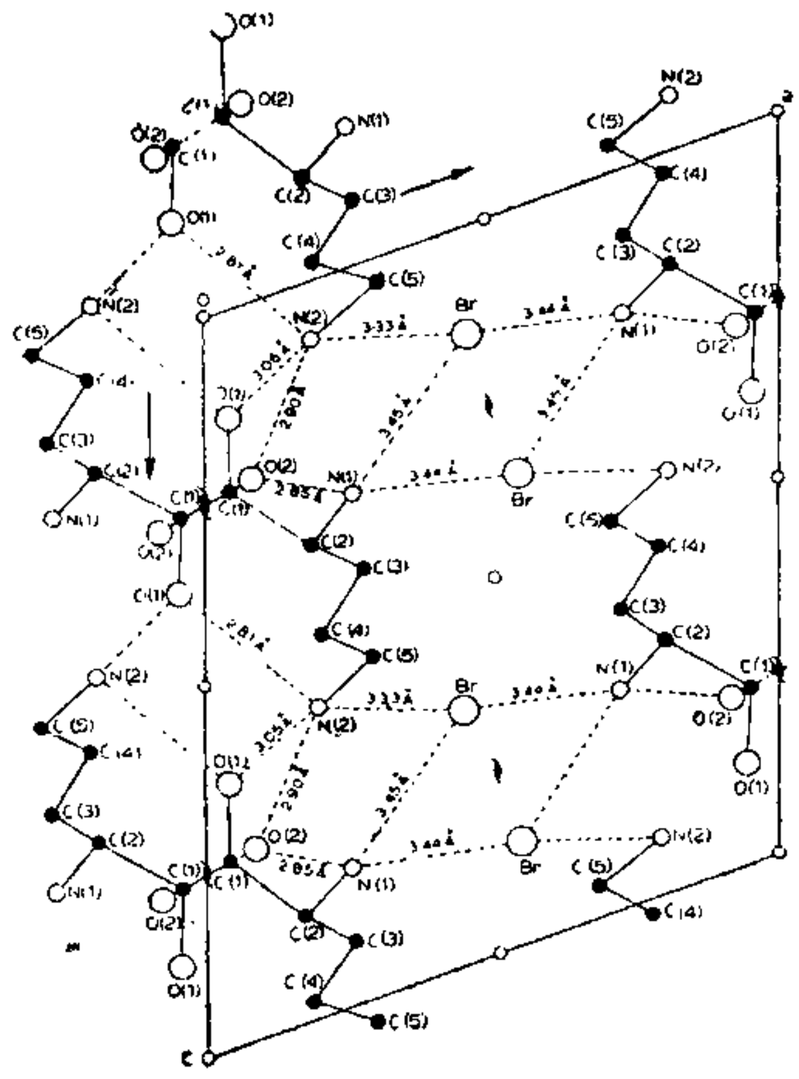

FIG. 1. A projection of the structures down the *b*-axis.

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STYLOCHEIRON INDICUS, A NEW EUPHAUSIID (CRUSTACEA: EUPHAUSIACEA) FROM INDIAN SEAS*

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IN the material of Euphausiacea in the deep-water plankton collections made with the Indian Ocean Standard net from the Indo-Norwegian Project Research Vessel *VARUNA* off the west coast of India, we have been able to identify 22 species of seven genera and an undescribed species of the genus *Stylocheiron* Sars for which a new name *Stylocheiron indicus* sp. nov. is proposed here. A description of the new species follows.

Stylocheiron indicus SP. NOV. (FIG. 1, *a-k*)

Material.—Holotype *male*, length 11·0 mm., R. V. *VARUNA* Sta. 2138 : 9° 00′ N., 75° 58′ E. on 18-3-1964, between 10·15–11·00 hours, 300 to 0 m. vertical haul ; Allotype *female*, length 13·25 mm., from same sample as holotype ; Paratypes are listed in Table II. The type specimens are deposited in the research collections of the Central Marine Fisheries Research Institute, Mandapam Camp.

Description.—Frontal plate produced as a short rostrum; latter declivous with a concavity dorsally, depressed at tip which is bluntly rounded (Fig. 1, *f-i*); rostrum slightly shorter in male, but not markedly as in other species of *Stylocheiron* ; gastric region of carapace with a well-developed keel or crest antero-dorsally.

First segment of peduncle of first antenna with an acute spine mid-ventrally at its distal end ; mid-dorsally segment wanting in spines or tooth-like structures at distal end, but a tuft of moderately elongate setæ on a slightly elevated lobe present ; second and third segments of antennular peduncle of almost equal length and normal ; *upper flagellum* of first antenna relatively shorter in both sexes, 7-jointed, its length not exceeding combined length of second and third peduncular segments ; flagellum distally depressed, first two segments short, third to fifth segments progressively longer, sixth segment as long as third segment and seventh segment short as first segment ; sensory setæ present at joints and tip of flagellum ; *lower flagellum* of first antenna 7-jointed, its length slightly exceeding combined length of

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