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PRELIMINARY CRYSTAL STRUCTURE DATA OF SOME AMINO ACIDS DERIVATIVES AND METAL COMPLEXES

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The determination of crystal structure by X-ray diffraction methods of the derivatives and metal complexes of amino acids, peptides and of other compounds of biological interest forms a major part of our research programme on the study of the structures and functions of biological molecules by various physico-chemical methods. In this project, we have already undertaken the structure determination of sarcosine hydrochloride, sarcosine hydrobromide, glycocyamine hydrochloride, glycocyamine hydrobromide, ornithine hydrochloride, copper-lysine and calcium EDTA and the present communication reports some of our preliminary structural data, e.g. unit cell dimensions, space groups etc. It may be noted that the structure of sarcosine hydrochloride has already been solved in our laboratory and reported in the Sixth International Congress on Crystallography held in Moscow in July, 1966. The structures of the rest of the above mentioned crystals are at different stages of progress.

Rotation and Weissenberg photographs of these crystals were taken using CuKα radiation. Density measurements were made by the method of floatation using a mixture of bromoform and benzene. Morphological studies were made by two-circle goniometer.

Sarcosine hydrochloride ($C_3H_7O_2N.HCl$)

Single crystals of this compound were obtained by allowing the solution of sarcosine in 40% hydrochloric acid to evaporate slowly at room temperature. The crystals thus obtained were needle shaped, transparent and hygroscopic. For taking X-ray photographs the crystals were sealed in special glass capillaries of 1.5 mm. diameter and 0.02 mm wall thickness. The crystals belong to the monoclinic system and the space group is $P2_1$. Work on the three dimensional refinement of the structure of this crystal is in progress.

Sarcosine hydrobromide ($C_3H_7O_2N.HBr$)

Single crystals of this compound were prepared in the same manner as sarcosine HCl. In this case also the crystals were found to be transparent, needle shaped and highly hygroscopic. The crystals belong to monoclinic system with space group $P2_1/c$.

Glycocyamine hydrochloride ($C_3H_7O_2N_3.HCl$)

Single crystals were grown from a solution of glycocyamine in 40% hydrochloric acid by the method of slow evaporation at room temperature. Needle shaped, translusecent crystals were obtained which belonged to tetragonal system. The space group is either $I\bar{4}2d$ or $I4_1md$.

Glycocyamine hydrobromide ($C_3H_7O_2N_3.HBr$)

Though the method used for growing the crystals was similar to that of glycocyamine HCl, two types of crystals were obtained.

Type I is isomorphous with glycocyamine hydrochloride, i.e. tetragonal with space group $I\bar{4}2d$ or $I4_1md$. Most of these crystals were found to be twins.

Type II crystals belong to monoclinic system and the space group is $P2_1/c$. Both types are unstable when exposed to air. As before, the crystals were mounted inside sealed glass capillaries for taking X-ray photographs.

Ornithine hydrochloride ($C_5H_{12}O_2N_2.HCl$)

On evaporating a solution of ornithine hydrochloride in water at room temperature, transparent and needle shaped single crystals were obtained. The crystals belong to the monoclinic system and the space group is $P2_1$.

Our grateful thanks are due to Messrs Kochlight Laboratories Ltd., England for making us a free gift of 5 gms of extra pure ornithine hydrochloride for our work.

Copper lysine Cu $(C_6H_{14}O_2N_2)_2\ Cl_2.2H_2O$

The compound was prepared by refluxing a mixture of lysine hydrochloride and cupric carbonate taken in stoichiometric proportions. The crystals were obtained by evaporating a solution of the compound in alcohal and water (50 : 50). The crystals thus obtained were blue and needle shaped. They belong to monoclinic system with space group $P2_1$.

Calcium EDTA ($CaC_{10}H_{13}O_8N_2.nH_2O$)

Calcium—EDTA was prepared by adding ethyl alcohol to a solution containing calcium carbonate and ethylene-diamine-tetra-acetate (EDTA) in equivalent molar proportions. Crystals were grown by slow evaporation of aqueous solution of Ca-EDTA. They were plate shaped and colourless. The crystals belong to triclinic system with space group $P\bar{1}$. Values of α, β and γ were obtained from zero layer Weissenberg photographs taken about [100], [010] and [001] axes respectively. The positive directions of a, b and c were chosen according to a $a < b < c$.

The results are given in tabular form in Table I, which contains the space group, dimensions of the unit cell, number of molecules per unit cell and the morphology of the crystals.

TABLE I

Unit cell dimensions and space group

Compound	Space group	a(Å)	b(Å)	c(Å)	α	β	γ	Number of Mol. (Z)	Morphology-Needle axis along [hkl]
Sarcosine Hydrochloride	$P2_1$	9 00	5 93	5 11	90	96°	90°	2	[010]
Glycocyamine Hydrochloride	$I\bar{4}2d$ or $I4_1md$	15.70	15 70	11 03	90	90°	90	16	[001]
Glycocyamine Hydrobromide	$P2_1/c$	5 53	13 52	9 24	90°	92°	90°	4	[100]
Ornithine Hydrochloride	$P2_1$	4 99	8 01	10 16	90°	96° 33′	90	2	[100]
Cu-lysine	$P2_1$	11 48	16 83	5 21	90°	93°36′	90°	2	[001]
Ca—EDTA	P1	9 88	11 14	13.37	131°58′	114°13′	77°2′	2	[100]