Molecular Configuration in Sodium Thymonucleate

Sodium thymonucleate fibres give two distinct types of X-ray diagrams. The first corresponds to a cylindrical form, structure A, obtained at about 22 per cent relative humidity; a study of this is described in detail elsewhere. At higher humidities a different structure, structure B, showing a lower degree of order, appears and persists over a wide range of ambient humidity. The change from A to B is reversible. The water content of structure B fibres which undergo this reversible change may vary from 8 to 30 per cent in several hundred per cent of the dry weight. Moreover, these fibres show structure B, and in these fibres B can be obtained with an even lower water content.

The X-ray diagrams of structure B fibres (see photographs shown in previous issue) show a reflection characteristic of helical structures, first worked out in this laboratory by Smith (unpublished) and by Clarke, Potts and Willatts. These fibres may be the new structure for nucleic acid in its usual state of nucleic acid fibres, although a helical structure has been previously described for X-ray studies of nucleoprotein and nucleic acid fibres.

While the X-ray evidence cannot, at present, be adduced in all cases that the structure is helical, other considerations discussed below make the existence of a helical structure highly probable. Structure B is derived from the cylindrical structure A when the sodium thymonucleate fibres take up 8 per cent of water in excess of about 40 per cent of their weight. The change is accompanied by an increase in about 70 per cent of the length of the fibre, and by a substantial rearrangement of the molecule. If therefore cannot be unreasonable to suppose that in structure B the structural units of sodium thymonucleate (molecules in groups of nucleotides) are relatively free from the influence of neighbouring molecules, each unit being separated by a sheet of water. Each unit is then free to take up its lowest energy configuration independently of its neighbours and, in view of the nature of the nucleic acid involved, it is highly likely that the spiral form of the helix is helical. If we adopt the hypothesis of a helical structure, it is immediately possible to fit the X-ray diagram of structure B, for under certain conditions, in the nature and dimensions of the helix.

The important maxima on the first, second, third and fifth layer lines are approximately on straight lines extending from the origin. For a smooth single-stranded helix the structure factor on the fifth layer line is given by:

$$F_n \approx \sin \frac{2\pi n a}{c}$$

where a is the pitch and c / 2\pi of the net of a, is the radius of the helix, and n is the radial and azimuthal co-ordinate in the spool coordinate system. The expression holds to an approximately linear array of intensity maximum of the type observed corresponding to the first maxima in the fourth, fifth, sixth, etc., layer lines.

If, instead of a smooth helix, we have a series of successive repeat planes along the helix, then the transform of the spool diagram treated by Dick, Potts and Willatts is quite complicated, but if there is a whole number of molecules per turn, the form of the transform is as for a smooth helix with the addition, only, of the same pattern repeated at the origin of the graph and...