rods being curved or kinked into a super helix, suggest themselves. In any case allowance must be made for the chains to turn corners.

The most important positive conclusion is that the length of the rods is probably rather small (15–20 Å). This suggests that globular proteins are really three-dimensional in their 'architecture', and not two-dimensional like the synthetic polypeptides. That is to say, whereas the broad structure of a synthetic polypeptide can be conveniently represented diagrammatically by a projection in the rod direction, a globular protein may be more like a three-dimensional framework, and may need a perspective drawing to show its main features. Whether this three-dimensional architecture conforms to a single general plan, or whether it is specific for each protein, or bit of a protein, remains to be seen.

Finally it must not be concluded that because of the poor quantitative agreement between observation and calculation we can immediately reject the rod model and α-helices. The method of calculation used is suitable for simple models, and becomes progressively more unreliable as we introduce complications. A more lengthy and accurate calculation would be needed to show whether the discrepancies in absolute height, projected shape, and asymmetry of the Patterson require a completely new model or whether they arise naturally out of simple modifications to the present model with short rods.

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Determination of Elastic Constants of Lithium Fluoride from Photographs of Diffuse Reflexions of X-rays

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A photographic method of determining elastic constants from the study of diffuse X-ray reflexions has been developed and applied to lithium fluoride. The results are as follows: $c_{11} = 9{\cdot}9 \times 10^{11}$, $c_{12} = 4{\cdot}3 \times 10^{11}$, $c_{44} = 5{\cdot}4 \times 10^{11}$ dyne cm^{-2}.

Thermal vibrations of the atoms in a crystal give rise in reciprocal space to scattering from regions other than the points of the reciprocal lattice. The theoretical distribution of this extra scattering density has been given by Jahn (1942) for cubic crystals, and it depends on the elastic constants of the crystal. Lonsdale & Smith (1941, 1942) have shown that there was qualitative agreement with this theory when the diffuse X-rays were photographically recorded, and Ramachandran & Wooster (1951*a*, *b*), using a Geiger counter, have obtained the elastic constants for several cubic crystals.

We have used the photographic method to study quantitatively the diffuse reflexions obtained with LiF. A camera of radius 10 cm. and monochromatized Cu $K\alpha$ radiation have been used, and the film blackening was measured with a Dobson microphotometer. Charts have been constructed to determine conveniently which point in reciprocal space corresponds to a given point of the diffuse spot (Hoerni & Wooster, in press). Although measurements at only three different points of the diffuse spot are in principle required to solve Jahn's equation for the elastic constants, many more observations have been made in order to check the results. The measurement of relative intensities within any one spot permits only the ratios of the constants to be determined. Observations around the 200 and 220 reciprocal points have given the following ratios:

$$c_{12}/c_{11} = 0{\cdot}43 \pm 0{\cdot}02,\ c_{44}/c_{11} = 0{\cdot}54 \pm 0{\cdot}02\ .$$

In order to obtain absolute values, we have followed Ramachandran & Wooster's method, which is to compare the intensity of the diffuse beam with that of the incident beam, using the Bragg integrated reflexion as an intermediate standard. The results are as follows:

$$c_{11} = 9{\cdot}9 \times 10^{11},\ c_{12} = 4{\cdot}3 \times 10^{11},$$
$$c_{44} = 5{\cdot}4 \times 10^{11} \text{ dyne cm.}^{-2}.$$

The absolute values, which have an accuracy of about 10%, are in good agreement with the results of Huntingdon (1947), but not with those of Rao (1949), who finds that LiF obeys the Cauchy relation ($c_{12} = c_{44}$).

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

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Interprétation simple du facteur de température artificielle employée dans l'analyse de structures.

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Afin de rendre les séries de Fourier convergentes et d'éviter les phénomènes de diffraction dus au nombre fini de termes, on utilise souvent l'artifice de multiplier les coefficients de Fourier par le facteur $\exp(-A \sin^2 \theta)$ qui par analogie avec le facteur de Debye correspondrait à l'introduction d'une température 'artificielle'. Nous en donnons ici une interprétation plus quantitative. Envisageons pour la simplicité des calculs le système orthorhombique et intégrons la densité électronique ϱ (1) dans le volume soustendu par le parallèlépipède $\boldsymbol{\varepsilon}_j$ (2), d'arêtes parallèles aux axes $\mathbf{a}_j$ du cristal et centré sur $\mathbf{r}_0$ (3).

$$\varrho(\mathbf{r}) = \sum_h F_h \exp(2\pi i \mathbf{hr}) \tag{1}$$

$$\boldsymbol{\varepsilon}_j = \eta_j \mathbf{a}_j \qquad j = 1, 2, 3 \tag{2}$$

$$\mathbf{r} = \mathbf{r}_0 + \boldsymbol{\varepsilon} \tag{3}$$

La valeur moyenne de ϱ dans ce volume, soit $\langle \varrho(\mathbf{r}_0) \rangle_\varepsilon$ sera (4):

$$\langle \varrho(\mathbf{r}_0)_\varepsilon \rangle = \sum F_h \frac{\sin(\pi h_1\eta_1) \,.\, \sin(\pi h_2\eta_2) \,.\, \sin(\pi h_3\eta_3)}{\pi h_1\eta_1 \,.\, \pi h_2\eta_2 \,.\, \pi h_3\eta_3} \exp(2\pi i \mathbf{hr}_0). \tag{4}$$

Omettons alors l'indice $_0$. $\langle \varrho(\mathbf{r}) \rangle_\varepsilon$ peut être considéré comme une fonction de $\mathbf{r}$ à laquelle nous pouvons encore appliquer le même procédé de moyenne. La deuxième moyenne dans le même volume et notée $\langle\langle \varrho(\mathbf{r}) \rangle_\varepsilon \rangle_\varepsilon$ sera par conséquent (5):

$$\langle\langle \varrho(\mathbf{r}) \rangle_\varepsilon \rangle_\varepsilon = \sum_h F_h \left(\frac{\sin \pi h_1\eta_1 \,.\, \sin \pi h_2\eta_2 \,.\, \sin \pi h_3\eta_3}{\pi h_1\eta_1 \,.\, \pi h_2\eta_2 \,.\, \pi h_3\eta_3}\right)^2 \exp(2\pi i \mathbf{hr})\ . \tag{5}$$

La fonction $\sin^2(\pi h\eta)/(\pi h\eta)^2$ de décroissance rapide, peut être approchée par une fonction de Gauss de même maximum et aire intégrée telle que $\exp(-\pi h^2\eta^2)$ de sorte que (5) peut s'écrire (6):

$$\langle\langle \varrho(\mathbf{r}) \rangle_\varepsilon \rangle_\varepsilon = \sum_h F_h \exp\left(-\pi \sum_j h_j^2\eta_j^2\right) \exp(2\pi i \mathbf{hr})\ . \tag{6}$$

Posons alors $|\varepsilon_1| = |\varepsilon_2| = |\varepsilon_3| = l$ ce qui revient à remplacer le parallèlepipède par un cube d'arête l. On montre alors aisément que

$$\sum_j h_j^2\eta_j^2 = l^2/d^2\ , \tag{7}$$

où d est la distance réticulaire (8) du plan (h_1, h_2, h_3).

$$d^{-2} = \sum_j h_j^2 a_j^{-2}\ . \tag{8}$$

D'après la loi de Bragg le facteur de température