The notation is that used by Klug *et al.* and the summation in (1*a*) extends over the values of n which satisfy the relation $l = tn + um$ and the summation in (1*b*) extends over the atoms in a set. In many instances (*e.g.* the α-helix) only one term is needed in (1*a*) for a particular value of l; this is the case considered here.

If a convenient axis Oz is chosen within the fibril we may suppose this to coincide with the helix axis of an imaginary reference molecule having some arbitrary rotation about Oz and displacement along Oz. The Fourier transform, F_o, of this reference molecule may then be calculated by expression (1). Each molecule in the fibril may generated from the reference molecule by a rotation α_v about Oz, a displacement z_v parallel to Oz and a displacement normal to Oz of magnitude r_v and azimuth φ_v. The transform of the fibril is thus

$$\begin{aligned} &F(R, \psi, l/c) \\ &= \sum_v F_o(R, \psi - \alpha_v, l/c) \exp \{2\pi i[Rr_v \cos(\psi - \varphi_v) + \zeta z_v]\} \end{aligned} \quad (2)$$

where the summation extends over the N molecules in the fibril and does not, of course, include the imaginary reference molecule. A similar expression, in cartesian coordinates, is implied in Section 4 of Cochran *et al.* (1952).

The intensity transform for the fibril is, from (1) and (2),

$$\begin{aligned} FF^*(R, \psi, l/c) = |G_{n,l}(R)|^2 \sum_v \sum_w \exp \{i[-n\alpha_{vw} \\ + 2\pi Rr_{vw} \cos(\psi - \varphi_{vw}) + 2\pi\zeta z_{vw}]\} \end{aligned} \quad (3)$$

where $\alpha_{vw} = \alpha_v - \alpha_w$, $z_{vw} = z_v - z_w$, r_{vw} is the magnitude of a vector normal to Oz joining the axes of the vth and wth molecules and φ_{vw} is the angle between this vector and the plane $\psi = 0$. In most instances the angular dependence of (3) is of no interest and the observable intensity is proportional to the cylindrically averaged value

$$\langle FF^*(R, \psi, l/c)\rangle_\psi = \int_0^{2\pi} FF^*(R, \psi, l/c) d\psi/2\pi. \quad (4a)$$

From (3), (4*a*) and the identity

$$J_o(x) = \int_0^{2\pi} \exp(ix \cos \theta) d\theta/2\pi$$

we obtain

$$\begin{aligned} &\langle FF^*(R, \psi, l/c)\rangle_\psi \\ &= |G_{n,l}(R)|^2 \sum_v \sum_w J_o(2\pi Rr_{vw}) \cos(-n\alpha_{vw} + 2\pi\zeta z_{vw}) \end{aligned} \quad (4b)$$

It may be noted that for $l = n = \zeta = 0$ the expression reduces to that derived by Oster & Riley (1952) for the equatorial scattering from assemblies of cylindrically symmetrical systems. Also for $N = 1$ (4*b*) reduces to $|G_{n,l}(R)|^2$ which is the result given by Klug *et al.* (1958) for a single molecule and a single value of n. The effect of interference between helical molecules in a fibril is thus the introduction of a double summation as in (4*b*).

This double summation implies the calculation of N^2 terms but in practice the maximum number required is N(N − 1)/2 at most as $\alpha_{vw} = -\alpha_{wv}$ and $z_{vw} = -z_{wv}$ and (4*b*) simplifies to

$$\begin{aligned} \langle FF^*(R, \psi, l/c)\rangle_\psi = |G_{n,l}(R)|^2 \{N + 2 \sum_{v=1}^{N} \sum_{w=v+1}^{N} J_o(2\pi Rr_{vw}) \\ \times \cos(-n\alpha_{vw} + 2\pi\zeta z_{vw})\} \end{aligned} \quad (5)$$

If, as frequently is the case, the molecules are symmetrically arranged within the fibril the number of terms in the double summation which need to be calculated is quite small.

We have shown elsewhere (Fraser, MacRae & Miller, 1964) that the Fourier transform of the coiled-coil model for α-fibrous proteins proposed by Crick (1953) may be written in the form

$$F(R, \psi, l/c) = G(R, m, \lambda) \exp[i\lambda(\psi + \tfrac{1}{2}\pi)] \quad (6)$$

where $l/c = \lambda/P + m/h$, P is the pitch of the major helix, h is the axial rise per seven residues and only a single combination of m and λ is needed for any particular l. $G(R, m, \lambda)$ is a complex number independent of ψ and so (6) is formally similar to (1). The analysis leading to (5) is thus equally valid in this case. Further it has been shown that when a number of coiled-coil structures are wound around a common axis to form a rope the Fourier transform of the rope can also be expressed in a form similar to (6) (Fraser *et al.*, 1964) and so (5) may also be applied to fibrils containing assemblies of coiled-coil ropes.

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A comment on centroid truncation procedures.

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A description of a truncation procedure for the determination of the centroid position of an X-ray diffraction line, and an account of the advantage of this procedure in dealing with the difficulties introduced by satellite lines, have recently been published (Taylor, Mack & Parrish, 1963; Parrish, Mack & Taylor, 1963).

A similar procedure, together with the results obtained when it is used to determine lattice parameters, has previously been described (Delf, 1963). This method is based on the approach due to Pike & Wilson (1959) but without the use of horizontal truncation. The only significant difference between this and the method of Taylor *et al.* (method D of Parrish *et al.*) is that, while both are symmetric-limit methods, the method described by Taylor *et al.* uses a symmetric wavelength range while that of Delf uses a symmetric angular range.

There may be a theoretical advantage in using symmetric wavelength ranges, but it is less convenient than symmetric angular ranges in practice, as line profiles are invariably recorded as angular intensity distributions in X-ray powder diffraction measurements. In practice the two methods will only differ significantly at high angles, where the centroid approach is unlikely to be of use because of the large dispersion effect and the nonlinearity, and increase in magnitude, of the background level.

There has been a certain amount of criticism of the centroid method of determining line positions as some truncation procedure has to be used to overcome the difficulties introduced by the Cauchy-like tails. It is, therefore, of interest that two laboratories have independently converged on essentially the same truncation procedure to give a reproducible measure of line position which can easily be related to the wavelength scale.

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Hydrogen bonding in (+)-demethanolaconinone hydroiodide trihydrate.

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The crystal structure of (+)-demethanolaconinone hydroiodide trihydrate, $C_{24}H_{31}O_4(OH)_4N.HI.3H_2O$, was determined by Przybylska (1961). A water molecule-iodine chain in the structure was somewhat later described by Clark (1963), who listed the hydrogen bonds and angles associated with that chain, and who quoted from a private communication from Przybylska as follows: *Considering the very low ionic character of* HI *and the fact that the iodine atom is situated at a distance of* 5 Å *from the nitrogen atom of the alkaloid, it seems unlikely that the hydrogen of* HI *is attached to nitrogen.* This suggestion cannot be accepted, however, because it ignores the fact that the alkaloid is a moderately strong organic base, and HI a strong acid, indeed, the strongest of the hydrogen halides.

Rather than discuss in detail the essentially incomplete suggestions of Przybylska (1961) and Clark (1963) regarding the hydrogen bonding, we shall instead discuss it from first principles in order to locate, if possible, the hydrogen atoms. This can be done in the following stepwise manner, with the help of Table 2 of Clark (1963):

1. We note first that there are eleven hydrogen atoms available for hydrogen bond formation: six water, four hydroxyl, and one $\geqslant N^+–H$.

2. There are five $I^- \cdots O$ distances in the range 3·52–3·62 Å. These are assumed to correspond to $O–H \cdots I^-$. Three of the oxygen atoms are hydroxyl. This fixes the hydrogen atoms of O(5), O(6), and O(7), and one each on the water oxygen atoms O(9) and O(10).

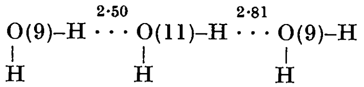
3. There are five $O \cdots O$ distances in the range 2·50–2·84 Å. These are assumed to correspond to $O–H \cdots O$.

4. One of these involves O(6), whose hydrogen atom is already assigned elsewhere. This gives $O(10)–H \cdots O(6)$.

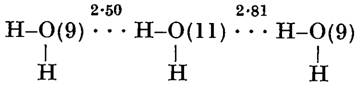
5. Both hydrogens of O(10) are now assigned. This gives $O(11)–H \cdots O(10)$.

6. The hydroxyl O(8) is involved in only one short $O \cdots O$ system. This gives $O(8)–H \cdots O(9)$.

7. Eight of the ten hydrogen atoms on oxygen have now been placed. For the remaining two there is an ambiguity:

either 

$$\underset{\mathrm{H}}{\mathrm{O(9)}}\text{–H} \overset{2\cdot50}{\cdots} \underset{\mathrm{H}}{\mathrm{O(11)}}\text{–H} \overset{2\cdot81}{\cdots} \underset{\mathrm{H}}{\mathrm{O(9)}}\text{–H}$$

or 

$$\text{H–}\underset{\mathrm{H}}{\mathrm{O(9)}} \overset{2\cdot50}{\cdots} \text{H–}\underset{\mathrm{H}}{\mathrm{O(11)}} \overset{2\cdot81}{\cdots} \text{H–}\underset{\mathrm{H}}{\mathrm{O(9)}}$$

8. The above considerations are made solely with regard to interatomic distances. *This criterion is not enough,* since it ignores covalent bond angles involving hydrogen. However, reference to Table 3 of Clark (1963) shows that all of the $C–O \cdots I$, $C–O \cdots O$, $O \cdots O \cdots O$ and $O \cdots O \cdots I$ angles implied by the above considerations are within the range of expectation for $C–OH \cdots I$, $C–OH \cdots O$, $O \cdots HOH \cdots O$, and $O \cdots HOH \cdots I$ interactions.

9. Finally, search for a hydrogen bond acceptor for the $\geqslant N^+–H$ group (and there is no reason why this should be an iodine ion) reveals an O(5) of a neighboring molecule at 3·05 Å, and with acceptable $C{\cdot}N \cdots O$ angles.

All of the foregoing, including the ambiguity of item 7 above, are shown in Fig. 1. It is concluded that, on the basis of interatomic distances and presumed interbond angles, nine of the eleven hydrogen atoms of the hydrogen bonds can be positioned. In the case of the remaining two, there is not a marked preference between the two possible arrangements, as may be seen from the values of the relevant angles in Fig. 1.

The discussion of Clark (1963) was mainly concerned with the hydrogen bonding involving the water molecules.