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Fourier transform of the collagen triple-helical structure and its significance*

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Abstract. The Fourier transforms of the collagen molecular structure have been calculated taking into consideration various side chain atoms, as well as the presence of bound water molecules. There is no significant change in the calculated intensity distribution on including the side chain atoms of non-imino-acid residues. Taking into account the presence of about two bound water molecules per tripeptide unit, the agreement with the observed x-ray pattern is slightly improved. Fourier transforms have also been calculated for the detailed molecular geometries proposed from other laboratories. It is found that there are no major differences between them, as compared to our structure, either in the positions of peak intensity or in the intensity distribution. Hence it is not possible to judge the relative merits of the various molecular geometries for the collagen triple helix from a comparison of the calculated transforms with the meagre data available from its x-ray fibre pattern. It is also concluded that the collagen molecular structure should be regarded as a somewhat flexible chain structure, capable of adapting itself to the requirements of the different side groups which occur in each local region.

Keywords. Collagen molecular structure; Fourier transforms; water-bound collagen triple helix.

1. Introduction

The molecular conformation of collagen has been determined primarily from an interpretation of its high-angle x-ray diffraction pattern, which was first characterised by Astbury (1938) as being different from the α-helical and the β-pleated sheet patterns. The x-ray pattern of an unstretched collagen fibre is rather diffuse and poor in detail. Its principal features are a strong meridional arc at about 2·9 Å and weaker arcs at 4·0 Å and 9·5 Å. There are also strong equatorial reflections with spacings corresponding to approximately 6 Å and 12 Å (which depend on the humidity), and a diffuse distribution of intensity around 4·5 Å, mainly near the equator. This pattern is greatly improved in orientation and detail if the fibre is kept stretched during the x-ray exposure (Cowan *et al* 1953; Ramachandran and Ambady 1954).

The general distribution of intensity in the collagen pattern is of the type given by helical structures. An interpretation of this pattern in terms of the helix diffraction theory of Cochran *et al* (1952) led to the conclusion that the collagen helix has a unit height of approximately 3 Å, the number of units per turn being close to 10/3, which corresponds to a unit twist of 108°. A more accurate measurement later of the

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