PREFACE

This thesis embodies the results of the investigations carried out by the author during 1960 to 1965 at the Department of Physics, University of Madras. As a part of the programme of research work on structure of compounds of biological interest undertaken in this laboratory, studies on polypeptide and polysaccharide chain conformations and X-ray studies on biological fibres like collagen and chitin have been made and reported in this thesis. The structure of the polysaccharide chitin has been completely worked out from X-ray and stereochemical data.

The methods and the results of the investigations are discussed in the five chapters of the thesis, while some of the special techniques employed are described in the appendices.

At the time the author joined the department, preliminary work on the polypeptide chain conformation had been made by Dr. V. Sasisekharan making use of van der Waals contact distances as a primary criteria for determining allowed conformations. The work was continued and extensive calculations were made to determine the allowed conformations of two linked
peptide groups making use of a set of minimum contact distances. These are described in Chapter 1, along with a brief review of the earlier attempts and postulates of polypeptide chain conformations. For comparison of the theory with observation, data have been obtained from known simple peptides and polypeptides and the results are discussed.

Chapter 2 deals with the evaluation of the helical parameters for regular helical polypeptides. Two methods are described, one a graphical method making use of stereographic projection and the other using rotation matrices.

In Chapter 3, a re-examination of the X-ray diffraction pattern of collagen is described with a view to obtain precise helical parameters for the structure of collagen. The Fourier transform calculations have been made for the proposed models described in the chapter, and it is shown that the two-bonded structure of collagen proposed by Professor Ramachandran agrees best with the calculated Fourier transform.

The stereochemistry of polysaccharide chain conformation is described in Chapter 4. A standard
set of coordinates has been obtained for the sugar residues from an analysis of the available crystallographic data on sugars. The allowed conformations for the polysaccharide chain have been worked out near the region where a good intra-chain hydrogen bond is formed. It is shown that the chain conformation in chitin and cellulose is likely to be buckled rather than straight.

The structure of chitin as such is described in detail in Chapter 5. The previously proposed models were critically examined both on the grounds of stereochemistry and X-ray intensity data. A set of refined coordinates for the atoms in the asymmetric unit of chitin has been given. The structure closely resembles the one proposed by Carlstrom.

Appendix 1 describes the stereographic projection method used for conversion of coordinates from one system to another.

In Appendix 2, a brief description of the programmes written for the Elliott-803 and IBM 1620 digital computers are given.

The Figures, Tables and Equations are numbered separately in each Chapter. All the references are collected at the end of the thesis.
The work described in Chapters 1, 2, 4 and 5 was done independently by the author under the guidance of the supervisors. The work described in Chapter 3 was carried out in collaboration with Dr. B.H. Lakshmanan. Mr. Y.T. Thathachari's name has been included in the paper for his earlier work which did not give any significant result.

Based on some of the investigations described in this thesis, the following is the list of papers published or being sent for publication. Available reprints are enclosed.

(1) X-ray Diffraction Pattern of Collagen and the Fourier Transform of Collagen Structure

by

B.H. Lakshmanan, C. Ramakrishnan, V. Sasishekharan and Y.T. Thathachari


(2) The Structure of Chitin

by

G.N. Ramachandran and C. Ramakrishnan


(3) Stereoschemistry of Polypeptide and Polysaccharide Chain Conformations

by

G.N. Ramachandran, C. Ramakrishnan and V. Sasishekharan
(4) Stereochemistry of Polypeptide Chain Configurations
by
G.N. Ramachandran, C. Ramakrishnan and V. Sasisekharan
J. Mol. Biol. 7, 95, (1963)

(5) Stereochemical Criteria for Polypeptide and
Protein Chain Conformations - Part I -
Evaluation of Helical Parameters
by
C. Ramakrishnan
Proc. Indian Acad. Sci., A59, 327, (1964)

(6) Stereochemical Criteria for Polypeptide and
Protein Chain Conformations - Part II -
Allowed Conformations

(Being sent for Publication)

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