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Unit-cell dimensions and space groups of synthetic peptides. III. Glycyl-L-valine hydrobromide, glycyl-L-valine hydrochloride and DL-alanyl-DL-methionine. By T. C. TRANTER, *Wool Industries Research Association, Torridon, Headingley, Leeds 6, England*

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Table 1. *Crystallographic data*

Peptide	Crystal system	Space group	Unit-cell dimensions	Density (g.cm. ⁻³)	Molecules/unit-cell
Glycyl-L-valine HCl.H ₂ O NH ₂ .HCl.CH ₂ .CO.NH.CH.(CH ₂) ₂ .COOH.H ₂ O	Monoclinic	P2 ₁	a = 6.06, b = 8.69, c = 11.52 Å β = 102° 0'	1.278	2.00
Glycyl-L-valine HBr.H ₂ O NH ₂ .HBr.CH ₂ .CO.NH.CH.(CH ₂) ₂ .COOH.H ₂ O	Monoclinic	P2 ₁	a = 6.10, b = 8.91, c = 11.43 Å β = 101° 8'	1.480	1.99
DL-Alanyl-DL-methionine NH ₂ .CH.CH ₂ .CO.NH.CH.(CH ₂ .CH ₂ .SCH ₃).COOH	Monoclinic	P2 ₁ /c	a = 13.30, b = 5.32, c = 15.99 Å β = 107° 13'	1.347	3.98

In pursuance of the research programme recently initiated by the Wool Industries Research Association (Tranter, 1952) with its main object the determination of the crystal structures of synthetic peptides, preliminary X-ray data have now been obtained for the following peptide or peptide derivatives containing heavy atoms: the hydrobromide and hydrochloride of glycyl-L-valine and DL-alanyl-DL-methionine.

Source of peptides

Glycyl-L-valine was prepared by the chloroacetyl method (Fischer & Otto, 1903) and the hydrobromide and hydrochloride were prepared as described in an earlier note (Tranter, 1953). Found, 15.24% Cl; calculated for glycyl-L-valine HCl.H₂O, 15.54%. The hydrobromide was not analysed.

Glycyl-L-valine hydrobromide and *glycyl-L-valine hydrochloride* both crystallized readily from aqueous solution. Unit-cell dimensions were obtained from rotation photographs about the principle crystallographic axes and the β angle by measurements of the [101] axis. Moving-film photographs on an equi-inclination Weissenberg goniometer were employed in the space-group determinations. The only systematic absence observed was 0k0 with k odd so that the probable space group is P2₁. The crystals contained water of crystallization. Loss in weight on drying at 100° C. *in vacuo*:

Glycyl-L-valine HCl, 6.9%; calculated for glycyl-L-valine HCl.H₂O, 7.9%.

DL-*Alanyl-DL-methionine* was obtained from British Drug Houses, Poole, England, and yielded acicular crystals from aqueous solution with b as the needle axis. The crystals showed pronounced cleavage parallel to (100) and (001). Systematic absences observed were h0l with l odd and 0k0 with k odd giving P2₁/c as the probable space group.

These results are summarized in Table 1.

The hydrobromide and hydrochloride of glycyl-L-valine are apparently isomorphous and the crystal structures of these derivatives and of DL-alanyl-DL-methionine are being examined in detail.

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References

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