LETTERS TO THE EDITORS

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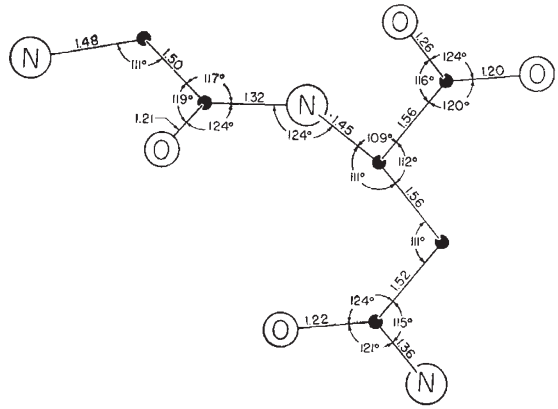
Configuration of the Peptide Link and of Asparagine in Glycyl-L-Asparagine

Since the geometrical problem of protein structure is mainly that of the configuration of the polypeptide chains, the geometry of the peptide link itself is a matter of prime importance. However, very few crystal-structure data have yet been published from which precise dimensions of the peptide link may be derived. We have recently carried out a three-dimensional X-ray analysis of the structure of glycyl-L-asparagine which provides an additional source of these data. Our analysis also provides information concerning the molecular configuration of asparagine, an amino-acid the structure of which has recently been discussed in *Nature* by Steward and Thompson[1].

The crystal data for glycyl-L-asparagine are: density, 1·506 (by flotation); space group, $P2_12_12_1$ (orthorhombic); unit-cell dimensions, $a = 4·81$, $b = 12·85$ and $c = 13·52$ A.; number of molecules per unit cell, 4. The intensities of all observable copper $K\alpha$ reflexions (more than a thousand) were estimated visually. These data were used to prepare a sharpened three-dimensional Patterson synthesis, from which, aided by application of the vector convergence method[2,3], we were able to deduce a satisfactory model for the molecule. Refinements of the thirty-nine positional parameters (excluding hydrogens) were made by using two- and three-dimensional Fourier synthesis and least squares methods. Most of the calculations were carried out with I.B.M. machines. The average standard error in the final parameters is 0·010 A.

The molecule of glycyl-L-asparagine (see diagram) can be described most simply by reference to two planes approximately at right angles to each other. One plane contains the succinamic acid part. The other contains the five atoms of the peptide group; the C—N bond to the amino-nitrogen atom points 8° out of this plane. One carbon atom is common to both planes. As is found in other amino-acids and peptides, the molecule of glycyl-L-asparagine contains the charged groups $-NH_3^+$ and $-COO^-$.



A drawing of the molecule of glycyl-L-asparagine viewed along the *a*-axis of the crystal. Bond-lengths are given in angströms

The dimensions of the peptide (see diagram) agree, within the limits of error of the structure determination, with those postulated by Pauling and Corey[4] in their models of proteins. In particular, their assumption of planarity for the peptide group is supported, since we find the average distance of the atoms from a plane to be 0·002 A. The atoms of the asparagine residue, excluding its α-amino-nitrogen atom, form a nearly planar extended chain. Thus, our structure does not conform to the cyclic structure proposed by Steward and Thompson[1] for free asparagine, and visualized by them as a possibility also when the molecule occupies the terminal position at the carboxyl end of a peptide chain.

There is a significant difference in the lengths of the C—O bonds of the carboxyl group. This difference is consistent with the distribution of hydrogen bonds; the oxygen atom of the longer bond participates in three N—H···O bonds, the other oxygen atom in only one. The carboxyl group is co-planar as expected. The same is true of the terminal amide group, and its bond-lengths are close to those found in the peptide amide group. However, the bond-angles around the carbon atom of the terminal amide group are significantly different from the corresponding angles in the peptide amide group; their magnitudes are reminiscent of those reported for the molecule of acetamide[5].

Of the six possible hydrogen bonds, five are found to have satisfactory lengths (2·75–2·93 A.) and bond-angles. The sixth, which involves the amino-nitrogen atom, has a length of 2·99 A. but is open to question, because its angles with the other H-bonds deviate appreciably from the tetrahedral.

We wish to thank Dr. John Leonard for the preparation of the glycyl-L-asparagine and for his assistance in reading the intensities. We are indebted to Dr. Jerry Donohue for valuable discussions and for instruction in the I.B.M. computing techniques.

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Behaviour of a Synthetic Polypeptide analogous to Protein Denaturation

Some observations made recently in this laboratory suggest a considerable resemblance, in certain respects, between poly DL-alanine and the soluble form of silk obtained from solution in cupriethylene diamine or lithium bromide solution[1,2].

Poly DL-alanine (degree of polymerization estimated from end-group analysis, about 500) is readily soluble in cold water, giving a mobile solution from which coherent films may be cast. The infra-red spectrum of these films (Fig. 1) shows a single C=O stretching mode at 1,662 cm.$^{-1}$, the frequency corresponding to a folded polypeptide chain[3]. If the solution is heated, a gel quickly separates out; this gel is not redissolved