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Unit-cell dimensions and space groups of some simple peptides*.

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Introduction

Preliminary studies of six crystalline peptides were made with the purpose of selecting those which might be especially suitable for a complete structure determination by X-ray diffraction methods. This work is part of an extensive survey which has been in progress in these laboratories (Carpenter, 1949; Leonard & Pasternak, 1952; Pasternak & Leonard, 1952; Pasternak, 1954).

The specimens of leucyl-aspartic acid and leucyl-alanyl-glycine were kindly provided by Prof. H. O. L. Fischer; for specimens of the other peptides examined we are indebted to Dr J. R. Vaughan, Jr, of the American Cyanamid Company.

The space-group determinations were based on data from Weissenberg photographs and, in some cases, precession photographs. All the crystals studied were found to be orthorhombic with space group $P2_12_12_1$.

The unit-cell dimensions were determined from Weissenberg photographs taken with Cu $K\alpha$ radiation. On each film a powder pattern of sodium chloride was recorded for calibration of the effective radius of the camera. The densities were determined by flotation of the crystal in mixtures of chlorobenzene and bromobenzene. The numerical data obtained for these crystals are listed in Table 1. The unit-cell dimensions are accurate to about 0·5%.

Phenylalanyl-glycine

Crystals of phenylalanyl-glycine were grown by slow evaporation of an aqueous solution. They crystallized as fine fibrous needles (typical dimensions, $0{\cdot}02 \times 0{\cdot}1 \times 2$ mm.).

Leucyl-aspartic acid

Leucyl-aspartic acid crystallized as fine needles (typical dimensions, $0{\cdot}03 \times 0{\cdot}05 \times 1$ mm.) from an aqueous solution to which a small amount of ethanol had been added. The crystals tended to grow together in bunches and it was difficult to obtain a single crystal.

Leucyl-asparagine

Rectangular prisms (typical dimensions, $0{\cdot}4 \times 0{\cdot}5 \times 3$ mm.) of leucylasparagine were grown by evaporation of aqueous solutions. The crystals were unstable in air and lost water of crystallization, becoming powdery after 5–6 days at room temperature.

Glycyl-phenylalanyl-glycine

Long fine needles (typical dimensions, $0{\cdot}05 \times 0{\cdot}1 \times 6$ mm.) were grown by slow cooling of a saturated aqueous solution.

Leucyl-alanyl-glycine

Crystals (typical dimensions, $0{\cdot}2 \times 0{\cdot}2 \times 2$ mm.) were obtained by slow evaporation of aqueous solutions.

Glycyl-tyrosine ethyl ester hydrobromide

Large flat plates (typical dimensions, $0{\cdot}2 \times 2 \times 3$ mm.) were grown by rapid evaporation of an aqueous solution. This compound is very soluble in water and readily forms glasses and gums. The crystals, although very irregular in shape, were found to be single.

A complete determination of the structure of glycyl-phenylalanyl-glycine is now in progress in the laboratories of this Institute.

References

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Table 1. *Crystallographic data*

Peptide	Configuration	Unit-cell dimensions a (Å)	b (Å)	c (Å)	Density (g.cm.$^{-3}$)	Number of molecules per unit cell
Phe.-Gly.H_2O	—	24·34	17·84	8·35	1·304	11·85
Leu.-Asp.H_2O	2L	19·82	14·04	5·19	1·299	4·00
Leu.-Asp.H_2O | NH_2	2L	17·55	14·28	5·55	1·261	4·01
Gly.-Phe.-Gly.H_2O	DL	29·72	9·98	4·90	1·334	4·00
Leu.-Ala.-Gly.	—	$16{\cdot}79_5$	$15{\cdot}17_5$	5·47	1·237	3·99
Gly.-Tyr.-OEt.HBr	L	30·53	18·22	8·54	1·471	12·12