with $a_0 = 12{\cdot}52$ A. was also reported by Phragmén, and solid solutions between it and the manganese compound have been investigated by Phragmén and by Pratt and Raynor.

The work on these phases is being continued and a detailed report will be published later.

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Invariant Characteristics of X-Ray Fourier Syntheses

It has been suggested by Bernal[1] that the presence of certain variations in the intensity of the X-ray reflexions from protein crystals imposes upon the Fourier density map, which results from their combination, certain features which are to some extent independent of the particular set of *phases* which are associated with these amplitudes. In this note it is proposed to show how a certain 'average' picture can be obtained, and that it is derivable from a well-known form of synthesis.

First consider the case of a structure containing a centre of symmetry; the electron density ρ_s is given, in terms of the structure factors F_s, by the well-known expression[2],

$$\rho_s = \frac{1}{V} \sum_3 F_s \cos \theta.$$

The suffix s indicates that a particular set of phases, s, has been chosen.

Next let an average be taken over all possible combinations of sign:

$$\bar{\rho} = \frac{1}{\Sigma s} \Sigma \rho_s = \frac{1}{V \Sigma s} \sum_s \sum_3 F_s \cos \theta \rightarrow \frac{F(000)}{V},$$

No useful information emerges from this, because to every group of signs there exists an exact negative. Suppose, however, that $\bar{\rho}^2$ is considered. Here:

$$\bar{\rho}^2 = \frac{1}{\Sigma s} \Sigma \rho_s^2 = \frac{1}{V \Sigma s} \sum_s \Sigma F^2 \cos^2 \theta + F_s F_t \cos \theta_s \cos \theta_t$$
$$\rightarrow \frac{1}{V} \sum_3 F^2 \cos^2 \theta$$
$$= \frac{1}{2V} \sum_3 F^2 \cos 2\theta + F^2,$$

so that the average features are given, apart from an additive constant, by the ordinary Patterson synthesis on *twice* the normal scale. It is to be noted that in this interpretation of the Patterson synthesis, maxima may in fact correspond to minima in real space.

Secondly, consider the case in which no centre of symmetry is present. Here, with an obvious change in notation:

$$\rho_a = \frac{1}{V} \sum_3 |F| \cos (\theta - \alpha)$$
$$\rho \rightarrow F(000)/V$$

and

$$\bar{\rho}^2 = \frac{1}{V \Sigma \alpha} \sum_a \sum_3 |F|^2 \cos^2 (\theta - \alpha) + |F_1||F_2| \cos (\theta_1 - \alpha_1) \cos (\theta_2 - \alpha_2)$$
$$\rightarrow \frac{1}{V \Sigma \alpha} \sum_a \sum_3 |F|^2 \cos^2 (\theta - \alpha)$$
$$= \frac{1}{2V \Sigma \alpha} \sum_a \sum_3 |F|^2 \cos (2\theta - 2\alpha) + |F|^2 = \Sigma |F|^2 / 2V,$$

since the average value of $\cos (2\theta - 2\alpha)$ is zero. So that, as might be expected on intuitive grounds, there are no 'average' features other than a uniform plateau.

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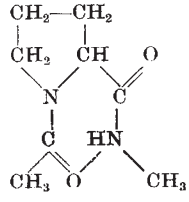
Infra-red Spectra of Acetylproline N-Methylamide and the Configuration of a Proline Residue in a Polypeptide Chain

We have recently determined by infra-red and dielectric measurements the molecular configuration of acetylproline N-methylamide, from which we can conclude the configuration of a proline residue contained in a polypeptide chain.

In a dilute carbon tetrachloride solution (0·0001 mol./l.) this substance showed only one absorption peak at 3,350 cm.$^{-1}$ in the 3-μ region which can be assigned to the hydrogen-bonded NH vibration. The frequency of the absorption peak remained the same when we changed the concentration from 0·0001 to 0·1 mol./l., and the temperature from 30° to 60° C.

This result is quite different from what we obtained for such a substance as acetylglycine N-methylamide; this showed two absorption peaks at 3,440 and 3,350 cm.$^{-1}$ which were assigned to the free and hydrogen-bonded NH vibrations, respectively, the intensity ratio of these two bands changing considerably with temperature[1,2]. Therefore we can conclude that practically all the molecules of this substance take the folded configuration as shown in the accompanying formula, in contrast to the case of acetylglycine N-methylamide, etc., the molecules of which take both the folded and the extended configurations. This conclusion is compatible with the fact that acetylproline N-methylamide is much more soluble in carbon tetrachloride than acetylglycine N-methylamide or acetylalanine N-methylamide, since in the folded configuration all the hydrogen bonds are intramolecular[3]. From this result we consider that the proline residue takes only the folded configuration in a polypeptide chain, although many other kinds of residues can take both the extended and folded configurations.



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